Quantum Physics
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Lecture No. # 07

Let us know how we could write down the evolution equation for the state vector Schrödinger equation for a simple model system namely; that of a particle moving in one dimension. That will give us a hint to what this Schrödinger equation should look like in more complicated cases. Let me look at a free particle moving on a line. This is the simplest of motions. This does not involve potential of any kind. So let's start by writing down the following.

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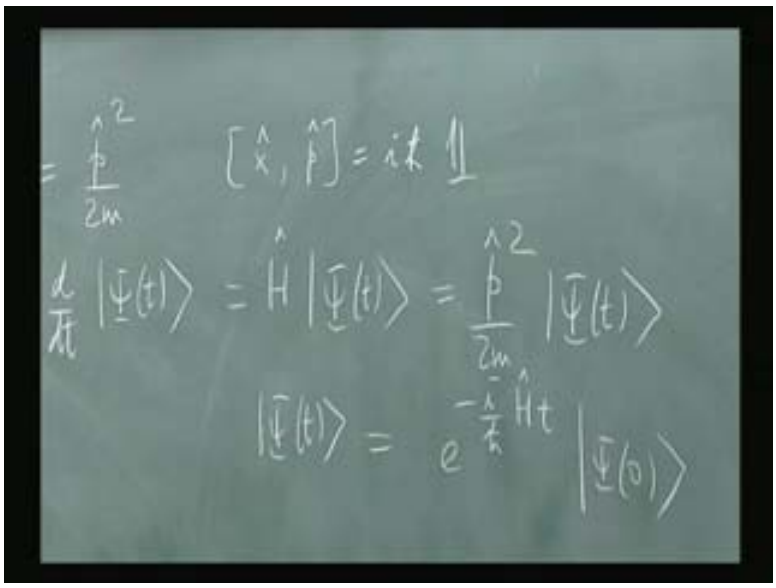

Let's write the Hamiltonian of the system of a particle moving on a line which is along the x axis. The way you go about it is to write classical Hamiltonian down which is p squared over 2 m. It's a single component. So there is no vector here. It is just on the x axis and that is the Hamiltonian. There is no potential energy at all. The version of this is the classical Hamiltonian. The quantum version of this is to say that the Hamiltonian operator is p operator squared. This is the momentum operator over 2m. Now remember that with every physical observable by postulate, we associate a self adjoint operator with real Eigen values. So this operator is a function of that operator here (Refer Slide Time: 02:55 min). Now we would like to write down the Schrödinger equation. The Schrödinger equation for this particle could be ih cross d over dt psi of t, that's a capital psi of t for the state vector, is equal to the Hamiltonian operator acting on psi of t. and we have to solve this equation and of course this is equal to p operator squared over 2m on

psi of t and one would like a solution to this equation given the initial state. The formal solution states that psi of t at any instant of time is equal to e to the - i over h cross H operator t acting on psi of 0. So you have to take the momentum squared operator multiplied by this constants, exponentiate it and act on the initial state in order to find this state at a latter instant of time. This is quite a formidable task but what is it we finally want to look at and what are the attributes of this particle? Well it's a particle moving in one dimension, then classically it has a coordinate x and a momentum p and these are the canonically conjugate variables such that this is equal to 1. That's the classical Poisson bracket relation. Quantum mechanically, this would become x operator p operator = ih cross times the unit operator because according to a rule for quantization, Poisson brackets go to commutators divided by ih cross. So we would like to find out how to exponentiate this operator here and how to act on that. Now whenever you have operators, vectors and so on.

You always choose a coordinate system. Only then can you write down the actual components of a vector. In exactly the same way, whenever you have an abstract problem of this kind in quantum mechanics, you must choose a basis set in terms of which you express everything else. As you realize, once you give me a cartesian frame, I could write down the numerical values of the components of a vector. Otherwise the vector remains an abstract vector. In exactly the same way, I would like to choose a basis. Now we have to choose the basis that would be convenient for this problem. Well the basis consisting of eigen states of some physical quantity are associated with the particle. Now its position and its momentum are the physical quantities associated with this particle. It has no other physical attributes whatsoever. Everything else is derived as a function of these two things. Therefore one would like to use a basis and let me call it the position basis.

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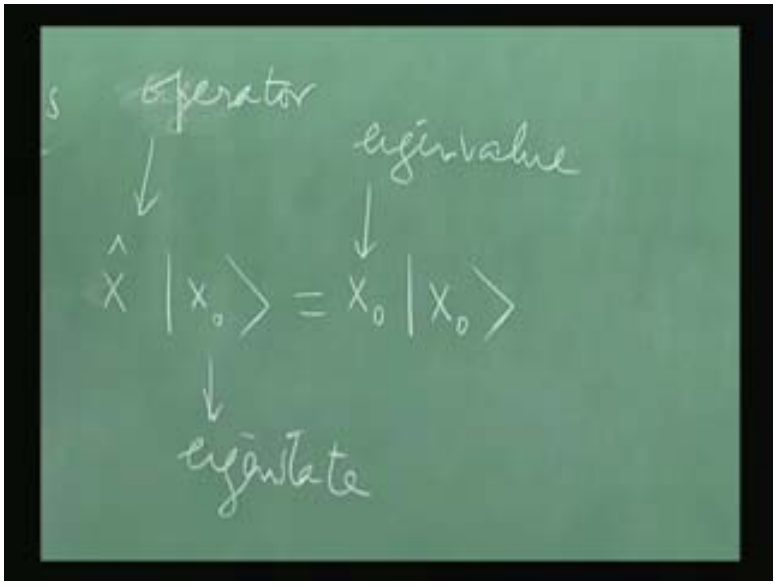

Of ket vectors which are eigenstates of the position but what are the possible values of the position. It's every number from - infinity to infinity. Therefore I introduce a set of vectors and let me denote it by just x here. Let me introduce a set of basis vectors such that x operator acting on a particular x say $x_{0.}$

This is an eigen basis, in the sense the position operator acting on this ket vector labeled by x_0 gives you just x_0 acting on x_0. This is an eigenvalue equation. I should really put psi here and put subscript x_0 to show you that this is the state vector corresponding to position x_0 but that's just a clutter of notation. So whatever is inside the bracket is already the label for the corresponding Eigen value. Minus infinity to infinity are the possible values that x_0 can take. I formerly introduced such a basis. Now this basis is different from the ones you have been used to a little earlier. It's a continuous basis because its not labeled by 1, 2,3,4,5, etc. Now therefore if I orthonormalize it and there are technical problems here with the continuous basis but we will not worry about them for the moment.

