Physics 137B, Fall 2007, Moore
Problem Set 5 Solutions

1.

Our unperturbed Hamiltonian is \( H_0 = \frac{g \mu_B B}{\hbar} S_z \), with eigenstates

\[
|\downarrow\rangle, \quad E_\downarrow = -\frac{g \mu_B B}{2} \equiv -\epsilon, \\
|\uparrow\rangle, \quad E_\uparrow = +\frac{g \mu_B B}{2} = +\epsilon.
\]

At time \( t = 0 \) we introduce the perturbation \( H' = \frac{g \mu_B B'}{\hbar} S_x \), whose eigenstates we will label as

\[
|1\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle - |\uparrow\rangle), \quad E_1 = -\frac{g \mu_B B'}{2}, \\
|2\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle + |\uparrow\rangle), \quad E_2 = +\frac{g \mu_B B'}{2}.
\]

(a) We start in the state \( |\psi(0)\rangle = |\downarrow\rangle \) at time \( t = 0 \). According to the formalism of time-dependent perturbation theory, we can expand our state \( |\psi(t)\rangle \) for \( t > 0 \) as

\[
|\psi(t)\rangle = c_\downarrow(t) e^{-i E_\downarrow t/\hbar} |\downarrow\rangle + c_\uparrow(t) e^{-i E_\uparrow t/\hbar} |\uparrow\rangle.
\]

To first order, the time-dependent coefficients \( c_\downarrow(t) \) and \( c_\uparrow(t) \) are given by

\[
c_\downarrow(t) = 1 + (i\hbar)^{-1} \int_0^t \langle \downarrow | H' | \downarrow \rangle \, dt' \\
= 1,
\]
\[ c_1(t) = (\imath \hbar)^{-1} \int_0^t \langle \uparrow | H' | \downarrow \rangle e^{\imath \omega t'} dt' \]
\[ = \frac{1}{\imath \hbar} \frac{g \mu_B B'}{2} \int_0^t e^{\imath \omega t'} dt' \]
\[ = \frac{1}{\imath \hbar} \frac{g \mu_B B'}{2} \frac{1}{\imath \omega} (e^{\imath \omega t} - 1) \]
\[ = -i \frac{B'}{B} e^{\imath \omega t/2} \sin \frac{\omega t}{2} , \]
where \( \omega = (E_1 - E_\downarrow)/\hbar = 2\epsilon/\hbar \) is the Bohr frequency. Thus our time-evolved state can be written to first order as
\[ |\psi(t)\rangle = e^{\imath \epsilon t/\hbar} |\downarrow\rangle + \left( -i B'/B e^{\imath \omega t/2} \sin \frac{\omega t}{2} \right) e^{-\imath \epsilon t/\hbar} |\uparrow\rangle \]
\[ = e^{\imath \omega t/2} |\downarrow\rangle - i B'/B \sin \frac{\omega t}{2} |\uparrow\rangle . \]

The transition probability is given by
\[ P_{\uparrow\downarrow}(t) = |\langle \uparrow | \psi(t) \rangle|^2 = \left( \frac{B'}{B} \right)^2 \sin^2 \frac{\omega t}{2} , \]

exactly as you calculated in the previous homework assignment.

To calculate the expectation value of \( H_0 \), we need
\[ \langle \psi(t) | H_0 | \psi(t) \rangle = \left( e^{-\imath \omega t/2} |\downarrow\rangle + i \frac{B'}{B} \sin \frac{\omega t}{2} |\uparrow\rangle \right) \left( e^{-\imath \omega t/2} (-\epsilon) |\downarrow\rangle + i \frac{B'}{B} \sin \frac{\omega t}{2} (+\epsilon) |\uparrow\rangle \right) \]
\[ = -\epsilon \left[ 1 - \left( \frac{B'}{B} \right)^2 \sin^2 \frac{\omega t}{2} \right] . \]

This is of order \((B'/B)^2\), whereas \( |\psi(t)\rangle \) is only normalized to order \( B'/B \). So we should divide by
\[ \langle \psi(t) | \psi(t) \rangle = 1 + \left( \frac{B'}{B} \right)^2 \sin^2 \frac{\omega t}{2} . \]

Expanding the denominator to leading order we obtain the expectation value
\[ \langle H_0 \rangle = \frac{\langle \psi(t) | H_0 | \psi(t) \rangle}{\langle \psi(t) | \psi(t) \rangle} = -\epsilon \left[ 1 - 2 \left( \frac{B'}{B} \right)^2 \sin^2 \frac{\omega t}{2} \right] . \]
The factor of 2 before \((B'/B)^2\) is crucial.

