CS191 – Fall 2014
Lecture 15: Open quantum systems: Hamiltonian formulation and master equations

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Open quantum systems are ones that are coupled to an environment that we cannot control or observe completely and therefore must average over in our modeling. In the last lecture we saw how to represent open quantum system dynamics in terms of the Kraus representation (also referred to as a CPTP map, or operator sum representation (OSR)). This representation let us write the reduced state of the system after some evolution time t, in terms of the initial reduced state of the system. The Kraus operators encode the effect of coupling to the environment during the evolution. In this lecture we will cover another common way to model open quantum system dynamics: master equations.

Recall that in deriving the OSR for a physical process we require knowledge of U_{SE}, the unitary coupling between the system and environment. In many settings it is infeasible to extract the form of this coupling unitary from the underlying physics. Instead, it may be more realistic to extract the Hamiltonian of the system and environment, H_{SE}, which generates time evolution, from examining the physical interactions. We know $U_{SE}(t) = \exp(-\frac{i}{\hbar}H_{SE}(t))$, but computing this exponential may not be computationally feasible. In such settings, it is more natural to derive an equation of motion describing the time evolution of the reduced state of the system rather than a map. The conceptual idea behind this approach is illustrated in the diagram in figure 1

The most general form of a master equation is not very useful in practice. Instead, we usually work with more specialized master equations that incorporate some assumptions but are computationally useful. In this lecture we will present one such specialized master equation, the *Lindblad master equation*, that is widely applicable in atomic and optical physical systems, and also has very strong mathematical underpinnings.

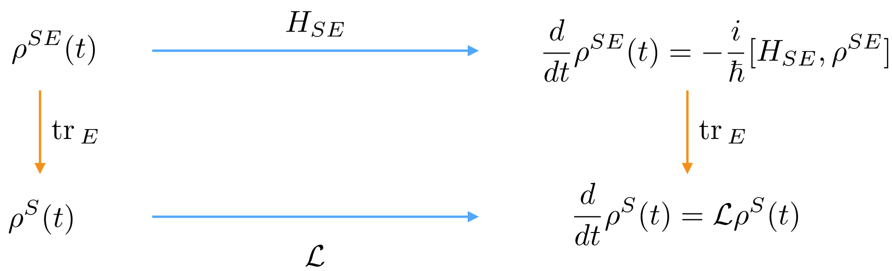

FIG. 1: The conceptual idea behind master equations. Just as the joint Hamiltonian, H_{SE} and the von-Neumann equation prescribe how a joint density matrix of the system and environment evolves in time, a master equation describes how the reduced state of the system evolves in time in the presence of coupling to an environment (this coupling and the environment must satisfy the assumptions used in deriving the master equation). We denote the generator of master equation evolution by $\mathcal{L}$.

I. SYSTEM-ENVIRONMENT HAMILTONIAN

Before presenting the Lindblad master equation let us review the form of the system-environment Hamiltonian. The system environment coupling is written in one of two forms:

$$H_{SE} = H_S + H_E + H_I = h_0^S \otimes I^E + I^S \otimes h_0^E + \sum_{k=1}^{K} h_k^S \otimes h_k^E \tag{1}$$

$$H_S(t) = H_S + H_{\text{noise}} = h_0^S + \sum_{k=1}^{K} \lambda_k(t) h_k^S \tag{2}$$

In these equations h_i^S are operators on the system, h_i^E are operators on the environment, and $\lambda_k(t)$ are (possibly time-dependent scalars) that are unknown – *e.g.*, a random process. Eq. (1) is a model of the system environment coupling where we explicitly specify the environment and its Hamiltonian and dynamics, whereas Eq. (2) is a model of the system environment coupling where we say the effect of the environment is some (possibly time-dependent) fluctuations of the system Hamiltonian represented by $\lambda_k(t)$. Eq. (2) is actually an approximation to Eq. (1) where the quantum environment is approximated by a classical fluctuating process. The conditions under which this approximation is valid depend on the type of the physical environment (*e.g.*, a collection of neighboring spins, or a vibrational environment, etc.). I will not specify exactly when Eq. (2) is a valid approximation, since it is not important for the proceeding discussion. What is important is that a Lindblad master equation can be derived for both models of system environment coupling under the physical approximations that will be specified below.

