QUANTUM INFORMATION

- A quantum state, $|\psi\rangle = c_0 |0\rangle + c_1 e^{i\phi} |1\rangle$, encodes information which can be processed, stored, or controlled, provided the state is sufficiently long-lived

- There are two primary mechanisms that we think about for how this information can be lost:

  (a) c_0 and c_1: the relatively probabilities of each state can change

  (b) $e^{i\phi}$: the phase or coherence can change

- We will consider these two processes in the simplest cases

AMPLITUDE DAMPING WITH KRAUS OPERATORS

> **Learning Objective**
>
> Demonstrate the loss of information from a quantum state due to an amplitude damping channel as it relates to T_1 relaxation of a system.

- Exercises 1-3 to derive Kraus operators for amplitude damping: $M_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}$ and

$M_1 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix}$

- We can caculate the dynamics of a generic density matrix,

$$\rho_S(0) = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}, \tag{1}$$

using the operator-sum formulation,

$$\rho_S(t) = M_0 \rho_S(0) M_0^\dagger + M_1 \rho_S(0) M_1^\dagger \tag{2}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} + \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ \sqrt{p} & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \rho_{00} & \rho_{01}\sqrt{1-p} \\ \rho_{10}\sqrt{1-p} & \rho_{11}(1-p) \end{pmatrix} + \begin{pmatrix} \rho_{11}p & 0 \\ 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \rho_{00} + p\rho_{11} & \rho_{01}\sqrt{1-p} \\ \rho_{10}\sqrt{1-p} & \rho_{11}(1-p) \end{pmatrix}.$$

- There is no time dependence in the above so the operators need to be applied iteratively.

Considering just the excited state population,

$$\rho_{11} \longrightarrow (1-p)^n \rho_{11}. \tag{3}$$

- Assume $p = \gamma dt$ where γ is the rate of population relaxation, which we can call $\gamma = \frac{1}{T_1}$,

$$(1 - \gamma dt)^{\frac{t}{dt}} \rho_{11} \approx e^{-\gamma t} \rho_{11} = e^{-\frac{t}{T_1}} \rho_{11}, \tag{4}$$

- This process yields population relaxation occuring at a rate of $\frac{1}{T_1}$

- This process also yields change in the off-diagonal or coherence terms,

$$\rho_{10} \longrightarrow \sqrt{1-p}\rho_{10} \tag{5}$$

- Following the same definition of $p = \gamma dt$ and $\gamma = \frac{1}{T_1}$,

$$(\sqrt{1 - \gamma dt})^{\frac{t}{dt}} \rho_{10} \approx e^{-\frac{\gamma t}{2}} = e^{-\frac{t}{2T_1}} \tag{6}$$

- Note here that through the iterative application of the operators, we have made a Markovian approximation in our dynamics and these results are therefore only valid within this parameter space

Key Take-Away

An amplitude-damping channel causes population relaxation at a rate proportional to $\frac{1}{T_1}$ and coherence relaxation at a rate of $\frac{1}{2T_1}$.

PHASE DAMPING WITH KRAUS OPERATORS

Learning Objective

Demonstrate the loss of information from a quantum state due to a phase damping channel and define decoherence.

- Exercise 4-6 to derive Kraus operators for phase damping:

$$M_0 = \begin{pmatrix} \sqrt{1-p} & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} \qquad M_1 = \begin{pmatrix} \sqrt{p} & 0 \\ 0 & 0 \end{pmatrix} \qquad M_2 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix} \tag{7}$$

- Starting with a general initial density matrix,

$$\rho_S = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}, \tag{8}$$

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using the operator sum formulation,

$$\rho(t) = \sum_k M_k \rho M_k^\dagger$$

$$= M_0 \rho M_0^\dagger + M_1 \rho M_1^\dagger + M_2 \rho M_2^\dagger$$

$$= \begin{pmatrix} \sqrt{1-p} & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} \begin{pmatrix} \sqrt{1-p} & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} + \begin{pmatrix} \sqrt{p} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} \begin{pmatrix} \sqrt{p} & 0 \\ 0 & 0 \end{pmatrix}$$

