

Relativistic Quantum Mechanics
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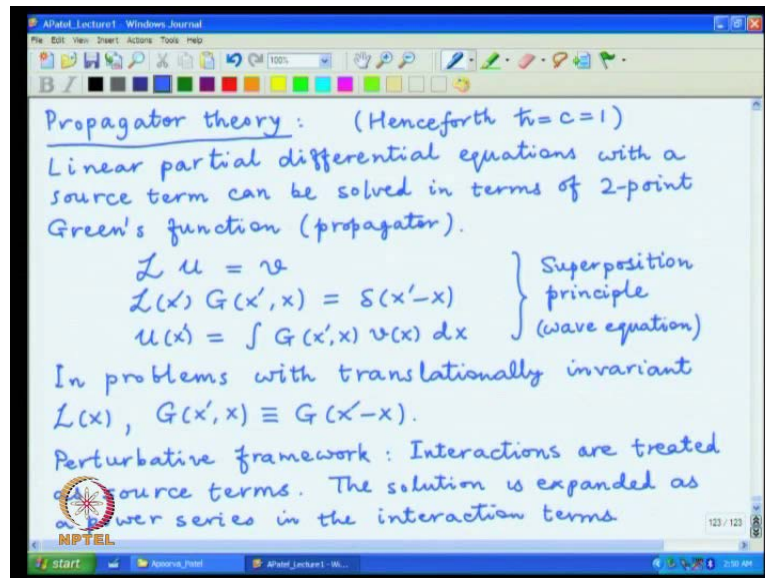
Lecture - 26
Propagator theory, Non-relativistic case and causality

So far in the course we have discussed two major topics; one is the relativistic wave equations in particular Dirac equation, and its solutions for simple potentials. And second topic was the analysis of Lorentz group; which provides important constraints on the type of consequences of the theory even when you do not want all the details of the dynamics. And now this 2 pieces can be put together to construct a framework in which we can deal with problems of electrons interacting with electromagnetic field in arbitrary instances.

And this framework is known as the theory of quantum electrodynamics; it can be formulated in many different ways. But I am going to follow the historical route where known the ingredients namely Dirac equation, Maxwells equations and Lorentz symmetry the features; where combined into a perturbation theory structure. And that allowed calculations and predictions of the theory in many instances where the interactions strength was sufficiently small.

This framework now a day has been extended to a more powerful framework which is formulated in terms of lagrangian and path integrals. And from which even Non-Perturbative predictions of any theory can be derived. But I will not go into those details in this particular course I will stick to the portability formulation. And that formulation can be obtained rather easily from the ingredients which we already constructed. And that analysis requires a fundamental quantity which is known as the propagator.

(Refer Slide Time: 03:01)



So, the next topic which I want to discuss is the so called propagator theory; which is essentially the description of how wave functions evolves in presence of various sources in the background. And if one can do that than, one can include more and more complicated features of the theory in a Perturbative framework to get higher and higher order accuracy in the solution; one thing which I will use is a framework which simplifies the notation. And that I am ask to choosing the units where plunges constantans speed of light are set to unity.

So, what does this propagator theory amount to it is essentially solution for the wave equation in presence of the source; and there is a general framework available for; so called linear partial differential equations; that the equations in presence of a source can be solved in terms of what are known as greens functions or mass specifically 2 point greens function. And this object is what will call the propagator; and it is a rather straight forward scheme where you have say some linear operator acting on some function u which produces the source v on the right hand side.

For any generic way the solution is obtained by defining the greens function; let me put the indices explicitly it is a same operator. But now acting on a object which has 2 arguments x prime and x . And the result is now not the arbitrary source; but a specific source, rather the delta function or a point object the reason for doing this is; that because the operator is linear we have the general principal of superposition available. So, you

can calculate the result for any arbitrary source by just clear a super positions; of many delta functions sources located that different points.

And, so the general solution now can be written as u at x is equal to integral G or other it should be x prime G x prime x, v, x integrated over $d x$. The reason it was now is quite obvious to see if you act on the left side by l of x prime. So, we have a $l u$ on the right hand side l of x prime on the greens function produces a delta function; the integral of delta function with v will just produce v of x prime and that is a original equation. So, all that has gone in this is basically the superposition principal; which is a simple property of any linear partial differential equation. And in general a problems, which we are going to deal with are all problems of wave mechanics; they will all have linear partial differential equation and they will obey the property of superposition.

