HW #4 Chem 2430 Answers

1. $B_e = 0.5\ cm^{-1}$

$$J_{max} = \frac{1}{2}\sqrt{\frac{2(kT)}{B_e}} - \frac{1}{2} \approx \frac{1}{2}\sqrt{\frac{2(200)}{0.5}} - \frac{1}{2} \approx 14$$

2. Show that Y_1^0 and Y_2^0 are $\perp$.

$Y_1^0 \sim \cos\theta$, $Y_2^0 \sim (3\cos^2\theta - 1)$

$$\int_0^{\pi} (\cos\theta)(3\cos^2\theta - 1)\sin\theta\, d\theta = \int_0^{\pi}(3\cos^3\theta - \cos\theta)\sin\theta\, d\theta$$

$$= -\frac{3}{4}(\cos\theta)^4 + \frac{(\cos\theta)^2}{2}\Big|_0^{\pi} = 0$$

Show that Y_1^0 and Y_1^{-1} are orthogonal

$$\int_0^{2\pi} e^{-i\phi} e^{-i\phi}\, d\phi = 0$$

3. Show that Y_1^0, Y_1^1, and Y_1^{-1} have the same energy

$Y_1^0 \sim \cos\theta$, $Y_1^{\pm 1} \sim \sin\theta\, e^{\pm i\phi}$

$$\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta}\right]\cos\theta = -\cos\theta - \cot\theta\sin\theta = -2\cos\theta$$

$$\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\sin\theta\, e^{i\phi}$$

$$= \left[-\sin\theta + \cot\theta\cos\theta + \frac{\sin\theta}{\sin^2\theta}(-1)\right]e^{i\phi}$$

$$= -2\sin\theta\, e^{i\phi}$$

obviously, the same result is obtained for Y_1^{-1}

4. Spherical well. Are $j_0(ar)$ and $j_1(ar)$ solutions

$j_0 = \frac{\sin ar}{r}$. I dropped the "a" from the denominator

$$\frac{\partial}{\partial r}\frac{\sin(ar)}{r} = \frac{a\cos(ar)}{r} - \frac{\sin(ar)}{r^2}$$

$$\frac{\partial^2}{\partial r^2}\frac{\sin(ar)}{r} = -\frac{a^2\sin(ar)}{r} - \frac{a\cos(ar)}{r^2} - \frac{a\cos(ar)}{r^2} + \frac{2\sin(ar)}{r^3}$$

$$-\frac{1}{2}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right]j_0 = -\frac{1}{2}\left[-\frac{a^2\sin(ar)}{r} - \frac{2a\cos(ar)}{r^2} + \frac{2\sin(ar)}{r^3}\right]$$

$$-\frac{1}{r}\left[\frac{a\cos(ar)}{r} - \frac{\sin(ar)}{r^2}\right] = \frac{1}{2}a^2\frac{\sin(ar)}{r}.\ \text{So it works.}$$