Begin 02-08-2024

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
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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)

(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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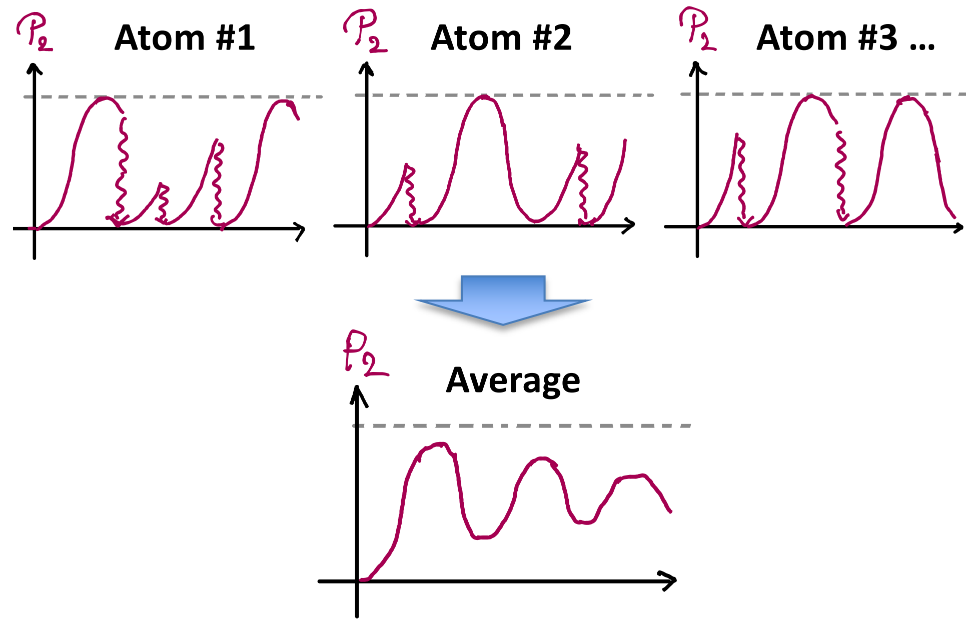
(5) Example: Quantum Trajectories

- 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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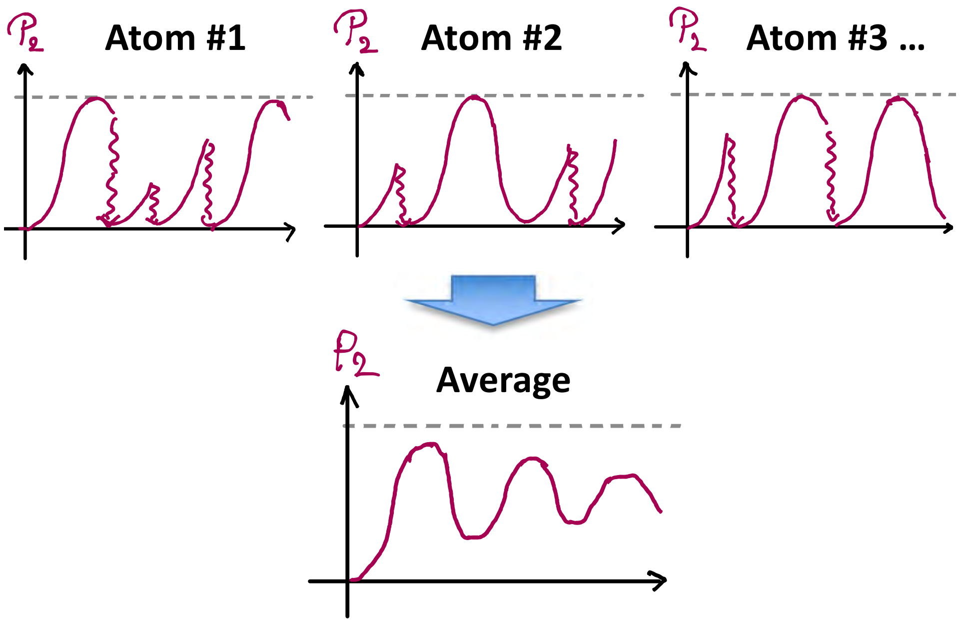

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Shorthand for non-mixed state: pure state

Definition: Density Operator for pure states

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

Definition: Density Matrix

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

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

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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Definition: Density Operator for mixed states

$$\rho(t) = \sum_{\vec{k}} \eta_k\,\rho_k(t), \quad \rho_k = |\psi_k(t)\rangle\langle\psi_k(t)|$$

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

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

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

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

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

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

Density Matrix Description of 2-Level Atoms

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Let A be an observable w/eigenvalues a_n

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

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

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

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

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Let A be an observable w/eigenvalues a_n

