# Density Matrices and Open Quantum Systems

ECE 590.01

Quantum Engineering with Atoms

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# But first… Atom-light Interaction Recap!

Atom-light interactions:

$$\hat{H}_I = -\frac{q}{m} A_0 e^{-i\omega t} \exp(i\vec{k}\cdot\hat{\boldsymbol{r}})\hat{\epsilon}\cdot\hat{\boldsymbol{p}}$$

$$= -\frac{q}{m} A_0 e^{-i\omega t} (\boxed{1} + i\vec{k}\cdot\hat{\boldsymbol{r}} + \ldots)\hat{\epsilon}\cdot\hat{\boldsymbol{p}}$$

$$\hat{H}_I^{(\mathrm{E1})} = -\frac{q}{m}\frac{E_0}{i\omega} e^{-i\omega t}\hat{\epsilon}\cdot\hat{\boldsymbol{p}}$$

$$[\hat{\boldsymbol{r}}, \hat{H}_0] = \frac{i\hbar}{m}\hat{\boldsymbol{p}}$$

$$\hat{H}_I^{(\mathrm{E1})} = \frac{q}{\hbar\omega} E_0 e^{-i\omega t}\hat{\epsilon}\cdot(\hat{\boldsymbol{r}}\hat{H}_0 - \hat{H}_0\hat{\boldsymbol{r}})$$

$$\omega_{fi} \approx \omega$$

$$\hat{H}_I = -q\vec{E}(0,t)\cdot\hat{\boldsymbol{r}}$$

Electric dipole (E1) interaction

# First-order Interaction Term

$$\hat{H}_I = -\frac{q}{m} A_0 e^{-i\omega t}(1 + i\vec{k}\cdot\hat{\boldsymbol{r}} + \dots)\hat{\epsilon}\cdot\hat{\boldsymbol{p}}$$

$$H_I^{(1)} = -i\frac{q}{m} k A_0 e^{-i\omega t}(\hat{k}\cdot\hat{\boldsymbol{r}})(\hat{\epsilon}\cdot\hat{\boldsymbol{p}})$$

$$(\vec{A}\cdot\vec{B})(\vec{C}\cdot\vec{D}) = (\vec{A}\times\vec{C})\cdot(\vec{B}\times\vec{D}) + (\vec{B}\cdot\vec{C})(\vec{A}\cdot\vec{D})$$

$$H_I^{(1)} = -i\frac{q}{m} k A_0 e^{-i\omega t}\left[(\hat{k}\times\hat{\epsilon})(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{p}}) + (\hat{\epsilon}\cdot\hat{\boldsymbol{r}})(\hat{k}\cdot\hat{\boldsymbol{p}})\right]$$

$$H_I^{\mathrm{M1}} = -\frac{q}{m}\vec{B}(0,t)\cdot\hat{\boldsymbol{L}}$$

$$= -\frac{q}{m}\vec{B}(0,t)\cdot(\hat{\boldsymbol{L}} + g_s\hat{\boldsymbol{S}})$$

Magnetic dipole (M1) interaction

$$H_I^{(\mathrm{E2})} = i\frac{qk}{\hbar\omega}\left(\vec{E}(0,t)\cdot\hat{\boldsymbol{r}}\right)\left[\hat{k}\cdot(\hat{\boldsymbol{r}}\hat{H}_0 - \hat{H}_0\hat{\boldsymbol{r}})\right]$$

$$= -iq(\vec{E}(0,t)\cdot\hat{\boldsymbol{r}})(\vec{k}\cdot\hat{\boldsymbol{r}})$$

Electric quadrupole (E2) interaction

# Wave Functions vs Density Matrices

| | Wave function | Density Matrix |
|---|---|---|
| **Notation:** | $\|\psi(t)\rangle$ | $\rho(t)$ |
| **Applies to:** | Pure states | Pure or mixed states |
| **Size:** | $N \times 1$ vector | $N \times N$ matrix |
| **Evolution:** | Schrodinger equation | von Neuman equation |
| **Superposition** | $\|\psi\rangle = \frac{1}{\sqrt{2}}(\|0\rangle + \|1\rangle)$ | $\rho_p = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ vs $\rho_m = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ |

