Problem Set # 10, Due: Wednesday April 5 by 11:00am

PHY 362K - Quantum Mechanics II, UT Austin, Spring 2017
(Dated: April 5, 2017)

More perturbation theory (time dependent and independent) and midterm review

I. $3d$ HARMONIC POTENTIAL – PERTURBATION THEORY

Consider a single massive particle moving in $3d$, in a harmonic potential:

$$\hat{H}_0 = \frac{|\hat{\vec{p}}|^2}{2m} + \frac{1}{2}m\omega^2|\hat{\vec{r}}|^2 \tag{1}$$

where $\hat{\vec{r}} = \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix}$, etc...

A. Single and multi-particle states of $\hat{H}_0$

1. Find the eigenstates and eigenvectors of $\hat{H}_0$ by introducing three sets of creation an annihilation operators, one each for the x, y, and z directions. What is the ground-state for a single particle?

   Solution: Notice that we can write this hamiltonian as

$$\begin{aligned}\hat{H}_0 &= \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right) + \frac{1}{2}m\omega^2\left(\hat{x}^2 + \hat{y}^2 + \hat{z}^2\right) \\ &= \left(\frac{\hat{p}_x^2}{2m} + \frac{1}{2}\hbar\omega\hat{x}\right) + \left(\frac{\hat{p}_y^2}{2m} + \frac{1}{2}\hbar\omega\hat{y}\right) + \left(\frac{\hat{p}_z^2}{2m} + \frac{1}{2}\hbar\omega\hat{z}\right)\end{aligned}$$

   If we now introduce creation and annihilation operators, $\hat{a}_j = \frac{1}{\sqrt{2\hbar m\omega}}\left(m\omega\hat{j} - i\hat{p}_j\right)$ and $\hat{a}_j^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}\left(m\omega\hat{j} + i\hat{p}_j\right)$, where $j = x, y, z$, then we can write this hamiltonian as

$$\begin{aligned}\hat{H}_0 &= \hbar\omega\left(\hat{a}_x^\dagger\hat{a}_x + \frac{1}{2}\right) + \hbar\omega\left(\hat{a}_y^\dagger\hat{a}_y + \frac{1}{2}\right) + \hbar\omega\left(\hat{a}_z^\dagger\hat{a}_z + \frac{1}{2}\right) \\ &= \hbar\omega\left(\hat{a}_x^\dagger\hat{a}_x + \hat{a}_y^\dagger\hat{a}_y + \hat{a}_z^\dagger\hat{a}_z + \frac{3}{2}\right)\end{aligned}$$

   Now, we know that the solutions to the one dimensional harmonic oscillator are $|n\rangle$ with energy $E_n = \hbar\omega(n + \frac{1}{2})$. We can write these states as $|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle$. Also, since $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$, we know that $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$. Since the hamiltonian was transformed into a sum of 3 independent one dimensional harmonic oscillators, we know that its solution is a tensor product of three one dimensional harmonic oscillator eigenstates, one for each direction, $|n\rangle \otimes |l\rangle \otimes |m\rangle$, where the $|n\rangle$ state corresponds to the x harmonic oscillator, $|l\rangle$ corresponds to the y oscillator, and $|m\rangle$ corresponds to the z oscillator. We will denote these states as $|n,l,m\rangle$ for ease of notation. Carrying over results from the 1D oscillator, we can write $|n,l,m\rangle = \frac{(\hat{a}_x^\dagger)^n(\hat{a}_y^\dagger)^l(\hat{a}_z^\dagger)^m}{\sqrt{n!l!m!}}|0,0,0\rangle$. It follows that

$$\begin{aligned}\hat{H}_0|n,l,m\rangle &= \hbar\omega\left(\hat{a}_x^\dagger\hat{a}_x|n,l,m\rangle + \hat{a}_y^\dagger\hat{a}_y|n,l,m\rangle + \hat{a}_z^\dagger\hat{a}_z|n,l,m\rangle + \frac{3}{2}|n,l,m\rangle\right)\\ &= \hbar\omega\left(n+l+m+\frac{3}{2}\right)|n,l,m\rangle\end{aligned}$$

Therefore the energy of an $|n,l,m\rangle$ state is $E_{n,l,m} = \hbar\omega\left(n+l+m+\frac{3}{2}\right)$. It follows that the ground state energy for a single particle is $E_{0,0,0} = \hbar\omega\left(0+0+0+\frac{3}{2}\right) = \frac{3}{2}\hbar\omega$ which corresponds to the state $|0,0,0\rangle$.

2. What are the symmetries of this Hamiltonian (please list at least 3)?

   Solution: The Hamiltonian is symmetric under:

   (a) Mirror reflections in the $x, y,$ and z directions.

   (b) Parity

   (c) Rotations about any axis

3. What are the first-excited states for a single particle? What is the degeneracy of the first excited states? the second excited states?

   Solution: The first excited states for a single particle are the states with energy $E_1 = \hbar\omega(0+0+1+\frac{3}{2}) = \frac{5}{2}\hbar\omega$. There are three states with this energy: $|1,0,0\rangle, |0,1,0\rangle, |0,0,1\rangle$ and so the first excited state is three-fold degenerate.

   The second excited states for a single particle are the states with energy $E_2 = \hbar\omega(2+0+0+\frac{3}{2}) = \frac{7}{2}\hbar\omega$. There are six states with this energy: $|2,0,0\rangle, |0,2,0\rangle, |0,0,2\rangle, |1,1,0\rangle, |1,0,1\rangle, |0,1,1\rangle$ and so the second excited state is six-fold degenerate.

4. Suppose instead of just one particle, we had N (non-interacting) identical particles. For N=2,3,6,7,12, and 13, what are the ground-state energy and degeneracy if:

   (a) the particles are spin-1 bosons?