In order to specify the relevant physical approximations we must first transform Eq. (1) into an interaction frame with respect to the free environment Hamiltonian $H_E = I^S \otimes h_0^E$. Recall that operators in the interaction frame with respect to an operator G are defined as

$$\tilde{O}(t) = e^{iGt} O(t) e^{-iGt}, \tag{3}$$

where we use the tilde to denote operators in the interaction frame. If a state in the bare frame evolves according to

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H + G, \rho], \tag{4}$$

then the state in the interaction frame with respect to G evolves according to

$$\frac{d}{dt}\tilde{\rho}(t) = -\frac{i}{\hbar}[\tilde{H}(t), \tilde{\rho}], \tag{5}$$

where the interaction frame Hamiltonian is defined as:

$$\tilde{H}(t) = e^{iGt}(H + G)e^{-iGt} - G = e^{iGt} H e^{-iGt} \tag{6}$$

Given these definitions, the system environment Hamiltonian in the interaction frame with respect to H_E is

$$\tilde{H}_{SE}(t) = H_S + \tilde{H}_I(t) = h_0^S \otimes I^E + \sum_{k=1}^{K} h_k^S \otimes \tilde{h}_k^E(t), \tag{7}$$

with $\tilde{h}_k^E(t) = e^{ih_0^E t} h_k^E e^{-ih_0^E t}$.

Note that in this interaction frame the similarity between $\tilde{H}_{SE}$ and Eq. (2) becomes more apparent. While Eq. (2) has fluctuating parameters ($\lambda_k(t)$) coupled to the system, Eq. (7) has time-dependent environment operators ($h_k^E(t)$) coupled to the system. As we mentioned above, in some circumstances it is appropriate to approximate the time-dependent environment operator with a classical fluctuating variable and thus we obtain Eq. (2).

II. LINDBLAD MASTER EQUATION

Given the interaction frame representation $\tilde{H}_{SE}$ we are not in a position to specify the conditions under which a Lindblad master equation can be derived, which are:

1. The system environment coupling is weak compared to system energies, the so-called *Born approximation.* Mathematically this means that $||h_k^E(t)|| \ll ||h_0^S||, \quad \forall k,t$ for Eq. (7), and $|\lambda_k(t)| \ll ||h_0^S||, \quad \forall k,t$ for Eq. (2).

2. The environment evolves at much faster timescales than the system, the so-called *Markov approximation.* Intuitively this condition is equivalent to saying that the environment has no memory and quickly relaxes to its steady state despite the interaction with the system.

Given these two assumptions, the evolution of the system is given by the *Lindblad master equation* [1]:

$$\begin{aligned} \frac{d}{dt}\rho^S(t) &= \mathrm{tr}_E\left\{\frac{d}{dt}\rho^{SE}(t)\right\} \\ &= -\frac{i}{\hbar}[h_0^S + h_{LS}^S, \rho^S(t)] + \sum_{k=1}^{K'} \gamma_k \left(L_k \rho^S(t) L_k^\dagger - \frac{1}{2} L_k^\dagger L_k \rho^S(t) - \frac{1}{2}\rho^S(t) L_k^\dagger L_k\right), \end{aligned} \tag{8}$$

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[1] The equation is named after Göran Lindblad, who was one of the first to derive it. In fact, this equation was derived by a number of authors in the fields of physics and mathematical physics around the same time. If we are to attribute credit fairly, the equation should called the *Lindblad-Gorini-Kossakowski-Sudarshan* master equation. We will avoid that mouthful and just refer to it as the Lindblad master equation.

where the operators L_k are called Lindblad operators and are arbitrary time-independent operators on the system Hilbert space and γ_k are time-independent real numbers.