# Density Matrix – General Form

$$\rho = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

Pure state: $p_i = \delta_{ik}$ for a single specific $k$

Normalization:

$$\begin{aligned}\mathrm{Tr}(\rho) &= \sum_j \left\langle\psi_j\right| \rho \left|\psi_j\right\rangle \\ &= \sum_j \left\langle\psi_j\right| \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i|\psi_j\right\rangle \\ &= \sum_i p_i \equiv 1\end{aligned}$$

Interpretation: $p_i$ is probability to be in state $|\psi_i\rangle$

# Density Matrix – Expectation Values

$$\langle \hat{O} \rangle = \sum_i p_i \langle \psi_i | \hat{O} | \psi_i \rangle \qquad \mathbb{1} = \textstyle\sum_j |\psi_j\rangle \langle \psi_j|$$

$$= \sum_j \sum_i p_i \langle \psi_i | \psi_j \rangle \langle \psi_j | \hat{O} | \psi_i \rangle$$

$$= \sum_i \sum_i p_j \langle \psi_i | \psi_j \rangle \langle \psi_j | \hat{O} | \psi_i \rangle$$

$$= \sum_i \langle \psi_i | \left( \sum_j p_j |\psi_j\rangle \langle \psi_j | \hat{O} \right) | \psi_i \rangle$$

$$= \sum_i \langle \psi_i | \rho \hat{O} | \psi_i \rangle = \mathrm{Tr}(\rho \hat{O})$$

$$\langle \hat{O} \rangle = \mathrm{Tr}(\rho \hat{O}) = \mathrm{Tr}(\hat{O} \rho)$$

(Trace is cyclical)

# Density Matrix – Pure vs Mixes States

$$\mathrm{Tr}(\rho^2) = \sum_k \langle\psi_k| \sum_j p_j |\psi_j\rangle \langle\psi_j| \sum_i p_i |\psi_i\rangle \langle\psi_i|\psi_k\rangle$$

$$= \sum_k \sum_j \sum_i \delta_{kj}\delta_{ji}\delta_{ik} p_j p_i$$

$$= \sum_i p_i^2 \qquad \begin{array}{ll} = 1 \Leftrightarrow p_i = \delta_{ik} & \text{(pure state)} \\ < 1 & \text{(mixed state)} \end{array}$$

The trace of $\rho^2$ is necessary and sufficient to determine state purity.

In general: $\frac{1}{d} \leq Tr(\rho) \leq 1$ where $d$ is the dimension of the Hilbert space

# Density Matrix – Matrix Representation

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} & \cdots & \rho_{0N} \\ \rho_{10} & \rho_{11} & \cdots & \rho_{00} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{N0} & \rho_{00} & \cdots & \rho_{NN} \end{pmatrix}$$

$\rho_{ii} \in (\mathbb{R} \geq 0)$ are called the *populations* $\quad \sum_{i=1}^{N} \rho_{ii} = 1$

$\rho_{ij} \in \mathbb{C}$ are called the *coherences* $\quad \rho_{ij} = \rho_{ji}^{*}$

# Density Matrix – Time Evolution

$$\rho = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

$$\frac{d\rho}{dt} = \sum_i p_i \left[\left(\frac{d}{dt}\left|\psi_i\right\rangle\right)\left\langle\psi_i\right| + \left|\psi_i\right\rangle\left(\frac{d}{dt}\left\langle\psi_i\right|\right)\right]$$

$$= \sum_i p_i \left[\frac{H}{i\hbar}\left|\psi_i\right\rangle\left\langle\psi_i\right| + \left|\psi_i\right\rangle\left\langle\psi_i\right|\frac{H}{-i\hbar}\right]$$

