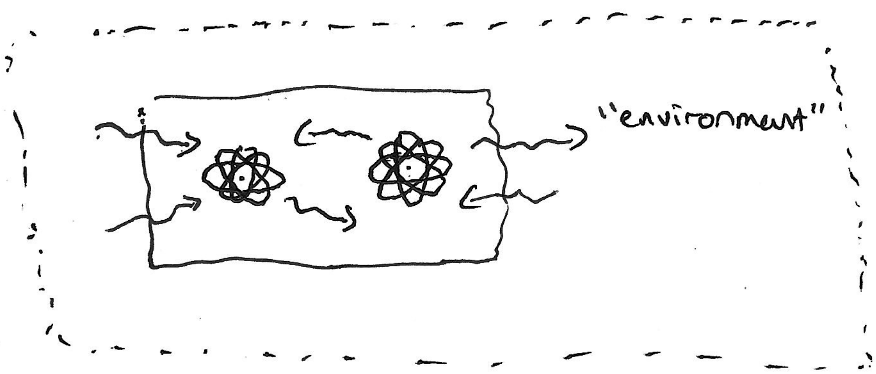
Open Quantum Systems:

- Up until now, we have only formally treated the behavior and dynamics of atoms either semi-classically, or quantum mechanically with the Skhrödinger equation, and "pure states" $|\psi\rangle$, which only captures the unitary dynamics of a closed system.

- This cannot capture a number of important processes that occur in any experiment, such as:

  - Spontaneous emission
  - noise from the environment
  - errors in state preperation, gates, or measurement
  - interactions with other uncontrolled/macroscopic systems

- These processes are all examples of "open quantum systems," or in other words dynamics that result from the system under consideration (and control) interacting with the rest of the universe:



- Interactions with macroscopic systems cause non-unitary dynamics through a "collapse of the wave function," or by becoming entangled with unknown/uncertain degrees of freedom.

- There are two ways to handle this:

  - Expand your system to include the environment (almost never a realistic/practical option)

  - introduce a new formalism for treating "open quantum systems."

- We will now take the second approach, by introducing the "density matrix" or "density operator" $\hat{\rho}$, and the corresponding concepts of "pure" and "mixed" states.

- The density operator for a system is defined as

$$\hat{\rho} \equiv \sum_{\alpha} P_{\alpha} |\psi_{\alpha}\rangle\langle\psi_{\alpha}|$$

where P_{α} is the probability to find the state in state $|\psi_{\alpha}\rangle$.

- If there exists a basis where $\hat{\rho} = |\phi\rangle\langle\phi|$ for some state $|\phi\rangle$, then the system is in a "pure state."

- If no such basis exists, the system is in a "mixed state," and has lost some of its quantum mechanical character.

- The density matrix/operator has some important properties:

i) $\hat{\rho} = \hat{\rho}^{\dagger}$ (hermitian)

ii) $Tr[\hat{\rho}] = \sum_n \langle n|\hat{\rho}|n\rangle = 1$ for any orthonormal basis $\{|n\rangle\}$
(conservation of probability)

iii) $Tr[\hat{\rho}^2] \leq 1$
$\uparrow$ $=1$ if and only if $\hat{\rho} = |\phi\rangle\langle\phi|$, pure state.

- Operator expectation values can be calculated directly from the density operator as:

$$\langle \hat{A} \rangle = Tr[\hat{\rho}\hat{A}]$$

This follows from:

$$\begin{aligned}
\langle \hat{A} \rangle &= Tr[\hat{\rho}\hat{A}] \\
&= \sum_n \langle n|\hat{\rho}\hat{A}|n\rangle \\
&= \sum_n \langle n| \sum_\alpha P_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|\hat{A}|n\rangle \\
&= \sum_\alpha \sum_n P_\alpha \langle n|\psi_\alpha\rangle\langle\psi_\alpha|\hat{A}|n\rangle \\
&= \underline{\sum_n} \sum_\alpha P_\alpha \langle\psi_\alpha|\underline{n\rangle\langle n}|\hat{A}|\psi_\alpha\rangle
\end{aligned}$$

