

A brief introduction to quantum master equations in the weak-coupling regime

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Lecture 1

1 Introduction

1.1 Philosophy of open systems

What is an open system? An open system is any object that interacts with its environment. So what is an environment? Strictly speaking, everything that is not part of what we define as the system is lumped into the environment. Therefore everything in the universe is an open system, the only system that is truly closed (i.e. not open) is the universe itself. Clearly, such a definition is too broad if we want to be successful at modelling open systems because it just ‘forces’ us to consider too many objects in our theory, even ones

that have no influence on our system. Nevertheless, it at least suggests that a realistic (i.e. nonidealised) description of physical systems should in some way incorporate the system's environment.

The question as to what should be defined as the environment depends on the system in question and what sort of interactions it has with its surrounding. It may also depend on what we want to know about the system. In general there are two guiding principles about how to divide many degrees of freedom into those that belong to a system Hilbert space \mathbb{H}_S , and those belonging to a bath¹ Hilbert space \mathbb{H}_B :

1. The effect of the environment on the system simply cannot be ignored but neither are we interested in tracking how the environment changes in time.
2. The environment is typically a large system. It may consist of many spins, many atoms, or say many bosonic degrees of freedom. Therefore keeping track of the environment is simply out of the question even if one wants to. The size of the environment is an especially important problem for quantum open systems (as opposed to classical open systems) because the state of a quantum system is described in a Hilbert space, whose dimension scales exponentially in the number of degrees of freedom (or systems in the environment). For example, if the environment has N two-state particles, then we need 2^N dimensions.

The philosophy of open-systems theory is thus to develop some methods that allows us to describe the system evolution accurately and effectively without having to track the environment. To be more concrete, if we denote the full Hamiltonian for the system and environment (including their interaction) by \hat{H} , and their joint state by $\rho(t)$ in $\mathbb{H}_S \otimes \mathbb{H}_B$, then we would like to know, starting from some initial system-bath state $\rho(0)$, the system state $\rho_S(t)$ at some future time t where

$$\rho_S(t) = \text{Tr}_B[\rho(t)] . \quad (1)$$

Note that we are using Tr_B to denote a partial trace over the environment. Clearly, it is possible to obtain $\rho_S(t)$ from

$$\frac{d}{dt} \rho_S(t) = -\frac{i}{\hbar} \text{Tr}_B\left\{[\hat{H}, \rho(t)]\right\} . \quad (2)$$

But this is not helpful as the right-hand side of (2) still involves $\rho(t)$. It is equivalent to evolving the joint system-bath state from $\rho(0)$ to $\rho(t)$ and then taking the partial trace over the environment. The aim is thus to write the right-hand side of (2) as a function of $\rho_S(t)$ only:

$$\frac{d}{dt} \rho_S(t) = \mathcal{L}_S(t) \rho_S(t) . \quad (3)$$

An equation in the form of (3) is called a master equation. In (3) we have denoted the functional dependence on $\rho_S(t)$ by using a superoperator $\mathcal{L}_S(t)$ which acts on \mathbb{H}_S . A superoperator acts on an operator and returns an operator. Superoperators will be written in calligraphic font except for the identity, which we will write as $\mathbb{1}$. The master equation reduces the problem of solving for $\rho(t)$ to one of solving for $\rho_S(t)$. Hence (3) is also referred to as an equation of motion for the reduced state, where the reduced state is simply $\rho_S(t)$.

1.2 Markovian evolution

An important point about (3) is that its right-hand side depends on the system state at the present time t . This means that if we are given the system state at multiple times, say $\{\rho_S(t_k)\}_{k=1}^K$ where $t_1 < t_2 < \dots < t_K < t$, then only the most recent specification given by $\rho_S(t_K)$ is required for us to say what $\rho_S(t)$ is for any future time i.e. for any $t > t_K$. Systems that have this property are said to be Markovian and the corresponding differential equation is said to be time local. Equation (3) is thus referred to as a time-local master equation. Another commonly used terminology is to say that (3) has the property of being memoryless.

