Chemn221a : Solution Set 7

David W.H. Swenson

November 16, 2007

Problem 1

(a) First we calculate the density operator for this ensemble. By definition, the density operator is

$$\hat{\rho} = \sum_i w_i |\alpha_i\rangle \langle\alpha_i| \tag{1}$$

where w_i is a weighting factor. In the specific case we are given for this problem, the states $|\alpha_i\rangle$ are either $|S_z;+\rangle$ or $|S_x;+\rangle$, with associated weights 75% and 25%, respectively. Plugging this in:

$$\hat{\rho} = \frac{3}{4} |S_z;+\rangle \langle S_z;+| + \frac{1}{4} |S_x;+\rangle \langle S_x;+| \tag{2}$$

Plugging that into the $|\pm\rangle$ basis, we obtain:

$$\hat{\rho} = \frac{1}{4}\left(3|+\rangle\langle+| + \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)\frac{1}{\sqrt{2}}(\langle+| + \langle-|)\right) \tag{3}$$

$$= \frac{1}{4}\left(3|+\rangle\langle+| + \frac{1}{2}(|+\rangle\langle+| + |+\rangle\langle-| + |-\rangle\langle+| + |-\rangle\langle-|)\right) \tag{4}$$

$$= \frac{7}{8}|+\rangle\langle+| + \frac{1}{8}|+\rangle\langle-| + \frac{1}{8}|-\rangle\langle+| + \frac{1}{8}|-\rangle\langle-| \tag{5}$$

From this, we can immediately write the matrix version in the $|\pm\rangle$ basis:

$$\hat{\rho} \doteq \begin{pmatrix} 7/8 & 1/8 \\ 1/8 & 1/8 \end{pmatrix} \tag{6}$$

Now for ensemble averages. We have equivalent two ways of doing this:

$$[\hat{A}] = \sum_i w_i \left\langle \alpha_i \middle| \hat{A} \middle| \alpha_i \right\rangle \tag{7}$$

$$[\hat{A}] = \mathrm{tr}\left(\hat{\rho}\hat{A}\right) \tag{8}$$

Using the first technique:

$$
\begin{aligned}
[S_x] &= \frac{3}{4}\langle S_z;+|S_x|S_z;+\rangle + \frac{1}{4}\langle S_x;+|S_x|S_x;+\rangle && (9)\\
&= \frac{3}{4}0 + \frac{1}{4}\frac{\hbar}{2} = \frac{\hbar}{8} && (10)\\
[S_y] &= \frac{3}{4}\langle S_z;+|S_y|S_z;+\rangle + \frac{1}{4}\langle S_x;+|S_y|S_x;+\rangle && (11)\\
&= \frac{3}{4}0 + \frac{1}{4}0 = 0 && (12)\\
[S_z] &= \frac{3}{4}\langle S_z;+|S_z|S_z;+\rangle + \frac{1}{4}\langle S_x;+|S_z|S_x;+\rangle && (13)\\
&= \frac{3}{4}\frac{\hbar}{2} + \frac{1}{4}0 = \frac{3\hbar}{8} && (14)
\end{aligned}
$$

Using the second technique:

$$
\begin{aligned}
[S_x] &= \operatorname{tr}\left(\frac{\hbar}{16}\begin{pmatrix}7 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right) && (15)\\
&= \frac{\hbar}{16}\operatorname{tr}\begin{pmatrix}1 & 7\\ 1 & 1\end{pmatrix} = \frac{\hbar}{8} && (16)\\
[S_y] &= \operatorname{tr}\left(\frac{i\hbar}{16}\begin{pmatrix}7 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\right) && (17)\\
&= \frac{i\hbar}{16}\operatorname{tr}\begin{pmatrix}1 & -7\\ 1 & -1\end{pmatrix} = 0 && (18)\\
[S_z] &= \operatorname{tr}\left(\frac{\hbar}{16}\begin{pmatrix}7 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right) && (19)\\
&= \frac{\hbar}{16}\operatorname{tr}\begin{pmatrix}7 & -1\\ 1 & -1\end{pmatrix} = \frac{3\hbar}{8} && (20)
\end{aligned}
$$

(b) We begin by calculating the density operator for this ensemble.

$$
\begin{aligned}
\hat{\rho} &= \sum_i w_i |\alpha_i\rangle\langle\alpha_i| && (21)\\
&= \frac{1}{2}|\psi_1\rangle\langle\psi_i| + \frac{1}{2}|\psi_2\rangle\langle\psi_2| && (22)\\
&= \frac{1}{2}\left(\frac{1}{2}(|0\rangle + |1\rangle)(\langle 0| + \langle 1|) + \frac{1}{2}(|1\rangle + |2\rangle)(\langle 1| + \langle 2|)\right) && (23)\\
&= \frac{1}{4}\left((|0\rangle\langle 0| + |1\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 1|) + (|1\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 1| + |2\rangle\langle 2|)\right) && (24)\\
&= \frac{1}{4}\left(|0\rangle\langle 0| + |1\rangle\langle 0| + |0\rangle\langle 1| + 2|1\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 1| + |2\rangle\langle 2|\right) && (25)
\end{aligned}
$$

Although the space of harmonic oscillator energy eigenstates is of infinite (but countable) dimension, this specific system is fully described by a basis of only the three lowest energy states ($|0\rangle$, $|1\rangle$, and $|2\rangle$). So we give the density matrix represented in that subspace:

$$\hat{\rho} \doteq \begin{pmatrix} 1/4 & 1/4 & 0 \\ 1/4 & 1/2 & 1/4 \\ 0 & 1/4 & 1/4 \end{pmatrix} \tag{26}$$

Now let's calculate the ensemble's averaged energy. We know the energy eigenvalues of the harmonic oscillator, so we can immediately write down the matrix representation of the Hamiltonian in this subspace:

$$[E] = \mathrm{tr}(\hat{\rho}\hat{H}) \tag{27}$$

$$= \mathrm{tr}\left(\frac{1}{4}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{pmatrix} \hbar\omega \begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 3/2 & 0 \\ 0 & 0 & 5/2 \end{pmatrix}\right) \tag{28}$$

$$= \frac{\hbar\omega}{8}\,\mathrm{tr}\begin{pmatrix} 1 & 3 & 0 \\ 1 & 6 & 5 \\ 0 & 3 & 5 \end{pmatrix} = \frac{12\hbar\omega}{8} = \frac{3\hbar\omega}{2} \tag{29}$$

The final question we need to answer is whether this energy differs from a totally incoherent ensemble with the same populations. That is to say, from an ensemble where each state $\{|0\rangle, |1\rangle, |2\rangle\}$ contributes independently to the ensemble, with probability corresponding to its probability in the ensemble given in the problem.

