

**Introduction to Quantum Mechanics**  
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**Lecture - 02**

**Equivalence of the Heisenberg and the Schrodinger formulations - The x and p operators and the quantum condition**

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Schrodinger Equation Solutions

$$\int \psi_m^* \psi_n dx = \delta_{mn}$$

$$\sum_n \psi_n^*(x) \psi_n(x') = \delta(x-x')$$

Quantum Condition

$$p x - x p = \frac{\hbar}{i} = \frac{h}{2\pi i}$$

$$\sum_l (p_{ml} x_{ln} - x_{ml} p_{ln}) = \frac{\hbar}{i} \delta_{mn}$$

Step 1

$$\frac{d}{dx}(x f) - x \frac{d}{dx} f = f$$

$$\cancel{x \frac{d}{dx} f} + f - \cancel{x \frac{d}{dx} f} = f$$

What you have learned in the previous lecture is that for the Schrodinger equation solutions, we have integration  $\psi_m^* \psi_n dx = \delta_{mn}$ . So, we are assuming we have normalized the wave functions and summation  $\sum_n \psi_n^*(x) \psi_n(x') = \delta(x-x')$  and we are going to use these 2 properties to show the equivalence of Heisenberg's and Schrodinger's approach and then see how to connect the 2.

So, remember the main thing in Heisenberg's approach is quantum condition which says that  $p x - x p$  is equal to  $\hbar/i$  which is  $h/2\pi i$ . In matrix form this means that  $p_{ml} x_{ln} - x_{ml} p_{ln}$ ; that means, I am taking the  $m n$  component of this matrix  $p x - x p$  is summed over  $l$  is equal to  $\hbar/i \delta_{mn}$ . Can we get the same condition from Schrodinger picture and what does it mean to have it coming from there. So, let us see that. So, to get this first recognize step one that if I take this operation  $d/dx$  times  $x f$  some function  $f$  minus  $x d/dx f$  this is equal to  $f$  alone.

So, how do we see that from the first term we get  $x \frac{d}{dx} f$  by  $\frac{d}{dx} x$  plus  $f$  and second term is minus  $x \frac{d}{dx} f$  by  $\frac{d}{dx} x$  and the first term and the last term cancel and you get  $f$ .

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$$\frac{d}{dx} x - x \frac{d}{dx} = 1$$

If I take  $f = \psi_n(x)$

$$\left\{ \frac{d}{dx} (x \psi_n) - x \frac{d \psi_n}{dx} \right\} = \{ \psi_n \} \times \frac{\hbar}{i}$$

$$\int dx \psi_m^*(x) \left[ \frac{\hbar}{i} \frac{d}{dx} (x \psi_n) - x \frac{\hbar}{i} \frac{d \psi_n}{dx} \right] = \frac{\hbar}{i} \psi_m$$

$$\int_{-\infty}^{\infty} dx \psi_m^* \frac{\hbar}{i} \frac{d}{dx} (x \psi_n) - \int_{-\infty}^{\infty} dx \psi_m^* x \frac{\hbar}{i} \frac{d \psi_n}{dx} = \frac{\hbar}{i} \delta_{mn}$$

$$\text{LHS} = \int_{-\infty}^{\infty} dx \psi_m^*(x) \frac{\hbar}{i} \frac{d}{dx} \underbrace{\int_{-\infty}^{\infty} \delta(x-x') dx' x' \psi_n(x')}_{x \psi_n(x)} - \int_{-\infty}^{\infty} dx \psi_m^* x \underbrace{\int_{-\infty}^{\infty} \delta(x-x') dx' \frac{\hbar}{i} \frac{d \psi_n(x')}{dx'}}_{\frac{\hbar}{i} \frac{d \psi_n(x)}$$

Therefore I can write that  $\frac{d}{dx} x$  operating on a function by that I mean  $\frac{d}{dx} x$  will act on first on  $x$  and then  $f$  both this operating on a function means I will multiply  $x$  and  $f$  and then take the derivative minus  $x \frac{d}{dx}$  is like multiplying by one in particular, if I take  $f$  to be the  $n$ th I can function of the solution of the Schrodinger equation, I am going to have  $\frac{d}{dx} x$  of  $x \psi_n$  minus  $x \frac{d}{dx} \psi_n$  is equal to  $\psi_n$ .

