Path Integral Methods in Physics & Finance Prof. J. P. Singh Department of Management Studies Indian Institute of Technology, Roorkee

Lecture - 19 Basic Machinery of Quantum Mechanics

Welcome back. So, in the last lecture having completed the statistical formalism of the Path Integral we moved over to it is spectrum of applications the initial applications that I proposed to explore is in the field of Quantum Mechanics.

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IT ROORKEE ONLINE CERTIFICATION COURSE

 The principle of the path integral formalism is that a particle/wave (such as an electron) traveling a path (world line in space-time) between two events could actually be considered to be traveling along all possible paths (infinite in number) between those events.

It is in the context of quantum mechanics that the path integral enjoys the pride of position for working out the transition amplitudes in the context of quantum mechanical problems.

The principle as propounded by Feynman on the basis of a earlier work done by Dirac and his own ingenuity is that for a given a particle or equivalently a wave that travels a path which is a world line in space time between two events; then we could view it as comprising of we could view the transition as comprising of all infinite paths moving from the initial point to the destination point.

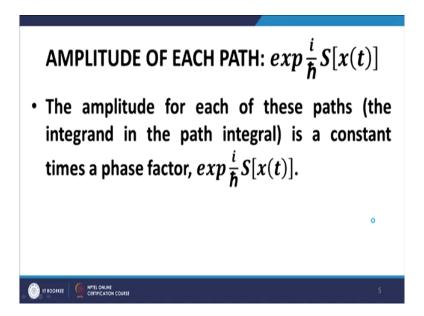
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PATH INTEGRAL FORMALISM

- · In the path integral, formulation of QM,
- the amplitude to find the particle at the final position x at time t, given that it was at x₀ at time t₀
 = 0,
- is a sum (the path integral) of amplitudes corresponding to all intermediate possibilities, that is, all paths connecting the two endpoints.



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However, each of those paths need to be weighted by a factor which is related to the classical action and which is given by exponential i upon h bar S of x of t. So, this is the weighting factor with which each path is weighted and then we arrive at the expression for the transition amplitude.

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THE QUANTUM STATE $|\psi>$

- It encodes all measurable information about an isolated physical state;
- $|\psi>$ at a given time is represented by a state vector in an infinite dimensional Hilbert space \mathcal{H} .
- It is an abstract object.



Now, and then I moved over to the discussion on the construction of a moving basis, but a bit of a preliminary knowledge would help in that context. The first thing that we encounter of course, is the quantum state in contrast to the classical state of a system which is usually represented either in configuration space or in phase space velocity or momentum phase space.

In contrast the quantum state which encodes all the measurable information about the physical state is represented in a Hilbert space and which is a complete space with an inner product defined on it.

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WAVEFUNCTION

 When the state vector is expanded in a basis (for example: position or momentum), the components or the coefficients of such basis vectors, say in position/momentum, are called the position or momentum wave functions.



The second important term that makes it is present frequently in quantum mechanics is the concept of wave function. If we expand the state vector in a particular basis for example, the position basis or the momentum basis, then the components or the coefficients of that basis vectors represent the wave functions in that particular basis and they are called the position or momentum wave functions.

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WAVEFUNCTION IN POSITION SPACE
$$|\Psi\rangle = \left(\int_{-\infty}^{+\infty} dq \, |q\rangle\langle q|\right) |\Psi\rangle$$

$$= \left(\int_{-\infty}^{+\infty} dq \, |q\rangle\langle q|\Psi\rangle\right) = \int_{-\infty}^{+\infty} dq \Psi(q) |q\rangle$$
where $\langle q|\Psi\rangle = \Psi(q)$.

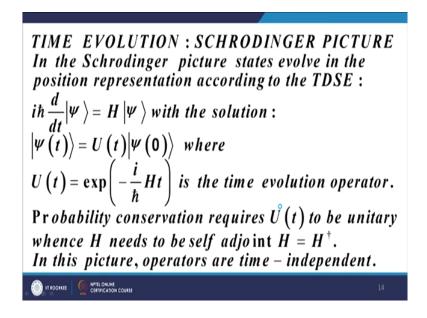
For example if I have a state vector represented by the ket phi as psi ket psi then we can obtain the wave functions corresponding or the coefficients representing the wave functions at various basis points by the integral of this expression which clearly shows the expansion of this state vector in terms of these wave functions on a basis represented by the kets q.