   Solution: If the particles are spin-1 bosons, all of the particles will settle into the ground state. Therefore the ground state energy for N spin-1 bosons will be $NE_0 = \frac{3}{2}N\hbar\omega$. Also, each particle has three possible spin states, and since bosons can all be in the same state there is no restriction on what spins are allowed. Therefore the degeneracy for N spin-1 bosons is 3^N. Therefore, we can construct the following table:

N	Energy	Degeneracy
2	$2\left(\frac{3}{2}\hbar\omega\right) = 3\hbar\omega$	$3^2 = 9$
3	$3\left(\frac{3}{2}\hbar\omega\right) = \frac{9}{2}\hbar\omega$	$3^3 = 27$
6	$6\left(\frac{3}{2}\hbar\omega\right) = 9\hbar\omega$	$3^6 = 729$
7	$7\left(\frac{3}{2}\hbar\omega\right) = \frac{21}{2}\hbar\omega$	$3^7 = 2187$
12	$12\left(\frac{3}{2}\hbar\omega\right) = 18\hbar\omega$	$3^{12} = 531441$
13	$13\left(\frac{3}{2}\hbar\omega\right) = \frac{39}{2}\hbar\omega$	$3^{13} = 1594323$

(b) the particles are spin-1/2 fermions?

Solution: If the particles are spin-1/2 fermions, then no two particles can share the same state. For spin-1/2, there are two possible spin states, so every $|n, m, l\rangle$ state can hold two particles. Therefore there are 2 states with energy $E_0 = \frac{3}{2}\hbar\omega$, 6 states with energy $E_1 = \frac{5}{2}\hbar\omega$, and 12 states with energy $E_2 = \frac{7}{2}\hbar\omega$. The fermions will settle into the lowest energy states available. We can use this information to construct the following table:

N	Energy	Degeneracy
2	$2\left(\frac{3}{2}\hbar\omega\right) = 3\hbar\omega$	No Degeneracy
3	$2\left(\frac{3}{2}\hbar\omega\right) + 1\left(\frac{5}{2}\hbar\omega\right) = \frac{11}{2}\hbar\omega$	$\binom{6}{1} = 6$
6	$2\left(\frac{3}{2}\hbar\omega\right) + 4\left(\frac{5}{2}\hbar\omega\right) = 13\hbar\omega$	$\binom{6}{4} = 15$
7	$2\left(\frac{3}{2}\hbar\omega\right) + 5\left(\frac{5}{2}\hbar\omega\right) = \frac{31}{2}\hbar\omega$	$\binom{6}{5} = 6$
12	$2\left(\frac{3}{2}\hbar\omega\right) + 6\left(\frac{5}{2}\hbar\omega\right) + 4\left(\frac{7}{2}\hbar\omega\right) = 32\hbar\omega$	$\binom{12}{4} = 495$
13	$2\left(\frac{3}{2}\hbar\omega\right) + 6\left(\frac{5}{2}\hbar\omega\right) + 5\left(\frac{7}{2}\hbar\omega\right) = \frac{71}{2}\hbar\omega$	$\binom{12}{5} = 792$

B. Single-particle plus perturbing potential

Consider adding the potential $\hat{V} = \lambda\left(\hat{x}\hat{y} + \hat{y}\hat{z} + \hat{x}\hat{z}\right)$.

1. Compute the matrix elements of $\hat{V}$ in the basis of eigenstates of $\hat{H}_0$.

Solution: The matrix elements of $\hat{V}$ are given by

$$\begin{aligned}\langle n', l', m'|\hat{V}|n, l, m\rangle &= \lambda\langle n', l', m'|\left(\hat{x}\hat{y} + \hat{y}\hat{z} + \hat{x}\hat{z}\right)|n, l, m\rangle \\ &= \lambda\left(\langle n', l', m'|\hat{x}\hat{y}|n, l, m\rangle + \langle n', l', m'|\hat{y}\hat{z}|n, l, m\rangle + \langle n', l', m'|\hat{x}\hat{z}|n, l, m\rangle\right)\end{aligned}$$

We will now compute $\langle n', l', m'|\hat{x}\hat{y}|n, l, m\rangle$. We know that we can write $\hat{x}$ and $\hat{y}$ in terms of the creation and annihilation operators as $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_x + \hat{a}_x^\dagger\right)$ and $\hat{y} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_y + \hat{a}_y^\dagger\right)$. Therefore, we can write:

$$\begin{aligned}\langle n', l', m'|\hat{x}\hat{y}|n, l, m\rangle &= \frac{\hbar}{2m\omega}\langle n', l', m'|\left(\hat{a}_x + \hat{a}_x^\dagger\right)\left(\hat{a}_y + \hat{a}_y^\dagger\right)|n, l, m\rangle \\ &= \frac{\hbar}{2m\omega}\langle n', l', m'|\left(\hat{a}_x + \hat{a}_x^\dagger\right)\left(\sqrt{l}|n, l-1, m\rangle + \sqrt{l+1}|n, l+1, m\rangle\right) \\ &= \frac{\hbar}{2m\omega}\langle n', l', m'|\left(\sqrt{nl}|n-1, l-1, m\rangle + \sqrt{n(l+1)}|n-1, l+1, m\rangle + \right. \\ &\qquad \left. \sqrt{l(n+1)}|n+1, l-1, m\rangle + \sqrt{(n+1)(l+1)}|n+1, l+1, m\rangle\right) \\ &= \frac{\hbar}{2m\omega}\delta_{m',m}\left[\delta_{n',n-1}\left(\sqrt{nl}\delta_{l',l-1} + \sqrt{n(l+1)}\delta_{l',l+1}\right) + \right. \\ &\qquad \left. \delta_{n',n+1}\left(\sqrt{l(n+1)}\delta_{l',l-1} + \sqrt{(n+1)(l+1)}\delta_{l',l+1}\right)\right]\end{aligned}$$