Let me now multiply both sides by  $\hbar$  cross over  $i$  and write  $\hbar$  cross over  $i$   $\frac{d}{dx} x \psi_n$  minus  $x \hbar$  cross over  $i$   $\frac{d}{dx} \psi_n$  is equal to  $\hbar$  cross over  $i$   $\psi_n$ . Next, let me multiply both sides by  $\psi_m^*$  and integrate over  $x$ . So, that I am going to get on the left hand side, I am going to get integration minus infinity to infinity  $\psi_m^* \hbar$  cross over  $i$   $\frac{d}{dx} x \psi_n$  and  $x$  minus  $\psi_m^* \hbar$  cross over  $i$   $\frac{d}{dx} \psi_n$  is equal to  $\hbar$  cross over  $i$   $\delta_{mn}$  this we have seen in the previous lecture that  $\psi_m$  actually orthogonal. So, orthogonality here is important.

Now, I am going to use something else and that is completeness. So, what I am going to do now write this as minus infinity to infinity, there is an integration over  $dx$ , I have  $\psi_m^* x$ , I have  $\hbar$  cross over  $i$   $\frac{d}{dx}$ , I am going to write the inner integral inner portion as minus infinity to infinity  $\delta(x-x') dx' x' \psi_n(x')$  because of the delta function is nothing, but  $x \psi_n(x)$ , but I am doing it. So, that I can

write delta x minus x prime using completeness in terms of size again.

And second term is therefore, going to be similarly minus integral minus infinity to infinity d x psi m star x integration minus infinity to infinity delta x minus x prime d x prime h cross over i d by d x prime of psi n x prime, I am only writing this left hand side. So, this is my left hand side again because this term in the second integral because of the delta function is nothing, but h cross over i d by d x of psi n x, all right. So, this is what we have done now I am going to use completeness.

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The image shows a whiteboard with handwritten mathematical expressions. At the top, it is labeled 'LHS:'. Below this, there are two integrals. The first integral is  $\int_{-\infty}^{\infty} dx \psi_m^*(x) \frac{1}{i} \frac{d}{dx} \int_{-\infty}^{\infty} \delta(x-x') dx' x' \psi_n(x')$ . The second integral is  $-\int_{-\infty}^{\infty} dx \psi_m^*(x) x \int_{-\infty}^{\infty} \delta(x-x') dx' \frac{1}{i} \frac{d}{dx'} \psi_n(x')$ . Below these, the completeness relation is written in red:  $\delta(x-x') = \sum_n \psi_n(x) \psi_n^*(x')$ . Then, the first integral is rewritten as  $\sum_l \left[ \int_{-\infty}^{\infty} dx \psi_m^*(x) \frac{1}{i} \frac{d}{dx} \psi_l(x) \right] \left[ \int_{-\infty}^{\infty} dx' \psi_l^*(x') x' \psi_n(x') \right]$ . The second integral is rewritten as  $\sum_l \left[ \int_{-\infty}^{\infty} dx \psi_m^*(x) x \psi_l(x) \right] \left[ \int_{-\infty}^{\infty} dx' \psi_l^*(x') \frac{1}{i} \frac{d}{dx'} \psi_n(x') \right]$ . Brackets labeled 'ml' and 'ln' are used to group terms in the summations.

So, let me write this left hand side again. So, that we can complete the whole thing, right. Here I have integration d x psi n star h cross over i d by d x integration of delta x minus x prime d x prime x prime psi n x prime minus integration d x psi m star x integration. This is all minus infinity to infinity minus infinity to infinity minus infinity to infinity minus infinity to infinity delta x minus x prime d x prime h cross over i d by d x prime psi n x prime that is my left hand side and now use completeness to write delta of x minus x prime as summation psi n x psi n star x prime, I am going to substitute this for delta function. So, that the left hand side now becomes integration minus infinity to infinity d x psi m star that will be very careful, right. This variable inside is x h cross over i d by d x of integration minus infinity to infinity, there is a summation over let me change the index because I am using m and n. So, I am going to write this as n psi l x.

