Dynamics of Classical and Quantum Fields: An Introduction

Prof. Girish S. Setlur
Department of Physics
Indian Institute of Technology, Guwahati

Path Integrals
Lecture - 27
Quantum Mechanics using Lagrangians

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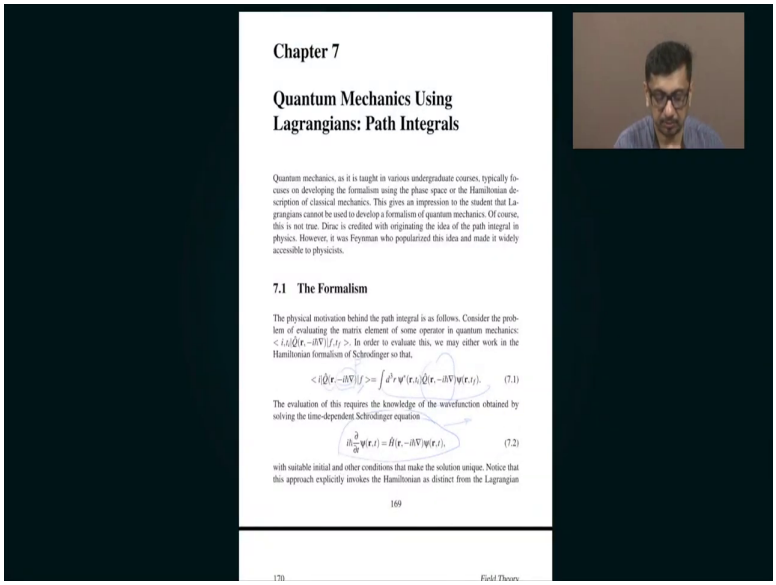

Ok. So, let us start this lecture with, this topic that I had briefly mentioned towards the end of the earlier lecture; and that is Quantum Mechanics using Lagrangians, which is another way of speaking of Path Integrals. So, normally you know in your undergraduate quantum mechanics you would have been taught quantum mechanics basically the subject using Hamiltonians; so that means, you would have been told that, in order to study quantum mechanics, you start with the Hamiltonian and you look at the generalized coordinates and generalized momenta.

And you now think of them as operators and you introduce commutation rules between the coordinates and momenta, and then your Hamiltonian becomes an operator and so on. So, that is the usual way in which quantum mechanics is taught. But then, that gives you a kind of biased view of quantum mechanics, as if somehow you cannot do quantum mechanics with Lagrangians.

Because after all you know in classical mechanics, it is a Lagrangian formalism that is taught first and the Hamiltonian formalism is usually less familiar to most students; because, we usually learn and especially in when solving problems, we use Lagrangians quite extensively in classical mechanics.

The Hamiltonian approach is used less frequently, but in quantum mechanics, it seems like it is the reverse, but that is not really an accurate statement or a meaning; even if that is the case, but it should not give you the impression that somehow Lagrangians cannot be used to study quantum mechanics. So, the whole purpose of this present today's lecture is to convince you that you can do quantum mechanics, with Lagrangians just as well as you can do quantum mechanics with Hamiltonians.

Of course, there is a catch in the sense that, there is a catch; obviously, because otherwise it would have been included in all your syllabus by now. So, the reason it why it is not frequently encountered in your syllabus that is discussing quantum mechanics from a Lagrangian perspective the reason why that is not included in many syllabi, at least at the MSc level is because, to do that you need to understand or you should already know how to do functional integrals.

So, that is exactly why I introduced that topic in the last few lectures and explain to you how to do functional integrals. It is only after you have developed some familiarity with that rather novel concept called integrating over function spaces, then only you are equipped to understand how to do quantum mechanics using Lagrangians. So, that is the reason why people do not discuss it that frequently. But now that, we know how to do functional integrals, we should not hesitate to understand how to do quantum mechanics using Lagrangians. So, let us proceed that way.

