

Statistical Thermodynamics for Engineers
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Lecture 15
Supplementary Video 4 Operator Theory 2

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Operator Theory

Recap: Function (Functions of a single real variable)

$y = f(x)$ function f : as a mapping from a set of input to a set of outputs.

$x \in \mathbb{R} \longrightarrow f \longrightarrow y \in \mathbb{R}$

input set of all inputs (Domain) set of all outputs (Range)

$x \longrightarrow \boxed{f} \longrightarrow y$

Ex: ① $f(x) = x^2$ $x \longrightarrow \boxed{f} \longrightarrow y$
 $2 \longrightarrow \boxed{f} \longrightarrow 4$

Ex: ② $g(x) = \sqrt{x}$ $x \longrightarrow \boxed{g} \longrightarrow y$
 $4 \longrightarrow \boxed{g} \longrightarrow 2$

Function of two variables $f(x, y) = z \longrightarrow \mathbb{R}$

$\mathbb{R} \quad \mathbb{R}$

Domain: $\mathbb{R}^2 \longrightarrow \mathbb{R}$

$f(x, y) = x^2 + y^2$ $\begin{matrix} 0 \\ 0 \end{matrix} \longrightarrow \boxed{f} \longrightarrow 0$

$f(x, y) = x^2 + y^2$

$\begin{matrix} 0 \\ 0 \end{matrix} \rightarrow \begin{matrix} \boxed{f} \\ \rightarrow 0 \end{matrix}$

$\begin{matrix} (x, y) \\ \mathbb{R}^2 \end{matrix} \begin{matrix} 1 \\ 2 \end{matrix} \rightarrow \begin{matrix} \boxed{f} \\ \rightarrow 5 \end{matrix}$

$F = F(x_1, x_2, x_3, \dots, x_N)$

\downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow

Real number. N -tuple Vector Matrix Vector

$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_N \end{pmatrix}_{N \times 1} \rightarrow \begin{matrix} \boxed{\text{Matrix}} \\ M \end{matrix} \rightarrow \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_M \end{pmatrix}_{N \times 1}$

$X \quad M \quad Y$

$M \times Y = Y$

$\begin{matrix} - & - & - \end{matrix}$

What happens when $N \rightarrow \infty$
 i.e. we are dealing with an infinite dimensional vectors

An infinite dimensional vector can be realized as a function.

$\begin{matrix} \text{Input} \\ \boxed{\hat{A}} \\ \text{Output} \end{matrix}$

$\hat{A} f(x) = g(x)$

$\hat{A} =$ Set of all inputs is known as a Function Spaces.

\hat{A} as a function spaces.

Operator

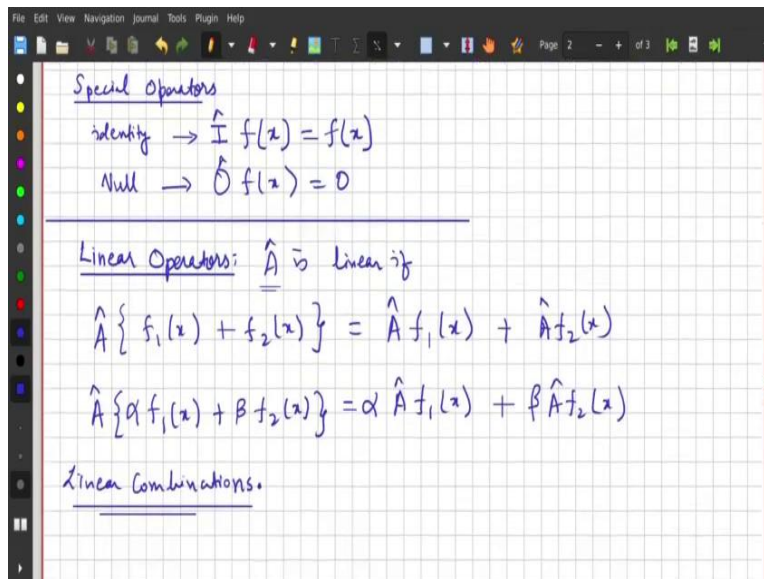
Basic Rules of Operator Algebra

- $\hat{A} C f(x) = C \hat{A} f(x)$; C is a constant.
- $(\hat{A} + \hat{B}) f(x) = \hat{A} f(x) + \hat{B} f(x)$
- $\hat{A} \hat{B} f(x) = \hat{A} \{\hat{B} f(x)\}$
- $(\hat{A} + \hat{B}) + \hat{C} = \hat{A} + (\hat{B} + \hat{C})$
- $\hat{A} + \hat{B} = \hat{B} + \hat{A}$ ($\hat{A} \hat{B} \neq \hat{B} \hat{A}$) Quantum Mechanics

