Density Matrix Description of 2-Level Atoms

More about the Density Matrix

Choose a basis $|\psi_k\rangle = \sum_j c_j^{(k)} |u_j\rangle$. We define

Populations: (real-valued) $\rho_{nn} = \sum p_k c_n^{(k)} c_n^{(k)*} = \sum_k p_k |c_n^{(k)}|^2$

Single system: Prob of finding state $|u_n\rangle$

Ensemble: $|u_n\rangle$ occurs with freq. ρ_{nn}

Coherences: (complex-valued) $\rho_{np} = \langle c_n^{(k)} c_p^{(k)*} \rangle_k$

Note: Defining $c_q = |c_q| e^{i\theta_q}$ we have

$$\langle c_n^{(k)} c_p^{(k)*} \rangle_k = \langle |c_n^{(k)}||c_p^{(k)}| e^{i(\theta_n^{(k)} - \theta_p^{(k)})} \rangle_k \le \langle |c_n^{(k)}||c_p^{(k)}| \rangle_k$$

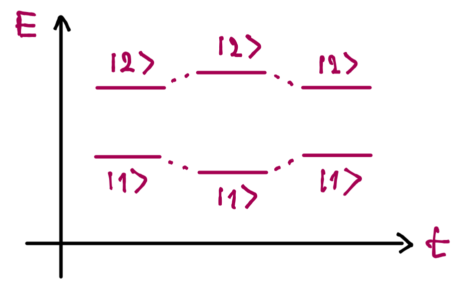
It follows that

$$\rho_{np}\rho_{pn} \le \rho_{nn}\rho_{pp}$$

with = for pure states

$$\rho = \begin{pmatrix} \rho_{nn} & \cdots & \rho_{np} \\ \vdots & \ddots & \vdots \\ \rho_{pn} & \cdots & \rho_{pp} \end{pmatrix}$$

Example: 2-level atom w/random perturbations



Perturbing events cause random phase shifts $e^{i\theta}$ between states.

The ensemble average $\rho_{np} = \sum_j p_j c_n c_p^* e^{i\theta_j}$ is reduced by the randomly fluctuating phase

Dipole Radiation:

$$\langle \hat{\vec{p}} \rangle = Tr[\rho \hat{\vec{p}}] = Tr\left[\begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}\begin{pmatrix} 0 & \vec{p}_{12} \\ \vec{p}_{21} & 0 \end{pmatrix}\right]$$

$$= \rho_{12}\vec{p}_{21} + \rho_{21}\vec{p}_{12} = 2Re[\rho_{12}\vec{p}_{21}]$$

For an ensemble of pure states w/different θ_k

$$\langle \hat{\vec{p}} \rangle = 2\sum_k p_k \underbrace{Re[\rho_{12}^{(k)} \vec{p}_{21}]}$$

Oscillating dipole w/phase that varies between atoms with different perturbation history

Density Matrix Description of 2-Level Atoms

Time Evolution of the Density Matrix

<u>Challenge</u>: We need "equations of motion" that combine the Schrödinger Equation with the effect of processes that can change $\mathrm{Tr}\,\rho^2$ (measure of purity)

<u>Approach</u>: We do not have time for a rigorous derivation, so will rely on plausible arguments to justify the equations

<u>Schrödinger Evolution</u>: In general, we have

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

matrix elements

$$(*) \quad \dot{\rho}_{nm} = -\frac{i}{\hbar}\sum_{k=1,2}(H_{nk}\rho_{km} - \rho_{nk}H_{km})$$

2-Level Atom $\Rightarrow$ $\begin{cases} \text{2 populations} \\ \text{2 coherences} \end{cases}$

Consider the 2-Level Rabi problem with

$$H = H_0 + V \quad \& \quad V_{12} = -\frac{1}{2}\hbar(\chi_{12}e^{-i\omega t} + \chi_{21}^* e^{i\omega t})$$

$$H = \hbar\begin{pmatrix} 0 & -\frac{1}{2}(\chi_{12}e^{-i\omega t} + \chi_{21}^* e^{i\omega t}) \\ -\frac{1}{2}(\chi_{21}e^{-i\omega t} + \chi_{12}^* e^{i\omega t}) & \omega_{21} \end{pmatrix}$$

Substitute in (*), set $\rho_{12} = \tilde{\rho}_{12}e^{i\omega t}$

slow variable

(For a pure state $\rho_{12} = a_1 a_2^* = c_1(c_2 e^{-i\omega t})^*$)