So the first this we need to do is find the probability of finding each individual state in the ensemble. This is given by:

$$P_n = \sum_i w_i \left|\langle n|\alpha_i\rangle\right|^2 \tag{30}$$

For this ensemble:

$$P_n = \frac{1}{2}\left|\langle n|\left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right)\right|^2 + \frac{1}{2}\left|\langle n|\left(\frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)\right)\right|^2 \tag{31}$$

$$= \frac{1}{4}\left(|\langle n|0\rangle + \langle n|1\rangle|^2 + |\langle n|1\rangle + \langle n|2\rangle|^2\right) \tag{32}$$

Plugging in the values of n:

$$P_{n=0} = \frac{1}{4}\left(|\langle 0|0\rangle + \langle 0|1\rangle|^2 + |\langle 0|1\rangle + \langle 0|2\rangle|^2\right) = \frac{1}{4} \tag{33}$$

$$P_{n=1} = \frac{1}{4}\left(|\langle 1|0\rangle + \langle 1|1\rangle|^2 + |\langle 1|1\rangle + \langle 1|2\rangle|^2\right) = \frac{1}{2} \tag{34}$$

$$P_{n=2} = \frac{1}{4}\left(|\langle 2|0\rangle + \langle 2|1\rangle|^2 + |\langle 2|1\rangle + \langle 2|2\rangle|^2\right) = \frac{1}{4} \tag{35}$$

So now we want the density matrix of an ensemble made up of 25% $|0\rangle$, 50% $|1\rangle$, and 25% $|2\rangle$. It's density operator is given by:

$$\hat{\rho} = \frac{1}{4}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| + \frac{1}{4}|2\rangle\langle 2| \tag{36}$$

We represent it in this basis by the matrix

$$\hat{\rho} \doteq \begin{pmatrix} 1/4 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/4 \end{pmatrix} \tag{37}$$

Now we calculate the ensemble average of energy for this modified ensemble:

$$[E] = \mathrm{tr}(\hat{\rho}\hat{H}) = \mathrm{tr}\left(\frac{\hbar\omega}{8}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix}\right) \tag{38}$$

$$= \frac{\hbar\omega}{8}\,\mathrm{tr}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 5 \end{pmatrix} = \frac{12\hbar\omega}{8} = \frac{3\hbar\omega}{2} \tag{39}$$

So the fully decoherent ensemble has the same ensemble average energy as the ensemble with coherences.

Problem 2

(a) First, let's recall how we express a coordinate q and momentUM p in terms of the creation and annihilation operators:

$$q = \sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger + a\right) \tag{40}$$

$$p = i\sqrt{\frac{m\hbar\omega}{2}}\left(a^\dagger - a\right) \tag{41}$$

Let's calculate L_z using those:

$$L_z = xp_y - yp_x \tag{42}$$

$$= i\sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{m\hbar\omega}{2}}\left((a_x^\dagger + a_x)(a_y^\dagger - a_y) - (a_y^\dagger + a_y)(a_x^\dagger - a_x)\right) \tag{43}$$

$$= i\frac{\hbar}{2}\left((a_x^\dagger a_y^\dagger + a_x a_y^\dagger - a_x^\dagger a_y - a_x a_y) - (a_y^\dagger a_x^\dagger + a_y a_x^\dagger - a_y^\dagger a_x - a_y a_x)\right) \tag{44}$$

$$= i\frac{\hbar}{2}(2a_x a_y^\dagger - 2a_x^\dagger a_y) \tag{45}$$

$$= i\hbar(a_x a_y^\dagger - a_x^\dagger a_y) \tag{46}$$

In doing this, we have made use of the fact that creation/annihilation operators from one subspace (x or y) commute with operators from the other subspace. If that doesn't seem obvious, it can be easily determined from the definitions of the creation and annihilation operators in terms of positions and momenta.

Now let's calculate the commutator $[H, L_z]$:

$$\begin{aligned}
[H, L_z] &= [\hbar\omega(N_x + N_y + 1), L_z] && (47)\\
[H, L_z] &= \hbar\omega[N_x + N_y, i\hbar(a_x a_y^\dagger - a_x^\dagger a_y)] + \hbar\omega[1, L_z] && (48)\\
&= i\hbar^2\omega\left([N_x, a_x a_y^\dagger] - [N_x, a_x^\dagger a_y] + [N_y, a_x a_y^\dagger] - [N_y, a_x^\dagger a_y]\right) && (49)\\
&= i\hbar^2\omega\left(([N_x, a_x]a_y^\dagger + a_y^\dagger[N_x, a_x]) - (-[N_x, a_x^\dagger]a_y - a_y[N_x, a_x^\dagger]) + \right. && (50)\\
&\qquad \left.(-a_x[N_y, a_y^\dagger] - [N_y, a_y^\dagger]a_x) - (a_x^\dagger[N_y, a_y] + [N_y, a_y]a_x^\dagger)\right) && (51)\\
&= i\hbar^2\omega\left(2a_x a_y^\dagger - 2a_x^\dagger a_y - 2a_x a_x^\dagger + 2a_y a_x^\dagger\right) && (52)\\
&= 0 && (53)
\end{aligned}$$

(b) In order to find the simultaneous eigenkets of $\hat{H}$ and $\hat{L}_z$, we'll start out by representing those operators as matrices. Right now, I'll define the basis $\mathfrak{B} = \{|0,0\rangle, |1,0\rangle, |0,1\rangle\}$. The order, in particular, is important. This basis will be used for the rest of this problem.