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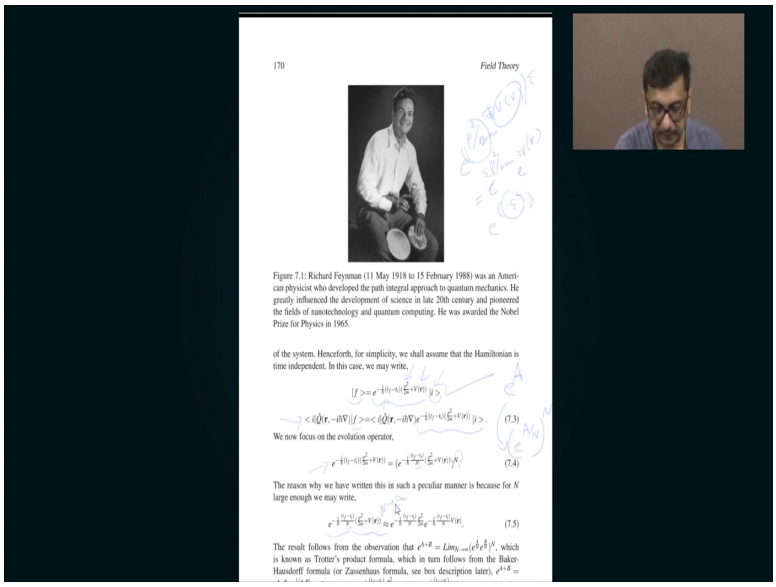

And so, if you remember towards the end of the last lecture I was pointing out, these facts that; so, in other words, see if you want to it is not clear entirely how we should proceed; because, see there is this Hamiltonian approach which involves eigen states and matrix elements right and expectation values and so on. So, the implication is that, you should be able to somehow reinterpret those concepts in a systematic way, such that you reach a stage where you are now discussing the same concepts now using functional integrals; rather than these more traditional concepts.

So, the idea is to start with familiar concepts like matrix elements and so on and systematically rework those familiar ideas, until you reach a stage where, now you are reinterpreting that, in terms of not only in terms of Lagrangians, but also in terms of integrals over function spaces. So, let us see how to do that. So, you see, in general, the in quantum mechanics, in the traditional way of doing quantum mechanics is the Hamiltonian approach to quantum mechanics, you are typically called upon to evaluate something like a matrix element like this.

So, for example, you could be asked to do a matrix element of this sort. So, for example, suppose q is the operator and you want to find the matrix elements of, of this operator between two states; I mean initial state and final state. So, the initial state could be for example, the initial state of some quantum mechanical system which evolves according

to some Hamiltonian; so and, so the initial state after a while becomes the final state which is f.

And now maybe you are called upon to find the matrix element of some operator which could depend on r and t; remember what that is that is just p vector; that is p operator. So, there is some observable perhaps Q r coma p; and you want to find the matrix element with from the with respect to the initial and final state. So, the final state determined by the time evolved initial state.

So, in other words the idea is that you have so to determine the final state, from the initial state you will have to necessarily solve an equation of this type. And, you know what that is; you know what 7.2 is that is basically, the time dependent Schrodinger equation. So, that if somebody tells you that this is the initial state, so this is the first order equation in time. So, you solve that and you get the final state.

So, the point is that formally you can always write this; in other words, the final state can always be written in a very especially, if the Hamiltonian is time independent. So, if you assume that, say the Hamiltonian is described by a kinetic energy like p squared by 2 m and a potential energy; I am talking about one particle ok. So, there is one quantum particle subjected to some force which depends on it is position.

So, it is a very simple example; it just meant to illustrate, how to get to the idea of path integrals from your traditional ideas of matrix elements Hamiltonians and so on. So, for that purpose, I am focusing on a problem that is incredibly simple; which is just one quantum particle subject to some force, which is derivative from a potential energy called V of r.

So, and that too that forces time independent; so your potential energy is time independent. So, if it is time independent then the final state is a very simple unitary time evolution of the initial state ok. So, that is all very familiar to us from our prerequisites; that is your elementary quantum mechanics.

You see now what we do is, now that you know what the final state is, because it is the time evolved version of the initial state; you insert that here and that is going to be your

actual matrix element of that observable Q that you are interested in. But now, keep in mind that if any operator ok so anything like any operator like this, can always be written as e raised to A by N whole raised to N; that is a trivial identity, because there is nothing; nobody will question this.

So, that is what I have written here ok. But the key is the following, that because I have put an N downstairs and I and this capital N is anything I want it to be; for any capital N this is an identity. So, specifically I will make, I will now pretend that N is really, really large. So, if N is very large, I can make this approximation. So, I can see normally I cannot write e raised to p squared by 2 m plus V of r as e raised to p squared by 2 m into, e raised to V of r, I cannot do that; regardless of whatever else is there.

See the reason is that, because these two do not commute; kinetic energy and potential energy do not commute right. So, because of that I cannot do this. So, if in classical mechanics I can do that, but in quantum mechanics, I cannot do that; so, they do not commute. But however, if I because there is an N next to it.