Make RWA, drop ~, and set $\chi_{21} = \chi$, $\chi_{21}^* = \chi^*$

$$\dot{\rho}_{11} = -\frac{i}{2}(\chi\rho_{12} - \chi^*\rho_{21})$$

$$\dot{\rho}_{22} = \frac{i}{2}(\chi\rho_{12} - \chi^*\rho_{21})$$

$$\dot{\rho}_{12} = i\Delta\rho_{12} + i\frac{\chi^*}{2}(\rho_{22} - \rho_{11}) = \dot{\rho}_{21}^*$$

Rabi Eqs. for pure and mixed states

Density Matrix Description of 2-Level Atoms

Consider the 2-Level Rabi problem with

$$H = H_0 + V \quad \& \quad V_{12} = -\tfrac{1}{2}\hbar\left(\chi_{12}e^{-i\omega t} + \chi_{21}^{*}e^{i\omega t}\right)$$

$$H = \hbar\begin{pmatrix} 0 & -\frac{1}{2}\left(\chi_{12}e^{-i\omega t}+\chi_{21}^{*}e^{i\omega t}\right) \\ -\frac{1}{2}\left(\chi_{21}e^{-i\omega t}+\chi_{12}^{*}e^{i\omega t}\right) & \omega_{21} \end{pmatrix}$$

Substitute in (*), set $\rho_{12} = \tilde{\rho}_{12}e^{i\omega t}$

slow variable

(For a pure state $\rho_{12} = a_1 a_2^{*} = c_1\left(c_2 e^{-i\omega t}\right)^{*}$)

Make RWA, drop ~, and set $\chi_{21} = \chi$, $\chi_{21}^{*} = \chi^{*}$

$$\dot{\rho}_{11} = -\frac{i}{2}\left(\chi\rho_{12} - \chi^{*}\rho_{21}\right)$$

$$\dot{\rho}_{22} = \frac{i}{2}\left(\chi\rho_{12} - \chi^{*}\rho_{21}\right)$$

$$\dot{\rho}_{12} = i\Delta\rho_{12} + i\frac{\chi^{*}}{2}\left(\rho_{22} - \rho_{11}\right) = \dot{\rho}_{21}^{*}$$

Rabi Eqs. for pure and mixed states

Next: Non-Hamiltonian evolution

Types of events

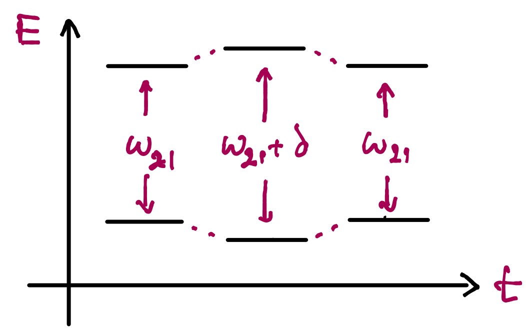
(i) Elastic collisions: No change in energy

(ii) Inelastic collisions: Atom loss

(iii) Spontaneous decay: Transition $|2\rangle \rightarrow |1\rangle$

Simple Model of Elastic Collisions

Two atoms near each other ➡ energy levels shift, free evol. of ρ_{12} changed



(Paradigm for perturbations that do not lead to net change in energy)

Density Matrix Description of 2-Level Atoms

Next: Non-Hamiltonian evolution

Types of events

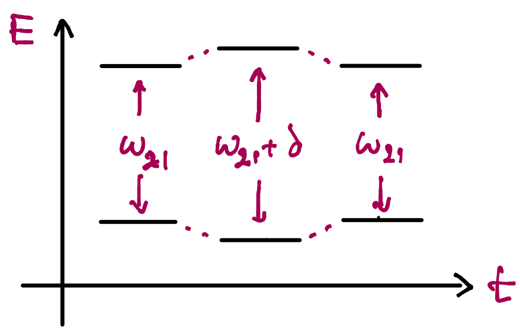
(i) Elastic collisions: No change in energy

(ii) Inelastic collisions: Atom loss

(iii) Spontaneous decay: Transition $|2\rangle \to |1\rangle$

Simple Model of Elastic Collisions

Two atoms near each other → energy levels shift, free evol. of ρ_{12} changed



(Paradigm for perturbations that do not lead to net change in energy)

Evolution of coherence (fast variables)

$$\dot{\rho}_{12} = -i\left[\omega_{21} + \delta\omega(t)\right]\rho_{12}$$

collisional history

$$\Rightarrow \rho_{12}(t) = \rho_{12}(0)\, e^{-i\omega_{21}t}\, e^{-i\int_0^t dt'\,\delta\omega(t')}$$