Special Operators

identity $\rightarrow \hat{I} f(x) = f(x)$

$\hat{A} f(x) = 0$



Hello everyone. So, welcome to the second supplementary lectures on operator theory. So, we were discussing the basics about what an operator is, and we saw the development of how we generalise the idea from a one dimensional function of a real variable to functions of 2 variables, N variables. And then we generalise the idea to a matrix vector operations.

So, here you see a matrix acting on a vector to provide another vector. So, there we thought of the matrix as an operator, and then we took another limiting case where we allowed N, in case with the vector what we are taking as an input was from an infinite dimensional vector space. And then we have the realisation of that an infinite dimensional vector space can be realised as a function.

And using that idea, we came to appreciate the fact that an operator is an any object that takes a function as its input, any function as its input and provides another function as an output. And we also said that the set from which all these functions were chosen are part of a space known as function spaces.

And then we covered some basic rules of operator algebra, where we said how the with respect to basic operations like addition, operator, operators are associative and commutative. And then we said, two special operators, the identity operator, null operators, we understood the concept of linearity of operators. So, from we will take some examples right from here, so that we get more clarity on what we were, what we mean.

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Null $\rightarrow \hat{O} f(x) = 0$

Linear Operators: \hat{A} is linear if

$$\hat{A}\{f_1(x) + f_2(x)\} = \hat{A}f_1(x) + \hat{A}f_2(x)$$
$$\hat{A}\{\alpha f_1(x) + \beta f_2(x)\} = \alpha \hat{A}f_1(x) + \beta \hat{A}f_2(x)$$

Linear Combinations.

Ex: ① \hat{A} is multiplication by x

$$\hat{A}f(x) = g(x) \Rightarrow x f(x) = g(x)$$

② $\hat{A} = \frac{d}{dx}$ $\hat{A}f(x) = g(x) \Rightarrow \frac{df(x)}{dx} = g(x)$

$\frac{d}{dx}$ operator is a linear operator

$$\frac{d}{dx} (\alpha f(x) + \beta g(x)) = \alpha \frac{d}{dx} f(x) + \beta \frac{d}{dx} g(x)$$

Example of a non-linear operator

① \hat{A} is square root operator

$$\hat{A}(f(x) + g(x)) = \hat{A}f(x) + \hat{A}g(x) \quad \text{--- ①}$$

$\hat{A} \equiv$ Square root operator

LHS of Eqn ①

$$\left. \begin{aligned} \text{LHS} &= \sqrt{f(x) + g(x)} \\ \text{RHS} &= \sqrt{f(x)} + \sqrt{g(x)} \end{aligned} \right\} \text{LHS} \neq \text{RHS}$$

So let us say, let us take the first example. So let us say A is multiplication by x . So, that means what we have in our mind is, remember, it is the operator acting on a function provides another function. So in this case, the operator since is multiplication by x , that means what we have in mind is x times f of x is g of x .

So, that is a very simple example of what that operator can be an operate, it can be as simple as just multiplication by let us say x here. Another very useful example and that I think we have seen disguise before in our calculus courses, where we can think about the derivative itself as an operator. So, what we can do is, we can ask, so, A hat is the derivative operator.

So, that means what the things that we are seeing is A hat acting on f is g of x , and this translates to the derivative of f of x is g of x . We will, we have seen how an, what characterises a linear operator? So, you see a operator is linear if it satisfies this following rule.

And remember for example, the derivative operator, we have seen that the derivative operator d/dx operator is a linear operator. Why? Because exactly it satisfies that rule, like if you know from our basics understanding of derivatives of functions. So, if we want to take the derivative of a function, let us say α times f of x plus β times g of x , this is exactly the same as α times derivative of f of x plus β times the derivative of g of x . So, here you see the derivative operator is hence a linear.