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Similarly, in momentum space:
$$\langle p|\Psi\rangle = \tilde{\Psi}(p)$$
Also $|\Psi\rangle = \frac{1}{2\pi\hbar} \left(\int_{-\infty}^{+\infty} dp |p\rangle \langle p|\right) |\Psi\rangle$

$$= \frac{1}{2\pi\hbar} \left(\int_{-\infty}^{+\infty} \tilde{\Psi}(p) dp |p\rangle\right)$$

Similarly, we can have in momentum space; we can have the wave function representation in the momentum space as well it is parallel to what we have in the position space right. (Refer Slide Time: 03:53)

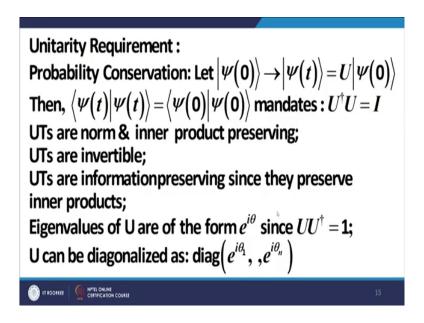


Now, as far as time evolution is concerned again there are two actually there are three pictures, but we have the Schrodinger picture, we have the Heisenberg picture and we have the interaction picture, for the moment let us focus on the Schrodinger and the Heisenberg picture.

In the Schrodinger picture the time evolution is captured by the time dependent Schrodinger equation which is given in this slide the first equation on this slide. And, this solution to this slide takes the form of the state vector and the time dependent state vector or time evolve state vector which is given by phi psi of t is equal to U t psi of 0 value is the evolution operator.

And, U is given U has to be unitary first of all in order to preserve probabilities and secondly, U t is given by exponential minus i upon h; i upon h bar into H t where a capital H is the Hamiltonian and the unitarity of U t requires or mandates that H needs to be self adjoint.

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The unity unitarity requirement follows directly from the requirement of conservation of probability, conservation of inner product. And, in order that the inner product we conserve it is necessary that the unitarity of the evolution operator time evolution operator be preserved which corresponds to the fact that the Hamiltonian should be a self adjoint operator.

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EQUIVALENCE OF SCHRODINGER & HEISENBERG PICTURES

- In the Schrödinger picture,
- the expectation value of a given operator $\widehat{0}$ (which itself is frozen in time) is defined as follows (with $\psi(t)$ the wavefunction of our system at time t) as:
- $\langle \boldsymbol{O}(t) \rangle = \langle \boldsymbol{\psi}(t) | \hat{\boldsymbol{O}} | \boldsymbol{\psi}(t) \rangle$
- which is just the average value of the observable corresponding to \widehat{O} if a measurement is made at time t.



Now, we see in the context of quantum mechanics is basically a statistical theory and the quantities that are relevant for us are expectation values. For example, if we want to work out the expectation value of an observable we make use of the formula that is given on your slide.

The expectation value of an observable represented by the operator at a point in time t O of t is given by a sandwiching O the operator representing that observable between the time in time evolved wave functions phi psi t and psi t at the point at which the observation is to be made.

Now, the important point here is if you look at this carefully the operator does not carry any time dependence O which is given in this expression does not carry any time dependence. The time dependence is captured by the wave vector or the state vector, quantum state which incorporate which embeds the time dependence, the operator is time independent this is called the Schrodinger picture.

In the Schrodinger picture the evolution is such the state vector evolves in time whereas, operator representing the observable does not evolve in time that is the fundamental. Now, let us see what happens in the Heisenberg picture.

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$$Now, \langle \hat{O}(t) \rangle = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle$$

$$= \langle \Psi(0) | U^{\dagger}(t,0) \hat{O} U(t,0) | \Psi(0) \rangle$$

$$= \langle \Psi(0) | (U^{\dagger}(t,0) \hat{O} U(t,0)) | \Psi(0) \rangle$$

$$= \langle \Psi(0) | \hat{O}(t) | \Psi(0) \rangle$$

We can write the above expression for the expectation value of the operator O t as this was which was there in the earlier slide we can write it in the form of by introducing a unitary transformation. We can write it in the form psi of 0 U conjugate t 0 O U t 0 psi of 0, where we have incorporated.

