A Modern Approach to Quantum Mechanics by Townsend - Solutions

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9 Translational and Rotational Symmetry in the Two-Body Problem

9.1

First we expand both $\hat{T}_x\hat{T}_y$ and $\hat{T}_y\hat{T}_x$, keeping only up to second order terms.

$$\hat{T}_x \hat{T}_y = \left(1 - \frac{i\hat{p}_x a_x}{\hbar} - \frac{\hat{p}_x^2 a_x^2}{2\hbar^2}\right) \left(1 - \frac{i\hat{p}_y a_y}{\hbar} - \frac{\hat{p}_y^2 a_y^2}{2\hbar^2}\right)$$

$$= 1 - \frac{i}{\hbar} \left(\hat{p}_y a_y + \hat{p}_x a_x\right) - \frac{a_x a_y}{\hbar^2} \hat{p}_x \hat{p}_y - \frac{1}{2\hbar^2} \left(\hat{p}_y^2 a_y^2 + \hat{p}_x^2 a_x^2\right) + \dots$$

$$\hat{T}_y \hat{T}_x = \left(1 - \frac{i\hat{p}_y a_y}{\hbar} - \frac{\hat{p}_y^2 a_y^2}{2\hbar^2}\right) \left(1 - \frac{i\hat{p}_x a_x}{\hbar} - \frac{\hat{p}_x^2 a_x^2}{2\hbar^2}\right)$$

$$= 1 - \frac{i}{\hbar} \left(\hat{p}_x a_x + \hat{p}_y a_y\right) - \frac{a_y a_x}{\hbar^2} \hat{p}_y \hat{p}_x - \frac{1}{2\hbar^2} \left(\hat{p}_x^2 a_x^2 + \hat{p}_y^2 a_y^2\right) + \dots$$

Here we see that, when we subtract the two products, everything cancels out except one term, which must equal zero.

$$[\hat{T}_x, \hat{T}_y] = \hat{T}_x \hat{T}_y - \hat{T}_y \hat{T}_x = -\frac{a_y a_x}{\hbar^2} \left(\hat{p}_x \hat{p}_y - \hat{p}_y \hat{p}_x \right) = -\frac{a_y a_x}{\hbar^2} [\hat{p}_x, \hat{p}_y] = 0$$

This implies that $[\hat{p}_x, \hat{p}_y] = 0$.

9.2

$$\langle p|\Psi|p|\Psi\rangle = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\hbar\pi}} e^{\frac{-ipx}{\hbar}} \langle x|\Psi|x|\Psi\rangle$$
 (6.57a)

$$\langle x|\Psi|x|\Psi\rangle = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\hbar\pi}} e^{\frac{ipx}{\hbar}} \langle p|\Psi|p|\Psi\rangle$$
 (6.57b)

In 3-dimensions,

$$|\vec{r}\rangle = |x, y, z\rangle \,, \ |\vec{p}\rangle = |p_x, p_y, p_z\rangle \,,$$

$$\langle \vec{r}|\vec{p}|\vec{r}|\vec{p}\rangle = \left(\frac{1}{\sqrt{2\hbar\pi}}e^{\frac{-ip_x x}{\hbar}}\right) \left(\frac{1}{\sqrt{2\hbar\pi}}e^{\frac{-ip_y y}{\hbar}}\right) \left(\frac{1}{\sqrt{2\hbar\pi}}e^{\frac{-ip_z z}{\hbar}}\right) = \frac{1}{(2\hbar\pi)^{\frac{3}{2}}}e^{\frac{-i\vec{p}\cdot\vec{r}}{\hbar}}$$
(0.25)

Therefore,

$$\langle \vec{p} | \Psi | \vec{p} | \Psi \rangle = \int_{-\infty}^{\infty} \langle \vec{p} | \vec{r} | \vec{p} | \vec{r} \rangle \, \langle \vec{r} | \Psi | \vec{r} | \Psi \rangle \, d\vec{r} = \int_{-\infty}^{\infty} \frac{1}{(2\hbar\pi)^{\frac{3}{2}}} e^{\frac{-i\vec{p}\cdot\vec{r}}{\hbar}} \, \langle \vec{r} | \Psi | \vec{r} | \Psi \rangle \, d\vec{r}$$

$$\langle \vec{r} | \Psi | \vec{r} | \Psi \rangle = \int_{-\infty}^{\infty} \langle \vec{r} | \vec{p} | \vec{r} | \vec{p} \rangle \, \langle \vec{p} | \Psi | \vec{p} | \Psi \rangle \, d\vec{r} = \int_{-\infty}^{\infty} \frac{1}{(2\hbar\pi)^{\frac{3}{2}}} e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \, \langle \vec{p} | \Psi | \vec{p} | \Psi \rangle \, d\vec{r}$$

9.3

Conservation of energy arises from invariance under time translations. Consider $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$, the generator of finite time translations. We wish to show $\left[\hat{H},\hat{U}(t)\right] = 0$.

$$\left[\hat{H}, e^{-i\hat{H}t/\hbar}\right] = \left[\hat{H}, \sum_{k=0}^{\infty} \frac{(-i\hat{H}t/\hbar)^k}{k!}\right]$$
$$= \sum_{k=0}^{\infty} \frac{\left[\hat{H}, (-i\hat{H}t/\hbar)^k\right]}{k!} = 0$$

It is clear that \hat{H} commutes with any exponential of itself times some scalars, and so indeed $\left[\hat{H},\hat{U}(t)\right]=0$.

9.4

To make life a little easier, let's define two constants, $c_i = \frac{m_i}{m_1 + m_2}$, where i = 1, 2 and $c_1 + c_2 = 1$. We now expand out \hat{P}_j , \hat{p}_j , \hat{X}_i , and \hat{x}_i . Note that $\hat{R}_i \to \hat{X}_i$ and $\hat{r}_i \to \hat{x}_i$.

$$\hat{P}_{j} = \hat{p}_{1j} + \hat{p}_{2j}$$

$$\hat{p}_{j} = c_{2}\hat{p}_{1j} - c_{1}\hat{p}_{2j}$$

$$\hat{X}_{i} = c_{1}\hat{x}_{1i} + c_{2}\hat{x}_{2i}$$

$$\hat{x}_{i} = \hat{x}_{1i} - \hat{x}_{2i}$$

$$\begin{split} [\hat{x}_i, \hat{P}_j] &= [\hat{x}_{1i} - \hat{x}_{2i}, \hat{p}_{1j} + \hat{p}_{2j}] \\ &= [\hat{x}_{1i}, \hat{p}_{1j}] + [\hat{x}_{1i}, \hat{p}_{2j}] + [-\hat{x}_{2i}, \hat{p}_{1j}] + [-\hat{x}_{2i}, \hat{p}_{2j}] \\ &= [\hat{x}_{1i}, \hat{p}_{1j}] - [\hat{x}_{2i}, \hat{p}_{2j}] \\ &= i\hbar \delta_{ij} - i\hbar \delta_{ij} \\ &= 0 \end{split}$$

$$\begin{split} [\hat{x}_i, \hat{p}_j] &= [\hat{x}_{1i} - \hat{x}_{2i}, c_2 \hat{p}_{1j} - c_1 \hat{p}_{2j}] \\ &= [\hat{x}_{1i}, c_2 \hat{p}_{1j}] + [\hat{x}_{1i}, -c_1 \hat{p}_{2j}] + [-\hat{x}_{2i}, c_2 \hat{p}_{1j}] + [-\hat{x}_{2i}, -c_1 \hat{p}_{2j}] \\ &= [\hat{x}_{1i}, c_2 \hat{p}_{1j}] + [\hat{x}_{2i}, c_1 \hat{p}_{2j}] \\ &= c_2 i \hbar \delta_{ij} + c_1 i \hbar \delta_{ij} \\ &= i \hbar \delta_{ij} \end{split}$$

