Quantization of Energy

The break through that led to satisfactory explanations of a number of phenomena, which had not been explained with the use of classical physics, was made by Planck in 1990 who put the basis of the quantum physics.

Hydrogen atom spectrum, blackbody radiation, photoelectric effect, and other unexplained observations by classical physics were explained on the assumption that energy is quantized in discrete packets (called quanta), each of magnitude $h\nu$.

$$E = nh\nu$$

h : Planck's constant $= 6.626 \times 10^{-34}$ J.S

and $\Delta E = h\nu$

All spectra are governed by this equation suggested by Planck

The quantum states (or energy levels) are determined from the solution of the Schrödinger wave equation.

For one particle in one dimension:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\hat{H}\psi = E\psi$$

$\hat{H}$ is the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V \quad = T + V$$

V : Potential energy

m: mass of particle.

For one particle in three dimension:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

∇^2 is Laplacian operator

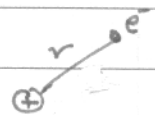
$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\nabla^2 = \frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin\phi}\frac{\partial^2}{\partial\phi^2}\right)\right]$$

Hydrogen Atom Solution from Schrödinger Equation

Schrödinger equation can be solved for a hydrogen atom

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + V\psi = E\psi$$



μ is the reduced mass $= \frac{m_1 m_2}{m_1 + m_2}$

$$\mu = \frac{m_e m_p}{m_e + m_p}$$

$$m_e << m_p$$

$$\therefore \mu \cong m_e$$

$$V = -\frac{Ze^2}{4\pi\epsilon_0 r} = -\frac{e^2}{4\pi\epsilon_0 r}$$

(Z for H atom is 1)

ϵ_0 is vacuum permitivity

After the equation is solved:

$$E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2 n^2}$$

where $n = 1, 2, 3, \ldots$ (quantum number)

$$E_n = -R_H / n^2$$

R: Rydberg constant $= 109677.576\ cm^{-1}$

$$\Delta E = E_2 - E_1 = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$= h\nu$$

The first five series (Lyman, Balmer, Paschen, Brackett, and Pfund) with $n'' = 1, 2, 3, 4,$ and 5 can be shown with this solution.

Using spherical polar coordinates instead of The cartesian coordinate has an advantage That The wave function can be factorized into two parts:

$$\Psi(r, \Theta, \phi) = R_{n\ell}(r)\, Y_{\ell m_\ell}(\Theta, \phi)$$

$R_{n\ell}$: Radial wave function and it is used to determine energy levels and probabilities of finding electrons at particular areas in space

$Y_{\ell m_\ell}$: Angular wave function and it is used to determine The shapes of orbitals and spins for electrons.

$Y_{\ell m_\ell}$ is sometimes called "spherical harmonic" as it determines The distribution of the wave function of a hydroget atom over a surface of a sphere at given r.

n : The quantum number that determines The quantized energy levels. It takes values: $1, 2, \ldots$

ℓ : called The azimuthal quantum number and can take values $\ell = 0, 1, 2, \ldots, (n-1)$

Electron orbitals are lableled with n and ℓ.
The symbols $s, p, d, f, g, \ldots$ maybe also used
$\ell = 0, 1, 2, 3, 4, \ldots$

Thus, we speak of $1s, 2s, 3p, 3d, \ldots$ orbitals.