Two- and Three-Dimensional Rotationally-Symmetric Potentials

The three-dimensional potential well is pretty hard to solve. We'll start off with the two-dimensional one.

The Two-Dimensional Schrödinger Equation in Polar Coordinates

We'll get bogged down if I try to show you the Schrödinger Equation in Polar Coordinates. I will just give it to you:

$$E_n\,\psi(r,\,\phi) = -\frac{\hbar^2}{2\,m}\left[\frac{d^2\,\psi(r,\phi)}{dr^2} + \frac{1}{r}\,\frac{\mathrm{d}\psi(r,\phi)}{dr} + \frac{1}{r^2}\,\frac{d^2\,\psi(r,\phi)}{d\phi^2}\right] + V(r,\,\phi)\,\psi(r,\,\phi)$$

If you want to derive this thing, you have to use multi-variable calculus rules to convert the $\frac{d^2}{dx^2} + \frac{d^2}{dy^2}$ that appears in Schrodinger's equation in Cartesian coordinates into $\frac{d^2}{dr^2} + \frac{1}{r}\,\frac{d}{dr} + \frac{1}{r^2}\,\frac{d^2}{d\phi^2}$. If you really want, here is somebody who wrote it up, and you'll see why I am not doing it for you: https://www.-math.ucdavis.edu/~saito/courses/21C.w11/polar-lap.pdf.

The Rotationally Symmetric Case and the Separation of Variables Ansatz

If the potential is rotationally symmetric it doesn't depend on ϕ, so we have:

$$E_n\,\psi(r,\,\phi) = -\frac{\hbar^2}{2\,m}\left[\frac{d^2\,\psi(r,\phi)}{dr^2} + \frac{1}{r}\,\frac{\mathrm{d}\psi(r,\phi)}{dr} + \frac{1}{r^2}\,\frac{d^2\,\psi(r,\phi)}{d\phi^2}\right] + V(r)\,\psi(r,\,\phi)$$

The ansatz for solving this is

$$\psi(r,\,\phi) = \psi(r)\,\Phi(\phi)$$

where $\Phi(\phi)$ is an unknown function of ϕ.

$$E_n\,\psi(r)\,\Phi(\phi) = -\frac{\hbar^2}{2\,m}\left[\left[\frac{d^2\,\psi(r)}{dr^2} + \frac{1}{r}\,\frac{\mathrm{d}\psi(r)}{dr}\right]\Phi(\phi) + \frac{1}{r^2}\,\frac{d^2\,\Phi(\phi)}{\mathrm{d}\phi^2}\,\psi(r)\right] + V(r)\,\psi(r)\,\Phi(\phi)$$

Multiply through by $\frac{r^2}{R(r)\,\Phi(\phi)}$

$$r^2\,E_n = -\frac{\hbar^2}{2\,m}\left[r^2\,\frac{d^2\,R(r)}{dr^2} + r\,\frac{dR(r)}{dr}\right]\frac{1}{R(r)} - \frac{\hbar^2}{2\,m}\,\frac{1}{\Phi(\phi)}\,\frac{d^2\,\Phi(\phi)}{\mathrm{d}\phi^2} + r^2\,V(r)$$

Rearrange

$$r^2 E_n + \frac{\hbar^2}{2m}\left[r^2 \frac{d^2 R(r)}{dr^2} + r \frac{dR(r)}{dr}\right]\frac{1}{R(r)} - r^2 V(r) = -\frac{\hbar^2}{2m}\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2}$$

All of the ϕ-dependence is on the RHS and all of the r-dependence is on the LHS. The LHS and the RHS must be constant!

Let’s call the constant $\frac{\hbar^2}{2m} l^2$. Of course, it could be negative, and I am predisposing you against that by putting in l^2, but you’ll see that it is positive in a moment. With this constant,

$$-\frac{\hbar^2}{2m}\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2} = \frac{\hbar^2}{2m} l^2$$

or

$$\frac{d^2\Phi(\phi)}{d\phi^2} = -l^2\,\Phi(\phi)$$

The $\Phi(\phi)$ that does this is $\Phi(\phi) = e^{i\,l\,\phi}$. If the constant had been negative, then $\Phi(\phi)$ would have grown exponentially.