$$\begin{split} [\hat{X}_i, \hat{P}_j] &= [c_1 \hat{x}_{1i} + c_2 \hat{x}_{2i}, \hat{p}_{1j} + \hat{p}_{2j}] \\ &= [c_1 \hat{x}_{1i}, \hat{p}_{1j}] + [c_1 \hat{x}_{1i}, \hat{p}_{2j}] + [c_2 \hat{x}_{2i}, \hat{p}_{1j}] + [c_2 \hat{x}_{2i}, \hat{p}_{2j}] \\ &= [c_1 \hat{x}_{1i}, \hat{p}_{1j}] + [c_2 \hat{x}_{2i}, \hat{p}_{2j}] \\ &= c_1 i \hbar \delta_{ij} + c_2 i \hbar \delta_{ij} \\ &= i \hbar \delta_{ij} \end{split}$$

$$\begin{split} [\hat{X}_i, \hat{p}_j] &= [c_1 \hat{x}_{1i} + c_2 \hat{x}_{2i}, c_2 \hat{p}_{1j} - c_1 \hat{p}_{2j}] \\ &= [c_1 \hat{x}_{1i}, c_2 \hat{p}_{1j}] + [c_1 \hat{x}_{1i}, -c_1 \hat{p}_{2j}] + [c_2 \hat{x}_{2i}, c_2 \hat{p}_{1j}] + [c_2 \hat{x}_{2i}, -c_1 \hat{p}_{2j}] \\ &= [c_1 \hat{x}_{1i}, c_2 \hat{p}_{1j}] + [c_2 \hat{x}_{2i}, -c_1 \hat{p}_{2j}] \\ &= c_1 c_2 i \hbar \delta_{ij} - c_1 c_2 i \hbar \delta_{ij} \\ &= 0 \end{split}$$

$$\hat{P}^2 = \hat{p}_1^2 + \hat{p}_1\hat{p}_2 + \hat{p}_2\hat{p}_1 + \hat{p}_2^2$$

$$\hat{p}^2 = \left(\frac{\mu}{m_1}\hat{p}_1 - \frac{\mu}{m_2}\hat{p}_2\right)^2 = \mu^2 \left(\frac{\hat{p}_2^2}{m_2^2} - \frac{\hat{p}_1\hat{p}_2}{m_1m_2} - \frac{\hat{p}_2\hat{p}_1}{m_1m_2} + \frac{\hat{p}_1^2}{m_1^2}\right)$$

$$\begin{split} \frac{\hat{P}^2}{2M} + \frac{\hat{p}^2}{2m} &= \frac{1}{2M} \left(\hat{p}_1^2 + \hat{p}_1 \hat{p}_2 + \hat{p}_2 \hat{p}_1 + \hat{p}_2^2 \right) \\ &+ \frac{\mu}{2} \left(\frac{\hat{p}_2^2}{m_2^2} - \frac{\hat{p}_1 \hat{p}_2}{m_1 m_2} - \frac{\hat{p}_2 \hat{p}_1}{m_1 m_2} + \frac{\hat{p}_1^2}{m_1^2} \right) \\ &= \left(\frac{1}{2M} + \frac{\mu}{2m_1^2} \right) \hat{p}_1^2 + \left(\frac{1}{2M} + \frac{\mu}{2m_2^2} \right) \hat{p}_2^2 \\ &+ \left(\frac{1}{2M} - \frac{\mu}{m_1 m_2} \right) \hat{p}_1 \hat{p}_2 + \left(\frac{1}{2M} - \frac{\mu}{2m_1 m_2} \right) \hat{p}_1 \hat{p}_2 \end{split}$$

A little algebra reveals that the first two terms in parenthesis reduce to $1/2m_1$ and $1/2m_2$, respectively, and the second two terms reduce to 0. Hence, we have

$$\frac{\hat{P}^2}{2M} + \frac{\hat{p}^2}{2m} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2}$$

9.6

9.7

$$\begin{split} \hat{L}^2 &= \hat{L} \cdot \hat{L} = \sum_i \hat{L}_i \hat{L}_i \\ &= \left(\sum_{ijk} \varepsilon_{ijk} \hat{x}_j \hat{p}_k \right) \left(\sum_{ilm} \varepsilon_{ilm} \hat{x}_l \hat{p}_m \right) \\ &= \sum_{jklm} \left(\sum_i \varepsilon_{ijk} \varepsilon_{ilm} \right) \hat{x}_j \hat{p}_k \hat{x}_l \hat{p}_m \\ &= \sum_{jklm} \left(\delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl} \right) \hat{x}_j \hat{p}_k \hat{x}_l \hat{p}_m \\ &= \sum_{jklm} \delta_{jl} \delta_{km} \hat{x}_j \hat{p}_k \hat{x}_l \hat{p}_m - \delta_{jm} \delta_{kl} \hat{x}_j \hat{p}_k \hat{x}_l \hat{p}_m \end{split}$$

Before we continue we should notice two things. In the first expression, we can rewrite $\hat{x}_l\hat{p}_m$ as $\hat{p}_m\hat{x}_l+i\hbar\delta_{lm}$ from the commutation relation. Also, we can rearrange the second expression by pulling the second Kronecker delta into the middle, sum over k,l (which equates to $\hat{r}\cdot\hat{p}$), and do the same thing with j,m.

$$\delta_{jm}\delta_{kl}\hat{x}_{j}\hat{p}_{k}\hat{x}_{l}\hat{p}_{m} = \delta_{jm}\hat{x}_{j} \left(\delta_{kl}\hat{p}_{k}\hat{x}_{l}\right)\hat{p}_{m}$$

$$= \delta_{jm}\hat{x}_{j} \left(\hat{r} \cdot \hat{p}\right)\hat{p}_{m}$$

$$= \hat{r} \cdot \hat{p} \left(\delta_{jm}\hat{x}_{j}\hat{p}_{m}\right)$$

$$= \left(\hat{r} \cdot \hat{p}\right)^{2}$$

$$\begin{split} &= \sum_{jklm} \delta_{jl} \delta_{km} \hat{x}_{j} \hat{p}_{k} \left(\hat{p}_{m} \hat{x}_{l} + i\hbar \delta_{lm} \right) - (\hat{r} \cdot \hat{p})^{2} \\ &= \sum_{jklm} \delta_{jl} \delta_{km} \hat{x}_{j} \hat{p}_{k} \hat{p}_{m} \hat{x}_{l} i\hbar \delta_{lm} + i\hbar \delta_{jl} \delta_{km} \delta_{lm} \hat{x}_{j} \hat{p}_{k} - (\hat{r} \cdot \hat{p})^{2} \\ &= \sum_{jklm} \left(\delta_{jl} \hat{x}_{j} \hat{x}_{l} \right) \left(\delta_{km} \hat{p}_{k} \hat{p}_{m} \right) + i\hbar \left(\delta_{jk} \hat{x}_{j} \hat{p}_{k} \right) - (\hat{r} \cdot \hat{p})^{2} \end{split}$$

From here it's easy to see how the sums reduce all expressions.

$$\hat{L}^2 = \hat{r}^2 \hat{p}^2 - (\hat{r} \cdot \hat{p})^2 + i\hbar \left(\hat{r} \cdot \hat{p}\right)$$

9.8

First we note that $\hat{L}_i = \hat{x}_j \hat{p}_k - \hat{x}_k \hat{p}_j$ and $\hat{L}_j = \hat{x}_k \hat{p}_i - \hat{x}_i \hat{p}_k$. Thus we have

$$\begin{split} [\hat{L}_i, \hat{L}_j] &= [\hat{x}_j \hat{p}_k - \hat{x}_k \hat{p}_j, \hat{x}_k \hat{p}_i - \hat{x}_i \hat{p}_k] \\ &= [\hat{x}_j \hat{p}_k, \hat{x}_k \hat{p}_i] - [\hat{x}_j \hat{p}_k, \hat{x}_i \hat{p}_k] - [\hat{x}_k \hat{p}_j, \hat{x}_k \hat{p}_i] + [\hat{x}_k \hat{p}_j, \hat{x}_i \hat{p}_k] \\ &= A - B - C + D \end{split}$$

9.9

a) What is the wavelength of a photon emitted in a vibrational transition?