So, because of the coefficient next to this are very very small, I can do this because the whatever corrections, whatever mistakes I have encountered, I have incurred by doing this, will be actually small by a factor of epsilon. So, that mistake tends to 0 as 1 by n tends to 0. So that means, if capital N is very large I can still do this. So, this becomes exact as capital N tends to infinity.

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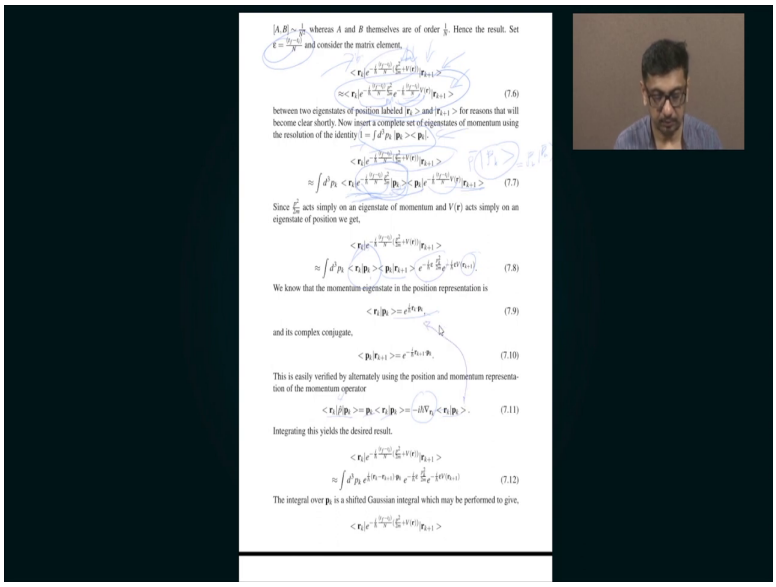

So, that is the reason why I introduced that capital N in the denominator. So, it is only then you can and you can justify this. So, this is called trotter product formula, this is an exact mathematical result, which says that e raised to A plus B, where A and B are operators that do not necessarily commute with each other.

So, if you have e raised to A plus B, you cannot simply blindly write it as e raised to A into e raised to B, because A and B do not commute, but if they do not commute you can still write it as something which only has A and something only has B, but only in this way. So, in other words, you have to write it as e raised to A divided by N, into e raised to B divided by N; then you have to whole raise it to N; then only it is correct and N tends to infinity.

So, you might be wondering why am I doing all this, and I mean obviously, I am doing this, because I know that by following this procedure, I will get to what I am interested in; and you should never lose track of what you are interested in. And what we are interested in is basically, going from a Hamiltonian description of quantum mechanics to a Lagrangian description of quantum mechanics. So, that is what we are interested in and the claim is that if you follow this procedure, you will get there sooner or later ok. So, let me go ahead and proceed that way.

So, now what I am going to do is that, I am going to imagine that there are certain; so, regardless of what I am going to introduce some new states, which I call r of k. So, r of k is basically some state some eigen state of position of that particle, where the eigenvalue of the position comes out as r vector subscript k.

So, if you act the position operator on this, this is going to be r of k acting on r of k; so that means, this is the eigen value. So, I am going to introduce this; so, you just have to bear with me because a whole bunch of new concepts that I am throwing at you, and it is not clear what the motivation is; that I am just saying consider this, let us imagine that this is there and so on.

But, you will soon see why I am doing all this. So, if suppose I introduce an eigen state of position of the sort, then the matrix element of this object, between two eigen states like r of k and r of k plus 1 ok; so the implication now is that, that k is some kind of a discrete index. So, the matrix element between these two is what I want to evaluate.

But to evaluate this, I am going to use my simple trotter type of decomposition. So, I am going to write an operator which involves these two non-commuting operators in the exponent, which is the kinetic energy p squared by 2 m and the potential energy which is V of r ok; these two are non-commuting, but then; so, they appear as a sum in the exponent, but the claim is that I can still write them as products; means, they do not have to retain them as some in the exponent.

I can write them as a product of two operators, one is only involving kinetic energy; the other involves only the potential energy. So, that is because a capital N is sufficiently large and any mistakes I make are of the order of 1 by N smaller than the what is correct ok. And, the mistakes tends to 0 as n tends to infinity. So, this is now; so, evaluating this is same as evaluating this. So that means, evaluating the matrix elements of this unitary operator which describes time evolution is same as doing this.

So, the reason why doing this one is simpler than the starting original question, is because now you see, now that I have written it as a product of two things, I can insert a complete set. So, I can insert a identity written in this funny way. So, you all know that;

so, I can think of p of k now as an eigen states of the momentum operator, whose eigen value is now p of k ok. So, this is what that is.

