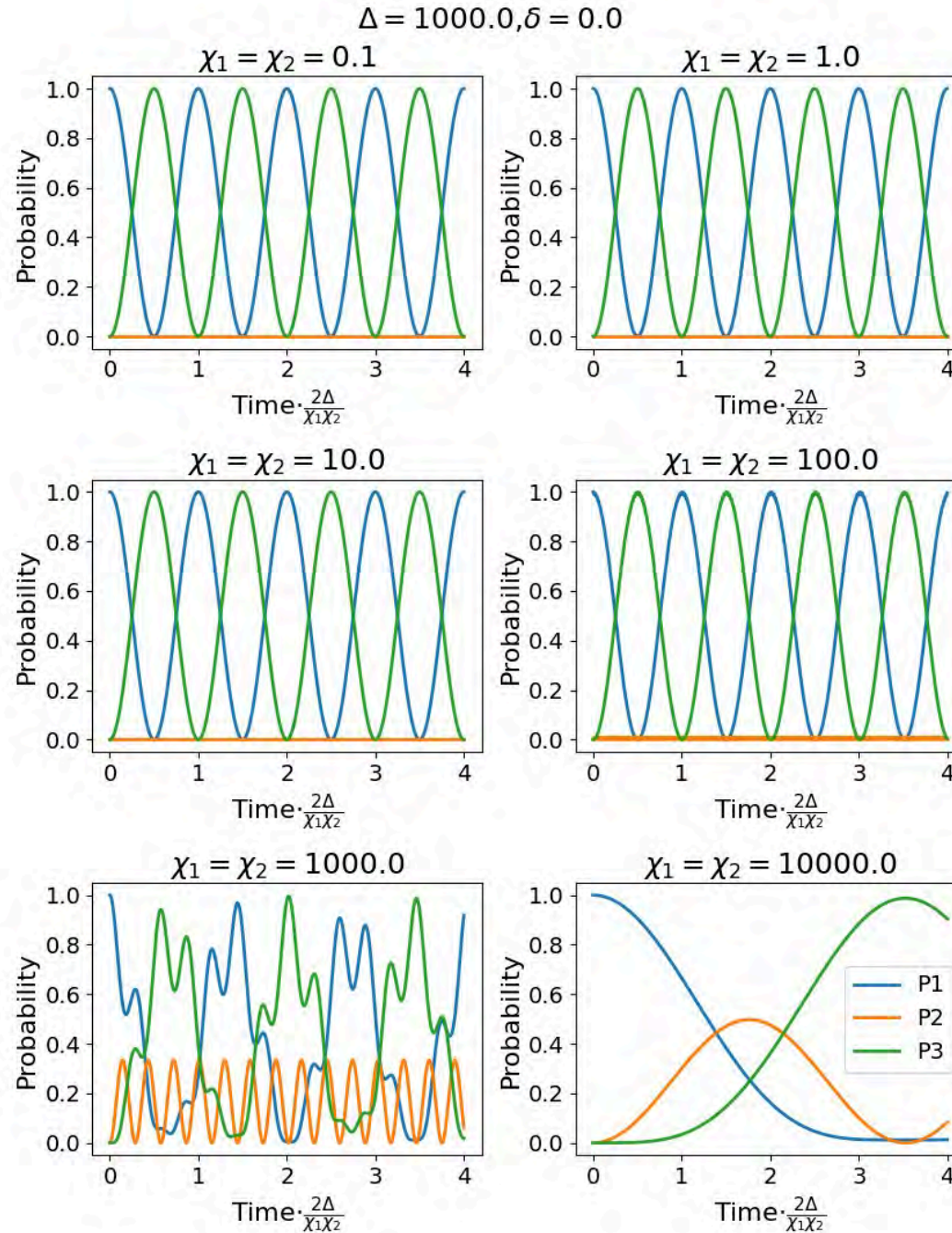


Numerical integration of the equations for the probability amplitudes in a 3-level Lambda system with zero Raman Detuning ($\delta = 0$).