This is nothing that you do not already know about ordinary differential equations. So what is special about Markovianity? The reason why this is interesting is that (3) is derived from (2) and how this can be achieved is quite nontrivial. That is to say, we would not make a big fuss about Markovianity if we were interested in closed systems, because all closed systems evolve according to the Schrödinger equation which

¹Often the word 'environment' is used interchangeably with 'bath', (the latter being more common in statistical mechanics) and so will we. In this case it makes sense to use a subscript 'B' for operations acting on the bath.

is a time-local equation. Therefore all unitary evolution is trivially Markovian. Note the converse statement, i.e. all Markovian evolution are unitary is not true because not all physically permissible² time-local equations for $\rho_S(t)$ have to be unitary. It should not be hard to accept that $\mathcal{L}_S(t)$ in (3) will be more than a simple commutator with a Hermitian operator so that it describes non-unitary evolution. Here we have reached a fundamental difference between open systems and closed systems: For open systems, Markovian evolution is non-unitary and is understood as an emergent, or special property.

2 A perturbative treatment of the reduced dynamics

We now show how it is possible to arrive at a time-local equation like (3) if certain conditions are fulfilled.

2.1 Definitions

2.1.1 Interaction picture

Let us write the full Hamiltonian as

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{V}, \quad (4)$$

where \hat{H}_S is the free Hamiltonian for the system and acts only on the system Hilbert space \mathbb{H}_S while \hat{H}_B is the free Hamiltonian for the bath and acts only on the bath Hilbert space \mathbb{H}_B . The interaction Hamiltonian \hat{V} accounts for their interaction and acts on the joint space $\mathbb{H}_S \otimes \mathbb{H}_B$. We also define the joint system-bath state in $\mathbb{H}_S \otimes \mathbb{H}_B$ as $\rho(t)$. In the Schrödinger picture the evolution of $\rho(t)$ is thus given by

$$\frac{\partial}{\partial t} \rho(t) = -\frac{i}{\hbar} [\hat{H}, \rho(t)]. \quad (5)$$

Our derivation of the master equation will be a perturbative one where the time evolution due to \hat{H}_0 is known (which is typically the case) and we regard \hat{V} as a perturbation. In this case it will be convenient to define

$$\hat{H}_0 = \hat{H}_S + \hat{H}_B, \quad (6)$$

and transform (5) into the interaction picture where \hat{H}_0 does not appear. This gives

$$\frac{\partial}{\partial t} \tilde{\rho}(t) = -\frac{i}{\hbar} [\tilde{V}(t), \tilde{\rho}(t)] \equiv \tilde{\mathcal{L}}(t) \tilde{\rho}(t). \quad (7)$$

Remember that an arbitrary operator \hat{A} and an arbitrary state ρ in the interaction picture is defined with respect to the Schrödinger picture by

$$\tilde{A}(t) = e^{i\hat{H}_0 t/\hbar} \hat{A}(0) e^{-i\hat{H}_0 t/\hbar}, \quad \tilde{\rho}(t) = e^{i\hat{H}_0 t/\hbar} \rho(t) e^{-i\hat{H}_0 t/\hbar}. \quad (8)$$

We would like to express the evolution of the system, now given in the interaction picture as

$$\tilde{\rho}_S(t) = \text{Tr}_B[\tilde{\rho}(t)], \quad (9)$$

as a perturbative series in the interaction Hamiltonian. To make the order of interaction strength easy to track we introduce a constant α into \hat{V} by hand:

$$\hat{V} \longrightarrow \alpha \hat{V}. \quad (10)$$

This simply changes the interaction picture evolution to

$$\boxed{\frac{\partial}{\partial t} \tilde{\rho}(t) = \alpha \tilde{\mathcal{L}}(t) \tilde{\rho}(t)}. \quad (11)$$

This allows us to simply read off the order of the perturbative expansion from the power of α and in the end set $\alpha = 1$.

²This opens up a can of worms because it now begs an answer to how ‘physically valid’ should be captured mathematically. This will lead us to a discussion about theorems in open systems which we will not go into. I am simply sweeping this entire branch of open-systems theory under the rug here.

