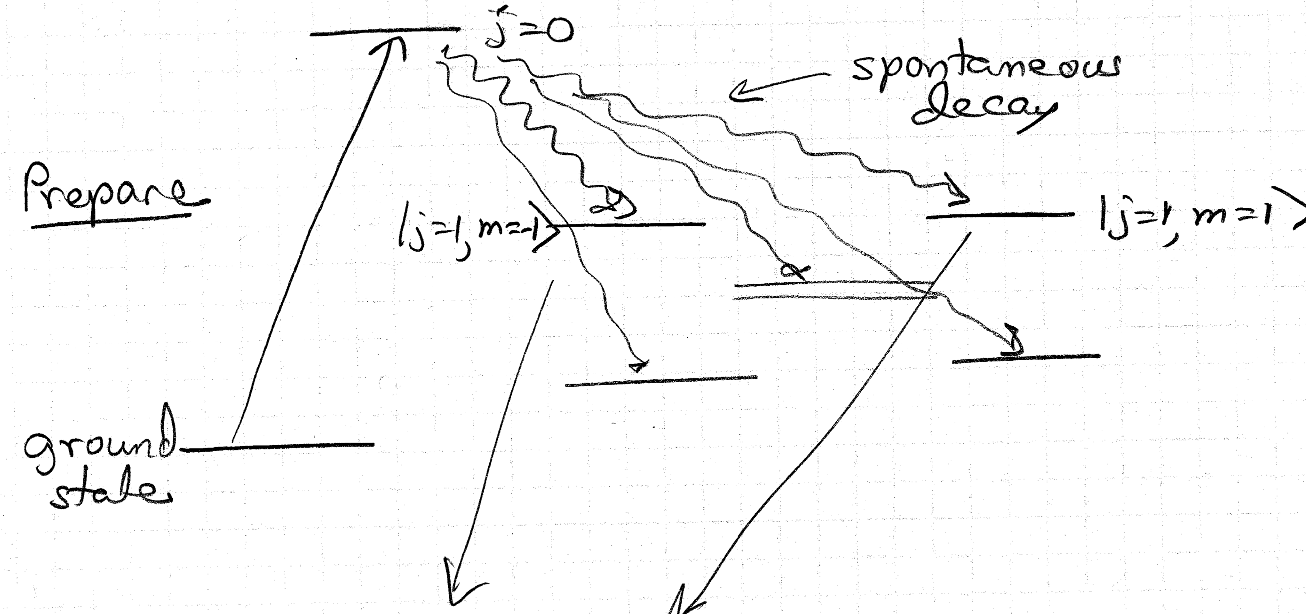
Density Operator

ACME edm state preparation — "dark state" in problems



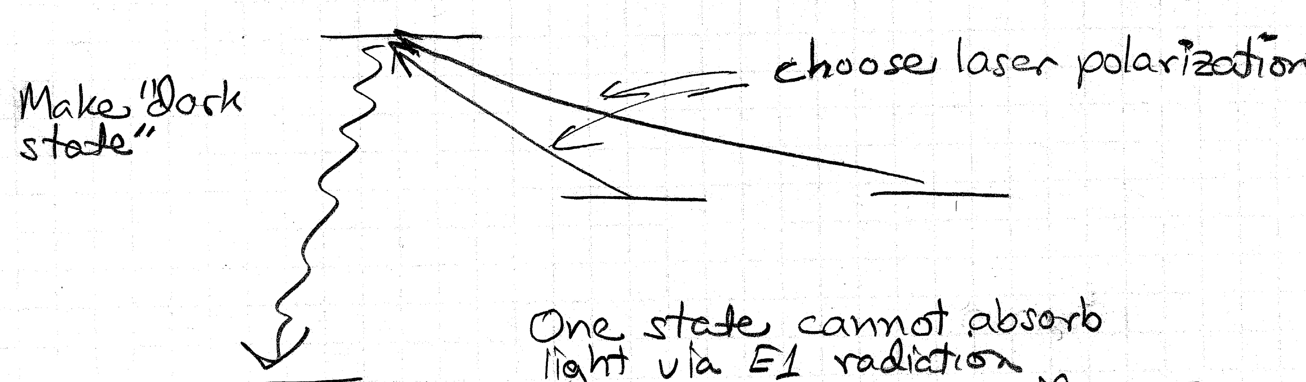
every excitation of those two states has no definite phase relation

cannot describe with a w.f.

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left[|1\,1\rangle + e^{i\delta}|1\,-1\rangle\right]$$

different for every excited molecule

"incoherent superposition"



One state cannot absorb light via E1 radiation

can describe with a w.f.

