

Statistical Thermodynamics for Engineers

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Lecture 16 Supplementary Video 5 Operator Theory 3

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

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

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

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

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

$\hat{A} = \frac{d^2}{dx^2}$

$\frac{d^2 f}{dx^2} = a f$ eigenvalue.

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So, hello everyone, welcome to another segment on supplementary video series. So, in the last session we were discussing about the basic idea of eigen value problem. So, we were able to establish what do we mean by an Eigen value? So, we are discussing about Eigen values Eigen values and Eigen functions of our operator and we showed an example of the second derivative operator and showed how the trigonometric functions like for example, here you see the $f_1 \sin, \sin \alpha x$ and $\cos x$ where the Eigen functions for the second derivative operates. So, we will be discussing a very another important property of various kinds, and specifically to quantum mechanics and that is the idea of Hermitian operators. So, that is the topic of the segment.

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Hermitian Operators
 An operator \hat{A} is Hermitian if it satisfies the following property:
 $\int g^* \hat{A} f d\tau = \int (\hat{A} g)^* f d\tau$ \hat{A} $f \& g$ are arbitrary functions.
 In general, the functions $f \& g$ are general & could be complex functions. $d\tau$ is the appropriate volume element/massive dimensionality & coordinate system in use.
 $*$ \rightarrow Complex conjugation

\rightarrow Complex Conjugation System in use.
 $z = x + iy$; $z^* = x - iy$
 Ex: check whether $\frac{d}{dx}$ is Hermitian or not ??
 $\int g^* \hat{A} f d\tau = \int (\hat{A} g)^* f d\tau$ $\hat{A} = \frac{d}{dx}$
 LHS = $\int g^* \frac{df}{dx} dx$ $\frac{d}{dx} (g^* f) = g^* \frac{df}{dx} + f \frac{dg^*}{dx}$
 $g^* \frac{df}{dx} = \frac{d}{dx} (g^* f) - f \frac{dg^*}{dx}$

$\int g^* \hat{A} f d\tau = \int (\hat{A} g)^* f d\tau$ $\hat{A} = \frac{d}{dx}$
 LHS = $\int g^* \frac{df}{dx} dx$ $\frac{d}{dx} (g^* f) = g^* \frac{df}{dx} + f \frac{dg^*}{dx}$
 $g^* \frac{df}{dx} = \frac{d}{dx} (g^* f) - f \frac{dg^*}{dx}$
 $\int \left[\frac{d}{dx} (g^* f) - f \frac{dg^*}{dx} \right] dx = \int \frac{d}{dx} (g^* f) dx - \int f \frac{dg^*}{dx} dx$
 Normally, the functions f & g vanish at the boundaries
 $= g^* f \Big|_1^2 - \int f \frac{dg^*}{dx} dx = - \int f \frac{dg^*}{dx} dx$

So, we were discussing about Hermitian operators. So, what do we mean by Hermitian operators? So, the definition is, so, operator. An operator \hat{A} let us say is Hermitian if it satisfies the following definition if it satisfies the following property so, let us write down the property that is so, let us say we want to test with the operator \hat{A} is Hermitian then if it is Hermitian then it should satisfy the property integral of g^* times $\hat{A} f d\tau$ should be equal to the integral of $\hat{A} g$ the whole conjugate $f d\tau$.

So, here remember we are testing for whether \hat{A} is Hermitian or not. So, \hat{A} is the operator that we are testing for and f and g are arbitrary functions and $d\tau$ is the appropriate volume element is a measure that depends on the dimensionality and the coordinate system. So, this depends on the dimensionality which coordinate system use coordinate system in use,

so, that is the generic identity that a Hermitian operator should satisfy. So, remember here like in general the functions f and g are general and could be complex functions.

So, that is a very important thing, because you will see that is the reason hermitian operators are so useful in quantum mechanics because you will see these Eigen functions are inherently complex and the wave function specifically like saying it is a complex valued function in general. So, that is the generic idea of what we are meaning by a Hermitian operator A , where one thing to keep in mind the star, this means complex conjugation, complex conjugation.

So, that means let us say we have a complex number Z , which is $x + iy$. The conjugate Z^* is defined as $x - iy$. So, that what we mean by complex conjugation. Same thing like is valid for any function. So, let us use this definition and see whether let us check for some operators whether they are Hermitian or not? So, for example, let us check whether the first derivative of the d/dx , d/dx is Hermitian or not, check whether the d/dx is Hermitian or not, so how we will be to that?