We need the ensemble average of $\rho_{12}(t)$

Assumptions:

- From atom to atom $\delta\omega(t)$ is a Gaussian Random Variable
- Averaged over the ensemble $\langle \delta\omega(t)\rangle_{e} = 0$
- Collisions have no memory over time, $\langle \delta\omega(t)\,\delta\omega(t')\rangle_t = \frac{2}{\tau}\,\delta(t-t')$

Can show that, averaged over time and the ensemble

$$\left\langle e^{-i\int_0^t dt'\,\delta\omega(t')} \right\rangle = e^{-t/\tau}$$

Density Matrix Description of 2-Level Atoms

It follows that: $\rho_{12}(t) = \rho_{12}(0)\, e^{-i\omega_{21}t}\, e^{-t/\tau}$

Add this decay to the equation of motion to get

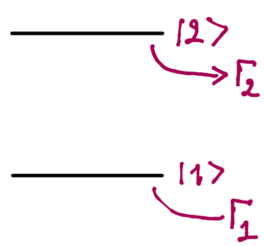
$$\boxed{\dot{\rho}_{12} = (\dot{\rho}_{12})_{S.E.} + (\dot{\rho}_{12})_{E.C.} = -(i\omega_{21} - 1/\tau)\rho_{12}}$$

Simple Model of Inelastic Collisions

As modeled by, e. g., Milloni & Eberly, this is a steady loss of atoms

$$\dot{\rho}_{11} = (\dot{\rho}_{11})_{S.E.} - \Gamma_1 \rho_{11}$$

$$\dot{\rho}_{22} = (\dot{\rho}_{22})_{S.E.} - \Gamma_2 \rho_{22}$$



This is strange because $Tr\,\rho(t)$ is not preserved

Convenient when working with quantities

$N\langle\vec{\mu}\rangle \propto N(\vec{\mu}_{12}\rho_{21} + \vec{\mu}_{21}\rho_{12})$??

Effect on probability amplitudes

Populations are ensemble averages of the type

$$\rho_{11}(t) = \langle |a_1(t)|^2 \rangle = \langle |a_1(0)|^2 \rangle e^{-\Gamma_1 t}$$

$$\rho_{22}(t) = \langle |a_2(t)|^2 \rangle = \langle |a_2(0)|^2 \rangle e^{-\Gamma_2 t}$$

When the populations decay, the averages of the probability amplitudes must decay accordingly,

$$\langle |a_1(t)| \rangle = \langle |a_1(0)| \rangle e^{-\Gamma_1/2\, t}$$

$$\langle |a_2(t)| \rangle = \langle |a_2(t)| \rangle e^{-\Gamma_2/2\, t}$$

Thus, for the coherences

$$\rho_{12}(t) = \langle a_1(t) a_2(t)^* \rangle = \langle a_1(0) a_2(0)^* \rangle e^{-\Gamma_1/2\, t} e^{-\Gamma_2/2\, t}$$

This gives us

elastic inelastic

$$\boxed{\dot{\rho}_{12} = (\dot{\rho}_{22})_{S.E.} - 1/\tau\, \rho_{12} - \frac{\Gamma_1 + \Gamma_2}{2}\rho_{12}}$$

Density Matrix Description of 2-Level Atoms

Effect on probability amplitudes

Populations are ensemble averages of the type

$$\rho_{11}(t) = \langle |a_1(t)|^2 \rangle = \langle |a_1(0)|^2 \rangle e^{-\Gamma_1 t}$$

$$\rho_{22}(t) = \langle |a_2(t)|^2 \rangle = \langle |a_2(0)|^2 \rangle e^{-\Gamma_2 t}$$

When the populations decay, the averages of the probability amplitudes must decay accordingly,

$$\langle |a_1(t)| \rangle = \langle |a_1(0)| \rangle e^{-\Gamma_1/2\, t}$$

$$\langle |a_2(t)| \rangle = \langle |a_2(t)| \rangle e^{-\Gamma_2/2\, t}$$

Thus, for the coherences

$$\rho_{12}(t) = \langle a_1(t) a_2(t)^* \rangle = \langle a_1(0) a_2(0)^* \rangle e^{-\Gamma_1/2\, t} e^{-\Gamma_2/2\, t}$$

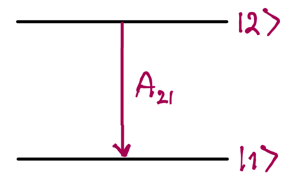
This gives us

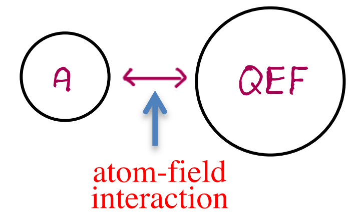
elastic inelastic

$$\boxed{\dot{\rho}_{12} = (\dot{\rho}_{22})_{S.E.} - 1/\tau\, \rho_{12} - \frac{\Gamma_1 + \Gamma_2}{2} \rho_{12}}$$

Spontaneous Decay

This process occurs due to interaction between the Atom and the Quantized Electromagnetic Field





Warm-up: A Bayesian recipe for Mixed States

Alice has two 2-level atoms in the ground state.

