Homework 10

Due: April 20 at 11:59 PM. Submit on Canvas.

Problem 1: Consider an alternate universe where we replace the dipole interaction between non-relativistic quantum systems and electromagnetic radiation, with a more generic kind of interaction $V(\mathbf{r})$, such that the spontaneous emission rate of photons between energy levels $E_\mathrm{i} > E_\mathrm{f}$ becomes:

$$R^\mathrm{se}_\mathrm{i\to f} = \frac{\omega^3_\mathrm{if}}{\pi\epsilon_0 \hbar c^3}|\langle \mathrm{f}|V|\mathrm{i}\rangle|^2. \tag{1}$$

20   **A:** Suppose that the interaction

$$V = C\left(x^2 - y^2\right). \tag{2}$$

    A1. Explain why this interaction V contains spherical harmonics with $l = 2$ and $m = \pm 2$.[1]

    A2. Follow Lecture 32 and argue that the selection rules for this interaction are (at least as strict as) $\Delta l = 0, 1, 2$, $\Delta m = \pm 2$.

    A3. What is the lowest energy state of hydrogen that can decay to the ground state $|100\rangle$? Explain what these states are, but do not calculate their lifetime!

20   **B:** Now, consider the perturbation

$$V = gr^2. \tag{3}$$

    B1. What are the selection rules in this case?

    B2. Show that there is a single $n = 2$ level of hydrogen that could decay to $|100\rangle$.

    B3. Take the state that is allowed to decay to $|100\rangle$, and calculate the time scale over which spontaneous emission would occur.

20   **Problem 2:** Consider the time-dependent Hamiltonian $H(t) = H_0 + V(t)$, with

$$H_0 = \begin{pmatrix} A & 0 & 0 \\ 0 & 2A & 0 \\ 0 & 0 & 3A \end{pmatrix}, \tag{4a}$$

$$V(t) = \begin{pmatrix} \epsilon & i\epsilon & 0 \\ -i\epsilon & 4\epsilon & 3\epsilon \\ 0 & 3\epsilon & -\epsilon \end{pmatrix} e^{-t/\tau}. \tag{4b}$$

If the initial wave function is $|\psi(0)\rangle = |1\rangle$, what is the probability of finding the particle in each of the three eigenstates of H_0 at $t = \infty$. Use first-order time-dependent perturbation theory to provide your answer.

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[1] *Hint:* You may find it helpful to look up results from McIntyre Chapter 7.

Problem 3 (Greenhouse gases): Greenhouse gases are molecules that, when in the gaseous atmosphere, interact strongly with thermal electromagnetic radiation emitted by the finite temperature surface of the Earth. To understand what molecules have strong interactions, recall that we have seen that fluctuations of the length of a covalent bond in a molecule are well approximated by a quantum harmonic oscillator.

In a molecule, we really have to study *coupled* harmonic oscillators associated with the individual motions of each atom. In this problem, you will be provided the solution to the coupled oscillator problem for two different relevant molecules.

20 **A:** Before talking about molecules, however, let us discuss what happens for a single harmonic oscillator:

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\Omega^2 x^2. \tag{5}$$

Take the dipole moment operator to be $\mathfrak{p} = \alpha x$. Describe the possible interactions of this oscillator with electromagnetic radiation within the electric dipole approximation (Lecture 31).

A1. Suppose that the initial state is the oscillator ground state $|0\rangle$. Show that the absorption rate of photons of frequency Ω is given by

$$R = \rho(\Omega) \times \frac{\pi\alpha^2}{6\epsilon_0\hbar m\Omega}. \tag{6}$$

A2. Into what states can the oscillator be excited, if it starts in $|0\rangle$?

A3. If the oscillator starts in any other state $|n\rangle$, is there any other frequency of photons (besides Ω) that will be absorbed?

10 **B:** On Homework 2, we discussed the normal modes of the carbon dioxide (CO_2) molecule. CO_2 is a greenhouse gas, meaning that it interacts efficiently with electromagnetic radiation. Let us see why. Consider the motion of the three atoms in a single line: let x_0 denote the position of the carbon atom, while $x_\pm$ denote the positions of the oxygens on either side. The dipole operator is

$$\mathfrak{p} = \alpha_O\left(x_+ + x_-\right) + \alpha_C x_0. \tag{7}$$

If $X_{1,2,3}$ denote the position operators for CO_2 normal modes, we found on Homework 2 that

$$x_- = X_1 - X_2 + X_3, \tag{8a}$$

$$x_0 = X_1 - \frac{2m_O}{m_C}X_3, \tag{8b}$$

$$x_+ = X_1 + X_2 + X_3. \tag{8c}$$

If k is the spring constant of the C-O covalent bond, the normal mode frequencies are

$$\Omega_1 = 0, \tag{9a}$$

$$\Omega_2 = \frac{k}{m_O}, \tag{9b}$$

$$\Omega_3 = k\left(\frac{1}{m_O} + \frac{2}{m_C}\right). \tag{9c}$$

B1. Express $\mathfrak{p}$ in terms of $X_{1,2,3}$.