2.1.2 Projection operators

A perturbative expansion for $\tilde{\rho}_S(t)$ can be arrived at systematically by using projection operators which act on any $\rho \in \mathbb{H}_S \otimes \mathbb{H}_B$. The projection operators are defined for an arbitrary reference state $\rho_B \in \mathbb{H}_B$, and an arbitrary joint state ρ as

$$\mathcal{P}\rho = \text{Tr}_B[\rho] \otimes \rho_B = \rho_S \otimes \rho_B, \quad (12)$$

$$\mathcal{Q}\rho = \rho - \rho_S \otimes \rho_B. \quad (13)$$

We define the reference state to be normalised so that ρ_S may be extracted directly from $\mathcal{P}\rho$ by taking the partial trace over \mathbb{H}_B . For us the reference state will be a bath state which we will specify later. Note that \mathcal{P} and \mathcal{Q} are defined to satisfy

$$(\mathcal{P} + \mathcal{Q})\rho = \rho. \quad (14)$$

Often one calls $\mathcal{P}\rho$ the relevant part of ρ , and $\mathcal{Q}\rho$ the irrelevant part. We will follow this terminology here as well. It can be shown from (12) and (13) that \mathcal{P} and \mathcal{Q} are projection operators

$$\mathcal{P}^2\rho = \mathcal{P}(\mathcal{P}\rho) \quad (15)$$

$$= \text{Tr}_B[\rho_S \otimes \rho_B] \otimes \rho_B \quad (16)$$

$$= \rho_S \otimes \rho_B = \mathcal{P}\rho, \quad (17)$$

$$\mathcal{Q}^2\rho = \mathcal{Q}(\mathcal{Q}\rho) \quad (18)$$

$$= \mathcal{Q}(\rho - \rho_S \otimes \rho_B) \quad (19)$$

$$= \mathcal{Q}\rho - \mathcal{Q}(\rho_S \otimes \rho_B) = \mathcal{Q}\rho. \quad (20)$$

Clearly we also have

$$\mathcal{Q}\mathcal{P}\rho = \mathcal{Q}(\rho_S \otimes \rho_B) = 0, \quad (21)$$

$$\mathcal{P}\mathcal{Q}\rho = \mathcal{P}\rho - \mathcal{P}(\rho_S \otimes \rho_B) = 0. \quad (22)$$

Let us summarise these as operator identities which we will use in our perturbative expansion.

$$\mathcal{P} + \mathcal{Q} = \mathbb{1}, \quad (23)$$

$$\mathcal{P}^2 = \mathcal{P}, \quad \mathcal{Q}^2 = \mathcal{Q}, \quad (24)$$

$$\mathcal{Q}\mathcal{P} = \mathcal{P}\mathcal{Q} = 0. \quad (25)$$

Note also that \mathcal{P} and \mathcal{Q} are linear and time-independent so that they will commute with differential and integral operators in time.

2.2 Time-local master equation

2.2.1 Exact time-local evolution for the relevant part

We first project the evolution of $\tilde{\rho}(t)$ into its relevant and irrelevant parts:

$$\frac{d}{dt} \mathcal{P}\tilde{\rho}(t) = \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\tilde{\rho}(t), \quad (26)$$

$$\frac{d}{dt} \mathcal{Q}\tilde{\rho}(t) = \alpha \mathcal{Q}\tilde{\mathcal{L}}(t)\tilde{\rho}(t). \quad (27)$$

It is not possible to do anything with these equations because their right-hand sides are not functions of the relevant and irrelevant parts. However, we can express their right-hand sides in terms of $\mathcal{P}\tilde{\rho}(t)$ and $\mathcal{Q}\tilde{\rho}(t)$ by inserting an identity in front of $\tilde{\rho}(t)$ and using (23):

$$\frac{d}{dt} \mathcal{P}\tilde{\rho}(t) = \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\mathbb{1}\tilde{\rho}(t) \quad (28)$$

$$= \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}(t) + \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{Q}\tilde{\rho}(t), \quad (29)$$

$$\frac{d}{dt} \mathcal{Q}\tilde{\rho}(t) = \alpha \mathcal{Q}\tilde{\mathcal{L}}(t)\mathbb{1}\tilde{\rho}(t) \quad (30)$$

$$= \alpha \mathcal{Q}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}(t) + \alpha \mathcal{Q}\tilde{\mathcal{L}}(t)\mathcal{Q}\tilde{\rho}(t). \quad (31)$$