The matrix representation of $\hat{H}$ in $\mathfrak{B}$ is trivial:

$$\hat{H} \doteq \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{54}$$

It takes a little more work to get the matrix representation of $\hat{L}_z$. First we operate of each of the kets with $\hat{L}_z = i\hbar(a_x a_y^\dagger - a_x^\dagger a_y)$:

$$\begin{aligned}
i\hbar(a_x a_y^\dagger - a_x^\dagger a_y)\,|0,0\rangle &= 0 && (55)\\
i\hbar(a_x a_y^\dagger - a_x^\dagger a_y)\,|1,0\rangle &= i\hbar(\sqrt{1}\sqrt{0+1}\,|0,1\rangle + 0) = i\hbar\,|0,1\rangle && (56)\\
i\hbar(a_x a_y^\dagger - a_x^\dagger a_y)\,|0,1\rangle &= i\hbar(0 - \sqrt{0+1}\sqrt{1}\,|1,0\rangle) = -i\hbar\,|1,0\rangle && (57)
\end{aligned}$$

From this, we can easily obtain the matrix representation of $\hat{L}_z$ in the $\mathfrak{B}$ basis:

$$\hat{L}_z \doteq i\hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \tag{58}$$

Immediately we see that $\hat{L}_z$ has an eigenvalue of 0 for the same space in which the eigenvalue of $\hat{H}$ is $\hbar\omega$, *i.e.*, the space spanned by $|0,0\rangle$. The remaining subspace is degenerate for $\hat{H}$, so any linear combination of kets from this subspace will also be an eigenket for $\hat{H}$. This means that when we find the eigenkets of $\hat{L}_z$ for this subspace, we will have found simultaneous eigenkets of $\hat{H}$ and $\hat{L}_z$.

So we just have to diagonalize the 2×2 submatrix:

$$\begin{pmatrix} 0 & i\hbar \\ -i\hbar & 0 \end{pmatrix} \tag{59}$$

This is a matrix we've seen before, and will probably see again. Let's find its eigenvalues:

$$0 = \det\begin{pmatrix} \lambda & -i\hbar \\ i\hbar & \lambda \end{pmatrix} \tag{60}$$
$$= \lambda^2 - \hbar^2 \tag{61}$$
$$= (\lambda - \hbar)(\lambda + \hbar) \tag{62}$$

So the eigenvalues are $\pm\hbar$.

Let's find the eigenvectors for each eigenvalue. First, for $\lambda = +\hbar$:

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \hbar & -i\hbar \\ i\hbar & \hbar \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \implies -ix_1 = x_2 \implies \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix} \tag{63}$$

And for $\lambda = -\hbar$:

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -\hbar & -i\hbar \\ i\hbar & -\hbar \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \implies ix_1 = x_2 \implies \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} \tag{64}$$

So putting all of these together, and labelling the simultaneous eigenkets according to first the eigenvalue of $\hat{H}$ and then the eigenvalue of $\hat{L}_z$, our final set of simultaneous eigenkets is:

$$\left\{ |\hbar\omega, 0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |2\hbar\omega, +\hbar\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}, |2\hbar\omega, -\hbar\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix} \right\} \tag{65}$$

(c) I will find the time-dependent expectation values by first determining a matrix representation for the operators, the finding the time-dependent state, and then putting those together to get the expectation values. You could also do this whole problem in bra-ket notation, but why write out that mess?

First, let's find the matrix representation for $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a_x^\dagger + a_x)$.

$$\sqrt{\frac{\hbar}{2m\omega}}\left\langle n_x', n_y'\middle| a_x^\dagger + a_x \middle| n_x, n_y\right\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\left\langle n_x', n_y'\middle| a_x^\dagger \middle| n_x, n_y\right\rangle + \left\langle n_x', n_y'\middle| a_x \middle| n_x, n_y\right\rangle\right) \tag{66}$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n_x+1}\,\delta_{n_x', n_x+1} + \sqrt{n_x}\,\delta_{n_x', n_x-1}\right)\delta_{n_y', n_y} \tag{67}$$

In the subspace of interest, represented in the $\mathfrak{B}$ basis, we have:

$$\hat{x} \doteq \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{68}$$

Similarly, we can show that the matrix representation of $\hat{y}$ in this basis is

$$\hat{y} \doteq \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{69}$$

With the matrices determined, let's find the time dependent state:

$$
\begin{align}
|\psi(t)\rangle &= e^{i\hat{H}t/\hbar}\left(\frac{1}{2}\left(\sqrt{2}\,|0,0\rangle + e^{i\alpha}\,|1,0\rangle + e^{i\beta}\,|0,1\rangle\right)\right) \tag{70}\\
&= \frac{1}{2}\left(\sqrt{2}e^{-i(E_0+E_0)t/\hbar}\,|0,0\rangle + e^{i\alpha}e^{-i(E_1+E_0)t/\hbar}\,|1,0\rangle + e^{i\beta}e^{-i(E_0+E_1)t/\hbar}\,|0,1\rangle\right) \tag{71}
\end{align}
$$

Remembering that $E_0 = \frac{1}{2}\hbar\omega$ and $E_1 = \frac{3}{2}\hbar\omega$, we get:

$$
\begin{align}
|\psi(t)\rangle &= \frac{1}{2}\left(\sqrt{2}e^{-i(2\omega)t}\,|0,0\rangle + e^{i(\alpha-2\omega t)}\,|1,0\rangle + e^{i(\beta-2\omega t)}\,|0,1\rangle\right) \tag{72}\\
&= \frac{e^{i\omega t}}{2}\left(\sqrt{2}\,|0,0\rangle + e^{i(\alpha-\omega t)}\,|1,0\rangle + e^{i(\beta-\omega t)}\,|0,1\rangle\right) \tag{73}
\end{align}
$$

Now we can plug all these things together in order to get the expectation values:

$$
\begin{align}
\langle x(t)\rangle &= \langle\psi(t)|x|\psi(t)\rangle \tag{74}\\
&\doteq \frac{e^{i\omega t}}{2}\begin{pmatrix}\sqrt{2} & e^{-i(\alpha-\omega t)} & e^{-i(\beta-\omega t)}\end{pmatrix}\sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}\frac{e^{-i\omega t}}{2}\begin{pmatrix}\sqrt{2}\\ e^{i(\alpha-\omega t)}\\ e^{i(\beta-\omega t)}\end{pmatrix} \tag{75}\\
&= \sqrt{\frac{\hbar}{32m\omega}}\begin{pmatrix}\sqrt{2} & e^{-i(\alpha-\omega t)} & e^{-i(\beta-\omega t)}\end{pmatrix}\begin{pmatrix}e^{i(\alpha-\omega t)}\\ \sqrt{2}\\ 0\end{pmatrix} \tag{76}\\
&= \sqrt{\frac{\hbar}{32m\omega}}\left(\sqrt{2}e^{i(\alpha-\omega t)} + \sqrt{2}e^{-i(\alpha-\omega t)} + 0\right) \tag{77}\\
&= \frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}\cos(\alpha-\omega t) \tag{78}\\
\langle y(t)\rangle &= \langle\psi(t)|y|\psi(t)\rangle \tag{79}\\
&\doteq \sqrt{\frac{\hbar}{32m\omega}}\begin{pmatrix}\sqrt{2} & e^{-i(\alpha-\omega t)} & e^{-i(\beta-\omega t)}\end{pmatrix}\begin{pmatrix}0 & 0 & 1\\ 0 & 0 & 0\\ 1 & 0 & 0\end{pmatrix}\begin{pmatrix}\sqrt{2}\\ e^{i(\alpha-\omega t)}\\ e^{i(\beta-\omega t)}\end{pmatrix} \tag{80}\\
&= \sqrt{\frac{\hbar}{32m\omega}}\begin{pmatrix}\sqrt{2} & e^{-i(\alpha-\omega t)} & e^{-i(\beta-\omega t)}\end{pmatrix}\begin{pmatrix}e^{i(\beta-\omega t)}\\ 0\\ \sqrt{2}\end{pmatrix} \tag{81}\\
&= \sqrt{\frac{\hbar}{32m\omega}}\left(\sqrt{2}e^{i(\beta-\omega t)} + \sqrt{2}e^{-i(\beta-\omega t)}\right) \tag{82}\\
&= \frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}\cos(\beta-\omega t) \tag{83}
\end{align}
$$

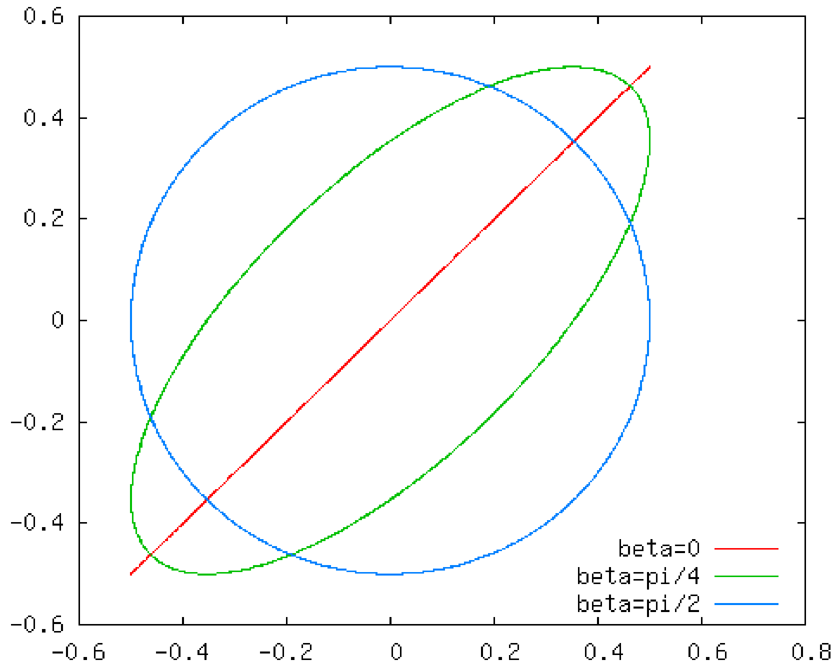

Figure 1: Parametric plots of the time dependent expectation values for $\alpha = 0$ and various values of β

Problem 3

(a) Let's start out by recalling how to write each of these dot products in spherical coordinates:

$$\langle \boldsymbol{\mu} \cdot \hat{z} \rangle = |\mu| \left\langle \cos(\hat{\theta}) \right\rangle \tag{84}$$

$$\langle \boldsymbol{\mu} \cdot \hat{x} \rangle = |\mu| \left\langle \sin(\hat{\theta}) \cos(\hat{\phi}) \right\rangle \tag{85}$$

$$\langle \boldsymbol{\mu} \cdot \hat{y} \rangle = |\mu| \left\langle \sin(\hat{\theta}) \sin(\hat{\phi}) \right\rangle \tag{86}$$

Each of these is an expectation value with respect to the state $|l, m\rangle$. We'll solve them by using the fact that we know how to write the wavefunction for $|l, m\rangle$ in the (θ, ϕ) representation.

Let's start with $\langle \boldsymbol{\mu} \cdot \hat{x} \rangle$:

$$\begin{aligned}
\langle \boldsymbol{\mu} \cdot \hat{x} \rangle &= |\mu| \left\langle l, m \middle| \sin(\hat{\theta}) \cos(\hat{\phi}) \middle| l, m \right\rangle & (87) \\
&= |\mu| \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin(\theta) \left\langle l, m \middle| \theta, \phi \right\rangle \left\langle \theta, \phi \middle| \sin(\hat{\theta}) \cos(\hat{\phi}) \middle| l, m \right\rangle & (88) \\
&= |\mu| \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin(\theta) \langle l, m | \theta, \phi \rangle \sin(\theta) \cos(\phi) \langle \theta, \phi | l, m \rangle & (89) \\
&= |\mu| \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin^2(\theta) \cos(\phi) Y_l^{m*}(\theta, \phi) Y_l^m(\theta, \phi) & (90) \\
&= |\mu| \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin^2(\theta) \cos(\phi) P_l^{m*}(\cos(\theta)) e^{-im\phi} P_l^m(\cos(\theta) e^{im\phi} & (91) \\
&= |\mu| \underbrace{\int_0^{2\pi} \mathrm{d}\phi \, \cos(\phi)}_{0} \int_0^{\pi} \mathrm{d}\theta \, \sin^2(\theta) \left| P_l^m(\cos(\theta)) \right|^2 & (92) \\
&= 0 & (93)
\end{aligned}$$

The integral over ϕ is zero because the function being integrated, $\cos(\phi)$, is periodic over the interval of the integrand (2π).

Similarly, we can see that $\langle \boldsymbol{\mu} \cdot \hat{y} \rangle$ is also zero, since $\sin(\phi)$ is also 2π-periodic.