Density Matrix Description of 2-Level Atoms

Begin 02-20-2025

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Mental Warmup: What is a probability?

(1) Example: Coin toss

- We can describe physical states by probability distributions
- Probabilities are assigned based on prior knowledge, updated when additional info becomes available
- As such, probability distributions are subjective (states of knowledge)

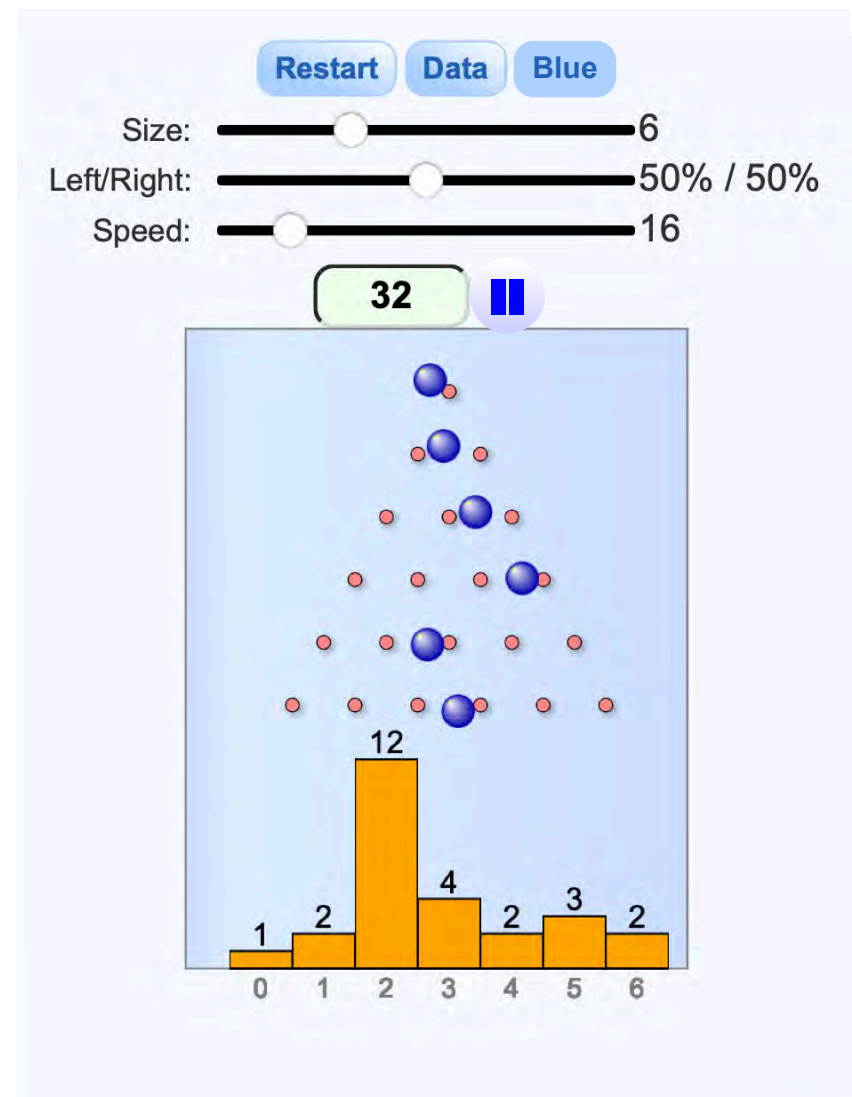
(2) Example: Quincunx

<https://www.mathsisfun.com/data/quincunx.html>

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This is the Bayesian Interpretation of Probability

