Density Matrix Description of 2-Level Atoms

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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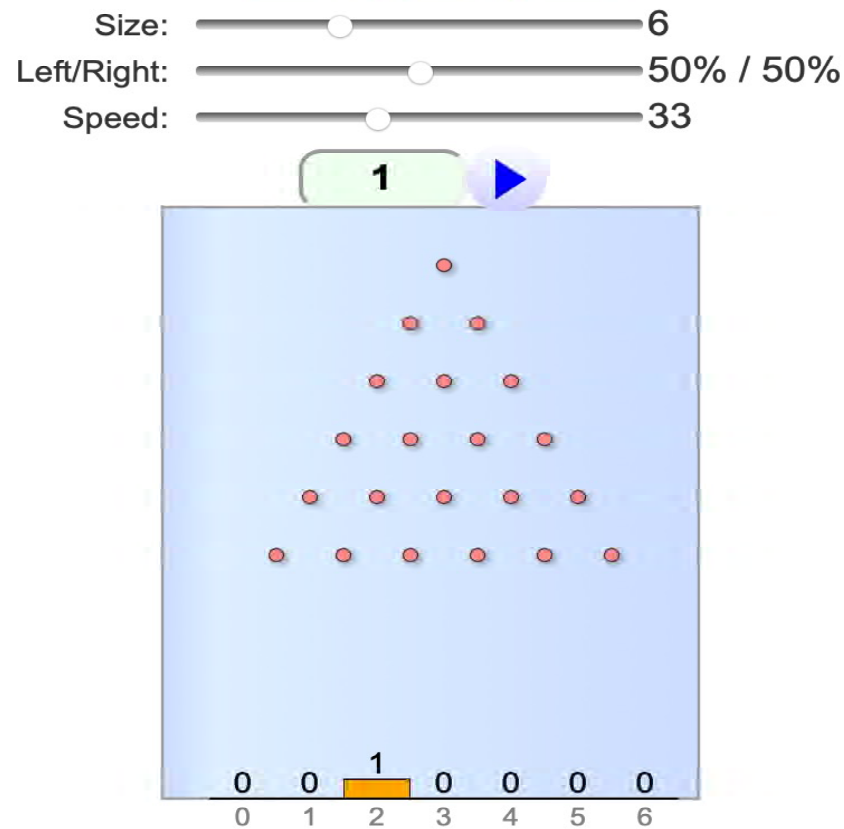
This is the Bayesian Interpretation of Probability

Quincunx



Note: We might do a coin flip to choose the Quincunx configuration (e. g., size)

Probability distribution over probability distributions !

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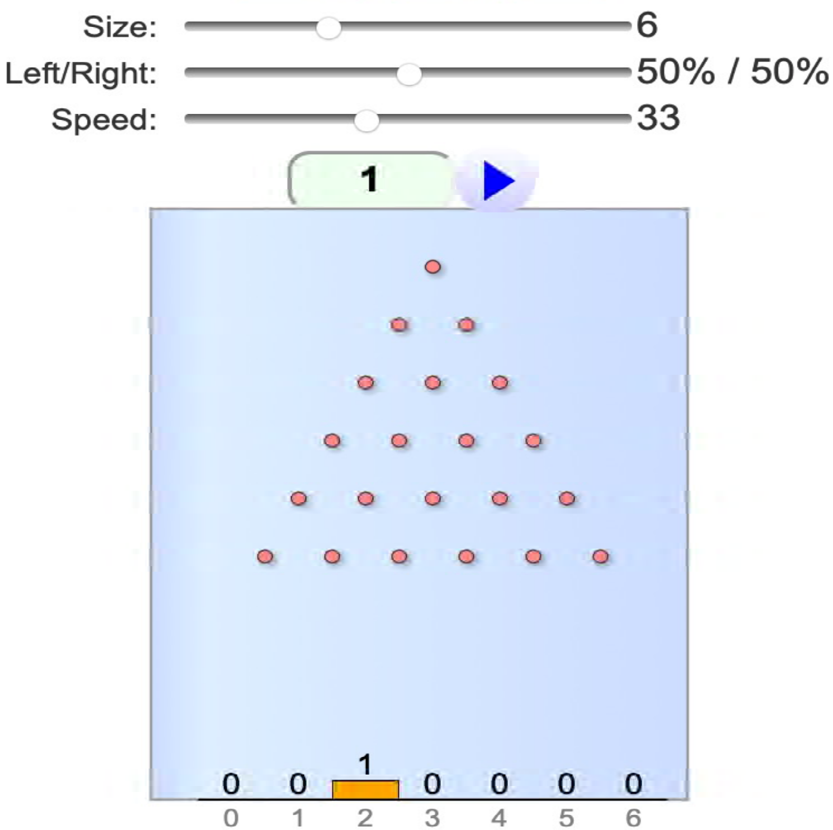
Quincunx



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Probability distribution over probability distributions !

