Ministry of Higher Education
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College of Science

Department of Chemistry

# Quantum Chemistry

- Fourteenth lecture -

Stage 4

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**3)** Particle **out put the box case:**

The function that represents the ()ψ system and the other property to be identified is the energy of that influencer used, which is hamilton's effect.

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

The equation used to solve the Schrodenker equation represents the equation of self-value.

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

*Compensate (1) in (2)*

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

$$v = \infty$$

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

Energy $E\psi$ is of neglected value compared to ()$\infty\, \psi_{(x)}$ so the relationship becomes

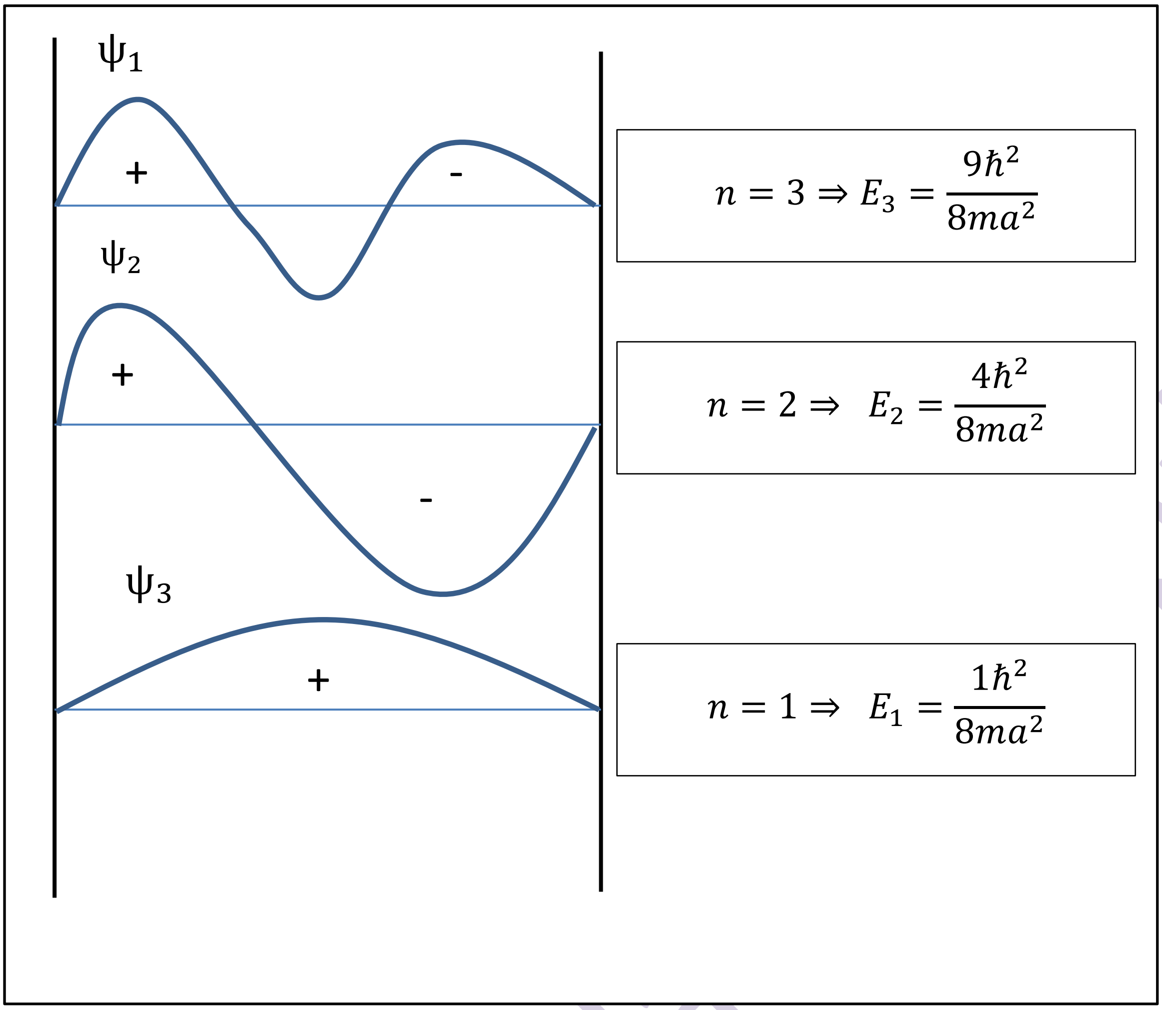
$$\frac{-\hbar^2}{2m} \cdot \frac{\partial^2}{\partial x^2} = \infty\, \psi_{(x)} \_\_\_\_\_\_ (5)$$

From the equation(5),  the function should be equal to zero because there is no  endless power system.

