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

- 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)

This is the Bayesian Interpretation of Probability

(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
- As such, quantum states are subjective (states of knowledge)

(3) Mixed Quantum & Classical Case

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

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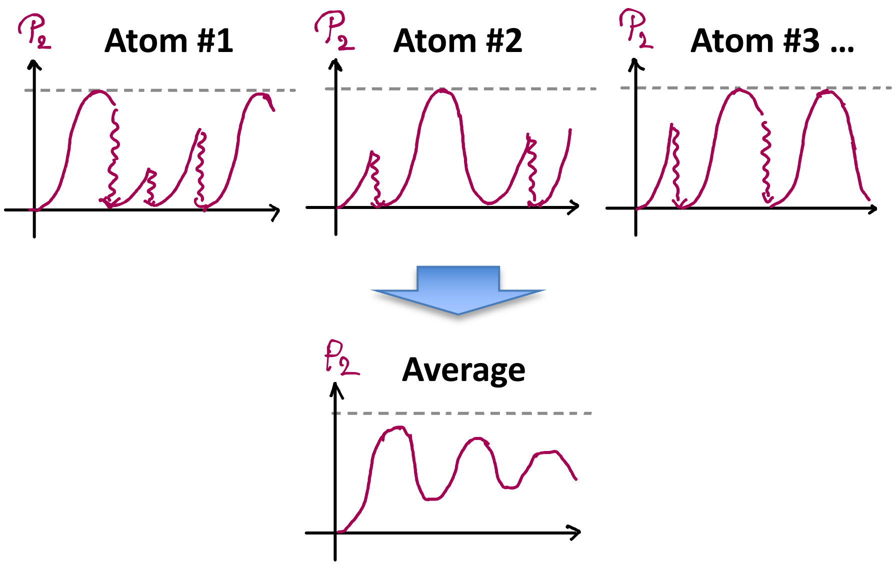
(4) Example: Quantum Trajectories

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



Definition: A system for which we know only the probabilities η_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

Definition: Density Operator for pure states

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

Definition: Density Matrix

$$|\psi(t)\rangle = \sum_n c_n(t)|u_n\rangle \Rightarrow$$

$$\rho_{pn}(t) = \langle u_p|\rho(t)|u_n\rangle = c_p(t)\,c_n^*(t)$$

The terms Density Operator and Density Matrix are used interchangeably

Definition: Density Operator for mixed states

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

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

Density Matrix Description of 2-Level Atoms

Let A be an observable with $\begin{cases} \text{eigenvalues} & a_n \\ \text{eigenvectors} & |a_n^{(j)}\rangle \end{cases}$

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

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

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

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

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

$= \mathrm{Tr}[\rho(t)A]$

(iii) P_n projector on subspace of a_n

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

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

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

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

Let A be an observable with $\begin{cases} \text{eigenvalues} & a_n \\ \text{eigenvectors} & |a_n^{(j)}\rangle \end{cases}$

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

For a <u>mixed</u> state, $\rho(t) = \sum_k \eta_k \rho_k(t)$, $\rho_k = |\psi_k(t)\rangle\langle\psi_k(t)|$

Density Operator formalism is general

(i) $\mathrm{Tr}\,\rho(t) = \sum_k \eta_k \mathrm{Tr}\,\rho_k(t) = 1$

(ii) $\langle A\rangle = \sum_k \eta_k \langle\psi_k(t)|A|\psi_k(t)\rangle$

$= \sum_k \eta_k \mathrm{Tr}[\rho_k(t)A]$

$= \mathrm{Tr}[\rho(t)A]$

(iii) P_n projector on subspace of a_n

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

(iv) $\dot{\rho}(t) = \sum_k \eta_k \left(|\dot{\psi}_k(t)\rangle\langle\psi_k(t)| + |\psi_k(t)\rangle\langle\dot{\psi}_k(t)|\right)$

$= \sum_k \eta_k \frac{1}{i\hbar}\left(H|\psi_k(t)\rangle\langle\psi_k(t)| - |\psi_k(t)\rangle\langle\psi_k(t)|H\right)$

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

Density Matrix Description of 2-Level Atoms

Some important properties of the Density Operator

(1) ρ is Hermitian, $\rho^\dagger = \rho$ ⇨ 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

⇨ $\mathrm{Tr}\,\rho^2$ is conserved
pure states stay pure
mixed states stay mixed