(3) Example: Quantum Quincunx

- We can describe physical states by quantum wavefunctions (state vectors)
- Quantum states are assigned based on prior knowledge, updated when additional info becomes available
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(4) Mixed Quantum & Classical Case

- We can easily envision a hybrid Quincunx that is part classical, part quantum.
- Physics needs an efficient description these kinds of intermediate situations

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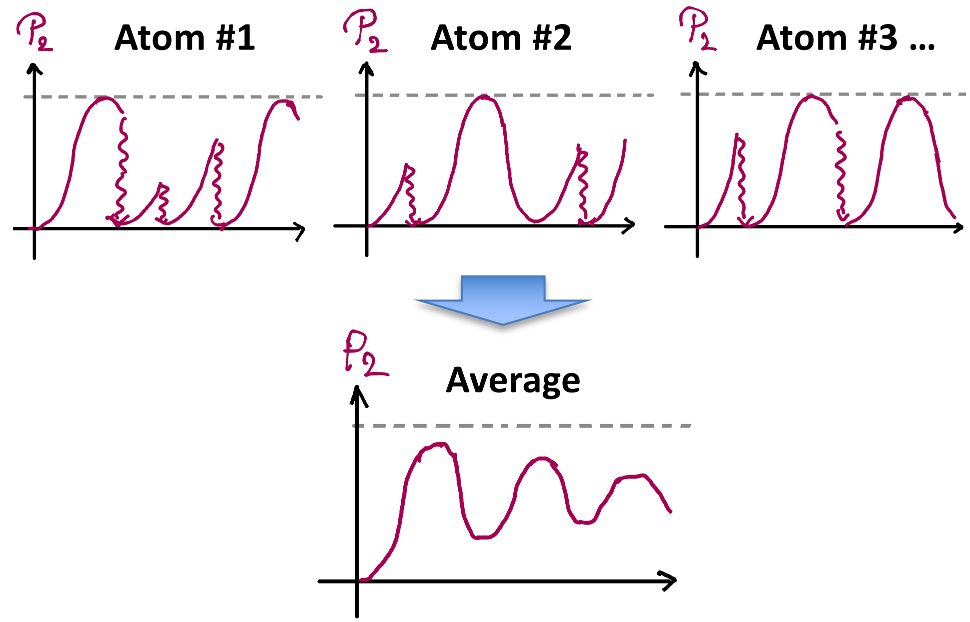
(5) Example: Quantum Trajectories

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



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

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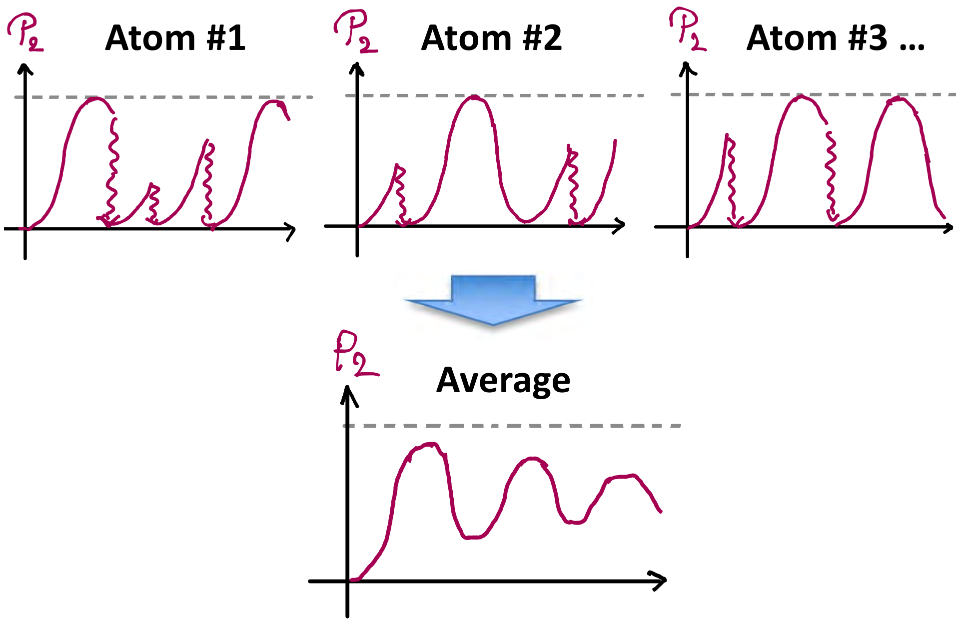

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Definition: Density Operator for pure states

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

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.