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

Integrate directly: $$\boxed{\rho(t) = e^{-iHt/\hbar}\rho(0)e^{iHt/\hbar}}$$

# Density Matrix – Time Evolution

$$
\begin{aligned}
\rho(t) &= \sum_i p_i \left|\psi_i(t)\right\rangle \left\langle\psi_i(t)\right| \\
&= \sum_i p_i e^{-iHt/\hbar} \left|\psi_i(0)\right\rangle \left\langle\psi_i(0)\right| e^{iHt/\hbar} \\
&= e^{-iHt/\hbar} \rho(0) e^{iHt/\hbar}
\end{aligned}
$$

# Density Matrix – Partial Trace

$$\mathrm{Tr}_B(\rho_{AB}) = \rho_A \qquad \mathcal{H}_A \otimes \mathcal{H}_B \longrightarrow \mathcal{H}_A$$

- Partial trace effectively averages over system B to yield the state of system A.
  - Typically used if we can't probe system B
- Must behave correctly: $\mathrm{Tr}(X\rho_A) = \mathrm{Tr}[(X \otimes \mathbb{1}_B)\rho_{AB}]$

$$\begin{aligned}
\mathrm{Tr}[(X \otimes \mathbb{1}_B)\rho_{AB}] &= \sum_a \sum_b (\langle a| \otimes \langle b|)(X \otimes \mathbb{1}_B)\rho_{AB}(|a\rangle \otimes |b\rangle) \\
&= \sum_a \sum_b \sum_{b'} (\langle a| \otimes \langle b|)(X \otimes |b'\rangle \langle b'|)\rho_{AB}(|a\rangle \otimes |b\rangle) \\
&= \sum_a \sum_b \langle a| X \langle b|\rho_{AB}|b\rangle (|a\rangle \\
&= \sum_a \langle a|X\rho_A|a\rangle = \mathrm{Tr}(X\rho_A)
\end{aligned}$$

# Open Quantum Systems – Problem Definition

Open quantum systems allow for coupling between the system of interest with an environment (bath)

- Bath often has infinite degrees of freedom
- Cannot perform measurements on bath
- No control over bath
- Goal is to describe system and eliminate bath dependence

$$\mathbb{1} \otimes H_B$$

$$H_T = H + H_B + H_{SB}$$

$$H \otimes \mathbb{1}_B$$

interaction

$$H_0$$

$$\dot{\rho}_T = -\frac{i}{\hbar}\left[H + H_B + H_{SB}, \rho_{SB}\right]$$

$$\tilde{\rho}_T = e^{-iH_0 t/\hbar} \rho_T e^{iH_0 t/\hbar}$$

(interaction picture)

# Open Quantum Systems – Interaction Picture

$$\dot{\tilde{\rho}}_T = e^{iH_0t/\hbar}\left(i\frac{H_0}{\hbar}\rho_T + \dot{\rho}_T - i\rho_T\frac{H_0}{\hbar}\right)e^{-iH_0t/\hbar}$$

$$= -\frac{i}{\hbar}e^{iH_0t/\hbar}\left(-H_0\rho_T + [H_0 + H_{SB}, \rho_T] + \rho_T H_0\right)e^{-iH_0t/\hbar}$$

$$= -\frac{i}{\hbar}e^{iH_0t/\hbar}\left(H_{SB}\rho_T - \rho_T H_{SB}\right)e^{-iH_0t/\hbar}$$

$$= -\frac{i}{\hbar}e^{iH_0t/\hbar}\left(H_{SB}e^{-iH_0t/\hbar}e^{iH_0t/\hbar}\rho_T - \rho_T e^{-iH_0t/\hbar}e^{iH_0t/\hbar}V\right)e^{-iH_0t/\hbar}$$

$$= -\frac{i}{\hbar}\left[\tilde{H}_{SB}, \tilde{\rho}_T\right]$$

# Open Quantum Systems – Time Evolution

$$\dot{\tilde{\rho}}_T = -\frac{i}{\hbar}\left[\tilde{H}_{SB}, \tilde{\rho}_T\right]$$

$$\tilde{\rho}_T(t) = \tilde{\rho}_T(0) - \frac{i}{\hbar}\int_0^t dt' \left[\tilde{H}_{SB}(t'), \tilde{\rho}_T(t')\right]$$

$$\dot{\tilde{\rho}}_T = -\frac{i}{\hbar}\left[\tilde{H}_{SB}, \tilde{\rho}_T(0)\right] - \frac{1}{\hbar^2}\int_0^t dt' \left[\tilde{H}_{SB}(t), \left[\tilde{H}_{SB}(t'), \tilde{\rho}_T(t')\right]\right]$$

