Separability of the 2D Particle in a Circle Problem

If we don't assume that the 2D rigid rotor has a fixed "r" then we are solving the particle-in-a-circle problem. It's just like a particle in a 2D box except the box is round.

This problem still uses cylindrical coordinates and is of the form $\hat{H}\Psi = E \cdot \Psi$

$$\frac{-\hbar^2}{2 \cdot \text{mass}}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right)\Psi = E \cdot \Psi$$

We assumed that $\Psi(r, \phi) = \Psi(r) \cdot \Psi(\phi)$, i.e. the solution is separable. Can you show that the Hamiltonian above is in fact separable?

Answer: First, bring over the constants:

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right)\Psi = \left(\frac{2 \cdot \text{mass}}{-\hbar^2}E\right) \cdot \Psi$$

And apply the separated wavefunction on the right and divide by the same on the left:

$$\frac{1}{\Psi(r) \cdot \Psi(\phi)}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right)\Psi(r) \cdot \Psi(\phi) = \frac{1}{\Psi(r) \cdot \Psi(\phi)}\left(\frac{2 \cdot \text{mass}}{-\hbar^2}E\right) \cdot \Psi(r) \cdot \Psi(\phi)$$

$$\frac{\Psi(\phi)}{\Psi(r) \cdot \Psi(\phi)}\frac{\partial^2 \Psi(r)}{\partial r^2} + \frac{\Psi(\phi)}{\Psi(r) \cdot \Psi(\phi) \cdot r}\frac{\partial \Psi(r)}{\partial r} + \frac{\Psi(r)}{\Psi(r) \cdot \Psi(\phi) \cdot r^2}\frac{\partial^2 \Psi(\phi)}{\partial \phi^2} = \left(\frac{2 \cdot \text{mass}}{-\hbar^2}E\right)$$

Simplify a bit more:

$$\frac{1}{\Psi(r)}\frac{\partial^2 \Psi(r)}{\partial r^2} + \frac{1}{\Psi(r) \cdot r}\frac{\partial \Psi(r)}{\partial r} + \frac{1}{\Psi(\phi) \cdot r^2}\frac{\partial^2 \Psi(\phi)}{\partial \phi^2} = \left(\frac{2 \cdot \text{mass}}{-\hbar^2}E\right)$$

Now multiply by r^2:

$$\frac{r^2}{\Psi(r)}\frac{\partial^2 \Psi(r)}{\partial r^2} + \frac{r}{\Psi(r)}\frac{\partial \Psi(r)}{\partial r} + \frac{1}{\Psi(\phi)}\frac{\partial^2 \Psi(\phi)}{\partial \phi^2} = \left(\frac{2 \cdot \text{mass}}{-\hbar^2}E\right) \cdot r^2$$

And you can now bring the Energy term to the right to group it with the radial part:

$$\left(\frac{r^2}{\Psi(r)}\frac{\partial^2 \Psi(r)}{\partial r^2} + \frac{r}{\Psi(r)}\frac{\partial \Psi(r)}{\partial r} + \frac{2 \cdot \text{mass}}{\hbar^2}E \cdot r^2\right) + \left(\frac{1}{\Psi(\phi)}\frac{\partial^2 \Psi(\phi)}{\partial \phi^2}\right) = 0$$

You are now left with two differential equations:

$$\frac{1}{\Psi(\phi)}\frac{\partial^2 \Psi(\phi)}{\partial \phi^2}$$

and:

$$\frac{r^2}{\Psi(r)}\frac{\partial^2 \Psi(r)}{\partial r^2} + \frac{r}{\Psi(r)}\frac{\partial \Psi(r)}{\partial r} + \frac{2 \cdot \text{mass}}{\hbar^2}E \cdot r^2$$

the sum of which is equal to a constant, which is 0.

Angular Part:

If we assume that $\Psi(\phi) = e^{i \cdot m \cdot \phi}$, the first mini-Schrodinger equation is:

$$\frac{1}{\Psi(\phi)}\frac{\partial^2\Psi(\phi)}{\partial\phi^2} = \frac{1}{e^{i\cdot m\cdot\phi}}\frac{\partial^2 e^{i\cdot m\cdot\phi}}{\partial\phi^2} = \frac{-m^2}{e^{i\cdot m\cdot\phi}}e^{i\cdot m\cdot\phi} = -m^2$$

There isn't anything else to examine with this part of the problem, especially because the radial one is the part that determines the energy.

Radial Part:

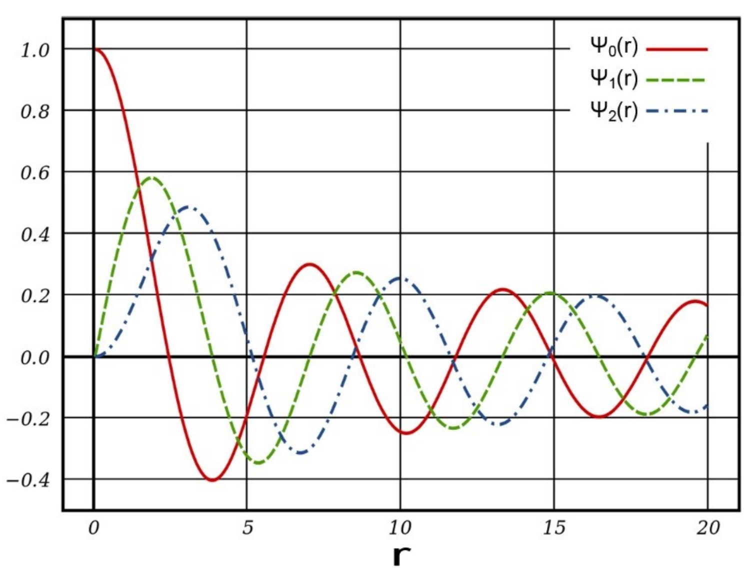
We are left with the radial equation:

$$\frac{r^2}{\Psi(r)}\frac{\partial^2\Psi(r)}{\partial r^2} + \frac{r}{\Psi(r)}\frac{\partial\Psi(r)}{\partial r} + \frac{2\cdot \text{mass}}{\hbar^2}E\cdot r^2 = m^2$$

where m is still 0, ±1, ±2, etc. Note how the radial is equal to $+m^2$, so it can effectively "wipe out" the effect of the rotational energy and still yield the total energy E. You can make it look more like a Schrodinger equation by bringing $\Psi(r)$ over to the right:

$$r^2\frac{\partial^2\Psi(r)}{\partial r^2} + r\frac{\partial\Psi(r)}{\partial r} = \left(m^2 - \frac{2\cdot \text{mass}}{\hbar^2}E\cdot r^2\right)\Psi(r)$$

The solution $\Psi_m(r)$ is called a Bessel function, which is like an "erf" in that there isn't a simple analytical way to express it. There is a solution for $\Psi_m(r)$ for every value of m. Shown here are a few Bessel functions, were you can see a different wavefunction for every m value. To solve the energy, you have to know where $\Psi_m(r) = 0$ (a boundary condition), which then gives you the energy. The graph below shows that $\Psi_{m=0}(r) = 0$ for the m=0 state occurs at $r = 2.4048$. This allows you to calculate its energy via: $E_0 = \frac{\hbar^2}{2\cdot \text{mass}}\left(\frac{2.4048}{\text{radius}}\right)^2$, where the radius of the box is the boundary condition.



References:

Bessel function adapted from: By Inductiveload - Own work, made with Inkscape, Public Domain, https://commons.wikimedia.org/w/index.php?curid=3564725