If I pretend that I can define rigorously a continuous basis, then the orthonormality relation what would that look like x with x prime = 0 unless x = x prime but it's continuous. So instead of the Kronecker delta we have the Dirac delta. So this is delta of (x - x prime) where x and x prime refer to the Eigen values corresponding to ket and bra here in this problem. They are numbers. These quantities inside the ket or bra are labels. This is orthonormality (Refer Slide Time: 09:29). Let's go back and look at the relations, phi $_n$ phi $_m$ = delta $_{nm}$ and summation over n phi $_n$ phi $_n$ = the unit operator. The first relation is orthonormality and the latter is completeness. You would need an integral instead of a summation here which becomes integral dx x with x = unit operator. This is completeness.

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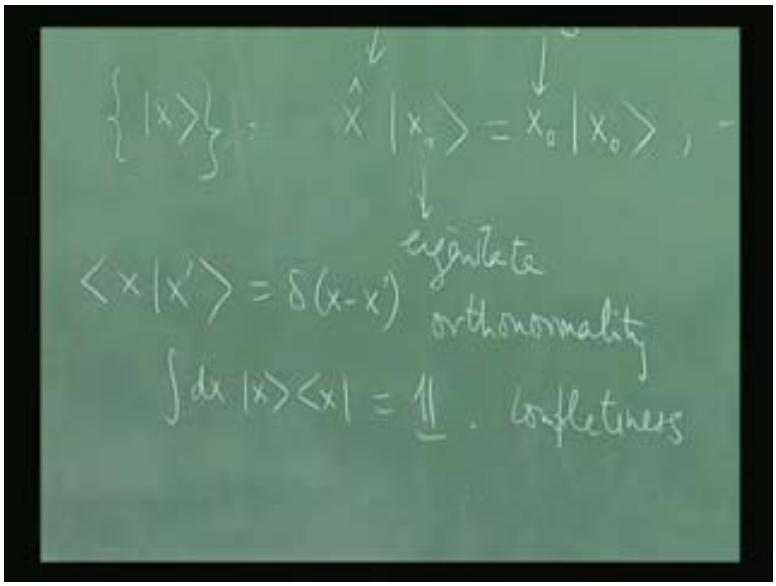

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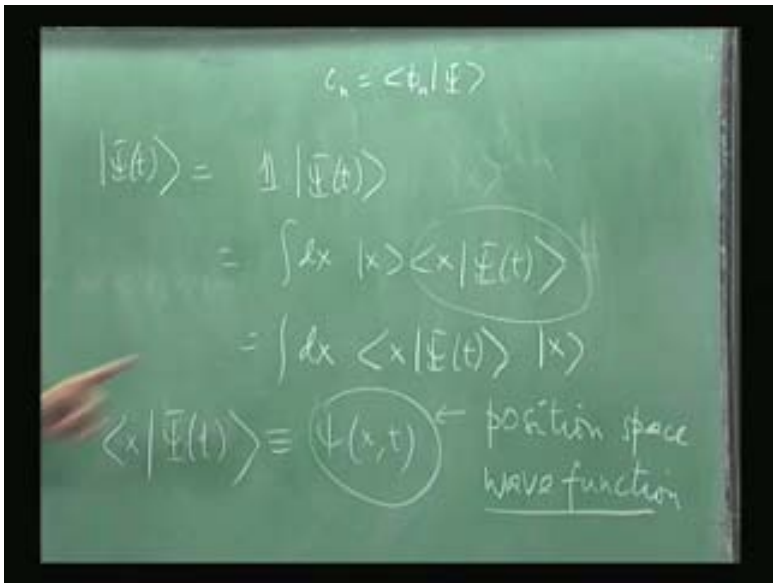

Now come to the probability interpretation because if you give an arbitrary state of the system, psi of t, i can expand this in the orthonormal basis. Therefore I can write this as equal to a summation over n if I have an orthonormal basis, labeled by a number n its of the form c_n phi $_n$. That is the way you normally would expand this but now I must replace this by an expansion in continuous basis. Therefore I have an integral over dx here (Refer Slide Time: 11:19), an x here and c_n was equal to phi $_n$ psi. So in the place of c_n, I put a

bra vector x and psi of t. please notice I could have moved it to the right hand side and use this fact that ket x bra x is just the unit operator.

I mean that you could have written psi of t = one times psi of t = integral dx, x, x, psi of t. but that is equal to integral dx x, psi of t with x because this is just a complex number. Therefore you can move it back and forth. but the coefficients are not labeled by a discrete number n but by a continuous index x. x psi of t = some coefficient c_x of t and this can be replaced by psi of x,t since it is the expansion of the vector psi on the left. The t dependence comes from the t dependence of the state vector and the x dependence comes from this scalar product of this state. This quantity is the probability amplitude that when this system is in the state psi of t, it is in the position Eigen state with label x. The mod squared of this is the probability amplitude or rather probability amplitude density because it is now a continuous variable that the position lies between x and (x + dx).

If I multiplied by dx, I get the probability that the position lies between x and (x + dx). Bra x ket psi = psi of x, t and we call psi of x, t as the wave function in quantum mechanics. We will write down differential equations for it and so on but it's just the coefficient in the expansion of an abstract state vector in the position basis. Since it is in the position basis, I call it position space wave function. It is the wave function in the position basis. It is it is the coefficient in the expansion of the state vector of a system in the position basis. Of course if you are working in three dimensions, then it's not label by just one number here but by x, y, z or r, theta, phi. You could express this coefficient either in polar coordinate, spherical coordinate or Cartesian coordinates.

So please appreciate the fact that the t dependence here comes from the dependence on t of the state vector. That's dynamics. The x dependence comes because you happen to have chosen the position basis in which you expand your state vector. Now after all, this particle has a momentum, you can choose the momentum basis and the Eigen states of momentum. So the Eigen value equation would have ket vectors p labeled by p such that p operator acting on some particular momentum Eigen state p_0 would give you p_0 times ket p_0. And this (Refer Slide Time: 17:45) immediately becomes p with p prime = delta of (p - p prime). This would be integral dp and then a p with p which is the unit operator.

Now this can be expanded as we did it with position basis and I get psi integral dp p with psi of t p ket vector.