$\tilde{\rho}_S = \mathrm{Tr}_B(\tilde{\rho}_T) \equiv \tilde{\rho}$ + system and bath start out uncorrelated

$$\dot{\tilde{\rho}} = -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_B\left(\left[\tilde{H}_{SB}(t), \left[\tilde{H}_{SB}(t'), \tilde{\rho}_T(t')\right]\right]\right)$$

# Open Quantum Systems – Approximations

$$\dot{\tilde{\rho}} = -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_B\left(\left[\tilde{H}_{SB}(t),\left[\tilde{H}_{SB}(t'),\tilde{\rho}_T(t')\right]\right]\right)$$

Weak system-bath interaction
"Large" bath
(Born approximation)

$$= -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_B\left(\left[\tilde{H}_{SB}(t),\left[\tilde{H}_{SB}(t'),\tilde{\rho}(t')\otimes\tilde{\rho}_B(0)\right]\right]\right)$$

System kernel only depend
on current state
(Born-Markov approximation)

$$= -\frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_B\left(\left[\tilde{H}_{SB}(t),\left[\tilde{H}_{SB}(t'),\tilde{\rho}(t)\otimes\tilde{\rho}_B(0)\right]\right]\right)$$

# Open Quantum System – System-Bath Separation

$$\tilde{H}_{SB}(t) = \hbar \sum_i S_i(t) \otimes B_i(t) = \hbar \sum_i S_i^\dagger(t) \otimes B_i^\dagger(t)$$

(Equivalent due to Hermiticity)

$$\dot{\tilde{\rho}} = -\frac{1}{\hbar^2} \int_0^t \mathrm{Tr}_B \left( \left[ \tilde{H}_{SB}(t), \left[ \tilde{H}_{SB}(t'), \tilde{\rho}(t) \otimes \tilde{\rho}_B(0) \right] \right] \right)$$

$$\begin{aligned}
\dot{\tilde{\rho}} = -\sum_i \sum_j \int_0^t dt' \{ & S_i^\dagger(t) S_j(t') \tilde{\rho}(t) \,\mathrm{Tr}_B \left[ B_i^\dagger(t) B_j(t') \tilde{\rho}_B(0) \right] \\
& - S_i(t) \tilde{\rho}(t) S_j^\dagger(t') \,\mathrm{Tr}_B \left[ B_i(t) \tilde{\rho}_B(0) B_j^\dagger(t') \right] \\
& - S_j(t') \tilde{\rho}(t) S_i^\dagger(t) \,\mathrm{Tr}_B \left[ B_j(t') \tilde{\rho}_B(0) B_i^\dagger(t) \right] \\
& + \tilde{\rho}(t) S_j^\dagger(t') S_i(t) \,\mathrm{Tr}_B \left[ \tilde{\rho}_B(0) B_j^\dagger(t') B_i(t) \right] \}
\end{aligned}$$

Free to choose either substitution

# Open Quantum Systems – Fast Bath Dynamics

$$\mathrm{Tr}\left[B_j(t')\tilde{\rho}_B B_i^\dagger(t)\right] = \mathrm{Tr}\left[\tilde{\rho}_B B_i^\dagger(t) B_j(t')\right] = \mathrm{Tr}\left[B_i^\dagger(t) B_j(t')\tilde{\rho}_B\right] \equiv \frac{h_{ij}}{2}\delta(t'-t)$$

$$\mathrm{Tr}\left[B_i(t)\tilde{\rho}_B B_j^\dagger(t')\right] = \mathrm{Tr}\left[\tilde{\rho}_B B_j^\dagger(t') B_i(t)\right] = \mathrm{Tr}\left[B_j^\dagger(t') B_i(t)\tilde{\rho}_B\right] \equiv \frac{h_{ji}}{2}\delta(t'-t)$$