(3) Example: Quantum Quincunx

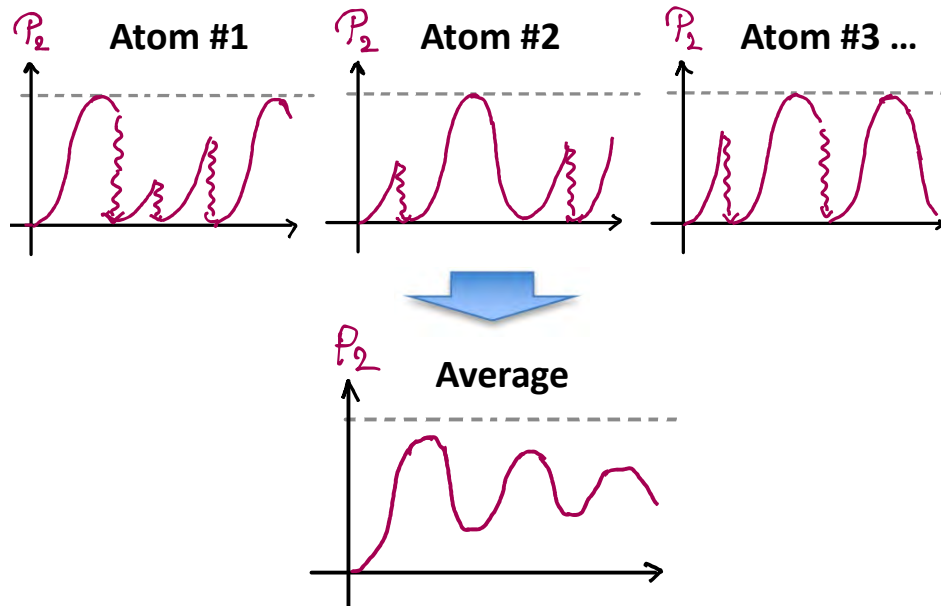


Density Matrix Description of 2-Level Atoms

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(5) Example: Quantum Trajectories

- Ensemble of 2-level atoms undergoing Rabi oscillation with random decays



Definition: Density Operator for pure states

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)|$$

Definition: Density Matrix

$$|\psi(t)\rangle = \sum_n C_n(t) |u_n\rangle \rightarrow$$

$$\rho_{pn}(t) = \langle u_p | \rho(t) | u_n \rangle = C_p(t) C_n^*(t)$$

Definition: Density Operator for mixed states

$$\rho(t) = \sum_k p_k \rho_k(t), \quad \rho_k = |\psi_k(t)\rangle\langle\psi_k(t)|$$

Note: A pure state is just a mixed state for which one $p_k = 1$ and the rest are zero.

Definition: A system for which we know only the probabilities p_k of finding the system in state $|\psi_k\rangle$ is said to be in a statistical mixture of states. Shorthand: mixed state.

Shorthand for non-mixed state: pure state

The terms Density Operator and Density Matrix are used interchangeably

Density Matrix Description of 2-Level Atoms

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The terms Density Operator and Density Matrix are used interchangeably

Let A be an observable w/eigenvalues a_n

Let P_n be the projector on the eigen-subspace of a_n

For a pure state, $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$, we have

$$(*) \quad \text{Tr} \rho(t) = \sum_n \rho_{nn}(t) = \sum_n |c_n|^2 = 1$$

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(*) Let P_n be the projector on eigensubspace of a_n

$$P(a_n) = \langle \psi(t) | P_n | \psi(t) \rangle = \text{Tr} [\rho(t) P_n]$$

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Density Matrix Description of 2-Level Atoms

Begin 02-20-2025

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Density Operator formalism is general !

Important properties of the Density Operator

(1) ρ is Hermitian, $\rho^\dagger = \rho \Rightarrow \rho$ is an observable

$\Rightarrow \exists$ basis in which ρ is diagonal

In this basis a pure state has one diagonal element = 1, the rest = 0

(2) Test for purity.