The energy of each photon is equal to the spacing of each energy, or the transition energy:

$$E = \hbar\omega = \frac{hc}{\lambda}$$

Therefore the photon wavelength is given by:

$$\lambda = \frac{hc}{E} = \frac{1240 \frac{\text{eV}}{\text{nm}}}{.37 \,\text{eV}} = 3351 \,\text{nm}$$

b) What is the effective spring constant k for this molecule?

Recall from classical mechanics that the angular frequency of this vibration can be written:

$$w = \sqrt{\frac{k}{m}} = \sqrt{\frac{k}{\mu}}$$

Thus, combining this with Equation 9.152 (a) we can find the spring constant to be:

$$k = w^{2}\mu = \left(\frac{2\pi c}{\lambda}\right)^{2}\mu$$
$$= \left(\frac{2\pi 3 \times 10^{8} \frac{\text{m}}{\text{s}}}{3351 \times 10^{-9} \text{m}}\right)^{2} 1.62 \times 10^{-27} \text{kg} = 513 \frac{\text{kg}}{\text{s}^{2}} = 513 \frac{\text{N}}{\text{m}}$$

c) What resolution is required for a spectrometer to resolve the presence of H 35 Cl and H 37 Cl molecules in the vibrational spectrum?

Following the derivation (Townsend 9.101 - 9.103) the generalized energy spacing is:

$$E = \hbar \left(\frac{1}{\mu} \left(\frac{d^2 V}{dr^r} \right)_{r=r_0} \right)^{\frac{1}{2}} \sim \left(\frac{m_e}{M_N} \right)^{\frac{1}{2}} \left(\frac{m_e e^4}{(4\pi\epsilon_0 \hbar)^2} \right)$$

where $\left(\frac{m_e e^4}{\hbar^2}\right)$ is the approximate energy scale of an electron. For each molecule, the transition energy is:

$$\begin{split} E_{\,\mathrm{H}^{35}\mathrm{Cl}} &\sim \left(\frac{m_e}{M_N}\right)^{\frac{1}{2}} \left(\frac{m_e e^4}{(4\pi\epsilon_0\hbar)^2}\right) \\ &= \left(\frac{(9.11\times10^{-31}\,\mathrm{kg})}{\frac{(7.07\times10^{-4}\,\frac{\mathrm{kg}}{\mathrm{mol}})}{(6.02\times10^{23}\,\frac{\mathrm{atoms}}{\mathrm{mol}})}}\right)^{\frac{1}{2}} \\ &\times \left(\frac{(9.11\times10^{-31}\,\mathrm{kg})(1.602\times10^{-19}\,\mathrm{C})^4}{(4\pi\,8.85\times10^{-12}\,\frac{\mathrm{s}^2\mathrm{C}^2}{\mathrm{kgm}^3}\,1.05\times10^{-34}\,\frac{\mathrm{kgm}^2}{\mathrm{s}})^2}\right) \\ &= 1.22\times10^{-19}\,\frac{\mathrm{kg}\,\mathrm{m}^2}{\mathrm{s}^2} \\ &= .764\,\mathrm{eV} \end{split}$$

$$\begin{split} E_{\,\mathrm{H}^{37}\mathrm{Cl}} &\simeq \left(\frac{(9.11 \times 10^{-31}\,\mathrm{kg})}{\frac{(7.27 \times 10^{-4}\,\frac{\mathrm{kg}}{\mathrm{mol}})}{(6.02 \times 10^{23}\,\frac{\mathrm{atoms}}{\mathrm{mol}})}} \right)^{\frac{1}{2}} \\ &\qquad \times \left(\frac{(9.11 \times 10^{-31}\,\mathrm{kg})(1.602 \times 10^{-19}\,\mathrm{C})^4}{(4\pi\,\,8.85 \times 10^{-12}\,\frac{\mathrm{s}^2\mathrm{C}^2}{\mathrm{kgm}^3}\,\,1.05 \times 10^{-34}\,\frac{\mathrm{kgm}^2}{\mathrm{s}})^2} \right) \\ &= 1.21 \times 10^{-19}\,\frac{\mathrm{kg}\,\mathrm{m}^2}{\mathrm{s}^2} \\ &= .754\,\mathrm{eV} \end{split}$$

And now if we follow the same procedure as in (a), we can find the respective wavelengths:

$$\begin{split} \lambda_{\,\mathrm{H^{35}Cl}} &= \frac{hc}{E} = \frac{1240 \frac{\mathrm{eV}}{\mathrm{nm}}}{.764 \, \mathrm{eV}} = 1621 \, \mathrm{nm} \\ \lambda_{\,\mathrm{H^{37}Cl}} &= \frac{hc}{E} = \frac{1240 \frac{\mathrm{eV}}{\mathrm{nm}}}{.754 \, \mathrm{eV}} = 1644 \, \mathrm{nm} \end{split}$$

And the difference between these wavelengths is the minimum size required to resolve transitions from both molecular isotopes.

$$\Delta \lambda = 23 \, \text{nm}$$

The resolution is then

$$\frac{\lambda}{\Delta\lambda} = \frac{(3351\,\mathrm{nm})}{(23\,\mathrm{nm})} = 145$$

a) Show that the population of rotational energy levels first increases and then decreases with increasing l.

The degeneracy for each level increases as the energy increases. The energy of each level depends on the quantum number l as:

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

where I is the moment of inertia of the molecule defined in terms of the reduced mass (μ) and position of minimum potential (r_0) as $I = \mu r_0^2$. We can expand ?? as a power series about l such that

$$\frac{n_l}{n_0} \sim (2l+1) \left(1 - l - \frac{l^2}{2} - \frac{5l^3}{6} - O(l^4) \right)$$
$$= 1 + l - \frac{3l^2}{2} - \frac{l^3}{6} - O(l^4)$$

Therefore at first order the ratio of states increases linearly with l, but quickly higher order terms are much larger and negative, so the ratio will rapidly decrease as l increases (see Figure 1).

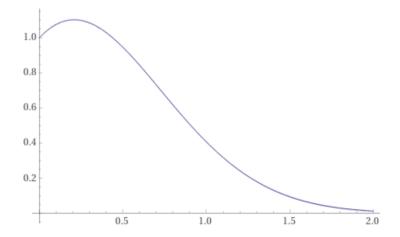


Figure 1: Sketch of the ratio of molecules with energy E_l to energy E_0 as a function of l.

b) Which energy level will be occupied by the largest number of molecules for HCl at room temperature? Compare your result with the intensities of the absorption spectrum in Fig. 9.9. What do you deduce about the temperature of the gas?