A similar argument can be applied to the other terms to give:

$$\begin{aligned}\langle n', l', m'|\hat{y}\hat{z}|n, l, m\rangle &= \frac{\hbar}{2m\omega}\delta_{n',n}\Big[\delta_{l',l-1}\left(\sqrt{ml}\delta_{m',m-1} + \sqrt{l(m+1)}\delta_{m',m+1}\right) + \\ &\qquad \delta_{l',l+1}\left(\sqrt{m(l+1)}\delta_{m',m-1} + \sqrt{(m+1)(l+1)}\delta_{m',m+1}\right)\Big] \\ \langle n', l', m'|\hat{x}\hat{z}|n, l, m\rangle &= \frac{\hbar}{2m\omega}\delta_{l',l}\Big[\delta_{n',n-1}\left(\sqrt{nm}\delta_{m',m-1} + \sqrt{n(m+1)}\delta_{m',m+1}\right) + \\ &\qquad \delta_{n',n+1}\left(\sqrt{m(n+1)}\delta_{m',m-1} + \sqrt{(m+1)(n+1)}\delta_{m',m+1}\right)\Big]\end{aligned}$$

Therefore, the matrix element is given by:

$$\begin{aligned}\langle n', l', m'|\hat{V}|n, l, m\rangle = \frac{\hbar\lambda}{2m\omega}\Big\{&\delta_{m',m}\Big[\delta_{n',n-1}\left(\sqrt{nl}\delta_{l',l-1} + \sqrt{n(l+1)}\delta_{l',l+1}\right) + \\ &\quad \delta_{n',n+1}\left(\sqrt{l(n+1)}\delta_{l',l-1} + \sqrt{(n+1)(l+1)}\delta_{l',l+1}\right)\Big] + \\ &\delta_{n',n}\Big[\delta_{l',l-1}\left(\sqrt{ml}\delta_{m',m-1} + \sqrt{l(m+1)}\delta_{m',m+1}\right) + \\ &\quad \delta_{l',l+1}\left(\sqrt{m(l+1)}\delta_{m',m-1} + \sqrt{(m+1)(l+1)}\delta_{m',m+1}\right)\Big] + \\ &\delta_{l',l}\Big[\delta_{n',n-1}\left(\sqrt{nm}\delta_{m',m-1} + \sqrt{n(m+1)}\delta_{m',m+1}\right) + \\ &\quad \delta_{n',n+1}\left(\sqrt{m(n+1)}\delta_{m',m-1} + \sqrt{(m+1)(n+1)}\delta_{m',m+1}\right)\Big]\Big\}\end{aligned} \tag{2}$$

2. When can we treat λ as a small perturbation?

   Solution: λ has units of energy per square length. The energy scale of the problem is $\hbar\omega$ and the length scale of the problem is $\sqrt{\frac{\hbar}{2m\omega}}$. Therefore the energy per square length scale of the problem is $\hbar\omega\left(\frac{m\omega}{\hbar}\right) = m\omega^2$. Therefore, we can treat λ as a small perturbation when $\lambda \ll m\omega^2$.

3. Compute the ground-state energy of a single particle with Hamiltonian $\hat{H}_0+\hat{V}$ perturbatively to second order in λ.

   Solution: The ground state energy of the bare hamiltonian is $E_0^0 = \frac{3}{2}\hbar\omega$. The first order correction to the ground state energy is $E_0^1 = \langle 0, 0, 0|\hat{V}|0, 0, 0\rangle$. Using the expression for the matrix element given in equation 2, we find that $E_0^1 = 0$.

   The second order correction to the ground state energy is:

$$E_0^2 = \sum_{\substack{n=0 \\ (n,l,m)\neq(0,0,0)}}^{\infty}\sum_{m=0}^{\infty}\sum_{l=0}^{\infty}\frac{\left|\langle n, l, m|\hat{V}|0, 0, 0\rangle\right|^2}{E_0^0 - E_{n,l,m}^0}$$

   Using the expression for the matrix element given by equation 2, we can write the energy correction as

$$
\begin{aligned}
E_0^2 &= \left(\frac{\hbar\lambda}{2m\omega}\right)^2 \sum_{\substack{n=0 \\ (n,l,m)\neq(0,0,0)}}^{\infty} \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \frac{|\delta_{m,0}\delta_{n,1}\delta_{l,1} + \delta_{n,0}\delta_{l,1}\delta_{m,1} + \delta_{l,0}\delta_{n,1}\delta_{m,1}|^2}{\frac{3}{2}\hbar\omega - \hbar\omega(n+m+l+\frac{3}{2})} \\
&= -\frac{1}{\hbar\omega}\left(\frac{\hbar\lambda}{2m\omega}\right)^2 \sum_{\substack{n=0 \\ (n,l)\neq(0,0)}}^{\infty} \sum_{m=0}^{\infty} \left[\frac{|\delta_{n,1}\delta_{m,1}|^2}{n+m} + \frac{|\delta_{m,0}\delta_{n,1} + \delta_{n,0}\delta_{m,1}|^2}{n+m+1}\right] \\
&= -\frac{\hbar\lambda^2}{4m^2\omega^3} \sum_{n=0}^{\infty} \left[\frac{|\delta_{n,1}|^2}{n+1} + \frac{|\delta_{n,1}|^2}{n+1} + \frac{|\delta_{n,0}|^2}{n+2}\right] \\
&= -\frac{\hbar\lambda^2}{4m^2\omega^3}\left[\frac{1}{2} + \frac{1}{2} + \frac{1}{2}\right] \\
&= -\frac{3\hbar\lambda^2}{8m^2\omega^3}
\end{aligned}
$$

Therefore, to second order in λ, the ground state energy is

$$
\boxed{E_0 = \frac{3}{2}\hbar\omega - \frac{3\hbar\lambda^2}{8m^2\omega^3}} \tag{3}
$$

