Homework H15 Solution

1. Using the formulas for x, y, and z show that $\varphi = \tan^{-1}\left(\frac{y}{x}\right)$ and $\theta = cos^{-1}\left(\frac{Z}{R}\right)$.

Solution:

Transformation between rectangular and spherical polar coordinates give,

$x = Rsin\theta cos\varphi$ (1)

$y = Rsin\theta sin\varphi$ (2)

and $z = Rcos\theta$. (3)

Therefore $\frac{y}{x} = \tan\varphi$, $\varphi = tan^{-1}\left(\frac{y}{x}\right)$

and, $\theta = cos^{-1}\left(\frac{Z}{R}\right)$

Turn in 2.

a. Prove that the $\widehat{H}_{rot}$ presented in lecture is the same as the one on page 87 of the textbook (equations A5.1 and A5.2).

Gruebele said that this equation should be solvable by a product wavefunction, so if the solution is called $Y_{lM}(\theta\phi)$, it can be written as a product $Y_{lM}(\theta\phi) = P_{lM}(\theta)\frac{1}{\sqrt{2\pi}}e^{iM\phi}$. The last part of the wavefunction is just the solution we previously found for rotation on a surface. **Note**: the $\frac{1}{\sqrt{2\pi}}$ normalization could also just be included with $P_{lM}(\theta)$.

b. Insert this $P_{lM}(\theta)\frac{1}{\sqrt{2\pi}}e^{iM\phi}$ wavefunction into $\widehat{H}_{rot}$ to prove that it solves the rotational eigenvalue equation $\widehat{H}_{rot}Y_{lM}(\theta,\phi) = E_{lM}Y_{lM}(\theta,\phi)$. Thus prove that $P_{lM}(\theta)$ satisfies the one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2mr^2}\left\{\frac{\partial^2}{\partial\theta^2} + cot\theta\frac{\partial}{\partial\theta} - \frac{M^2}{sin^2\theta}\right\}P_{lM}(\theta) = E_{lM}P_{lM}(\theta)$$

The solutions of this equations are the functions like $P_{10} \sim cos\theta$ or $P_{20} \sim 3cos^2\theta - 1$ in the table in the N15 lecture notes. Multiply them together with the $e^{iM\phi}$ part, and you get the whole rotational wavefunctions. As always, these wavefunctions have high probability in the same places where a classical particle would, as we discussed in Monday's lecture.

Solution:

a. We consider,

$$\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right) = \frac{1}{sin\theta}\frac{\partial(sin\theta)}{\partial\theta}\left(\frac{\partial}{\partial\theta}\right) + \frac{1}{sin\theta}sin\theta\frac{\partial}{\partial\theta}\left(\frac{\partial}{\partial\theta}\right) = \frac{cos\theta}{sin\theta}\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\theta^2}$$

$$\Rightarrow \frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{sin^2\theta}\frac{\partial^2}{\partial\varphi^2} = cot\theta\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\theta^2} + \frac{1}{sin^2\theta}\frac{\partial^2}{\partial\varphi^2}.$$

This suggests that the two forms are equivalent.

b. $\hat{H}_{rot} Y_{lM}(\theta\phi) = -\frac{\hbar^2}{2mr^2}\left\{\frac{\partial^2}{\partial\theta^2} + cot\theta\frac{\partial}{\partial\theta} + \frac{1}{sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\} P_{lM}(\theta)\frac{1}{\sqrt{2\pi}}e^{iM\phi}$

$$= -\frac{\hbar^2}{2mr^2}\left\{\frac{\partial^2}{\partial\theta^2} + cot\theta\frac{\partial}{\partial\theta} - \frac{M^2}{sin^2\theta}\right\} P_{lM}(\theta)\frac{1}{\sqrt{2\pi}}e^{iM\varphi} = E_{lM}P_{lM}(\theta)\frac{1}{\sqrt{2\pi}}e^{iM\varphi}$$

Only $\frac{\partial^2}{\partial\varphi^2}$ acts on $\frac{1}{\sqrt{2\pi}}e^{iM\varphi}$, giving $-M^2\frac{1}{\sqrt{2\pi}}e^{iM\varphi}$ inside the brackets. Thus this product wavefunction satisfies the eigenvalue equation of the rotational Hamiltonian.
The $\frac{1}{\sqrt{2\pi}}e^{iM\varphi}$ part of the wavefunction is the only place where φ shows up on both sides of the equation, so we can just divide by it and obtain:

$$-\frac{\hbar^2}{2mr^2}\left\{\frac{\partial^2}{\partial\theta^2} + cot\theta\frac{\partial}{\partial\theta} - \frac{M^2}{sin^2\theta}\right\} P_{lM}(\theta) = E_{lM}P_{lM}(\theta).$$

You can try out functions like $P_{20}{\sim}3cos^2\theta - 1$ and will see that they solve the equation (in that particular case for ℓ=2 and M=0).