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:

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

If you want to derive this thing, you have to use multi-variable calculus rules to convert the $\frac{d^2}{d\,x^2} + \frac{d^2}{d\,y^2}$ 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:

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

The ansatz for solving this is

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

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

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

Multiply through by $\frac{r^2}{\psi(r)}\Phi_{(\phi)}$

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

Rearrange

$$r^{2} E_{n} + \frac{\hbar^{2}}{2m} \left[r^{2} \frac{d^{2} \psi(r)}{d r^{2}} + r \frac{d \psi(r)}{d r} \right] \frac{1}{\psi(r)} - r^{2} V(r) = -\frac{\hbar^{2}}{2m} \frac{1}{\Phi_{(\phi)}} \frac{d^{2} \Phi(\phi)}{d \phi^{2}}$$

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,

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

or

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

The $\Phi(\phi)$ that does this is $\Phi(\phi) = e^{i |\phi|}$. 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.

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

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

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

or

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

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

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