So, now if this is the eigen state of the momentum, then it obeys a completeness condition. So, this is called a completeness condition. So, you should know all these things I mean, quantum mechanics is a prerequisite for this course. So, I am going to assume you know what I am talking about.

So, if that is the case, then because this is identity; I can simply insert an identity here, I can insert identities wherever I want; but specifically I am going to insert it in between this operator, which involves only the kinetic energy and this is operator that are only involves the potential energy.

So, if I inserted here, so now, answering the original question which is what is the matrix element of the time evolution operator between r k and r k plus 1, answering that question is the same as, first finding the matrix element of the sort which is between a position eigen state and a momentum eigen state of an operator that only involves the kinetic energy, times a similar matrix element involving only the potential energy.

So, the bottom line is that this is easy to do, because you see because p k is an eigen state of momentum, this particular whatever I am circling now, has a very simple answer and that very simple answer is, it is just replace this operator p squared by p of k, squared; because you see p is now an operator which acts on the eigen state of momentum; it just simply becomes, it is eigenvalue and it goes outside and then you just get this one.

So, r of k p k, times this one ok and epsilon is basically this t f minus t i by n ok. So, epsilon is that t f minus t i by n. So, that is what you get. So, this simply becomes, this matrix element; the first matrix element of this evolution involving only the kinetic energy, between r k and p k is simply the matrix element of r k and p k times something which involves the eigen value p k ok.

So, similarly the matrix element of the time evolution involving only the potential energy, between p k and r k plus 1 is also simple; because now you see, V of r involves the position operator r, but now it is acting on an eigen state of position, whose

eigenvalue is r k plus 1. So, what does that mean; that means, we can simply replace, the position operator r, even though it is inside b of r; you can simply replace it by its eigen value which is r k plus 1.

So, instead of having operator V of r, we will have this number V of r k plus 1; because, r k plus 1 is the eigen value of r operator. So, now, it just becomes a number which is V of r k plus 1; and then you get back your matrix element which is remaining; which is p k and r k plus 1. But now you all know from your quantum mechanics that, the matrix elements of r and p is just this exponential e raised to i r dot p by h bar.

If you have forgotten how to conclude that, it is, it comes from this; that, suppose you want to calculate this, this is same as; because p acts on p k and produces p k as the eigenvalue, but alternatively in the position representation, it is just this. And, the dependence of r k is only this. So, it does I mean in the position representation, I mean the operator acts on r k not on p k. So, you get this. So, since these two have to be equal, this is equal only if this is true ok.

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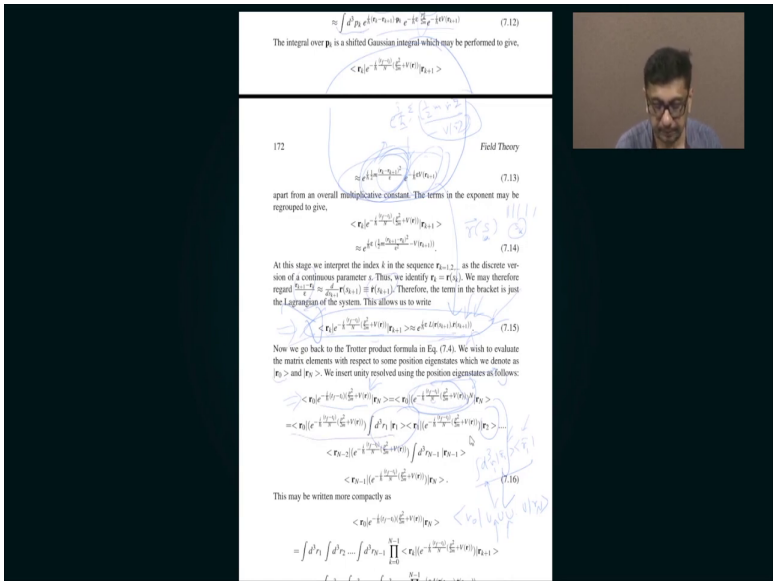

So, I am going to assume you know all that; that is just quantum mechanics; it is not part of this course, it is prerequisite. So, bottom line is the matrix element that I was originally interested in finding which is the entire evolution operator, between r k and r k

plus 1 is now, therefore, given by this integral over that complete basis, which is integral over all the p k's times whatever it is that we have, found along the way; which is this times this times with the rest of it ok, which is this.

