Physics 4261: Lectures for week 8

Prof. Colin V. Parker (cparker@gatech.edu)
Georgia Institute of Technology

8.1 Our loss rate in terms of Bloch equations

In order to obey the superposition principal, we must have a set of linear equations for the time evolution of ρ. Each component (u, v, or w), can have a derivative proportional to each of the other two components, to itself, or it can be constant (this is still linear in ρ since it can be technically proportional to Tr $\rho = 1$). The matrix defining the derivates of ρ in terms of ρ is called the Lindblad superoperator. One obvious type of equation we can write is unitary evolution:

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho].$$

As there are only three types of Hermitian Hamiltonian for two by two matrices (the Pauli matrices), we have, for example

$$\begin{aligned}
\dot{\rho} = -i[\sigma_z, \rho] &= -\frac{i}{2}\left[\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1+w & u+iv\\ u-iv & 1-w\end{pmatrix} - \begin{pmatrix}1+w & u+iv\\ u-iv & 1-w\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right],\\
\dot{\rho} &= \begin{pmatrix}0 & v-iu\\ v+iu & 0\end{pmatrix},\\
\begin{pmatrix}\dot{u}\\ \dot{v}\\ \dot{w}\end{pmatrix} &= \begin{pmatrix}v\\ -u\\ 0\end{pmatrix}.
\end{aligned}$$

This accounts for three possible types of time-evolution (one for each direction). Note that if we start within the Bloch sphere (as we must), we stay there. Removing the single minus sign causes the solutions to grow arbitrarily large, so we cannot have that, so another three types of evolution can be crossed off. There are then three copies of equations like $\dot{w} = -w$, and three equations like $\dot{w} = 1$. These determine the non-unitary evolution.

Let us see how our decay of the excited state fits in. As the excited state decays, we evolve toward the pure state $|1\rangle$, which has $w = 1$. Therefore, this is a steady state of the system, so we must have $\dot{w} = \Gamma(1-w)$, for $\Gamma > 0$. This is the only term which has $|1\rangle$ as a stable steady state. But can this term exist by itself? No, because if we started with $(u, v, w) = (\epsilon, 0, \sqrt{1-\epsilon^2})$, we would flow to $(\epsilon, 0, 1)$, which has magnitude greater than one (now I am paying attention to higher order terms). So we need to introduce some Γ' to cause decay of the u and v components to keep things sane. We insist the derivative of $u^2 + v^2 + w^2$ be non-positive for this initial state, leading to

$$\begin{aligned}
2\dot{u}u + 2\dot{v}v + 2\dot{w}w &\le 0,\\
-2\Gamma'\epsilon^2 + \Gamma\epsilon^2 + \mathcal{O}(\epsilon^4) &\le 0,\\
\Gamma &\le 2\Gamma'.
\end{aligned}$$

Therefore the most basic possible mechanism for decay is

$$\dot{u} = -\frac{\Gamma}{2}u,$$
$$\dot{v} = -\frac{\Gamma}{2}v,$$
$$\dot{w} = -\Gamma(w-1).$$

Note that this is the *only* possible equation that can describe our atom's decay and agree for small excited fraction with classical electromagnetism. It is possible to add other terms to the Lindblad superoperator (for example, we can add faster decay of the coherences), but this would not agree with the classical solution for small values of the excitation. So the fundamental observation is that, if we start with a quantum system which agrees with classical physics for small excited state populations, we are forced to have decay of the excited state (by the superposition principal) *even though the classical decay of the excited state is zero!*

8.2 Moment of a superposition state

An atom in a superposition of two states $|\psi\rangle = |1\rangle + c_2|2\rangle$ (here c_2 is so small that we ignored the terms of order c_2^2 in the normalization) possesses a time-dependent dipole moment (in the z direction) equal to

$$\begin{aligned} p_0 &= c_2 \langle 1|\, er\cos\theta\, |2\rangle + c_2^* \langle 2|\, er\cos\theta\, |1\rangle\,, \\ &= 2e|c_2||X_{12}|\cos(\omega t), \end{aligned}$$

with $X_{12} = Z_{12} = \langle 1|\, r\cos\theta\, |2\rangle$.

The classical power radiated from this system follows the formula

$$\begin{aligned} P &= \frac{p_0^2\omega^4}{12\pi\epsilon_0 c^3} = \frac{4e^2\omega^4}{12\pi\epsilon_0 c^3}|c_2|^2|X_{12}|^2 = A_{21}|c_2|^2\hbar\omega, \\ A_{21} &= \frac{4e^2\omega^3}{12\pi\epsilon_0\hbar c^3}|X_{12}|^2 = \frac{4\alpha}{3c^2}\times\omega^3|X_{12}|^2, \end{aligned}$$

where A_{21} is the rate of decay of the excited state.