4. Compute the first excited state energies of $\hat{H}_0 + \hat{V}$ to first order in λ.

   Solution: The first excited energy of the bare hamiltonian is $E_1^0 = \frac{5}{2}\hbar\omega$. There are three eigenstates of the bare hamiltonian that share this energy, $|1,0,0\rangle, |0,1,0\rangle, |0,0,1\rangle$. To begin finding the first order corrections, we will find the matrix elements of the perturbation in the degenerate subspace. Using the expression for a general matrix element given by equation 2, we can show that:

$$
\begin{aligned}
&\langle 1,0,0|\hat{V}|1,0,0\rangle = 0, \qquad \langle 1,0,0|\hat{V}|0,1,0\rangle = \frac{\hbar\lambda}{2m\omega}, \qquad \langle 1,0,0|\hat{V}|0,0,1\rangle = \frac{\hbar\lambda}{2m\omega} \\
&\langle 0,1,0|\hat{V}|1,0,0\rangle = \frac{\hbar\lambda}{2m\omega}, \qquad \langle 0,1,0|\hat{V}|0,1,0\rangle = 0, \qquad \langle 0,1,0|\hat{V}|0,0,1\rangle = \frac{\hbar\lambda}{2m\omega} \\
&\langle 0,0,1|\hat{V}|1,0,0\rangle = \frac{\hbar\lambda}{2m\omega}, \qquad \langle 0,0,1|\hat{V}|0,1,0\rangle = \frac{\hbar\lambda}{2m\omega} \qquad \langle 0,0,1|\hat{V}|0,0,1\rangle = 0
\end{aligned}
$$

   Therefore, the matrix representation of $\hat{V}$ in the degenerate subspace is

$$
\frac{\hbar\lambda}{2m\omega}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}
$$

   Now, to find the eigenvalues of the matrix, we will set

$$
0 = \det\begin{pmatrix} -x & \frac{\hbar\lambda}{2m\omega} & \frac{\hbar\lambda}{2m\omega} \\ \frac{\hbar\lambda}{2m\omega} & -x & \frac{\hbar\lambda}{2m\omega} \\ \frac{\hbar\lambda}{2m\omega} & \frac{\hbar\lambda}{2m\omega} & -x \end{pmatrix}
$$

$$
0 = -x\left(x^2 - \left(\frac{\hbar\lambda}{2m\omega}\right)^2\right) + \frac{\hbar\lambda}{2m\omega}\left(\frac{\hbar\lambda}{2m\omega}x + \left(\frac{\hbar\lambda}{2m\omega}\right)^2\right) + \frac{\hbar\lambda}{2m\omega}\left(\frac{\hbar\lambda}{2m\omega}x + \left(\frac{\hbar\lambda}{2m\omega}\right)^2\right)
$$

solving this cubic gives that the eigenvalues of the matrix are $x_{1,2} = -\frac{\hbar\lambda}{2m\omega}$ and $x_3 = \frac{\hbar\lambda}{m\omega}$
Now, we can find the eigenvectors, $\vec{v}_i$, of this matrix by solving the system

$$\begin{pmatrix} -x_i & \frac{\hbar\lambda}{2m\omega} & \frac{\hbar\lambda}{2m\omega} \\ \frac{\hbar\lambda}{2m\omega} & -x_i & \frac{\hbar\lambda}{2m\omega} \\ \frac{\hbar\lambda}{2m\omega} & \frac{\hbar\lambda}{2m\omega} & -x_i \end{pmatrix} \vec{v}_i = \vec{0}$$

for $x_i = x_{1,2}$, we obtain

$$\frac{\hbar\lambda}{2m\omega} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \vec{v} = \vec{0}$$

This has two solutions,

$$\vec{v}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad \vec{v}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

for $x_i = x_3$ we obtain

$$\frac{\hbar\lambda}{2m\omega} \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} \vec{v} = \vec{0}$$

This has the solution

$$\vec{v}_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Therefore we have the states $|a\rangle = \frac{1}{\sqrt{2}}\left(|1,0,0\rangle - |0,1,0\rangle\right)$ with energy $E_a = \frac{5}{2}\hbar\omega - \frac{\hbar\lambda}{2m\omega}$,
$|b\rangle = \frac{1}{\sqrt{2}}\left(|1,0,0\rangle - |0,0,1\rangle\right)$ with energy $E_b = \frac{5}{2}\hbar\omega - \frac{\hbar\lambda}{2m\omega}$,
and $|c\rangle = \frac{1}{\sqrt{3}}\left(|1,0,0\rangle + |0,1,0\rangle + |0,0,1\rangle\right)$ with energy $E_c = \frac{5}{2}\hbar\omega + \frac{\hbar\lambda}{m\omega}$

5. Suppose the particle is initially in the ground-state of H_0, and at time $t = 0$, we suddenly switch on a time-dependent potential $\hat{V}(t) = \lambda(t)\left(\hat{x}\hat{y} + \hat{y}\hat{z} + \hat{x}\hat{z}\right)$, with $\lambda(t) = \lambda_0 \cos\Omega t$. Using 1st order time-dependent perturbation theory, compute the probability the particle transitions into an excited state a time t later. Sketch your answer as a function of t.