We now have a set of coupled differential equations for the relevant and irrelevant parts of $\tilde{\rho}(t)$. Hence we first solve (31) for $\mathcal{Q}\tilde{\rho}(t)$ first. The solution for (31) is

$$\mathcal{Q}\tilde{\rho}(t) = \mathcal{N}_{\mathcal{Q}}(t, t_0) \mathcal{Q}\tilde{\rho}(t_0) + \alpha \int_{t_0}^t dt' \mathcal{N}_{\mathcal{Q}}(t, t') \mathcal{Q}\tilde{\mathcal{L}}(t') \mathcal{P}\tilde{\rho}(t'), \quad (32)$$

where we have defined $\mathcal{N}_{\mathcal{A}}(t, t_0)$ as a time-evolution superoperator generated by $\mathcal{A}\tilde{\mathcal{L}}(t)$ for any \mathcal{A} :

$$\mathcal{N}_{\mathcal{A}}(t, t_0) = \mathbb{T}_{\triangleleft} \left\{ \exp \left[\alpha \int_{t_0}^t dt' \mathcal{A}\tilde{\mathcal{L}}(t') \right] \right\}, \quad t > t_0. \quad (33)$$

This is a superoperator Dyson series where $\mathbb{T}_{\triangleleft}$ is the chronological time-ordering operator. This is defined, for any $\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_N$, by

$$\mathbb{T}_{\triangleleft} [\mathcal{O}_1(t_1) \mathcal{O}_2(t_2) \cdots \mathcal{O}_N(t_N)] = \mathcal{O}_N(t_N) \cdots \mathcal{O}_2(t_2) \mathcal{O}_1(t_1), \quad \forall t_1 < t_2 < \cdots < t_N. \quad (34)$$

Note that $\mathbb{T}_{\triangleleft}$ does nothing if its argument is already ordered with time increasing from right to left.

Exercise: Check that (32) is a solution to (31).

Normally one would substitute (32) back into (29). However, we can see from (32) that $\mathcal{Q}\tilde{\rho}(t)$ depends on the history of $\mathcal{P}\tilde{\rho}(t)$ so that a time-local equation cannot be reached simply by plugging (32) in (29). In order to get a time-local equation we express $\tilde{\rho}(t')$ in the integral of (32) in terms of $\tilde{\rho}(t)$ for $t > t'$. Since we know $\tilde{\rho}(t) = \mathcal{N}_{\mathbb{1}}(t, t') \tilde{\rho}(t')$ for $t > t'$ we can simply invert this equation to obtain

$$\tilde{\rho}(t') = \mathcal{N}_{\mathbb{1}}^{-1}(t, t') \tilde{\rho}(t). \quad (35)$$

One may also write the time-reversed evolution superoperator as

$$\mathcal{N}_{\mathbb{1}}^{-1}(t, t_0) = \mathbb{T}_{\triangleright} \left\{ \exp \left[-\alpha \int_{t_0}^t dt' \tilde{\mathcal{L}}(t') \right] \right\}, \quad t > t_0, \quad (36)$$

where $\mathbb{T}_{\triangleright}$ is the antichronological time-ordering operator defined by

$$\mathbb{T}_{\triangleright} [\mathcal{O}_1(t_1) \mathcal{O}_2(t_2) \cdots \mathcal{O}_N(t_N)] = \mathcal{O}_N(t_N) \cdots \mathcal{O}_2(t_2) \mathcal{O}_1(t_1), \quad \forall t_1 > t_2 > \cdots > t_N. \quad (37)$$

Exercise: Verify that $\mathcal{N}_{\mathbb{1}}^{-1}(t, t_0)$ can be written explicitly in terms of $\mathbb{T}_{\triangleright}$ as in (36). Note the time-evolution superoperator has the property that $\mathcal{N}_{\mathbb{1}}^{-1}(t, t_0) = \mathcal{N}_{\mathbb{1}}(t_0, t)$.

We now substitute (35) into (32), and using again (23),

$$\mathcal{Q}\tilde{\rho}(t) = \mathcal{N}_{\mathcal{Q}}(t, t_0) \mathcal{Q}\tilde{\rho}(t_0) + \alpha \int_{t_0}^t dt' \mathcal{N}_{\mathcal{Q}}(t, t') \mathcal{Q}\tilde{\mathcal{L}}(t') \mathcal{P}\mathcal{N}_{\mathbb{1}}^{-1}(t', t) \tilde{\rho}(t) \quad (38)$$