Some comments about this equation:

1. We will not derive this equation from the underlying dynamics of the system and environment, given by Eq. (1) or Eq. (2). If you're interested in the derivation see the References and further reading section for some literature that covers this.

2. Just like the Kraus operators in the OSR could be related to the unitary U_{SE}, the Lindblad operators can be related to the underlying physical coupling represented by H_{SE}.

3. Notice that part of the first component of Eq. (8), $-\frac{i}{\hbar}[h_0^S, \rho^S(t)]$, is exactly what the system evolution would be if there was no coupling to the environment. The system-environment coupling induces the terms with the Lindblad operators, L_k, and also an additional Hamiltonian, h_{LS}^S, which is typically called the Lamb shift Hamiltonian for historical reasons.

4. Eq. (8) defines a linear differential equation for the density matrix for the system. We often denote this evolution as

$$\frac{d}{dt}\rho^S(t) = \mathcal{L}\rho^S(t), \tag{9}$$

   for convenience. The term $\mathcal{L}$ is the called the *Lindblad generator*.

5. Just as the OSR has desirable mathematical properties such as trace preservation and positivity preservation, the Lindblad master equation satisfies mathematical properties we expect from a valid description of system dynamics. It preserves the trace, hermiticity and positivity of a density matrix. Also, just like the OSR, it can be derived from purely mathematical considerations as well as the more physical arguments we gave above.

6. Similar to the OSR, the Lindblad operators are not uniquely defined for a particular master equation. There are two classes of transformation under which the master equation dynamics remain invariant. The first is given by scaling of the Lindblad operators and the Lamb shift Hamiltonian:

$$L_k \to L_k + \alpha_k I, \quad H_{LS} \to H_{LS} + \frac{1}{2i}\sum_k (\alpha_k^* L_k - \alpha_k L_k^\dagger) + \beta I, \tag{10}$$

   where α_k and β are arbitrary scalars. The second transformation under which the master equation remains invariant is an arbitrary unitary transformation of the Lindblad operators:

$$L_k \to \sum_j u_{kj} L_j, \tag{11}$$

   where u_{kj} are the elements of a unitary matrix.

7. The solution to any Lindblad equation can be represented as a CPTP map, *i.e.*, as a Kraus representation. However, the converse is not true. That is, not every CPTP map is generated by a Lindblad master equation. This is because there are CPTP maps for system environment dynamics that do not satisfy the approximations used in deriving the Lindblad master equation. Therefore, such maps have more complicated generators of evolution.

8. The mapping from master equation to CPTP map is not unique. That is, many master equations can generate the same CPTP map.

9. The Lindblad master equation is only one generator of open system dynamics. It is possible to derive other master equations that generate dynamics under fewer or different approximations than the ones listed above. In fact, in many systems where the above approximations are invalid (*e.g.*, many solid-state systems) there is a lot of research into deriving more accurate master equations.

   Exercise: Prove that a general Lindblad master equation preserves trace and Hermiticity of the state.

III. EXAMPLE

A physical process that satisfies the approximations required for deriving the Lindblad master equation is spontaneous emission into a broadband vacuum. The environment here is the continuum of modes in an electromagnetic field. For a two-level system (*e.g.*, an approximation of an atomic system where we only model the two energy levels that are relevant, the excited state and the ground state), the Lindblad master equation describing these dynamics is

$$\frac{d}{dt}\rho(t) = \gamma\left(\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\sigma_+\sigma_-\rho(t) - \frac{1}{2}\rho(t)\sigma_+\sigma_-\right),$$

where $\rho(t)$ is a 2×2 density matrix:

$$\rho(t) = a(t)\left|0\right\rangle\left\langle 0\right| + b(t)\left|0\right\rangle\left\langle 1\right| + b^*(t)\left|1\right\rangle\left\langle 0\right| + c(t)\left|1\right\rangle\left\langle 1\right|, \tag{12}$$

with $\left|0\right\rangle$ being the ground state, $\left|1\right\rangle$ being the excited state and $a(t)+c(t)=1\ \ \forall t$. $\sigma_- = \left|0\right\rangle\left\langle 1\right|$ and $\sigma_+ = \left|1\right\rangle\left\langle 0\right|$. We have assumed that there is no free Hamiltonian for the system ($h_0^S + h_{LS}^S = 0$) for simplicity.