Such an equation is not mathematically correct unless the value multiplied in it (0 =)∞  i.e. the function $\psi_{(x)}$= zero i.e. the particle does not exist outside the box and thus can find a relationship between the shape of the wave function and the energy by the number of quantity according to the following relationship

$$\psi_{n(x)} = \sqrt{\frac{2}{a}}\, Sin\frac{8\pi x}{a}$$

Therefore, to determine the value of the wave function at any point and at any quantitative number, you must enter the number of quantity and location in equation 1,  as in the forms of the following wave function.




The difference between two levels of energy such as $E_1, E_2$

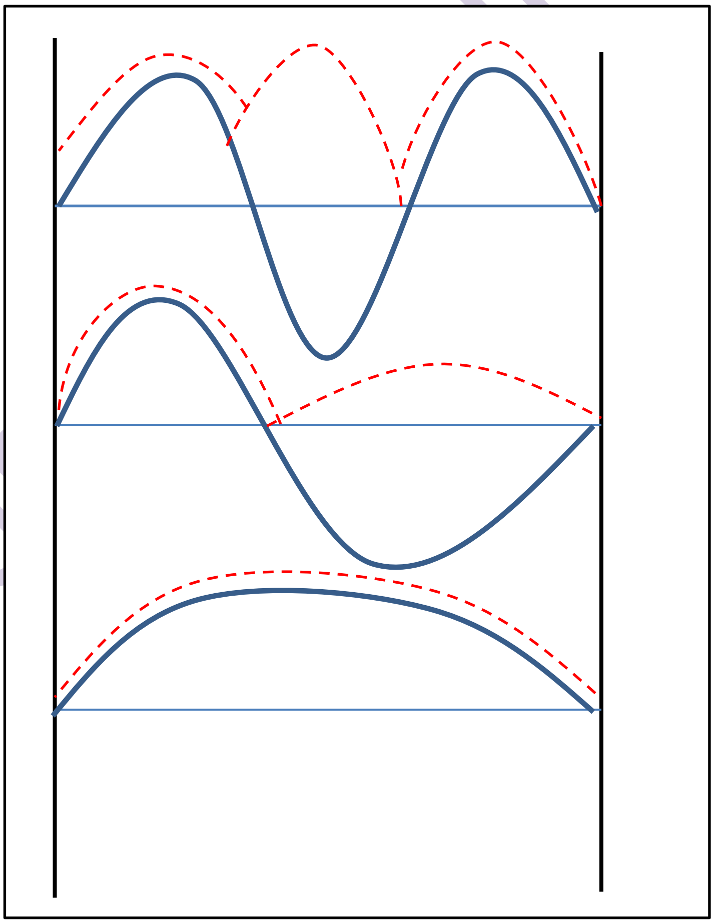
$$\Delta E = E_2 - E_1$$

$$E_{1,2} = \frac{4\hbar^2}{8\,m\,a^2} - \frac{\hbar^2}{8ma^2}$$

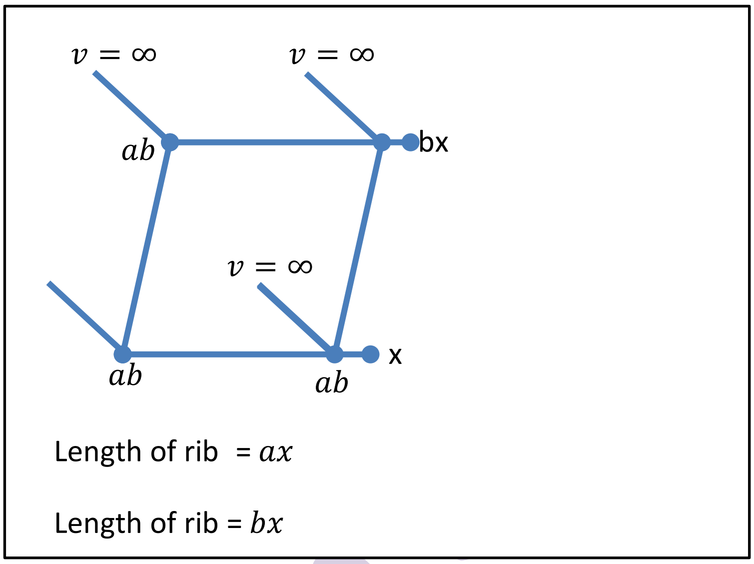
$$= \frac{4\hbar^2}{8ma^2}$$

By drawing the first case, the line that represents the acceptable function.

