Physical Chemistry

Quantum mechanics Formula

There are many mathematical aspects of quantum mechanics that need to be understood in quantum mechanics. These can help explain why systems behave the way that they do and the importance of some of the variables that may be present in a system.

A wavelength for any particle (λ) can be given by Plank's constant (h) and its momentum (p). Its speed here is represented c to avoid confusion with v and v meaning velocity and frequency.

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

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

$$E = \frac{P^2}{2m}$$

It is also important to remember the rules of kinetic energy etc.

$$E = \frac{1}{2}mc^2$$

Uncertainty principle

With the use of Plank's constant the uncertainty can be given by:

$$\Delta X.\Delta P \geq \frac{h}{4\pi}$$

$$\Delta X = \frac{h}{\Delta P 4\pi}$$

Wave functions

Explaining the wave function

A particle moving along the x axis with a constant momentum has a complex wave function:

$$\Psi = Ae^{ikx} = A(\cos kx + \mathrm{i}\sin kx)$$

If an equation of the wave function is assumed to be for simplistic sake:

$$\Psi = A\sin kx \;\; or\; A\cos kx$$

When a particle is adjusted by one phase in the x direction the following equations are formed.

$$\Psi = A\sin k(x + \lambda) \;\; or\; A\cos k(x + \lambda)$$

$$\Psi = A\sin kx + k\lambda \;\; or\; A\cos kx + k\lambda$$

This is a complete phase change which means that:

$$k\lambda = 2\pi$$

$$k = \frac{2\pi}{\lambda}$$

As de Broglie states

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

$$p = \frac{hk}{2\pi}$$

$$E = \frac{(\hbar k)^2}{2m}$$

As:

$$\Psi = Ae^{ikx} \pm Ae^{-ikx}$$

$$\Psi = Ae^{ikx} = A(\cos kx + \mathrm{i}\sin kx)$$

And:

$$\Psi = Ae^{-ikx} = \cos(-kx) + i\sin -kx = \cos kx - i\sin kx$$

IMPORTANT

$$\Psi = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}$$

$$E = \frac{n^2\hbar^2\pi^2}{2mL^2} \quad or \quad E = \frac{n^2h^2}{8mL^2}$$

Quantum tunnelling

For a particle travelling towards a barrier: (with potential V and length L) in the first energy level with a given energy (E). The following equations are used:

$$K_{II} = \left(\frac{2m(V-E)}{\hbar^2}\right)^{\frac{1}{2}}$$

$$T = \left\{1 + \frac{\left(e^{k_{II}L} - e^{-k_{II}L}\right)^2}{16\left(\frac{E}{V}\right)\left[1 - \left(\frac{E}{V}\right)\right]}\right\}^{-1}$$

The simple Hamiltonian wave function is given as: This is where $\hat{H}$ is an operator, $\mathit{\Psi}$ is an eigen function and the eigenvalue is given as Ψ.

$$\hat{H}\mathit{\Psi} = E\mathit{\Psi}$$