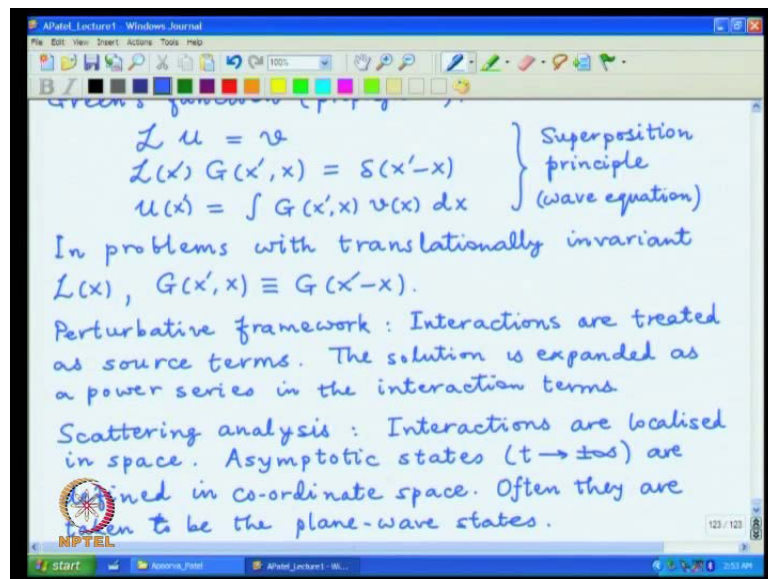
So, we just have to cast our problem in this generic frame work and the greens function is extremely useful because it is a solution of the equation; not in presence of any arbitrary force; but the solution presence of a point source. And the point source solutions are generally very easy to obtained one other feature; which is all pervasive in our analysis is in problems with Translational invariance; the greens function cannot depend on 2 arguments independently. But it depends only on the difference; it is a consequence of a translational symmetry. And it is extremely useful in simplifying the detail calculation you do not need to have an absolute frame of coordinates only the relative coordinates matter ok.

There are other features which are also useful and one of them is the so called Perturbative framework; in which the interactions are treated as source terms which means, the linear operator which occurs in the equation; is the so called Hamiltonian without any interaction it will become the free particle Hamiltonian. And all the interactions will be moved in this equation on to the right hand side. And treated by this Perturbative framework; it becomes very convenient to expand the solution the a power series in the interaction terms.

So, it means that the leading order contribution will be no interaction at all. Then the next correction will be 1 interaction; the next correction will be 2 interaction and so on and so forth. And the interaction is sufficiently small these construct the series which makes reasonable sense in terms of predicting quantities; which can be compared with

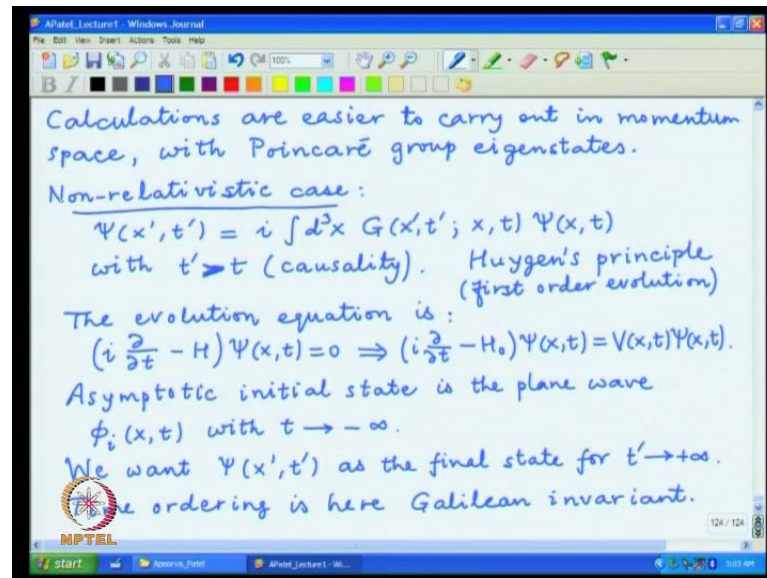
experimental result to better and better accuracy. This is a generic framework which we are going to use I also want to say that the formulation here; is written in terms of the space time coordinates. And for that reason it is convenient to construct this solutions in terms of boundary conditions; which are specified at infinity in the position and the time coordinates. Then one can ask what happens in the detailed solution where the interactions are localized in a certain region; this framework is what is known as a scattering analysis.