Now let's calculate $\langle \boldsymbol{\mu} \cdot \hat{z} \rangle$:

$$\begin{aligned}
\langle \boldsymbol{\mu} \cdot \hat{z} \rangle &= |\mu| \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin(\theta) Y_l^{m*}(\theta, \phi) \cos(\theta) Y_l^m(\theta, \phi) & (94) \\
&= |\mu| \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin(\theta) Y_l^{m*}(\theta, \phi) \cos(\theta) Y_l^m(\theta, \phi) & (95)
\end{aligned}$$

There are several ways of solving this integral. I'll show two of them: first let's use the recursion relation given on the problem set. Ignoring the exact values of the constants (which won't be necessary to us), we can write the recursion relation as:

$$\cos(\theta) Y_l^m(\theta, \phi) = k_- Y_{l-1}^m(\theta, \phi) + k_+ Y_{l+1}^m(\theta, \phi) \tag{96}$$

Plugging this into equation (95):

$$\begin{aligned}
\langle \boldsymbol{\mu} \cdot \hat{z} \rangle &= |\mu| \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin(\theta) Y_l^{m*}(\theta, \phi) \left(k_- Y_{l-1}^m(\theta, \phi) + k_+ Y_{l+1}^m(\theta, \phi) \right) & (97) \\
&= |\mu| \Bigg(k_- \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin(\theta) Y_l^{m*}(\theta, \phi) Y_{l-1}^m(\theta, \phi) \\
&\qquad + k_+ \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin(\theta) Y_l^{m*}(\theta, \phi) Y_{l+1}^m(\theta, \phi) \Bigg) & (98) \\
&= 0 & (99)
\end{aligned}$$

The final equality comes about by invoking the orthogonality of the spherical harmonics (and the fact that $l \neq l \pm 1$).

The other method to solve the integral in equation (95), which I think is a little more elegant, is to make the change of variables $x = \cos(\theta)$, which means that $\mathrm{d}x = \mathrm{d}\theta\,\sin(\theta)$. Starting from equation (95):

$$\langle \boldsymbol{\mu} \cdot \hat{z} \rangle = |\mu| \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta\, \sin(\theta)\cos(\theta)\, \left|P_l^m(\cos(\theta))\right|^2 \tag{100}$$

$$= -2\pi\,|\mu| \int_{-1}^{1} \mathrm{d}x\, x\, \left|P_l^m(x)\right|^2 \tag{101}$$

$$= 0 \tag{102}$$

Since $P_l^m(x)$ is always either even or odd, $\left|P_l^m(x)\right|^2$ is even, and the whole integrand is odd. So the integral is zero.

So why are these all zero? Probably the easiest way to think of it is that since there is no preferred direction for the molecules, their dipole moments are equally likely to point in any direction. Therefore, the expectation value of the dipole moment is zero.

(b) Now we are to calculate the z-component of the dipole moment in a specific coherent superposition state (instead of the general eigenstate from the previous part).

This is another example of a problem that can be done either with a lot of bra-ket notation or by finding a matrix representation. As usual, I prefer the matrix representation. So let's start out by finding a matrix representation of $\cos(\hat{\theta})$, which we'll obtain by using (the corrected form of) the recursion formula given in the problem:

$$\left\langle l', m' \middle| \cos(\hat{\theta}) \middle| l, m \right\rangle = \left\langle l', m' \middle| \sqrt{\frac{l^2 - m^2}{4l^2 - 1}} \middle| l-1, m \right\rangle + \left\langle l', m' \middle| \sqrt{\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1}} \middle| l+1, m \right\rangle \tag{103}$$

$$= \left(\sqrt{\frac{l^2 - m^2}{4l^2 - 1}}\,\delta_{l',l-1} + \sqrt{\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1}}\,\delta_{l',l+1} \right) \delta_{m',m} \tag{104}$$

Since all components of our initial state have $m = 0$, and the matrix elements of $\cos(\hat{\theta})$ require that $\Delta m = 0$, we can look at just the $m = 0$ subspace.

Further, since the states $|l, m\rangle$ are eigenstates of the Hamiltonian, we know that even in the time dependent case, only the energy eigenstates which contribute to the initial state will ever be populated (the time evolution involves no coupling between energy eigenstates). So we can reduce our system to the subspace spanned by $|1, 0\rangle$ and $|2, 0\rangle$. Writing the basis in that order, we can represent $\cos(\hat{\theta})$ as:

$$\cos(\hat{\theta}) \doteq \begin{pmatrix} 0 & \sqrt{\frac{2^2 - 0}{4(2^2) - 1}} \\ \sqrt{\frac{(1+1)^2 - 0}{4(1+1)^2 - 1}} & 0 \end{pmatrix} = \frac{2}{\sqrt{15}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{105}$$

So let's go ahead and find the expectation value at $t = 0$. In the same basis as above, this gives us:

$$
\begin{aligned}
\left\langle \psi(t=0) \middle| \boldsymbol{\mu} \cdot \cos(\hat{\theta}) \middle| \psi(t=0) \right\rangle &= |\mu| \frac{2}{\sqrt{15}} \frac{1}{2} \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} && (106) \\
&= \frac{|\mu|}{\sqrt{15}} \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} && (107) \\
&= \frac{2\,|\mu|}{\sqrt{15}} && (108)
\end{aligned}
$$

Now let's get the time-dependent version of the our state. We know that $E_l = Bl(l+1)$ for the rigid rotor, so:

$$
\begin{aligned}
|\psi(t)\rangle &= e^{-i\hat{H}t/\hbar} \frac{1}{\sqrt{2}} \left(|1,0\rangle + |2,0\rangle \right) && (109) \\
&= \frac{1}{\sqrt{2}} \left(e^{-i(B(1)(2))t/\hbar} \, |1,0\rangle + e^{-i(B(2)(3))t/\hbar} \, |2,0\rangle \right) && (110) \\
&= \frac{1}{\sqrt{2}} \left(e^{-2iBt/\hbar} \, |1,0\rangle + e^{-6iBt/\hbar} \, |2,0\rangle \right) && (111)
\end{aligned}
$$

With that, we can calculate the time dependent expectation value:

$$
\begin{aligned}
|\mu| \left\langle \psi(t) \middle| \cos(\hat{\theta}) \middle| \psi(t) \right\rangle &= \frac{|\mu|}{\sqrt{15}} \begin{pmatrix} e^{2iBt/\hbar} & e^{6iB/\hbar} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-2iBt/\hbar} \\ e^{-6iB/\hbar} \end{pmatrix} && (112) \\
&= \frac{|\mu|}{\sqrt{15}} \begin{pmatrix} e^{2iBt/\hbar} & e^{6iB/\hbar} \end{pmatrix} \begin{pmatrix} e^{-6iBt/\hbar} \\ e^{-2iB/\hbar} \end{pmatrix} && (113) \\
&= \frac{|\mu|}{\sqrt{15}} \left(e^{-4iBt/\hbar} + e^{4iBt/\hbar} \right) && (114) \\
&= \frac{2\,|\mu|}{\sqrt{15}} \cos\left(\frac{4B}{\hbar} t \right) && (115)
\end{aligned}
$$

When $t = 0$, this reduces to our previous result. That's a goodd sign that we're on the right path.