We can’t have discontinuity between $\phi = 0$ and $\phi = 2\pi$, so l has to be an integer.

Now that we know l, from solving the ϕ equation, we put it back in to the r equation.

$$r^2 E_n + \frac{\hbar^2}{2m}\left[r^2 \frac{d^2 R(r)}{dr^2} + r \frac{dR(r)}{dr}\right]\frac{1}{R(r)} - r^2 V(r) = -\frac{\hbar^2}{2m} l^2$$

Multiplying through by $\frac{R(r)}{r^2}$ we have

$$E_n R(r) + \frac{\hbar^2}{2m}\left[\frac{d^2 R(r)}{dr^2} + \frac{1}{r}\frac{dR(r)}{dr}\right] - V(r) R(r) = -\frac{\hbar^2}{2m} l^2 \frac{R(r)}{r^2}$$

or

$$E_n R(r) = -\frac{\hbar^2}{2m}\left[\frac{d^2 R(r)}{dr^2} + \frac{1}{r}\frac{dR(r)}{dr}\right] + V(r)\,\psi(r) + \frac{\hbar^2}{2m} l^2 \frac{R(r)}{r^2}$$

This last equation is often a bear to solve, but the nice thing is that it looks just like a 1-d Schrodinger equation. There are two constants in it that change from solution to solution. They are E_n and l. We emphasize that the wave function will depend on these things by subscripting it as $R_{n,l}(r)$. E_n might depend on l, so we give it a subscript too.

$$E_{n,l}\,R_{n,l}(r) = -\frac{\hbar^2}{2\,m}\left[\frac{d^2\,R_{n,l}(r)}{dr^2} + \frac{1}{r}\,\frac{dR_{n,l}(r)}{dr}\right] + V(r)\,R_{n,l}(r) + \frac{\hbar^2}{2\,m}\,l^2\,\frac{R_{n,l}(r)}{r^2}$$

The next thing that is generally done is to define a new dimensionless radial coordinate:

$$\rho \equiv \frac{\sqrt{2\,m\,E_{n,l}}}{\hbar}\,r$$

Then the equation is:

$$E_{n,l}\,R_{n,l}(\rho) = -\frac{\hbar^2}{2\,m}\,\frac{2\,m\,E_{n,l}}{\hbar^2}\left[\frac{d^2\,R_{n,l}(\rho)}{d\,\rho^2} + \frac{1}{\rho}\,\frac{dR_{n,l}(\rho)}{d\,\rho}\right] + V\left(\frac{\hbar}{\sqrt{2\,m\,E_{n,l}}}\,\rho\right)R_{n,l}(\rho) + \frac{\hbar^2}{2\,m}\,l^2\,\frac{2\,m\,E_{n,l}}{\hbar^2}\,\frac{R_{n,l}(\rho)}{\rho^2}$$

or, dividing through by $E_{n,l}$

$$R_{n,l}(r) = -\left[\frac{d^2\,R_{n,l}(\rho)}{d\,\rho^2} + \frac{1}{\rho}\,\frac{dR_{n,l}(\rho)}{d\,\rho}\right] + \frac{V\left(\frac{\hbar}{\sqrt{2\,m\,E_{n,l}}}\,\rho\right)R_{n,l}(\rho)}{E_{n,l}} + l^2\,\frac{R_{n,l}(\rho)}{\rho^2}$$

or,

$$\left(\rho^2 - l^2\right)R_{n,l}(r) + \left[\rho^2\,\frac{d^2\,R_{n,l}(\rho)}{d\,\rho^2} + \rho\,\frac{dR_{n,l}(\rho)}{d\,\rho}\right] - \rho^2\,\frac{V\left(\frac{\hbar}{\sqrt{2\,m\,E_{n,l}}}\,\rho\right)R_{n,l}(\rho)}{E_{n,l}} = 0$$