(Refer Slide Time: 13:22)



Which means, that interaction are localized in space and asymptotic states in particularly t going to plus or minus infinity are defined in co ordinate space. And since these are the states which are far away from the interactions; they will be the solutions of the free part of the Hamiltonian. And in this particular case of wave equations this states are often selected to be the plane wave states. So, this also is a important part of the framework in the Perturbative analysis it typically calculate processes; which can be expressed in the scattering scenario.

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One more comment I would like at the general principals; which is a there the problem is formulated in space time coordinates. The calculations are easier to carry out in momentum space the reason being; that this allows us to use the full power of the Poincare group in the sense; that we know the Eigen states of Poincare group are specified by momentum and the spin. And so we can explicitly label what happens to it particular Eigen state in this framework it is also useful; that the plane wave are also Poincare group Eigen states in absence of an a interactions in the problems which we handle. And then the calculations become straight forward and of course one can go from the momentum space to position space and back whenever required by simple for your transforms. But it just that one framework is more convenient then the other in case of calculations.

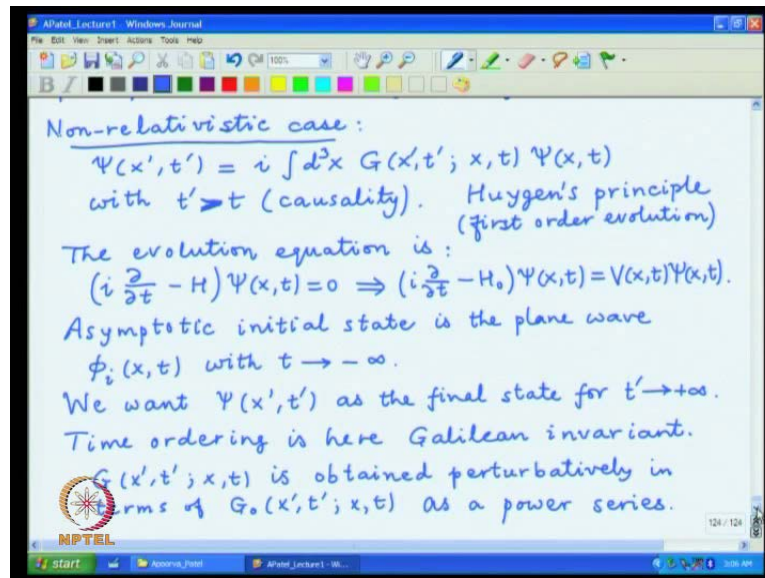
Now, let us look at the setting of the whole problem in case of quantum mechanics; particularly the non relativistic quantum mechanics would using the language of this propagators or 2 point game function. The problem here is written in terms of the greens function language which I can now express as wave function at some time t prime. And position x prime is an integral of the green function times the source which was the initial wave function. So, the green function contains all the changes which can occur in the wave function due to whatever interactions there may be and this is a evaluation; which is arrange to go from past to the future also called the principal of causality.

This is just analogous to the solution; I wrote down for generic linear equation on the previous slide and these factors of I and integral so position etc; they are all taken according to some convention many times, these kinds of expression is referred to as Huygens principal for wave propagation. And it is correct to apply it in particular form because the evolution equation, we will deal with are first order in time. So, given description at a past time you can go to the next step in the future time; some made a mistake there is a greater than sign in this causality not equal to sign.

So, this is a solution which we want we have a corresponding equation; which now can be rewritten in terms of the Hamiltonian and interaction the original equation is $i \delta t \text{ minus } H \text{ acting on } \psi(x, t) \text{ is equal to } 0$. We are going to rewrite this form by separating the free and the interacting parts. And the purpose of the formalism is given that we can easily obtain the solutions of H_0 which are typically the plane wave state how to obtain the solutions for some arbitrary potential if we. And that is what the greens functions allow us to do conveniently; on top of that we have the boundary conditions; the asymptotic initial state is the plane wave we can give it some label ϕ_i at x and t with t going to minus infinity.

And, we want ψ at x' , t' as the final state for t' going to plus infinity it is useful in this particular framework; that the time ordering is a here, Galilean invariants. So, if we unsure that the prime is greater than t in one particular frame it will always be true in any arbitrary frame. And so the causality is little easier to deal with we have to find a particular frame; where it holds and then you do not have to worry about it in any other frame this essentially is a set of the problem now we need. So, solve this machinery so far it is only a formal machinery. But now we want to convert this expression to what will happen to the greens function?