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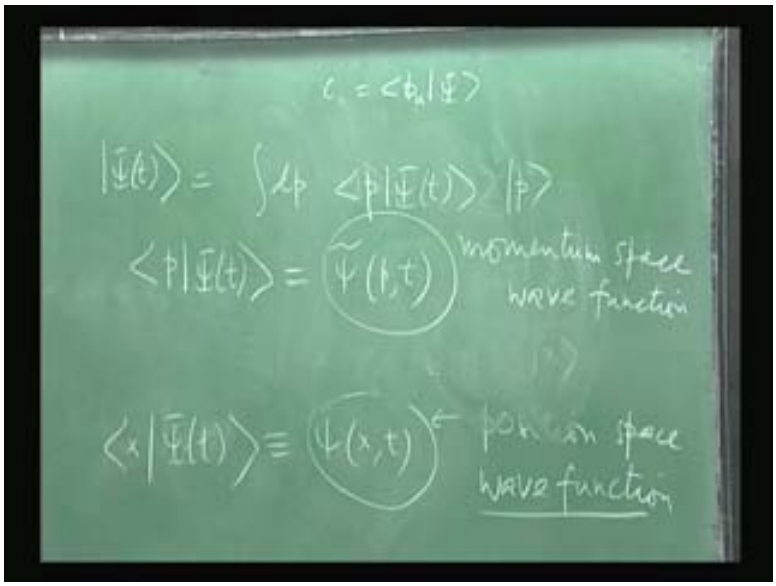

This wave function in momentum space can be called as psi tilde of p,t. This is called as momentum space wave function for the same state. What would the mod square of this be? It is the probability density that the momentum has a specific value p. You could ask what is the value of the position in that momentum eigenstate. We come to that slowly. They cannot be simultaneously made sharp. The point is momentum eigenstate cannot be a position eigenstate and a position eigenstate cannot be a momentum eigen state which brings us to the next question if I give you two operators corresponding to a physical system, can I find the simultaneously eigen state for them or not. we are going to answer that very important question shortly but first let us know the relation between psi of x,t and psi tilde of p,t. It is just a change of basis so we can knock this off right way.

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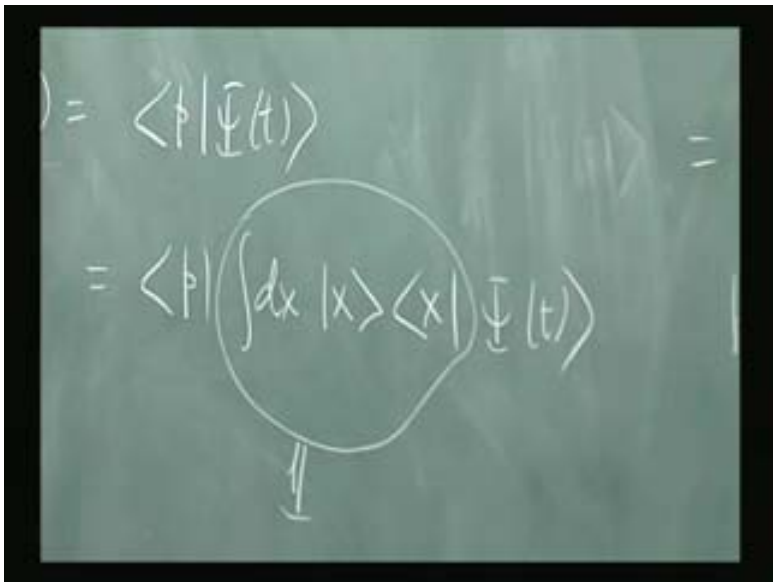

Psi tilde of p , t = p with psi of t and I want to relate it to psi of x , t. Let me insert the unit operator which can be written as integral dx ket x with bra x acting on psi of t. Bra x with psi of t is the position wave function psi of x,t. so we have this crucial relation which says psi tilde of p , t = integral over dx p, x psi of x , t. So the momentum space wave function is related to the position space wave function by this relationship. And what does the physical meaning of p, x is the probability amplitude when the position of the particle is x, its momentum is p. and of course we know at back of our minds we are going to prove this. we are going to find that number p,x. this thing here you know from the uncertainty principle that if you specify x sharply, the uncertain thing p becomes infinity because when delta x goes to 0, delta p must be infinite so that the product can be remain greater than h cross over 2.

This means all possible p's must contribute and that this is a number whose modulus squared is independent of p. we will compute the number p,x backwards from the commutation relation. This number will turn out to be e to the power I p x over h cross where p and x are numbers. They are numbers here because of the labels here. These are kets corresponding to certain labels. If integral over x e to the ipx psi of x, t this is the result, you call it the Fourier transform.

Then psi of x, t as a function of psi p, t in terms of psi tilde would look like exactly the same thing. Psi of x, t = all p's x with p , x with p and psi tilde of p,t. x, p is the complex conjugate of p, x. The number x, p would be e to the power – i p x over h cross. Therefore it's the inverse Fourier transform. One can see how for canonically conjugate variables like x and p; coordinate and it's generalize momentum, Fourier transforms automatically enter the picture. The description of the abstract state either in the position

basis or in the momentum basis is completely equivalent. You might want to do one or you might want to do the other depending on which ever is easier in given problem.

In most cases, it's easier to work in the position basis for a reason which will become clear very shortly but it's not necessarily always true. there are important problems where it doesn't matter which basis you work in. and if I look at the motion of a particle in a potential, so the Hamiltonian now is p squared over 2 m + a potential energy which is a function of the position operator. When you have a Hamiltonian like this, if I take a particular x_0, a position ket vector and I apply H to it. So H acting on it is p squared acting on x_0 over 2 m + V of x acting on x_0.

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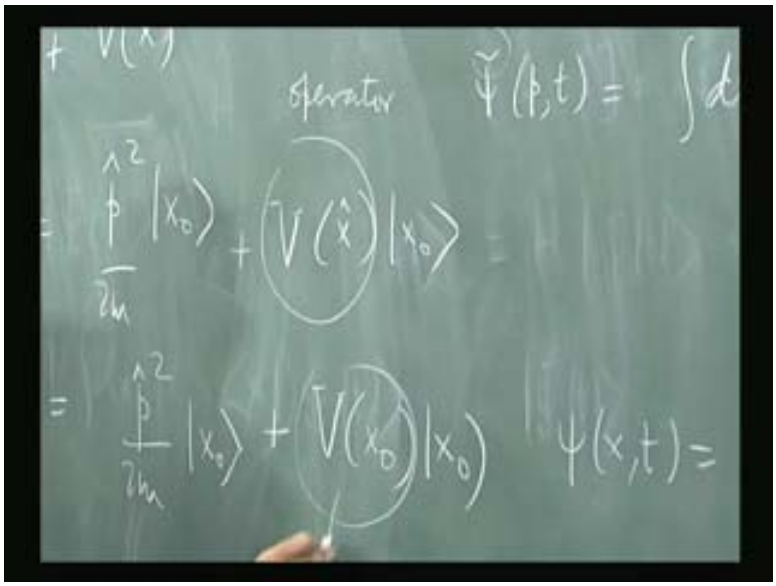

We don't know a priory what is the first term equal to because we don't know action of p on that. Well, x operator acting on x_0 produces x_0 times x_0. So any function of x operator produces the same c number function. So the second term becomes equal to V of x_0 on x_0. This (Refer Slide Time: 28:03) is an operator and this is just a function because this is an eigenstate of the position operator. Therefore any function of the position operator is still an eigenstate. This step is crucial. If you did the same thing with the momentum eigenstate, I apply H to a p_0, we would have a p_0 here and p operator acting on it. So would just be p_0 squared upon p_0. The second term is V of x acting on p_0. Unless you tell me what is the effect of x operator on a momentum eigen state, I can't proceed further. But you immediately see that this V of x could be quite complicated. On the other hand, the kinetic energy is always p squared over 2 m in this situation.