Correlation within bath don't last

$$\begin{aligned}\dot{\tilde{\rho}} = -\sum_i\sum_j\int_0^t dt'\{ & S_i^\dagger(t)S_j(t')\tilde{\rho}(t)\,\mathrm{Tr}_B\left[B_i^\dagger(t)B_j(t')\tilde{\rho}_B(0)\right] \\ & -S_i(t)\tilde{\rho}(t)S_j^\dagger(t')\,\mathrm{Tr}_B\left[B_i(t)\tilde{\rho}_B(0)B_j^\dagger(t')\right] \\ & -S_j(t')\tilde{\rho}(t)S_i^\dagger(t)\,\mathrm{Tr}_B\left[B_j(t')\tilde{\rho}_B(0)B_i^\dagger(t)\right] \\ & +\tilde{\rho}(t)S_j^\dagger(t')S_i(t)\,\mathrm{Tr}_B\left[\tilde{\rho}_B(0)B_j^\dagger(t')B_i(t)\right]\}\end{aligned}$$

$$\dot{\tilde{\rho}} = -\sum_i\sum_j\left\{\frac{h_{ij}}{2}\left[S_i^\dagger(t)S_j(t)\tilde{\rho}(t) - S_j(t)\tilde{\rho}(t)S_i^\dagger(t)\right] + \frac{h_{ji}}{2}\left[\tilde{\rho}(t)S_j^\dagger(t)S_i(t) - S_i(t)\tilde{\rho}(t)S_j^\dagger(t)\right]\right\}$$

# Open Quantum Systems – First Lindblad Form

$$\dot{\tilde{\rho}} = -\sum_i \sum_j \left\{ \frac{h_{ij}}{2} \left[ S_i^\dagger(t) S_j(t) \tilde{\rho}(t) - S_j(t) \tilde{\rho}(t) S_i^\dagger(t) \right] + \frac{h_{ji}}{2} \left[ \tilde{\rho}(t) S_j^\dagger(t) S_i(t) - S_i(t) \tilde{\rho}(t) S_j^\dagger(t) \right] \right\}$$

$$= -\sum_i \sum_j \left\{ \frac{h_{ij}}{2} \left[ S_i^\dagger S_j \tilde{\rho} - S_j \tilde{\rho} S_i^\dagger \right] + \frac{h_{ij}}{2} \left[ \tilde{\rho} S_i^\dagger S_j - S_j \tilde{\rho} S_i^\dagger \right] \right\}$$

$$= \sum_i \sum_j h_{ij} \left\{ S_j \tilde{\rho} S_i^\dagger - \frac{1}{2} \left( S_i^\dagger S_j \tilde{\rho} + \tilde{\rho} S_i^\dagger S_j \right) \right\}$$

# Open Quantum System – Standard Lindblad Form

$$\dot{\tilde{\rho}} = \sum_i \sum_j h_{ij} \left\{ S_j \tilde{\rho} S_i^\dagger - \frac{1}{2} \left( S_i^\dagger S_j \tilde{\rho} + \tilde{\rho} S_i^\dagger S_j \right) \right\}$$

Using an appropriate unitary transform $d$:

$$\Gamma = d h d^\dagger \quad \begin{cases} \Gamma_i = \sum_k \sum_l d_{ik} h_{kl} d_{li}^* \\ L_i = \sum_k d_{ik} S_k \end{cases}$$

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \sum_i \Gamma_i \left[ L_i \rho L_i^\dagger - \frac{1}{2} \left( L_i^\dagger L_i \rho + \rho L_i^\dagger L_i \right) \right]$$

$$\tilde{L}_i = \sqrt{\Gamma_i} L_i$$

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \sum_i \left[ \tilde{L}_i \rho \tilde{L}_i^\dagger - \frac{1}{2} \left( \tilde{L}_i^\dagger \tilde{L}_i \rho + \rho \tilde{L}_i^\dagger \tilde{L}_i \right) \right]$$