(Refer Slide Time: 25:22)



So, G of x prime t prime G here is a greens function of the complete problem; we will not be able to solve it in full generalities, we will actually solve it perturbatively x prime, t prime, x . And t is obtained perturbatively in terms of the solution in absence of any interaction which I will denote as G_0 . It is a solution for the problem where the potential part v is 0. And H_0 is the only evolution part in the dynamics this essentially will describe how a plane wave evolves.

And, so G will then be expressed as a power series in terms of G_0 as usual with solutions of linear homogenous equation; the generic solution is a arbitrary solution of the homogenous part plus a particular solution corresponding to in how much in a s part. So, arbitrary greens function G will be G_0 as a solution of the homogenous part plus all the effects which come as the particular solution involving the interaction v ; one can now easily see that the equation as a simple form the source term now is v times ψ on the right hand side. And so the equation for G will look the same except the there is a delta function its 1 of the whole v then one can go back and forth between the equation for ψ and the equation for the G ; they look very similar.

(Refer Slide Time: 28:03)

The formal general solution is

$$G(x'; x) = G_0(x'; x) + \int d^4x_1 G_0(x', x_1) V(x_1) G(x_1, x).$$

Iterative expansion gives

$$G(x', x) = G_0(x'; x) + \int d^4x_1 G_0(x', x_1) V(x_1) G_0(x_1, x) + \int d^4x_1 d^4x_2 G_0(x', x_1) V(x_1) G_0(x_1, x_2) V(x_2) G_0(x_2, x) + \dots$$

Space-time diagrams:

$x \xrightarrow{G_0} x'$ + $x \xrightarrow{G_0} x_1 \xrightarrow{G_0} x'$ + $x \xrightarrow{G_0} x_1 \xrightarrow{G_0} x_2 \xrightarrow{G_0} x'$ + ...

$$\Psi(x', t') = \phi_i(x', t') + \int d^4x_1 G_0(x', t'; x_1, t_1) V(x_1, t_1) \Psi(x_1, t_1)$$

Can also be expanded iteratively.

Generically, this solution can be rewritten as the formal structure is G with x prime and x . I will omit to many indices as long as notation is on ambiguous here; it is written as whole dimensions the solutions for the homogenous part plus. Then homogenous contribution V times G is now the source. And multiplied by this homogenous equations greens functions G_0 will give this result one can easily apply the operator on both sides to get back the original term; where the operator is just $\text{id} + d^4x_1 H$ this is a general solution it does not solve anything in any detail because the unknown part G is appearing on both the sides.

And, so the way it is used is actually iteratively; where one gets G equal to G_0 plus integral the first time one just take a leading term here; and substitutes and this expressions. So, it is $G_0(x', x_1) V(x_1) G_0(x_1, x)$ to x . Then the next order one takes this whole result which came out of the expansion and puts it back that gives a next order term and so on and so forth. And this is the way the actual calculations are done; the greens function for the free particle is known or other evaluate explicitly what it comes out to be the interaction is also known; and the interaction is use in a power series expansion assuming that it is localized as well as small, and so one has the final result accurate up to certain order in the interaction strength b .

And, this framework also is conveniently describe many times in terms of space time diagrams; where one has some initial point x , final point x prime. And the leading

contribution is just G_0 next order involves 1 interaction which here is at point x_1 . And then on either side of it is again the free propagator. So, this is a first order correction then one can have more elaborator schemes so on and so forth.

And, structure is simple enough to remember, that in calculation of this greens function there is basically an alternating sequence of a propagator followed by a interaction vertex another propagator, another interaction vertices till you go to the final point. And the calculation is done up to a finite number of steps in terms of this interaction vertex. And higher order accuracy will result if you include more such terms this is now the strategy in case of non relativistic quantum mechanics; one can do the whole analysis of scattering from a potential in this framework. The final result comes out again in terms of this power series or the formal expansion that we wanted $\psi(x', t')$ we sent in some initial wave.

And, ψ_i at x', t' is just the initial way provided nothing happened during the whole evolution. So, it is a solution of the homogenous part of the equation then the effect of the interaction is now given by this propagator G_0 ; which follows the interaction of the complete solution acts the point x_1, t_1 . This is a superposition principal connected with the definition of the greens function above V times ψ_i is the source we apply a greens function. And then you get the in homogenous part of the solution ψ_i is just the homogenous part of the solution; again this is a complete description.

