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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

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Start with the Hamiltonian

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

For the case $I = I_1 = I_2 \neq I_3$, the Hamiltonian becomes

$$H = \frac{\hbar^2}{2I}\left(J_x^2 + J_y^2\right) + \frac{\hbar^2}{2I_3}J_z^2$$

Introduce the raising/lowering operators J_+ and J_-

$$J_+ = \left(J_x + iJ_y\right) \qquad J_- = \left(J_x - iJ_y\right)$$

Solve for J_x and J_y in terms of J_+ and J_-

$$J_x = \frac{1}{2}\left(J_x + J_-\right) \qquad J_y = \frac{1}{2i}\left(J_x - J_-\right)$$

One can now write

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

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

The Hamiltonian becomes

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

Recall the action of operators on state |j,m>

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

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

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

So we have

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

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

$$J_+J_-\left|j,m\right\rangle = \sqrt{j^2(j+1)^2 - 2m(m-1)j(j+1) + m^2(m-1)^2}\left|j,m\right\rangle$$

$$J_+J_-\left|j,m\right\rangle = \left[j(j+1) - m(m-1)\right]j,m\rangle \qquad \text{(i)}$$

Similarly

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

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

$$J_-J_+\left|j,m\right\rangle = \left[j(j+1) - m(m+1)\right]j,m\rangle \qquad \text{(ii)}$$

Combining results (i) and (ii) yields

$$\left(J_+J_- + J_-J_+\right)j,m\rangle = \left[2j(j+1) - 2m^2\right]j,m\rangle$$

The energy states are thus given by

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

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

Rewrite the Hamiltonian as

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

Now write the middle term as

$$\frac{\hbar^2}{2I_1}\left(1-\frac{2\Delta}{I_1}\right)^{-1} J_y^2$$

and use the binomial theorem to get

$$\frac{\hbar^2}{2I_1}\left(1+\frac{2\Delta}{I_1}\right)J_y^2$$

So the new Hamiltonian is given by

$$H_{new} = H_0 + \frac{\hbar^2\Delta}{I_1^2}J_y^2$$

Note that

$$J_y^2 = \frac{1}{4}\left(J_+J_- + J_-J_+ - J_+^2 - J_-^2\right)$$

The first order shift in energies is given by

$$\frac{\hbar^2\Delta}{I_1^2}\langle j,m|J_y^2|j,m\rangle$$

For j=0, m=0:

$$\Delta E_{0,0} = \frac{\hbar^2\Delta}{4I_1^2}\langle 0,0|J_-J_+|0,0\rangle = 0$$

For j=1, m=+1:

$$\Delta E_{1,1} = \frac{\hbar^2\Delta}{4I_1^2}\langle 1,1|J_+J_-|1,1\rangle = \frac{\hbar^2\Delta}{2I_1^2}$$

For j=1, m=0:

$$\Delta E_{1,0} = \frac{\hbar^2\Delta}{4I_1^2}\langle 1,0|J_+J_- + J_-J_+|1,0\rangle = \frac{\hbar^2\Delta}{I_1^2}$$

For j=1, m=-1:

$$\Delta E_{1,-1} = \frac{\hbar^2\Delta}{4I_1^2}\langle 1,-1|J_-J_+|1,-1\rangle = \frac{\hbar^2\Delta}{2I_1^2}$$