Applied Physics 216 — Assignment #3

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Due: **10:20am + 10 min grace period**, Feb 24th, 2017; slide your work under through the door at Maxwell-Dworkin Room 131.

Problem 1 (200 pt): 2-level atoms with electric dipolar transitions

Consider a one-electron 2-level atom. The electronic Hamiltonian H_0 has eigenstates of $|1\rangle$ and $|2\rangle$ with energy eigenvalues of $\mathcal{E}_1$ and $\mathcal{E}_2$. Each of $|1\rangle$ and $|2\rangle$ has either even or odd parity. $\mathcal{E}_1 - \mathcal{E}_2 = \hbar\omega_0$. The electric dipole moment operator is $\vec{\tilde{\mu}} = -e\vec{r}$, or, $\tilde{\mu}_x = -ex$, $\tilde{\mu}_y = -ey$, and $\tilde{\mu}_z = -ez$ (note the tilde for the dipole moment operators).

(a) Consider, as an example, $|1\rangle = |100\rangle$ and $|2\rangle = |210\rangle$ where $|nlm\rangle$ denotes electron wave functions in hydrogen. Show that $\langle 1|\tilde{\mu}_x|2\rangle = \langle 1|\tilde{\mu}_y|2\rangle = 0$ on the one hand, and $\langle 1|\tilde{\mu}_z|2\rangle = \langle 2|\tilde{\mu}_z|1\rangle \neq 0$ on the other hand. Define these non-vanishing identical matrix elements as μ_z (note no tilde here as it is a value, not an operator), that is, $\mu_z \equiv \langle 1|\tilde{\mu}_z|2\rangle = \langle 2|\tilde{\mu}_z|1\rangle$ (you don't have to calculate μ_z here; we will just call these matrix elements μ_z).

(b) With the example of (a), find the two eigenstates $|a\rangle$ and $|b\rangle$ of $\tilde{\mu}_z$ (as superpositions of $|1\rangle$ and $2\rangle$) and their corresponding eigenvalues (in terms of μ_z). Polar plot the spatial electron (probability) distribution $|\psi_a(r,\theta,\phi)|^2$ and $|\psi_b(r,\theta,\phi)|^2$, where $\psi_a(r,\theta,\phi) = |a\rangle$ and $\psi_b(r,\theta,\phi) = |b\rangle$. Do you identify definite electric dipole moments with states $|a\rangle$ and $|b\rangle$? Show that the electron initially prepared in $|a\rangle$ vibrates with frequency ω_0 between $|a\rangle$ and $|b\rangle$, calculate the associated $\langle\tilde{\mu}_z\rangle(t)$, and show that $\langle\vec{\tilde{\mu}}\rangle(t)$ flips up and down with ω_0. This is the fast ω_0 electric dipole oscillation.

(c) In the example of (a), we apply an electric field at the resonance frequency ω_0: $\vec{E}_1(t) = \hat{z}E_1\cos(\omega_0 t)$. The electronic state at time t is $|\psi(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle$. Solve, in the coherent (strong-signal) regime, the Schrödinger equation to show the occurrence of the Rabi oscillation at frequency $\omega_1 = |\mu_z|E_1/\hbar$. Consider a half period of one Rabi cycle where the electron makes a downward transition from $|2\rangle$ to $|1\rangle$. During this transition, calculate $\langle\tilde{\mu}_z\rangle$(t), $P_a(t)$ and $P_b(t)$ to show that the fast ω_0 electric dipolar oscillation underlies the slow ω_1 Rabi transition. *Optional - not to be graded*: this dipole oscillation will emit a light: what is the polarization and phase of the electric field of this emitted light? Will the emitted electric field add to or subtract from the excitation electric field? Is the excitation electric field doing the work to the atom, or the other way around?

(d) Now take another example for $|1\rangle$ and $|2\rangle$, that is, $|1\rangle = |100\rangle$ and $|2\rangle = |211\rangle$. Show that

$$\langle 1|\tilde{\mu}_x|2\rangle = \langle 2|\tilde{\mu}_x|1\rangle = a \quad (1)$$

$$\langle 1|\tilde{\mu}_y|2\rangle = \langle 2|\tilde{\mu}_y|1\rangle^* = ia \quad (2)$$

$$\langle 1|\tilde{\mu}_z|2\rangle = \langle 2|\tilde{\mu}_z|1\rangle = 0 \quad (3)$$

where a is a certain real number, which you can calculate but I am not asking you to. Define $\mu_\perp \equiv a$. Assume that the electron is initially at one of the two eigenstates of $\tilde{\mu}_x$, whose corresponding eigenvalue indicates a dipole towards a positive x direction. Evaluate $\langle\tilde{\mu}_x\rangle(t)$ and $\langle\tilde{\mu}_y\rangle(t)$ and from these, describe the nature of the electric dipole oscillation (frequency and polarization of the electric field emitted). Consider the following three excitation fields:

$$\vec{E}_1(t) \sim \hat{x}\cos\omega_0 t \quad (4)$$

$$\vec{E}_1(t) \sim \hat{x}\cos\omega_0 t + \hat{y}\sin\omega_0 t \quad (5)$$

$$\vec{E}_1(t) \sim \hat{x}\cos\omega_0 t - \hat{y}\sin\omega_0 t \quad (6)$$

Show that to obtain the same Rabi frequency, the second field requires only half the power of the first field while the third excitation cannot effectively induce transitions in the atom. Can you explain why?