The expectation value of \(H'\) can be calculated in a similar fashion, and one finds
\[
\langle H' \rangle = -2\epsilon \left( \frac{B'}{B} \right)^2 \sin^2 \frac{\omega t}{2}.
\]
Thus the total energy expectation value is
\[
\langle H_0 + H' \rangle = -\epsilon \left[ 1 - 2 \left( \frac{B'}{B} \right)^2 \sin^2 \frac{\omega t}{2} \right] - 2\epsilon \left( \frac{B'}{B} \right)^2 \sin^2 \frac{\omega t}{2}
= -\epsilon = -\frac{g\mu_B B}{2}.
\]
This is independent of time, as we expect for the total energy expectation value, since
for \(t > 0\) the total Hamiltonian is time-independent.

(More generally, Ehrenfest’s theorem states for any observable \(A\) we have
\[
\frac{d\langle A \rangle}{dt} = (i\hbar)^{-1} \langle [A, H] \rangle + \left\langle \frac{dA}{dt} \right\rangle.
\]
If \(A\) commutes with the Hamiltonian \(H\) and has no explicit time dependence, then
\(d\langle A \rangle/ dt = 0.\))

(b) In the sudden approximation, we assume that the Hamiltonian switches abruptly
from \(H_0\) for \(t < 0\) to
\[
H = H_0 + H' = \frac{g\mu_B B}{2} \left( \begin{array}{cc} 1 & \frac{B'/B}{2} \\ \frac{B'/B}{2} & -1 \end{array} \right) = \epsilon \left( \begin{array}{cc} 1 & \alpha \\ \alpha & -1 \end{array} \right)
\]
for \(t > 0\), where we have defined \(\alpha = B'/B\) and \(\epsilon = g\mu_B B/2\), as before. The eigenvalues and eigenvectors of \(H\) can be obtained in the usual way. The algebra
isn’t nice, but the results are
\[
E_+ = +\epsilon \sqrt{1 + \alpha^2}, \quad |\phi_\rangle = \frac{1}{2^{1/2}(1 + \alpha^2 - \sqrt{1 + \alpha^2})^{1/2}} \left( \begin{array}{c} \alpha \\ \sqrt{1 + \alpha^2} - 1 \end{array} \right),
\]
\[
E_- = -\epsilon \sqrt{1 + \alpha^2}, \quad |\phi_-\rangle = \frac{1}{2^{1/2}(1 + \alpha^2 - \sqrt{1 + \alpha^2})^{1/2}} \left( \begin{array}{c} 1 - \sqrt{1 + \alpha^2} \\ \alpha \end{array} \right).
\]
If we start out in the state \(|\psi(0)\rangle = |\downarrow\rangle\), the time-evolved state is
\[
|\psi(t)\rangle = d_+ e^{-iE_+ t/\hbar} |\phi_\rangle + d_- e^{-iE_- t/\hbar} |\phi_-\rangle,
\]
where
\[ d_+ = \langle \downarrow | \phi_+ \rangle = \frac{\sqrt{1 + \alpha^2} - 1}{2^{1/2}(1 + \alpha^2 - \sqrt{1 + \alpha^2})^{1/2}}, \]
\[ d_- = \langle \downarrow | \phi_- \rangle = \frac{\alpha}{2^{1/2}(1 + \alpha^2 - \sqrt{1 + \alpha^2})^{1/2}}. \]

Expressed in terms of the original basis \{ |\uparrow\rangle , |\downarrow\rangle \}, this is
\[ |\psi(t)\rangle = \frac{1}{2(1 + \alpha^2 - \sqrt{1 + \alpha^2})} \left[ \left( \sqrt{1 + \alpha^2} - 1 \right)e^{-iE_{+}t/\hbar} \left( \frac{\alpha}{\sqrt{1 + \alpha^2} - 1} \right) + \alpha e^{-iE_{-}t/\hbar} \left( 1 - \frac{\sqrt{1 + \alpha^2}}{\alpha} \right) \right] \]
\[ = \frac{1}{2(1 + \alpha^2 - \sqrt{1 + \alpha^2})} \left( \frac{\alpha(\sqrt{1 + \alpha^2} - 1)(e^{-iE_{+}t/\hbar} - e^{-iE_{-}t/\hbar})}{2 - 2\sqrt{1 + \alpha^2} + \alpha^2}e^{-iE_{+}t/\hbar} + \alpha^2e^{-iE_{-}t/\hbar} \right) \]
\[ = \ldots \]
\[ = \left( \frac{-i\sqrt{1 + \alpha^2}}{\sqrt{1 + \alpha^2}} \sin \frac{\sqrt{1 + \alpha^2} t}{\hbar} + \frac{\alpha}{\sqrt{1 + \alpha^2}} \sin \frac{\sqrt{1 + \alpha^2} t}{\hbar} \right). \]

