Ministry of Higher Education and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

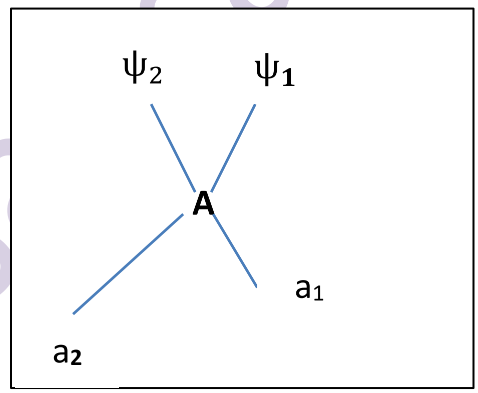
- Thirteenth lecture –

Stage 4

Prof. Dr Hassan sabih

Function Linear Combination

If we have two functions ($\psi 1$, $\psi 2$) that may be similar or different to one effect, it $\hat{A}$has two self-vacuum values (a1,a2) so it is:



Therefore, the two functions can be represented by a single function, the linear union of them, written as follows:

$\Psi = C_1\psi_1 + C_2\psi_2$

$C_{1,C2}$ transactions for the two medals of the linear union

How do we prove that the function is not subjective to effect A.

Note the following:

1 of the equation of linear union of the wali

$\Psi = C_1\psi_1 + C_2\psi_2$ 1

2 We affect the function with the effect $\hat{A}$

$$\hat{A}\,\Psi = \hat{A}\,(C_1\psi_1 + C_2\psi_2) \;\dots\dots\dots 2$$

3 In order for the function to be a subjective function of the influencer, we $\hat{A}$mustachieve thecondition by self-value a.

$$\hat{A}(C_1\psi_1 + C_2\psi_2) = a\,(C_1\psi_1 + C_2\psi_2) \;\dots\dots..3$$

4 In order for the two functions to be self-fulfilling, the following equations must be achieved.

$$\left.\begin{array}{l}\hat{A}\,\psi_1 = a_1\,\psi_1\\ \hat{A}\,\psi_2 = a_2\,\psi_2\end{array}\right\} \quad \dots\dots\dots 4$$

But when you go back to the equation (3) and open the brackets we notice

$$\hat{A}(C1\psi1 + C2\psi2) = C1\hat{A}\psi1 + C2\hat{A}\psi2$$
$$= C1\,a\,\psi1 + C2\,a\,\psi2 \;\ldots\ldots..5$$

Therefore, the equation cannot be written as follows, i.e. the function is not subjective:

$$\hat{A}\,(C_1\psi_1 + C_2\psi_2) = a\,(C_1\psi_1 + C_2\psi_2)$$

Exact solution of schrodinger equation for some simple system

M/ Precise solutions to schrodker equation for simple systems

Through our study of previous chapters, the Schrodniker equation can be written for any physical system consisting of several particles, but the solution of the Schrodniker equation is limited to simple systems, thus helping us to understand many basic concepts of quantum mechanics, including the study of the free particle system, the particle system in a single- and multi-dimensional box, and the harmonic oscillator system.

1 Free partical

We take a particle that moves freely into space so that its potential energy is fixed or equal to zero. If the particle is only one way (x)

So Hamilton's influence can be written with this particle.

$$\hat{H} = T + V \qquad , \text{if } V=0$$

$$\hat{H} = T$$

$$\because \hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \quad \dots\dots\dots (1)$$

$$\because \hat{H}\,\psi = E\psi \quad \dots\dots\dots (2)$$

Compensate (1) in (2)

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi = E\psi \quad \dots\dots\dots (3)$$

Equation organization (3)

$$\left(\frac{-\hbar^2}{2\mathrm{m}}\frac{\partial^2}{\partial \mathrm{x}^2}\right)\psi - E\psi = 0 \ldots\ldots (4)$$

we care about the limit $\left(\frac{\partial^2}{\partial \mathrm{x}^2}\right)$ so we have to get rid of $\left(\frac{-\hbar^2}{2\mathrm{m}}\right)$

So we multiply $\left(\frac{-\hbar^2}{2\mathrm{m}}\right)$ in, so the equation becomes the following.

$$\frac{\partial^2\psi}{\partial \mathrm{x}^2} + \frac{2mE}{\hbar}\psi = 0 \ldots\ldots .5$$

We impose the constant. $k^2 = \frac{2mE}{\hbar} \ldots\ldots 6$

We make up 5 in 6.

$$\frac{\partial^2\psi}{\partial \mathrm{x}^2} + k^2\psi = 0 \ldots\ldots 7$$

$$\left(\frac{\partial^2}{\partial \mathrm{x}^2} + k^2\right)\psi = 0 \ldots\ldots 8$$

Thus, a stimulating equation can be written that represents the equation of a wave after compensating for the constants with the abbreviation and arrangement, which is associated with a particle moving towards the axis.

$$\boxed{\psi_{(x)} = Ce^{\pm ik_x}}$$

Signal + ← indicates an object moving towards the positive X axis

Signal - ← indicates an object moving towards negative X

2 particles in particle in box:

An object moving from zero ←a on the x axis has only kinetic energy (latent energy = zero) so an end must be put to no end so as not to exceed site A (we place a barrier and bar the particle instead of outside the barrier limits)

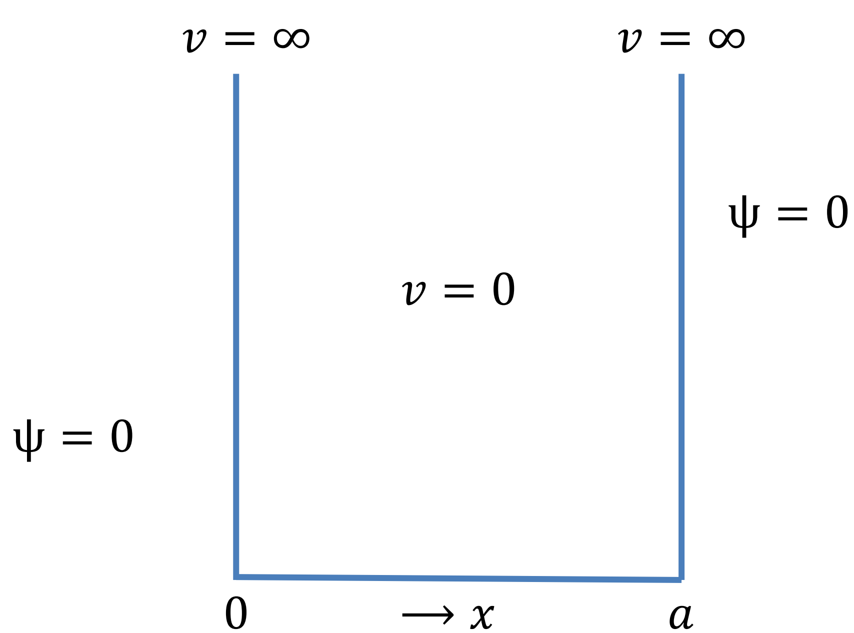
The function is ψ=0 so use the Schrodenker equation in the simplest systems

she:

1 particle condition restricted movement in a box and one way from 0 ← a

2 We impose the energy inherent inside and outside the box = zero and outside = infinity

3 The properties to be determined by the power and self-function of the system and this is done according to the conditions



$$v(x)\begin{cases} v = 0, & 0 \le x \le a \\ v = \infty, & 0 > x > a \end{cases}$$

So Hamilton's influencer is written for a particle in a box.

$$\because \hat{H} = \frac{-\hbar^2}{2\mathrm{m}} \cdot \frac{\partial^2}{\partial \mathrm{x}^2} + v(x) \_\_\_\_(1)$$

As for the Schrodinger equation.

$$\because \hat{H}\psi_{(x)} = E\psi \_\_\_(2)$$

Compensate (1) in (2)

$$\frac{-\hbar^2}{2\mathrm{m}} \cdot \frac{\partial^2 \psi}{\partial \mathrm{x}^2} + v(x) = E\psi \_\_\_(3)$$

$$v = 0$$

$$\frac{-\hbar^2}{2\mathrm{m}} \cdot \frac{\partial^2 \psi}{\partial \mathrm{x}^2} = E\psi \_\_\_(4)$$

we multiply in $\frac{-2m}{\hbar^2}$

$$\frac{\partial^2 \psi}{\partial \mathrm{x}^2} = \frac{-2m}{\hbar^2} E\psi \_\_\_(5)$$

$$\frac{\partial^2 \psi}{\partial \mathrm{x}^2} + \frac{2m}{\hbar^2} E\psi = 0 \_\_\_(6)$$

we impose $\frac{2m}{\hbar^2} E = k^2$

$$\frac{\partial^2 \psi}{\partial \mathrm{x}^2} + k^2\psi = 0 \_\_\_(7)$$

When conducting the necessary mathematical processes, both the energy and the wave function can be set.

a) Set the wave function in the next relationship

$$\psi_{A(x)} = \sqrt{\frac{2}{a}}\, Sin \frac{n\pi x}{a}$$

b) Power set

$$E_n = \frac{n^2 \hbar^2}{8\pi a_2}$$

n: Represents the slowest energy, i.e. the body is found at zero, called zero **point energy.**

is the energy that the body has when it is at the lowest energy levels i.e. n=0 so

$$E = \frac{\hbar^2}{8\pi a_2}$$

So we conclude:

1) The state of the body in the box of electron similarity in a metal wire any electron effort remains constant in the wire but until it reaches the end of the wire increases its effort sharply i.e. the launch of the electron needs very high energy but not indefinitely

2) The model is used to study electrons π in successive polydynaines and when calculating the energy with which the electron moves for all dual bonds

$$-\mathrm{C}=\mathrm{C}-\mathrm{C}=\mathrm{C}=\mathrm{C}=\mathrm{C}-$$

Conjugat polyenes