Problem 4

(a) As always, the first task is to find the matrix representation of this Hamiltonian. We use the basis in which $\hat{L}_z$ is diagaonal because that tends to be the standard basis to use in quantum mechanics.

Before giving a proper quantum mechanical derivation, I'd like to look at a classical picture which should give us some guidance. Let's remember that classically, the angular momentum vector is the vector which represents the axis around which the system is rotating. So we can think of the resulting coordinate system that same way we would think about simple vectors. This problem asks us to rotate the system by 45°. The resulting system is shown in figure 2, where we mark the points where vectors along **u** and **v** have unit length.

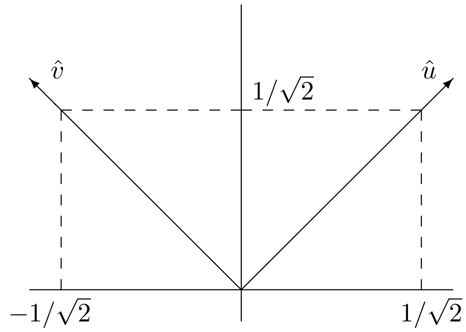

Figure 2: Classical vector picture of the rotation

From this picture, we can quickly obtain the results

$$\hat{u} = \frac{1}{\sqrt{2}}\left(\hat{z} + \hat{x}\right) \tag{116}$$

$$\hat{v} = \frac{1}{\sqrt{2}}\left(\hat{z} - \hat{x}\right) \tag{117}$$

While this is suggestive, it is definitely not a fully quantum mechanical proof. Now let's do one of those.

We didn't talk much about using angular momentum as the generator of rotation, but to generate a rotation of $\pi/4$ about the y-axis, we use a trick similar to what we did previously in a problem about translation. But first, let me prove two lemmas.

Lemma 1 (Recursion relation for even n-fold commutators)**.** We intend to prove:

$$\left[L_y, L_x\right]_{2n} = \hbar^{2n} L_x \tag{118}$$

We will perform this proof by induction. First, we will prove the inductive step (that is, show that if that is satisfied for $n' = n - 1$, then it is also satisfied for n). Then we will show that it is satisfied for $n = 0$, and therefore for all $n > 0$.

To show that if this is satisfied for $n' = n - 1$, then it is satisfied for n, we simply assume that it is satisfied for $n - 1$:

$$\begin{aligned}
\left[L_y, L_x\right]_{2n} &= \Big[L_y, \Big[L_y \left[L_y, L - x\right]_{2n-2}\Big]\Big] && (119)\\
&= \left[L_y, \left[L_y, \hbar^{2n-2} L_x\right]\right] && (120)\\
&= \hbar^{2n-2}\left[L_y, \left[L_y, L_x\right]\right] && (121)\\
&= \hbar^{2n-2}\left[L_y, i\hbar\varepsilon_{yxz} L_z\right] && (122)\\
&= \hbar^{2n-2}(-i\hbar)\left[L_y, L_z\right] && (123)\\
&= \hbar^{2n-2}(-i\hbar)(i\hbar\varepsilon_{yzx}) L_x && (124)\\
&= \hbar^{2n-2}(\hbar^2) L_x && (125)\\
&= \hbar^{2n} L_x && (126)
\end{aligned}$$

To show that this is, in fact, true for all values of $n \geq 0$, we just need to show that it is true for $n = 0$, which is trivial (since $[L_y, L_x]_0 = L_x$).

Lemma 2 (Recursion relation for odd n-fold commutators)**.** Now we will prove a similar result for odd commutators:

$$[L_y, L_x]_{2n+1} = -i\hbar^{2n+1} L_z \tag{127}$$

We'll simplify the proof of this by using the result of the previous lemma.

$$\begin{aligned}
[L_y, L_x]_{2n+1} &= \left[L_y, [L_y, L_x]_{2n}\right] && (128)\\
&= \left[L_y, \hbar^{2n} L_x\right] && (129)\\
&= \hbar^{2n}(i\hbar)\varepsilon_{yxz} L_z && (130)\\
&= -i\hbar^{2n+1} L_z && (131)
\end{aligned}$$

With those lemmas out of the way, let's really start on this problem. First, remember that $\hat{L}_u$ is given by rotating $\hat{L}_x$ by $\pi/4$ about the axis which corresponds to $\hat{L}_y$. So we can write it as:

$$\hat{L}_u = e^{i\hat{L}_y \frac{\pi}{4}/\hbar} L_x e^{i\hat{L}_y \frac{\pi}{4}/\hbar} \tag{132}$$

Using the result from a previous problem set, this becomes:

$$\begin{aligned}
\hat{L}_u &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i\pi}{4\hbar}\right)^n [L_y, L_x]_n && (133)\\
&= \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left(\frac{i\pi}{4\hbar}\right)^{2n} [L_y, L_x]_{2n} + \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left(\frac{i\pi}{4\hbar}\right)^{2n+1} [L_y, L_x]_{2n+1} && (134)\\
&= \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left(\frac{i\pi}{4\hbar}\right)^{2n} \hbar^{2n} \hat{L}_x + \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left(\frac{i\pi}{4\hbar}\right)^{2n+1} (-i\hbar^{2n+1}) \hat{L}_z && (135)\\
&= \hat{L}_x \sum_{n=0}^{\infty} \frac{1}{(2n)!} (-1)^n \left(\frac{\pi}{4}\right)^{2n} + \hat{L}_z (-i) \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} i \, (-1)^n \left(\frac{\pi}{4}\right)^{2n+1} && (136)\\
&= \hat{L}_x \sum_{n=0}^{\infty} \frac{1}{(2n)!} (-1)^n \left(\frac{\pi}{4}\right)^{2n} + \hat{L}_z \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} (-1)^n \left(\frac{\pi}{4}\right)^{2n+1} && (137)\\
&= \hat{L}_x \cos\left(\frac{\pi}{4}\right) + \hat{L}_z \sin\left(\frac{\pi}{4}\right) && (138)\\
&= \frac{1}{\sqrt{2}} \left(\hat{L}_z + \hat{L}_x\right) && (139)
\end{aligned}$$