Step (1) **She applies a Hamiltonian that drives the evolution**

$$|1\rangle_A |1\rangle_B \rightarrow a_1 |1\rangle_A |1\rangle_B + a_2 |2\rangle_A |2\rangle_B$$

Step (2) **She gives atom B to Bob and asks him to measure if it is in $|1\rangle_B$ or $|2\rangle_B$ and keep the result secret forever.**

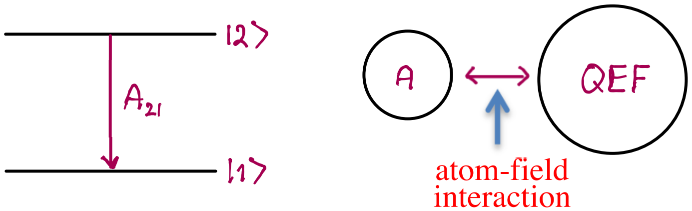
Result: **Alice now has a 2-level atom in the state**

$$\rho = |a_1|^2 |1\rangle_{BB}\langle 1| + |a_2|^2 |2\rangle_{BB}\langle 2|$$

Density Matrix Description of 2-Level Atoms

Spontaneous Decay

This process occurs due to interaction between the Atom and the Quantized Electromagnetic Field



Warm-up: A Bayesian recipe for Mixed States

Alice has two 2-level atoms in the ground state.

Step (1) She applies a Hamiltonian that drives the evolution

$$|1\rangle_A|1\rangle_B \rightarrow a_1|1\rangle_A|1\rangle_B + a_2|2\rangle_A|2\rangle_B$$

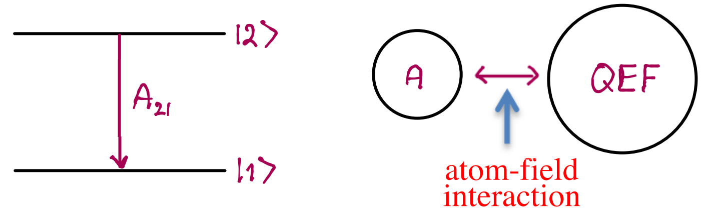
Step (2) She gives atom B to Bob and asks him to measure if it is in $|1\rangle_B$ or $|2\rangle_B$ and keep the result secret forever.

Result: Alice now has a 2-level atom in the state

$$\rho = |a_1|^2\,|1\rangle_{BB}\langle 1| + |a_2|^2\,|2\rangle_{BB}\langle 2|$$

Spontaneous Decay

This process occurs due to interaction between the Atom and the Quantized Electromagnetic Field



Final OPTI 544 Lectures: interaction drives the evolution

$$|\psi(0)\rangle = |2\rangle_A \otimes |vac\rangle_{QEF}$$

Evolution for time *t*

$$|\psi(t)\rangle = C_{2,0}(t)\,|2\rangle_A|vac\rangle_{QEF} + \sum_k C_{1,1_k}(t)\,|1\rangle_A|n_k=1\rangle_{QEF}$$

photon "in the atom" photon in field mode *k*

Cannot recover info in continuum of field modes

Probability $|C_{2,0}(t)|^2$ of having **no decay**

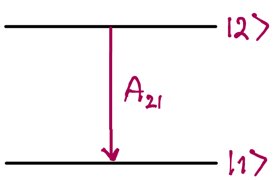
Probability $\sum_k |C_{1,1_k}(t)|^2$ of having **decay**

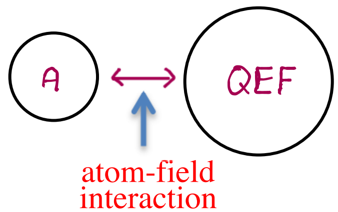
<u>No Coherence</u> established between states $|1\rangle, |2\rangle$

Density Matrix Description of 2-Level Atoms

Spontaneous Decay

This process occurs due to interaction between the Atom and the Quantized Electromagnetic Field