So, let us apply the definition of an Hermitian operator. So, let us say that is g^* , $A f$ $d\tau$ is $A g$ whole complex conjugate $f d\tau$. And this is, and for our specific example, here A hat is the derivative operator d/dx , so let us see. Let us apply, so, let us see the left hand side of this thing. So, the LHS let the LHS becomes the integral of $g^* df/dx$, let us do it in one dimension, so $d\tau$ becomes just dx .

That is the LHS, and so let us draw on a very important thing. And that is, let us keep in mind, let us write what is d/dx of $g^* f$. And we can use a product rule to write this thing down. So, this is $g^* df/dx + f dg^*/dx$. And you see here we have $g^* df/dx$ here we have $d^* df/dx$. So, let us make that let us take that out and write it in terms of this.

So, let us write that $g^* df/dx$ that becomes d/dx of $g^* f$ minus $f dg^*/dx$. So, then using this thing using this here the left hand side becomes the integral of d/dx $g^* f$ minus $f dg^*/dx$ all multiplied by dx this becomes the integral of d/dx of $g^* f dx$ minus the integral $f dg^*/dx dx$.

So, one very important thing about the functions that we did so, normally these functions f and g normally, the functions f and g vanish at the boundaries, so, therefore, you will see this term goes to 0 because this becomes just $g^* f$ at the boundaries. So, let us call and let us

say this is integrated between two points 1 and 2, 1 and then 2 and that is the boundary. Let us say that is the domain boundary.

This is the point 1, 2, this is like let us call that x_1 and x_2 . So, at these two points. The functions themselves has to vanish so f of x_1 has to be 0. f of x_2 has to be 0. Similarly, for g , so this is like point 1 to 2 minus the integral f 1 to 2, $d g^* dx$. So, using the idea that this function f and g vanishes at the boundary, this term goes to 0 goes to 0, so we are just left with so the left hand side becomes minus integral $f dg^* dx dx$. So, that is the left hand side let us write down the right hand side.

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$$\text{LHS} = \int_{x_1}^{x_2} \left\{ \frac{d}{dx}(g^* f) - f \frac{dg^*}{dx} \right\} dx = \int_{x_1}^{x_2} \frac{d}{dx}(g^* f) dx - \int_{x_1}^{x_2} f \frac{dg^*}{dx} dx$$

Normally, the functions f & g vanish at the boundaries

$$= g^* f \Big|_{x_1}^{x_2} - \int_{x_1}^{x_2} f \frac{dg^*}{dx} dx = - \int_{x_1}^{x_2} f \frac{dg^*}{dx} dx$$

$$\text{RHS} = \int_{x_1}^{x_2} \left(\frac{d}{dx} g \right)^* f dx = + \int_{x_1}^{x_2} f \frac{dg^*}{dx} dx \quad \text{LHS} \neq \text{RHS}$$

$\frac{d}{dx}$ is not a Hermitian operator.

The right hand side if you see is integral of A the operator which is $d dx$. And if you see it is $ag^* dx$, $f dx$ if you see this is what this is what the right hand side where we are using a one dimensional so $d \tau$ is dx . So, this becomes, this becomes integral $f dg^* dx dx$ and you see, LHS is not equal to RHS as you can see because you see the LHS is the positive sign here you see.

And if you see the left hand side, so left hand side is negative as you can see that because the underlined term is the same but if you see there is a difference in sign. Hence, the derivative operator the first derivative operator $d dx$ is not an Hermitian operator you see. So, therefore, we prove that $d dx$ is not an Hermitian operator.

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Normally, the functions f & g vanish at the boundaries

$$= \int_1^2 f g^* dx - \int_1^2 f \frac{dg^*}{dx} dx = - \int_1^2 f \frac{dg^*}{dx} dx$$

RHS = $\int_1^2 (\frac{d}{dx} g)^* f dx = \int_1^2 f \frac{dg^*}{dx} dx$ LHS \neq RHS