The maxima of Equation ?? will give the energy level with the most number of molecules:

$$\frac{d}{dl}\frac{n_l}{n_0} = \left(2 - \frac{\hbar^2 (1+2l)^2}{2Ik_b T}\right) \exp\left\{\left(\frac{E_0 - \frac{l(l+1)\hbar^2}{2I}}{k_b T}\right)\right\} = 0$$

Which has real solutions

$$l = -\frac{1}{2} \pm \frac{\sqrt{Ik_bT}}{\hbar} =$$

$$-\frac{1}{2} \pm \frac{\sqrt{(2.64 \times 10^{-47} \text{ kg m}^2)(1.38 \times 10^{-23} \frac{\text{m}^2\text{kg}}{\text{s}^2\text{K}})(293 \text{ K})}}{1.054 \times 10^{-34} \frac{\text{m}^2\text{kg}}{\text{s}}}$$

$$\simeq 3 \text{ and } -4$$

We only care about the positive solution since the quantum number l must be greater than or equal to zero. As seen in Figure 2, the spectra is centered on the zeroth transition with transition levels of the same quantum number reflections of one another about this center. Therefore it is clear that Figure 9.9 in the text has maximum transmission for the l=3 states. The HCl must then have a temperature of 293 K, which which we have calculated to produce maxma at l=3 transitions.

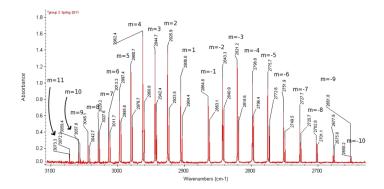


Figure 2: Total HCl spectra in the mid-infrared with both vibrational and rotational components

9.12

The first four spherical harmonics (l = 0, 1) can be written in Cartesian coordinates as

$$Y_{0,0}(\theta,\phi) = \sqrt{\frac{1}{4\pi}}$$

$$Y_{1,\pm 1}(\theta,\phi) = \mp \sqrt{\frac{3}{8\pi}} e^{\pm i\phi} \sin \theta = \mp \sqrt{\frac{3}{8\pi}} \frac{(x \pm iy)}{r}$$

$$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}} \cos \theta = \sqrt{\frac{3}{4\pi}} \frac{z}{r}$$

with linear combinations

$$\frac{(Y_{1,-1} - Y_{1,1})}{\sqrt{2}} = \sqrt{\frac{3}{4\pi}} \frac{x}{r} \qquad \frac{i(Y_{1,1} + Y_{1,-1})}{\sqrt{2}} = \sqrt{\frac{3}{4\pi}} \frac{y}{r}$$

If we sum together the $Y_{1,0}$ harmonic and linear combinations in the correct ratios we can produce the wave function

$$\begin{split} \Psi(\mathbf{r}) &= (x+y+z)f(r) = \sqrt{\frac{4\pi}{3}} \left(\sqrt{\frac{3}{4\pi}} \frac{z}{r} + \sqrt{\frac{3}{4\pi}} \frac{y}{r} + \sqrt{\frac{3}{4\pi}} \frac{z}{r} \right) r f(r) \\ &= \sqrt{\frac{4\pi}{3}} \left(\frac{(Y_{1,-1} - Y_{1,1})}{\sqrt{2}} + \frac{i(Y_{1,1} + Y_{1,-1})}{\sqrt{2}} + Y_{1,0}(\theta,\phi) \right) r f(r) \\ &= \sqrt{\frac{4\pi}{6}} \left(Y_{1,-1}(1+i) + Y_{1,1}(i-1) + \sqrt{2} Y_{1,0}(\theta,\phi) \right) r f(r) \end{split}$$

Now to normalize this wavefunction we must force it to follow the normalization condition

$$\int_{-\infty}^{\infty} \infty |\Psi(\mathbf{r})|^2 dr = 1$$

For which we simply choose any f(r) which satisfies that condition

 \mathbf{L}^2 : Because $\Psi(r)$ is made up of only $Y_{1,m}$ spherical harmonics, a measurement of \mathbf{L}^2 could only yield $l(l+1)\hbar^2=2\hbar^2$ with a 100% probability.

 \hat{L}_z : $\Psi(r)$ is made up of $Y_{1,1}$, $Y_{1,0}$, $Y_{1,-1}$ spherical harmonics, which means that the possible measurements of \hat{L}_z are $m\hbar = \hbar$, 0, and $-\hbar$, each with a 1/3 probability

$$\begin{split} \left\langle \Psi(\mathbf{r}) | \hat{L}_z | \Psi(\mathbf{r}) \right\rangle &= \left\langle \Psi(\mathbf{r}) \left| \hat{L}_z \right| \left(\sqrt{\frac{1}{6}} Y_{1,-1} (1+i) \right. \\ &+ \sqrt{\frac{1}{6}} Y_{1,1} (i-1) + \sqrt{\frac{1}{3}} Y_{1,0} (\theta,\phi) \right) \right\rangle \\ &= \left(\frac{1}{3} \right) \hbar - \left(\frac{1}{3} \right) \hbar + \left(\frac{1}{3} \right) 0 \hbar \end{split}$$

We can begin by finding the appropriate expectation values in terms of the angular momentum raising and lowering operators

$$\Delta L_x = \langle l, m | (\hat{L}_x - \langle L_x | L_x \rangle) | l, m \rangle$$

$$= \langle l, m | \left(\frac{1}{2} (\hat{L}_+ + \hat{L}_-) - \langle l, m | \frac{1}{2} (\hat{L}_+ + \hat{L}_-) | l, m \rangle \right) | l, m \rangle$$

$$\Delta L_y = \langle l, m | (\hat{L}_y - \langle L_y | L_y \rangle) | l, m \rangle$$

$$= \langle l, m | \left(\frac{1}{2i} (\hat{L}_+ - \hat{L}_-) - \langle l, m | \frac{1}{2i} (\hat{L}_+ - \hat{L}_-) | l, m \rangle \right) | l, m \rangle$$

where,

$$\hat{L}_{+} = \hbar \sqrt{l(l+1) - m(m+1)} |l, m+1\rangle$$

$$\hat{L}_{-} = \hbar \sqrt{l(l+1) - m(m-1)} |l, m-1\rangle$$

The state $|l,m\rangle$ must be a superposition for ΔL_z and ΔL_y to be non-zero and to satisfy the uncertainty relation.

Or we can recall from Chapter 3 Section 5 that $[\hat{A}, \hat{B}] = i\hat{C}$ implies $\Delta A \Delta B \geq \frac{1}{2} |\langle C|C \rangle|$. starting with the Schwartz inequality

$$\langle L_x | L_x | L_x | L_x \rangle \langle L_y | L_y | L_y | L_y \rangle \ge |\langle L_x | L_y | L_x | L_y \rangle|^2$$

where,

$$\langle L_x|L_x|L_x|L_x\rangle = (\Delta L_x)^2 \qquad \langle L_y|L_y|L_y|L_y\rangle = (\Delta L_y)^2 \qquad \langle L_x|L_y|L_x|L_y\rangle = \left\langle l,m|\hat{O}|l,m\right|l,m|\hat{O}|l,m\rangle$$

And because any operator can be written as $\hat{O} = \frac{\hat{F}}{2} + \frac{i\hat{G}}{2}$, assuming \hat{F} and \hat{G} have real expectation values, we find

$$|\langle L_x|L_y|L_x|L_y\rangle|^2 = \left|\frac{1}{2}\left\langle l,m|\hat{F}|l,m\Big|l,m|\hat{F}|l,m\right\rangle + \frac{i}{2}\left\langle l,m|\hat{L}_z|l,m\Big|l,m|\hat{L}_z|l,m\right\rangle\right|^2$$

$$= \frac{\left|\left\langle l,m|\hat{F}|l,m\Big|l,m|\hat{F}|l,m\right\rangle\right|^2}{4} + \frac{\left|\left\langle l,m|\hat{L}_z|l,m\Big|l,m|\hat{L}_z|l,m\right\rangle\right|^2}{4} \ge \frac{\left|\left\langle L_z|L_z\right\rangle\right|^2}{2}$$