Therefore if I find what p operator does on x_0, all I have to do is to find what p squared does. That's a fairly simple task but V of x could be a horrible function which may involve exponentials, logs and functions and that would have to act as operator on p_0.

This is why since the kinetic energy is always just the square of the momentum, but the potential energy is not a simple function of x in general, you have problems. the harmonic oscillator is the situation one can think of where it doesn't matter which basis you use because that is the case in which you get x operator squared and its completely symmetrical. Now you see the special role played by the harmonic oscillator. That is one in which the position and momentum basis are completely equally difficult or equally simple. So it is a very special Hamiltonian because this quadratic formed in x and p it's completely symmetric under the interchange of x with p. that doesn't happen in other problems. This is why a normal potential problems, you always use the position basis but it's not necessary. You could use the momentum or other basis but for a particle moving on a line, it's just the position and momentum. For three dimensional motions, there are other things like angular momentum and so on. We then have to ask what are the operators which commute with each other. So now let me make a few statements about mutually commuting operators. After that we have to come back and address this question of what is p on x_0.

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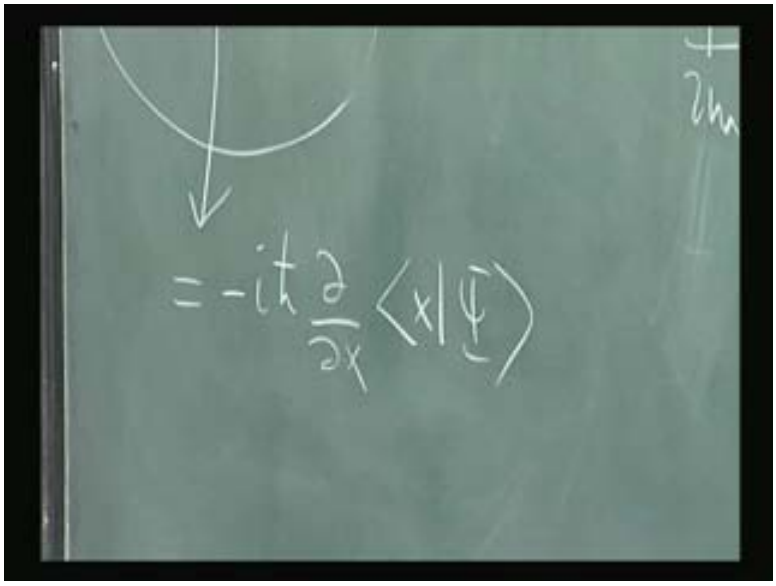

Actually we don't need to answer this question. It's not relevant because clearly p operator or any operator acting on a ket vector is going to take you to some other ket vector. In this case what we are interested in always is working in the position basis. When you say I am going to work in a basis, it means you are always going to take a scalar product on the left hand side with another basis vector belonging to the basis. So it is clear that I am not so interested in question of what is p operator x_0 because always going to work in the position basis. So I am going to do scalar product with this x.

It will turn out that this will involve the partial derivative with respect to x. it will turn out to be - ih cross d over dx of x with x_0. More generally if you have an arbitrary state psi

here (Refer Slide Time: 32:37). This will turn out to be - ih cross delta over delta x, x with psi. But this (Refer Slide Time: 32:50) is what you call the wave function in the position basis. So this is the reason why one identifies the momentum operator with - ih cross the gradient operator because that is the representation for it in the position basis. When acting on position space wave functions, the momentum operator acts as if it is just - ih cross the gradient operator. It's a representation of this operator.

Let's write down a few key results. Talking about simultaneous Eigen states, I will drop this cap on top of these symbols for simplicity. Suppose you have an operator A and an operator B belonging to a certain physical system, they are both self adjoint hermitian operators so A = A dagger and B = B dagger. The first result we need to ask is can I find simultaneous eigen states for A and B. Can I find eigen functions and eigenstates which are common to both these operators.

In general, the answer is you may not be able to do this. If you just give me two arbitrary operators, there is no reason why the eigenstates of one should be the eigenstates of the other at all. But you might expect that some eigen states of one are some eigenstates of the other. There may be some overlap between them. Now we want to make this precise. the first question is, given the fact that these operators are hermitian and self adjoint, does it mean I can always find their eigenvalues and eigenstates and the answer is yes. Let's do this from matrix theory. Given a matrix A; an n by n matrix, under what conditions can you diagonalize this matrix. Because I would like to diagonalize it, find the eigenvalues and find the eigenvectors. Finding the eigenvalues is a trivial algebraic exercise in principle but finding the eigenvalues and the eigenvectors diagonalization means finding the eigen states of this matrix. It is not always a trivial exercise. Under what conditions can you diagonalize a matrix?

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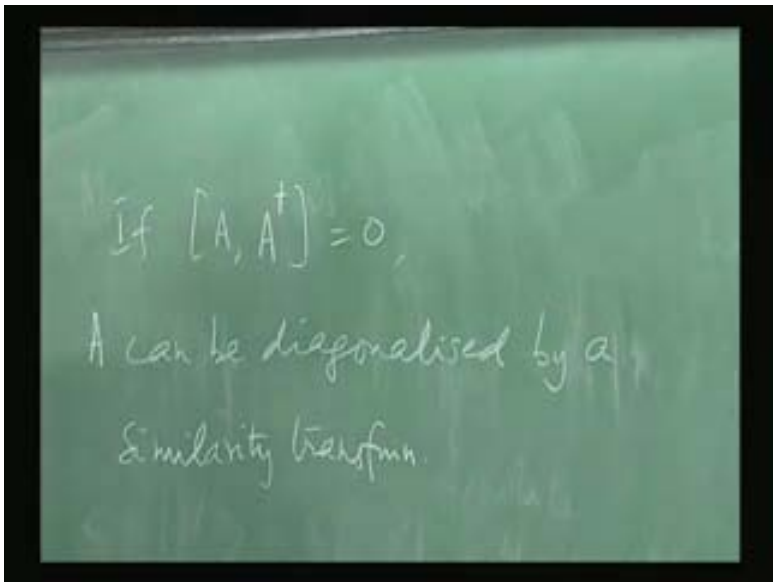