$\frac{d}{dx}$ is not a Hermitian operator. $i^* = -i$

$i \frac{d}{dx}$ = Hermitian

LHS = $-i \int_1^2 f \frac{dg^*}{dx} dx$

RHS = $\int_1^2 (i \frac{d}{dx} g)^* f dx = -i \int_1^2 f \frac{dg^*}{dx} dx$

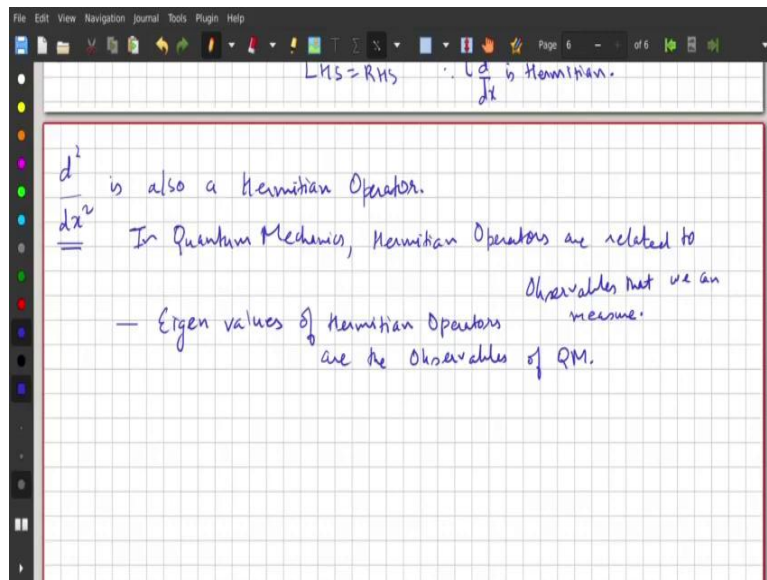
LHS = RHS $\therefore i \frac{d}{dx}$ is Hermitian.

What about other operators? Let us say we have another example where we have operator $i \frac{d}{dx}$ this i is the imaginary number. This is square root of minus 1. What about this, this entire operator is this Hermitian. We all see this is Hermitian, this is an Hermitian operator. And if you do the same procedure we can check that will become Hermitian, how can you see that?

So, if you see the left hand side will just become if we just skip the steps but I will just write the LHS. So the LHS will become minus just like before nothing changes. So, it will become minus integral minus i integral $f dg^* dx$ that is the left hand side because now you remember the operator is $i \frac{d}{dx}$ so therefore, we (i)(13:25) an extra i factor and the right hand side will become the integral of $i \frac{d}{dx}$ of g complex conjugate multiplied by $f dx$.

And now if you see when we do the complex conjugation, so, i complex conjugate is minus i if you see so, this will become minus i integral $f dg^* dx$. So, therefore, you see your LHS becomes equal to RHS, LHS is equal to RHS and hence we show that $i \frac{d}{dx}$ is Hermitian. That is the basic idea about what do we mean by Hermitian operators.

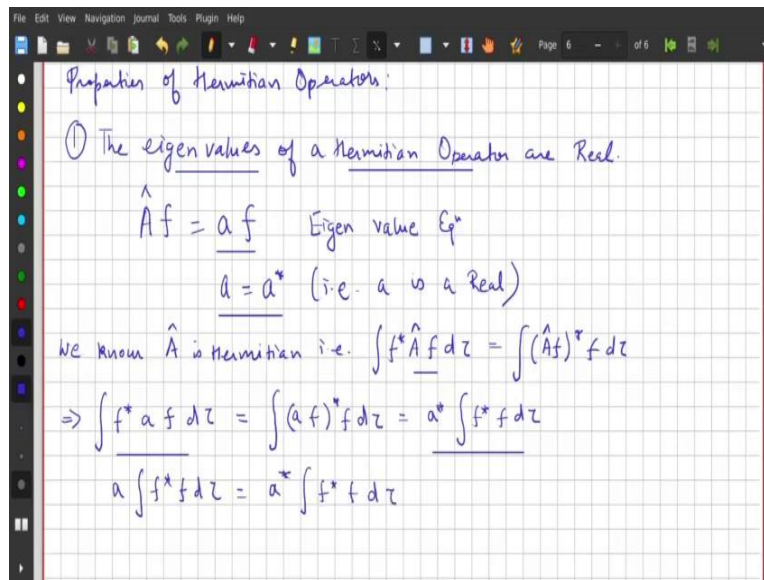
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Similarly, we can show let us say the operator the secondary derivative operator $\frac{d^2}{dx^2}$ is also a Hermitian operator so Hermitian operator and this you can test it yourself, test it out just by looking at this expression you will see now you have to do this. This so this is if you think about the step that we did this was basically integration by parts in disguise, and we have to do this twice. So, we will pull an extra minus. So, that minus sign will be absorbed. So, when we will compare the LHS and RHS both will be now positive.