But now, so, you see now things are beginning to look up; because, we have looked at I mean looks doable now and in fact, it is doable, because you see certainly the integral over p k is what we have to do and that is very doable. Because, it is just a shifted Gaussian, there is a Gaussian e raised to something times p squared, and there is a something involving only the linear term; and that is very easy to do and it just a shifted Gaussian and you simply do it.

And when you do it you get this answer ok. So, the answer to that original question what is the matrix element between r k and r k plus 1 of the entire evolutionary operator, the answer is this ok. So, now, you see, now I am going to do the following. So, I am going to assume, that this k in this sequence that I have introduced, is actually the discrete version of some continuous parameter right.

So, I am going to assume that r depends continuously on s and I have divided this s into various pieces and r k means, the piece where that r depends upon that particular value of s at the index k. So, in other words, r k is basically; so, you will have to imagine that r is now following some path, parameterized by s.

And now that path has been broken up into pieces, which is why it is called r k. So, r k is the k th location of that path ok. So, I mean I am entitled to make that re interpretation because it was I who introduced that concept of r k and I can choose to give it whatever meaning I desire. So, I decided to I decide that is the meaning, that , I am entitled to do interpret it and any way I want ok; because I was the one who introduced that.

So, the point is that r k plus 1 minus r k by epsilon, therefore, now has this interpretation, of the slope of the path along; basically, it is the slope of the path as parameterized by s. So, it has that meaning ok. So, that is the meaning of this ratio. So, if you interpret it that way and that is how we are going to interpret it; this is going to be, like this. And why is that? Because you see; now this is going to look like see what is this? It is e raised to i by h bar, times epsilon, into 1 half m into r dot squared because you see this.

So, what is going to be here is r k plus 1 minus, r k divided by epsilon whole squared and what is r k plus 1 minus r k divided by epsilon it is r dot. So, basically what you will get is, r dot squared. So, that is what this one, this will become. So, this whole term will become e raised to i by h bar into epsilon into half m r dot squared. And what is half m r dot squared? It is basically, the kinetic energy; and now, what is this? This is nothing but minus V of r.

So, now, you see there are no operators; keep in mind that, now we are dealing with matrix elements; so, after calculating matrix elements, there are no operators left; we have explicitly evaluated them. So, these are all numbers now; no operators are here; r k is an eigenvalue, r k plus 1 is also an eigen value. V of r k plus 1 is the value of V at the eigenvalue r k plus 1. So, they are all numbers basically.

So, therefore, I can happily put this in I mean; now there is no issue like e raised to A plus B, not being equal to e raised to A into e raised to B, that issue does not arise because, these are actually numbers now not operators. So, in that case, you simply combine it this way, and now you know what that is; once you combine its half m V square into r dot squared minus V of r. And what is that? It is obviously the Lagrangian; because, half m r dot squared is half m V squared; which is kinetic energy and V of r is potential energy.

So, that is basically the Lagrangian, which is what I have written here. So, it is e raised to I, i by h bar into epsilon into the Lagrangian ok. So, that is as far as the answer to this question is concerned. But that was not my very starting original question; this is some intermediate step. So, I asked what is the answer to this so, what is the answer to the matrix elements between r k and r k plus 1 of this evolution operator raised to 1 by N and the answer is this.

So, it is nice to know; is it not because this is this involves a Hamiltonian, because it is p squared by 2 m plus V of r, which is basically Hamiltonian and the matrix elements of that between r k and r k plus 1; there is a position vectors eigenvalues, that matrix involves the Lagrangian now. So, the left hand side involves Hamiltonian, right hand side involves Lagrangian. So, now, you see where we are getting at.

So, in other words, I told you the whole purpose of today's lecture; and that is, to do quantum mechanics using Lagrangians. So, the original question involves matrix elements involving Hamiltonians, which is the left hand side of this. But then, with a suitable interpretation and you know by series sequence of steps, I now I am gradually converting that question to something involving only Lagrangians ok.

So, the Hamiltonians have gone away and in the place of that, I am getting Lagrangians ok. But still that is not the whole story; that is just an intermediate step. And, what is that an intermediate step of. So, the and it is the intermediate step in the following sense, that it is basically, so this is what I originally wanted right, I wanted to know, what is this. So, instead of calculating this, I have written this in this way, and then I am calculating the matrix element of only one of them; not the whole raised to N.

So, now I have to answer the original question; what is the matrix element of Q? That was the original question. So, this is some interesting intermediate step. So, let us go back to 7.4 ok. So, this is so this is what whose, in fact, we want the matrix elements. So, typically we can always think of this as for example, suppose i was some initial position.