You can always diagonalize a matrix by a similarity transformation. if [A, A dagger]=0, in other words, if a matrix commutes with its hermitian conjugate, it is called a normal matrix and such a matrix can always be diagonalized by similarity transformation. This is a sufficiency condition and is not actually necessary. Of course A dagger is same A and therefore A commutes with itself in a normal matrix. So, all physical operators can be diagonalized. We can always find their eigen values and eigen states in principle. So that question is not going to bother us. Under what conditions can A and B be simultaneously diagonalized? The answer is if A and B commute with each other, then you can simultaneously diagonalize. If [A, B] =0, they can be simultaneously diagonalized. The similarity transformation can be used to diagonalize both. It means I can take this matrix of the same order, say an n by m matrix, take matrices A and B and use the same similarity transformation S, such that SA S inverse is diagonal and SB S inverse is also diagonal.

By simultaneous, I don't mean in the sense of time but with the same similarity transformation. Now what happens when A and B don't commute? It's a common misconception to assume that if you have two operators A and B in a quantum mechanical system which don't commute with each other, then you cannot find simultaneous eigenstates. That's not true. The statement is you cannot find a complete set of common eigen states. You may find one given eigen state which is common to both of them. For example, 0 may be an eigenstate of both operators but not a full set of eigenstates. Incidentally if they commute with each other, does it imply that every eigenstate of A is an eigenstate of B? This does mean that at all.

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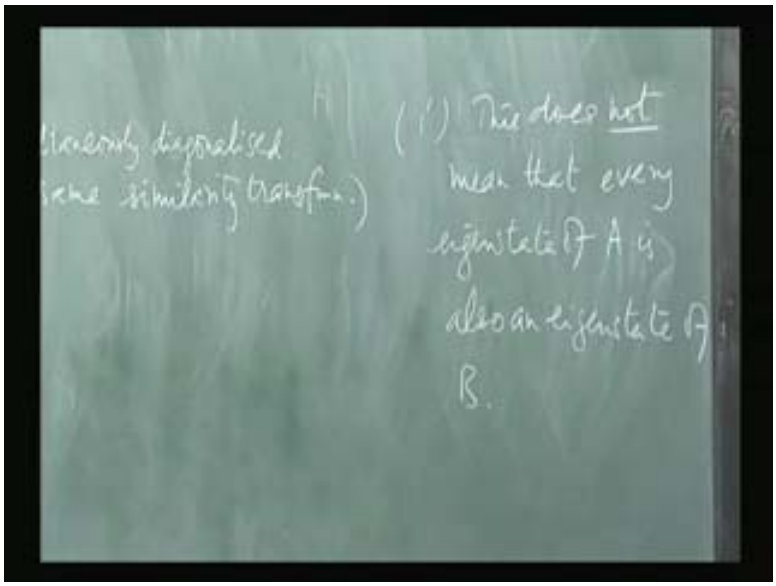

Let me give you a very trivial example. Take all possible functions on a line. Then we know that in this function space, the identity operator acting on f of x is f of x itself. So every function is an eigenstate of the identity operator with eigenvalue 1. Now consider the parity operator p such that p f (x) = f (- x). It changes x to – x.

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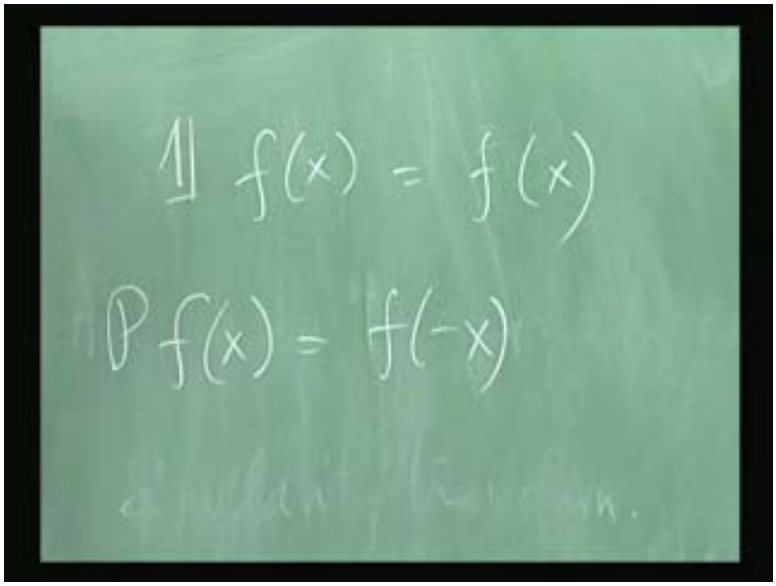

That is the parity operator. What happens if you apply this parity operator twice? p squared f (x) = p acting on f (-x). Therefore it brings you back to f (x). It means that the square of the parity operator is the identity operator. Therefore the parity operator commutes with the identity operator. P commutes with p squared. Even functions or odd functions are the parity eigen functions. Because an eigen function of the parity operator if I call it phi of x, then it says p phi of x = phi of (- x) and but this must also be equal to lambda times phi of x.

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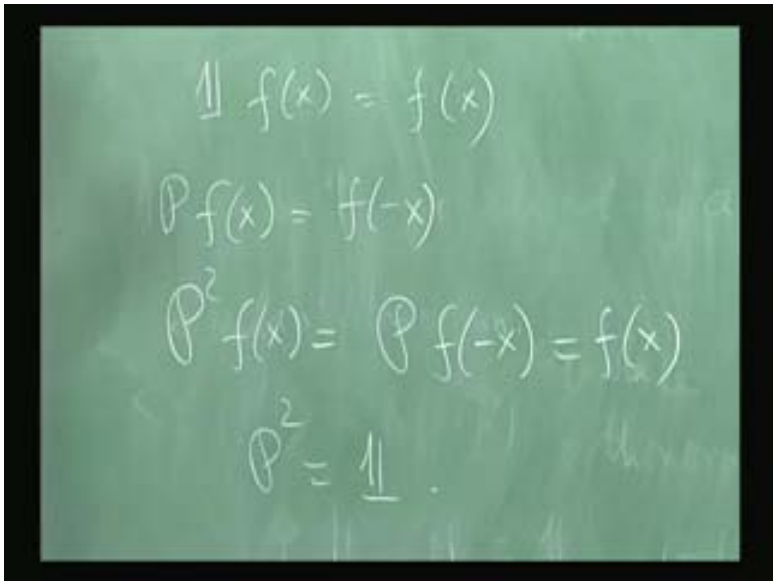

Moreover if you apply twice, it implies p squared phi of x = lambda squared phi of x and p squared is the identity operator. So this is equal to phi of x itself. This immediately implies that lambda equal to ± 1. In the case lambda = + 1, they are called even functions and in the case, -1, you call it odd functions. So even functions are eigen functions of the parity operator and odd functions are functions of the parity operator. But every function is an eigenstate of p squared.