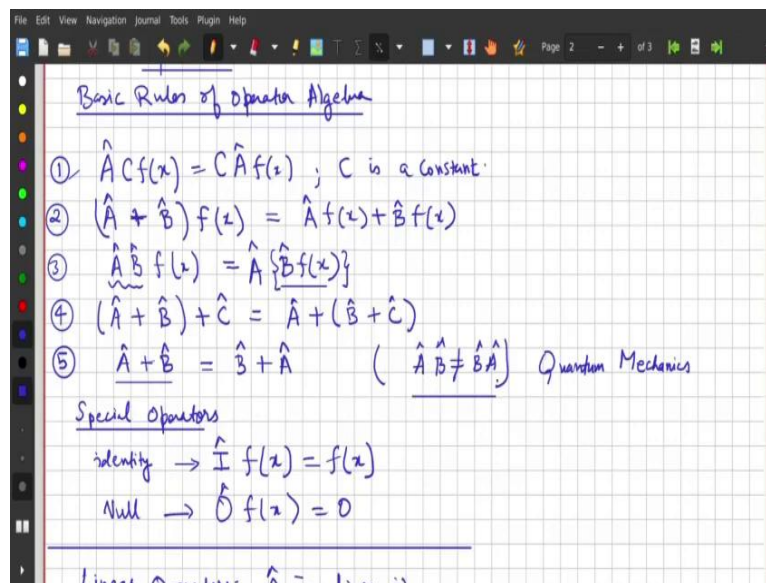
Because it satisfies the definition of linearity as you can see, so, this is the definition, the general definition of linearity that we discussed before. So, those are some of the very basic and simple examples of what do we mean and what kind of operators that we will be dealing with. In general, not all operators are linear by the way for example, I will give you another example of a nonlinear operator. And very common example of that is, let us say the square root operator, A hat is the square root operator. Now, think about the idea, let us say that if you want to take the square root, or let us write first it in terms of how we think about operators.

So, let us write it what we mean. So let us say we have A hat. And let us see why it is nonlinear. So let us impose a definition of linearity right away. So, let us have f of x plus g of x . And if A is linear, this should become A hat f of x plus, A hat g of x . And then let us does this idea whether this works for the square root operator or not. So, remember, in this case, A hat is square root operator. Let us call this equation 1. So, let us write the left hand side of

equation 1, and so the left hand side using the idea that A hat, A square root is becomes square root of f of x plus g of x.

And you see that what is the right hand side, the right hand side is square root of f of x, plus the square root of g of x, and now you can readily see that for any generic functions LHS is not equal to RHS. Hence, the definition of linearity is not being satisfied. So that is a very important idea. So, square root is a kind of an operator which is a nonlinear operator as you can see here.

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So, there can be various kinds of operators, linear, nonlinear, and we will see more important ideas about various important ideas operator, where here we saw an case where the addition operator are being commutative. Like the, if you see the operators A and B were commutative under addition, but we also discussed this fact that there are some operators and in specific, in general with respect to multiplication, the operators themselves are non-commutative and we will see that idea coming next.

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RHS = $\sqrt{f(x)} + \sqrt{g(x)}$

Commutative Properties of Operator

* In general, operators are non-commutative over the operation multiplication.

$$\hat{A}\hat{B} \neq \hat{B}\hat{A} \text{ in general}$$

Concept of Commutator → Basically gives a measure of the degree of commutativity of two operators.

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Concept of Commutator → Basically gives a measure of the degree of commutativity of two operators.

$$[\hat{A}, \hat{B}] \equiv \text{Commutator of operator } \hat{A} \text{ and } \hat{B}$$
$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \neq 0$$

As a special case of this, there can be some set of operators that are commutative over multiplication.

i.e. $[\hat{A}, \hat{B}]f(x) = 0 \Rightarrow \hat{A}$ and \hat{B} commutes.