8.3 Excitation by an external field

The previous section introduced us to the dissipative part of OBE. Now we will calculate (quantum mechanically) the excitation by an oscillating field. We will do this with time-dependent perturbation theory, but note that we could use a similar low-amplitude classical argument and get the same result. Furthermore, we could have calculated the decay in the previous sections by quantizing the radiation field and treating the decay of the atom fully quantum mechanically. To do the perturbation approach, we use the Hamiltonian $H = H_0 + H_I(t)$, were H_0 is constant and presumably solvable, and the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi.$$

The eigenspectrum of H_0 is denoted $|\,\Psi_n(t)\rangle\,=|\,\psi_n\rangle\,e^{-iE_nt/\hbar}$. Since we have again a two level system n takes the values 1 and 2. Any system can be written as a superposition of these states:

$$|\,\Psi(t)\rangle\,=c_1(t)\,|\,1\rangle\,e^{-i\omega_1 t}+c_2(t)\,|\,2\rangle\,e^{-i\omega_2 t}.$$

We have a perturbing Hamiltonian given by the dipole operator times the applied field

$$H_I(t)=e\mathbf{r}\cdot\mathbf{E}\cos(\omega t).$$

The matrix elements of H_I are given by

$$\langle 1|\,H_I\,|1\rangle\,=\langle 2|\,H_I\,|2\rangle\,=0,$$

because of parity, and

$$\langle 1|\,H_I\,|2\rangle\,=eEX_{12}\cos(\omega t)=\hbar\Omega\cos(\omega t),$$

where Ω is called the Rabi rate ($\Omega/2\pi$ is the Rabi frequency if you want to keep angular frequencies well-identified). Now, let's plug this form into the Schrödinger equation,

$$\begin{aligned} i\dot{c_1} &= \Omega\cos(\omega t)e^{-i\omega_0 t}c_2,\\ i\dot{c_2} &= \Omega^*\cos(\omega t)e^{i\omega_0 t}c_1, \end{aligned}$$

$$\begin{aligned} i\dot{c_1} &= \frac{\Omega}{2}c_2\left\{e^{-i(\omega_0-\omega)t}+e^{-i(\omega_0+\omega)t}\right\},\\ i\dot{c_2} &= \frac{\Omega^*}{2}c_1\left\{e^{i(\omega_0-\omega)t}+e^{i(\omega_0+\omega)t}\right\}, \end{aligned}$$

where $\omega_0\,=\,\omega_2-\omega_1$. This very important trick is called the rotating wave approximation, and life would be very difficult without it. Taking $c_1(t)\,=\,1$, and $c_2(0)\,=\,0$, we will integrate these equations for small amplitudes of c_2.

$$\begin{aligned} c_2(t) &\approx -i\frac{\Omega^*}{2}\int_0^t\left\{e^{i(\omega_0-\omega)t'}+e^{i(\omega_0+\omega)t'}\right\}dt',\\ c_2(t) &\approx 1-\frac{\Omega^*}{2}\left\{\frac{e^{i(\omega_0-\omega)t}}{\omega_0-\omega}+\frac{e^{i(\omega_0+\omega)t}}{\omega_0+\omega}\right\}. \end{aligned}$$

We are now going to throw away the terms containing $\omega_0+\omega$. This makes sense if you start to integrate the equations, the denominator for some terms will be $\omega_0-\omega$, and we assume this to be much smaller than $\omega_0+\omega$. This leads to

$$\begin{aligned} |c_2(t)|^2 &= |\Omega|^2\frac{\sin^2\{(\omega_0-\omega)t/2\}}{(\omega_0-\omega)^2},\\ |c_2(t)|^2 &= \frac{1}{4}|\Omega|^2t^2\frac{\sin^2(x)}{x^2}, \qquad x=\frac{(\omega_0-\omega)t}{2}. \end{aligned}$$

8.4 The Einstein B coefficients (Foot 7.2)

Now we are going to follow the book and derive the excitation rate integrated over frequency when the transition is driven not by a single frequency source but by blackbody radiation. We begin with the frequency dependent component of the excited state (for small excited state fractions):

$$|c_2(t,\omega)|^2 = \frac{e^2E^2(\omega)|X_{12}|^2}{4\hbar^2}t^2\frac{\sin^2(x)}{x^2},$$

where x has implicit ω dependence. Substitute in the electromagnetic energy density $\rho(\omega) = \epsilon_0 E(\omega)^2/2$:

$$|c_2(t)|^2 = \frac{e^2|X_{12}|^2}{2\epsilon_0\hbar^2}t^2\int_0^\infty \rho(\omega)\frac{\sin^2(x)}{x^2}d\omega,$$

