Ministry of Higher Education and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

# Quantum Chemistry

## - The Twelfth lecture –

Stage 4

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# Hermitem (op) properties properties

1) The subjective value of pyramidal effects is real, this change is made using variables to represent observed quantities because the values of these properties are physical and are therefore considered accurate properties.
   We assume that the function is a real function of the $(\psi_n)$pyramidal effect so as to achieve the equation of self-value.

$$\hat{A}\psi_n = an\ \psi_n$$

Where $a_n$ represents the subjective value of the function.

The true value of the pyramidal effect can thus be demonstrated as follows:

a. We multiply the equation with the motor function. $\psi_n^*$

$$\psi_n^*\ \hat{A}\ \psi_n = a_n \int \underline{\psi_n^*\ \psi_n}\ d\tau$$

صفحة السواء تساي 1

The hierarchical adjective can be applied to this function

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$$\int \psi_n^* \hat{A} \psi_n = \int \Big(\psi_n^* \underbrace{\hat{A} \psi_n}_{a_n \psi_n}\Big)^* = a_n^* \int \underline{\psi_n^* \psi_n d\tau}$$

صفحة السواء تساي 1

$$a_n = \underbrace{a_n^*}_{Hermitim\ actual}$$

**2)** Self-worth functions are different with the influence of two pyramids orthogonal pleasures. Tostabilize this property, take two different functions $(\psi_n, \psi_m)$where

$$a_m \psi_m = \hat{A} \psi_m$$

$$a_n \psi_n = \hat{A} \psi_n$$

$$\int \psi_m^* \underbrace{\hat{A} \psi_n}_{A_n \psi_n} d\tau = an \int \psi_m^* \psi_n d\tau \ \_\_\_\_\_(1)$$

The effect $\hat{A}$affects the function according to the $(\psi_n)$self-value equation.

The influencer wouldn't have$\hat{A}$ influenced my pyramid, so we could take the alternative of the hierarchical character, which is

$$\int \psi_n^* \hat{A} \psi_m d\tau = \int \Big(\psi_n^* \underbrace{\hat{A}\psi_m}_{A_m \text{ دالة } m}\Big)^* \ d\tau \ a_m \int \psi_m^* \psi_n d\tau \ \_\_\_\_(2)$$



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The two equations can be equated

$$a_n \int \psi_m^* \, \psi_n d\tau = a_m \int \psi_m^* \, \psi_n d\tau$$

$$a_n - a_m \int \psi_m^* \, \psi_n d\tau \qquad hermetion\ orthogonality$$

**3)** Commute Interchange

*To show theeffects* $(\hat{A}, \hat{B})$*have the same unknown of subjective functions where the effecter's function* is subjective to $\hat{A}$*function* $\psi_n$*as follows: -*

$$\hat{A}\psi_n = a_n\psi_n$$

*An:- Represents the subjective value of the influencer.*$\hat{A}$

$\because$*and since it* $\hat{A}$*fits in with*$\hat{B}$ $\qquad \hat{A}\hat{B} = \hat{B}\hat{A}$

*So we can prove the following:*

$$\hat{A}\hat{B}\psi_n = \hat{B}\hat{A}\,\psi_n$$

$$\hat{A}\psi_n = a_n\,\psi_n$$

$$\hat{B}\psi_n = b_n\psi_n$$



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$$\hat{A}\hat{B}\psi_n = \hat{A}\left(\underline{\hat{B}\psi_{\mathrm{n}}}\right) = b_n\underline{\hat{A}\psi_n} = b_n a_n \psi_{\mathrm{n}}$$

$$\hat{B}\hat{A}\psi_n = \hat{B}\left(\underline{\hat{A}\psi_n}\right) = a_n\,\underline{\hat{B}\,\psi_n} = a_n\,b_n\,\psi_n$$

$$a_n\,b_n\,\psi_n = b_n\,a_n\,\psi_n \text{ Hermetim Comnute}$$

## 3) *Third hypothesis* third pastulate

*If it $A$represents a certain amount and has a set of subjective functions that achieve the following equation:-*

$$\hat{A}\psi_n = a_n\,\psi_n$$

If a series of practical measurements of this amount ($a_n$) are made, they should all give one value, $a_{n.}$