Pure: $\rho^2 = \rho \Rightarrow \text{Tr} \rho^2 = 1$

Mixed: $\rho^2 \neq \rho \Rightarrow \text{Tr} \rho^2 < 1$

(3) Schrödinger evolution does not change the p_k

\Rightarrow $\left\{ \begin{array}{l} \text{Tr} \rho^2 \text{ is conserved} \\ \text{pure states stay pure} \\ \text{mixed states stay mixed} \end{array} \right.$

Changing pure \Rightarrow mixed requires non-Hamiltonian evolution – see Cohen Tannoudji D_{III} & E_{III}

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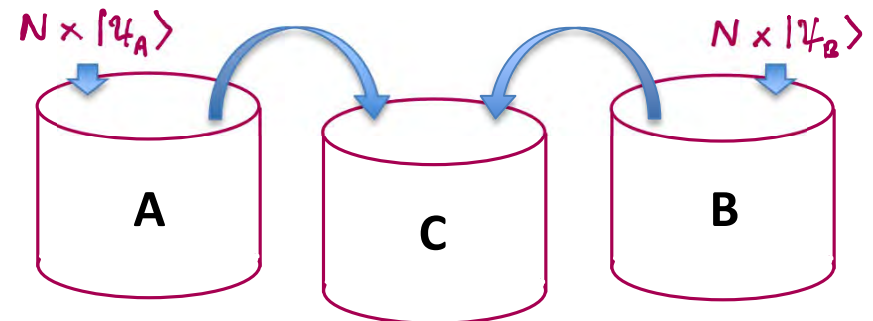
A cooks recipe – interpretations of ρ

Step 1 Add N atoms in state $|\psi_A\rangle$ to bucket A
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We now have two ensembles, each of which consist of N atoms in a known pure state

Step 2 Add buckets A and B to bucket C and stir.



Pick an atom from C

Which is Correct?

The atom is in a pure state but we don't know if it is in $|\psi_A\rangle$ or $|\psi_B\rangle$

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$$\rho = \frac{1}{2} |\psi_A\rangle\langle\psi_A| + \frac{1}{2} |\psi_B\rangle\langle\psi_B|$$

Density Matrix Description of 2-Level Atoms

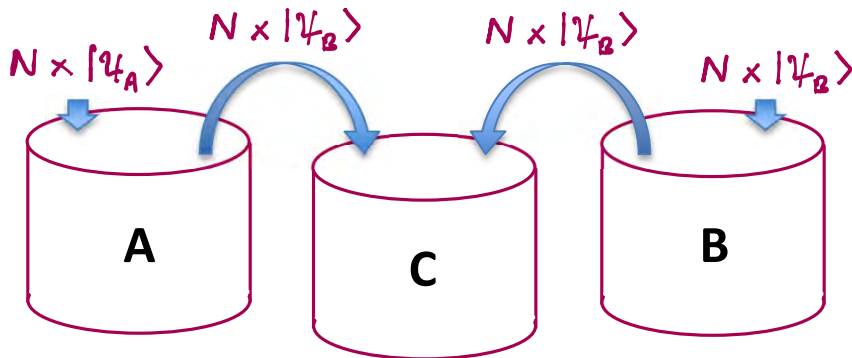
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There is no difference!

The two interpretations lead to identical predictions for any measurement we can do on atoms from C

Quantum Mechanics:

If two descriptions lead to identical predictions for observable outcomes then they are identical

Loosely, (i) is a *frequentist view*
 (ii) is a *Bayesian view*

Quantum Bayesianism

Quantum States are States of Knowledge
 (subjective)

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(*) Note: The notation $\langle \cdot \rangle_k$ is used on the following pages to indicate an ensemble average.

More about the Density Matrix

In the orthonormal basis $\{|u_j\rangle\}$ the elements of a pure density matrix are $\langle u_n | \rho | u_p \rangle = c_n c_p^*$. For a mixed state, $\rho = \sum_k \eta_k \rho_k$, we have $\rho_{np} = \sum_k \eta_k c_n^{(k)} (c_p^{(k)})^*$. Here and elsewhere, the index k indicates members of the ensemble that are distinct due to, e. g., different preparation.