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

(*) $\mathrm{Tr}\,\rho(t) = \sum_n \rho_{nn}(t) = \sum_n |C_n|^2 = 1$

(*) $\langle A\rangle = \langle\psi(t)|A|\psi(t)\rangle = \sum_p \langle\psi(t)|A|u_p\rangle\langle u_p|\psi(t)\rangle$

$= \sum_p \langle u_p|\psi(t)\rangle\langle\psi(t)|A|u_p\rangle = \sum_p \langle u_p|\rho(t)A|u_p\rangle$

$= \mathrm{Tr}[\rho(t)A]$ ($|u_p\rangle$ basis in $\mathcal{H}$)

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

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

(*) $\dot{\rho}(t) = |\dot{\psi}(t)\rangle\langle\psi(t)| + |\psi(t)\rangle\langle\dot{\psi}(t)|$

$= \frac{1}{i\hbar}H|\psi(t)\rangle\langle\psi(t)| - \frac{1}{i\hbar}|\psi(t)\rangle\langle\psi(t)|H$

$= \frac{1}{i\hbar}[H,\rho]$

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Density Operator formalism is general !

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Density Operator formalism is general !

Important properties of the Density Operator

(1) ρ is Hermitian, $\rho^+ = \rho$ ⇨ ρ is an observable

⇨ $\exists$ basis in which ρ is diagonal

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

(2) Test for purity.

Pure: $\rho^2 = \rho$ ⇨ $\mathrm{Tr}\,\rho^2 = 1$

Mixed: $\rho^2 \neq \rho$ ⇨ $\mathrm{Tr}\,\rho^2 < 1$

(3) Schrödinger evolution does not change the p_k

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

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

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A cooks recipe – interpretations of ρ

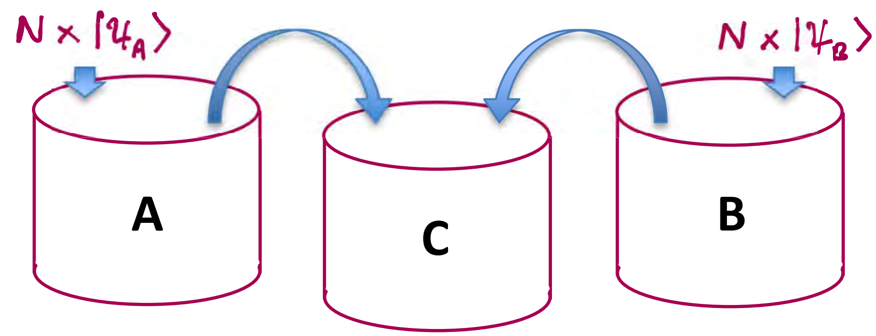
Step 1 Add N atoms in state $|\psi_A\rangle$ to bucket A

Add N atoms in state $|\psi_B\rangle$ to bucket B

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 mix

(Mixing does not affect the state of a given atom)



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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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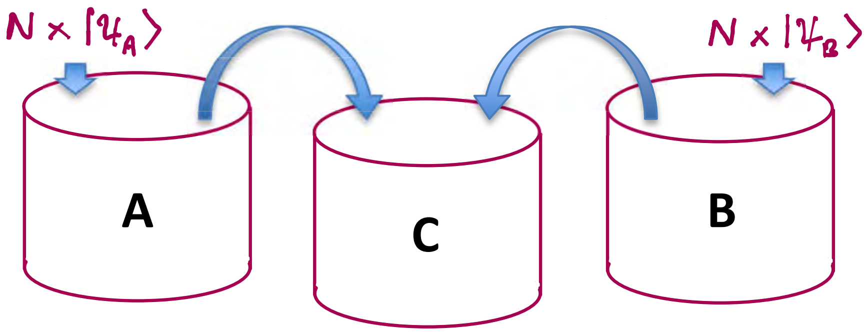

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There is no difference!