   Solution: After a time t, the particle is in the state $|\psi\rangle = \sum_{n=0}^{\infty} c_{n,l,m}(t)|n,l,m\rangle$. It is a standard result in time-dependent perturbation theory that these coefficients are given to first order by

$$c_{n,l,m} = \frac{1}{i\hbar}\int_{t_1}^{t_2} \langle n,l,m|\hat{V}|n',l',m'\rangle e^{i\frac{E_n - E_k}{\hbar}t'} dt'$$

where t_1 is the initial time, $|n', l', m'\rangle$ is the initial state, t_2 is the final time and $|n, l, m\rangle$ is the final state. For this problem, $t_1 = 0$, $t_2 = t$, and the initial state is $|0, 0, 0\rangle$. Therefore, these coefficients in this problem are given by

$$c_{n'l'm} = \frac{1}{i\hbar} \int_0^t \langle n, l, m|\hat{V}|0, 0, 0\rangle e^{i\frac{\hbar\omega(n+m+l+\frac{3}{2})-\frac{3}{2}\hbar\omega}{\hbar}t'} dt'$$

simplifying and using the expression for the matrix element given by equation 2, we find

$$\begin{aligned}
c_{n'l'm} &= \frac{1}{i\hbar}\left(\frac{\hbar}{2m\omega}\right) \int_0^t \left(\delta_{m,0}\delta_{n,1}\delta_{l,1} + \delta_{n,0}\delta_{l,1}\delta_{m,1} + \delta_{l,0}\delta_{n,1}\delta_{m,1}\right) e^{i(n+m+l)\omega t'} \lambda(t')dt' \\
&= -\left(\frac{i\lambda_0}{2m\omega}\right) \int_0^t \left(\delta_{m,0}\delta_{n,1}\delta_{l,1} + \delta_{n,0}\delta_{l,1}\delta_{m,1} + \delta_{l,0}\delta_{n,1}\delta_{m,1}\right) e^{i(n+m+l)\omega t'} \cos(\Omega t')dt' \\
&= -\left(\frac{i\lambda_0}{2m\omega}\right) \left(\delta_{m,0}\delta_{n,1}\delta_{l,1} + \delta_{n,0}\delta_{l,1}\delta_{m,1} + \delta_{l,0}\delta_{n,1}\delta_{m,1}\right) \int_0^t \cos((n+m+l)\omega t')\cos(\Omega t') \\
&\quad + i\sin((n+m+l)\omega t')\cos(\Omega t')dt'
\end{aligned}$$

Now using the results $\int_0^t \cos(ax)\cos(bx)dx = \frac{a\sin(at)\cos(bt)-b\cos(at)\sin(bt)}{a^2-b^2}$ and $\int_0^t \sin(ax)\cos(bx)dx = \frac{a-b\sin(at)\sin(bt)-a\cos(at)\cos(bt)}{a^2-b^2}$, we can write

$$\begin{aligned}
c_{n,l,m} = &-\left(\frac{i\lambda_0}{2m\omega}\right) \left(\delta_{m,0}\delta_{n,1}\delta_{l,1} + \delta_{n,0}\delta_{l,1}\delta_{m,1} + \delta_{l,0}\delta_{n,1}\delta_{m,1}\right) \\
&\times \left[\frac{(n+m+l)\omega\sin((n+m+l)\omega t)\cos(\Omega t) - \Omega\cos((n+m+l)\omega t)\sin(\Omega t)}{(n+m+l)^2\omega^2 - \Omega^2}\right. \\
&\left. + i\left(\frac{(n+m+l)\omega - \Omega\sin((n+m+l)\omega t)\sin(\Omega t) - (n+m+l)\omega\cos((n+m+l)\omega t)\cos(\Omega t)}{(n+m+l)^2\omega^2 - \Omega^2}\right)\right]
\end{aligned}$$

Now, the probability of transitioning to an excited state is given by

$$P = \sum_{\substack{n=0 \\ (n,l,m)\neq(0,0,0)}}^{\infty} \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} |c_{n,l,m}|^2$$

But

$$\begin{aligned}
|c_{n,l,m}|^2 = &\left(\frac{\lambda_0}{2m\omega}\right)^2 \left(\delta_{m,0}\delta_{n,1}\delta_{l,1} + \delta_{n,0}\delta_{l,1}\delta_{m,1} + \delta_{l,0}\delta_{n,1}\delta_{m,1}\right)^2 \\
&\times \left[\left(\frac{(n+m+l)\omega\sin((n+m+l)\omega t)\cos(\Omega t) - \Omega\cos((n+m+l)\omega t)\sin(\Omega t)}{(n+m+l)^2\omega^2 - \Omega^2}\right)^2\right. \\
&\left. + \left(\frac{(n+m+l)\omega - \Omega\sin((n+m+l)\omega t)\sin(\Omega t) - (n+m+l)\omega\cos((n+m+l)\omega t)\cos(\Omega t)}{(n+m+l)^2\omega^2 - \Omega^2}\right)^2\right]
\end{aligned}$$

and so

$$
\begin{aligned}
P = & \sum_{\substack{n=0 \\ (n,l,m)\neq(0,0,0)}}^{\infty} \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} \left(\frac{\lambda_0}{2m\omega}\right)^2 \left(\delta_{m,0}\delta_{n,1}\delta_{l,1} + \delta_{n,0}\delta_{l,1}\delta_{m,1} + \delta_{l,0}\delta_{n,1}\delta_{m,1}\right)^2 \\
& \times \left[\left(\frac{(n+m+l)\omega \sin((n+m+l)\omega t)\cos(\Omega t) - \Omega \cos((n+m+l)\omega t)\sin(\Omega t)}{(n+m+l)^2\omega^2 - \Omega^2}\right)^2\right. \\
& \left. + \left(\frac{(n+m+l)\omega - \Omega \sin((n+m+l)\omega t)\sin(\Omega t) - (n+m+l)\omega \cos((n+m+l)\omega t)\cos(\Omega t)}{(n+m+l)^2\omega^2 - \Omega^2}\right)^2\right] \\
= & \frac{3\lambda_0^2}{4m^2\omega^2}\left[\left(\frac{2\omega \sin(2\omega t)\cos(\Omega t) - \Omega\cos(2\omega t)\sin(\Omega t)}{4\omega^2 - \Omega^2}\right)^2 + \left(\frac{2\omega - \Omega \sin(2\omega t)\sin(\Omega t) - 2\omega \cos(2\omega t)\cos(\Omega t)}{4\omega^2-\Omega^2}\right)^2\right]
\end{aligned}
$$

Using Mathematica, we can plot this transition probability as a function of time.

