Ministry of Higher Education
and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

-The ninth lecture-

Stage 4

Prof. Dr Hassan sabih

Quantum mechanic

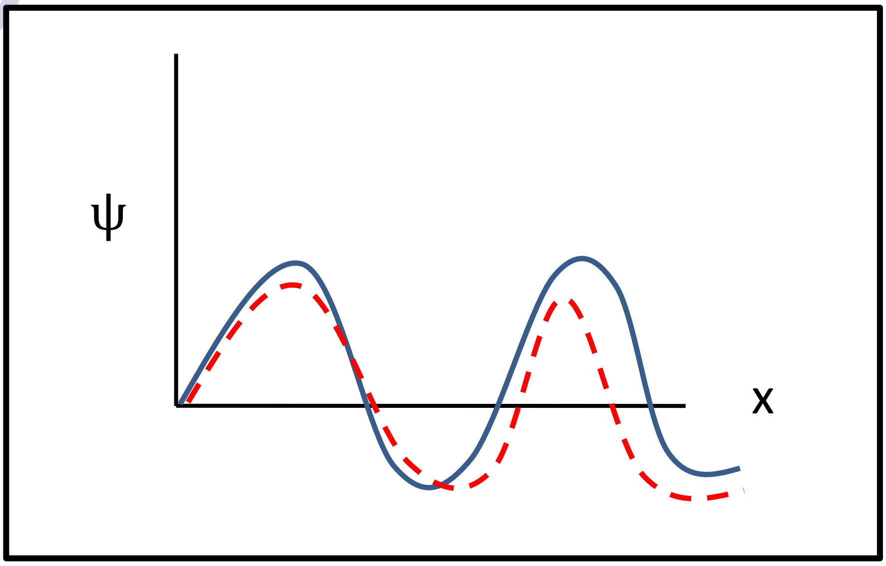
It became clear that the movement of particles is not subject to the laws of traditional mechanics, so quantitative mechanics based on quantum theory must be formulated where:

1) The German scientist Heisenberg made his first attempt to formulate a quantum mechanics in 1925 and relied on mathematical units called Matrix arrays called matrix mechanics.

2) Austrian physicist Schrodinger revealed a wave equation called schrodinger equation in 1926

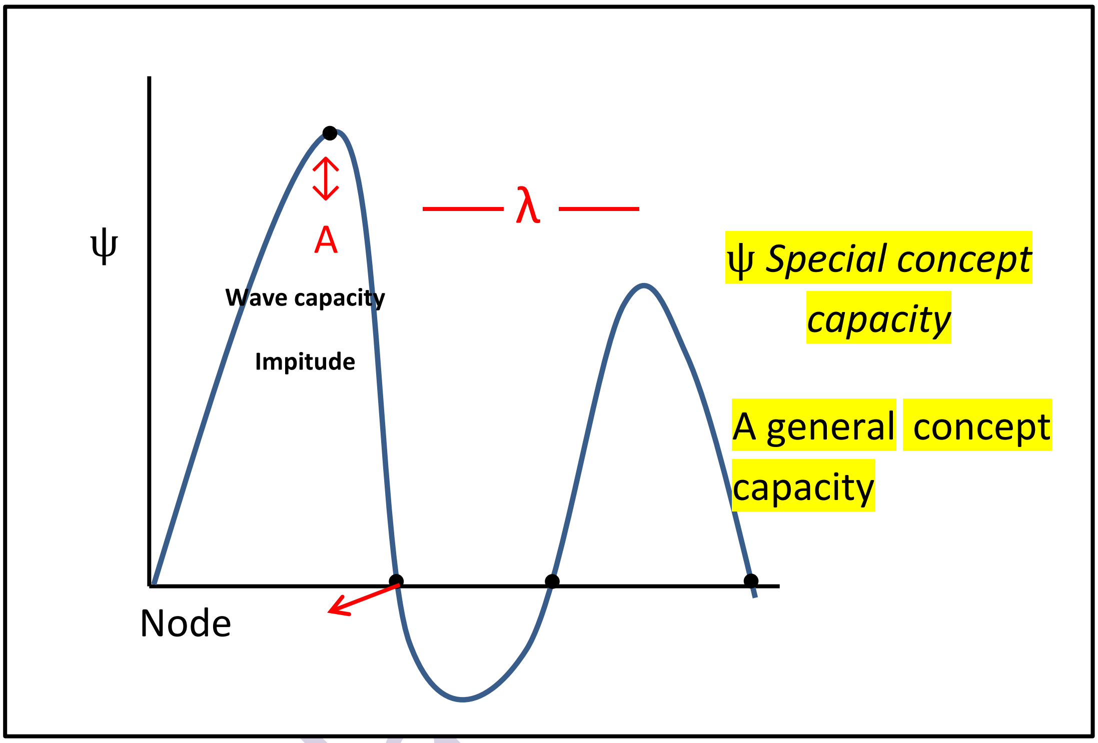
As is known, there are two types of waves.