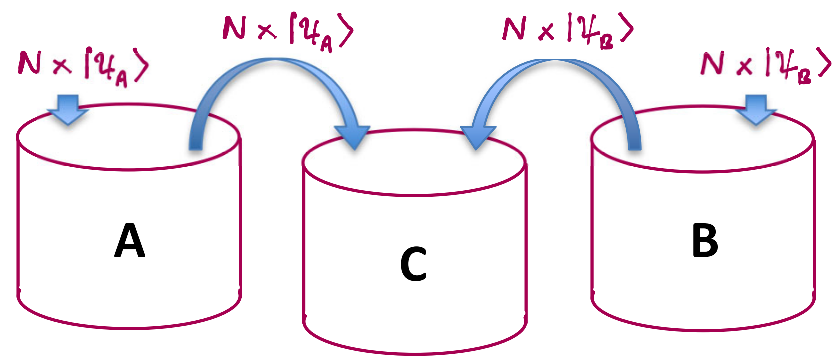
Changing pure ⇨ mixed requires non-Hamiltonian evolution – see Cohen Tannoudji D_{III} & E_{III}

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 know 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 well



Pick an atom from C

Which is Correct?

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

The atom is in a mixed state

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

Density Matrix Description of 2-Level Atoms

There is no difference!

The two interpretations lead to identical predictions for any measurement we can do on atoms drawn 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)

Density Matrix Description of 2-Level Atoms

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 $\mathrm{Tr}\,\rho^2$ (measure of purity)

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

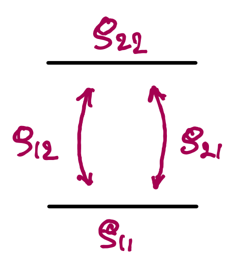
Schrödinger Evolution: In general, we have

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

matrix elements

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

2-Level Atom ⇨ 2 populations, 2 coherences



Consider the 2-Level Rabi problem with

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

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

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

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Next: Non-Hamiltonian evolution

Types of events

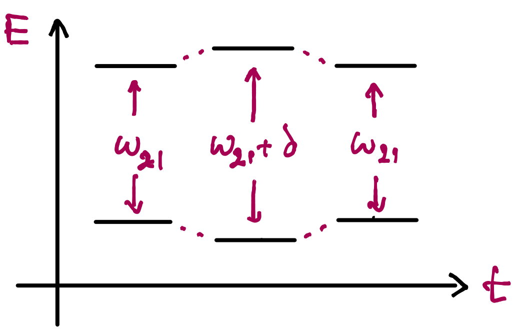
(i) Elastic collisions: No change in energy

(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

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

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

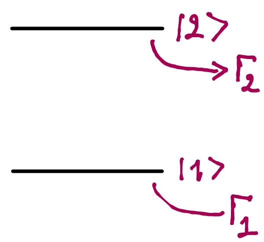
Add this decay to the equation of motion to get

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

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

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

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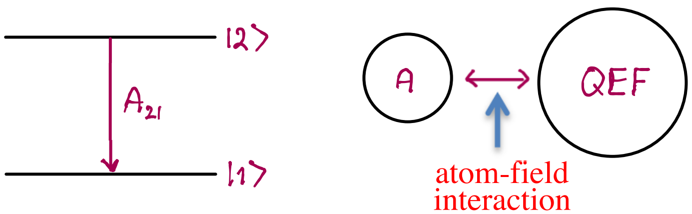
Spontaneous Decay

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**

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

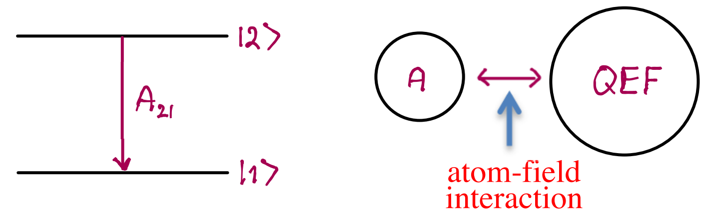
Step (2) **She gives atom B to Bob and asks him to measure if it is in $|1\rangle_B$ or $|2\rangle_B$ and keep the result secret forever.**

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

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

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*

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

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 $|1\rangle, |2\rangle$

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

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

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

Putting it all together:

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

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

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

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

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