Now what are we done we are simply represented the bras and kets psi t in terms of their respective values at psi 0 or in respect of the evolution from psi 0 to psi t it. The unitary operators U represent the evolution of this state vectors from t equal to 0 to t equal to the given point at which the identification is being considered.

Now we can write this in the form of psi 0 and we can identify instead of identifying O as it is we identify O with the transformation U conjugate O U the operator is now evolving. Now the operator carries the time dependence earlier we had the operator time independent operator has not evolved it was the state vectors which had evolved and we had applied the evolved state vector on the operator which was time independent to get the average value.

Now, what has happened is, the states are the states at t equal to 0 the states remain the states at t equal to 0; however, the operator instead of being the operator at t equal to 0 has now evolved in time according to this to it is value or to it is expression at time t equal to the given observation point and we can write it in this form.

We are now O t is the evolved operator acting on the initial state. So, we have two situations very clearly seen from here one situation where the operator is time independent operator does not evolve in time it acts on the state which evolves in time.

On the other hand the other situation is the states do not evolved in evolve in time and the operator evolves in time and the evolved operator acts on the state which is fixed in time. So, and we can see that both these schemes or the both these interpretations lead us to the same expectation value of O t.

So, they are and now as I mentioned at the start it is the expectation values that are relevant in the context of quantum mechanics it is a statistical theory. So, because we arrive at the same expectations so in the context of both the formalisms it follows, it follows that the two formalisms are equivalent.

The first formalism where the state vector evolves the operator does not evolve is called the Schrodinger picture and in the second formalism where the where the state vector does not evolve and the operator evolves in time operative representing the given observable the operator evolves in time is called the Heisenberg picture right.

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- We can relate the operator in the Schrödinger picture with that of Heisenberg picture by:
- $\widehat{\pmb{O}}_{\pmb{h}}(t) = \pmb{U}^\dagger(t,0) \widehat{\pmb{O}}_{\pmb{s}} \widehat{\pmb{U}}(t,0)$ operating on
- $\psi(0) = \psi_h$
- In other words, $\widehat{O}_h(t) = U^\dagger(t,0) \widehat{O}_s \widehat{U}(t,0)$ operating on $\psi(0) = \psi_h$ is equivalent to $\widehat{O} = \widehat{O}(0) = \widehat{O}_s$ operating on $\psi(t)$.

So, that is basically the difference between the two and they are equivalent as I mentioned is, this is the expression in the red font summarises what we have discussed, the operator is evolving like this and it acts on the state vector at t equal to 0. And this gives us the same expression where the operator is unevolved, but it acts on the state vector which has evolved at t as per the time evolution captured by the Hamiltonian.

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$$\hat{q}_{h}(t) = e^{i\hat{H}t}\hat{q}_{h}(0)e^{-i\hat{H}t} : \text{Heisenberg picture}$$

$$\hat{q}_{h}(t) = e^{i\hat{H}t}\hat{q}_{s}e^{-i\hat{H}t} \text{ since } \hat{q}_{h}(0) = \hat{q}_{s}$$

$$\hat{q}_{s}|q\rangle = q|q\rangle : \text{ Schrodinger picture}; \text{ and }$$

$$e^{i\hat{H}t}|q\rangle = |q,t\rangle : \text{ Schrodinger picture}$$

$$\hat{q}_{h}(t)|q,t\rangle = e^{i\hat{H}t}\hat{q}_{s}e^{-i\hat{H}t}e^{i\hat{H}t}|q\rangle$$

$$= e^{i\hat{H}t}\hat{q}_{s}|q\rangle = qe^{i\hat{H}t}|q\rangle = q|q,t\rangle$$

Now, in the last lecture we discuss the preliminary work with respect to the construction of the moving basis and we discussed the important point that the operator q Heisenberg operator will be operating in the Heisenberg picture, the Heisenberg operator the time evolved operator acts on the time evolved state and we again get the eigenvalue q with respect to the time evolve state.

In other words given that we have a Schrodinger state at t equal to 0 with the eigenvalue q if we given that we have a Schrodinger state or a t as state at t equal to 0 acted on an operator which yields an eigenvalue q; if the operator is evolved in time and the state vector is also evolved in time we get another expression where we get the same eigenvalue q of on in consequence of a measurement made on the time evolved state vector right.