So p squared is a much bigger set of eigenstates than p itself. p and p squared commute but all eigenstates of p squared are not eigenstates of p. the converse is true. All eigenstates of p are a subset of the eigenstates of p squared. So this is again something you must watch out for. It doesn't mean that every eigenstate of A is an eigenstate of p. it just means that when you take the one with the smallest subset and if that forms a complete set, then you are through. But if they don't commute which happens more often, all you can say is that they cannot be simultaneously diagonalized.

And you cannot find a complete set of eigenstates belonging to both. But you may have some overlap. You may find a few eigenstates which are eigenstates of p of A as well as p because in a sense you see diagonalization means finding all the eigenvalues and

eigenvectors. But they may share one or more common eigenstates. Let me give you an example from quantum mechanics which you already know. if you look at the angular momentum in the hydrogen atom problem, you know that states are labeled by a principle quantum number n, orbital angular momentum quantum number l and magnetic quantum number m.

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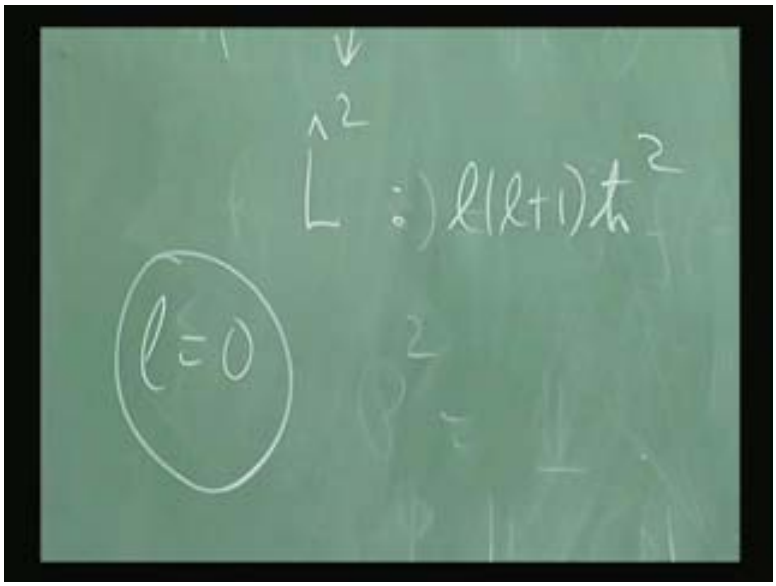

Now we know that this corresponds to the eigenvalues of the one of the components of the angular momentum. Let's call it L_z. so you know that L_z operator has a eigenvalues mh cross. This corresponds to the total angular momentum operator L square. And this has eigenvalues l (l + 1) h cross squared. Now you know that L_x and Ly don't commute with each other. L_x commutator Ly is actually ih cross times L_z.

They commute with each other. Therefore you cannot find the complete set of eigenstates of L_x, L_y and L_z simultaneously. Suppose you look at the ground state in which l =0, since L squared has a value 0, it's clear that every component must also have the value 0. Therefore the ground state is an eigenstate of L_x, L_y and L_z, all with eigenvalues 0 even though you cannot find a complete set of eigenstates. So they share one state but that's a trivial ground state eigenstate. It is not true that if they don't commute with each other they cannot have a common eigenstate. What is true is that if they commute, they can be simultaneously diagonalized. If they don't commute, that can be done. So we are going to use this statement.

Now the fact is if you back to our position and momentum example, x with p is not 0. It's an ih cross from the unit operator. Then it turns out they cannot be simultaneously diagonalized. A position eigen function cannot be a momentum eigen function and vice versa. They do not share any eigenstate. And then the question is what about

uncertainties? Well that's not hard to answer because the uncertainties are just standard deviations.

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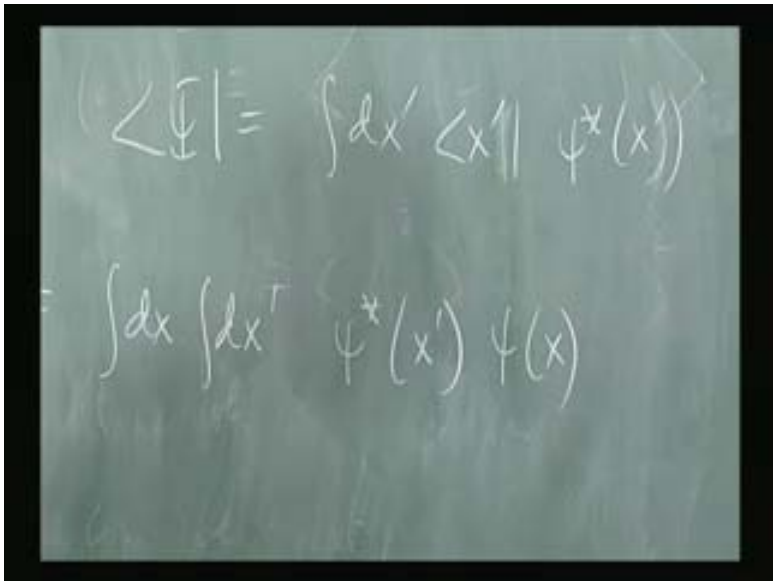

So the uncertainty in an observable in a quantum system is the following. if this variable is A and is represented by an operator A, then the expectation value of A in a state psi = state psi A psi. A squared = psi A squared psi. Now what do you call the uncertainty delta A whole squared? This quantity is nothing but the expectation value of A - A whole squared which is also equal to A squared. It is just the standard deviation. It is a square root of the variance. The only difference is these expectation values are taken with respect to a quantum state and you need to compute this number. The way you do is to get to a particular basis in the case of a particle moving in space under potential. For example, I would work in the position basis, represent this state psi by the position space wave function and compute these numbers. For instance, suppose I want to do in the position basis for an abstract operator A, what would that be reduced to?