$$\begin{aligned} &= \mathcal{N}_{\mathcal{Q}}(t, t_0) \mathcal{Q}\tilde{\rho}(t_0) + \left[\alpha \int_{t_0}^t dt' \mathcal{N}_{\mathcal{Q}}(t, t') \mathcal{Q}\tilde{\mathcal{L}}(t') \mathcal{P}\mathcal{N}_{\mathbb{1}}(t', t) \right] \mathcal{P}\tilde{\rho}(t) \\ &\quad + \left[\alpha \int_{t_0}^t dt' \mathcal{N}_{\mathcal{Q}}(t, t') \mathcal{Q}\tilde{\mathcal{L}}(t') \mathcal{P}\mathcal{N}_{\mathbb{1}}(t', t) \right] \mathcal{Q}\tilde{\rho}(t). \end{aligned} \quad (39)$$

This motivates us to define

$$\boxed{\mathcal{S}(t) = \alpha \int_{t_0}^t dt' \mathcal{N}_{\mathcal{Q}}(t, t') \mathcal{Q}\tilde{\mathcal{L}}(t') \mathcal{P}\mathcal{N}_{\mathbb{1}}(t', t)} \quad . \quad (40)$$

Equation (39) can then be written compactly as

$$[\mathbb{1} - \mathcal{S}(t)] \mathcal{Q}\tilde{\rho}(t) = \mathcal{N}_{\mathcal{Q}}(t, t_0) \mathcal{Q}\tilde{\rho}(t_0) + \mathcal{S}(t) \mathcal{P}\tilde{\rho}(t). \quad (41)$$

Assuming $\mathbb{1} - \mathcal{S}(t)$ to be invertible, we may write

$$\mathcal{Q}\tilde{\rho}(t) = [\mathbb{1} - \mathcal{S}(t)]^{-1} \mathcal{N}_{\mathcal{Q}}(t, t_0) \mathcal{Q}\tilde{\rho}(t_0) + [\mathbb{1} - \mathcal{S}(t)]^{-1} \mathcal{S}(t) \mathcal{P}\tilde{\rho}(t). \quad (42)$$

This now allows us to obtain a time-local equation of motion for $\mathcal{P}\tilde{\rho}(t)$. Substituting (42) into (29) we arrive at the following equation of motion for the relevant part of $\tilde{\rho}(t)$:

$$\boxed{\frac{d}{dt} \mathcal{P}\tilde{\rho}(t) = \mathcal{K}(t) \mathcal{P}\tilde{\rho}(t) + \mathcal{I}(t) \mathcal{Q}\tilde{\rho}(t_0)} \quad , \quad (43)$$

where $\mathcal{K}(t)$ and $\mathcal{I}(t)$ are defined, on using the projector property (24), by

$$\boxed{\mathcal{K}(t) = \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P} + \alpha \mathcal{P}\tilde{\mathcal{L}}(t)[\mathbb{1} - \mathcal{S}(t)]^{-1}\mathcal{S}(t)\mathcal{P} \quad ,} \quad (44)$$

$$\boxed{\mathcal{I}(t) = \alpha \mathcal{P}\tilde{\mathcal{L}}(t)[\mathbb{1} - \mathcal{S}(t)]^{-1}\mathcal{N}_{\mathcal{Q}}(t, t_0)\mathcal{Q} \quad .} \quad (45)$$

The form of $\mathcal{K}(t)$ now makes the relevant part independent of its own history. For this reason $\mathcal{K}(t)$ is also called a time-convolutionless generator for the relevant part. The irrelevant part at the initial time in (43) makes the evolution of the relevant part inhomogeneous $\mathcal{I}(t)$ is often called the inhomogeneity superoperator. It plays the role of a forcing term. Note that (43) [along with (44) and (45)] expresses the relevant dynamics exactly. However, it is also extremely complicated. This is where the expansion in terms of powers of α that we mentioned in Sec. 2.1.1 becomes useful. It is possible, under certain assumptions, to express the evolution of the relevant part [i.e. the right-hand side of (43)] as a superoperator power series in α and approximate the dynamics of the relevant part by truncating the series.

