Quantum Mechanics 2

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Central Fields

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Central Potential Schrodinger Equation

Central fields (potential) constitute another class of problems with separable Schrodinger Equation. By definition, central fields are those with potentials $V(r)$ that depend on distance $r = \sqrt{x^2 + y^2 + z^2}$ only. Thus, the Schrodinger equation is best expressed in spherical coordinates

$$-\frac{\hbar^2}{2m}\nabla^2 u(r,\theta,\varphi) + V(r)u(r,\theta,\varphi) = Eu(r,\theta,\varphi)$$

Laplacian in spherical polar coordinates is

$$\nabla^2 u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 u}{\partial\varphi^2}$$

If we separate the wave functions

$$u(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$$

Separated Schrodinger Equation

The Schrodinger equation becomes

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right]+V(r)RY=ERY$$

Multiplying by r^2/YR, we have

$$-\frac{\hbar^2}{2m}\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right]+[V(r)-E]r^2=0$$

which separates into the radial equation

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2m}{\hbar^2}[V(r)-E]r^2R=\lambda R$$

and the angular equation

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}=-\lambda Y$$

Rotational Symmetry

The potential is found only in the radial equation. Thus, the specific dynamics of the system is contained in the radial equation.

On the other hand, all central field systems have the same angular equation.

Because the potential depends on r only, the system has rotational symmetry. By Noether's Theorem, there must be a conserved quantity, and that is the angular momentum.

It is thus worth looking at angular momentum.

Angular Momentum

Angular momentum is defined by

$$L = r \times p$$

In coordinate representation, the linear momentum operator is

$$p = \frac{\hbar}{i} \nabla$$

Thus,

$$L_x = yp_z - zp_y = i\hbar \left[z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z} \right]$$

$$L_y = zp_x - xp_z = i\hbar \left[x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x} \right]$$

$$L_z = xp_y - yp_x = i\hbar \left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \right]$$

Coordinate Transformation

The coordinate transformation between Cartesian and spherical coordinates are as follows:

$$x = r\sin\theta\cos\varphi$$

$$y = r\sin\theta\sin\varphi$$

$$z = r\cos\theta$$

and the partial derivatives transform as [see partial derivatives – Cartesian to polar]

$$\frac{\partial}{\partial x} = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

Angular Momentum in Spherical Coordinates

Angular momentum operators may the be expressed in spherical coordinates as

$$L_x = i\hbar\left[\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right]$$

$$L_y = i\hbar\left[-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right]$$

$$L_z = -i\hbar\frac{\partial}{\partial\varphi}$$

and

$$L^2 = L_x^2 + L_y^2 + L_z^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

The angular equation is therefore none other than the eigenvalue equation for the operator L^2

$$L^2 Y = \lambda\hbar^2 Y$$