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$$\hat{q}_h(t)$$
 has a complete set of eigenstates: $\hat{q}_h(t)|q,t\rangle = q|q,t\rangle$ which evolve in time as: $|q,t\rangle = e^{i\hat{H}t}|q\rangle$: Schrodinger picture These eigenstates $|q,t\rangle$ form a MOVING BASIS.

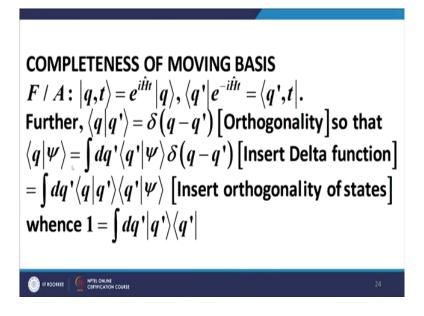
So, this is what is called moving basis, basis where we have a functional dependence on time. Now the operator q h t, h represents it is a Heisenberg operator and carries the time dependence.

So, q h t has a complete set of eigenstates this is clearly seen from the expression the last expression on the previous slide. This q h t is equal to q q h t operating on the ket q comma t ket q comma t that time evolved ket gives you q into the q comma t this; in other words we are getting a eigenvalue q with the measurement performed by the operator q h t on this.

This is the working it is quite straightforward not much of explanation involved here, but it gives us this outcome and this outcome clearly shows that. Firstly, this q h t has the this states

q t this because the state q form the complete set of states of the operator q s therefore, q h t or q t also forms the complete set of states of the operator q h t right.

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So, that is one part, the second part is and as a consequence of this what I have mentioned we also have this expression that the identity operator can be written as the in the completeness relation as the integral of dq dash q dash t dash which will as you will see instead of q dash t dash we can also use the expression q dash t dash and the ket and the bra in this form in this form q dash t dash and q dash and t dash.

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ORTHONORMALITY
$$1 = \int dq' |q'\rangle \langle q'| \text{ which gives}$$

$$\int dq' |q',t\rangle \langle q',t| = \int dq' e^{+i\hat{H}t} |q'\rangle \langle q'| e^{-i\hat{H}t}$$

$$= e^{+i\hat{H}t} e^{-i\hat{H}t} = 1. \text{ Also,}$$

$$\langle q',t|q,t\rangle = \langle q'|e^{-i\hat{H}t} e^{i\hat{H}t} |q\rangle = \langle q'|q\rangle = \delta(q-q')$$

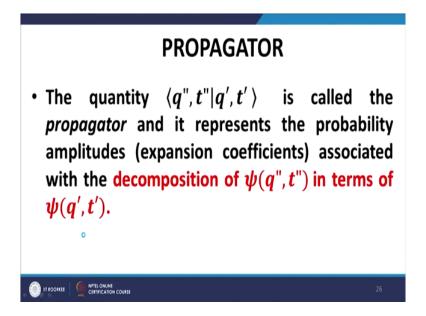
In other words this moving basis q comprising of these eigenstates q comma t is a complete basis that is the first part. The second part it is the orthonormality to see the orthonormality it is easily seen because the original states the Schrodinger states q dash form a complete set there can be written as a partition of unity.

And thereafter or as a consequences that you are multiplying or introducing these factors e to the power plus iHt e to the power minus iHt in the form as shown in this equation we find the time evolve state also obeying the relation of incompleteness integral dq dash q dash t q dash t is equal to 1 that is one part.

And the inner product as you can see also the inner product is unchanged as the states evolve q dash t of forming a inner product with q t gives us the direct delta function of q minus q

dash. So, the states that the basis that, we have talked about comprising of q comma t is complete and it is also orthonormal right.

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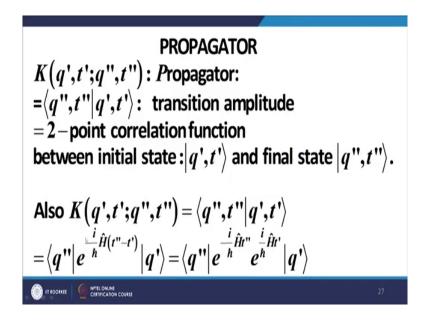
Now, we talk about the propagator, the transition amplitude represented by this expression the scalar product of q dash t dash q dash q double dash t dash and q dash t dash is what we call the propagator, it basically the transition amplitude and it is also given the name of the propagator. It represents the probability amplitudes associated with the decomposition of psi q double dash t double dash in terms of psi q dash t dash.