So, I can write psi l x outside because inside the integration it does not really matter and

then I am going to write  $\psi_l^* x \psi_n$  that is the first term for the second term I am going to write again summation over  $l$  from minus infinity to infinity  $\int dx \psi_n^* x \psi_l$  integration minus infinity to infinity  $\int dx \psi_l^* x \psi_n$  I am going to put the  $x$  index inside. So,  $\psi_l^* x \psi_n$  cross over  $l$  by  $\int dx \psi_n^* x \psi_l$  and out here, I get  $\psi_l^* x$ , let me now put some brackets. So, that terms are easy to identify, I will put one bracket here, second bracket in the second term one bracket here and second one for the second integer, this first term is like a matrix element with  $m$  and  $l$  indices this term is also a matrix element with  $l$  and  $n$  indices.

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The image shows a whiteboard with handwritten mathematical derivations. The top part shows the commutator of the position operator  $x$  and the momentum operator  $p$  in matrix mechanics. The first line is:

$$\sum_l \left[ \left\{ \int_{-\infty}^{\infty} dx \psi_m^* \frac{\hbar}{i} \frac{d\psi_l(x)}{dx} \right\} \left\{ \int_{-\infty}^{\infty} dx \psi_l^*(x) x \psi_n(x) \right\} - \left\{ \int_{-\infty}^{\infty} dx \psi_m^*(x) x \psi_l(x) \right\} \left\{ \int_{-\infty}^{\infty} dx \psi_l^*(x) \frac{\hbar}{i} \frac{d\psi_n(x)}{dx} \right\} \right]$$

The second line shows the result of the commutator:

$$= \frac{\hbar}{i} \delta_{mn}$$

Below this, the text "If we identify" is written in red. The next line defines the position matrix element  $x_{ml}$ :

$$x_{ml} = \int_{-\infty}^{\infty} \psi_m^*(x) x \psi_l(x) dx$$

Then, the text "And" is written in green. The next line defines the momentum matrix element  $p_{ml}$ :

$$p_{ml} = \int_{-\infty}^{\infty} \psi_m^*(x) \frac{\hbar}{i} \frac{d\psi_l(x)}{dx} dx$$

The final line shows the commutator in terms of these matrix elements:

$$\sum_l [p_{ml} x_{ln} - x_{ml} p_{ln}] = \frac{\hbar}{i} \delta_{mn}$$

To the right of this equation, the text "Matrix Mechanics Quantum Condition" is written in red.

This is a matrix element with  $m$  and  $l$  indices. This is a matrix element with  $l$  and  $n$  indices, I have summation over  $l$  and I will put this whole thing in a big bracket and I have the first integral minus infinity to infinity  $\int dx \psi_n^* x \psi_l$  over  $\int dx \psi_l^* x \psi_n$ , second one is integration minus infinity to infinity  $\int dx \psi_l^* x \psi_n$ , but since these a dummy variable, I can still write this as  $\int dx \psi_l^* x \psi_n$  and integration minus infinity to infinity  $\int dx \psi_l^* x \psi_n$  cross over  $l$  by  $\int dx \psi_n^* x \psi_l$  and recall all this is equal to  $\hbar$  cross over  $i$  delta  $m n$ .

Now, let me assert if we identify  $x_{ml}$  as integration  $\int dx \psi_m^* x \psi_l$  and  $p_{ml}$  as minus infinity to infinity  $\int dx \psi_m^* \frac{\hbar}{i} \frac{d\psi_l}{dx}$ , we identify it like this, what does this reduce to it reduces to the summation over  $l$  inside the bracket

i have p m l second term is x l n minus i get x m l p l n is equal to h cross over i delta m n and this is matrix mechanics quantum condition. So, if you want to have the 2 formulism equivalent then there is a particular way of defining the matrix elements of Heisenberg's approach to quantum mechanics using the wave function in a very particular way and that way is now called through operators.

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To have equivalence of Heisenberg's and Schrodinger's theory,  $p_{mn}$   $x_{mn}$  are defined from the wavefunction using multiplication ( $x$ ) or differential ( $p$ ) "operators"

$$\text{for } p_{ml} = \int \psi_m^* \hat{p}_{op} \psi_l \, dx$$

$$\hat{p}_{op} = \frac{\hbar}{i} \frac{d}{dx}$$

$$x_{ml} = \int \psi_m^* \hat{x} \psi_l \, dx$$

$$\hat{x} = x$$

So, to have equivalence of Heisenberg's and Schrodinger's theory  $p_{m n}$  and  $x_{m n}$  are defined from the wave functions using multiplicative that is four  $x$  or differential for  $p$  operators.