Combining these definitions with the Schwartz inequality

$$(\Delta L_x)^2 (\Delta L_y)^2 \ge \frac{\hbar}{4} |\langle L_z | L_z \rangle|^2$$
$$\Delta L_x \Delta L_y \ge \frac{\hbar}{4} |\langle L_z | L_z \rangle|$$

9.15

Using the general solution to the spherical harmonics

$$Y_{l,m}(\theta,\phi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} e^{im\phi} \frac{1}{\sin^m \theta} \frac{d^{l-m}}{d(\cos \theta)^{(l-m)}} \sin^{2l} \theta$$

Then applying the parity operator, which is achieved by inverting the wavefunction coordinates, we find

$$\hat{P}Y_{l,m}(\theta,\phi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} e^{im(\phi+\pi)} \frac{1}{\sin^m(\pi-\theta)} \frac{d^{l-m}}{d(\cos(\pi-\theta))^{(l-m)}} \sin^{2l}(\pi-\theta)$$

$$= \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} (-1)^m e^{im\phi} \frac{1}{\sin^m \theta} \frac{d^{l-m}}{d(-\cos \theta)^{(l-m)}} \sin^{2l} \theta$$

$$= \frac{(-1)^{2l}}{2^l l!} \sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} e^{im\phi} \frac{1}{\sin^m \theta} \frac{d^{l-m}}{d(\cos \theta)^{(l-m)}} \sin^{2l} \theta = (-1)^l Y_{l,m}(\theta,\phi)$$

where,

$$e^{i\pi} = -1$$
$$\cos(\pi - \theta) = -\cos\theta$$
$$\sin(\pi - \theta) = \sin\theta$$

9.16

a) We already know that

$$Y_{1,1}(\theta,\phi) = -\sqrt{\frac{3}{8\pi}} e^{i\phi} \sin(\theta) = \langle \theta, \phi | 1, 1 | \theta, \phi | 1, 1 \rangle, \qquad (9.152 \text{ (a)})$$

$$\hat{L}_{\pm} \to \frac{\hbar}{i} e^{\pm i\phi} \left(\pm i \frac{\partial}{\partial \theta} - \cot(\theta) \frac{\partial}{\partial \phi} \right). \qquad (9.142)$$

Applying the lowering operator as instructed,

$$\begin{split} \left\langle \theta, \phi | \hat{L}_{-} | 1, 1 \middle| \theta, \phi | \hat{L}_{-} | 1, 1 \right\rangle &= -\frac{\hbar}{i} \sqrt{\frac{3}{8\pi}} e^{-i\phi} \left(-i\frac{\partial}{\partial \theta} - \cot(\theta) \frac{\partial}{\partial \phi} \right) e^{i\phi} \sin(\theta) \\ &= -\frac{\hbar}{i} \sqrt{\frac{3}{8\pi}} e^{-i\phi} (-2i\cos(\theta)) e^{i\phi} \\ &= \hbar \sqrt{\frac{3}{2\pi}} \cos(\theta). \end{split}$$

According to Eq. 9.147,

$$\hat{L}_{-}|1,1\rangle = \sqrt{2}\hbar |1,0\rangle.$$

Together with the above calculation, this implies that

$$\sqrt{2}\hbar Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{2\pi}}\hbar\cos(\theta)$$
$$\Rightarrow Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos(\theta)$$

b) In position space, the Laplacian \hat{L}^2 takes the form

$$\hat{L}^2 \to -\hbar^2 \left[\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right]$$
(9.129)

so applying this to the state $|1,1\rangle$ we get

$$\begin{split} \langle \theta, \phi | \, \hat{L^2} \, | 1, 1 \rangle &= \hbar^2 \sqrt{\frac{3}{8\pi}} \left[\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \cos(\theta) e^{i\phi} \right) + \frac{1}{\sin^2(\theta)} (i^2 e^{i\phi} \sin(\theta)) \right] \\ &= \hbar^2 \sqrt{\frac{3}{8\pi}} \left[\left(\frac{-\sin^2(\theta) + \cos^2(\theta)}{\sin(\theta)} \right) e^{i\phi} - \frac{e^{i\phi}}{\sin(\theta)} \right] \\ &= \hbar^2 \sqrt{\frac{3}{8\pi}} e^{i\phi} \left[\frac{-\sin^2(\theta) + \cos^2(\theta) - \sin^2(\theta) - \cos^2(\theta)}{\sin(\theta)} \right] \\ &= -2\hbar^2 \sqrt{\frac{3}{8\pi}} e^{i\phi} \sin(\theta) \\ &= 2\hbar^2 \langle \theta, \phi | 1, 1 | \theta, \phi | 1, 1 \rangle \end{split}$$

To begin this problem we will perform a substitution of $u = \cos \theta$ in the eigenvalue equation, where $du = -\sin \theta d\theta$. We can first expand the derivatives

$$\frac{\delta}{\delta\theta} = \frac{\delta}{\delta u} \frac{\delta u}{\delta\theta} = -\frac{\delta}{\delta u} \sqrt{1 - u^2}$$

Which we can then substitute in the equation, with the second order term ignored, in order to produce Legendre's equation

$$-\left[\frac{-1}{\sqrt{1-u^2}}\sqrt{1-u^2}\frac{\delta}{\delta u}\left(-\sqrt{1-u^2}\sqrt{1-u^2}\frac{\delta}{\delta u}\right)\right]\Theta_{\lambda,m}(\theta) = \lambda\Theta_{\lambda,m}(\theta)$$
$$-\left[\frac{\delta}{\delta u}\left((1-u^2)\frac{\delta}{\delta u}\right)\right]\Theta_{\lambda,m}(\theta) = \lambda\Theta_{\lambda,m}(\theta)$$
$$(1-u^2)\frac{d\Theta_{\lambda,0}}{du^2} - 2u\frac{d\Theta_{\lambda,0}}{du} + \lambda\Theta_{\lambda,0} = 0$$

Now to do the power series. The first and second derivatives of the possible power series solution are

$$\frac{d\Theta_{\lambda,0}}{du} = \sum_{k=0}^{\infty} (k+1)a_{k+1}u^k \qquad \frac{d^2\Theta_{\lambda,0}}{du^2} = \sum_{k=0}^{\infty} (k+1)(k+2)a_{k+2}u^k$$

Which we can now plug into the Legendre equation

$$(1 - u^2) \sum_{k=0}^{\infty} (k+1)(k+2)a_{k+2}u^k - 2u \sum_{k=0}^{\infty} (k+1)a_{k+1}u^k + \lambda \sum_{k=0}^{\infty} a_k u^k = 0$$
$$\sum_{k=0}^{\infty} (k+1)(k+2)a_{k+2}u^k - \sum_{k=0}^{\infty} (k+1)(k+2)a_{k+2}u^{k+2}$$
$$-2\sum_{k=0}^{\infty} (k+1)a_{k+1}u^{k+1} + \lambda \sum_{k=0}^{\infty} a_k u^k = 0$$

$$2a_2u^0 + 6a_3u^1 + \sum_{k=2}^{\infty} (k+1)(k+2)a_{k+2}u^k - \sum_{k=2}^{\infty} (k-1)(k)a_ku^k$$
$$-2a_1u^1 - 2\sum_{k=2}^{\infty} (k)a_ku^k + \lambda a_0u^0 + \lambda a_1u^1 + \lambda \sum_{k=2}^{\infty} a_ku^k = 0$$

$$u^{0}(2a_{2} + \lambda a_{0}) + u^{1}(6a_{3} - 2a_{1} + \lambda a_{1}) + \sum_{k=2}^{\infty} [(k+1)(k+2)a_{k+2} - (k-1)ka_{k} - 2ka_{k} + \lambda a_{k}]u^{k} = 0$$