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

Single system: Prob of finding state $|u_n\rangle$
Ensemble: $|u_n\rangle$ occurs with freq. ρ_{nn}

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

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It follows that

$$\rho_{np} \rho_{pn} \leq \rho_{nn} \rho_{pp} \Rightarrow \rho =$$

with = for pure states

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Density Matrix Description of 2-Level Atoms

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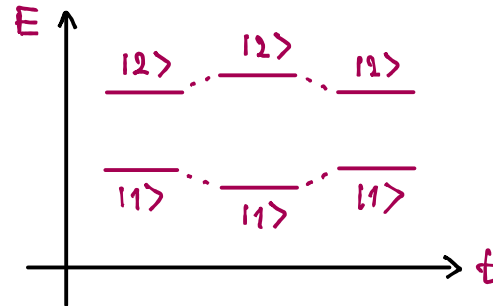
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Example: 2-level atom w/random perturbations



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

The ensemble average

$$\rho_{np} = \langle c_n c_p^* e^{i\theta} \rangle_k$$

is reduced by the randomly fluctuating phase

Dipole Radiation:

$$\begin{aligned} \langle \hat{n} \rangle &= \text{Tr}[\rho \hat{n}] = \text{Tr} \left[\begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \begin{pmatrix} 0 & \vec{n}_{12} \\ \vec{n}_{21} & 0 \end{pmatrix} \right] \\ &= \rho_{12} \vec{n}_{21} + \rho_{21} \vec{n}_{12} = 2 \text{Re}[\rho_{12} \vec{n}_{21}] \end{aligned}$$

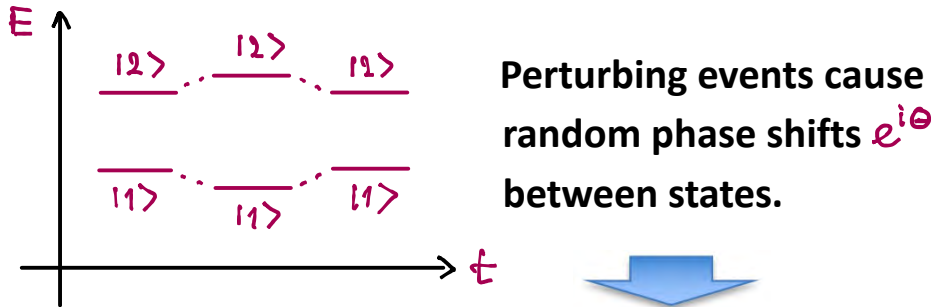
For an ensemble of pure states w/different θ

$$\langle \hat{n} \rangle = \langle \text{Re}[\rho_{12}^{(k)} \vec{n}_{21}] \rangle_k$$

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

Density Matrix Description of 2-Level Atoms

Example: 2-level atom w/random perturbations



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Time Evolution of the Density Matrix

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

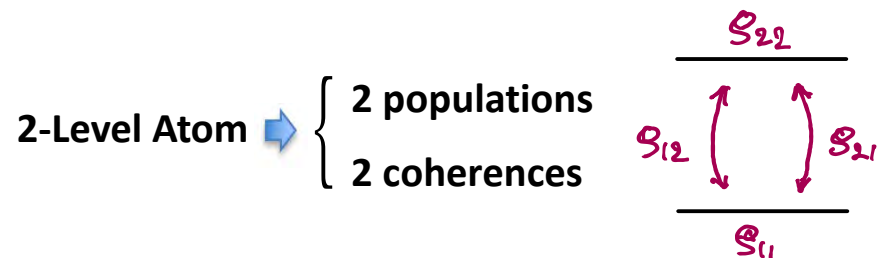
Approach: We do not have time for a rigorous derivation, so will rely on plausible arguments to justify the equations

Schrödinger Evolution: In general, we have

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

matrix elements

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



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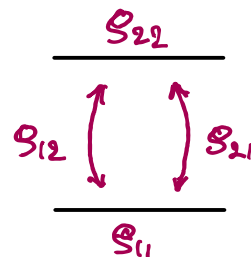
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2-Level Atom

- 2 populations
- 2 coherences



Consider the 2-Level Rabi problem with

$$H = H_0 + V \quad \& \quad V_{12} = \frac{1}{2} \hbar X_{12} e^{-i\omega t} + c.c.$$