So, I am introducing a term called operator these are known as operators. So, for  $p_{m l}$  and is this equal to integration  $\psi_m^*$  then I apply  $p$  operator, sometimes it is written with a hat on top  $\psi_l \, dx$  where  $p$  operator is equal to  $\hbar$  cross over  $i$   $d$  by  $d x$  for  $x_{m l}$   $x_{m l}$  i have  $\psi_m^* x$  operator i put a hat  $\psi_l \, dx$  where  $x$  operator is nothing, but just  $x$  and multiply by that what about  $p$  square and  $x$  square.

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What about

$$x^2: \quad x_{mn}^2 = \sum_l x_{ml} x_{ln}$$

$$= \sum_l \left\{ \int \psi_m^*(x) x \psi_l(x) dx \right\} \left\{ \int \psi_l^*(x') x' \psi_n(x') dx' \right\}$$

$$= \int \psi_m^*(x) x dx \left( \sum_l \int \psi_l(x) \psi_l^*(x') dx' \right)$$

$\downarrow$   
 $\delta(x-x')$

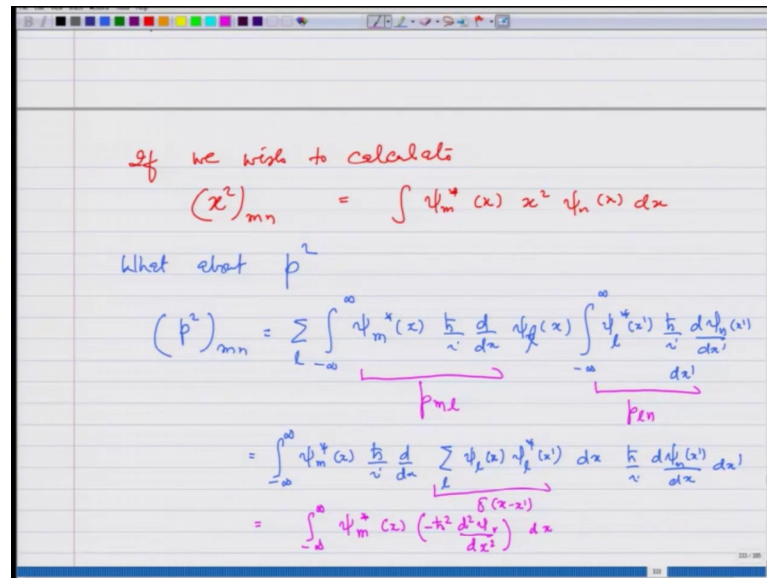
$$= \int \psi_m^*(x) x^2 \psi_n(x) dx$$

Operator for  $x^2$

So, let us now check what about  $x$  square remember in Heisenberg's mechanics  $x$  square  $m$   $n$  would be equal to  $x$   $m$   $l$   $x$   $l$   $n$  summation over  $l$  which would be same as summation over  $l$  integration  $\psi_m^* x \psi_l$  multiplied by integration  $\psi_l^* x' \psi_n$  let me write this as  $x$  prime  $x$  prime  $\psi_n$  and again using completeness i can write this as integration  $\psi_n^* x$  times  $x$   $\delta(x-x')$  i will use summation over  $l$   $\psi_l x \psi_l^* x$  prime then there is an  $x$  prime  $\psi_n$  this is an  $x$  prime  $x$  prime  $\delta(x-x')$ .

This is nothing, but  $\delta(x-x')$  this is  $\delta(x-x)$ . So, this becomes integration  $\psi_m^* x^2 \psi_n$ .