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## 4) Fourth hypothesis fourth pastulate

If the effect represents a reduced amount of a $\widehat{\mathrm{H}}$system described by the function $\psi_n$and is not a subjective function of the effect, a series of $\hat{A}$practical measurements of the amount an does not give a single value but a set of different values distributed around a numerical average called expectation value

$$(E_{exp}) = \frac{\int \psi_m^* \,\hat{A}\, \psi_n d\tau}{\psi_m^* \,\psi_n d\tau} = \frac{\langle n|\hat{A}|m\rangle}{\langle n|m\rangle}$$

If the function is together, the denominator = 1

The third hypothesis is a special case of the fourth hypothesis because when the function is $\psi_n$subjective to the influencer, $\hat{A}$the expected value is subjective.

**Ex:- Calculate the expectation value for on if you know ?$\frac{d}{dx} e^{-\alpha x}\psi^* = e^{-i\alpha x}, \quad \psi = e^{+i\alpha x}$**

**solu**

$$\langle E_{exp}\rangle = \frac{\int \psi_m^* \,\hat{A}\, \psi_n d\tau}{\int \psi_m^* \,\psi_n d\tau} = \frac{\int \psi^* \frac{\partial}{\partial x} \;\psi\, dx}{\int \psi^* \,\psi\, dx}$$

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$$= \frac{\int e^{-i\alpha x} \frac{d}{dx} \, e^{+i\alpha x} \, dx}{\int e^{-i\alpha x} \, e^{+i\alpha x} \, dx} = \frac{\int e^{-i\alpha x} \frac{d}{dx} \, e^{+i\alpha x} \, dx}{\int e^{0} \, dx}$$

$$= \frac{\int e^{-i\alpha x} \, \alpha x \, e^{+i\alpha x} \, dx}{\int dx} = \frac{\alpha x \int e^{-i\alpha x} \quad e^{+i\alpha x} \, dx}{\int \, dx}$$

$$\frac{\alpha x \int e^{0} \quad dx}{\int \, dx} = \frac{\alpha x \, dx}{dx} = \frac{\alpha x}{x}$$

$$\therefore \langle E_{exp} \rangle = \alpha x$$

## 5) Fifth pastulate hypothesis

It is a collection of many issues in quantum mechanics and spectroscopy that are concerned with time-based phenomena. In this case, we use the time-based Schrodenker equation to describe a particular time-based system according to quantum mechanics.

$$\hat{H}\psi(x, y) = -\frac{\hbar}{i} \cdot \frac{\psi}{\psi_t} \, \_\_\_\_\_\_ (1)$$

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In general, it is difficult to find a solution to the time-based Schrodinger equation, but the separation of variables is as follows:

$$-\frac{\hbar^2}{2m}\cdot\frac{\partial^2\,\psi(x,t)}{\partial x^2}+v(x)\psi_{(x,y,z)}=\frac{-\hbar}{i}\cdot\frac{\psi}{\psi_t}\ \_\_\_\_(2)$$

Variables can be separated

$$\psi_{(x,t)}=\psi_{(x)}\cdot f(t)\_\_\_\_(3)$$

We make up 2 in 3 and divide.$\psi_{(x)}, f(t)$

$$-\frac{\hbar^2}{2m}\cdot\frac{1}{\psi_{(x)}}\cdot\frac{\partial^2\,\psi_{(x)}}{\partial x^2}+v\,\psi_{(x,y,z)}$$

$$=\frac{-\hbar^2}{t}\cdot\frac{1}{f(t)}\cdot\frac{df(t)}{dt}\ \_\_\_\_(4)$$

∵ the two sides of the last equation depends on two different variables the right end includes (t) and the left depends on (x)) so each of the terminal equals a constant and thus the equation becomes as follows:

$$-\frac{\hbar^2}{2m}\cdot\frac{1}{\psi_{(x)}}\cdot\frac{\partial^2\,\psi_{(x)}}{\partial x^2}+v=E\ \_\_\_\_(5)$$

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It is the equation of Schrodenker..... Time-based, therefore, can be written regularly as follows: -

$$\hat{H}\,\psi_{(x)} = E_{\psi_{(x)}}$$

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