We now have a representation of the coefficients of each u term, which we know must equal zero. Thus we can set up a system of equations

$$2a_2 + \lambda a_0 = 0$$

$$6a_3 - 2a_1 + \lambda a_1 = 0$$

$$\sum_{k=2}^{\infty} [(k+1)(k+2)a_{k+2} - (k+1)ka_k + \lambda a_k] = 0$$

We then know that your choice of a_0 and a_1 is arbitrary, but we can create a chart of the rest of the solutions

$$\begin{array}{|c|c|c|c|} \hline k & \text{equation} \\ \hline 2 & 12a_4 - 6a_2 + \lambda a_2 = 0 \\ 3 & 20a_5 - 12a_3 + \lambda a_3 = 0 \\ 4 & 30a_6 - 20a_4 + \lambda a_4 = 0 \\ \vdots & \vdots \\ \hline \end{array}$$

The series of l(l+1) goes 1, 2, 6, 12, 20. And unless λ is one of these series, it is not possible for all the coefficients to be zero, and therefore the series will diverge.

The solutions to this eigenvalue problem are in fact the Legendre polynomials

$$P_0 = 1$$

$$P_1 = \cos \theta$$

$$P_2 = \frac{1}{2}(\cos^2 \theta - 1)$$

which have exactly the same form as the spherical harmonics, times their respective normalizations which are a function of the degeneracy of their energy level

$$Y_{0,0}(\theta,\phi) = \sqrt{\frac{1}{4\pi}}$$

$$Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_{2,0}(\theta,\phi) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$\begin{split} \left\langle \theta, \phi | \hat{L}_{-} | l, l \middle| \theta, \phi | \hat{L}_{-} | l, l \right\rangle &= \hbar \sqrt{l(l+1) - l(l-1)} Y_{l,l-1} \\ &= \hbar \sqrt{2l} Y_{l,l-1} \\ &= \frac{\hbar}{i} \frac{(-1)^{l}}{2^{l} l!} \sqrt{\frac{(2l+1)!}{4\pi}} e^{-i\phi} \left(-i \frac{\partial}{\partial \theta} - \cot(\theta) \frac{\partial}{\partial \phi} \right) \left(e^{il\phi} \sin^{l}(\theta) \right) \\ &= \frac{\hbar}{i} \frac{(-1)^{l}}{2^{l} l!} \sqrt{\frac{(2l+1)!}{4\pi}} e^{-i\phi} \left(-il \sin^{l-1}(\theta) \cos(\theta) e^{il\phi} - \frac{\cos(\theta)}{\sin(\theta)} (ile^{il\phi}) \sin^{l}(\theta) \right) \\ &= \frac{\hbar}{i} \frac{(-1)^{l}}{2^{l} l!} \sqrt{\frac{(2l+1)!}{4\pi}} e^{i\phi(l-i)} \left(-2il \sin^{l-1}(\theta) \cos(\theta) \right) \\ &= -2l\hbar \frac{(-1)^{l}}{2^{l} l!} \sqrt{\frac{(2l+1)!}{4\pi}} e^{i\phi(l-i)} \left(\sin^{l-1}(\theta) \cos(\theta) \right) \\ &\Rightarrow Y_{l,l-1} = -\sqrt{2l} \frac{(-1)^{l}}{2^{l} l!} \sqrt{\frac{(2l+1)!}{4\pi}} e^{i\phi(l-i)} \left(\sin^{l-1}(\theta) \cos(\theta) \right) \end{split}$$

We now want to compare this result to the general expression;

$$\begin{split} Y_{l,m} &= \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} e^{im\phi} \frac{1}{\sin^m(\theta)} \left(\frac{d^{l-m}}{d(\cos(\theta))^{l-m}} \sin^{2l}(\theta) \right) \\ \Rightarrow Y_{l,l-1} &= \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)!}{(2l)4\pi}} e^{i\phi(l-1)} \frac{1}{\sin^{l-1}(\theta)} \left(\frac{\frac{d}{d\theta} \sin^{2l}(\theta)}{\frac{d}{d\theta} \cos(\theta)} \right) \\ &= \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)!}{(2l)4\pi}} e^{i\phi(l-1)} \frac{1}{\sin^{l-1}(\theta)} \left(\frac{2l \sin^{2l-1}(\theta) \cos(\theta)}{-\sin(\theta)} \right) \\ &= -\sqrt{2l} \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}} e^{i\phi(l-1)} (\sin^{l-1}(\theta) \cos(\theta)) \end{split}$$

The two results agree, as expected.

9.19

9.20

a) What is $\langle \theta, \phi | \Psi(t) \rangle$?

Recall that the time evolution of a wavefunction is given by:

$$|\Psi(t)\rangle = e^{i\hat{H}t/\hbar} |\Psi(0)\rangle$$

We must then write this in terms of the spherical harmonics so we know how to act the Hamiltonian upon the state. First, note the Euler identity defines that

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

We can use this to express the wavefunction in terms of the spherical harmonics

$$\begin{split} \langle \theta, \phi | \Psi(0) \rangle &= \sqrt{\frac{3}{4\pi}} \sin \theta \sin \phi = \sqrt{\frac{3}{4\pi}} \sin \theta \frac{e^{i\phi}}{2i} - \sqrt{\frac{3}{4\pi}} \sin \theta \frac{e^{-i\phi}}{2i} \\ &= \sqrt{\frac{3}{8\pi}} e^{-i\phi} \frac{i \sin \theta}{\sqrt{2}} - \sqrt{\frac{3}{8\pi}} e^{i\phi} \frac{i \sin \theta}{\sqrt{2}} = \frac{i(Y_{1,1} + Y_{1,-1})}{\sqrt{2}} \end{split}$$

This is now in a form we can act on with the Hamiltonian to produce the state's eigenenergies, and thus the time-evolved state

$$\begin{split} |\Psi(t)\rangle &= e^{i\hat{\mathbf{L}}^2 t/2I\hbar} \, |\Psi(0)\rangle = e^{il(l+1)\hbar t/2I} \bigg| \frac{i(Y_{1,1} + Y_{1,-1})}{\sqrt{2}} \bigg\rangle \\ &= \frac{i}{\sqrt{2}} e^{i\hbar t/I} \, |Y_{1,1}\rangle + \frac{i}{\sqrt{2}} e^{i\hbar t/I} \, |Y_{1,-1}\rangle \end{split}$$

The initial state is an energy eigenstate, so the state just picks up an overall phase as time progress. For t = 0, we recover the state vector at t = 0.

b) What values of L_z will be obtained if a measurement is carried out and with what probability will these values occur?

Recall that \hat{L}_z acting on some state is given by

$$\hat{L}_z |\Psi_{l,m}\rangle = m\hbar |\Psi_{l,m}\rangle$$

Therefore for our system, a measurement will produce values of $\pm \hbar$ with sign corresponding to the m value. The probabilities are given by

$$P = |c_{\Psi}|^2$$

where c_{Ψ} is the coefficient of each state. Therefore, both measurements have a $^{1}/_{2}$ probability of occurring.

c) What is $\langle L_x \rangle$ for this state?