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if we wish to calculate

$$(x^2)_{mn} = \int \psi_m^*(x) x^2 \psi_n(x) dx$$

What about  $p^2$

$$(p^2)_{mn} = \sum_l \int_{-\infty}^{\infty} \psi_m^*(x) \frac{\hbar}{i} \frac{d}{dx} \psi_l(x) \int_{-\infty}^{\infty} \psi_l^*(x') \frac{\hbar}{i} \frac{d}{dx'} \psi_n(x') dx$$

$$= \int_{-\infty}^{\infty} \psi_m^*(x) \frac{\hbar}{i} \frac{d}{dx} \sum_l \psi_l(x) \psi_l^*(x') dx \frac{\hbar}{i} \frac{d}{dx'} \psi_n(x')$$

$$= \int_{-\infty}^{\infty} \psi_m^*(x) \left( -\hbar^2 \frac{d^2}{dx^2} \right) \psi_n(x) dx$$

So, operator for x square is x square. So, if we wish to calculate x square m n this is going to be nothing, but square of psi m star x x square psi n x d x. Let us see what about p square p square m n is going to be integration minus infinity to infinity psi m star x h cross over i d by d x on psi n or l x times minus infinity to infinity psi l star x prime h cross over i d psi m by d x prime this is all prime d x prime summed over l because the first term is nothing, but this is p m l and this is nothing, but p l n.

So, by the rule of matrix multiplication this is what it is and this again I can write as minus infinity to infinity psi m star x h cross over i d by d x operating on summation over l psi l x psi l star x prime, I can write it like this because d by d x does not act on x prime, there is an integration over x and then i have h cross over i d psi n x prime over d x d x prime.

But again this term is delta x minus x prime. And therefore, this whole thing becomes minus infinity to infinity psi m star x h cross square d 2 psi by d x square d x.

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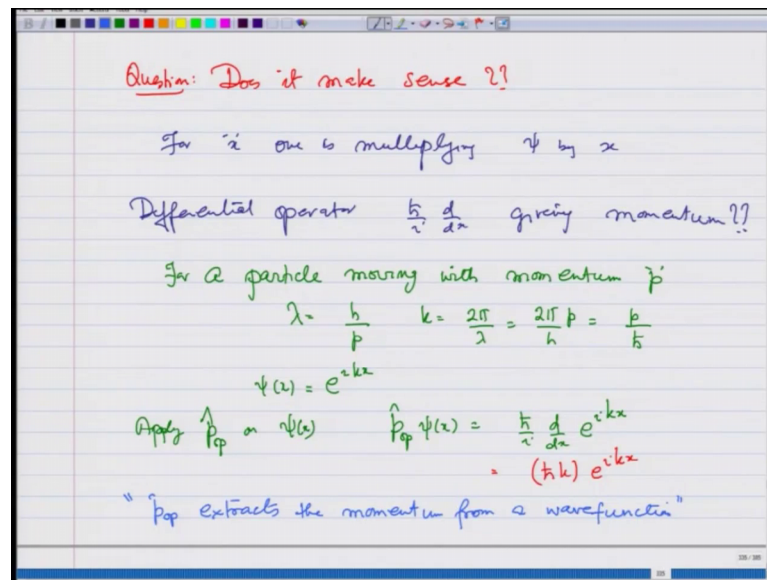
$$\begin{aligned}
 (p^2)_{mn} &= \sum_l p_{ml} p_{ln} \\
 &= \int \psi_m^* \frac{\hbar}{i} \frac{d\psi_l}{dx} \int_{-\infty}^{\infty} \psi_l^*(x') \frac{\hbar}{i} \frac{d\psi_n}{dx'} dx' \\
 &= \int \left( \psi_m^*(x) - \hbar^2 \frac{d^2}{dx^2} \psi_n(x) \right) dx \\
 &\quad \uparrow \\
 &\quad \hat{p}^2 \\
 p^2_{\text{operator}} &= p \cdot p \\
 (p^2) &= \int \psi_m^*(x) - \hbar^2 \frac{d^2}{dx^2} \psi_n(x) dx
 \end{aligned}$$

So, for  $p^2$   $m n$  I did  $p_{ml} p_{ln}$  summed over  $l$  and this I wrote as integration  $\psi_m^*$   $\hbar$  cross over  $i$   $d \psi_l$  over  $dx$  and this is minus infinity to infinity  $\psi_l^*$   $\hbar$  cross over  $i$   $d \psi_n$  over  $dx'$  this is all prime  $dx'$  then, I use the orthogonality condition to show that this is equal to  $\psi_m^* x$  minus  $\hbar^2$   $d^2$  by  $dx^2$   $\psi_n$   $dx$  integration this therefore, is the operator for  $p^2$  and you can see that  $p^2$  operator is nothing, but  $p$  times  $p$  operator. So, if I want to calculate  $p^2$  I do not really have to go through the matrix suit, I can straightaway write this is equal to  $\psi_m^* x$   $p^2$  operator which is minus  $\hbar^2$   $d^2$  by  $dx^2$   $\psi_n$   $dx$ .