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left[|1\,1\rangle + e^{i\delta}|1\,-1\rangle\right]$$

light pol. chooses this

"coherent superposition"

Both cases $\longrightarrow$ equal prob. for each of the two states

Incoherent superposition

$$\langle O \rangle = \frac{1}{2} \left| \langle \overbrace{\tfrac{1}{2}\,\tfrac{1}{2}}^{\psi_1} | O | \tfrac{1}{2}\,\tfrac{1}{2} \rangle \right|^2 + \frac{1}{2} \left| \langle \overbrace{\tfrac{1}{2}\,-\tfrac{1}{2}}^{\psi_2} | O | \tfrac{1}{2}\,-\tfrac{1}{2} \rangle \right|^2$$

extra probability

Coherent superposition

$$\langle O \rangle = (1) \left| \langle \psi | O | \psi \rangle \right|^2$$

Both have the form

$$\langle O \rangle = \sum_i P_i \left| \langle \psi_i | O | \psi_i \rangle \right|^2$$

Formalize the averaging

$$\langle \mathcal{O} \rangle_\psi = \langle \psi | \mathcal{O} | \psi \rangle$$

$$\langle \mathcal{O} \rangle = \sum_\psi P_\psi \langle \psi | \mathcal{O} | \psi \rangle$$

$$= \sum_{k\ell} \sum_\psi P_\psi \langle \psi | k \rangle \langle k | \mathcal{O} | \ell \rangle \langle \ell | \psi \rangle$$

$$= \sum_{k\ell\psi} P_\psi \langle \ell | \psi \rangle \langle \psi | k \rangle \langle k | \mathcal{O} | \ell \rangle$$

$$= \sum_{k\ell} \langle \ell | \underbrace{\left[\sum_\psi P_\psi | \psi \rangle \langle \psi | \right]}_{} | k \rangle \langle k | \mathcal{O} | \ell \rangle$$

Density Operator $\boxed{\rho \equiv \sum_\psi P_\psi | \psi \rangle \langle \psi |}$

$$= \sum_{k\ell} \langle \ell | \rho | k \rangle \langle k | \mathcal{O} | \ell \rangle$$

$$= \sum_\ell \langle \ell | \rho \mathcal{O} | \ell \rangle$$

$$\boxed{\langle \mathcal{O} \rangle = \mathrm{tr} \{ \rho \mathcal{O} \}}$$

eg. Unpolarized spins

$$\rho = \sum_{\psi} P_{\psi} \left[\frac{1}{\sqrt{2}} |\tfrac{1}{2}\tfrac{1}{2}\rangle + \frac{1}{\sqrt{2}} e^{i\delta_{\psi}} |\tfrac{1}{2}\,{-\tfrac{1}{2}}\rangle \right] \left[\frac{1}{\sqrt{2}} \langle\tfrac{1}{2}\tfrac{1}{2}| + \frac{1}{\sqrt{2}} e^{-i\delta_{\psi}} \langle\tfrac{1}{2}\,{-\tfrac{1}{2}}| \right]$$

$$= \frac{1}{2} \sum_{\psi} P_{\psi} \Big(|\tfrac{1}{2}\tfrac{1}{2}\rangle\langle\tfrac{1}{2}\tfrac{1}{2}| + |\tfrac{1}{2}\,{-\tfrac{1}{2}}\rangle\langle\tfrac{1}{2}\,{-\tfrac{1}{2}}| \cancel{+ e^{i\delta_{\psi}} |\tfrac{1}{2}\,{-\tfrac{1}{2}}\rangle\langle\tfrac{1}{2}\tfrac{1}{2}|} \cancel{+ e^{-i\delta} |\tfrac{1}{2}\tfrac{1}{2}\rangle\langle\tfrac{1}{2}\,{-\tfrac{1}{2}}|} \Big)$$

These phase factor average to zero for unpolarized case

$$= \frac{1}{2} \underbrace{\sum_{\psi} P_{\psi}}_{1} \left[|\tfrac{1}{2}\tfrac{1}{2}\rangle\langle\tfrac{1}{2}\tfrac{1}{2}| + |\tfrac{1}{2}\,{-\tfrac{1}{2}}\rangle\langle\tfrac{1}{2}\,{-\tfrac{1}{2}}| \right]$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

What is the average value of S_z?

