

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

$$(0.1) \quad -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

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

$$(0.2) \quad \Psi(x, y, z, t) = \psi(x, y, z)e^{-iEt/\hbar}$$

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:

$$(0.3) \quad -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

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:

$$(0.4) \quad \frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) - \frac{2mr^2}{\hbar^2} (V - E) = l(l+1)$$

$$(0.5) \quad \frac{1}{Y \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{Y \sin^2 \theta} \left(\frac{\partial^2 Y}{\partial \phi^2} \right) = -l(l+1)$$

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:

$$(0.6) \quad Y_l^m(\theta, \phi) = \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} e^{im\phi} P_l^m(\cos \theta)$$

They obey the normalization condition

$$(0.7) \quad \int_0^{2\pi} \int_0^\pi (Y_l^m)^* Y_{l'}^{m'} \sin \theta d\theta d\phi = \delta_{ll'} \delta_{mm'}$$

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 :

$$(0.8) \quad \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{2mr^2}{\hbar^2} (V - E)R = l(l+1)R$$

We can now make the substitution

$$(0.9) \quad u(r) \equiv rR$$

$$(0.10) \quad R = \frac{u}{r}$$

$$(0.11) \quad \frac{dR}{dr} = -\frac{u}{r^2} + \frac{u'}{r}$$

$$(0.12) \quad = \frac{1}{r^2} (ru' - u)$$

$$(0.13) \quad \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = u' + ru'' - u'$$

$$(0.14) \quad = ru''$$

The radial equation then becomes

$$(0.15) \quad r \frac{d^2 u}{dr^2} - \frac{2mr}{\hbar^2} (V - E) u = l(l+1) \frac{u}{r}$$

$$(0.16) \quad -\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left(V + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right) u = Eu$$

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

$$(0.17) \quad V_{rad} = V + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$$

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:

$$(0.18) \quad F_{cent} = -\frac{d}{dr} \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$$

$$(0.19) \quad = \frac{\hbar^2}{m} \frac{l(l+1)}{r^3}$$

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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