Using bra-ket notation I will express the operator in terms of the raising and lowering operators.

$$\begin{split} \hat{L}_{+} \, | l, m \rangle &= (\hat{L}_{x} + i \hat{L}_{y}) \, | l, m \rangle = \hbar \sqrt{l(l+1) - m(m+1)} \, | l, m+1 \rangle \\ \hat{L}_{-} \, | l, m \rangle &= (\hat{L}_{x} - i \hat{L}_{y}) \, | l, m \rangle = \hbar \sqrt{l(l+1) - m(m-1)} \, | l, m-1 \rangle \\ \hat{L}_{x} \, | l, m \rangle &= \frac{1}{2} (\hat{L}_{-} + \hat{L}_{+}) \, | l, m \rangle \end{split}$$

Therefore the expectation value is

$$\begin{split} \langle \Psi | L_x | \Psi \rangle &= \left\langle \Psi \bigg| \frac{1}{2} (\hat{L}_- + \hat{L}_+) \bigg| \Psi \right\rangle \\ &= \left\langle \Psi \bigg| \frac{\hbar}{2} \left(\sqrt{l(l+1) - m(m-1)} + \sqrt{l(l+1) - m(m+1)} \right) \\ &\left(\frac{i}{\sqrt{2}} e^{i\hbar t/I} \left| Y_{1,1} \right\rangle + \frac{i}{\sqrt{2}} e^{i\hbar t/I} \left| Y_{1,-1} \right\rangle \right) = \sqrt{2}\hbar - \sqrt{2}\hbar = 0 \end{split}$$

d) If a measurement of L_x is carried out, what results(s) will be obtained? With what probability?

We can use the expressions for states $|1, m\rangle_x$

$$\begin{split} |1,1\rangle_x &= \frac{1}{2} \, |Y_{1,1}\rangle + \frac{\sqrt{2}}{2} \, |Y_{1,0}\rangle + \frac{1}{2} \, |Y_{1,-1}\rangle \\ |1,0\rangle_x &= \frac{\sqrt{2}}{2} \, |Y_{1,1}\rangle - \frac{\sqrt{2}}{2} \, |Y_{1,-1}\rangle \\ |1,-1\rangle_x &= \frac{1}{2} \, |Y_{1,1}\rangle - \frac{\sqrt{2}}{2} \, |Y_{1,0}\rangle + \frac{1}{2} \, |Y_{1,-1}\rangle \end{split}$$

to rewrite the state in terms making the measurement results more easily calculable.

$$\frac{i}{\sqrt{2}}\left|Y_{1,1}\right\rangle+\frac{i}{\sqrt{2}}\left|Y_{1,-1}\right\rangle=\frac{i}{\sqrt{2}}\left|1,1\right\rangle_x+\frac{i}{\sqrt{2}}\left|1,-1\right\rangle_x$$

Recall that \hat{L}_x acting on some state is given by

$$\hat{L}_x |\Psi_{l,m}\rangle = m\hbar |\Psi_{l,m}\rangle$$

and the probabilities are given by

$$P = |c_{\Psi}|^2$$

where c_{Ψ} is the coefficient of each state. Therefore such a measurement would produce values $\pm \hbar$ with probability $^{1}/_{2}$ for both.

We need to first rewrite $\langle \theta, \phi | \psi(0) | \theta, \phi | \psi(0) \rangle$ in terms of the orthogonal states Y_{lm} .

$$\langle \theta, \phi | \psi(0) | \theta, \phi | \psi(0) \rangle = \sqrt{\frac{3}{4\pi}} \sin(\theta) \sin(\phi)$$

$$= \sqrt{\frac{3}{4\pi}} \sin(\theta) \frac{e^{i\phi} - e^{i\phi}}{2i}$$

$$= \frac{\sqrt{2}}{2i} \left[\sqrt{\frac{3}{8\pi}} e^{i\phi} \sin(\theta) - \sqrt{\frac{3}{8\pi}} e^{-i\phi} \sin(\theta) \right]$$

$$= i \frac{\sqrt{2}}{2} (Y_{1,1} + Y_{1,-1})$$

$$= i \frac{\sqrt{2}}{2} (|1,1\rangle + |1,-1\rangle)$$

We need to figure out how the Hamiltonian behaves on both basis states. Remember that $\hat{L}^2 | l, m \rangle = l(l+1)\hbar^2 | l, m \rangle$ and $\hat{L}_z | l, m \rangle = m\hbar | l, m \rangle$.

$$\begin{split} \hat{H} \left| 1, 1 \right\rangle &= \left(\frac{\hbar}{I} + \omega_0 \right) \left| 1, 1 \right\rangle \\ \hat{H} \left| 1, -1 \right\rangle &= \left(\frac{\hbar}{I} - \omega_0 \right) \left| 1, -1 \right\rangle \end{split}$$

$$\begin{split} \langle \theta, \phi | \psi(t) | \theta, \phi | \psi(t) \rangle &= \langle \theta, \phi | \hat{H} | \psi(0) \rangle \\ &= i \frac{\sqrt{2}}{2} \left(e^{-i()t} | 1, 1 \rangle + e^{-i()t} | 1, -1 \rangle \right) \\ &= i \frac{\sqrt{2}}{2} e^{-i\hbar t/I} \left(e^{-i\omega_0 t} | 1, 1 \rangle + e^{i\omega_0 t} | 1, -1 \rangle \right) \quad * \\ &= i \frac{\sqrt{2}}{2} e^{-i\hbar t/I} \left[-\sqrt{\frac{3}{8\pi}} e^{i(\phi - \omega_0 t)} \sin\left(\theta\right) + \sqrt{\frac{3}{8\pi}} e^{-i(\phi - \omega_0 t)} \sin\left(\theta\right) \right] \\ &= \sqrt{\frac{3}{4\pi}} e^{-i\hbar t/I} \sin\left(\theta\right) \left(\frac{e^{i(\phi - \omega_0 t)} - e^{-i(\phi - \omega_0 t)}}{2i} \right) \end{split}$$

This last term just reduces to a cosine function, so we are left with

$$\langle \theta, \phi | \psi(t) | \theta, \phi | \psi(t) \rangle = \sqrt{\frac{3}{4\pi}} e^{-i\hbar t/I} \sin(\theta) \cos(\phi - \omega_0 t)$$

To find the expectation value of the x-component of angular momentum, \hat{L}_x , we will refer to the equation marked with * from above. Remember also that \hat{L}_x can be written in terms of the raising and lowering operators and takes the

form $\hat{L}_x = \hat{L}_+ + \hat{L}_-$. We have that $\hat{L}_+ |1,1\rangle = \hat{L}_- |1,-1\rangle = 0$ and $\hat{L}_- |1,1\rangle = \hat{L}_+ |1,-1\rangle = \sqrt{2}\hbar \, |1,0\rangle$.

$$\begin{split} \left(\hat{L}_{+} + \hat{L}_{-}\right) |\psi(t)\rangle &= i\frac{\sqrt{2}}{2} e^{-i\hbar t/I} \left(\sqrt{2}\hbar e^{-i\omega_{0}t} \left|1,0\right\rangle + \sqrt{2}\hbar e^{i\omega_{0}t} \left|1,0\right\rangle\right) \\ &= i\hbar e^{-i\hbar t/I} \left(e^{-i\omega_{0}t} + e^{i\omega_{0}t}\right) |1,0\rangle \end{split}$$

The expectation value, $\langle \hat{L}_x \rangle$, is the inner product of $\langle \psi(t) |$ with the last expression. However, we see that this simply evaluates to 0 because $\langle 1, 1 | 1, 0 | 1, 1 | 1, 0 \rangle = \langle 1, -1 | 1, 0 | 1, -1 | 1, 0 \rangle = 0$.