1 diffusion wave diffusion wave



The spreading wave is similar to those from a rope movement where the cochlear is unstable and changes over time.

2 Standing Wave Standing Wave



The standing wave is similar to the chord waves in which the positions of the peaks and the hemophilia do not change, and you have fixed positionpoints (wave capacity = zero)

The node is called that point where the wave capacity = zero.

So when the electron that has a wave movement moves when we assume the wave is spreading, there is a destructive interference, i.e. energy is equal to zero, which is not true, so you use static waves.

Particles have wave qualities that can be described as a wave equation of a shaky wire. The Schrödinger equation was therefore based on the conventional wave equation, thus using static waves characterized by constant points, i.e. wave capacity equal to zero, i.e. the wave is not a function of time. And so Schrodinger found a second-rate reciprocal equation.

$$\frac{\partial^2 \Psi_{(x,t)}}{\partial x^2} = \frac{1}{v^2} \cdot \frac{\partial^2 \Psi_{(x,t)}}{\partial t^2} \quad \_\_\_\_\_\_ 1$$

Thus, wave capacity can be calculated through the general solution of the equation that has been made.

$$\Psi_{(x,t)} = Ae^{-i2\pi\left(\frac{x}{2}-yt\right)} \quad \_\_\_\_\_\_ 2$$

The capacity with the special concept $\psi()$ represents the height of the wave of the axis and varies with the difference in distance (coordinate and time) and during the measurement of this height such as a straight length in the middle so this line is called the maximum capacity and symbolizes it (A).

The systems studied are retention systems so we have to get rid of time so we do the fragmentation process in a way that separates the variables and as follows

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

$$\psi_{(x,t)} = Ae^{i2\pi\left(\frac{x}{\lambda}-yt\right)} \quad \_\_\_\_\_\_ 4$$

$$\psi_{(x,t)} = Ae^{i2\pi\frac{x}{\lambda}} \cdot e^{-i2\pi yt} \qquad \text{———} 5$$

$$\psi_{(x,t)} = \psi_{(x)} \cdot e^{i2\pi yt} \qquad \text{———} 6$$

We make up 6 in 1.

$$\sqrt{-1} = i$$

y = frequency

ϕ = Wavelength

x = axis (coordinates)

ψ = General concept capacity

A = Special concept capacity

$$\frac{\partial^2 \psi_{(x)} f(x)}{\partial x^2} = \frac{1}{v^2} \cdot \frac{\partial^2 \psi_{(x)} \cdot f(x)}{\partial t^2} \qquad \text{———} 7$$

$$\frac{\partial^2 \psi_{(x)}\, e^{i2\pi yt}}{\partial t^2} = \frac{1}{v^2} \cdot \frac{\partial^2 \psi_{(x)} \cdot f(x)}{\partial t^2} \qquad \text{———} 8$$

$$\frac{\delta^2\, \psi_{(x)}\, e^{-i2\pi yt}}{\delta x^2} = \frac{1}{v^2} \cdot \psi_x \frac{-i2\pi y\, e^{-i2\pi yt}}{\delta t} \qquad \text{———} 9$$