Well, simply expand this in the position basis. So write psi in the position basis as integral dx psi of x times x. so bra psi = integral dx bra x psi star. Therefore if I plug it in here you get two dx. So let's call x prime. So this would become dx dx prime and then I would have psi star of x prime, psi of x that comes from these coefficients. The bra vector is x prime on the left. This would be x prime A x. x prime A x is just a complex number. This is just the matrix element of the abstract operator A in the position basis. It's the x prime x matrix element if these were i and j. you would say this is aij but is the x prime x matrix element and x prime and x are continuous variables. And I would like to remind myself that this is a function which arises from the operator A so you permit me to write this as just A here (Refer Slide Time: 54:36) as a function of x prime and x. this quantity here by definition is this (Refer Slide Time: 54:40).

So if you tell me how the operator A is represented in the position basis, then it is just an integer. Now where does the t dependence coming in? The t dependence comes from here (Refer Slide Time: 55:01). This would become x prime, t and this would become x, t. So our task now is really is to find out what is the representation for p. how does p look in the position basis?

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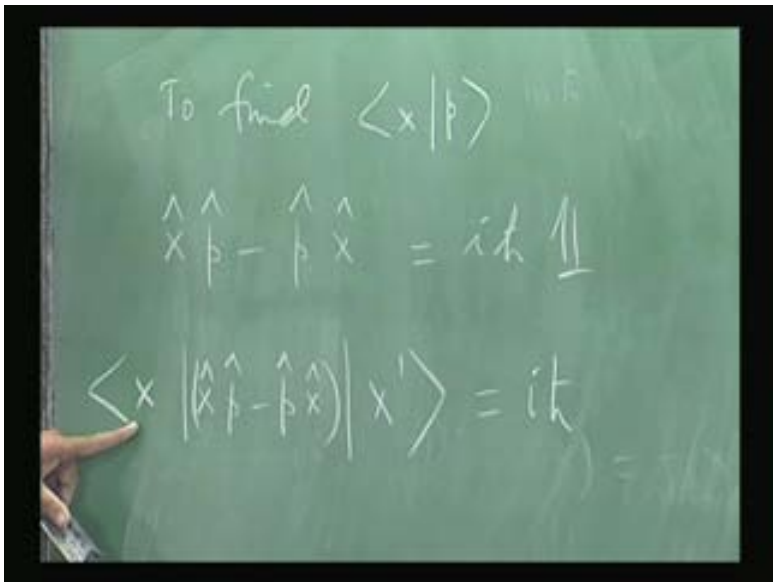

Let us compute x, p. I start by saying x p minus p x = ih cross times the unit operator. That's my input information. And now I am going to find the matrix element on both sides of this operator in the position basis. I take the scalar product with x prime on the right and x on the left. These are labels and that's equal to ih cross the matrix element with x unit operator x prime. But it is just x x prime because it's a unit operator there but by orthonormality, it is just the Dirac delta function, delta of (x - x prime).

What does x operator acting on x prime do? It just gives you number x prime. So it is – x prime x p x prime and x acting on xp will produce x star but x is a real number. So it just produces x x p x prime. So in fact it says x p x prime is a pretty singular object and it equal to ih cross delta of (x - x prime) divided by (x - x prime).

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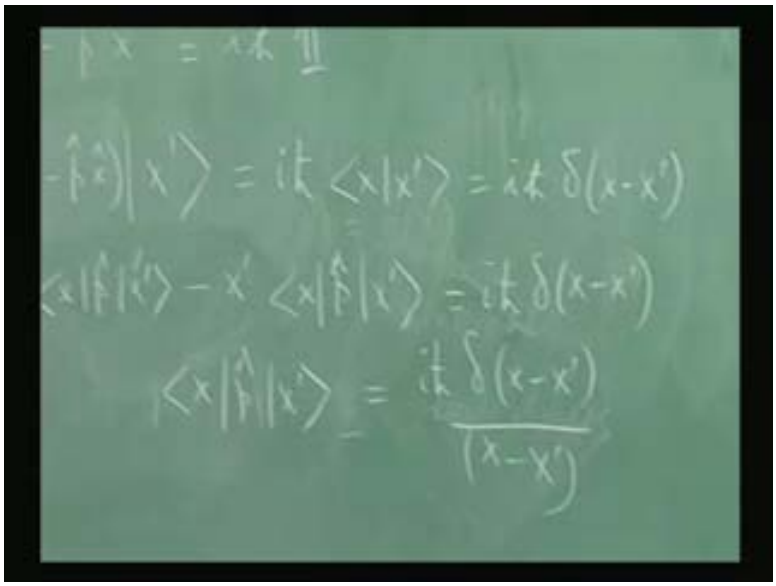

The delta function looks like a sharp spike. You know the width goes to zero the height goes to infinity in suitable manner.

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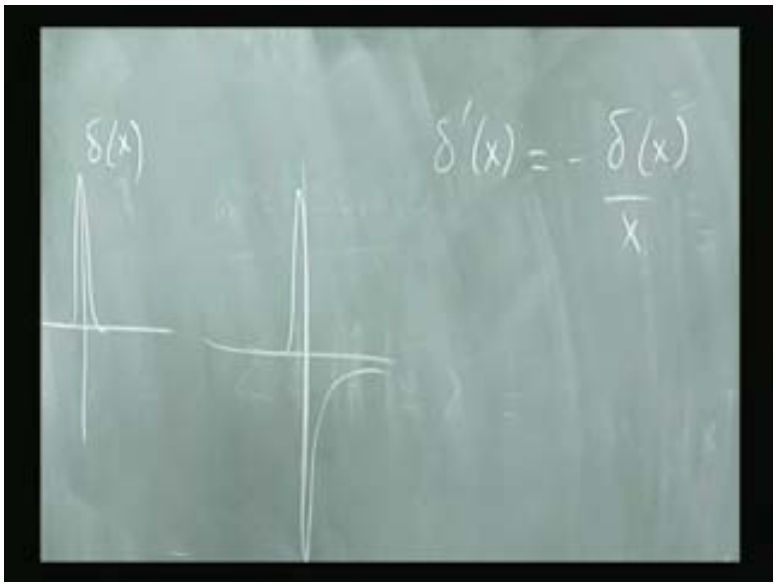

The derivative looks like this (Refer Slide Time: 01:00:02) where the slope is increasing, then goes to zero and then the slope is decreasing. So you can easily see that delta prime of x can be formally defined as - delta x over x. Delta x is an even function but the derivative is an odd function. It is anti symmetric function as you can see it goes up and

then goes up the other way. So this quantity here (Refer Slide Time: 01:56:00) is equal to - ih cross delta over delta x of delta(x- x prime) and that is equal to –ih cross delta over delta x of x with x prime. So if you now superpose a whole lot of x primes and integrate over x primes with some weight factor, that would be exactly the same a superposing all those quantities, taking the derivatives with respect to x of this weight factor.