$\hat{I}$

$$= \sum_\alpha P_\alpha \langle\psi_\alpha|\hat{A}|\psi_\alpha\rangle$$

- Note that this captures both pure and mixed states:

$\langle \hat{A} \rangle = \langle\phi|\hat{A}|\phi\rangle$, or $\langle \hat{A} \rangle = P_1 \langle\psi_1|A|\psi_1\rangle + P_2\langle\psi_2|A|\psi_2\rangle \ldots$
$= \sum P_\alpha \langle\psi_\alpha|\hat{A}|\psi_\alpha\rangle$

- We can write/understand the density matrix/operator as a matrix with elements $\rho_{n,m}$ such that

$$\hat{\rho} = \sum_{n,m} |n\rangle \underbrace{\langle n|\hat{\rho}|m\rangle}_{\rho_{n,m}} \langle m| \, , \quad \hat{\rho} = \begin{pmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1m} \\ \rho_{21} & \rho_{22} & \cdots & \rho_{2m} \\ \vdots & \vdots & & \vdots \\ \rho_{n1} & \rho_{n2} & \cdots & \rho_{nm} \end{pmatrix}$$

- These matrix elements have physical meaning.

  - Diagonal elements $\rho_{nn} = P_n$, the probability to occupy state $|n\rangle$.
    $\rho_{n,n} = \langle (|n\rangle\langle n|) \rangle$

  - Off diagonal elements correspond to the expectation value of the "coherence" between level $|n\rangle$ and $|m\rangle$, $\rho_{nm} = \langle (|n\rangle\langle m|) \rangle$, e.g. the atomic transition dipole operators.

    - Note that $\rho_{nm} = \rho_{mn}^*$.

- For example, consider a 2-level atom:

$$\hat{\rho} = \rho_{11} |1\rangle\langle 1| + \rho_{12} |1\rangle\langle 2| + \rho_{21} |2\rangle\langle 1| + \rho_{22} |2\rangle\langle 2|$$

or $\hat{\rho} = \frac{1}{2}(\hat{I} + \vec{S} \cdot \hat{\vec{\sigma}})$, in σ_z basis:

$$\hat{\rho} = \begin{pmatrix} 1 + \frac{S_z}{2} & \frac{S_x - iS_y}{2} \\ \frac{S_x + iS_y}{2} & \frac{1 - S_z}{2} \end{pmatrix}$$

- A pure state $|\psi\rangle = C_1|1\rangle + C_2|2\rangle$ has a density matrix

$\rho_{ij} = C_i C_j^*$

$$\Rightarrow |\rho_{ij}|^2 = \rho_{ii}\rho_{jj}$$

For mixed states, $\rho^2 < \rho$, and therefore

$$|\rho_{ij}|^2 \leq \rho_{ii}\rho_{jj}$$

- Lets consider a few examples:

If $|\psi\rangle = |1\rangle$, then $\hat{\rho} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ (in $\hat{\sigma}_z$ basis.)

Pure state.

If $|\psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ then $\rho = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$

Pure state.

If $\hat{\rho} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$, the state is a "maximally mixed" state or a "statistical mixture" of $|1\rangle$ and $|2\rangle$ with a 50/50 chance of finding it in each state.

- The density matrix is well-suited for treating a system composed of two parts when only one system is relevant. We can describe any system as a subsystem we are interested in and an environment. If we are only interested in operators $\langle\hat{S}\rangle$ that only act on the subsystem with states described by the density operator $\hat{\rho}_s$, then

$$\langle\hat{s}\rangle = Tr_s[\hat{s}\hat{\rho}_s]$$

If we have total density matrix $\hat{\rho}$ consisting of subsystem s and environment e, then the "reduced density matrix" $\hat{\rho}_s$ can be found by taking the partial trace:

$$\hat{\rho}_s = Tr_e[\hat{\rho}]$$

This is sometimes called "tracing out" the environment, and generally results in a partially mixed state if s interacts with e, meaning it is an "open" system.

- Using this, one can study the dynamics of an open system. If the system is closed/only undergoes coherent dynamics,

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

- If not, need extra terms.