2.2.2 Perturbative expansion of relevant dynamics

Let us first deal with the inverse of $\mathbb{1} - \mathcal{S}(t)$. If $\Lambda[\mathcal{S}(t)] \leq 1$, where $\Lambda(\mathcal{O})$ denotes the spectral radius³ of \mathcal{O} , then we can use a power series representation for the inverse of $\mathbb{1} - \mathcal{S}(t)$:

$$[\mathbb{1} - \mathcal{S}(t)]^{-1} = \sum_{n=0}^{\infty} \mathcal{S}^n(t) \quad . \quad (46)$$

We can see from (40) that $\mathcal{S}(t) = 0$ if either $\alpha = 0$ for any $t < \infty$, or $t = t_0$ for any $\alpha < \infty$. In general we will start with $\mathcal{S}(t_0) = 0$ for some nonzero but finite α (otherwise there is no interaction between the system and bath). In this case, the condition for $\Lambda[\mathcal{S}(t)] \leq 1$ can be guaranteed for sufficiently small $t - t_0$. The power series (46) then gives

$$[\mathbb{1} - \mathcal{S}(t)]^{-1}\mathcal{S}(t) = \sum_{n=0}^{\infty} \mathcal{S}^{n+1}(t) = \sum_{n=1}^{\infty} \mathcal{S}^n(t) \quad . \quad (47)$$

Using this we can then write the time-convolutionless generator $\mathcal{K}(t)$ as

$$\mathcal{K}(t) = \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P} + \alpha \mathcal{P}\tilde{\mathcal{L}}(t) \sum_{n=1}^{\infty} \mathcal{S}^n(t)\mathcal{P} \quad . \quad (48)$$

Ultimately $\mathcal{K}(t)$ must have the form of a power series in α so we define

$$\mathcal{K}(t) = \sum_{n=1}^{\infty} \alpha^n \mathcal{K}_n(t) \quad . \quad (49)$$

Note that $\mathcal{K}_n(t)$ for any value of n is defined to be independent of α so it will be convenient to also express $\mathcal{S}(t)$ as a power series in α . Evidently $\mathcal{S}(t)$ may also be written as

$$\mathcal{S}(t) = \sum_{n=1}^{\infty} \alpha^n \mathcal{S}_n(t) \quad , \quad (50)$$

where $\mathcal{S}_n(t)$ is independent of α for every value of n . We can therefore make the expansion of $\mathcal{K}(t)$ more systematic by substituting (50) into (48). This allows us to express the set of superoperator expansion

³The spectral radius of \mathcal{O} is the absolute value of the largest eigenvalue of \mathcal{O} .

coefficients $\{\mathcal{K}_n(t)\}_{n=1}^\infty$ in terms of $\{\mathcal{S}_n(t)\}_{n=1}^\infty$. Up to fourth order in α we have

$$\mathcal{K}_1(t) = \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}, \quad (51)$$

$$\mathcal{K}_2(t) = \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{S}_1(t)\mathcal{P}, \quad (52)$$

$$\mathcal{K}_3(t) = \mathcal{P}\tilde{\mathcal{L}}(t)[\mathcal{S}_1^2(t) + \mathcal{S}_2(t)]\mathcal{P}, \quad (53)$$

$$\mathcal{K}_4(t) = \mathcal{P}\tilde{\mathcal{L}}(t)[\mathcal{S}_1^3(t) + \mathcal{S}_1(t)\mathcal{S}_2(t) + \mathcal{S}_2(t)\mathcal{S}_1(t) + \mathcal{S}_3(t)]\mathcal{P}. \quad (54)$$

Exercise: Derive (51)–(54).

Thus to calculate the time-convolutionless generator we just have to find $\{\mathcal{S}_n(t)\}_{n=1}^\infty$. The higher the order of α we carry the expansion to, the more accurate $\mathcal{K}(t)$ will be for a fixed α . In what follows we will expand $\mathcal{K}(t)$ up to second order in which case only $\mathcal{S}_1(t)$ is required. This defines the weak-coupling regime (i.e. when the system and environment are not strongly interacting).

There is also the inhomogeneity in (43), so what about $\mathcal{I}(t)$? This can also be expanded as a power series in α but we note that $\mathcal{I}(t)$ acts on $\mathcal{Q}\tilde{\rho}(t_0)$, which depends on the initial state. For a system-bath state that is initially factorised, we have

$$\tilde{\rho}(t_0) = \tilde{\rho}_S(t_0) \otimes \rho_B = \mathcal{P}\tilde{\rho}(t_0), \quad (55)$$

and hence, by (25),

$$\mathcal{Q}\tilde{\rho}(t_0) = 0. \quad (56)$$

Thus for a factorised initial state the relevant dynamics is given by a homogeneous differential equation. The form of (55) says that our system starts in a state that is unentangled with the environment. This is a reasonable assumption for many systems as the system is usually prepared in a known state independently of the environment. We will assume this in the following. Although we will not be considering other non-factorised initial states, we highlight here that this case can in principle be handled perturbatively by the inhomogeneity superoperator $\mathcal{I}(t)$.

