SCHRÖDINGER EQUATION IN THREE DIMENSIONS - THE RADIAL EQUATION

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 4.1.3.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.2.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

When we considered the solution of the Schrödinger equation in three dimensions, we found that the general solution separated neatly into a product of three functions, one for each variable in spherical coordinates.

The Schrödinger equation in three dimensions can be written as

$$-\frac{\hbar^2}{2m}\nabla^2\Psi+V\Psi=i\hbar\frac{\partial\Psi}{\partial t} \tag{1}$$

If we assume that the potential $V=V(x,y,z)$ is independent of time, we can use the same separation of variables method that we used in one dimension to split off the time part of the solution to get

$$\Psi(x,y,z,t)=\psi(x,y,z)e^{-iEt/\hbar} \tag{2}$$

where, as before, the energy E takes on a set of discrete values for the bound states and a set of continuous values for the scattering, or unbound, states. The spatial wave function ψ satisfies the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=E\psi \tag{3}$$

So far, the analysis is the same as that for one dimension.

Using separation of variables in the form $\psi(r,\theta,\phi)=R(r)Y(\theta,\phi)$ we got two separated equations:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-\frac{2mr^2}{\hbar^2}(V-E) = l(l+1) \tag{4}$$

$$\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{Y\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\phi^2}\right) = -l(l+1) \tag{5}$$

where $l(l+1)$ is a constant term.

We found that the angular equation could be solved and that the solutions were the spherical harmonics:

$$Y_l^m(\theta,\phi)=\left[\frac{2l+1}{4\pi}\frac{(p-m)!}{(p+m)!}\right]^{1/2}e^{im\phi}P_l^m(\cos\theta) \tag{6}$$

They obey the normalization condition

$$\int_0^{2\pi}\int_0^{\pi}(Y_l^m)^*Y_{l'}^{m'}\sin\theta d\theta d\phi=\delta_{ll'}\delta_{mm'} \tag{7}$$

Returning to the radial function we find that we can actually make one further transformation of the equation that makes it a bit easier to solve in some cases. We can rewrite the equation using total derivatives, since $R(r)$ depends only on r:

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}(V-E)R=l(l+1)R \tag{8}$$

We can now make the substitution

$$u(r) \equiv rR \tag{9}$$

$$R = \frac{u}{r} \tag{10}$$

$$\frac{dR}{dr} = -\frac{u}{r^2}+\frac{u'}{r} \tag{11}$$

$$= \frac{1}{r^2}(ru'-u) \tag{12}$$

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = u'+ru''-u' \tag{13}$$

$$= ru'' \tag{14}$$

The radial equation then becomes

$$r\frac{d^2u}{dr^2}-\frac{2mr}{\hbar^2}(V-E)u = l(l+1)\frac{u}{r} \tag{15}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left(V+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u = Eu \tag{16}$$

In this form, the equation looks like the original one-dimensional Schrödinger equation with the wave function given by u and the potential given by

$$V_{rad}=V+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{17}$$

The extra term $\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$ is called the centrifugal term. Classically, the force due to this term is:

$$F_{cent} = -\frac{d}{dr}\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{18}$$

$$= \frac{\hbar^2}{m}\frac{l(l+1)}{r^3} \tag{19}$$

which is a force that tends to repel the particle from the origin (the force gets larger the closer to the origin we are). Thus it is analogous to the pseudo-force known as the centrifugal force in classical physics.

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