And hence, we can show that the second derivative operator will be an Hermitian operator that is a that is a very important operator that will be used in quantum mechanics because in general in quantum mechanics, mechanics Hermitian operators are related to observables that we measure in lab. The objects that we can measure basically, we will see that the Eigen values of Hermitian operators are the measurable. So, the I will write it down here the Eigen values Eigen values of Hermitian operators and operators are the observables the observables of quantum mechanics and this follows from a very important fact that we all we all just see.

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There are some very interesting properties of Hermitian operators I will write that down the properties of Hermitian operators. So, let us now study the some of the properties of Hermitian operators in general. So, one other very important and fundamental property of Hermitian operators are the Eigen values of a Hermitian operator are real, that is a very important property of Hermitian operators. And, let us see how can we prove this thing, that is a very simple proof, let us do it.

So, let us say so, you want to understand the Eigen values of a Hermitian operator, that means the Hermitian operator should pose a Eigen value problem. So, let us write the Eigen value problem first. So, that is let us say A an operator acting on a function f gives us scalar multiplier of the function f . So, here f is the Eigen function and a is the Eigen value this is the Eigen value equation. So, this is the Eigen value equation, and then what we have to prove is the equivalent mathematical statement of this is that we have to prove that a is the same as a star that means a is real, a is a real.

It is not complex, it is not a complex number, it is purely real number. So, a number whose complex conjugate is same as the number itself, that is a real number. So, we know that A is Hermitian. So, we know \hat{A} is Hermitian, that is, the integral $\int f^* \hat{A} f dz = \int (\hat{A} f)^* f dz$ so we just use the definition of an Hermitian operator. So, this can be rewritten as instead of $\hat{A} f$. Remember, this is the operator.

Yes, instead of $\hat{A} f$ we will be substituting this because it satisfies the Eigen value equation, so this becomes $\int f^* a f dz = \int (a f)^* f dz$ and instead of that we will again write $\hat{A} f$ becomes $\hat{A} f$

whole star f d tau this becomes then a star integral of f star f d tau if you see if you compare this and this. So, this becomes a integral f star f d tau is same as a star integral f star f d tau, so that means a minus a star integral f star f d tau equals 0 so, in general, this will not be equal to 0 is not equal to 0, we all see later, why.

So, this has to be equal to 0 that is to be equal to 0 then that is a equals a star. So, for any arbitrary function, you see f we are not arbitrary will say because this is an Eigen function, this is an Eigen function for the operator a you can function operator a real the Eigen values are real as you can see, so, that is a quite so, very important property of Hermitian operators Eigen values of a Hermitian operators are always real.

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$$\Rightarrow \int f^* a f d\tau = \int (a f)^* f d\tau = a^* \int f^* f d\tau$$

$$a \int f^* f d\tau = a^* \int f^* f d\tau$$

$$(a - a^*) \int f^* f d\tau = 0 \quad \text{i.e. } \boxed{a = a^*}$$

$$\int f^* f d\tau \neq 0 \quad \text{if } f \neq 0 \quad f^* f \text{ is +ve.}$$

$Z = x + iy$
 $Z^* = x - iy$
 $Z Z^* = x^2 + y^2 > 0 = |z|$

② The associated eigen functions form a complete orthogonal & normalizable set.
 If $\int g^* f d\tau = 0$ & $\int f^* f d\tau \neq 0$
 Then f & g are orthogonal.

$\int f^* f d\tau \neq 0 \quad \text{if } f \neq 0 \quad f^* f \text{ is +ve.}$

② The associated eigen functions form a complete orthogonal & normalizable set.
 If $\int g^* f d\tau = 0$ & $\int f^* f d\tau \neq 0$
 Then f & g are orthogonal.

$\hat{A} f = \lambda f ; \hat{A} g = t g \quad \text{if } \lambda \neq t \quad \text{then } \int g^* f d\tau = 0$