Problem 2 (150 pt): Spontaneous decay of 2-level atoms: electric v. magnetic dipole transitions

Again consider a one-electron 2-level atom with stationary states $|1\rangle$ and $|2\rangle$ and energy eigenvalues of $\mathcal{E}_1$ and $\mathcal{E}_2$. Each of $|1\rangle$ and $|2\rangle$ has either even or odd parity. $\mathcal{E}_1 - \mathcal{E}_2 = \hbar\omega_0$. This problem ultimately seeks to calculate the spontaneous decay rate of this 2-level atom of electric dipole character, and to compare it to the spontaneous decay rate of a 2-level atom of magnetic dipole character. We will go step by step, beginning at the beginning with stimulated transition rate calculation (to calculate Einstein B coefficient, from which Einstein A coefficient, or the spontaneous decay rate, can be immediately calculated).

(a) Assume an excitation electric field at a general frequency ω: $\vec{E}_1(t) = \hat{z}E_1\cos(\omega t)$. The electronic state at time t is $|\psi(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle$ while $c_1(0) = 1$ and $c_2(0) = 0$ (so we will be considering an upward transition here; the goal is to calculate the stimulated transition rate W, which is the same for upward and downward transition). Assume the weak-field (non-Rabi) regime, commensurate with the standard time-dependent perturbation regime (which also has much to do with the rate-equation regime). Starting from the known result of the time-dependent perturbation solution of the Schrödinger equation, show, to the first order, that

$$|c_2(t)|^2 = P_2(t) = (\frac{\mu_z E_1}{2\hbar})^2 \times F(\omega, t) \tag{7}$$

where $\mu_z = \langle 1|\tilde{\mu}_z|2\rangle = \langle 2|\tilde{\mu}_z|1\rangle$ as in Problem 1(a) and

$$F(\omega, t) \equiv \frac{\sin^2[(\omega - \omega_0)t/2]}{[(\omega - \omega_0)/2]^2} \tag{8}$$

(b) The situation of part (a) was the excitation field concentrated at one frequency ω. Think of now an excitation electric field of spread spectrum $\rho(\omega)$, which denotes the spectral energy density of the "*light*" plane wave whose electric field is used for the excitation; $\rho(\omega)$ has the unit of energy per unit bandwidth per unit volume. The plane light wave has also magnetic field, so $\rho(\omega)$ contains both the electric and magnetic energy. Only the electric dipolar interaction matters here, but we consider the total light energy density $\rho(\omega)$ simply because the Einstein B coefficient, which we seek to calculate, was defined in reference to $\rho(\omega)$ (no physics changes; it's just a matter of definition of B). Consider an infinitesimal frequency band $(\omega - d\omega/2, \omega + d\omega/2)$ and let the infinitesimal electric field intensity within this band be $d(E_1^2(\omega))$. Show

$$d(E_1^2(\omega)) = \frac{2}{\epsilon_0}\rho(\omega)d\omega. \tag{9}$$

(c) The infinitesimal probability for the electron to occupy the state $|2\rangle$ at time t due to the infinitesimal excitation signal of Eq. (9) is denoted as $dP_2(t)$. From Eqs. (7) and (9), show that

$$dP_2(t) = (\frac{\mu_z^2}{2\hbar^2\epsilon_0}) \times F(\omega, t) \times \rho(\omega)d\omega \tag{10}$$

(d) Plot $F(\omega, t)$ as a function of frequency ω and using t as a parameter. Show that with an increasing t, $F(\omega, t)$, which captures the atomic frequency response peaked at $\omega = \omega_0$, becomes increasingly sharp and tall. In contrast, $\rho(\omega)$ is typically of broader bandwidth. By integrating Eq. (10) over the entire frequency, calculate $P_2(t)$ and W, and from this, show that the Einstein B coefficient is given by

$$B = \frac{\pi}{\epsilon_0\hbar^2}\mu_z^2. \tag{11}$$

Now generalize the result above by considering the random orientation of the atom with respect to the excitation polarization, and show that

$$B = \frac{\pi}{3\epsilon_0\hbar^2}|\vec{\mu}|^2 \tag{12}$$

where $\vec{\mu} = \langle 1|\vec{\tilde{\mu}}|2\rangle = -e\langle 1|\vec{r}|2\rangle$.

(e) By using the Einstein's A-B coefficient relation, show that the spontaneous decay rate $\delta_r = A$ is

$$\delta_r = A = \frac{\omega_0^3}{3\pi\epsilon_0\hbar c^3}|\vec{\mu}|^2 = \frac{\omega_0^3}{3\pi\epsilon_0\hbar c^3}|\langle 1|e\vec{r}|2\rangle|^2 \tag{13}$$

(f) Repeat the calculation of parts (a)-(e) to calculate the spontaneous decay rate for the ^1H spin-1/2 in static magnetic field B_0 at the same frequency ω_0. Show that $\delta_r = A$ of the electric dipole transition is many orders of magnitude larger than that of the magnetic dipole transition. If you use the fine structure constant α, you can simplify the numerical comparison.