$$\frac{\partial^2 \psi_{(x)}\, e^{\overbrace{i}^{\sqrt{-1}}2\pi yt}}{\partial x} = \frac{1}{v^2}\, \psi_{(x)} \cdot i^{-2}\, 4\pi^2 y^2 \cdot e^{-i2\pi yt} \qquad \text{———} 10$$

$$= \frac{1}{v^2}\,\psi - 4\pi^2 y^2 \qquad \text{———}11$$

$$\frac{\partial^2\psi_{(x)}}{\partial x^2} = \frac{-4\pi^{2y^2}}{v^2}\psi_{(x)} \qquad \text{———}12$$

$$\because \lambda = \frac{y}{v}$$

$$\frac{\partial^2 x\psi_{(x)}}{\partial x^2} + \frac{4\pi^2}{\lambda^2} + \psi_{(x)} = 0 \qquad \text{———}13$$

$$\because \lambda = \frac{h}{p}$$

$$\frac{\partial^2\psi_{(x)}}{\partial x^2} + \frac{4\pi^2 p^2}{h^2}\psi_{(x)} = 0 \qquad \text{———}14$$

$$\frac{\partial^2\psi_{(x)}}{\partial x^2} + \frac{p^2}{\hbar^2}\psi_{(x)} = 0 \qquad \text{———}15$$

Equation 12, 15 differential equations that don't depend on time, so it's a static wave.

$$E_T = T + v$$

$$E = \frac{1}{2}\,m\,v^2 + v$$

$$E = \frac{m^2v^2}{2m} + v$$

$$E = \frac{p^2}{2m} + v$$

$$\frac{p^2}{2m} = E - v$$

$$p^2 = 2m\,(E - v) \qquad \text{———}16$$

We make up 16 in 15.

$$\frac{\partial^2 \psi_{(x)}}{\partial x^2} + \frac{2m}{\hbar^2}(E - v)\,\psi_{(x)} = 0 \qquad \text{———}17$$

Schrodenker's equation doesn't depend on time for amodernist x.

$$\frac{\partial^2 \psi_{(x,y,z)}}{\partial x^2} + \frac{\partial^2 \psi_{(x,y,z)}}{\partial y^2} + \frac{\partial \psi_{(x,y,z)}}{\partial z^2} + \frac{2m}{\hbar}(E - v)\psi_{(x)} = 0 \quad \text{——}18$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi_{(x,y,z)} + \frac{2m}{\hbar}(E - v)\psi_{(x)} = 0$$

$$\boxed{\nabla^2 \psi_{(x,y,z)} + \frac{2m}{\hbar^2}(E - v)\,\psi_{(x)} = 0 \text{ \_\_\_\_\_}19}$$

Schrodenker equation

1- Convert Schrodinger to Eigen value eqution

2- Exposition function

3- Pastulale for quantum mechanics

*** Turning the Schrodenker equation into a subjective value equation (derivation supplement)**

$$\frac{\partial^2 \psi_{(x)}}{\partial x^2} + \frac{2m}{\hbar^2}(E - v)\psi_{(x)} = 0 \ldots\ldots 1$$

$$\left(\frac{-\hbar^2}{2m}\right) \quad * \qquad \text{by beating}$$

$$\frac{-\hbar^2}{2m} \cdot \frac{\partial^2 \psi_{(x)}}{\partial x^2} - (E - v)\,\psi_{(x)} = 0 \qquad \ldots\ldots\ldots 2$$

$$\frac{-\hbar^2}{2m} \cdot \frac{\partial^2 \psi_{(x)}}{\partial x^2} - E\,\psi_{(x)} + v\ \psi_{(x)} = 0 \qquad \ldots\ldots\ldots\ldots 3$$

$$\frac{-\hbar^2}{2m} \cdot \frac{\partial^2 \psi_{(x)}}{\partial x^2} + v\ \psi_{(x)} = E\,\psi_{(x)} \qquad \ldots\ldots\ldots\ldots 4$$

$$A\psi = E\psi \qquad \ldots\ldots 5$$

$$H\psi = E\psi \qquad \ldots\ldots\ldots 6$$