Physical Chemistry

Wave functions: Building the knowledge

Introduction

The wave function is a highly useful piece of information for any form of chemistry it allows a deeper understanding of how molecules behave and how this can effect a system.

Developing the wave function

A wave function is a formula that explains how a particle behaves under certain conditions. The equations below represent how to derive a simple wave function for a particle in a box system.

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

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

This seems highly complicated but is the best way in which to describe a wave function. This will be explained below by using a more simple equation to explain the principles behind the final equation and the best ways in which to develop the thought experiment.

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:

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

And:

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

The above series of equations use some known facts about all wave equations and comes to some very important conclusions.

It is known that a wave will be in the same y position after one full phase (2π) whether this is a maximum or 0 is dependent on the wave function but this must occur. Once the relationship between this and the wavelength has been found the value of the constant k can be calculated. From this the wave function can be quantitatively solved.

The reason behind the use of the complex functions allows the direction of the wave to be seen. This means that:

$$\Psi = Ae^{-ikx} \text{ and } \Psi = Ae^{ikx}$$

Are distinct from one another.

Wave functions and probabilities

As the wave function has both real and complex parts it can be difficult to see where the significance of its value lies. The importance of this was found by multiplying the wavefunction by its complex conjugate.

A complex conjugate is where both functions have the same real parts but the part containing the complex number has an opposite sign. This means that in the multiplication of the two the complex term can usually be factored out of the equation.

This leave the equivalent of Ψ^2 and is a wholly real number.

With the wavefunction being a real number and being a square of itself it is fair to come to the conclusion that this could be a one dimensional probability density for the particle.

Wave function behaviour

To find the probability of finding the molecule in a certain area a graph needs to be plotted and then integrated. For a wave function to be accurately plotted the wavefunction must not tend to infinity across its given range. And must not have two points that equate to the same x value. It should also not be seen that there is a discontinuous value. When the wavefunction is integrated the discontinuous value may equal 0 or ∞.