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For a **mixed** state, $\rho(t) = \sum_k \eta_k \rho_k(t)$, $\rho_k = |\psi_k(t)\rangle\langle\psi_k(t)|$

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

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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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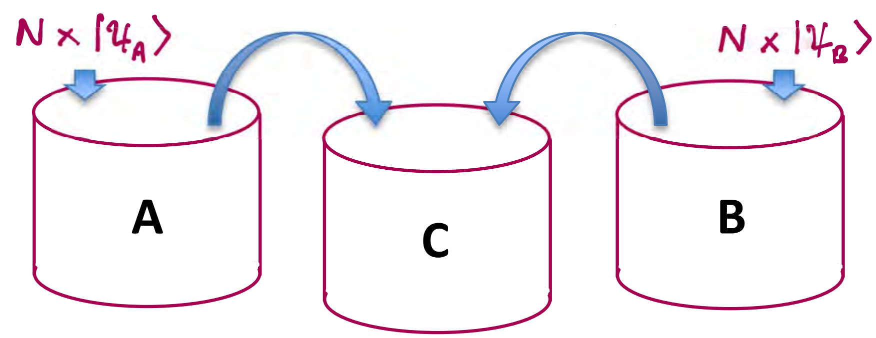
A cooks recipe – interpretations of ρ

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 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 $|\psi_B\rangle$
>
> The atom is in a mixed state
>
> $\rho = \frac{1}{2}|\psi_A\rangle\langle\psi_A| + \frac{1}{2}|\psi_B\rangle\langle\psi_B|$

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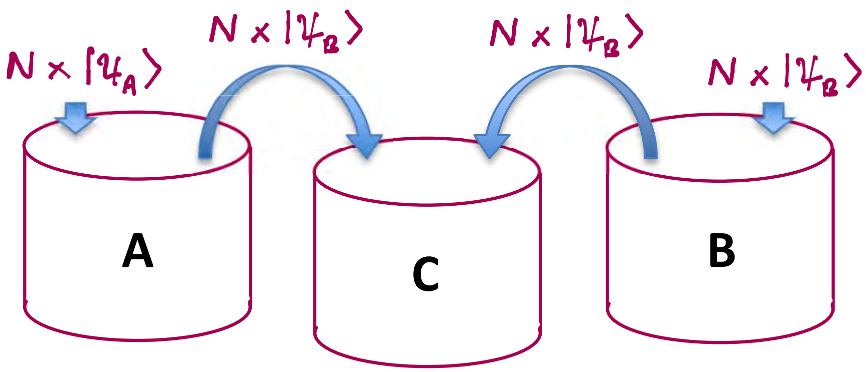

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There is no difference!

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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Quantum States are States of Knowledge
(subjective)

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

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

It follows that

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

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with = for pure states

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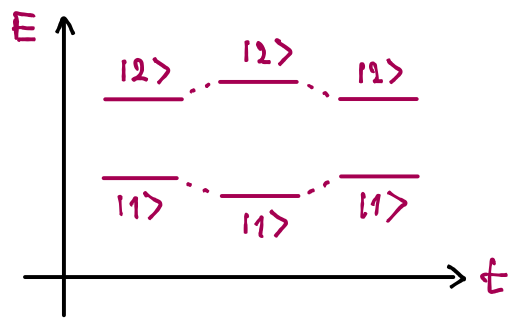
Example: 2-level atom w/random perturbations



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:

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

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

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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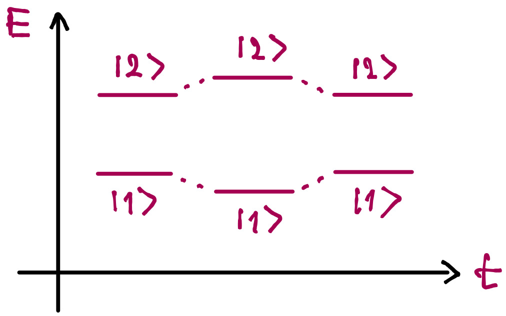
Example: 2-level atom w/random perturbations



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

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

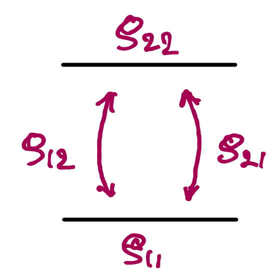
Schrödinger Evolution: In general, we have

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

matrix elements

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

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



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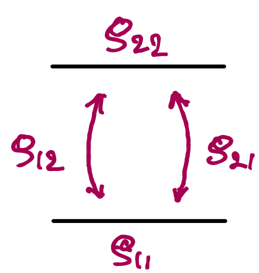

Consider the 2-Level Rabi problem with

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

⇩

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

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

slow variable

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

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

⇩

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

Rabi Eqs. for pure and mixed states

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