$$+ \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix}$$

$$= \begin{pmatrix} \sqrt{1-p} & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} \begin{pmatrix} \rho_{00}\sqrt{1-p} & \rho_{01}\sqrt{1-p} \\ \rho_{10}\sqrt{1-p} & \rho_{11}\sqrt{1-p} \end{pmatrix} + \begin{pmatrix} \sqrt{p} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \rho_{00}\sqrt{p} & 0 \\ \rho_{10}\sqrt{p} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix} \begin{pmatrix} 0 & \rho_{01}\sqrt{p} \\ 0 & \rho_{11}\sqrt{p} \end{pmatrix}$$

$$= \begin{pmatrix} \rho_{00}(1-p) & \rho_{01}(1-p) \\ \rho_{10}(1-p) & \rho_{11}(1-p) \end{pmatrix} + \begin{pmatrix} \rho_{00}p & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \rho_{11}p \end{pmatrix}$$

$$= \begin{pmatrix} \rho_{00} & \rho_{01}(1-p) \\ \rho_{10}(1-p) & \rho_{11} \end{pmatrix}$$

- There is no time dependence in the above so the operators need to be applied iteratively. Considering just the off-diagonal terms,

$$\rho_{01} \longrightarrow (1-p)^n \rho_{01} \tag{9}$$

- Assume $p = \gamma dt$ where γ is the rate of phase damping which we can call $\gamma = \frac{1}{T_\phi}$,

$$(1 - \gamma dt)^{\frac{t}{dt}} \rho_{01} \approx e^{-\gamma t} \rho_{01} = e^{-\frac{t}{T_\phi}} \rho_{01} \tag{10}$$

- This process yields phase relaxation occuring at a rate of $\frac{1}{T_\phi}$
- This process does not yield population relaxation
- Note here that again we are in the Markovian regime due to the assumption of iterative application of the probability for the time propagation

> **Key Take-Away**
>
> A phase-damping channel causes only causes phase damping, where the coherence is damped at a rate proportional to $\frac{1}{T_\phi}$ where T_ϕ is referred to as the **phase lifetime**.

DECOHERENCE

> **Learning Objective**
>
> Define decoherence and the alphabet soup of subscripts that arise in literature.

- Decoherence overall is defined by all the processes that cause loss in the coherence term of the density matrix

- If we assume dynamical decoupling to correct for static inhomogeneities then we can define the decoherence lifetime T_2 and the decoherence rate,

$$\frac{1}{T_2} = \frac{1}{2T_1} + \frac{1}{T_\phi} \tag{11}$$

- If the dephasing lifetime is infinite $(T_\phi = \infty)$ then we have,

$$\frac{1}{T_2} = \frac{1}{2T_1}, \tag{12}$$

which implies,

$$T_2 = 2T_1, \tag{13}$$

- If the dephasing lifetime is finite $(T_\phi < \infty)$ then we have,

$$T_2 < 2T_1 \tag{14}$$

which is often referred to as an upper limit on decoherence lifetimes.

- The lifetime of static inhomogeneities is often written as T_2' which yields a decoherence lifetime given by T_2^* and rates defined as,

$$\frac{1}{T_2^*} = \frac{1}{T_2} + \frac{1}{T_2'} \tag{15}$$

> **Key Take-Away**
>
> - T_1: Longitudinal relaxation
> - T_2: Transverse relaxation or decoherence with a Hahn-Echo to eliminate static inhomogeneities, $\frac{1}{T_2} = \frac{1}{2T_1} + \frac{1}{T_\phi}$, $T_2 \leq 2T_1$
> - T_2^*: Decoherence that includes contribution from static inhomogeneities, $\frac{1}{T_2^*} = \frac{1}{T_2} + \frac{1}{T_2'}$
> - T_2': Decoherence due to static inhomogeneities
> - T_ϕ: Pure dephasing

TRANSVERSE OR SPIN-SPIN RELAXATION

- Complicated to model so we often consider a toy model that we can then map into real systems
- The central spin model (or spin start) model are common starting points
- Methods can then be adapted to real systems:
  - ▷ Molecular systems: Often an electronic spin interacting with a nuclear spin bath of hydrogens
  - ▷ Material systems: A nitrogen-vacancy center interacting with a bath of ^{1}3C present in the diamond lattice
  - ▷ Quantum dots
- This problem, even in a toy model, is complicated because the spins are usually all interacting (N-body problem), there can be strong coupling, and there are often small baths
- The latter two challenges can cause non-Markovianity which is an additional computational challenge

AN ASIDE ON NON-MARKOVIAN DYNAMICS

> **Learning Objective**
>
> A broad strokes idea of what non-Markovianity is to lay the groundwork for the rest of the week.