But since I appears on the both sides of the equation you cannot directly solve it. Iterative procedure gives the solution in the same way, that you will take this ψ_i put it back on the right hand side which means, that right hand side will have ψ_i which is the initial state instead of the exact solution ψ_i . And one can do the calculation up to a certain order this also can be expanded iteratively; the central in all this calculation is basically to obtained the G_0 the interaction V . And then be able to do all the space time integrals in a clever way; we will see that this integrals are conveniently done not in positions space as I have written. But it momentum space; but let me give another definition which is also quite useful; and that is the so called scattering matrix element.

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The slide contains the following content:

Space-time diagrams: $x \xrightarrow{G_0} x'$ + $x \xrightarrow{G_0} x_1 \xrightarrow{G_0} x'$ + $x \xrightarrow{G_0} x_1 \xrightarrow{G_0} x_2 \xrightarrow{G_0} x'$ + ...

$$\Psi(x', t') = \phi_i(x', t') + \int d^3x_1 G_0(x', t'; x_1, t_1) V(x_1, t_1) \Psi(x_1, t_1)$$

Can also be expanded iteratively.

Scattering matrix elements are defined as

$$S_{fi} = \lim_{t' \rightarrow \infty} \int d^3x' \phi_f^*(x', t') \Psi^{(+)}(x', t')$$

↑ Forward propagating wave

$$= i \lim_{t' \rightarrow \infty} \lim_{t \rightarrow -\infty} \int d^3x' d^3x \phi_f^*(x') G(x', x) \phi_i(x)$$

$$= \delta^3(\mathbf{p}_f - \mathbf{p}_i) + \lim_{t' \rightarrow \infty} \int d^3x' d^3x \phi_f^*(x', t') G_0(x', t'; x, t) V(x, t) \Psi^{(+)}(x, t)$$

And, they are defined as what happens to the initial state? Then whatever comes out what is his projection on to a particular final state; we have to take this limit the t prime goes to plus infinity. And it is a overlap of some specific panel state bases 1 has to choose with whatever solution which came out from solving this equation. This one is often return with this index plus it means, this is forward propagating wave its equivalent to the boundary conditions; which we have used saying that the way goes from t to t prime only when t prime is larger than t.

And, now this can be formally rewritten in terms of the initial conditions which we have we will sticking this various constraints of initial state and final states. And then appear the integrals there are d cube, x prime, d cube, x phi, f star, x prime; the complete greens function from x prime to x; and then the initial state phi i. So, this is just rewriting this final wave function as a initial wave function multiplied by a complete greens function; when the complete greens function is broken up into the homogenous. And the Perturbative part this gets further simplified just take this above equation.

And, substitute G in terms of G 0; the first term is just overlap between phi f and phi i which produces delta function by definition of the greens function; that is a trivial part of the scattering matrix just means, that is a contribution corresponding to nothing at all happening to the initial wave in terms of matrix languages is identity matrix. And then there is a interaction correction which can be rewritten as final state. But now we do not

have G we have to prove $G \neq 0$. And then a potential appears then with the potential comes the wave function propagating forward in time.

This is a formal expression for what is called the scattering matrix; actually in the conventions which I have used there are some differences between the space and time integrals. But you can sort it out it is not very complicated this is a generic definition. And many results are expressed in terms of the non identity part of this particular scattering matrix; which is this second complicated integral. And which one has to evaluate again by expanding ψ plus iteratively one has now iterating sequence of propagators and vertices. But on either side those are evaluated as expectation values between some initial state and some final state wave function.

(Refer Slide Time: 43:53)

A Hermitian Hamiltonian will have a complete set of orthogonal eigenstates, and a unitary S -matrix. (The completeness sum includes any bound states if they exist.)

Causality is included using the step function

$$\Theta(\tau) = \begin{cases} 1, & \tau > 0 \\ 0, & \tau < 0 \end{cases}, \quad \frac{d\Theta(\tau)}{d\tau} = \delta(\tau).$$

For example,

$$\Theta(t'-t) \Psi(x') = i \int d^3x G(x', x) \Psi(x).$$

Using contour integration, we find that

$$\Theta(\tau) = \lim_{\epsilon \rightarrow 0} -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega \cdot \frac{e^{-i\omega\tau}}{\omega + i\epsilon}$$

is slightly below the real axis

And, that will produce this S - matrix what one finds is the Hermitian Hamiltonian will have a complete set of orthogonal Eigen states; this ψ_i and ψ_f are specific instances of them. And unitary S - matrix this is the standard feature of quantum theory Hermitian Hamiltonian and unitary evolution; one has to remember that this completeness sum includes any bound states; if they exist in particular the asymptotic states might be just plane waves. But in the intermediate steps if there is any sum over complete set of states; and if bound states exist they must be made part of the calculation to get a valid reason. So, this is all formal machinery.