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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02-15-2023

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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

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

ensemble average

It follows that

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

with = for pure states

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

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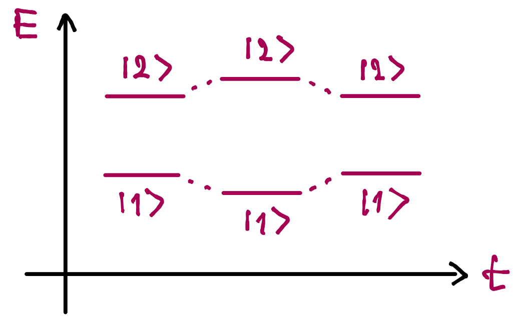
Example: 2-level atom w/random perturbations



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

The ensemble average $\rho_{nm} = \sum_k p_k c_n c_m^* e^{i\theta_k}$ 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

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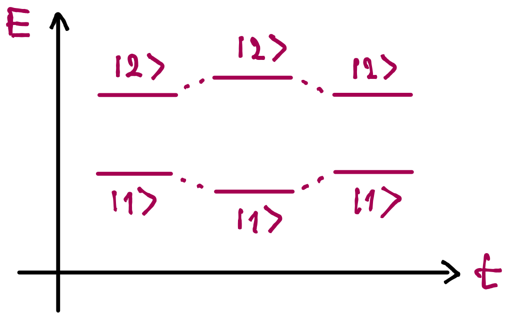

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Time Evolution of the Density Matrix

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

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

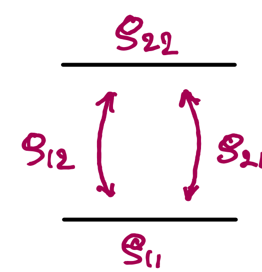
Schrödinger Evolution: In general, we have

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

matrix elements

$$\dot{\rho}_{nm} = -\frac{i}{\hbar}\sum_{j=1,2}(H_{nj}\rho_{jm} - \rho_{nj}H_{jm})$$

2-Level Atom ⇒ { 2 populations, 2 coherences }



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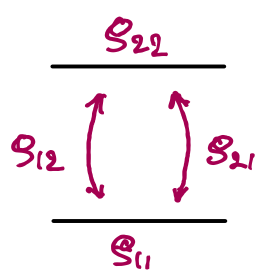

Consider the 2-Level Rabi problem with

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

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

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

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

Substitute in $(*)$, make RWA, and drop ~

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

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Rabi Eqs. for pure and mixed states

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Rabi Eqs. for pure and mixed states

Next: Non-Hamiltonian evolution

Types of events

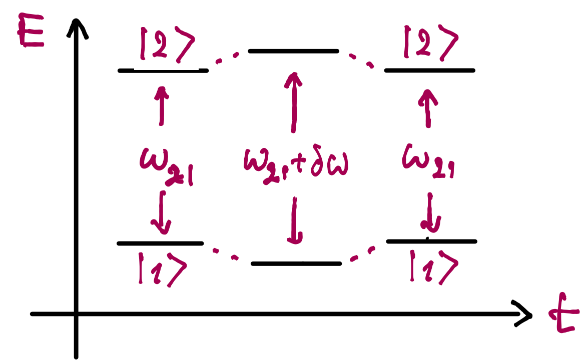
(i) Elastic collisions: No change in energy

(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)

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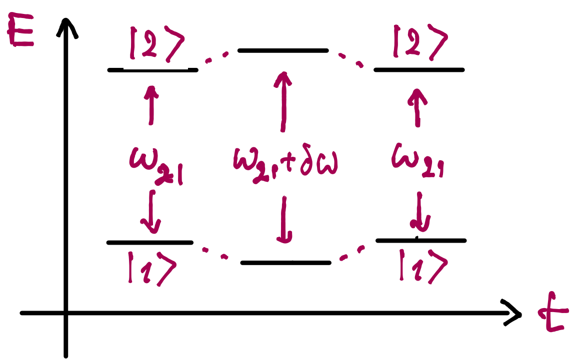


(Paradigm for perturbations that do not lead to net change in energy)

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 <u>ensemble average of</u> $\rho_{12}(t)$

<u>Assumptions</u>: (k : ensemble average)

- From atom to atom $\delta\omega(t)$ is a Gaussian Random Variable
- Averaged over the ensemble $\langle\delta\omega(t)\rangle_k = 0$
- Collisions have no memory over time,

$$\langle\delta\omega(t)\,\delta\omega(t')\rangle_k = \frac{2}{\tau}\,\delta(t-t')$$

Can show that, averaged over time and the ensemble

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

Density Matrix Description of 2-Level Atoms

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 <u>ensemble average of</u> $\rho_{12}(t)$

<u>Assumptions</u>: ($\mathcal{E}$: ensemble average)