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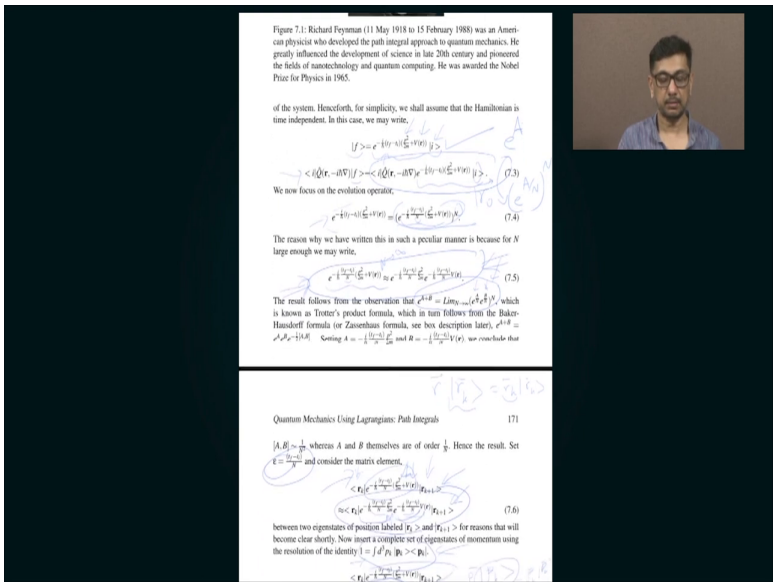

So, eigen state of some position vector; it could be anything, so for simplicity, we think of i as the initial state, as the eigen state of position with eigen value r 0. So, imagine,

suppose the initial state had a well-defined position; that means, the particle had a well-defined position and so, the initial state was prepared in such a way that the particle is exactly at r 0.

So, now, the question is, how would you; therefore, so, if that is the case, then you would typically answer such questions ok. So, I mean right now I will let me just keep it general. So, imagine that r 0 is my initial state so, in this path ok. So, this path, so remember that, r k is one of the pieces of the path. So, I have interpreted it like that. So, now, I want to suppose, I want to calculate the matrix element between r 0 and r n.

Because, I have decided to break it up into all these pieces. So, if this is the question I want to answer. So, I will tell you later, why this is a valid question to answer; right now it is not clear. But suppose, this is the question I want to answer; that is I want to calculate this matrix element ok.

If that is the question I want to answer, then answering this is same as writing like this, first; because, then I put in a N and raise it to N th power this is anyway; obviously, an identity. But now, you see what is this, this is something some operator raised to N. So, that is in other words is the same operator multiplied N times is the some operator, you know N copies of the same operator one next to the other.

But, so, instead of writing that as just N copies of the same operator U, U, U, U like that, I will simply insert an identity. So, I will resolve the identity and write like this. So, I will put identities here. So, I will put identities of this kind, I can put identities of any kinds, but specifically in the first gap between two of these U, U means this one. U means whatever is here; this is my U. So, this is U raised to N.

So, it is the matrix element of U raised to N between r 0 and r N; instead of inserting anything I want, I can insert any way of resolving the identity, but specifically, in the first gap between two U's I will insert that is I will resolve the identity in this way, involving eigen state r 1 and it is ad joint; and similarly, in the second gap I will put r 2 and so on and so forth. So, I will resolve using r 2 etcetera, etcetera. So, that is the whole idea. So, I have resolved it this way ok.

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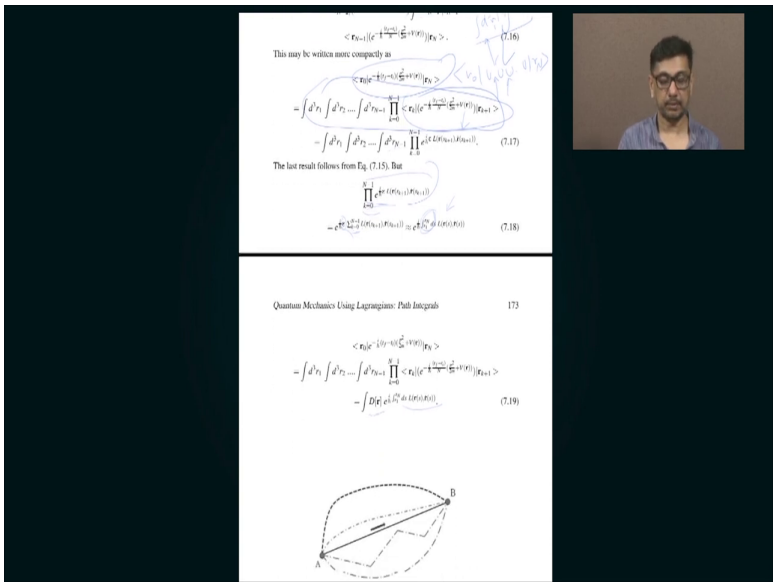