And, now one has to implemented in case of specific Hamiltonians. And what we need to


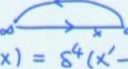
do little carefully is implement the constraint of causality; once we have done that we have the greens function solution. And that is a place which requires little mathematical tricks to be able to do the calculations; causality is included using the step function which has the behavior that it is equal to 1. And the argument is positive it is 0 when it is negative; related to this step function definition is a definition of the delta function of the same argument which is the derivative of the step function is the delta function.

We can now include this extra condition by just inserting in the differential equation factor of the step function by hand. And then you do not have to write that particular condition separately. And so the equation can also be written as $\phi(x, t')$ is $G(x, t')$ plus $\int_{-\infty}^t \psi(x, t-t')$ explicitly make sure that if t' is larger than t you have a actual solution; if t' is less than t then this whole integral over this function vanishes that is now convenient. Because the step function has many convenient integral representations which are easily written in terms of Fourier transform variables using contour integration.

We find that this $\theta(\tau)$ can also be written as an integral from minus infinity to infinity $d\omega e^{i\omega\tau}$ divided by $\omega + i\epsilon$; that is the crucial part of the prescription. So, the pole is $\omega = -i\epsilon$ this pole is slightly below the real axis. And that produces this step function behavior by closing the contour in different manners depending on whether τ is positive or negative and τ is positive. Then to make this exponential factor decay at infinity in the complex plane one must close the contour in the lower half of the plane.

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$\Theta(t'-t)\Psi(x') = i \int dx G(x', x)\Psi(x).$
 Using contour integration, we find that

$$\Theta(\tau) = \lim_{\epsilon \rightarrow 0} -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega \cdot \frac{e^{-i\omega\tau}}{\omega + i\epsilon}$$
 Pole is slightly below the real axis.
 $\tau > 0$: Contour closed as : Pole inside
 $\tau < 0$: Contour closed as : Pole outside
 Thus, $[i \frac{\partial}{\partial t} - H(x')] G(x'; x) = \delta^4(x' - x)$
 with non-relativistic $H_0 = -\frac{\nabla^2}{2m}$,
 leads to the non-relativistic propagator

$$G_0(p, \omega) = \frac{1}{\omega - \frac{p^2}{2m} + i\epsilon}$$

So, this is the integral from minus infinity to infinity. And one closes in the lower of the plane the pole is included in the region of integration residue theorem gives the result the $2\pi i$ coming from the residue theorem including a negative sign. Because the contour is closed clockwise exactly cancels out this factor in front. And all one is left with from the contribution of the simple pole is the result that it is 1; that is how when tau is positive the answer is 1. If tau is negative then the contour is closed in the upper half plane. Because then the imaginary part of tau gives exponentially dumpt phase at infinity. And this semicircle can be added to the contour without any problem; the integral over there vanishes.

But now the pole is outside and so does not contribute to the integral and literally 1 obtains 0. This is a kind of clever trick to write the step function as a integral over an energy variable. But now adding a pole which is slightly away from the real axis shifting is by this amount epsilon in and epsilon is going to 0. So, that at the pole this factor $e^{-i\omega t}$ basically becomes 1; this trick allows us to rewrite the result for the greens function which we are looking at in the non relativistic problem; we have the equation for the greens function.

And, the unperturbed part of the Hamiltonian can be written in coordinates space as minus Del square by 2 m. The propagator is easily obtained in momentum space the delta function Fourier transforms to that is 1. And for the greens function is nothing but the

reciprocal of the operator which we have on the left hand side; except that now we have to write this particular operator in momentum space; that becomes $1/\omega$ from $\nabla^2 t^2$ by $2m$ from H_0 .

And, on top of that we add this $i\epsilon$ prescription to ensure that this greens function is not 0; only if t' is bigger than t . Now, using this particular propagator together with a potential a calculation in non relativistic quantum mechanics of any scattering analysis can be carried out. So, this is a illustration of the formulism and a simple result we will build on it in the next lecture to look at a relativistic case.