Note how this compares to our classical solution for $\hat{u}$. A similar process gives us $\hat{L}_v$:

$$\hat{L}_v = \frac{1}{\sqrt{2}} \left(\hat{L}_z - \hat{L}_x\right) \tag{140}$$

Now let's use that to find the Hamiltonian in terms of $\hat{L}_z$ and $\hat{L}_x$:

$$\begin{aligned}
\hat{H} &= \frac{\omega_0}{\hbar}\left(\hat{L}_u^2 - \hat{L}_v^2\right) && (141)\\
&= \frac{\omega_0}{\hbar}\left(\left(\frac{1}{\sqrt{2}}(\hat{L}_z + \hat{L}_x)\right)^2 - \left(\frac{1}{\sqrt{2}}(\hat{L}_z - \hat{L}_x)\right)^2\right) && (142)\\
&= \frac{\omega_0}{2\hbar}\left((\hat{L}_z^2 + \hat{L}_z\hat{L}_x + \hat{L}_x\hat{L}_z + \hat{L}_x^2) - (\hat{L}_z^2 - \hat{L}_z\hat{L}_x - \hat{L}_x\hat{L}_z + \hat{L}_x^2)\right) && (143)\\
&= \frac{\omega_0}{\hbar}\left(\hat{L}_z\hat{L}_x + \hat{L}_x\hat{L}_z\right) && (144)
\end{aligned}$$

In order to get a matrix representation of this, we'll need matrix representations of $\hat{L}_z$ and $\hat{L}_x$ in the $\hat{L}_z$ diagonal basis. While we're at it, let's go ahead and also get the matrix representation of $\hat{L}_y$, which we'll need later.

The matrix representation of $\hat{L}_z$ in its diagonal basis is trivial:

$$\hat{L}_z \doteq \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix} \tag{145}$$

To calculate the matrix representations of $\hat{L}_x$ and $\hat{L}_y$, we recall their definitions in terms of the ladder operators:

$$\hat{L}_x = \frac{1}{2}\left(\hat{L}_+ + \hat{L}_-\right) \tag{146}$$

$$\hat{L}_y = \frac{1}{2i}\left(\hat{L}_+ - \hat{L}_-\right) \tag{147}$$

So really, we just need the matrix elements of the ladder operators. Using the definition given in the problem set, we can quickly see that the ladder operators have the matrix representations:

$$\hat{L}_+ \doteq \hbar\sqrt{2}\begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 1\\ 0 & 0 & 0\end{pmatrix} \tag{148}$$

$$\hat{L}_- \doteq \hbar\sqrt{2}\begin{pmatrix}0 & 0 & 0\\ 1 & 0 & 0\\ 0 & 1 & 0\end{pmatrix} \tag{149}$$

Therefore, we have

$$\hat{L}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix} \tag{150}$$

$$\hat{L}_y = \frac{\hbar}{i\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ -1 & 0 & 1\\ 0 & -1 & 0\end{pmatrix} \tag{151}$$

Returning to our Hamiltonian, we now have what we need to create its matrix representation, based on equation (144):

$$\hat{H} \doteq \frac{\omega_0}{\hbar}\frac{\hbar^2}{\sqrt{2}}\left(\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix} + \begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}\right) \tag{152}$$

$$= \frac{\hbar\omega_0}{\sqrt{2}}\left(\begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 0\\ 0 & -1 & 0\end{pmatrix} + \begin{pmatrix}0 & 0 & 0\\ 1 & 0 & -1\\ 0 & 0 & 0\end{pmatrix}\right) \tag{153}$$

$$= \frac{\hbar\omega_0}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & -1\\ 0 & -1 & 0\end{pmatrix} \tag{154}$$

By now, you probably can already guess the eigenvalues and eigenvectors of this matrix. Just in case you can't, I'll calculate them. Again. Defining $a = \hbar\omega_0/\sqrt{2}$:

$$0 = \det\begin{pmatrix}\lambda & -a & 0\\ -a & \lambda & a\\ 0 & a & \lambda\end{pmatrix} \tag{155}$$

$$= \lambda^3 - 2a^2\lambda \tag{156}$$

$$= \lambda(\lambda - a\sqrt{2})(\lambda + a\sqrt{2}) \tag{157}$$

So the possible eigenvalues are, in decreasing order, $\{\hbar\omega_0, 0, -\hbar\omega_0\}$. On to the eigenvectors. First, $|E_1 = \hbar\omega_0\rangle$:

$$\begin{pmatrix}a\sqrt{2} & -a & 0\\ -a & a\sqrt{2} & a\\ 0 & a & a\sqrt{2}\end{pmatrix}\begin{pmatrix}x_1\\ x_2\\ x_3\end{pmatrix} = \begin{pmatrix}0\\ 0\\ 0\end{pmatrix} \implies \begin{cases}x_2 = \sqrt{2}x_1\\ x_3 = x_1 - \sqrt{2}x_2\end{cases} \implies \begin{cases}x_2 = \sqrt{2}x_1\\ x_3 = -x_1\end{cases} \tag{158}$$

This gives us the normalized eigenket

$$|E_1 = \hbar\omega_0\rangle = \begin{pmatrix}1/2\\ 1/\sqrt{2}\\ -1/2\end{pmatrix} \tag{159}$$

Now for the ket $|E_2 = 0\rangle$:

$$\begin{pmatrix}0 & -a & 0\\ -a & 0 & a\\ 0 & a & 0\end{pmatrix}\begin{pmatrix}x_1\\ x_2\\ x_3\end{pmatrix} = \begin{pmatrix}0\\ 0\\ 0\end{pmatrix} \implies \begin{cases}x_2 = 0\\ x_3 = x_1\end{cases} \tag{160}$$

From those equations, we obtain the normalized eigenket

$$|E_2 = 0\rangle = \begin{pmatrix}1/\sqrt{2}\\ 0\\ 1/\sqrt{2}\end{pmatrix} \tag{161}$$