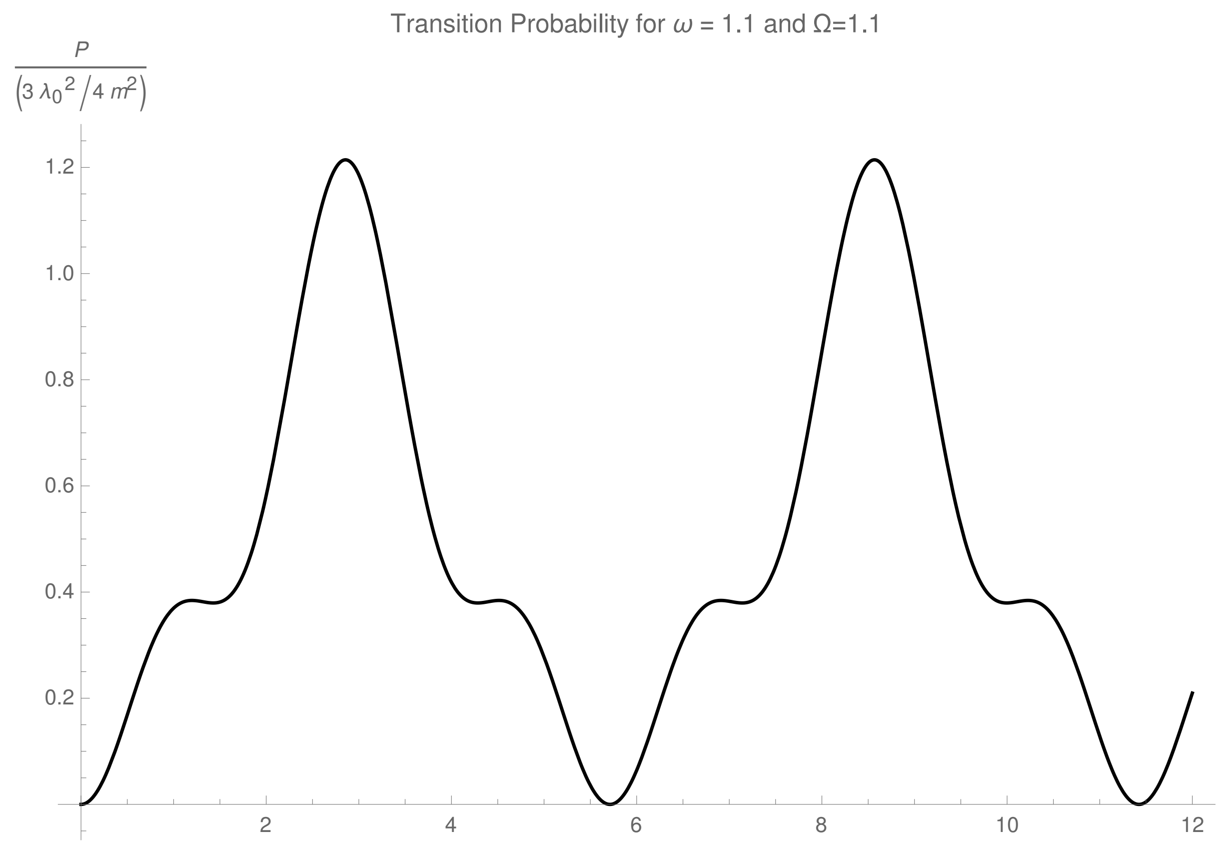

FIG. 1: Plot of the ratio of the transition probability, P to $\frac{3\lambda_0^2}{4m^2}$ vs t with $\omega = 1.1$ and $\Omega = 1.1$.