$$\langle \hat{L}_x \rangle = 0$$

9.22

We first write the Hamiltonian in terms of \hat{L}_x , \hat{L}_y , and \hat{L}_z . However, remember that $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \rightarrow \hat{L}_x^2 + \hat{L}_y^2 = \hat{L}^2 - \hat{L}_z^2$, meaning we can transform the Hamiltonian into a form in which the eigenstates are known.

$$\hat{H} = \frac{\hat{L}_x^2}{2I_3} + \frac{\hat{L}_y^2}{2I_1} + \frac{\hat{L}_z^2}{2I_1} = \frac{\hat{L}_z^2}{2I_3} + \frac{\hat{L}_x^2 + \hat{L}_y^2}{2I_1} = \frac{\hat{L}_z^2}{2I_3} + \frac{\hat{L}^2 - \hat{L}_z^2}{2I_1}$$

$$\hat{H}=\alpha_1\hat{L}_z^2+\alpha_2\hat{L}^2, \quad \text{where} \quad \alpha_1=rac{I_1-I_3}{2I_1I_3} \quad \text{and} \quad \alpha_2=rac{1}{2I_1}$$

In order to show that \hat{H} and \hat{L}_z commute, we use a commutator identity and the commutation relations of \hat{L}^2 and \hat{L}_z (i.e. \hat{L}_z commutes with itself and \hat{L}^2).

$$[\hat{H}, \hat{L}_z] = [\alpha_1 \hat{L}_z^2 + \alpha_2 \hat{L}^2, \hat{L}_z]$$

$$= \alpha_1 [\hat{L}_z^2, \hat{L}_z] + \alpha_2 [\hat{L}^2, \hat{L}_z]$$

$$= 0$$

Because the Hamiltonian is composed of \hat{L}^2 and \hat{L}_z^2 , it shares eigenstates with these two operators. Thus, we only need to know how \hat{L}^2 and \hat{L}_z^2 act on the state vector.

$$\begin{split} \hat{H} \left| l, m \right\rangle &= \alpha_1 \hat{L}_z^2 \left| l, m \right\rangle + \alpha_2 \hat{L}^2 \left| l, m \right\rangle \\ &= \alpha_1 m^2 \hbar^2 \left| l, m \right\rangle + \alpha_2 l (l+1) \left| l, m \right\rangle \\ &= (\alpha_1 m^2 \hbar^2 + \alpha_2 l (l+1)) \left| l, m \right\rangle \end{split}$$

The eigenstates of the Hamiltonian are $|l,m\rangle$ (or $Y_{l,m}$, the Legendre polynomials/spherical harmonics) and it's eigenvalues are

$$E_{l,m} = \left(\frac{I_1 - I_3}{I_1 I_3} + \frac{l(l+1)}{I_1}\right) \frac{\hbar^2}{2}.$$

To find the time evolved solution, we simply need to determine how the Hamiltonian acts on the individual basis states.

$$\hat{H}\left|0,0\right>=0\quad\text{and}\quad\hat{H}\left|1,1\right>=\left(\frac{I_{1}-I_{3}}{I_{1}I_{3}}+\frac{2}{I_{1}}\right)\frac{\hbar^{2}}{2}\left|1,1\right>$$

Finally, we have

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}|0,0\rangle + \frac{e^{-\frac{\alpha\hbar}{2}t}}{\sqrt{2}}|1,1\rangle$$
, where $\alpha = \left(\frac{I_1 - I_3}{I_1I_3} + \frac{2}{I_1}\right)\frac{\hbar^2}{2}$

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The exact position along the z-axis is arbitrary and the potential is only a function of ρ , the distance from the central axis. Thus, we know that the Hamiltonian must commute with the z-component of linear momentum, \hat{p}_z . Additionally, since the potential is only dependent on the magnitude of distance from the central axis, $|\rho|$, the Hamiltonian must be invariant under rotations about this axis. Thus, the Hamiltonian should commute with the z-component of the angular momentum, \hat{L}_z .

Because the Hamiltonian, z-component of angular momentum, and z-component of linear momentum all commute, they must share simultaneous eigenstates, $|\psi\rangle=|E,m,p_z\rangle$.

$$\begin{split} \langle \phi|E,m,p_z|\phi|E,m,p_z\rangle &= \Phi(\phi) \\ \langle \rho|E,m,p_z|\rho|E,m,p_z\rangle &= R(\rho) \\ \langle z|E,m,p_z|z|E,m,p_z\rangle &= Z(z) \\ &\downarrow \\ \langle \rho,\phi,z|E,m,p_z|\rho,\phi,z|E,m,p_z\rangle &= R(\rho)\Phi(\phi)Z(z) \end{split}$$

Consider Z(z) first (see Townsend chapter 6 section 6):

$$Z(z) = \frac{1}{\sqrt{\sqrt{\pi}a}} e^{-z^2/2a^2}$$

The z-component of the wavefunction is simply a Gaussian wave-packet along it's central axis. Next, consider the angular part of the wavefunction, $\Phi(\phi)$. We can use the fact that $\hat{L}_z |\psi\rangle = m\hbar |\psi\rangle$ and $\hat{L}_z |\psi\rangle = \frac{\hbar}{i} \frac{\partial}{\partial \phi} |\psi\rangle$.

$$\langle \phi | \hat{L}_z | \psi \rangle \to \langle \phi | \frac{\hbar}{i} \frac{\partial}{\partial \phi} | \psi \rangle = \langle \phi | m\hbar | \psi \rangle$$
$$\frac{\hbar}{i} \frac{\partial}{\partial \phi} \langle \phi | \psi | \phi | \psi \rangle = m\hbar \langle \phi | \psi | \phi | \psi \rangle$$

Solving this simple differential equation yields the angular equation,

$$\Phi(\phi) = e^{im\phi}$$

It will be useful to go ahead of find the second derivative of $\Phi(\phi)$ for the next part of the question.

$$\frac{\partial^2 \Phi}{\partial \phi^2} = -m^2 \Phi(\phi)$$

Now we want to find the radial equation. For this we will consider $\langle \rho, \phi, z | \hat{H} | \psi \rangle = E \langle \rho, \phi, z | \psi | \rho, \phi, z | \psi \rangle$. We can rewrite rewrite this equation in the form that is presented on page 330, equation 9.130, which makes use of the Laplacian.

$$\begin{split} \langle \rho, \phi, z | \, \hat{H} \, | \psi \rangle &= E \, \langle \rho, \phi, z | \psi | \rho, \phi, z | \psi \rangle \\ \langle \rho, \phi, z | \, \frac{\hat{p}^2}{2\mu} + V(\hat{\rho}) \, | \psi \rangle &= ER(\rho) \Phi(\phi) Z(z) \\ \left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(\hat{\rho}) \right] R(\rho) \Phi(\phi) Z(z) &= ER(\rho) \Phi(\phi) Z(z) \end{split}$$

We can now simply plug in for the cylindrical Laplacian.

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2}\right)+V(\hat{\rho})\right]R(\rho)\Phi(\phi)Z(z)=ER(\rho)\Phi(\phi)Z(z)$$

At this point we can separate out the z-component of the equation and distribute the $R(\rho)\Phi(\phi)$.

$$-\frac{\hbar^2}{2\mu}\left(\Phi(\phi)\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)R(\rho)+R(\rho)\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\Phi(\phi)\right)+R(\rho)\Phi(\phi)V(\hat{\rho})=ER(\rho)\Phi(\phi)$$

Recall from above that $\partial^2 \Phi / \partial \phi^2 = -m^2 \Phi(\phi)$, meaning we can substitute this into our equation and factor/cancel out $\Phi(\phi)$. This leaves us with the final form of the radial equation,

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{m^2}{\rho^2}\right)+V(\hat{\rho})\right]R(\rho)=ER(\rho)$$