- Non-Markovianity is generally defined as memory effects in a system which arise when the environment is slow to relax compared to the system
- One formal definition is the Breuer-Laine-Piilo (BLP) measure, [1]

$$\mathcal{N} = \max_{\rho_S^{1,2}(0)} \int dt \frac{d}{dt}\left(\frac{1}{2}||\rho_S^1(t) - \rho_S^2(t)||_1\right) \tag{16}$$

> **Key Take-Away**
>
> This is a big field with a lot of really nice resources if you want or need them. To higlight a few:
>
> 1. Ref. 2: C.-F. Li, G.-C. Guo and J. Piilo, "Non-Markovian quantum dynamics: What does it mean?", *EPL*, **127** 50001 (2019)
> 2. Ref. 3: I. de Vega and D. Alonso, "Dynamics of non-Markovian open quantum systems", *Rev. Mod. Phys.* **89**, 015001 (2017)

METHODS TO TREAT SPIN-SPIN DYNAMICS

- Many methods rely on a cluster or pair approximation, including two popular approaches:

  ▷ Cluster correlation expansion (CCE): Originally developed for general spin dynamics, more recently applied to nitrogen-vacancy centers and molecules [4–11]

  ▷ Analytical pair product approximation (APPA): [12] Commonly used, less commonly named

- Generally these start from a generic spin Hamiltonian where we will call our central spin e and our bath spins n,

$$\hat{H} = \hat{H}_e + \hat{H}_n + \hat{H}_{en} \tag{17}$$

- As one example, for a three-spin system (one central spin with two bath spins), in the large-field limit and invoking the secular Hamiltonian, we can write,

$$\hat{H} = \omega_e \hat{S}_z + \omega_n(\hat{I}_z^1 + \hat{I}_z^2) + \omega_{nn}\big(\hat{I}_z^1 \hat{I}_z^2 - \frac{1}{4}\big(\hat{I}_+^1 \hat{I}_-^2 + \hat{I}_-^1 \hat{I}_+^2\big)\big) + A_1 \hat{S}_z \hat{I}_z^1 + A_2 \hat{S}_z \hat{I}_z^2, \tag{18}$$

where A_i are hyperfine tensors representing the electromagnetic interaction between the electron (central) spin and the nuclear spins of the environment, w_{nn} is the nuclear dipole-dipole coupling (often written as b_{ij} for a more general case)

- Note on Hamiltonians: a reminder that each term in the Hamiltonian has to have the same dimensionality (the dimensionality of the whole Hilbert space) so each term has a bunch of Kronecker products that we rarely explicitly write. As an example:

$$\omega_e \hat{S}_z = \omega_e \hat{S}_z \otimes \mathbb{1} \otimes \mathbb{1} \tag{19}$$

- Another common approximation or trick used in the pure dephasing limit is to reorder the Hamiltonian such that,

$$\hat{H} = |0\rangle \langle 0| \hat{H}^{(0)} + |1\rangle \langle 1| \hat{H}^{(1)}, \tag{20}$$

where the Hamiltonian acts on the central spin in its up and down states independently. This is a valid approximation for pure dephasing because there is no energy exchange in the system, so the states $|0\rangle$ and $|1\rangle$ in the system are independent

CLUSTER CORRELATION EXPANSION

- To consider the cluster correlation expansion method, we will refer to a wonderful resource out of the Galli Group at the University of Chicago referred to as PyCCE which gives a nice overview of both conventional and general versions of the CCE.

- The general idea is to factorize the bath spins into clusters and consider the coherence due to different clusters, propagate the system and clustered environment in a unitary fashion, then trace out the bath spins to get the system coherence at some time t

A FEW APPLICATIONS

- A lot of methods to treat spin-induced dynamics are developed for general models, but can also be parametrized for molecular or material systems if the hyperfine and dipolar coupling terms are obtained through electronic structure theories
- Applications give us great insight into when our methods succeed and when they fail, which tells us which loss mechanisms we understand well and where are our gaps in understanding

EXERCISES

- Play around with the Jupyter notebook for CCE-1 and CCE-2
- Which interaction Hamiltonians result in CCE-1 and CCE-2 being the same?
- Is decoherence complete?
- How do you know if the calculation has converged?

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