

Quantum Mechanics II

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Contents

1	3D Schrodinger equation	4
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1 3D Schrodinger equation

- In QM the Hamiltonian is written in terms of operators. Momenta becomes $\mathbf{p} \rightarrow -i\hbar\nabla$ and the potential $V \rightarrow \hat{V}$ also an operator. So the Hamiltonian becomes:

$$\frac{-\hbar^2}{2m}\nabla^2 + \hat{V} \quad (1.1)$$

- The (time independent) Schrodinger equation is:

$$H\psi(x, y, z) = E\psi \quad (1.2)$$

- If we then have a central potential, that is $V = V(r)$, so rotation symmetry generated by a rotational group, we find it best to change co-ords to spherical co-ords. Here the Laplacian is:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial \Phi}{\partial \theta}) + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial^2 \Phi}{\partial \phi^2} = 0 \quad (1.3)$$

We then make the typical assumption of separation of variables, that is:

$$\psi = R(r)Y(\theta, \phi) \quad (1.4)$$

The Schrodinger equation then becomes:

$$\begin{aligned} -\frac{\hbar^2}{2m} \left[\frac{Y}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{R}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial Y}{\partial \theta}) + \frac{R}{r^2 \sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right] \\ + V(r)R(r)Y(\theta, \phi) = ER(r)Y(\theta, \phi) \end{aligned} \quad (1.5)$$

Dividing by $R(r)Y(\theta, \phi)$ and multiplying by r^2 , we get two terms, one a function of r only and one a function of θ and ϕ , adding to a constant E . This means that both these terms must themselves be constant. This gives us two separate equations.

$$\begin{aligned} -\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{2mr^2}{\hbar^2} [V(r) - E] &= l(l+1) \\ \frac{1}{Y} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial Y}{\partial \theta}) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right] &= -l(l+1) \end{aligned} \quad (1.6)$$

The choice $l(l+1)$ as a constant, may seem strange at first but makes sense later. On the later

equation we again perform separation of variables, $Y = \Theta(\theta)\Phi(\phi)$, so we get two more equations:

$$\begin{aligned} \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} &= -m^2 \\ \sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + (l(l+1) \sin^2 \theta - m^2) \Theta &= 0 \end{aligned} \tag{1.7}$$