- From atom to atom $\delta\omega(t)$ is a Gaussian Random Variable
- Averaged over the ensemble $\langle \delta\omega(t)\rangle_{\mathcal{E}} = 0$
- Collisions have no memory over time,

$$\langle \delta\omega(t)\,\delta\omega(t')\rangle_{\mathcal{E}} = \frac{2}{\tau}\,\delta(t-t')$$

Can show that, averaged over time and the ensemble

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

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

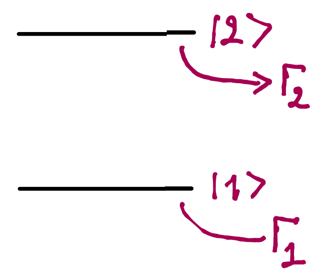
$$\boxed{\dot{\rho}_{12} = (\dot{\rho}_{12})_{S.E.} + (\dot{\rho}_{12})_{E.C.} = -(i\omega_{21} - 1/\tau)\rho_{12}}$$

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

Convenient when working with quantities

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

Density Matrix Description of 2-Level Atoms

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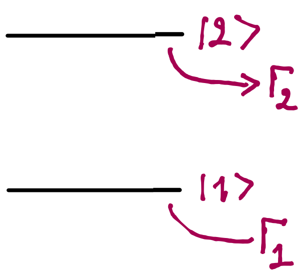

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Effect on probability amplitudes

Populations are ensemble averages of the type

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

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

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

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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

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

Density Matrix Description of 2-Level Atoms

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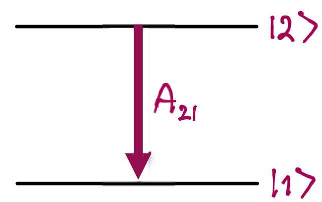
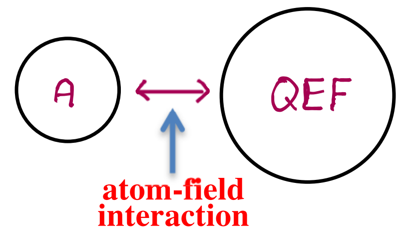
Spontaneous Decay

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

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

Density Matrix Description of 2-Level Atoms

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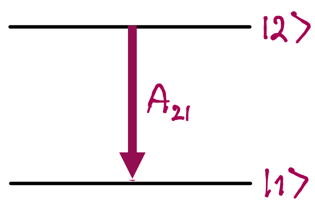

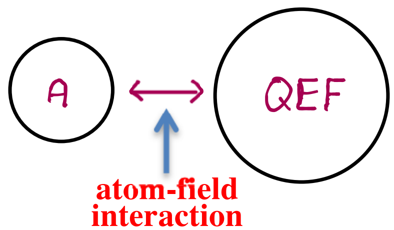

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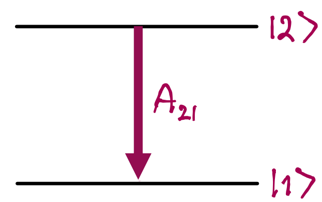

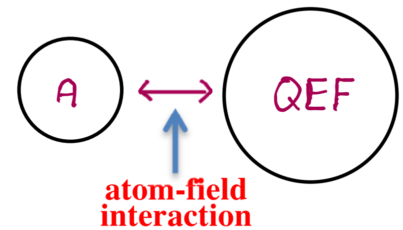

Final OPTI 544 Lectures:

$|\psi(0)\rangle = |2\rangle_A \otimes |Vac\rangle_{QEF}$ evolve for time t

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

excitation in the atom — excitation 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 $|1\rangle, |2\rangle$

Density Matrix Description of 2-Level Atoms

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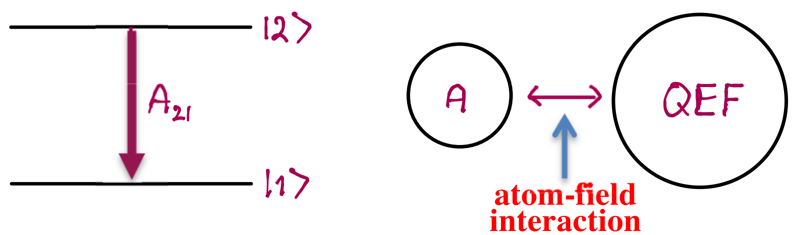

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Conclusion: Decay moves population $|2\rangle \rightarrow |1\rangle$ at rate A_{21}, damps coherence at rate $A_{21}/2$

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

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

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**