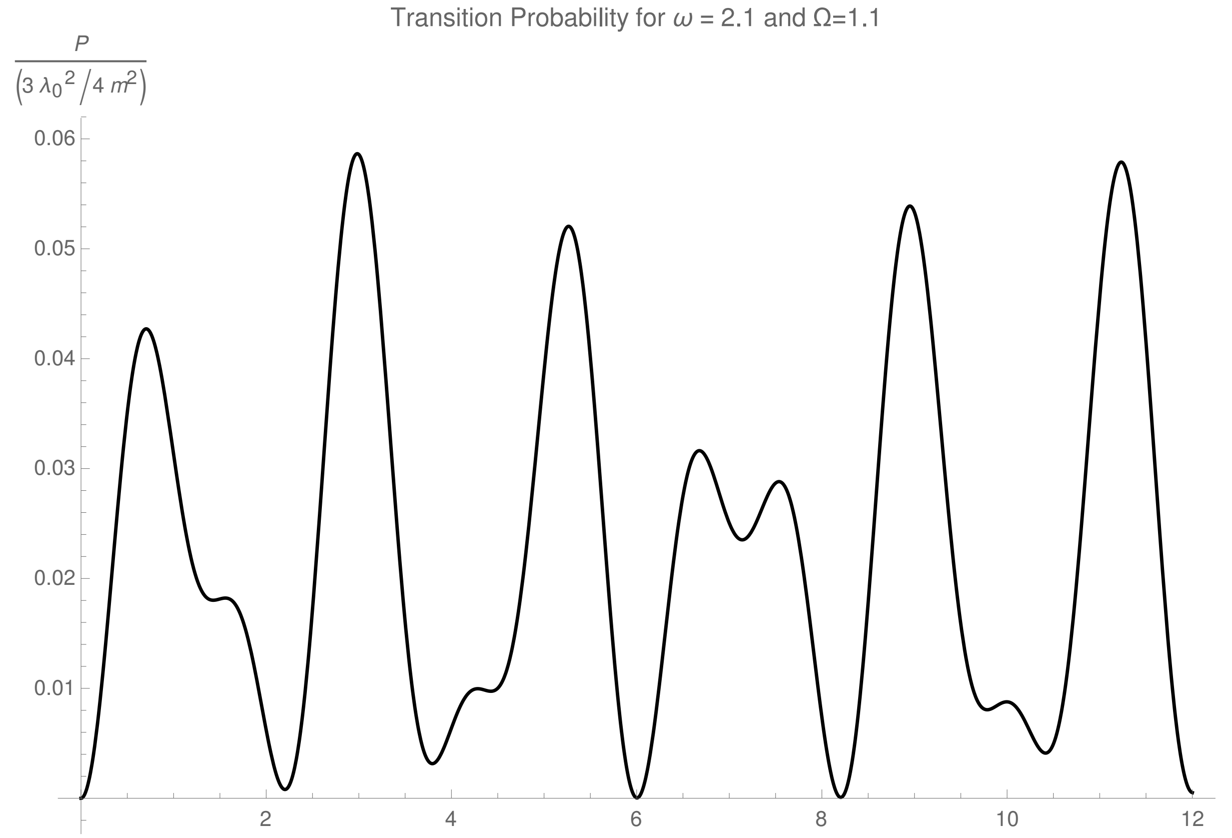

FIG. 2: Plot of the ratio of the transition probability, P to $\frac{3\lambda_0^2}{4m^2}$ vs t with $\omega = 2.1$ and $\Omega = 1.1$.

C. Electric field transitions

Suppose we apply an oscillating electric field of strength E_0 and frequency ω. For all of the following examples, treat this field within the dipole approximation.

1. Consider the ground state and first excited states of $\hat{H}_0$. Which transitions between these levels are "dipole allowed" (i.e. not forced to be zero by selection rules from parity and rotation symmetry) if the light is:

   (a) z-polarized?

   Solution: For z polarized light, the transition probabilities will involve a matrix element of the form $\langle n, l, m|\hat{z}|0, 0, 0\rangle$. We know that $M_z|0, 0, 0\rangle = |0, 0, 0\rangle$ and that $M_z|n, l, m\rangle = (-1)^m|n, l, m\rangle$, and also that $M_z\hat{z}M_z^\dagger = -\hat{z}$. Therefore

   $$\langle n, l, m|\hat{z}|0, 0, 0\rangle = \langle n, l, m|M_z^\dagger M_z\hat{z}M_z^\dagger M_z|0, 0, 0\rangle = (-1)^{m+1}\langle n, l, m|\hat{z}|0, 0, 0\rangle$$

   Therefore, if m is even, we have $\langle n, l, m|\hat{z}|0, 0, 0\rangle = -\langle n, l, m|\hat{z}|0, 0, 0\rangle \implies \langle n, l, m|\hat{z}|0, 0, 0\rangle = 0$. Therefore only transitions to states with odd values of m are allowed. So the only first excited state transition that is allowed is to the $|0, 0, 1\rangle$ state.

   (b) right-hand circularly polarized?

Solution: We will start by finding the matrix elements of L_z in the subspace spanned by the first excited states. We know that $M_x L_z M_x^\dagger = M_x(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)M_x^\dagger = -L_z$ and similarly, $M_y L_z M_y^\dagger = -L_z$. Now consider,

$$\langle n', l', m'|L_z|n, l, m\rangle = \langle n', l', m'|M_x^\dagger M_x L_z M_x^\dagger M_x|n, l, m\rangle = (-1)^{n'+n+1}\langle n', l', m'|L_z|n, l, m\rangle$$

Therefore it follows that if $n' = n$ this matrix element is zero. Similarly, consider:

$$\langle n', l', m'|L_z|n, l, m\rangle = \langle n', l', m'|M_y^\dagger M_y L_z M_y^\dagger M_y|n, l, m\rangle = (-1)^{l'+l+1}\langle n', l', m'|L_z|n, l, m\rangle$$

Therefore it follows that if $l' = l$ this matrix element is zero.

So for the frist excited state subspace, we only need to compute $\langle 1,0,0|L_z|0,1,0\rangle$ and $\langle 0,1,0|L_z|1,0,0\rangle$.

$$\begin{aligned}
\langle 1,0,0|L_z|0,1,0\rangle &= \langle 1,0,0|(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)|0,1,0\rangle \\
&= i\frac{\hbar}{2}\langle 1,0,0|\left[(\hat{a}_x + \hat{a}_x^\dagger)(\hat{a}_y^\dagger - \hat{a}_y) - (\hat{a}_y + \hat{a}_y^\dagger)(\hat{a}_x^\dagger - \hat{a}_x)\right]|0,1,0\rangle \\
&= i\frac{\hbar}{2}\left[\langle 1,0,0|(\hat{a}_x + \hat{a}_x^\dagger)(\sqrt{2}|0,2,0\rangle - |0,0,0\rangle) - \langle 1,0,0|(\hat{a}_y + \hat{a}_y^\dagger)|1,1,0\rangle\right] \\
&= i\frac{\hbar}{2}\left[\langle 1,0,0|(\sqrt{2}|1,2,0\rangle - |1,0,0\rangle) - \langle 1,0,0|(|1,0,0\rangle + \sqrt{2}|1,2,0\rangle)\right] \\
&= -i\frac{\hbar}{2} \times 2 = -i\hbar
\end{aligned}$$

Then, $\langle 0,1,0|L_z|1,0,0\rangle = \langle 1,0,0|L_z|0,1,0\rangle^* = i\hbar$. So the matrix of L_z in the first excited state subspace is

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

This matrix has the eigenvectors:

$$\begin{aligned}
|a\rangle &= |0,0,1\rangle \quad \text{with eigenvalue: } 0 \\
|b\rangle &= \frac{1}{\sqrt{2}}\left(-i|1,0,0\rangle + |0,1,0\rangle\right) \quad \text{with eigenvalue: } \hbar \\
|c\rangle &= \frac{1}{\sqrt{2}}\left(i|1,0,0\rangle + |0,1,0\rangle\right) \quad \text{with eigenvalue: } -\hbar
\end{aligned}$$