We can explicitly solve this master equation by evaluating the right hand side for a general $\rho(t) = \begin{pmatrix} a(t) & b(t) \\ b^*(t) & c(t)\end{pmatrix}$:

$$\begin{aligned}\begin{pmatrix} \dot{a}(t) & \dot{b}(t) \\ \dot{b}^*(t) & \dot{c}(t)\end{pmatrix} &= \gamma\left(\begin{pmatrix} c(t) & 0 \\ 0 & 0\end{pmatrix} - \frac{1}{2}\begin{pmatrix} 0 & 0 \\ b^*(t) & c(t)\end{pmatrix} - \frac{1}{2}\begin{pmatrix} 0 & b(t) \\ 0 & c(t)\end{pmatrix}\right) \\ &= \begin{pmatrix} \gamma c(t) & -\frac{\gamma}{2}b(t) \\ -\frac{\gamma}{2}b^*(t) & -c(t)\end{pmatrix}\end{aligned} \tag{13}$$

This matrix equation defines two scalar differential equations:

$$\begin{aligned}\dot{c}(t) &= -\gamma c(t) \\ \dot{b}(t) &= -\frac{\gamma}{2}b(t)\end{aligned}$$

Solving these and using $a(t)+c(t)=1$, gives us the density matrix at any time t:

$$\rho(t) = \begin{pmatrix} 1-e^{-\gamma t}c(0) & e^{-\frac{\gamma}{2}t}b(0) \\ e^{-\frac{\gamma}{2}t}b^*(0) & e^{-\gamma t}c(0)\end{pmatrix} \tag{14}$$

> **Exercise:** If we begin in the excited state ($\rho(0) = \left|1\right\rangle\left\langle 1\right|$) what is the state at long times? If we begin in an equal superposition of the excited and ground states ($\rho(0) = \left|+\right\rangle\left\langle +\right|$), what is the state at long times?

We mentioned above that the solution to any Lindblad master equation has a Kraus representation. Also, in the last lecture you saw that the OSR for a spontaneous emission process was the amplitude damping channel:

$$\mathcal{E}(\rho_0) = A_0\rho_0 A_0^\dagger + A_1\rho_0 A_1^\dagger, \tag{15}$$

with

$$A_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p}\end{pmatrix} \tag{16}$$

$$A_1 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0\end{pmatrix} \tag{17}$$

for some $0 \le p \le 1$. Applying the right hand side of Eq. (15) to a general input state yields

$$\rho(t) = \begin{pmatrix} a(0)+pc(0) & \sqrt{1-p}\,b(0) \\ \sqrt{1-p}\,b^*(0) & (1-p)c(0)\end{pmatrix} \tag{18}$$

Comparing this to Eq. (14) we can equate

$$\sqrt{1-p} = e^{-\frac{\gamma}{2}t} \Rightarrow p = 1-e^{-\gamma t} \tag{19}$$

Therefore the dynamics generated by the Lindblad master equation given in Eq. (12) is given by the amplitude damping process for $p = 1-e^{-\gamma t}$.

IV. REFERENCES AND FURTHER READING

1. Chapter 8.4.1 of Nielsen & Chuang.
2. Chapters 6.2 of Benenti, Casati, & Strini, Volume 2. This chapter sketches the derivation of the Lindblad master equation from physical principles and mathematical arguments.
3. Lecture 8 of MIT OpenCourseWare 22-51 "Quantum theory of radiation interactions":
   `http://ocw.mit.edu/courses/nuclear-engineering/22-51-quantum-theory-of-radiation-interactions-fall-2012/lecture-notes/MIT22_51F12_Ch8.pdf`
   These notes present a readable derivation of the Lindblad master equation, and also include some more advanced topics in the theory of open quantum systems.