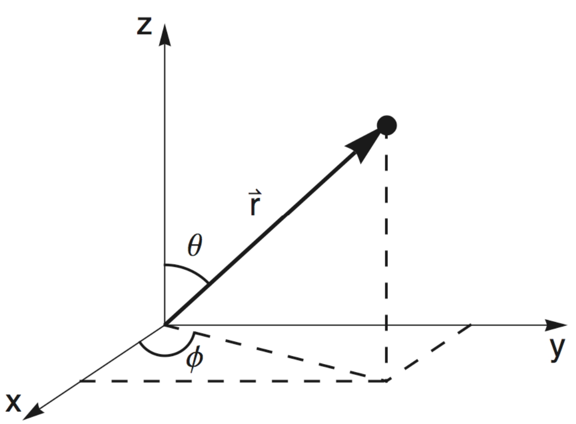
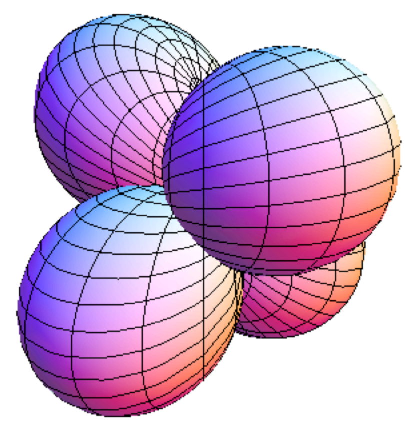
$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\,\Theta_\ell^m(\theta)\,\Phi_m(\phi)$$

$$\psi(r,\theta,\phi,t) = \sum_{n\ell m} c_{n\ell m} R_{n\ell}(r)\,\Theta_\ell^m(\theta)\,\Phi_m(\phi)\,e^{-iE_n t/\hbar}$$

The quantum central force problem: three dimensions & separation of variables

Reading: McIntyre 7.1-7.4, Appendix E





The 2-body problem

$$H = \left[\frac{\vec{\mathbf{p}}_1^2}{2m_1} + \frac{\vec{\mathbf{p}}_2^2}{2m_2} \right] + V(\vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2)$$

$$H = \left[\frac{\vec{\mathbf{P}}_{CM}^2}{2M} + \frac{\vec{\mathbf{p}}_{rel}^2}{2\mu} \right] + V(r)$$

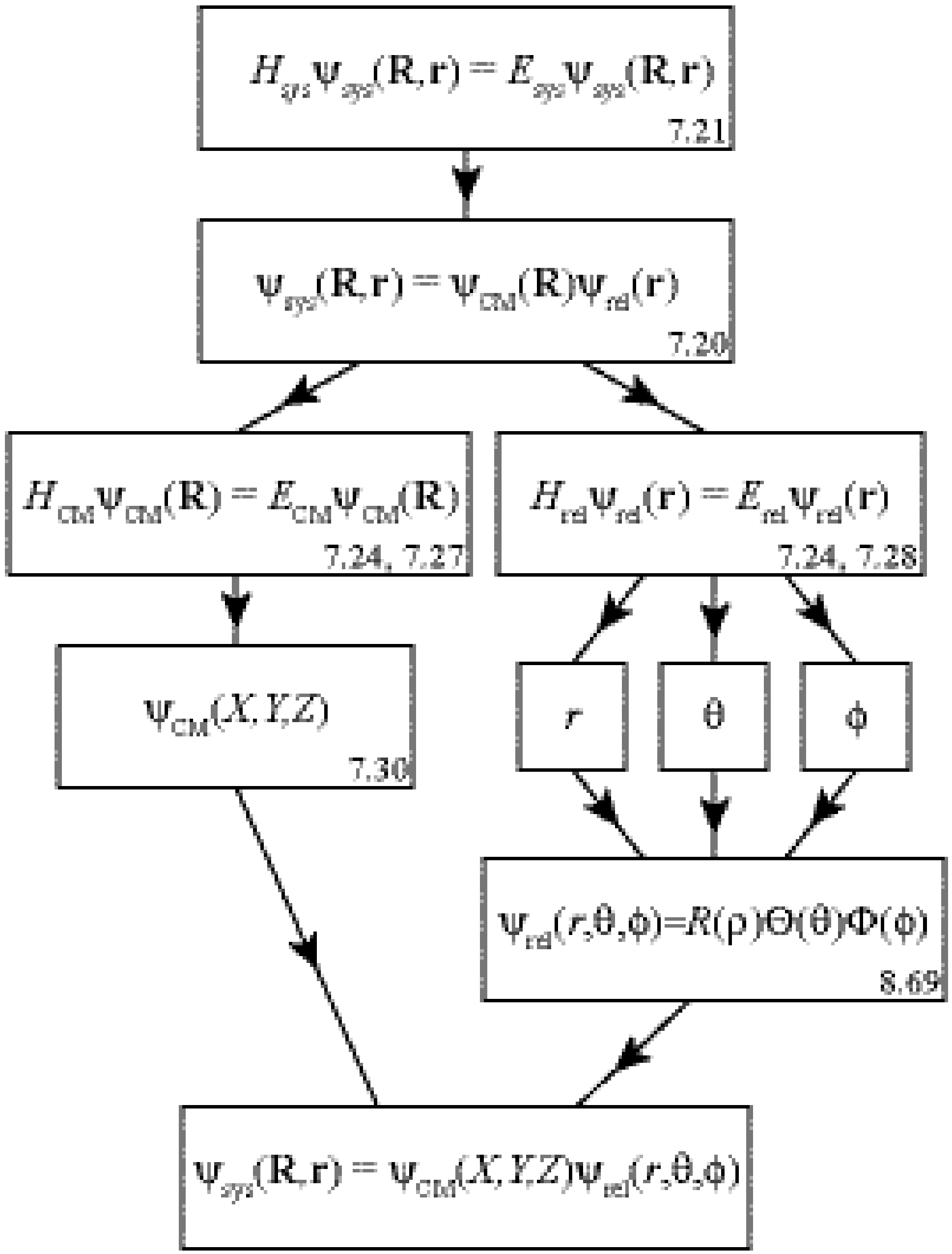
- Separates into a CoM part and a relative part with same definitions as in classical problem for center of mass, relative coordinates. Again, we will treat the CoM part of the problem as "solved".