Ex: $\hat{A} = x$; $\hat{B} = \frac{d}{dx}$

$$[\hat{A}, \hat{B}]\phi(x) = \hat{A}\hat{B}\phi(x) - \hat{B}\hat{A}\phi(x)$$
$$= x \frac{d\phi(x)}{dx} - \frac{d(x\phi(x))}{dx}$$
$$= x \frac{d\phi}{dx} - \left[x \frac{d\phi}{dx} + \phi \right] = x \frac{d\phi}{dx} - x \frac{d\phi}{dx} - \phi$$
$$[\hat{A}, \hat{B}]\phi(x) = -\phi \neq 0$$

∴ \hat{A} & \hat{B} i.e. $[x, \frac{d}{dx}] \neq 0$

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

$$= x \frac{d\phi}{dx} - \left[x \frac{d\phi}{dx} + \phi \right] = x \frac{d\phi}{dx} - x \frac{d\phi}{dx} - \phi$$

$$[\hat{A}, \hat{B}] \phi(x) = -\phi \neq 0$$

$\therefore \hat{A} \text{ \& \ } \hat{B} \text{ i.e. } \left[x, \frac{d}{dx} \right] \neq 0$ Quantum Mechanics.

Heisenberg Uncertainty principle is a direct result of certain Quantum Mechanical Operators that do not commute.

So, what we will talk next about is the commutative properties of operator, and the most important thing that we realised, I will say is in general operators are non-commutative over the operation multiplication. So, that is the general, generic idea. So, what we have in mind in mathematical notation is, let us say we have an operator A hat and we have another operator B hat. So, A hat, B hat is not equal to B hat, A hat in general.

That means for any arbitrary operators A and B that is what we meant. And based on this idea that the product of two operators are non-commutative in general, there is a very important concept, which is known as, or let us call that is the concept of commutator, and what this commutator does the idea of this commutator is? It basically gives a measure of the degree of commutativity of two operators.

So, what it does is, or the definition or, we will let us say we write so, this the symbol square brackets A hat comma B hat squared bracket close this means the commutator. This is read as the commutator of A and B, this is the commutator of operator A hat and B hat, and this definition of that is exactly the definition is exactly this what we understood it, is a measure of the degree of commutativity of two operators.

So, as you can see here in general A hat B hat is not the same as B hat A hat. So, the definition of this is basically A hat B hat minus B hat A hat. So, in general the commutator A hat, the commutator of A hat and B hat, this is not equal to 0, that is the most important idea that we are trying to come up with, that is the generic idea of what we mean by commutator.

As a special case of this as I will say as a special case of this, case of this, there can be some set of operators that are commutative over multiplication. That means in that case that is in

that case, the commutator of \hat{A} , \hat{B} acting, let us say on a function gives us 0. And if this is true, then we say that \hat{A} and \hat{B} commutes, let us take a very simple example.

Let us say our first operator \hat{A} is multiplication by x . And our second operator \hat{B} is the derivative operator. So, let us see whether what is the commutator of \hat{A} with \hat{B} . Let us say this acts on some function ϕ of x . So, let us find out whether the operators \hat{A} and \hat{B} commute or not. So, if they commute, this thing will go to 0. So, we have to evaluate what this, we have to evaluate this quantity.

So, let us apply the definition of the commutator. So, what that does, that does is $\hat{A}\hat{B}\phi$ of x minus $\hat{B}\hat{A}\phi$ of x . And let us now use the definition of what \hat{A} and \hat{B} is themselves are, which is this is x , \hat{B} is the derivative operator, minus \hat{B} is the derivative operator and \hat{A} is x times ϕ of x .

Now, you see what is happening here. So, this becomes $x \frac{d\phi}{dx}$ minus here you see let us use the because you see this is a product of two functions x and ϕ of x , we can use the product rule of differentiation. So, this will become $x \frac{d\phi}{dx}$ plus ϕ , because the derivative of x with x is 1. So, if you simplify further you see this becomes $x \frac{d\phi}{dx}$ minus $x \frac{d\phi}{dx}$ minus ϕ . So, these two cancels, so, what we are left with is minus ϕ .

So, what we shown was operator \hat{A} and \hat{B} acting on any arbitrary function ϕ provides that is not 0 you see, this is not equal to 0, this is minus of ϕ . So, therefore, we say operator \hat{A} and \hat{B} that is x and $\frac{d}{dx}$, the commutator of that is non 0, and x and $\frac{d}{dx}$ do not commute with each other. And this idea is very important in quantum mechanics in general.

If you remember the Heisenberg's uncertainty principle can be, or let us write it can be is a direct result of certain quantum mechanical operators, that do not commute with each other. That is the basic very, very basic understanding. That is one of the very important idea of commutator, and where commutator comes and handy in quantum mechanics, and we will see this later, in later videos that where this commutators comes in quantum mechanics.