Final OPTI 544 Lectures: **interaction drives the evolution**

$$|\psi(0)\rangle = |2\rangle_A \otimes |vac\rangle_{QEF}$$ Evolution for time *t*

$$|\psi(t)\rangle = C_{2,0}(t)\,|2\rangle_A\,|vac\rangle_{QEF} + \sum_k C_{1,1k}(t)\,|1\rangle_A\,|n_k = 1\rangle_{QEF}$$

photon "in the atom" photon in field mode *k*

Cannot recover info in continuum of field modes

Probability $|C_{2,0}(t)|^2$ of having **no decay**

Probability $\sum_k |C_{1,1k}(t)|^2$ of having **decay**

<u>No Coherence</u> established between states $|1\rangle, |2\rangle$

Conclusion: Decay moves population $|2\rangle \rightarrow |1\rangle$ at rate A_{21}, damps coherence at rate $A_{21}/2$

$$\dot{\rho}_{11} = A_{21}\,\rho_{22}, \quad \dot{\rho}_{22} = -A_{21}\,\rho_{11}$$

$$\dot{\rho}_{12} = -\frac{A_{21}}{2}\,\rho_{12} = \dot{\rho}_{21}^*$$

Putting it all together:

$$\dot{\rho}_{11} = -\Gamma_1\,\rho_{11} + A_{21}\,\rho_{22} - \frac{i}{2}\left(\chi\,\rho_{12} - \chi^*\rho_{21}\right)$$

$$\dot{\rho}_{22} = -\Gamma_2\,\rho_{22} - A_{21}\,\rho_{22} + \frac{i}{2}\left(\chi\,\rho_{12} - \chi^*\rho_{21}\right)$$

$$\dot{\rho}_{12} = (i\Delta - \beta)\,\rho_{12} + \frac{i\chi^*}{2}\left(\rho_{22} - \rho_{11}\right) = \dot{\rho}_{21}^*$$

where $\beta = \frac{1}{\tau} + \frac{A_{21}}{2} + \frac{\Gamma_1 + \Gamma_2}{2}$

These are our desired **Density Matrix Equations of Motion**

Emission and Absorption – Population Rate Equations

So far we have derived a set of Equations of Motion for the elements of the Density Matrix:

$$\dot{\rho}_{11} = -\Gamma_1 \rho_{11} + A_{21}\rho_{22} - \frac{i}{2}(X\rho_{12} - X^*\rho_{21})$$

$$\dot{\rho}_{22} = -\Gamma_2 \rho_{22} - A_{21}\rho_{22} + \frac{i}{2}(X\rho_{12} - X^*\rho_{21})$$

$$\dot{\rho}_{12} = (i\Delta - \beta)\rho_{12} + \frac{iX^*}{2}(\rho_{22} - \rho_{11}) = \dot{\rho}_{21}^*$$

where $\beta = \frac{1}{\tau} + \frac{A_{21}}{2} + \frac{\Gamma_1 + \Gamma_2}{2}$

(∗) These equations are difficult to solve in the general case. See, e. g., Allen & Eberly for a discussion of some special cases and a reference to original work by Torrey et al.

(∗) For ≥ 3 levels the Density Matrix Equations get very cumbersome and it is desirable to simplify the description when possible.

(∗) One such simplification takes the form of Rate Equations for the populations only.

Steady State Solutions: (requires $\Gamma_1 = \Gamma_2 = 0$)

Let $\dot{\rho}_{12} = 0$ ⇒

$$\begin{cases} \rho_{12} = \dfrac{iX^*/2}{\beta - i\Delta}(\rho_{22} - \rho_{11}) \\ \rho_{21} = \dfrac{-iX/2}{\beta - i\Delta}(\rho_{22} - \rho_{11}) \end{cases}$$

$$X\rho_{12} - X^*\rho_{21} = \frac{i|X|^2\beta}{\Delta^2 + \beta^2}(\rho_{22} - \rho_{11})$$

Plug into eqs for Populations to get

$$\boxed{\begin{aligned} \dot{\rho}_{11} &= A_{21}\rho_{22} + \frac{|X|^2\beta/2}{\Delta^2 + \beta^2}(\rho_{22} - \rho_{11}) = 0 \\ \dot{\rho}_{22} &= -A_{21}\rho_{22} - \frac{|X|^2\beta/2}{\Delta^2 + \beta^2}(\rho_{22} - \rho_{11}) = 0 \end{aligned}}$$

These eqs. let us find steady state values for the populations and coherences in terms of X, Δ, A_{21}, β when (and only when) $\dot{\rho}_{11} = \dot{\rho}_{22} = 0$