$$p_{(rel)} \doteq -i\hbar \left(\mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z} \right) = -i\hbar \nabla_{(rel)}$$

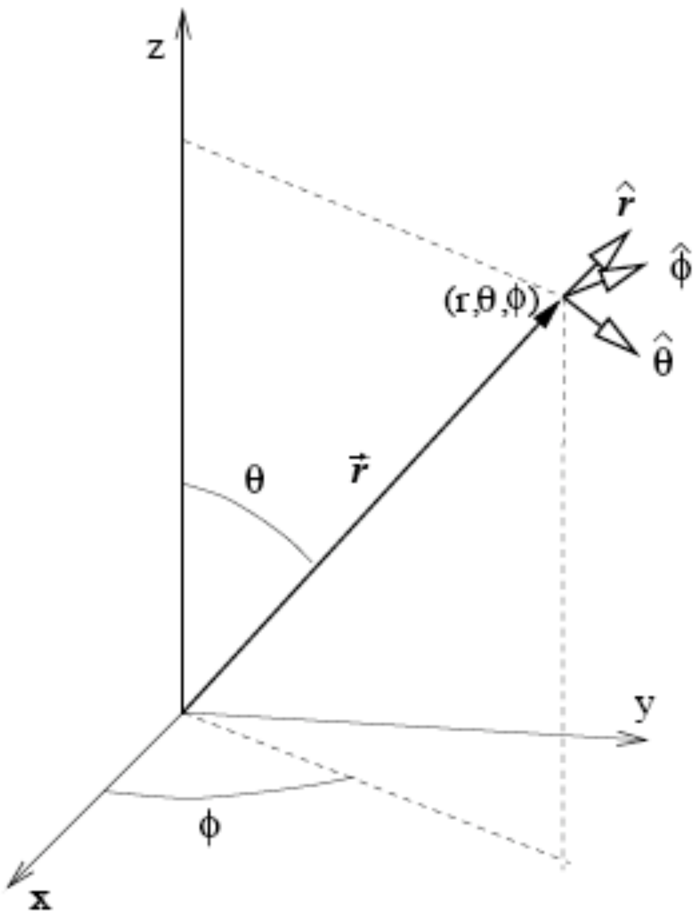
$$H_{(rel)} \doteq -\frac{\hbar^2}{2\mu} \nabla_{(rel)}^2 + V\left(r_{(rel)}\right)$$

Warning: always ask yourself -> is this an operator or a number? H, P and p are operators here.

