Ministry of Higher Education
and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

- tenth lecture -

Stage 4

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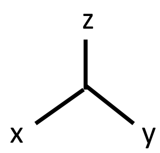
Explanation (function interpretation) Exposition function

First explanation - schrodinger explanation shrandinger exposition

The function (Ψ Represents the positive capacity associated with the movement of the system and is called the capacity function and I assume that the capacity function appears in three dimensions



So Schrodenker's interpretation doesn't apply to two bodies (so I faced rejection)

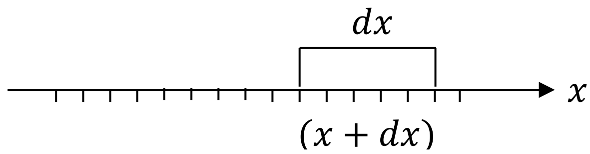
Explanation II - max born exposition Max Bourne

The German physicist explained that the function (Ψ)is a brobablity probability function while (Ψ^2) represents the probability density of this to find an object in a particular location in space, which is a valid expression of the probability function so when writing (Ψ^2) represents a real function or complex composite function but when writing ($\Psi * \Psi$) is either real or imaginary.

For a single object moving towards the axis (x), the function should be defined because it contains all particle specifications, so we conclude that:

1)ψ_r represents the probability function (case function) and is a general concept of the function.

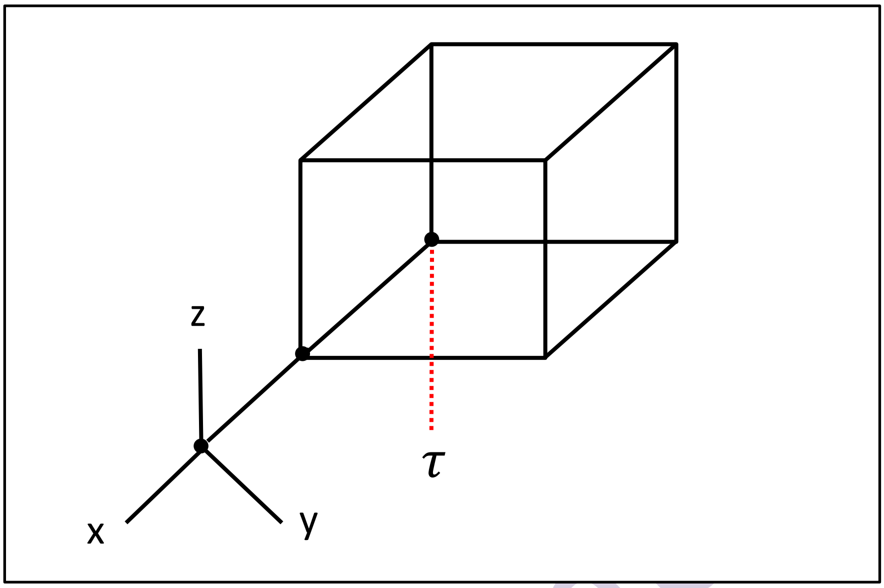
2)ψ_r^2 represents probability density and is a special concept of function so to locate the particle



3)$\Psi^2 dx$ The probability of the particle being within part of the axis (x) can be written as follows: $\psi_x^* \, \psi_x \, dx$

4) ψ^2,x, y, z represents the possibility of a particle in a space of its size so (dx, dy, dz)it writes as follows:$\left(\psi^2 x, y, z \quad (dx, dy, dx)\right)$

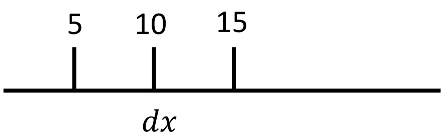
So when there are (x, y, z)perpendicular axes on each other, a parallel rectangles (cube) are formed as follows:



So it symbolizes the $dx, dy, dz(\ \tau\ )$ axes, so the function can be written as follows.

$$\psi^2 x, y, z \ = \ \tau$$

The older the condition, the greater the probability, as in the form



So everyone takes integration.

Thus, we conclude the total probability of the presence of the particle within the x axis *is as follows:*

$$\int_{-\infty}^{+\infty} \psi^2 x \, dx = 1$$

But if there's a particle in all the space,

$$\int_{-\infty}^{+\infty} \psi_{x,y,z}^2 \, dt = 1$$

Sometimes the function is not equal to one so you have to multiply in amount to make it equal to one.

If this function is equal to one, it's said to be a function *together.*

normalized function

Therefore, when the function is achieved, a condition is said together and the new equation is called both.

Wave function properties:

One of the most important characteristics of the wave function is that it is changing from physical reality to be characterized by certain characteristics that it is an acceptable function (the decline of the first chapter) which is as follows:

1) To be continuous, i.e. the first and second differentials must be continuous (a function with a differential).
2) The function is one-value.
3) The function has a specific value, i.e. it does not take infinity value
4) The total probability in space in this case is called a function together normalized function

$$\int_{-\infty}^{+\infty} \psi^2\psi \ d\tau = 1$$

So the function represents the probability density of the (ψ^2) *particle's presence for that total integration in space and should be equal to one because the body exists.*

5) *The function should be integratable and the function should have an integratable box, i.e.*

$$\int \psi_x^2 \, dx = 1 \_\_\_\_\_(1)$$

Therefore, if the function is not equal to one, you must calibrate this function and according to the following steps:

1. *If the function is not equal to one*

$$\int \psi\psi \, d\tau \neq 1 \_\_\_\_\_(2)$$

2. *We assume this amount* = k

$$\int \psi\psi \, d\tau = k \_\_\_\_\_(3)$$

3. *Multiply the function with calibration* (N) until *the function becomes calibration*

$$\int N\psi \, N\psi \, d\tau = 1 \qquad \_\_\_\_\_(4)$$

In order of this equation

$$N^2 \underbrace{\int \psi\psi \, d\tau}_{k} = 1 \qquad \_\_\_\_\_\_(5)$$

$$N^2 k = 1 \qquad \_\_\_\_\_\_(6)$$

$$N = \sqrt{\frac{1}{k}} \qquad \_\_\_\_\_\_(7)$$

Compensate (7) in (4)

$$\int \sqrt{\frac{1}{k}} \; \psi \; + \sqrt{\frac{1}{k}} \; \psi \, d\tau = 1 \; \_\_\_\_\_\_(8)$$

$$\frac{1}{k} \int \psi \, \psi \, \mathrm{d}\tau = 1 \qquad \_\_\_\_\_\_(9)$$