$$\langle S_z \rangle = \mathrm{tr}(\rho S_z) \qquad S_z = \tfrac{1}{2}\hbar\, \sigma_z = \tfrac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \mathrm{tr}\left\{ \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{2}\hbar \right\}$$

$$= \mathrm{tr}\left\{ \frac{\hbar}{4} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}$$

$$= 0 \quad \checkmark$$

Check: $\rho^2 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$= \frac{1}{2}\rho$ ⇐ note $\rho^2 \neq \rho$

eg. Completely polarized case $\longrightarrow$ i.e. wavefunction is also a good description

$$|\psi\rangle = \frac{|\tfrac{1}{2}\tfrac{1}{2}\rangle + e^{i\delta}|\tfrac{1}{2}-\tfrac{1}{2}\rangle}{\sqrt{2}}$$

$$\begin{aligned}
\rho &= (1)\,|\psi\rangle\langle\psi| \\
&= \tfrac{1}{2}\Big[\,|\tfrac{1}{2}\tfrac{1}{2}\rangle\langle\tfrac{1}{2}\tfrac{1}{2}| + |\tfrac{1}{2}\tfrac{1}{2}\rangle\langle\tfrac{1}{2}-\tfrac{1}{2}|\,e^{-i\delta} \\
&\qquad + |\tfrac{1}{2}-\tfrac{1}{2}\rangle\langle\tfrac{1}{2}-\tfrac{1}{2}| + |\tfrac{1}{2}-\tfrac{1}{2}\rangle\langle\tfrac{1}{2}\tfrac{1}{2}|\,e^{i\delta}\,\Big] \\
&= \tfrac{1}{2}\begin{pmatrix} 1 & e^{-i\delta} \\ e^{+i\delta} & 1 \end{pmatrix}
\end{aligned}$$

<u>What is the average value of S_z?</u>

$$S_z = \tfrac{1}{2}\hbar\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\begin{aligned}
\langle S_z\rangle &= \mathrm{tr}\{\rho S_z\} \\
&= \mathrm{tr}\left\{\tfrac{1}{2}\begin{pmatrix} 1 & e^{-i\delta} \\ e^{+i\delta} & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\tfrac{\hbar}{2}\right\} \\
&= \tfrac{\hbar}{4}\,\mathrm{tr}\left\{\begin{pmatrix} 1 & -e^{-i\delta} \\ e^{+i\delta} & -1 \end{pmatrix}\right\} \\
&= 0
\end{aligned}$$

<u>Check:</u>

$$\begin{aligned}
\rho^2 &= \tfrac{1}{2}\begin{pmatrix} 1 & e^{-i\delta} \\ e^{i\delta} & 1 \end{pmatrix}\tfrac{1}{2}\begin{pmatrix} 1 & e^{-i\delta} \\ e^{i\delta} & 1 \end{pmatrix} \\
&= \tfrac{1}{4}\begin{pmatrix} 1+1 & e^{-i\delta}+e^{-i\delta} \\ e^{i\delta}+e^{i\delta} & 1+1 \end{pmatrix} \\
&= \tfrac{1}{2}\begin{pmatrix} 1 & e^{-i\delta} \\ e^{i\delta} & 1 \end{pmatrix} \\
&= \rho \quad \Leftarrow \text{ interesting}
\end{aligned}$$

Density Operator Properties

Definition: $\boxed{\rho \equiv \sum_{\psi} P_{\psi} |\psi\rangle\langle\psi|}$

Normalization:
$$
\begin{aligned}
1 &= \sum_{\psi} P_{\psi} \\
&= \sum_{\psi} P_{\psi} \langle\psi|\psi\rangle \\
&= \sum_{k}\sum_{\psi} P_{\psi} \langle\psi|k\rangle\langle k|\psi\rangle \\
&= \sum_{k} \langle k| \Big[\sum_{\psi} P_{\psi} |\psi\rangle\langle\psi| \Big] |k\rangle
\end{aligned}
$$
$$\boxed{1 = tr\{\rho\}}$$

Pure state: Single known wavefunction: $P_{\psi} = 1$

$$\therefore \rho = |\psi\rangle\langle\psi|$$

Consider $\rho^2 = |\psi\rangle \underbrace{\langle\psi|\psi\rangle}_{1} \langle\psi| = |\psi\rangle\langle\psi| = \rho$

For "mixed" state:
$$
\begin{aligned}
\rho^2 &= \sum_{\psi} P_{\psi} |\psi\rangle\langle\psi| \sum_{\phi} P_{\phi} |\phi\rangle\langle\phi| \\
&= \sum_{\psi\phi} P_{\psi} P_{\phi} |\psi\rangle \underbrace{\langle\psi|\phi\rangle}_{\delta_{\psi\phi}} \langle\phi| \\
&= \sum_{\psi} (P_{\psi})^2 |\psi\rangle\langle\psi|
\end{aligned}
$$

