

# Spring 2000 # 12 (p 1 of 4)

Consider the Hamiltonian for a general top with principal moments of inertia  $I_1, I_2, I_3$ .

(a) For the symmetric top with  $I = I_1 = I_2 \neq I_3$ , derive all the energy levels

The general Hamiltonian for this system is given by (see Spring 2000 # 6)

$$H = \frac{\hbar^2}{2I_1} J_x^2 + \frac{\hbar^2}{2I_2} J_y^2 + \frac{\hbar^2}{2I_3} J_z^2$$

set  $\hbar=1$  and use what we are given that  $I = I_1 = I_2 \neq I_3$ . That is,

$$H = \frac{J_x^2 + J_y^2}{2I} + \frac{J_z^2}{2I_3} \quad (1)$$

We know that the  $J_i$ 's must satisfy the following commutation relation:

$$[J_i, J_j] = i \sum_k \epsilon_{ijk} J_k$$

From here we can construct the algebra in the basis of eigenstates  $|j, m\rangle$  of  $J^2$  and  $J_z$ . See Abers pp 77-80. So, we construct raising and lowering operators  $J_+$  &  $J_-$  such that

$$J_x = \frac{J_+ + J_-}{2} \quad \text{and} \quad J_y = \frac{J_+ - J_-}{2i} \quad (2)$$

if you have trouble remembering these think of the definitions of  $\cos x$  and  $\sin x$

$$\cos x = \frac{e^x + e^{-x}}{2} \quad \text{and} \quad \sin x = \frac{e^x - e^{-x}}{2i}$$

and note the similar form.

From eq (2), we know

$$\begin{aligned} J_x^2 + J_y^2 &= \frac{1}{4} \left( J_+^2 + J_-^2 + J_+ J_- + J_- J_+ \right) \\ &= \frac{1}{4} \left( 2J_+ J_- + 2J_- J_+ \right) \end{aligned}$$

from (2)

$$\Rightarrow J_x^2 + J_y^2 = \frac{1}{2} (J_+ J_- + J_- J_+)$$

substitute these results into eq (1)

$$H = \frac{1}{4I} (J_+ J_- + J_- J_+) + \frac{J_z^2}{2I_3}$$

Spring 2000 # 12 (p2 of 4)

recall (A bos eq 3.113a & 3.113b)

$$J_z |j, m\rangle = m |j, m\rangle$$

$$J_{\pm} |j, m\rangle = \sqrt{j(j+1) - m(m\pm 1)} |j, m\pm 1\rangle$$

so,

$$H |j, m\rangle = \left[ \frac{1}{4I} (J_+ J_- + J_- J_+) + \frac{J_z^2}{2I_3} \right] |j, m\rangle$$

$$= \frac{1}{4I} J_+ \sqrt{j(j+1) - m(m-1)} |j, m-1\rangle + J_- \sqrt{j(j+1) - m(m+1)} |j, m+1\rangle + \frac{m^2}{2I_3} |j, m\rangle$$

$$= \frac{1}{4I} \sqrt{j(j+1) - (m-1)m} \sqrt{j(j+1) - m(m-1)} |j, m\rangle + \frac{m^2}{2I_3} |j, m\rangle$$

$$+ \sqrt{j(j+1) - (m+1)m} \sqrt{j(j+1) - m(m+1)} |j, m\rangle$$

where  $\sqrt{j(j+1) - m(m\pm 1)} \sqrt{j(j+1) - m(m\pm 1)} = \sqrt{[j(j+1) - m(m\pm 1)]^2} = j(j+1) - m(m\pm 1)$

so,

$$H |j, m\rangle = \frac{1}{4I} \left[ j(j+1) - m(m-1) + j(j+1) - m(m+1) \right] |j, m\rangle + \frac{m^2}{2I_3} |j, m\rangle$$

$$= \frac{1}{2I} [j(j+1) - m^2] |j, m\rangle + \frac{m^2}{2I_3} |j, m\rangle$$

Thus,

$$E_{j,m} = \left[ \frac{j(j+1) - m^2}{2I} + \frac{m^2}{2I_3} \right]$$

(b) A slightly asymmetric top has  $2\Delta = I_1 - I_2 \neq 0$ ,  $2I = I_1 + I_2$  and  $\Delta \ll I$ , with  $I \ll I_3$ . compute the  $j=0$  and  $j=1$  energies up to and including first order in  $\Delta$ .

let's use what we know from part (a) and what we are given to make this as simple as possible.