CM Separation Flowchart



Spherical polar coordinates



Spherical Coordinates

$$\mathbf{r} = r\sin\theta\cos\phi\mathbf{i} + r\sin\theta\sin\phi\mathbf{j} + r\cos\theta\mathbf{k}$$

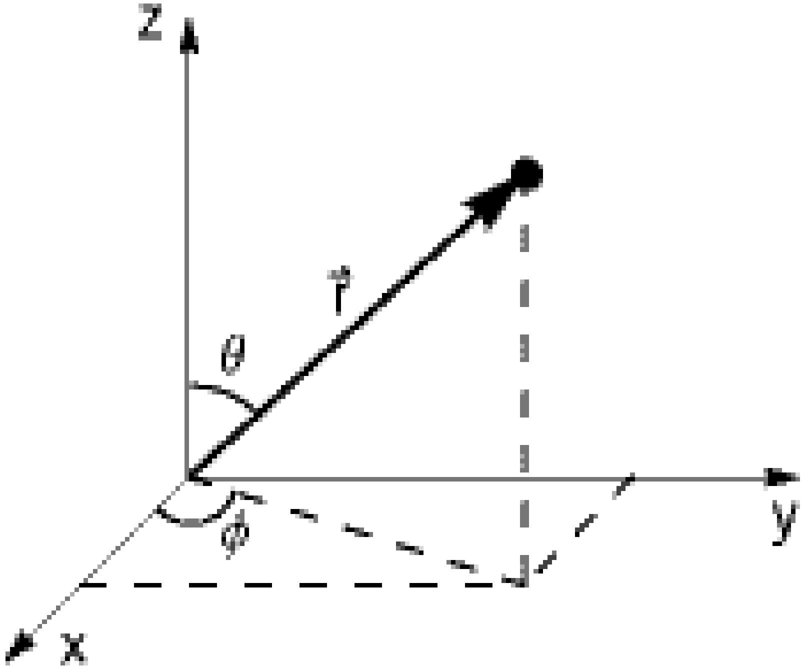
$$\hat{\mathbf{r}} = \sin\theta\cos\phi\mathbf{i} + \sin\theta\sin\phi\mathbf{j} + \cos\theta\mathbf{k}$$

$$\hat{\boldsymbol{\theta}} = \cos\theta\cos\phi\mathbf{i} + \cos\theta\sin\phi\mathbf{j} - \sin\theta\mathbf{k}$$

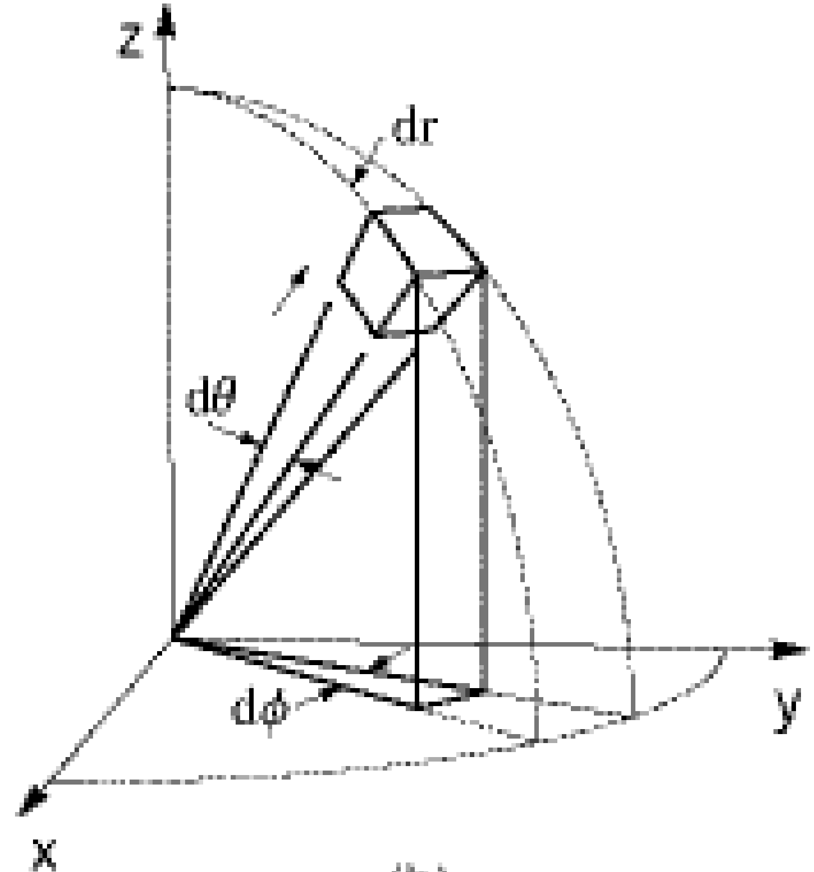
$$\hat{\boldsymbol{\phi}} = -\sin\phi\mathbf{i} + \cos\phi\mathbf{j}$$

$$\nabla = \hat{\mathbf{r}}\frac{\partial}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\boldsymbol{\phi}}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}$$