(Details omitted.) Thus the probability to find the system in the state \(|\uparrow\rangle\) at time \(t > 0\) is
\[ P_{\uparrow\downarrow}(t) = |\langle \uparrow | \psi(t) \rangle|^2 = \frac{\alpha^2}{1 + \alpha^2} \sin^2 \frac{\epsilon \sqrt{1 + \alpha^2} t}{h}. \]

The result above is exact. If \(B' \ll B\), then \(\alpha \ll 1\) and we can expand about \(\alpha = 0:\)
\[ \frac{\alpha^2}{1 + \alpha^2} = \alpha^2 + O(\alpha^4), \]
\[ \sin^2 \frac{\epsilon \sqrt{1 + \alpha^2} t}{h} = \sin^2 \frac{\epsilon t}{\hbar} + O(\alpha^2). \]

Thus
\[ P_{\uparrow\downarrow}(t) \approx \alpha^2 \sin^2 \frac{\epsilon t}{h} = \left( \frac{B'}{B} \right)^2 \sin^2 \frac{\omega t}{2}, \]

exactly as we found above.
2.

(a) The 1D harmonic oscillator has energies $E_n = \hbar \omega_0 (n + \frac{1}{2})$. The number of states with energies less than or equal to $E = E_n$ is

$$N(E) = n + 1 = \frac{E}{\hbar \omega_0} + \frac{1}{2}.$$  

For large $n$ (i.e. for $E \gg \hbar \omega_0$), we treat this function as a smooth function of the energy $E$. Then the density of states is

$$\rho(E) = \frac{dN}{dE} = \frac{1}{\hbar \omega_0}.$$  

(b) A 2D harmonic oscillator is equivalent to two independent 1D harmonic oscillators, so the eigenstates are labeled by pairs of non-negative integers $(n_x, n_y)$, with energy

$$E_{n_x, n_y} = \hbar \omega_0 (n_x + \frac{1}{2}) + \hbar \omega_0 (n_y + \frac{1}{2}) = \hbar \omega_0 (n_x + n_y + 1).$$

Let $n = n_x + n_y$. There are $n + 1$ energy eigenstates with energy equal to $E = \hbar \omega_0 (n + 1)$, namely

$$(n_x, n_y) = (n, 0), (n - 1, 1), \ldots, (1, n - 1), (0, n).$$

Thus the number of states with energy less than or equal to $E$ is

$$N(E) = \sum_{k=0}^{n} (k + 1) = \frac{1}{2} (n + 1)(n + 2) = \frac{1}{2} \left( \frac{E}{\hbar \omega_0} \right) (\frac{E}{\hbar \omega_0} + 1) \approx \frac{1}{2} \frac{E^2}{(\hbar \omega_0)^2}.$$  

where the last approximation is valid for $E \gg \hbar \omega_0$. The density of states is therefore

$$\rho(E) = \frac{dN}{dE} = \frac{E}{(\hbar \omega_0)^2}.$$  

(Note: Many of you inserted an extra factor of 2 for spin. For a 2D harmonic oscillator the particles are generally assumed to be spin 0, unless you are explicitly told otherwise.)
Consider the 1D harmonic oscillator, initially in the ground state, with a time-dependent perturbation $H' = -qx\mathcal{E}(t)$ added at $t = 0$, where $\mathcal{E}(t) = \mathcal{E}_0 e^{-t/\tau}$. The transition probabilities in first-order time-dependent perturbation theory are given by the usual formula:

$$P_{n0}(t) = \frac{1}{\hbar^2} \left| \int_0^t \langle n|H'(t')|0 \rangle e^{i\omega_{n0} t'} dt' \right|^2 = \frac{q^2 \mathcal{E}_0^2}{\hbar^2} \left| \frac{\langle n|x|0 \rangle}{\sqrt{2m\omega}} \right|^2 \left| \int_0^t dt' e^{-t'/\tau} e^{i\omega t'} \right|^2,$$

where $\omega_{n0} = (E_n - E_0)/\hbar = n\omega$.

The matrix element $\langle n|x|0 \rangle$ is most easily computed by introducing the raising and lowering operators $a^\dagger$ and $a$, in terms of which

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger).$$

Using the standard rules $a \langle n \rangle = \sqrt{n} \langle n - 1 \rangle$ and $a^\dagger \langle n \rangle = \sqrt{n + 1} \langle n + 1 \rangle$, we have

$$\langle n|x|0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n|a + a^\dagger|0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n|1 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \delta_{n1}$$

Therefore only transitions to the $n = 1$ state are allowed.