Solve for  $I_2$  from what was given:

$$I_2 = I_1 - 2\Delta$$

so the second term in the general Hamiltonian becomes

$$\frac{J_y^2}{2I_2} = \frac{J_y^2}{2(I_1 - 2\Delta)} = \frac{J_y^2}{2I_1(1 - \frac{2\Delta}{I_1})} \approx \frac{J_y^2}{2I_1} \left(1 + \frac{2\Delta}{I_1}\right)$$

binomial theorem  
since  $\Delta \ll I_1$

so, our Hamiltonian is

$$H = \frac{J_x^2}{2I_1} + \frac{J_y^2}{2I_1} + \frac{2\Delta}{2I_1^2} J_y^2 + \frac{J_z^2}{2I_3} = \frac{(J_x^2 + J_y^2)}{2I_1} + \frac{J_z^2}{2I_3} + \frac{\Delta J_y^2}{I_1^2}$$

$$\Rightarrow H = H_0 + \frac{\Delta J_y^2}{I_1^2} \quad \text{where } H_0 = \text{Hamiltonian from part (a)} \\ \text{with } I \rightarrow I_1$$

so, let's consider the "perturbed term" in the Hamiltonian

$$H' |j, m\rangle = \frac{\Delta}{I_1^2} J_y^2 |j, m\rangle = \frac{\Delta}{I_1^2} \left(\frac{J_+ - J_-}{2i}\right)^2 |j, m\rangle = \frac{\Delta}{4I_1^2} (J_+^2 + J_-^2 - J_+ J_- - J_- J_+) |j, m\rangle$$

$$= \frac{-\Delta}{4I_1^2} \left[ J_+ \sqrt{j(j+1) - m(m+1)} |j, m+1\rangle + J_- \sqrt{j(j+1) - m(m-1)} |j, m-1\rangle \right]$$

$$+ \left( j(j+1) - m(m-1) + j(j+1) - m(m+1) \right) |j, m\rangle$$

$$\Rightarrow \langle j, m | H' | j, m \rangle = + \frac{\Delta}{2I_1^2} [j(j+1) - m^2]$$

so, the energy is

$$E_{j,m} = \frac{j(j+1) - m^2}{2I_1} + \frac{\Delta j(j+1)}{2I_1^2} - \frac{\Delta m^2}{2I_1^2} + \frac{m^2}{2I_3}$$

Spring 2000 #12 (p 4 of 4)

→ For  $j=0, m=0$

$$\boxed{E_{00} = 0}$$

→ For  $j=1$

•  $m=+1$ ,

$$E_{11} = \frac{2-1}{2I_1} + \frac{2\Delta}{2I_1^2} - \frac{\Delta}{2I_1^2} + \frac{1}{2I_3} = \frac{1}{I_1} + \frac{1}{2I_3} + \frac{\Delta}{2I_1^2}$$

$$\therefore E_{11} = \left( \frac{1}{I_1} + \frac{1}{2I_3} \right) + \frac{\Delta}{2I_1^2}$$

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perturbed part

•  $m=0$ ,

$$E_{10} = \frac{2}{2I_1} - \frac{\Delta 2}{2I_1^2} + 0 + 0 = \boxed{\frac{1}{I_1} - \frac{\Delta}{I_1^2}}$$

•  $m=-1$

$$E_{1,-1} = \frac{2-1}{2I_1} + \frac{2\Delta}{2I_1^2} - \frac{\Delta}{2I_1^2} + \frac{1}{2I_3} = \boxed{E_{11}}$$