2.2.3 Weak-coupling master equation for an initially factorised state

For an initially unentangled system-bath state we have

$$\frac{d}{dt} \mathcal{P}\tilde{\rho}(t) = \mathcal{K}(t)\mathcal{P}\tilde{\rho}(t). \quad (57)$$

Up to second order in the system-bath interaction, valid in the weak-coupling regime, this is

$$\frac{d}{dt} \mathcal{P}\tilde{\rho}(t) = \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}(t) + \alpha^2 \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{S}_1(t)\mathcal{P}\tilde{\rho}(t). \quad (58)$$

To determine $\mathcal{S}_1(t)$ we need to go back to (40) and expand it in powers of α . This requires that we use (33) and (36) for $\mathcal{N}_{\mathcal{Q}}(t, t_0)$ and $\mathcal{N}_{\mathbb{1}}^{-1}(t, t_0)$. The result is simply

$$\mathcal{S}_1(t) = \int_{t_0}^t dt' \mathcal{Q}\tilde{\mathcal{L}}(t')\mathcal{P}. \quad (59)$$

Equation (58) now becomes

$$\frac{d}{dt} \mathcal{P}\tilde{\rho}(t) = \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}(t) + \alpha^2 \int_{t_0}^t dt' \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{Q}\tilde{\mathcal{L}}(t')\mathcal{P}\tilde{\rho}(t) \quad (60)$$

$$= \alpha \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\rho}(t) + \alpha^2 \int_{t_0}^t dt' \mathcal{P}\tilde{\mathcal{L}}(t)\tilde{\mathcal{L}}(t')\mathcal{P}\tilde{\rho}(t) - \alpha^2 \int_{t_0}^t dt' \mathcal{P}\tilde{\mathcal{L}}(t)\mathcal{P}\tilde{\mathcal{L}}(t')\mathcal{P}\tilde{\rho}(t). \quad (61)$$

where we used $\mathcal{Q} = \mathbb{1} - \mathcal{P}$ in the last line. Recall that for any \hat{A}

$$\tilde{\mathcal{L}}(t)\hat{A} = -\frac{i}{\hbar} [\tilde{V}(t), \hat{A}]. \quad (62)$$

The first term in (61) is thus

$$\mathcal{P} \tilde{\mathcal{L}}(t) \mathcal{P} \tilde{\rho}(t) = -\frac{i}{\hbar} \text{Tr}_B \left\{ [\tilde{V}(t), \tilde{\rho}_S(t) \otimes \rho_B] \right\} \otimes \rho_B \quad (63)$$

If $\tilde{V}(t)$ has zero mean then this term is zero. This will be the case when the bath operators which couple to the system have zero mean in the state ρ_B . This is commonly encountered in practice so we will assume this to be the case. However, even if it is not the case one can always make this true by redefining \hat{H}_0 and \hat{V} so that \tilde{V} always averages to zero.

Exercise: Show that $\tilde{V}(t)$ can always be arranged to have zero mean.

In this case,

$$\mathcal{P} \tilde{\mathcal{L}}(t) \mathcal{P} \tilde{\rho}(t) = \int_{t_0}^t dt' \mathcal{P} \tilde{\mathcal{L}}(t) \mathcal{P} \tilde{\mathcal{L}}(t') \mathcal{P} \tilde{\rho}(t) = 0. \quad (64)$$

Using (62) we obtain

$$\frac{d}{dt} \mathcal{P} \tilde{\rho}(t) = -\frac{1}{\hbar^2} \int_{t_0}^t dt' \text{Tr}_B \left\{ [\tilde{V}(t), [\tilde{V}(t'), \tilde{\rho}_S(t) \otimes \rho_B]] \right\} \otimes \rho_B. \quad (65)$$