The integral is easy to compute, but we must not forget the boundary term coming from the lower limit of integration. Setting $n = 1$, we have

$$I = \int_0^t dt' e^{-t'/\tau} e^{i\omega t'} = \int_0^t dt' e^{i\omega - 1/\tau t'} = \frac{1}{i\omega - 1/\tau} \left[ e^{(i\omega - 1/\tau)t} - 1 \right].$$

$$|I|^2 = \frac{1}{\omega^2 + 1/\tau^2} \left[ (e^{-t/\tau} \cos \omega t - 1)^2 + (e^{-t/\tau} \sin \omega t)^2 \right]$$

$$= \frac{1}{\omega^2 + 1/\tau^2} \left[ e^{-2t/\tau} - 2e^{-t/\tau} \cos \omega t + 1 \right].$$

Thus

$$P_{10}(t) = \frac{q^2 \mathcal{E}_0^2}{2\hbar m\omega} \frac{1}{\omega^2 + 1/\tau^2} \left[ e^{-2t/\tau} - 2e^{-t/\tau} \cos \omega t + 1 \right].$$
In the limit $t \to \infty$, this becomes
\[
P_{10}(\infty) = \frac{q^2 \mathcal{E}_0^2}{2\hbar m \omega^2 + 1/\tau^2}.
\]

4.

To use the sudden approximation in the limit $\tau \to \infty$, we again have to solve for the exact eigenfunctions for $t > 0$. If $\tau \to \infty$, our perturbation is just $H' = -q\mathcal{E}_0x$, so our total Hamiltonian is
\[
H = H_0 + H' = \frac{p^2}{2m} + \frac{1}{2}kx^2 - q\mathcal{E}_0x
\]
\[
= \frac{p^2}{2m} + \frac{1}{2}k \left( x - \frac{q\mathcal{E}_0}{k} \right)^2 - \frac{q^2 \mathcal{E}_0^2}{2k}
\]
\[
= \frac{p'^2}{2m} + \frac{1}{2}kx'^2 - \frac{q^2 \mathcal{E}_0^2}{2k},
\]
where $x' = x - q\mathcal{E}_0/k$. Up to an irrelevant offset $q^2 \mathcal{E}_0^2/2k$, this is just another 1D harmonic oscillator, but now centered around $a = q\mathcal{E}_0/k$ rather than about 0. The eigenfunctions, as functions of $x'$, are exactly the same as the usual 1D harmonic oscillator eigenfunctions.

Let us use the notation $|n\rangle$ to denote the original harmonic oscillator eigenstates centered around 0, and $|n'\rangle$ to denote the harmonic oscillator eigenstates centered around $a$. At $t = 0$, our initial state is $|\psi(0)\rangle = |0\rangle$. Since the $|n\rangle$'s are no longer energy eigenstates for $t > 0$, we need to expand this in the new basis. Thus, if we define $d'_n = \langle n'|0\rangle$, then our time-evolved state at time $t > 0$ is
\[
|\psi(t)\rangle = \sum_{n=0}^{\infty} d'_n e^{-iE'_n t/\hbar} |n'\rangle,
\]
where $E'_n = E_n = \hbar \omega_0 (n + \frac{1}{2})$, as usual. The probability of finding this system in an excited state is just 1 minus the probability of finding it in the ground state. Thus
\[
P_{\text{excited}} = 1 - P_0 = 1 - |\langle 0'|\psi(t)\rangle|^2 = 1 - |d'_0|^2.
\]
It is now straightforward to calculate
\[
d'_0 = \langle 0'|0\rangle = \int dx \psi^*_0(x - a) \psi_0(x)
\]
\[ \left( \frac{m \omega}{\pi \hbar} \right)^{1/2} \int_{-\infty}^{\infty} dx \ e^{-m \omega (x-a)^2/2\hbar} e^{-m \omega x^2/2\hbar} = \left( \frac{m \omega}{\pi \hbar} \right)^{1/2} \int_{-\infty}^{\infty} dx \ e^{-m \omega (2x^2-2ax+a^2)/2\hbar} = \left( \frac{m \omega}{\pi \hbar} \right)^{1/2} e^{-m \omega a^2/4\hbar} \int_{-\infty}^{\infty} dx \ e^{-m \omega (x-a/2)^2/\hbar} = e^{-m \omega a^2/4\hbar}. \]

Thus

\[ P_{\text{excited}} = 1 - |d_0'|^2 = 1 - e^{-m \omega a^2/2\hbar} = 1 - e^{-q^2 \xi_0^2/2\hbar m \omega^3}. \]

Note that this expression is \textit{exact}. In particular, we didn’t have to assume that the perturbation is small. If the perturbation \textit{is} small, then we can expand the exponential to first order to obtain

\[ P_{\text{excited}} = 1 - \left( 1 - \frac{q^2 \xi_0^2}{2\hbar m \omega^3} + \ldots \right) \approx \frac{q^2 \xi_0^2}{2\hbar m \omega^3}. \]

This is exactly what we get when we take \( \tau \to \infty \) in the result of Problem 3.