So then, so that is easy, because now you see it will then have this flavor; it will then have, it is the same as doing this. So, writing this now, after having resolved it like that, it is the same as now doing this. Because, it is now going to be a successive product of matrix element between r k and r k plus 1 which is what that is ok. So, now, this matrix element we have painstakingly evaluated and we have realized that basically even though it involves a Hamiltonian to start with it is answer involves now a Lagrangian ok

So, that is what that is. So, it will the final answer to that matrix element even though the original question involved a Hamiltonian; it is matrix element the final answer involves the Lagrangian. So, the final answer between these two r 0 and r N is actually an integral over all those intermediate positions of the particle, all the way starting from r 0 all the way up to r N. So, now, I am going to reinterpret this this type of product, this product of an exponential is really exponential of the summation clearly.

So, now you see the epsilon into sigma, has the quality of an integral; because, that is what the definition of integral is. It is just divide up into small pieces and each piece has size epsilon and you add up all of them, you get an integral; that is what integral means. So, I am just adding up all the small small epsilons so, when I, if I add up small small epsilons, I am effectively doing an integral. So, that is what that is.

So, rather than write it as a discrete sum, because now, N tends to infinity and there are infinitely many pieces, but then the distance is r 0 and r N; are the end points. See remember that N has to tend to infinity; because, otherwise that, that kind of separation is not valid; this is wrong if N is not tending to infinity. So, I have used this explicitly in my in all the steps.

So, I have no business to make this statement unless N is very large. So, it; so when N is very large you see, that all the summations become integrals and that path becomes smooth and continuous; rather than discrete. So, then you are integrating now over a path ok. So, and you are integrating over all the intermediate points in the path. So, that is why it is called the path integral ok; so, integrating over paths.

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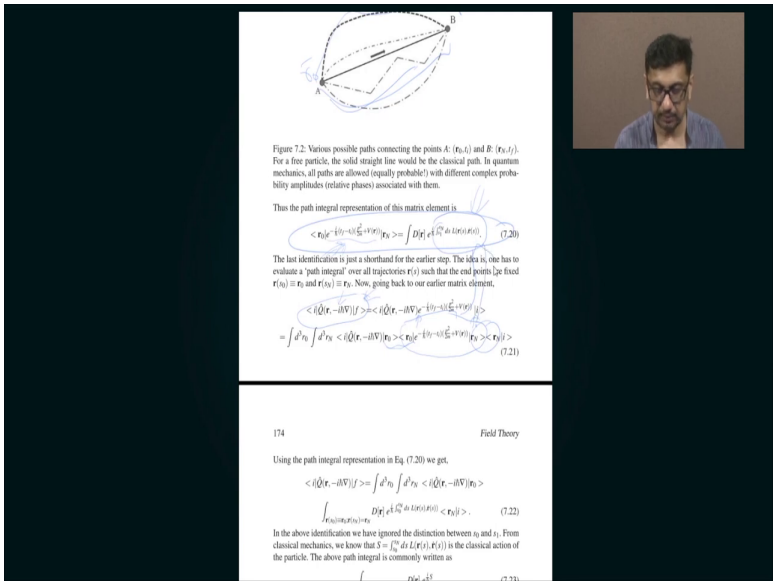

So, this is my r 0, this is my r N and you are integrating over all paths that connect r 0 and r N. So, that is what the. So, now you see, why I said you need functional integration; because, r is a function of some parameter s and you are integrating over all possible such functions.

So, that is what that path integral is; you are integrating over function spaces because, r is a function of a real variable called s. And you are not; you are integrating over s, but on top of that you are integrating over all such possible functions, which depend on s;

that is you are integrating over all possible r bracket s; all paths connecting r 0 and r N. So, that is the whole idea.

So, therefore, if you want to calculate a matrix element of an evolution operator like p squared by 2 m plus V of r; that means, an evolution operator corresponding to that Hamiltonian; and the matrix N element is between some initial position r 0 and final position r N. The answer is basically a path integral, of the integral of the e raised to i times the action, i by h bar times action. So, this is called the action ok.