In other words you have initial state q dash t dash and the state evolves to or is expected to evolve to a state q double dash t double dash then this quantity gives you the transition amplitude the square of which or the modulus of the square of the modulus will give you the

probability of the evolution of this state that is the state q dash t dash evolving to the state q double dash at time t double dash.

Given the initial state q dash t dash the probability of it is evolving to this state q double dash at time t double dash is captured by the probability amplitude which is the scalar product and which is also called the propagator. Now, this propagator is also called the transition amplitude as I mentioned it is also the 2 - point correlation function because it relates to 2-points in space time.

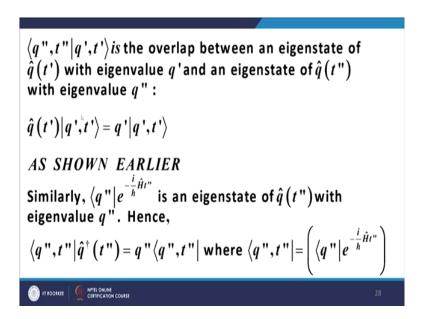
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And so that is the important at the we also use the notation in this form to represent this q double dash t double dash scale scalar produced product with q dash t dash in terms of the kernel or the green function which is K q dash t dash the initial state and q double dash t double dash.

So, the propagator is essentially the transition amplitude and it is also the 2 - point correlation function because it relates to 2 points in the space time continuum right.

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So, we can also express we also find because this is an inner product of these two states it is also the overlap between the an eigenstate of q t dash because the ket here is an eigenstate of q t dash and with eigenvalue q dash and an eigenstate of q t double dash with eigenvalue q double dash is quite simple to see that because of the property of the moving basis, the operator q t dash acting on this basis vector q dash t dash gives us the eigenvalue q dash.

Similarly, if we operate q double dash q t double dash on this particular operator q double dash t double dash we get the eigenvalue q double dash. So, the inner product is nothing, but the projection of the eigenstate of the operator q t double dash as a t dash with eigenvalue q

dash and the operator q t double dash with the eigenvalue q double dash. It is quite simple to see in using the property of the moving basis that we have done right.

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$$K(q',t';q'',t'') = \langle q'',t''|q',t'\rangle AS EVOLUTION OPERATOR$$

$$F/A, 1 = \int dq' e^{i\hat{H}t} |q'\rangle \langle q'| e^{-i\hat{H}t} = \int dq' |q',t\rangle \langle q',t|$$
so that
$$\Psi(q'',t'') = \langle q'',t''|\Psi\rangle = \int dq' \langle q'',t''|q',t'\rangle \langle q',t'|\Psi\rangle$$

$$= \int dq' \langle q'',t''|q',t'\rangle \Psi(q',t')$$

$$= \int dq' K(q',t';q'',t'') \Psi(q',t')$$

$$= \int dq' K(q',t';q'',t'') \Psi(q',t')$$

Now, the transition amplitude or the propagator that we have talked about is the represents the time evolution operator that is also easy to see here simple properties using the properties of the identity operator the completeness of the basis q dash and our moving basis q dash t dash subject to and q dash t dash the completeness of this basis and gives us this condition this decomposition of identity partitioning of identity.

And this that gives us what? That gives us that the wave function at q double dash t double dash which is the scalar product of q double dash t double dash with psi with the state vector psi, it can be written in this form by introducing the partition of identity. And this expression this part together with this integration gives us the partition of identity incorporating this

complete set of states in the moving basis we have this expression. And, now if you look carefully this expression is nothing, but the transition amplitude nothing, but the propagator.

So, this expression becomes the propagator and this expression is nothing, but the wave function at time t dash with position q dash. So, to repeat this integration over by introducing a complete set of states what we get here is q double dash t double dash q dash t dash q dash t dash phi psi and q double dash t double dash q dash t dash is nothing, but the propagator this part is the propagator. And q dash t dash subject to psi is nothing, but the nothing, but the wave function at q dash t dash.

So, what we end up with this expression and this expression can be written in this form and this is nothing, but our propagator. So, our propagator is nothing, but the time evolution operator, when this propagator acts on psi at q dash t dash we get the outcome of psi at q double dash t double dash. So, we can in some sense we can relate K q dash t dash q double dash t double dash as the time evolution operator, we will continue from here.

Thank you.