So, you see how things become very easy I do not really have to do matrix multiplication all the time and I can perform these operations, I can make operators for anything, they just multiply the operators and you get the answer. So, this now makes a equivalence of the Heisenberg picture with Schrodinger picture where now from the wave function I extract the matrix elements by applying the corresponding operators does it make sense.



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Let us see that; so the question; now I have question, does it make sense in particular for  $x$  1 is multiplying  $\psi$  by  $x$ . So, there it seems to be that if I want to calculate  $x$ , I just multiply by  $x$  that will be clear in the next lecture when I give the born interpretation for the wave function, but differential operator  $\hbar$  cross over  $i$   $d$  by  $d$   $x$  giving momentum that looks a little odd, but let us see does it make sense.

Recall for a particle moving with momentum  $p$  wave length is  $h$  over  $p$   $k$  which is  $2\pi$  over  $\lambda$  is  $2\pi$  over  $h$   $p$  which is  $p$  over  $h$  cross and the static part of the wave function is  $e$  raise to  $i$   $k$   $x$   $\psi$   $x$  it is a plane wave for a fixed momentum and let us now apply  $p$  operator on  $\psi$   $x$  and see what does it give. So, when I do  $p$  operator  $\psi$   $x$ , it gives me a crossover  $i$   $d$  by  $d$   $x$  operating on  $e$  raise to  $i$   $k$   $x$  and that gives me  $h$  cross  $k$   $e$  raised to  $i$   $k$   $x$ . So, in this case when the particle has a pure momentum  $p$  applying  $p$  operator on  $\psi$  gives me that momentum. So, it does make sense that  $p$  operator gives me momentum; that means; this is an operator that extracts right the momentum out of a wave function.

So, in a very loose statement I will just write this  $p$  operator extracts the momentum from a wave function and that is the formalism in Schrodinger that whenever you want to extract a quantity it has to have a corresponding operator that then acts on the wave function and gives you that quantity incidentally here since you get exact momentum. So, this is a momentum Eigen state with the Eigen value of the operator being  $h$  cross  $k$

let us look at it slightly differently what about the energy the Schrodinger equation is minus h cross over 2 m d 2 by d x square operating on psi n plus v x psi n is equal to E n psi n.

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The image shows a whiteboard with handwritten mathematical derivations. At the top, it is titled "Schrodinger equation". The first equation is  $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n + V(x) \psi_n = E_n \psi_n$ . The second equation is  $\frac{1}{2m} \left( -\hbar^2 \frac{d^2}{dx^2} \right) \psi_n + V(x) \psi_n = E_n \psi_n$ . The third equation is  $\left( \frac{\hat{p}^2}{2m} + \hat{V}(x) \right) \psi_n = E_n \psi_n$ . Below this, it says "Operator for the energy" and shows  $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$ . To the right, it shows  $e^{ikx} \hat{p} e^{ikx} = (p) e^{ikx}$  and  $\psi_n(x) \left( \frac{\hat{p}^2}{2m} + V(x) \right) \psi_n = E_n \psi_n$ . A purple oval at the bottom contains the word "HAMILTONIAN", with an arrow pointing to it from the operator expression above.