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

Set $X_{12} = X, X_{21} = X^*$, substitute $\rho_{12} = \tilde{\rho}_{12} e^{i\omega t}$
↗ slow variable

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

Substitute in (*) (LHS of the page), make RWA, and drop \sim **Homework Set 4 Assignment**



$$\begin{aligned} \dot{\rho}_{11} &= -\frac{i}{2} (X \rho_{12} - X^* \rho_{21}) \\ \dot{\rho}_{22} &= \frac{i}{2} (X \rho_{12} - X^* \rho_{21}) \\ \dot{\rho}_{12} &= -i\Delta \rho_{12} + i\frac{X^*}{2} (\rho_{22} - \rho_{11}) = \dot{\rho}_{21}^* \end{aligned}$$

Rabi Eqs. for pure and mixed states

Density Matrix Description of 2-Level Atoms

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$$\begin{aligned} \dot{\rho}_{11} &= -\frac{i}{2} (X \rho_{12} - X^* \rho_{21}) && \text{Rabi Eqs. for} \\ &&& \text{pure and} \\ &&& \text{mixed states} \\ \dot{\rho}_{22} &= \frac{i}{2} (X \rho_{12} - X^* \rho_{21}) \\ \dot{\rho}_{12} &= -i\Delta \rho_{12} + i\frac{X^+}{2} (\rho_{22} - \rho_{11}) = \dot{\rho}_{21}^* \end{aligned}$$

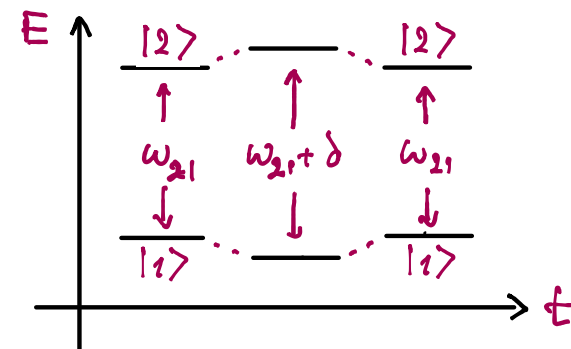
Next: Non-Hamiltonian evolution

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 \Rightarrow 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

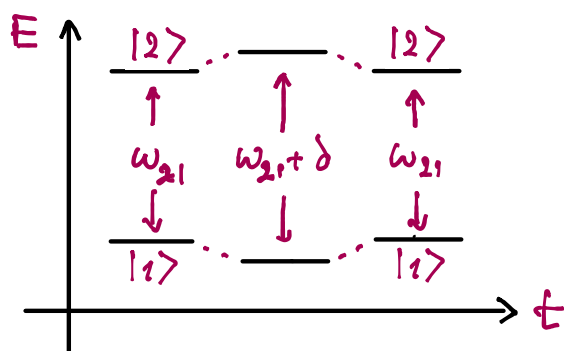
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Evolution of coherence (fast variables)

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

collisional history \downarrow

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

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 $\langle \delta\omega(t) \rangle_{\mathbb{R}} = 0$
- Collisions have no memory over time,

$$\langle \delta\omega(t) \delta\omega(t') \rangle_{\mathbb{R}} = \frac{2}{\tau} \delta(t-t')$$



Can show that, averaged over time and the ensemble

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

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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

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

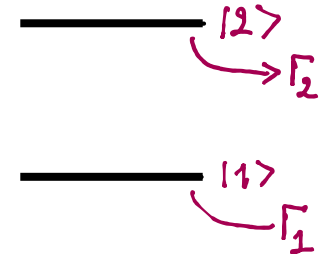
Simple Model of Inelastic Collisions

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 $\text{Tr} \rho(t)$ is not preserved

Convenient when working with quantities

$$N \langle \hat{n} \rangle \propto N (\vec{\eta}_{12} \rho_{21} + \vec{\eta}_{21} \rho_{12})$$