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$\therefore \hat{A} \& \hat{B}$ i.e. $[\hat{x}, \frac{d}{dx}] \neq 0$ Quantum Mechanics.

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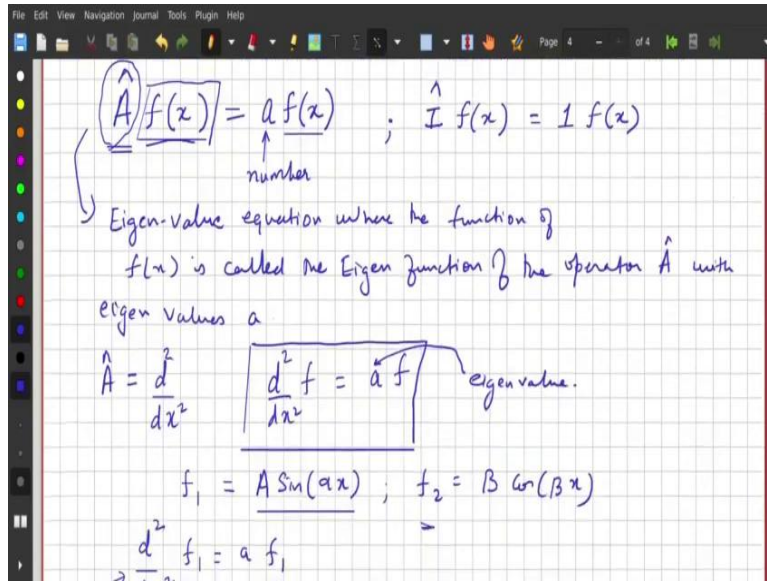
$$\hat{A} f(x) = a f(x) \quad ; \quad \hat{I} f(x) = 1 f(x)$$

↑
number

Eigen-value equation where the function $f(x)$ is called the Eigen function of the operator \hat{A} with eigen values a .

$$\hat{A} = \frac{d^2}{dx^2} \quad \boxed{\frac{d^2 f}{dx^2} = a f}$$
$$f_1 = A \sin(\alpha x) \quad ; \quad f_2 = B \cos(\beta x)$$
$$\frac{d^2}{dx^2} f_1 = a f_1$$
$$\frac{d}{dx} f_1 = A \alpha \cos(\alpha x) \quad ; \quad \frac{d^2 f_1}{dx^2} = -A \alpha^2 \sin(\alpha x)$$
$$f_1 = A \sin(\alpha x) \quad ; \quad f_2 = B \cos(\beta x)$$
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$$-A \alpha^2 \sin(\alpha x) = a A \sin(\alpha x) \Rightarrow a = -\alpha^2$$

$A \sin(\alpha x)$ & $B \cos(\beta x)$ are eigen functions for the second derivative operator with $-\alpha^2$ & $-\beta^2$ as the corresponding eigenvalues respectively.



So, we have a very good understanding of now what about the degree of commutativeness and that is expressed by the idea of a commutator. And based on that, we will be able to tell whether two operators in general commute with each other. So, now let us go to a, let us see one another very nice little thing, which is let us say think about a situation whether when you operate, we have an operator A, you act on a function f of x, and let us say you get a result which is a scalar multiple of the function itself, something like this, where this a is just a number, we have already seen one of such operators, a very trivial operator by the way, which is the identity operator, if you see the identity operator acting on the function f of any function f of x, gives a number which is 1 times the function itself.

So, we specifically want to look at these kinds of operators, which will act on a function provides the output which is a number times a function itself. And this, this the situation where you have an operator acting on a function gives you a number times the function itself, this equation is known as an eigenvalue equation, equation where the function f of x is called the eigenfunction of the operator A hat with eigenvalues a. So, what we are dealing with is an eigenvalue problem. So, let us take an very simple example. So, let us see. Let us find out.

Let us say we have an operator A, which is the second derivative operator d^2/dx^2 and let us say we apply this on to a function. So, let us write. So let us find out the eigenfunctions of this derivative operator. So, let us apply the definition of the eigenvalue equation. So, which is d^2/dx^2 acts on a function should give us a times the function itself.

So just by eyeballing the equation, you can see what we are looking at, we need a function whose second derivative is somehow related to the function itself. So, we can think of such one off such function is basically the trigonometric functions if you think about it. So it is so

$A \sin \alpha x$, and similarly, can have $B \cos \beta x$. So, if you see if you substitute f_1 or f_2 in the eigenvalue equation, so what we will have is, let us write that down, $d^2 x dx^2 f_1$ is a of f_1 .