Importantly, because energy is per unit frequency, we can imagine making t very long, and then the frequency bins become very narrow and the total power in each is very small. We can define $\rho(x)$ similarly, and then integrating over all x (this includes negative frequency, but we assume the integrand is very small at this range)

$$|c_2(t)|^2 = \frac{e^2|X_{12}|^2}{\epsilon_0\hbar^2}t\int_{-\infty}^\infty \rho(x)\frac{\sin^2(x)}{x^2}dx,$$

$$|c_2(t)|^2 = \frac{\pi e^2|X_{12}|^2}{\epsilon_0\hbar^2}t\rho(\omega_0),$$

where in the last step we used the function $x^{-2}\sin^2(x) = \pi\delta(x)$.This is valid because taking t to be long means that x is large except when $\omega = \omega_0$ or very nearby. The final thing we must check to make sure the approximations are valid is that t can be large compared to the relative variation in the blackbody spectrum (which is of order ω_0). This leads to an approximate relation

$$|c_2(t)|^2 \sim \frac{e^2|X_{12}|^2}{\epsilon_0\hbar^2}\frac{1}{\omega_0}\rho(\omega_0).$$

Since

$$\rho(\omega_0) = \frac{\hbar\omega_0^3}{\pi^2c^2}\frac{1}{e^{\hbar\omega/k_BT}-1}. \approx \frac{k_BT}{\hbar\omega_0}\frac{\hbar\omega_0^3}{\pi^2c^3},$$

with the high-temperature limit taken, we get (using $|X_12| \sim e^2/(4\pi\epsilon_0\omega_0)$).

$$|c_2(t)|^2 \sim \frac{e^2|X_{12}|^2}{\epsilon_0\hbar^2}\frac{1}{\omega_0}\frac{k_BT}{\hbar\omega_0}\frac{\hbar\omega_0^3}{c^3},$$

$$|c_2(t)|^2 \sim \alpha^3\frac{k_BT}{\hbar\omega_0}.$$

where we dropped small constants, like π and 4. But this is very small under reasonable conditions. In the sun, we might have $k_BT \sim \hbar\omega_0$, but even then the number is still small by α^3. Accepting the approximation now, this implies a transition rate

$$B_{12} = \frac{\pi e^2|X_{12}|^2}{\epsilon_0\hbar^2}.$$

The book writes things in terms of $|D_{12}|^2 = 3|X_{12}|^2$, which is an averaged-over-angles integral $\mathbf{D}_{12} = \langle 1|\,\mathbf{r}\,|2\rangle$, but we will keep things in terms of X_{12} for now. Furthermore, for a true two level system, we have to keep track of polarizatoin, so only $1/3$ of the blackbody energy will be in the "right" polarization state, hence it might be better to write:

$$\tilde{B}_{12} = \frac{\pi e^2 |X_{12}|^2}{3\epsilon_0 \hbar^2},$$

using special notation to distinguish the two-level system results.

8.5 Einstein's relation between A and B coefficients

We have already calculated the Einstein coefficients

$$\begin{aligned}\tilde{A}_{21} &= \frac{4\alpha}{3c^2} \times \omega^3 |X_{12}|^2 \\ \tilde{B}_{12} &= \frac{\pi e^2 |X_{12}|^2}{3\epsilon_0 \hbar^2} = \frac{4\alpha c \pi^2 |X_{12}|^2}{3\hbar}.\end{aligned}$$

Einstein wrote the following equation for the rate of change of the total excited state fraction:

$$\frac{dN_2}{dt} = N_1 B_{12} \rho(\omega_{12}) - N_2 B_{21} \rho(\omega_{12}) - N_2 A_{21} = 0.$$

This leads to

$$\rho(\omega_{12}) = \frac{A_{21}}{B_{21}} \frac{1}{\frac{N_1}{N_2}\frac{B_{12}}{B_{21}} - 1}.$$

From the Planck formula,

$$\rho(\omega_{12}) = \frac{\hbar \omega_{12}^3}{\pi^2 c^2} \frac{1}{e^{\hbar\omega/k_B T} - 1}.$$

We also have the thermal equilibrium relation

$$\frac{N_2}{g_2} = \frac{N_1}{g_1} e^{-\hbar\omega/k_B T},$$

where g_n is the degeneracy. From these we deduce

$$\begin{aligned}A_{21} &= \frac{\hbar \omega_{12}^3}{\pi^2 c^2} B_{21}, \\ B_{12} &= \frac{g_2}{g_1} B_{21}.\end{aligned}$$

Note that this agrees with the two-level case if $g_1 = g_2 = 1$. In other cases, one would be using averages over all possible polarizations, and in this case the degeneracy factors would be necessary to correct for the difference between averaging over polarizations in the excited state, and averaging over polarizations in the ground state.