

SCHRÖDINGER EQUATION IN THREE DIMENSIONS - THE RADIAL EQUATION

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Post date: 30 July 2021.

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

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

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

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

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:

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

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:

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

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

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:

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

They obey the normalization condition

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

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 :

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

We can now make the substitution

$$u(r) \equiv rR \quad (9)$$

$$R = \frac{u}{r} \quad (10)$$

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

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

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

$$= ru'' \quad (14)$$

The radial equation then becomes

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

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

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

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

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:

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

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

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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