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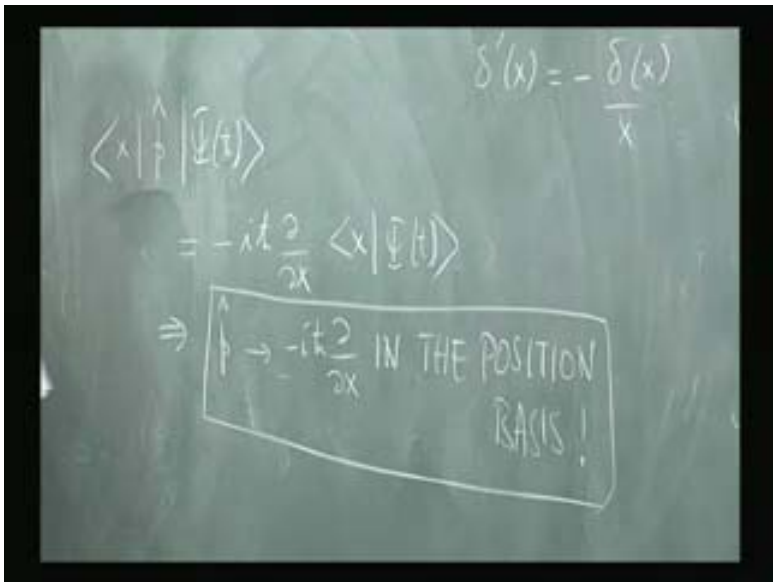

So that corresponds to saying that if you give me an arbitrary state psi of x of t and ask what happens to this matrix element, this is the same as - ih cross delta over delta x,x psi of t. This implies that the momentum operator can be written as - ih cross delta over delta x in the position basis. This is true for every ket vector x in this basis and is true as an identity. Now we are going to be able to convert things to differential equations but I want you to appreciate the fact that x operator in the position basis corresponds to just multiplying by x. but p operator in the position basis corresponds to differentiation. Suppose I worked in the momentum basis what would have happened? p operator corresponds to just multiplying by p but what would x position operator look like?

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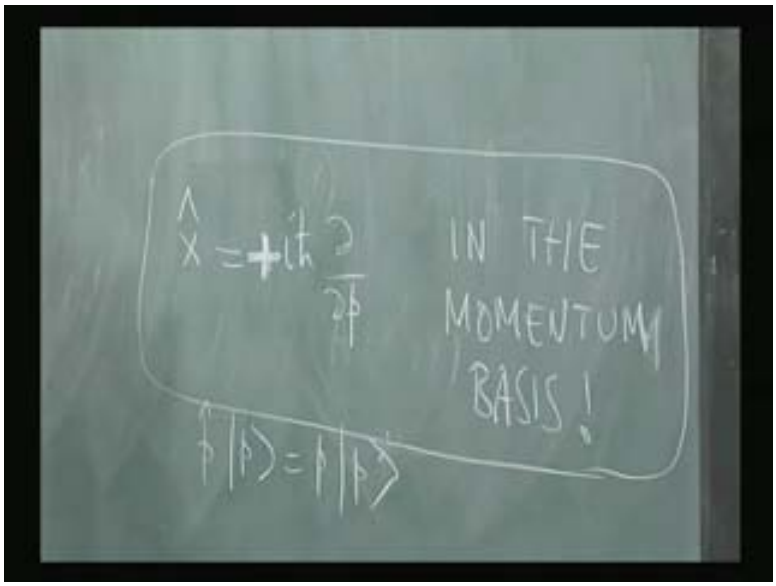

It's a similar argument with p. after all the input was just this (Refer Slide Time: 01:04:07). So x in the momentum basis = + ih cross delta over delta p. You differentiate with respect to the label p but the "plus" is because its x commutator ih cross and p commutator x is - ih cross. So this has an extra minus sign that you pickup and therefore there is a plus sign.

Now we will see what the consequences of this yeah [Conversation between the Student and Professor/not audible ((1:04:57))] yeah pardon me [Conversation between the Student and Professor/not audible ((1:05:00))] how did I do this? I did this essentially by waving my hands because this is not a rigorous argument but it's completely satisfying mean you can make this completely rigorous which part of it is missing. [Conversation between the Student and Professor/not audible ((1:05:18))] this one this relation here that's my fundamental input it arose because x p was equal to one implies in quantum mechanics when Iquantise a theory xp over ih cross equal to one [Conversation between the Student and Professor/not audible ((1:05:38))] that is the unite operator yeah yes that's input information that's my definition of canonically of a conjugate pair of variables in the quantum case [Conversation between the Student and Professor/not audible ((1:05:51))] in the discrete case yeah that would be [Conversation between the Student and Professor/not audible ((1:05:55))] what is the unite operator what is the unite operator that's really what he is asking what is the unite operator what is the element of the unite matrix in the discrete case suppose I have an n by m matrix and Iask what is one ij equal to what is this equal to it is the kronecher delta for the unite matrix for the unite operator in the continuous case these become labels so what is the corresponding element the direct delta function absolutely the direct that direct delta function of x minus x prime that is the x x prime the element if you like exactly because we know this we know if you took f of x delta of x minus x prime f of x prime the x prime this is equal to a x

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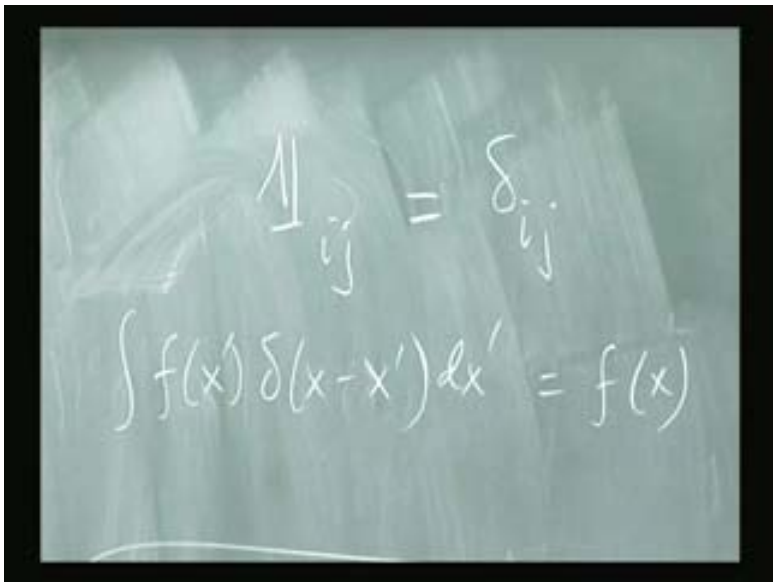

therefore this is the a unite operator the representation of a unite operator .now that's exactly what I have used there all right

So let me stop here. Thank you!