Spin Eigenstates, a review

$J^2 \longrightarrow S^2 \qquad J_z \longrightarrow S_z$

$$\hat{S}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle$$
$$\hat{S}_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle$$

$$m_s = -s, -s+1, \ldots, s-1, s$$

$$\hat{S} |\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle = \tfrac{3}{4}\hbar^2 |\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle$$

$$\hat{S}^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

$$S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \hat{S}_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Derivation of the AM operator in a spherical basis

$$\hat{L} = \hat{r} \times \hat{p} = -i\hbar\, r(\hat{r} \times \vec{\nabla}) = -i\hbar \begin{vmatrix} \hat{r} & \hat{\theta} & \hat{\varphi} \\ r & 0 & 0 \\ \frac{\partial}{\partial r} & \frac{\partial}{r\,d\theta} & \frac{\partial}{r\sin\theta\,\partial\varphi} \end{vmatrix}$$

$$\hat{L} = -i\hbar \left[\hat{\varphi} \frac{\partial}{\partial\theta} - \frac{\hat{\theta}}{\sin\theta} \frac{\partial}{\partial\varphi} \right]$$

$$\hat{L}_x = \hat{x} \cdot \hat{L} = -i\hbar \left(-\sin\phi \frac{\partial}{\partial\theta} - \cos\phi \cot\theta \frac{\partial}{\partial\phi} \right)$$
$$\hat{L}_y = \hat{y} \cdot \hat{L} = -i\hbar \left(\cos\phi \frac{\partial}{\partial\theta} - \sin\phi \cot\theta \frac{\partial}{\partial\phi} \right)$$
$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\phi}$$

Spherical Harmonics

$Y_{\ell m}(\theta, \varphi) \qquad \hat{L}^2 Y_{\ell m} = \hbar \ell(\ell+1) Y_{\ell m}(\theta, \varphi)$

$\qquad\qquad\qquad\quad L_z Y_{\ell m} = \hbar m Y_{\ell m}(\theta, \varphi)$

Separation of Vars

$$Y_{\ell m}(\theta,\varphi) = \Theta_{\ell m}(\theta)\,\Phi_m(\varphi)$$

$$-i\hbar \frac{\partial}{\partial\phi}\Phi_m(\varphi) = m\,\Phi_m(\varphi)$$

$$\hat{L}^2 Y_{\ell m}(\theta,\varphi) = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$$

$$\Theta(\theta)\ \frac{1}{\sqrt{2\pi}}e^{im\varphi} = \frac{\hbar\,\ell(\ell+1)}{\sqrt{2\pi}}e^{im\varphi}$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\Theta_{\ell m}(\theta)\right) + \left[\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right]\Theta_{\ell m}(\theta) = 0$$

Legendre Polynomials

$$\Theta_{\ell m}(\theta) = C_{\ell m}P_\ell^m(\cos\theta)$$

$$\boxed{\begin{aligned} P_\ell^m(\xi) &= (1-x^2)^{m/2}\frac{d^m}{dx^m}P_\ell(x) \\ P_\ell &= \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}(x^2-1)^\ell \end{aligned}}$$

Spherical Harmonics

$$\boxed{Y_\ell^m(\theta,\phi) = \sqrt{\left(\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}\right)}\,e^{im\phi}\,P_\ell^m(\cos\theta)}$$

Particle Motion constrained to a sphere

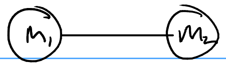
$$\hat{H} = \frac{|\vec{r}\times\vec{p}|^2}{2mr^2} = \frac{L^2}{2mr^2} = \frac{L^2}{2I}$$

$$\frac{L^2}{2I}Y_{\ell m} = E\,Y_{\ell m}$$

$$E_\ell = \frac{\hbar^2}{2I}\ell(\ell+1) \qquad \ell = 0, 1, 2, \ldots$$

$2\ell+1$ degen states per energy level.

Diatomic Molecule



$$\mu = \frac{m_1 m_2}{m_1 + m_2} \qquad L = I\omega = \mu r^2 \omega$$

$$I = \mu r^2$$

$$\hat{H} = \frac{\hat{L}^2}{2\mu r^2}$$

$$E_l = \frac{l(l+1)\hbar^2}{2\mu r^2}$$

electron orbital of a Hydrogen atom

$$V = -k\frac{e^2}{r}$$

$$-\left(+\frac{\hbar^2}{2m}\nabla^2 + k\frac{e^2}{r}\right)\Psi(r) = E\Psi(r)$$

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r} r - \frac{1}{\hbar^2 r^2}\hat{L}^2$$

$$-\left(\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial}{\partial r} r - \frac{\hat{L}^2}{2mr^2} + V(r)\right) = E\Psi$$

$$\Psi(\vec{r}) = R(r)\, Y_{lm}(\theta, \varphi)$$

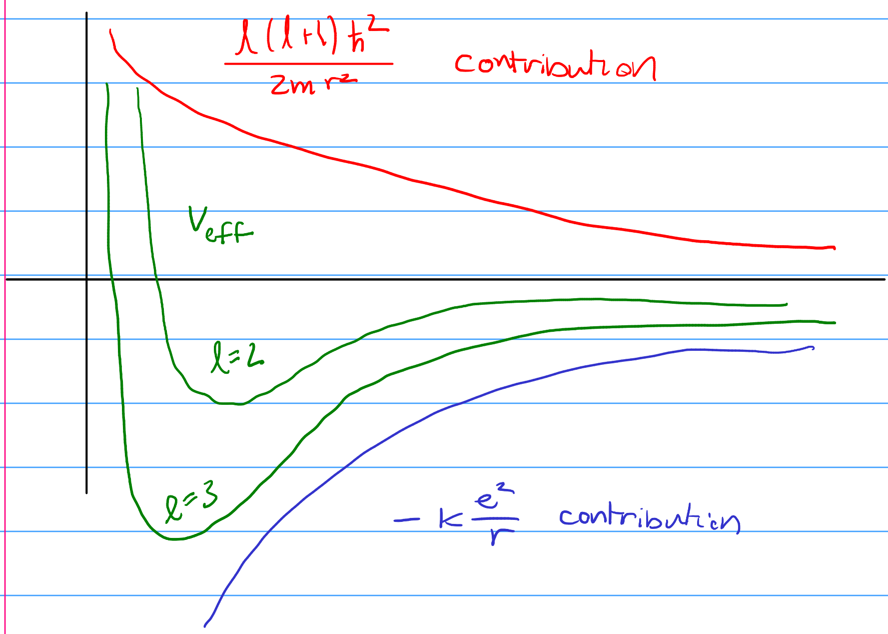
Ra

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\left(r R_{nl}(r)\right) + \left[V(r) + \frac{l(l+1)\hbar^2}{2mr^2}\right]\left(r R_{nl}(r)\right)$$

$$= E_n\left(r R_{nl}(r)\right)$$

V_{eff} !

Effective potential



$\longrightarrow$ Define $U_{nl}(r) \equiv r R_{nl}(r)$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}(U_{nl}(r)) + V_{eff}(r)\,U_{nl}(r) = E_n U_{nl}(r)$$

1D ODE