Spherical polar coordinates



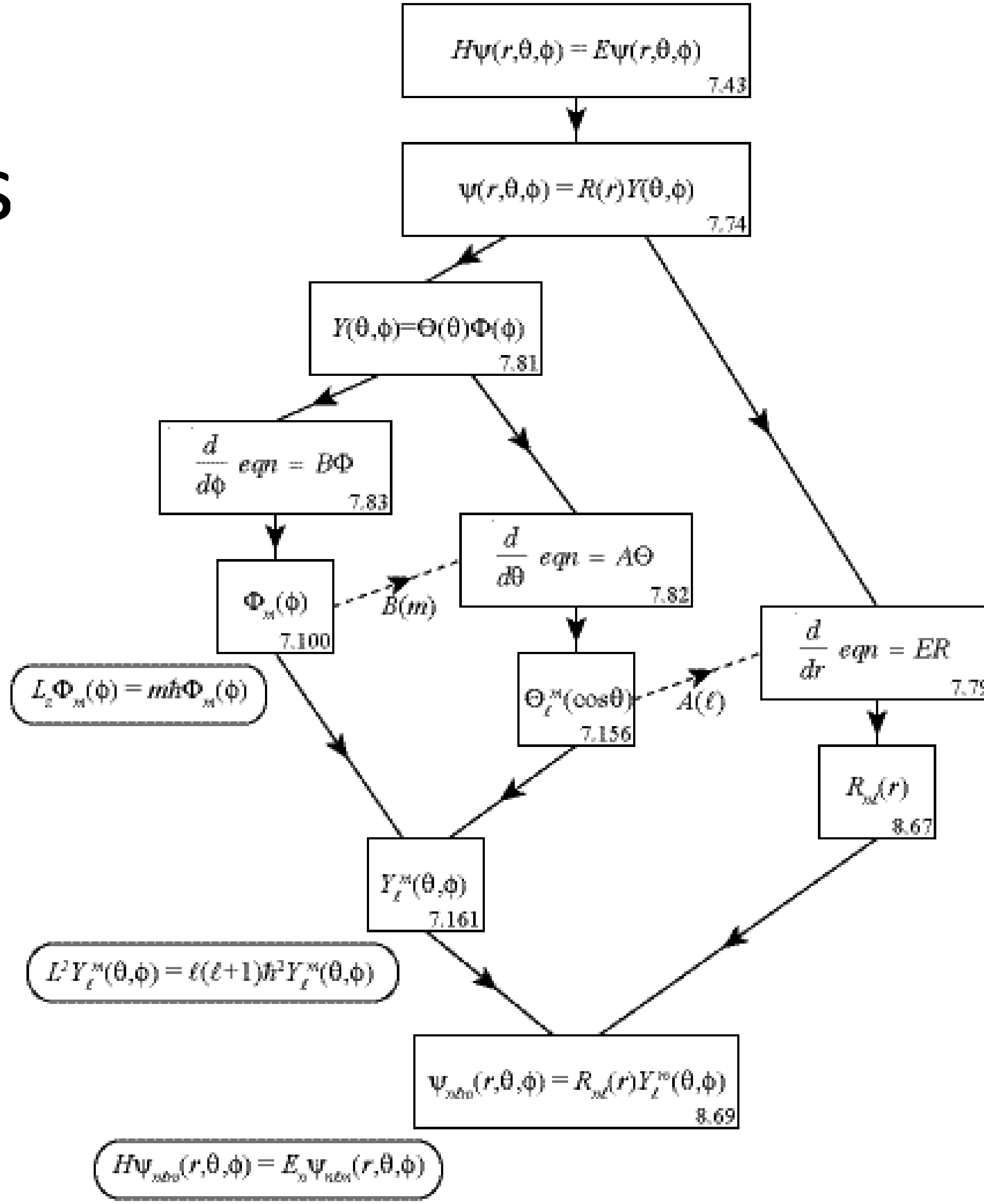
(a)



(b)

$$dV = r^2 \sin\theta \; d\theta \; d\phi \; dr$$
$$= (r \; d\theta)\,(r\sin\theta \; d\phi)\,(dr)$$
$$= (\sin\theta \; d\theta)\;\;(d\phi)\left(r^2 \; dr\right)$$
$$= r^2 \; dr \; d\Omega$$