$\int f^* \hat{A} g d\tau = \int (\hat{A} f)^* g d\tau \Leftarrow$

$\Rightarrow \int g^* \hat{A} f d\tau = \int (\hat{A} g)^* f d\tau$

$t \text{ is Real}$
 $t^* = t$

$$\text{If } \int g^* f d\tau = 0 \text{ \& } \int f^* f d\tau \neq 0$$

$$\text{Then } f \text{ \& } g \text{ are orthogonal.}$$

$$\hat{A}f = s f; \hat{A}g = t g \quad \text{if } s \neq t \text{ then } \int g^* f d\tau = 0$$

$$\int f^* \hat{A}g d\tau = \int (\hat{A}f)^* g d\tau \Leftrightarrow$$

$$\Rightarrow \int g^* \hat{A}f d\tau = \int (\hat{A}g)^* f d\tau \quad \begin{matrix} t \text{ is Real} \\ t^* = t \end{matrix}$$

$$\int g^* s f d\tau = \int (t g)^* f d\tau = t^* \int g^* f d\tau = t \int g^* f d\tau$$

$$(s - t) \int g^* f d\tau = 0 \Rightarrow \int g^* f d\tau = 0$$

And that comes to the second property again important property associated Eigen functions, Eigen functions form a complete orthogonal and normalizable set and part of this proof is here where when we said so, so when we are that let us. So, let us see, let us do it like this so if the integral of say $g^* f d\tau$ equals 0 and the integral of say $f^* f d\tau$ this is not equal to 0 we will see. So, then f and g are orthogonal, one important thing to realize here that when you multiply your function by its complex conjugate this is always a real number. This is a real positive quantity.

So, if f is not equal to 0, $f^* f$ is always positive. You can think about from complex analysis like let us say we have z is x plus iy and z^* is x minus iy . And the product $z^* z$ is x plus iy minus x . So, this just becomes x^2 plus y^2 this is this is a positive remember it is always positive, this is $\text{mod } z^2$. So, therefore this is never equal to 0 as you saw here. And using that idea and this idea, you can say when two functions are orthogonal.

So, let us see how we can tell whether you have an Hermitian operators the Eigen functions of the Hermitian operator will be orthogonal, so let us say we have A acting on the function f , it should provide f times f . It is an eigenvalue problem, correct. So, that is f there is one of the Eigen function and let us say we have another Eigen function, let us say that it is called g and it acts on to provide another Eigen value times Eigen function g .

And see if s is not the same as t that means these two are different Eigen values, then what we need to show is the integral $g^* f d\tau$ has to be equal to 0, so, that is the orthogonality condition. And again, like the easiest way to do is just by applying the definition of Hermitian

operators, let us do that. So, the integral of $f^* A g$ $d\tau$ is equal to integral $A f^* g$ $d\tau$ this can be rewritten as a think about just by using that $A f$ is sf and $A g$ is tg , we just use that substitution. This will become the integral.

Or let us let us write it in a little bit. Let us rewrite this in a different form because what we want to show here is $g^* f$. So, we all just slightly change the way we write the Hermitian operator, it is one in the same, so that will be $g^* A f$ $d\tau$ is equal to integral of $A^* g$ or $A^* g$ $d\tau$, so that is this statement is the same as basically the statement. There is no difference just the way how we are casting it to prove actually, so since here we want g^* , that is why we will we want to keep g^* here.

That is, that is why we are using this definition for writing the Hermitian operator definition. So, now we all just use the identity that we already have, which is $A f$ is sf and $A g$ is tg . So, that will become integral $g^* sf$ instead of $A f$ and this becomes $d\tau$ and that is equal to integral $A^* g$ instead of that we will write $g^* A f$ $d\tau$ and then this becomes $t^* \int g^* f d\tau$ and since, this is an Eigen value, we know that t is real from the previous property of Hermitian operator and we know that A is an Hermitian operator therefore, t^* is the same as t , this becomes just $t \int g^* f d\tau$.

Therefore, what we have is $s - t \int g^* f d\tau = 0$ and since we already told that s is not equal to t , that means this is not equal to 0 this is not equal to 0. So, the only way this can be 0 is this is to be 0 therefore, this implies that $\int g^* f d\tau = 0$ and hence we prove that f and g are orthogonal.

So, f and g are the two Eigen functions of the Hermitian operator and when we and then we showed using just the definition of Hermitian operators that f and g has to be orthogonal. That is the generic idea of Hermitian operators and Hermitian operators are very much useful in specifically in quantum mechanics, because as we discussed before it the Eigen values of the Hermitian operators are the quantum mechanical observable.

So, I think so that is what this segment was all about. So, we discussed about Hermitian operators, what are Hermitian operators and what we saw two important properties of Hermitian operators, that the Eigen values of the Hermitian operator are always real and the associated Eigen functions forms a complete orthogonal basis set. And if it is orthogonal we can easily show it is normalizable it is a matter of scaling that is what normalizable means. So,

I think so that is for this segment. Thank you for listening, so we will see in the next segment, thank you.