Density Matrix Description of 2-Level Atoms

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

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,

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

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

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

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

Density Matrix Description of 2-Level Atoms

Effect on probability amplitudes

Populations are ensemble averages of the type

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

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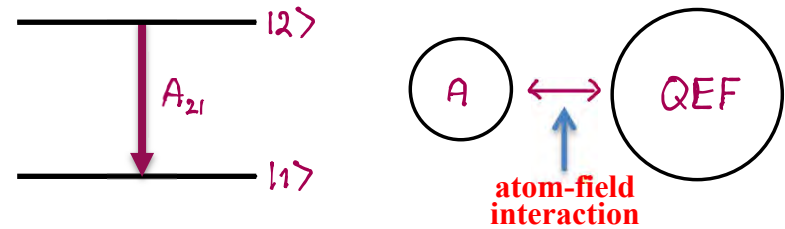
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$$\dot{S}_{12} = (\dot{S}_{12})_{S.E.} - 1/\tau S_{12} - \frac{\Gamma_1 + \Gamma_2}{2} S_{12}$$

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.

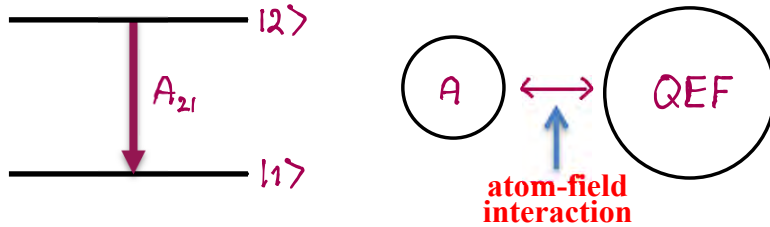
Result: Alice now has a 2-level atom in the state

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

Density Matrix Description of 2-Level Atoms

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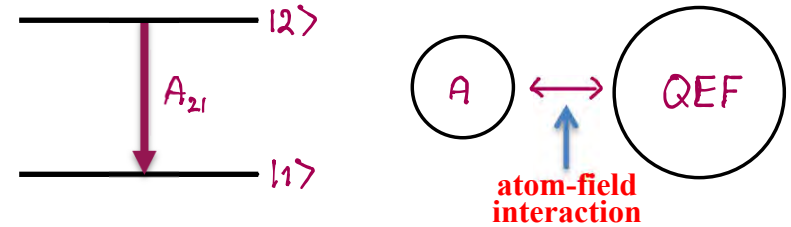
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$$\rho = |a_1|^2 |1\rangle_B \langle 1| + |a_2|^2 |2\rangle_B \langle 2|$$

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Final OPTI 544 Lectures:

$$|\psi(0)\rangle = |2\rangle_A |vac\rangle_{QEF} \xrightarrow{\text{evolution over time } t} |\psi(t)\rangle = c_{2,0}(t) |2\rangle_A |vac\rangle_{QEF} + \sum_k c_{1,1k}(t) |1\rangle_A |n_k=1\rangle_{QEF}$$

↑
↑
 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**

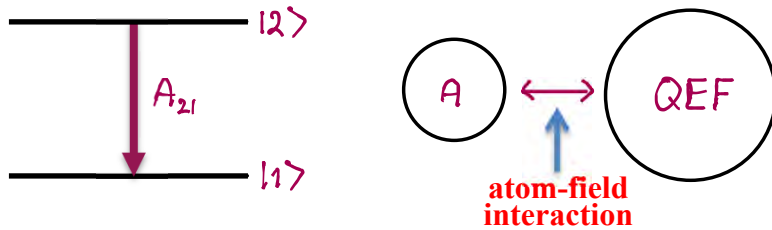
Probability $\sum_k |c_{1,1k}(t)|^2$ of having **decay**

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No Coherence 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:

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

$$\dot{\rho}_{22} = -\Gamma_2 \rho_{22} - A_{21} \rho_{11} + \frac{i}{2} (X \rho_{12} - X^* \rho_{21})$$

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

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

These are our desired

Density Matrix Equations of Motion

Emission and Absorption – Population Rate Equations