Separation of Variables Flowchart



Spherical coordinates

- Energy eigenvalue equation for reduced mass part of the 2-body problem with kinetic energy operator explicitly in spherical coordinates

$$\left[\underbrace{-\frac{\hbar^2}{2\mu}\nabla^2}_{\text{kinetic energy operator}} + \underbrace{V(r)}_{\text{potential energy operator}}\right]\underbrace{\psi(r,\theta,\phi)}_{\text{eigenfunction}} = \underbrace{E}_{\text{eigenvalue}}\underbrace{\psi(r,\theta,\phi)}_{\text{eigenfunction}}$$

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi$$

Angular momentum

- This is angular momentum in rectangular coordinates

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

$$L_x = yp_z - zp_y \doteq -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right)$$

$$L_y = zp_x - xp_z \doteq -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right)$$

$$L_z = ?$$

$$\mathbf{L}^2 = \mathbf{L}_x^2 + \mathbf{L}_y^2 + \mathbf{L}_z^2$$

$$\left[L_x, L_y \right] = i\hbar L_z$$

$$\left[L_y, L_z \right] = i\hbar L_x$$

$$\left[L_z, L_x \right] = i\hbar L_y$$

$$\left[\mathbf{L}^2, L_{x,y,z} \right] = 0$$

$$\mathbf{L}^2 \left| \ell m_\ell \right\rangle = \ell\left(\ell + 1 \right)\hbar^2 \left| \ell m_\ell \right\rangle$$

$$L_z \left| \ell m_\ell \right\rangle = m_\ell \hbar \left| \ell m_\ell \right\rangle$$

BUT JUST LIKE SPIN!

Angular momentum

- This is angular momentum in spherical coordinates (homework)

$$L_x \doteq i\hbar\left(\sin\phi\frac{\partial}{\partial\theta}+\cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_y \doteq i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta}+\sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_z \doteq -i\hbar\frac{\partial}{\partial\phi}$$

$$\mathbf{L}^2 \doteq -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

Angular momentum

- Here comes the big simplification:

$$H_{KE} = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\mathbf{L}^2\right]\psi(r,\theta,\phi) + V(r)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

- Assume a separable solution:

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

Separation of variables:

- Blue has angular dependence, red is radial:

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{1}{\hbar^2 r^2}\mathbf{L}^2\right]R(r)Y(\theta,\phi)+V(r)R(r)Y(\theta,\phi)$$

$$=ER(r)Y(\theta,\phi)$$

Algebra (follow book 7.4):

$$\underbrace{\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)-\frac{2\mu}{\hbar^2}(E-V(r))r^2}_{function\ of\ r\ only}=\underbrace{\frac{1}{\hbar^2}\frac{1}{Y(\theta,\phi)}\mathbf{L}^2Y(\theta,\phi)}_{function\ of\ \theta,\phi\ only}\equiv A$$

Separation of variables:

- Once we solve the (blue) angular problem, it is the solution to the angular part of ALL central force problems!

$$\frac{1}{\hbar^2}\mathbf{L}^2 Y(\theta,\phi) = A Y(\theta,\phi)$$

- Once we find *A* (and Y), plug back into red equation and solve to find *E* (and *R*(*r*)).

$$\frac{d}{dr}\left(r^2 \frac{dR(r)}{dr}\right) - \frac{2\mu}{\hbar^2}(E - V(r))r^2 R(r) \equiv A R(r)$$

Separate angular equation

- But we need to work on blue equation more, first.

$$\mathbf{L}^2 \doteq -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

$$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$$

$$\left[\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d}{d\theta} \right) - B \frac{1}{\sin^2\theta} \right] \Theta(\theta) = -A\Theta(\theta)$$

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

Summary

- Here's the plan:

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

$$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right) - B\frac{1}{\sin^2\theta}\right]\Theta(\theta) = -A\Theta(\theta)$$

$$\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) - \frac{2\mu}{\hbar^2}(E - V(r))r^2R(r) \equiv AR(r)$$

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\Theta_\ell^m(\theta)\Phi_m(\phi)$$

$$\psi(r,\theta,\phi,t) = \sum_{n\ell m} c_{n\ell m}R_{n\ell}(r)\Theta_\ell^m(\theta)\Phi_m(\phi)e^{-iE_nt/\hbar}$$

Summary

- Here's the plan:
- We'll consider 3 different systems, a ring (to solve the ϕ problem), a sphere (to solve the θ and ϕ problem), and the full hydrogen atom (to solve the (r, θ, ϕ problem)
- We'll find the quantum numbers and wave functions that solve each problem
- We'll apply all the things you've learned in PH424 and PH425
- <u>**Please read ahead**</u> – the math is much more intense (though not harder) than before