Estructura atómica: Modelo de la Mecánica Cuántica

La ecuación de onda de Schrödinger

Para el átomo de H (el más sencillo)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$$

Segunda derivada con respecto a X: $\frac{\partial^2 \psi}{\partial x^2}$

Función de onda de Schrödinger: ψ

Posición: x

Energía: E

Energía potencial: V

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \left(\operatorname{sen}\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\operatorname{sen}\phi}{r\operatorname{sen}\theta}\frac{\partial}{\partial\phi}\right)^2 + \left(\operatorname{sen}\theta\operatorname{sen}\phi\frac{\partial}{\partial r} + \frac{\cos\theta\operatorname{sen}\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\operatorname{sen}\theta}\frac{\partial}{\partial\phi}\right)^2 + \left(\cos\theta\frac{\partial}{\partial r} - \frac{\operatorname{sen}\theta}{r}\frac{\partial}{\partial\theta}\right)^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2}\frac{\cos\theta}{\operatorname{sen}\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\operatorname{sen}^2\theta}\frac{\partial^2}{\partial\phi^2} \quad (4)$$

$$\frac{d\Psi}{dx} = -C\frac{\alpha}{2}e^{-\alpha x^2/2}2x$$

$$\frac{d^2\Psi}{dx^2} = -C\alpha e^{-\alpha x^2/2} + C\alpha^2 x^2 e^{-\alpha x^2/2}$$

$$\frac{-\hbar^2}{2m}\left[-\alpha + \alpha^2 x^2\right]\Psi + \frac{1}{2}m\omega^2 x^2\Psi = E\Psi$$