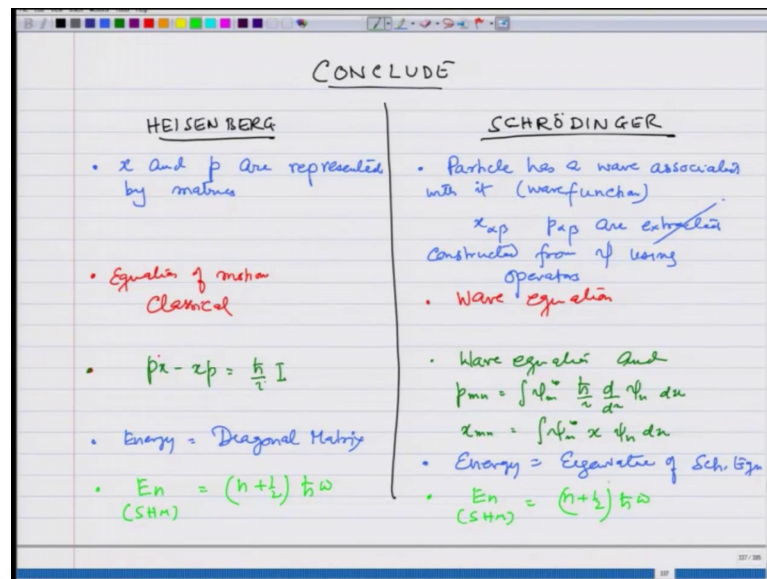
What did we say this operator was this is 1 over 2 m minus h cross square d 2 by d x square psi n plus v x. Now v x you can write as a polynomial or whatever and we saw that that also is like an operator operating on psi n is equal to E n psi n in operator language this will become this as p square. So, it will become p square operator divided by 2 m plus v operator which is a multiplicative operator acting on psi n gives me E n psi n and what is this p squared over 2 m plus v x it is like an operator for the energy.

So, operator for the energy acting on the wave function gives me the energy. So, this suddenly starts making sense that p operator being written as h cross over i d by d x in 2 instances, it has given me the right answer for e raise to i k x p acting on e raised y k s gave me the true momentum p times e raise to i k s and for psi n x p square over 2 m plus three x on psi n gave me the energy. So, this operator for the energy is known as the Hamiltonian and in this course this is an introductory course, I am not going to go more into details of why this is called Hamiltonian, but this is the Hamiltonian operator. So, Hamiltonian is the operator for energy it acts on psi n and Eigen function and gives you E n.

So, to conclude this lecture let me just make a comparative table for Heisenberg and

Schrodinger picture.

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So, I will conclude this lecture by making a table of Heisenberg Schrodinger in Heisenberg's picture the  $x$  and  $p$  are represented by matrices in the Schrodinger picture particle has a wave associated with it which is known as the wave function  $x_{\alpha\beta}$  or  $x_{mn}$  and  $p_{\alpha\beta}$  are extracted or I will use constructed from  $\psi$  using operators. So, if there are matrices in here you have to apply an operator on the function, now here the equation of motion is classical except that now this is written in terms of the matrices here is the wave equation here the quantum condition is  $p x$  minus  $x p$  equals  $h$  cross over  $i$ , the identity matrix again here I will write wave equation and  $p_{mn}$  equals  $\psi_m^*$  star  $h$  cross over  $i$   $d$  by  $d x$   $\psi_n$   $d x$   $x_{mn}$  being given as  $\psi_m^*$  star  $x$   $\psi_n$   $d x$ .

Here the energy for stationary systems or conservative systems is diagonal matrix and you have done that in the past for harmonic oscillator here the energy is Eigen value of Schrodinger equation; however, through all this finally, the energy for harmonic oscillator right  $s h m$  comes out to be  $n$  plus a half  $h$  cross  $\omega$  and here also we have solved this energy for  $s h m$  comes out to be  $n$  plus a half  $h$  cross  $\omega$  and the 2 are equivalent.

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What about diagonal terms?

$$x_{nn} = \int \psi_n^*(x) x \psi_n(x) dx$$
$$= \int |\psi_n(x)|^2 x dx$$
$$p_{nn} = \int \psi_n^*(x) \frac{h}{i} \frac{d\psi_n}{dx} dx$$

So, after this conclusion, I just want to leave you with a question what about diagonal terms for example,  $x$  and  $n$  which is integration  $\psi_n^* x \psi_n dx$  which is integration  $|\psi_n|^2 x dx$  and  $p_{nn}$  which is integration  $\psi_n^* \frac{h}{i} \frac{d\psi_n}{dx} dx$ . These terms we have not yet addressed what do they mean and we will address this in the next lecture when we discuss the interpretation of  $|\psi_n|^2$ .

So, I will leave you with that question in this lecture.