So, the time s is now, you can think of it as time if you want, but you do not have to, but basically it is some parameterization. So, it some parameterization such that, when s is the initial value it is r 0, is the value of r for the path, and it is r N; when it is the final value. So, that is certainly the action in some sense. So, in any case s has the dimensions of time; because, yeah that is how we have defined it right; because it is basically delta s is t f minus t i by N.

So, basically the matrix elements of this time evolution operator which involves only the Hamiltonian, is now a path integral over all possible paths connecting r 0 and r N. So, now, coming lastly to the my very original question; what was the original question. So, the claim was that in quantum mechanics, the most general question, that you can answer that is of practical utility is, find the matrix element between some initial and final state of some observable, some general observable Q, with a function of position and momentum.

So, now we are equipped to recast the answer to this question, in terms of a path integral. And why am I saying that. So, the reason is because now you can insert, your. So, here, I am going to insert a complete set. So, this; so that, I am going to insert an r 0 here, because now this is going to involve, integral over r 0 and now I am going to insert a r N here.

So, I am going to insert an r N there ok. So, when I do that; so, I can always do this because, these are complete sets. So, it is like inserting identities there. So, now, once I do that, I will now get this one. And this is what we have painstakingly just now evaluated; we have just evaluated that.

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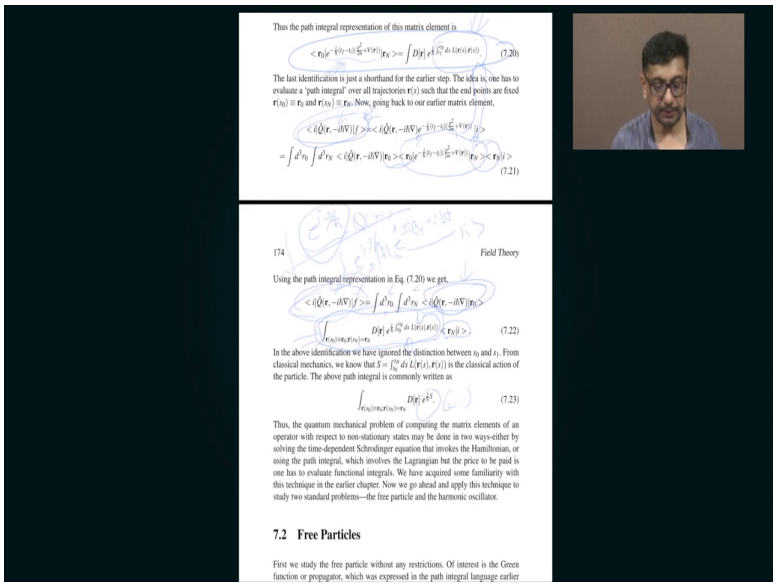

So, therefore, the answer to this question, that is what is the matrix element of some general observable Q, from some initial state some general initial state to some general final state, is basically given by integral over r 0, r N of, of the matrix element with respect of this Q from i to r 0 times this path integral over all paths connecting r 0 and r N, times this overlap and then finally, you do this integral.

So, so, once you; so, you see. So, the answer to this question involves, first doing this path integral and then doing the rest; I mean the rest is, not related to path integrals; but the important thing is that, somewhere in between you have to do a path integral and that path integral involves a Lagrangian rather than a Hamiltonian. So, that is the thing. So, so here the so, original question if you want to answer using your undergraduate level of quantum mechanics, you would write f as e raised to minus i, t f minus t i times h which is Hamiltonian right.

You would write it as initial state times evolution; evolution involves Hamiltonian. And then, you would evaluate this in the usual way. But now, I have rewritten this in terms of the Lagrangian rather than Hamiltonian, but the price I have to pay is that, instead of using familiar concepts like overlaps and operators and all that. Now, I have to work with a path integral over all the functional integral over all paths, connecting two points; and only then I can then evaluate this matrix element.

So, in general, the prescription is the following that, if you want to find the expectation value or basically anything, you just have to multiply that by this e raised to i by h bar into action; and integrate over all paths, keeping that next to that; whose, suppose you want to find the expectation value, it is very simple interpretation.

You think of this as your weight. So, expectation value of any quantity which depends on the path for example. So, you multiply that quantity which depends on that path, by this weight which is e raised to i by h bar into action, you integrate over all paths, then divide by the normalization. Normalization is e raised to i h bar divided by N times integrated over all paths ok. I think this is a good time to stop and in the next class, I will be discussing, the applications of the path integral approach ok.

Thank you.