Good morning student. I'm Apurva Narvekar, Assistant

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Today we're going to learn about commutator and commutation rule, model number 29

and it belong to the unit quantum chemistry.

So the outline of this presentation includes commutators, Commutation rules

and problems based on commutators.

Outcome of this module will be, you all will be understanding what is commutator,

What are different commutation rule and how to use it for different observables or

operators in quantum mechanics.

So first let's see what is commutators.

So if we have operators A&B then the

commutator of these two

operators A&B is operator C, which is denoted as A&B in the

square bracket and it is defined as a [A B.

So AB minus BA is equal to the commutator.

Now, if a AB is equal to BA, then commutator is equal to 0.

That means the operator A&B commute with each other.

If a AB is not equal to BA, then commutator is not equal to 0.

Then operators A&B does not commute with each other. If the

value of the commutator is close to zero, it determines to how much extent this operator commute. If it is very close to 0, then the

extent of commutation is higher.

So when we are solving a problem, we have to calculate a

AB & BA and see whether AB is equal to BA or not.

So let's see some examples, if operator A is d/dx and operator B is 7, then

let's calculate what is a AB and what is BA

Let's take one function f(x) on which these operators operate. So

AB of f(x) is equal to d/dx {7 f(x)}.

7 is constant, so AB of f(x) is equal to 7 d/dx f(x)

Now let's see what is BA f(x)

BA f(x) is equal to 7 d/dx f(x). Now if you see AB f(x) and BA f(x) both are equal.

Therefore d/dx and 7 commute with each other.

Now let's see example 2, A is d/dx & B is x, so let's

calculate what is AB f(x). So A is d/dx, B is x & function f(x).

So it is d/dx { x f(x) }.

Now here it is a derivative of the product of two values.

So we have to apply derivative multiplication rule that is d/dx {u v} = u d/dx (v) + v d/dx (u)

The same rule we will apply here.

So we get AB f(x) is equal to x d/dx f(x) + f(x) d/dx (x),

which gives x d/dx f(x) + f(x)

because d/dx (x) is equal to 1.

Now this is about AB f(x).

Now let's see BA f(x).

B is X and A is d/dx. So we write BA of f(x) is equal to x d/dx f(x).

Now if you see AB f(x) and BA f(x), both are not same.

Let's take out AB f(x) minus BA of f(x),

AB f(x) minus BA of f(x) is equal to

x d/dx f(x) + f(x) - x d/d/dx f(x)

Now if you see here x d/dx f(x) term 1

positive one negative, cancels out

AB f(x) - BA f(x) is equal to f(x) which is not equal to 0.

Therefore d/dx and x do not commute with each other. Let's see some

commutation rules. If you see here operator A

Commute with itself, and any power n of itself. where n = 1, 2, 3, 4.

Second, if we multiply any constant k to any

of the operator A or B, we get the commutator of this operator

is equal to the constant K into the commutator of AB.

The third one is if we find out the commutator of operator A

with that of the sum of the operator B&C. It is equal to

some of the commutator of operator AB and operator AC.

Similarly, commutator of operator A + B and C is

equal to some of the commutator of operator AC and BC, so this is called the property of linearity

Next, if we see.

In the 4th point, the commutator of operator A with

that of the product of operator B&C is equal to some of the

product of commutator of operator AB with that of

operator C and product of operator B with that of the

commutator of operator AC.Similarly for commutator of

product of operator AB and operator C. So this is called is

the distributive property, so

Commutation is distributive.

Next commutator of operator A with any scalar quantity b is equal to 0. Now let's see that.

If we switch the order of the computation of operator A&B to

operator B&A, the product is opposite. So let's prove this.

As per the definition of commutator, we have the

commutator of operator A B is equal to AB-BA and commutator

of operator B A is equal to BA-AB.

so let's rearrange the equation number (i), that is

we will put BA first. It is -BA+AB. Now if we

take the minus sign common we get - (BA - AB) which is equal to

the commutator of operator B A.

That is, commutator of operator AB is equal to minus of commutator of operator BA. So now in quantum

mechanics how commutators are useful for two observables if

the commutator is 0 then they can be measured simultaneously.

We all know about Heisenberg Uncertainity principle that we

cannot find the position and momentum of microscopic particle

simultaneously exactly.

That's the reason position and momentum operator do not

commute, so let's find out what is the commutator of position

and momentum operator. So the position operator is represented

as X hat and momentum operator is represented as Px hat, which

is equal to X Px - Px X.

let's take some function f(x) so the position operator x is equal to x and

momentum Operator Px is equal to h/i d/dx.

Now according to the definition of commutator, the computation of

operator x and Px is equal to operator x and operator Px minus

momentum operator PX into position operator x.

and the function is used to operate on it. OK, now this can

be written as x Px f(x) - Px x f(x)

So now when we substitute the values for x and Px,

we substitute for x as x and Px as h/i d/dx f(x)

Now here if you see

we have two in the second term it is d/dx {x f(x)}

So we have to similarly use derivative multiplication rule the the one which we use

while solving example #2. So according to this rule we write

d/dx {x f(x)} + f(x) d/dx x

So when you open the bracket that is once

you substitute d/dx x is equal to 1.

And then you open the bracket we get here x h/i d/dx f(x) - h/i x d/dx f(x)

+ * - = -, so we will get

-h/i f(x)

So if you see the first to terms

they are similar in values but opposite in sign, so they will

cancel out and the final value will be -h/i f(x)

Thus position and momentum operators do not commute.

This is a reference. I. N. Levin, Quantum Chemistry. Thank you.