So, you see, this equation will be satisfied when, so this will be satisfied. So, let us substitute this f_1 here. So, this will become the second derivative. So, let us take the first derivative. So, $d dx$ of f_1 is $A \alpha$ derivative of \sin is $\cos \alpha x$, that is the first derivative. And let us write the secondary derivative. So, the second derivative of f_1 with respect to x^2 is A and you get another factor of α , so that become α^2 and \cos , so that becomes $-\sin \alpha x$. So, let us now substitute this in to the eigenvalue equation here.

So, that becomes $-A \alpha^2 \sin \alpha x$ equals $\lambda A \sin \alpha x$. So, if you see what this implies is that the eigenvalue equations can be satisfied with f_1 , if and only if a very important $(\lambda) = -\alpha^2$ if and only if, λ equals $-\alpha^2$. That means if it is realise what was λ . So, this is the eigenvalue, that means what we are telling is the function $A \sin \alpha x$ is an eigenfunction of the operator $d^2 dx^2$, the second derivative with an eigenvalue $-\alpha^2$.

Similarly for f_2 . So, what we mean here is $A \sin \alpha x$ and $B \cos \beta x$ are eigenfunctions for the second derivative operator, with $-\alpha^2$ and $-\beta^2$ as the corresponding eigenvalues respectively. So, that is the generic idea for what do we mean by an eigenvalue equation and what is an eigenfunction for a given operator.

So, when you take an operator, you operate it on a function, the output that you get is a scaled version of the original function. That is that you do not get any. So, this is only very special functions, only some special functions for a special operator will have this property. This will not be true for all functions. So that is why for a given operator, the eigenfunctions are very, very special. And we will see later that the eigenfunctions acts as appropriate basis for function decomposition in general. So that is the generic idea of eigenvalue function.

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As a special case of this, there can be some set of operators that

LHS of Eqn ①

$$\text{LHS} = \sqrt{f(x) + g(x)}$$
$$\text{RHS} = \sqrt{f(x)} + \sqrt{g(x)}$$

} LHS \neq RHS

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Ex: $\hat{A} = x$; $\hat{B} = \frac{d}{dx}$

$$[\hat{A}, \hat{B}] \varphi(x) = \hat{A} \hat{B} \varphi(x) - \hat{B} \hat{A} \varphi(x)$$

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

$$= x \frac{d\varphi}{dx} - \left[x \frac{d\varphi}{dx} + \varphi \right] = x \frac{d\varphi}{dx} - x \frac{d\varphi}{dx} - \varphi$$

$$[\hat{A}, \hat{B}] \varphi(x) = -\varphi \neq 0$$

$\therefore \hat{A} \& \hat{B}$ i.e. $[x, \frac{d}{dx}] \neq 0$ Quantum Mechanics.

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Eigen-value equation where the function of $f(x)$ is called the Eigen function of the operator \hat{A} with eigen values a

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Eigen values a

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$$f_1 = A \sin(\alpha x) ; f_2 = B \cos(\beta x)$$

$$\rightarrow \frac{d^2}{dx^2} f_1 = a f_1$$

$$\frac{d^2 f_1}{dx^2} = A \alpha^2 \cos(\alpha x) ; \frac{d^2 f_1}{dx^2} = -A \alpha^2 \sin(\alpha x)$$

$$-A \alpha^2 \sin(\alpha x) = a A \sin(\alpha x) \Rightarrow a = -\alpha^2$$

So, that is the what we have covered in this small segment, where we saw the basic ideas of what do we mean by a commutator, we covered some ideas of nonlinear operator for example, the square root operator, then we came up with the idea of a commutator, and how it measured the degree of commutativity between two operators. We saw an example where let us say the function of the operator x and the derivative operators are not commutative.

And then we saw there is a, we discussed, we will discuss this in little bit more depth in later segments about the relationship about for example, the Heisenberg uncertainty principle in quantum mechanics with commutators. And then we discuss a basic idea about what do we mean by eigenvalues and eigenfunctions, and what do we mean by an eigenvalue equation, and we will see more specific concrete physical examples where these concepts will be understood better in later segments. So that is what for this segment. Thank you.