$\neq P_{\psi}$ except for pure state

$\therefore \boxed{\rho^2 = \rho}$ ← only for a pure state

<u>Hermiticity:</u> $\rho^\dagger = \sum_\psi P_\psi \left[|\psi\rangle\langle\psi|\right]^\dagger = \rho$ <u>hermitian</u>

<u>Time evolution:</u>

$$H|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$$

$$\underset{\overset{\|}{H}}{\langle\psi|H^\dagger} = -i\hbar\left\{\frac{\partial}{\partial t}\langle\psi|\right\}$$

$$\frac{\partial\rho}{\partial t} = \sum_\psi P_\psi\left[\underbrace{\frac{\partial|\psi\rangle}{\partial t}}_{\frac{H|\psi\rangle}{i\hbar}}\langle\psi| + |\psi\rangle\underbrace{\frac{\partial}{\partial t}\langle\psi|}_{\frac{\langle\psi|H}{-i\hbar}}\right]$$

$$= \frac{1}{i\hbar}\sum_\psi P_\psi\left[H|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|H\right]$$

$$\boxed{i\hbar\frac{\partial\rho}{\partial t} = [H,\rho]}$$

✓

<u>Time evolution of any other operator</u>

explicit time dep. in θ

$$\frac{\partial\langle\theta\rangle}{\partial t} = \frac{\partial}{\partial t}\mathrm{tr}\{\rho\theta\}$$

$$= \mathrm{tr}\{\dot\rho\theta\} + \mathrm{tr}\{\rho\dot\theta\}$$

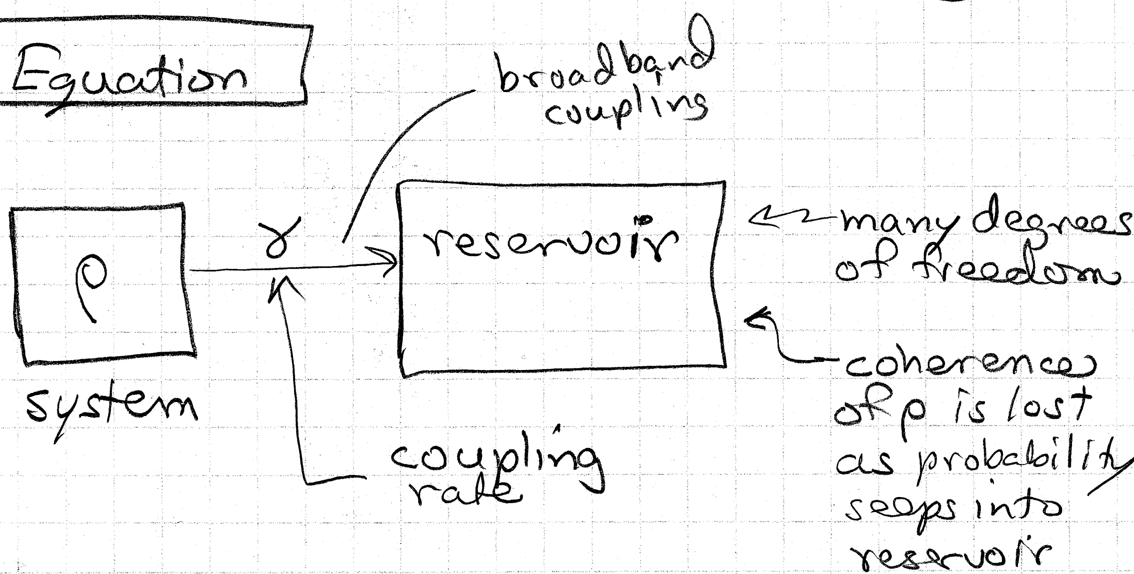
$$\dot\rho = \frac{[H,\rho]}{i\hbar}$$

$$i\hbar\frac{\partial\langle\theta\rangle}{\partial t} = \mathrm{tr}\{H\rho\theta\} - \mathrm{tr}\{\rho H\theta\} + \langle\dot\theta\rangle i\hbar$$

$$= \mathrm{tr}\{\rho[\theta,H]\} + i\hbar\langle\dot\theta\rangle$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\langle\theta\rangle = \langle[\theta,H]\rangle + i\hbar\langle\dot\theta\rangle}$$

Master Equation



eg. $$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H,\rho] \underbrace{- \frac{\gamma}{2}\left(a^{+}a\rho - 2a\rho a^{+} + \rho a^{+}a\right)}_{\text{nonlinear terms}}$$

↑ 2 state or harmonic osc.

$$V \sim a^{+}b + c.c.$$

a^{+}: raise system by a quantum

b: lower reservoir oscillator by a quantum