B2. Model the interaction of the molecule with radiation by sequentially assuming that only $X_1 \neq 0$ (while $X_2 = X_3 = 0$), and then "turning on" the other two normal modes. Combine the results of A1 and B1, and the fact that $\rho(0) = 0$, to show $R \neq 0$ only for the X_3 mode.

B3. Using $m_C \approx 2.4 \times 10^{-26}$ kg, $m_O \approx 3.2 \times 10^{-26}$ kg, $k \sim 200$ J/m^2, and the values of fundamental constants, numerically evaluate the frequency of radiation Ω_3 with which CO_2 strongly interacts with.

B4. The typical frequency emitted by an object at temperature T is $\omega_T = k_B T/\hbar$. Using $T \sim 300$ K for the surface of the Earth, evaluate ω_T for the Earth's thermal radiation. Compare to Ω_3.

C: Now, let us repeat this calculation for the N_2 molecule. Letting $x_\pm$ denote the displacements of the two nitrogen atoms, we find

$$x_\pm = X_1 \pm X_2 \tag{10}$$

and $\Omega_1 = 0$, while $\Omega_2 \neq 0$.

C1. In one or two sentences, argue that if you try to generalize (7) to N_2, you expect that $\mathfrak{p} = \alpha X_1$ for some constant α.

C2. Deduce that N_2 does not interact effectively with electromagnetic radiation.

These simple considerations allow us to see that CO_2 is a greenhouse gas, while N_2 (or O_2 etc.) are not. In fact, somewhat unfortunately, *only* diatomic A_2 molecules will, in general, not interact with radiation within the dipole approximation. Since our order of magnitude estimates for CO_2 also hold for more general molecules, this simple physical argument suggests that most molecules in the atmosphere can play a role in the greenhouse effect, contributing to climate change.

Problem 4 (Qubit decoherence): Consider a qubit encoded in quantum states $|0\rangle$ and $|1\rangle$: as one example, these may correspond to two particular energy levels in an atom. This atom (or any other qubit platform) will inevitably have *more* states in Hilbert space, which are unwanted and which we can decay in to. In this problem, let us consider just adding one more state $|b\rangle$ to the Hilbert space. Suppose that the encoded qubit is subject to Hamiltonian

$$H_0 = \epsilon_0 |0\rangle\langle 0| + \epsilon_1 |1\rangle\langle 1|, \tag{11}$$

i.e. $H_0 |b\rangle = 0|b\rangle$.

Now, let us consider the effect of environmental noise, which couples the logical qubit states to the bad state $|b\rangle$. We will model this noise with a time-dependent perturbation: $H = H_0 + V(t)$ where

$$V(t) = \delta \left(|0\rangle\langle b| + |1\rangle\langle b| + |b\rangle\langle 0| + |b\rangle\langle 1| \right) \xi(t). \tag{12}$$

Here ϵ is real, and $\xi(t)$ is **noise**: a random function obeying

$$\mathbb{E}[\xi(t)] = 0, \tag{13a}$$
$$\mathbb{E}\left[\xi(t)\xi(s)\right] = f(t-s). \tag{13b}$$

$\mathbb{E}[\cdots]$ denotes *averaging over classical noise*, and $f(t)$ is a function determined to the precise environmental dynamics giving rise to the noise.

1. Suppose that the qubit starts in state $|i\rangle$ $(i = 0, 1)$. Write a formal expression for the probability $P_{i\to b}(t)$ of transitioning to $|b\rangle$ at time t, within first-order time-dependent perturbation theory.

2. Average over the random noise, assuming that

$$f(t) = e^{-|t|/\tau}. \tag{14}$$

You may assume that $t \gg \tau$ if it helps you to simplify your expression for $P_{i\to b}(t)$.

3. Estimate the lifetime T of the qubit: i.e. the time scale T over which $|\langle b|\psi(T)\rangle| \ll 1$.