But in the second case, part of the function is below the line, which is a negative function (and each function is negative, so the importance of the function when it is(2) so we have to quarter$\psi$ the values that we have, so the drawing is in the following form (which is the function that expresses the system (2) $\psi$



## **Particle in a two-dimensional box:** Body in 2D box two-dimen sional




In the case of a two-dimensional particle, there are two quantitative numbers and energy pooling, so we deduce energy.

$$En_1(x) = \frac{n_1^2 \hbar^2}{8ma^2} \qquad \_\_\_\_(1)$$

$$En_2(x) = \frac{n_2^2 \hbar^2}{8mb^2} \qquad \_\_\_\_(2)$$

$$En_1, n_2\ (x)_\infty = \frac{n_1^2 \hbar^2}{8ma^2} + \frac{n_2 \hbar^2}{8mb^2}$$

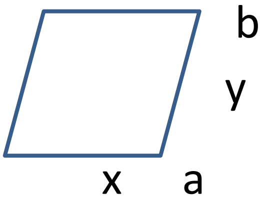
$$\text{بصورة عامة} = \frac{\hbar^2}{8m}\left(\frac{n_1}{a^2} + \frac{n_2}{b^2}\right) \qquad \_\_\_\_(3)$$

$$\because a = b$$

*In general* $\quad En_1, n_2\ (x)_\infty = \frac{\hbar^2}{8m}(n_1^2 + n_2^2) \qquad \_\_\_\_(4)$

$$E_{1,2} = \frac{\hbar^2}{8m}(1+4) \qquad \text{\_\_\_\_}(4)$$

## Wave function equation for a moving object Two directions:

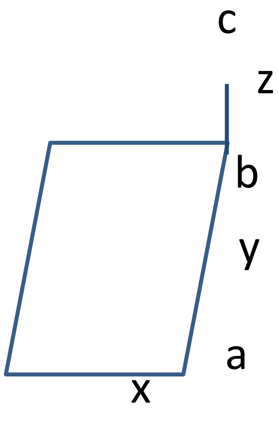



$$\psi\, nx, ny\,(x,y) = \sqrt{\frac{2}{a}} \cdot \sqrt{\frac{2}{b}}\, Sin \frac{nx\pi x}{a} \cdot Sin \frac{ny\pi y}{b}$$

$$Enx, ny\,(x,y) = Enx\,(x) + Eny\,(y)$$

$$\therefore E = \frac{n^2\hbar^2}{8ma^2}$$

## The equation of the wave function of a body moving in three directions:




$$\psi\, nx, ny, nz\,(x,y,z) = \sqrt{\frac{2}{a}} \cdot \sqrt{\frac{2}{b}} \cdot \sqrt{\frac{2}{c}}\, Sin \frac{nx\pi x}{a}$$

$$Sin\frac{ny\pi y}{b}\ Sin\frac{nz\pi z}{c}$$

المكعب $a = b = c$

$$\psi = \sqrt{\frac{8}{a}}\ Sin\frac{nx\pi x}{a}\ Sin\frac{ny\pi y}{b}\ Sin\frac{nz\pi z}{c}$$

## Degenrat

We impose a particle in a two-dimensional box so that a=b so we can find

Energy and wave function as follows:

$$E = \frac{n^2\hbar^2}{8ma^2} \qquad let\ n = 1, n = 2$$

$$E_{1,2} = \frac{\hbar^2}{8ma^2}(n_1^2 + n_2^2)\_\_\_\_(1)$$

$$= \frac{\hbar^2}{8ma^2}\cdot(1+4)\_\_\_\_(2)$$

$$E_{2,1} = \frac{\hbar^2}{8ma^2}\cdot(4n_2^2 + n_1^2)\_\_\_\_(3)$$

$$= \frac{\hbar^2}{8ma^2}\cdot(4+1)\_\_\_\_(4)$$

$$E_{2,1} = E_{1,2}$$

The wave function

$$\psi = \sqrt{\frac{2}{a}}\, Sin\frac{n\pi x}{a}$$

$$\psi_{1,2} = \sqrt{\frac{2}{a}}\, Sin\frac{\pi x}{a} \cdot \sqrt{\frac{2}{a}}\, Sin\frac{4\pi x}{a}$$

$$\psi_{2,1} = \sqrt{\frac{2}{a}}\, Sin\frac{4\pi x}{a} \cdot \sqrt{\frac{2}{a}}\, Sin\frac{\pi x}{a}$$

$$\therefore\ \psi_{1,2} = \psi_{2,1}$$

The two functions are equivalent $\psi_{1.2}$, $\psi_{2.1}$ because they are different and equal in energy, so they are said to be two dichotomy functions.