- In general, the dynamics of an open quantum system can be quite complex and hard to treat. Under certain simplifying assumptions we can still arrive at tractable equations. For example, if the "environment" is Markovian, meaning it has no memory, you can derive the Lindblad form of the "master equation":

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

$\frac{\partial}{\partial t} \hat{\rho}$

Anti-commutator

$\{a, b\} = ab + ba$

L_i are the "jump operators" describing the interaction between the system and the Markovian environment, and γ_i are the non-negative, real coefficients called the "damping rates."

- This can be used to describe absorption and emission of photons from a surrounding thermal bath/reservoir/environment.

- As a concrete example, lets consider the case we already considered of an atom experiencing a resonant, coherent drive and under-going Rabi oscillations. The master equation allows us to now include spontaneous emission due to the finite lifetime of the excited state, and absorption of thermal photons from the surrounding environment at temp T.

- Spontaneous emission is described by the operator

$$\hat{L} = \underbrace{|1\rangle\langle 2|}_{\sigma_{12},\ \sigma_{ij} = |i\rangle\langle j|} \quad \text{and occurs with rate } \gamma.$$

Thermal absorption and emission occurs at rate $\gamma\bar{n}$, where $\bar{n}$ is the average number of photons at frequency ω_0.

The coherent interaction with the driving field is given by

$$\hat{H}_S = -\hbar\delta |2\rangle\langle 2| + \hbar\Omega^* |1\rangle\langle 2| + \hbar\Omega|2\rangle\langle 1|$$

detuning

and ~~the dissipative part of~~ the master equation gives

$$\begin{aligned}
\dot{\hat{\rho}} = &-\frac{\gamma}{2}(\bar{n}+1)\, \sigma_{22}\hat{\rho} - \sigma_{12}\rho\,\sigma_{21} + \text{h.c.} \\
&-\frac{\gamma}{2}\bar{n}(\sigma_{11}\hat{\rho} - \sigma_{21}\rho\,\sigma_{12}) + \text{h.c.} \\
&+ \frac{1}{i\hbar}[\hat{H}_s, \hat{\rho}]
\end{aligned}$$

Taking the matrix elements $\langle i|\dot{\hat{\rho}}|j\rangle = \dot{\rho}_{ij}$ gives four differential equations:

$$\begin{aligned}
\dot{\rho}_{22} &= -\gamma(\bar{n}+1)\rho_{22} + \gamma\bar{n}\rho_{11} + i\Omega^*\rho_{21} - i\Omega\rho_{12} \\
\dot{\rho}_{11} &= \gamma(\bar{n}+1)\rho_{22} - \gamma\bar{n}\rho_{11} - i\Omega^*\rho_{21} + i\Omega\rho_{12} \\
\dot{\rho}_{12} &= -\frac{\gamma}{2}(2\bar{n}+1)\rho_{12} - i\delta\rho_{12} - i\Omega^*(\rho_{22}-\rho_{21}) \\
\dot{\rho}_{12} &= -\frac{\gamma}{2}(2\bar{n}+1)\rho_{21} + i\delta\rho_{21} + i\Omega(\rho_{22}-\rho_{21})
\end{aligned}$$

- These equations are known as the "optical Bloch equations."

  - Note that only 2 of the equations are independent,

    as $\rho_{11} + \rho_{22} = 1$, and $\rho_{12} = \rho_{21}^*$.

- These equations result in damping of the coherent Rabi oscillations, and decay of population/decoherence into a mixed state.

- Ignoring the oscillations (or set $\Omega = 0$) and considering the optical regime where $k_B T \ll \hbar\omega_0$ so $\bar{n} \approx 0$, we have only spontaneous emission. In this case we find

$$\frac{\partial \rho_{11}}{\partial t} = \gamma \rho_{22}$$

$$\frac{\partial \rho_{22}}{\partial t} = -\gamma \rho_{22}$$

$$\frac{\partial \rho_{12}}{\partial t} = -\frac{\gamma}{2} \rho_{12}$$

So population decays from out of $|2\rangle$ into $|1\rangle$ with $e^{-\gamma t}$, but interestingly coherence decays with $\gamma/2$.

The decay of population is labeled with time constant $T_1 = \frac{1}{\gamma}$, and the decay of ~~coh~~ coherence is labeled $T_2 = \frac{2}{\gamma} = 2T_1$.