In the $\{|a\rangle, |b\rangle, |c\rangle\}$ basis, we have $L_z|j\rangle = m_j\hbar$, where $j = a, b, c$ and $m_j = 0, 1, -1$. Now, the rotation operator acts on these states in the following way:

$$R_z(\theta)|j\rangle = e^{-iL_z\theta/\hbar}|j\rangle = e^{-im_j\theta}|j\rangle$$

and also that $R_z(\theta)|0,0,0\rangle = |0,0,0\rangle$. For right-hand circularly polarized light, the transition probabilities will involve a matrix element of the form $\langle j|(\hat{x} + i\hat{y})|0,0,0\rangle$. We know that $R_z(\theta)(\hat{x} + i\hat{y})R_z^\dagger(\theta) = e^{i\theta}$, and so

$$\begin{aligned}
\langle j|(\hat{x} + i\hat{y})|0,0,0\rangle &= \langle j|R_z^\dagger(\theta)R_z(\theta)(\hat{x} + i\hat{y})R_z^\dagger(\theta)R_z(\theta)|0,0,0\rangle \\
&= e^{i\theta(m_j+1)}\langle j|(\hat{x} + i\hat{y})|0,0,0\rangle
\end{aligned}$$

So if $m_j \neq -1$, then we have $\langle j|(\hat{x}+i\hat{y})|0,0,0\rangle = e^{i\phi}\langle j|(\hat{x}+i\hat{y})|0,0,0\rangle$, $\phi \neq 0$, which implies that $\langle j|(\hat{x}+i\hat{y})|0,0,0\rangle = 0$. Therefore the only allowed transition for right hand circularly polarized light is to the $|c\rangle = \frac{1}{\sqrt{2}}(i|1,0,0\rangle + |0,1,0\rangle)$ state.

(c) left-hand circularly polarized?

Solution: For left-hand circularly polarized light, the transition probabilities will involve a matrix element of the form $\langle j|(\hat{x}-i\hat{y})|0,0,0\rangle$. We know that $R_z(\theta)(\hat{x}-i\hat{y})R_z^\dagger(\theta) = e^{-i\theta}$, and so

$$\begin{aligned}\langle j|(\hat{x}+i\hat{y})|0,0,0\rangle &= \langle j|R_z^\dagger(\theta)R_z(\theta)(\hat{x}+i\hat{y})R_z^\dagger(\theta)R_z(\theta)|0,0,0\rangle \\ &= e^{i\theta(m_j-1)}\langle j|(\hat{x}+i\hat{y})|0,0,0\rangle\end{aligned}$$

So if $m_j \neq 1$, then we have $\langle j|(\hat{x}+i\hat{y})|0,0,0\rangle = e^{i\phi}\langle j|(\hat{x}+i\hat{y})|0,0,0\rangle$, $\phi \neq 0$, which implies that $\langle j|(\hat{x}+i\hat{y})|0,0,0\rangle = 0$. Therefore the only allowed transition for left hand circularly polarized light is to the $|b\rangle = \frac{1}{\sqrt{2}}(-i|1,0,0\rangle + |0,1,0\rangle)$ state.

(d) x-polarized?

Solution: For x polarized light, the transition probabilities will involve a matrix element of the form $\langle n,l,m|\hat{x}|0,0,0\rangle$. We know that $M_x|0,0,0\rangle = |0,0,0\rangle$ and that $M_x|n,l,m\rangle = (-1)^n|n,l,m\rangle$, and also that $M_x\hat{x}M_x^\dagger = -\hat{x}$. Therefore

$$\langle n,l,m|\hat{x}|0,0,0\rangle = \langle n,l,m|M_x^\dagger M_x\hat{z}M_x^\dagger M_x|0,0,0\rangle = (-1)^{n+1}\langle n,l,m|\hat{x}|0,0,0\rangle$$

Therefore, if n is even, we have $\langle n,l,m|\hat{x}|0,0,0\rangle = -\langle n,l,m|\hat{x}|0,0,0\rangle \implies \langle n,l,m|\hat{x}|0,0,0\rangle = 0$. Therefore only transitions to states with odd values of n are allowed. So the only first excited state transition that is allowed is to the $|1,0,0\rangle$ state.

2. For z-polarized light, what light frequency do we need to drive transitions from the ground-state to a first excited state? For this frequency, what is the transition rate (using Fermi's golden rule)?

Solution: The photons of light with frequency Ω carry an energy $E_p = \hbar\Omega$. In order to drive a transition from the ground to first excited states, the photon must carry an energy $E_1 - E_0 = \frac{5}{2}\hbar\omega - \frac{3}{2}\hbar\omega = \hbar\omega$. Therefore, the light must have frequency ω, the natural frequency of the harmonic oscillator.

We showed in the last problem that the only allowed transition is to the $|0,0,1\rangle$ state. Now, in the dipole approximation, z polarized light can be described by a potential $\hat{V} = qE_0\hat{z}$. For transition, Fermi's golden rule says:

$$\begin{aligned}\Gamma_{i\to f} &= \frac{2\pi}{\hbar}|\langle 0,0,1|qE_0\hat{z}|0,0,0\rangle|^2\delta(\hbar\omega) \\ &= \frac{2\pi}{\hbar}q^2E_0^2\,\frac{\hbar}{2m\omega}\bigg)\,|\langle 0,0,1|(\hat{a}_z+\hat{a}_z^\dagger)|0,0,0\rangle|^2\delta(\hbar\omega) \\ &= \frac{2\pi}{\hbar}q^2E_0^2\,\frac{\hbar}{2m\omega}\bigg)\,|\langle 0,0,1|0,0,1\rangle|^2\delta(\hbar\omega) \\ &= \frac{\pi q^2E_0^2}{m\omega}\delta(\hbar\omega)\end{aligned}$$

But if we know that the light is shining at the required frequency, we can neglect the delta function and find that the transition rate is

$$\boxed{\Gamma = \frac{\pi q^2E_0^2}{m\omega}} \tag{4}$$