Finally, we find the eigenket $|E_3 = -\hbar\omega_0\rangle$:

$$\begin{pmatrix} -a\sqrt{2} & -a & 0 \\ -a & -a\sqrt{2} & a \\ 0 & a & -a\sqrt{2} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \implies \begin{cases} x_2 = -\sqrt{2}x_1 \\ x_3 = x_1 + \sqrt{2}x_2 \end{cases} \implies \begin{cases} x_2 = -\sqrt{2}x_1 \\ x_3 = -x_1 \end{cases} \tag{162}$$

This gives us the normalized eigenket

$$|E_3 = -\hbar\omega_0\rangle = \begin{pmatrix} 1/2 \\ -1/\sqrt{2} \\ -1/2 \end{pmatrix} \tag{163}$$

Putting it all together, the energies and eigenkets are:

$$\left\{ |E_1 = \hbar\omega_0\rangle = \begin{pmatrix} 1/2 \\ 1/\sqrt{2} \\ -1/2 \end{pmatrix},\ |E_2 = 0\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{pmatrix},\ |E_3 = -\hbar\omega_0\rangle = \begin{pmatrix} 1/2 \\ -1/\sqrt{2} \\ -1/2 \end{pmatrix} \right\} \tag{164}$$

(b) We're given an initial state in terms of the eigenstates of $\hat{L}_z$, and asked to find its time dependence. As always, we get the time dependence by operating the time evolution operator on it. We also need to insert a sum of energy eigenstates.

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} \sum_i |E_i\rangle \langle E_i|\psi(0)\rangle \tag{165}$$

$$= \sum_i e^{-iE_i t/\hbar} |E_i\rangle \langle E_i|\psi(0)\rangle \tag{166}$$

$$= e^{-i\omega_0 t} |E_1\rangle \langle E_1|\psi(0)\rangle + e^0 |E_2\rangle \langle E_2|\psi(0)\rangle + e^{i\omega_0 t} |E_3\rangle \langle E_3|\psi(0)\rangle \tag{167}$$

$$\begin{aligned} &= e^{-i\omega_0 t} \begin{pmatrix} 1/2 \\ 1/\sqrt{2} \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 & 1/\sqrt{2} & -1/2 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix} \\ &\quad + \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix} \\ &\quad + e^{i\omega_0 t} \begin{pmatrix} 1/2 \\ -1/\sqrt{2} \\ -1/2 \end{pmatrix} \begin{pmatrix} 1/2 & -1/\sqrt{2} & -1/2 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix} \end{aligned} \tag{168}$$

$$= e^{-i\omega_0 t} \frac{1}{\sqrt{2}} \begin{pmatrix} 1/2 \\ 1/\sqrt{2} \\ -1/2 \end{pmatrix} + 0 + e^{i\omega_0 t} \frac{1}{\sqrt{2}} \begin{pmatrix} 1/2 \\ -1/\sqrt{2} \\ -1/2 \end{pmatrix} \tag{169}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{2}\left(e^{-i\omega_0 t} + e^{i\omega_0 t}\right) \\ \frac{1}{\sqrt{2}}\left(e^{-i\omega_0 t} - e^{i\omega_0 t}\right) \\ \frac{1}{2}\left(e^{-i\omega_0 t} + e^{i\omega_0 t}\right) \end{pmatrix} \tag{170}$$

$$= \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} \\ -i\sin(\omega_0 t) \\ \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \tag{171}$$

Therefore the probabilities of measuring each state at a given time t is given by:

$$Prob(L_z = +\hbar) = \frac{1}{2}\cos^2(\omega_0 t) \tag{172}$$

$$Prob(L_z = 0) = \sin^2(\omega_0 t) \tag{173}$$

$$Prob(L_z = -\hbar) = \frac{1}{2}\cos^2(\omega_0 t) \tag{174}$$

(c) We found the matrix representations of all of these operators earlier in this problem (see equation (145) for $\hat{L}_z$, equation (150) for $\hat{L}_x$, and equation (151) for $\hat{L}_y$). So we'll just plug those in to get our each time-dependent expectation value:

$$\left\langle \hat{L}_x(t) \right\rangle = \left\langle \psi(t) \middle| \hat{L}_x \middle| \psi(t) \right\rangle \tag{175}$$

$$= \frac{\hbar}{\sqrt{2}} \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} & i\sin(\omega_0 t) & \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} \\ -i\sin(\omega_0 t) \\ \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \tag{176}$$

$$= \frac{\hbar}{\sqrt{2}} \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} & i\sin(\omega_0 t) & \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \begin{pmatrix} -i\sin(\omega_0 t) \\ \sqrt{2}\cos(\omega_0 t) \\ -i\sin(\omega_0 t) \end{pmatrix} \tag{177}$$

$$= \frac{i\hbar}{2} \left(-\frac{1}{2}\cos(\omega_0 t)\sin(\omega_0 t) + \cos(\omega_0 t)\sin(\omega_0 t) - \frac{1}{2}\cos(\omega_0 t)\sin(\omega_0 t) \right) \tag{178}$$

$$= 0 \tag{179}$$

$$\left\langle \hat{L}_y(t) \right\rangle = \left\langle \psi(t) \middle| \hat{L}_y \middle| \psi(t) \right\rangle \tag{180}$$

$$= \frac{\hbar}{i\sqrt{2}} \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} & i\sin(\omega_0 t) & \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} \\ -i\sin(\omega_0 t) \\ \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \tag{181}$$

$$= \frac{\hbar}{i\sqrt{2}} \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} & i\sin(\omega_0 t) & \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \begin{pmatrix} -i\sin(\omega_0 t) \\ 0 \\ i\sin(\omega_0 t) \end{pmatrix} \tag{182}$$

$$= 0 \tag{183}$$

$$\left\langle \hat{L}_z(t) \right\rangle = \left\langle \psi(t) \middle| \hat{L}_z \middle| \psi(t) \right\rangle \tag{184}$$

$$= \hbar \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} & i\sin(\omega_0 t) & \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} \\ -i\sin(\omega_0 t) \\ \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \tag{185}$$

$$= \hbar \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} & i\sin(\omega_0 t) & \cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \begin{pmatrix} \cos(\omega_0 t)/\sqrt{2} \\ 0 \\ -\cos(\omega_0 t)/\sqrt{2} \end{pmatrix} \tag{186}$$

$$= 0 \tag{187}$$

So the expectation value $\langle L \rangle$ is time-independent — there is no motion. To paraphrase Fermat, "I have a truly marvellous explanation for this which this page is too narrow to contain." If you want to hear it, ask me.