Taking the partial trace over the bath and setting $\alpha = 1$ we finally arrive at

$$\boxed{\frac{d}{dt} \tilde{\rho}_S(t) = -\frac{1}{\hbar^2} \int_{t_0}^t dt' \text{Tr}_B \left\{ [\tilde{V}(t), [\tilde{V}(t'), \tilde{\rho}_S(t) \otimes \rho_B]] \right\} \equiv \tilde{\mathcal{L}}_S(t) \tilde{\rho}_S} \quad (66)$$

This now defines $\tilde{\mathcal{L}}_S(t)$ —the $\mathcal{L}_S(t)$ in (3) but in the interaction picture. Equation (66) is often used as a starting point for deriving the evolution of open systems. In the next lecture I will present a simple example and explore the physical consequences that such an equation describes.

Lecture 2

3 Example: Damped harmonic oscillator

3.1 Model Hamiltonian

Here we consider the dissipation of a single harmonic oscillator with frequency ω_0 . The system Hamiltonian is

$$\hat{H}_S = \hbar \omega_0 \hat{a}^\dagger \hat{a}, \quad (67)$$

where \hat{a} and \hat{a}^\dagger are annihilation and creation operators, defined by

$$[\hat{a}, \hat{a}^\dagger] = \hat{1}_S. \quad (68)$$

We choose our bath to be a collection of harmonic oscillators with the set of annihilation operators $\{\hat{c}_k\}_k$ with the corresponding set of frequencies $\{\omega_k\}_k$. The model for the bath is thus defined by the Hamiltonian

$$\hat{H}_B = \sum_k \hbar \omega_k \hat{c}_k^\dagger \hat{c}_k. \quad (69)$$

This is an infinite sum over k and the members of $\{\hat{c}_k\}_k$ satisfy the commutation relations

$$[\hat{c}_j, \hat{c}_k] = [\hat{c}_j^\dagger, \hat{c}_k^\dagger] = 0, \quad [\hat{c}_j, \hat{c}_k^\dagger] = \delta_{jk} \hat{1}_B. \quad (70)$$

We now assume that the system oscillator interacts with the k th bath oscillator with coupling constant g_k and that the system-bath interaction is such that we can apply the rotating-wave approximation to describe it. The interaction Hamiltonian is thus

$$\hat{V} = \sum_k \hbar (g_k^* \hat{a} \otimes \hat{c}_k^\dagger + g_k \hat{a}^\dagger \otimes \hat{c}_k). \quad (71)$$

This model can be used to describe the transfer of energy from a single-mode electromagnetic field (often engineered by an optical cavity) to free space (modes of the electromagnetic field outside the cavity). Finally, we need to specify the state of the bath. Here we will take it to be a multimode thermal state at temperature T , given by

$$\rho_{\text{B}} = \bigotimes_k \rho_k, \quad (72)$$

where ρ_k is a thermal state for the k th mode, defined by

$$\rho_k = e^{-\beta \hbar \omega_k \hat{c}_k^\dagger \hat{c}_k} (1 - e^{-\beta \hbar \omega_k}). \quad (73)$$

We have defined $\beta = 1/k_{\text{B}}T$ and k_{B} is the Boltzmann constant.

3.2 Master equation

There is in fact still some work that you have to do to simplify the form of $\tilde{\mathcal{L}}_{\text{S}}(t)$. I will outline the steps here but they are covered in most quantum-optics textbooks:

1. Expand the nested commutator $[\tilde{V}(t), [\tilde{V}(t'), \tilde{\rho}_{\text{S}}(t) \otimes \rho_{\text{B}}]]$ and work out $\tilde{V}(t)$.
2. Take the partial trace of the nested commutator over the bath. This gives rise to bath correlation functions of the form

$$C_{j,k}(t, t') \equiv \langle \tilde{b}_j(t) \tilde{b}_k(t') \rangle = \text{Tr}_{\text{B}} [\tilde{b}_j(t) \tilde{b}_k(t') \rho_{\text{B}}], \quad j, k = 1, 2, \quad (74)$$

where

$$\tilde{b}_1(t) = \hbar \sum_n g_n^* \hat{c}_n^\dagger e^{i\omega_n t}, \quad \tilde{b}_2(t) = \hbar \sum_n g_n \hat{c}_n e^{-i\omega_n t}. \quad (75)$$

Calculating the partial trace amounts to calculating the bath correlation functions.

3. Calculate the time integral by assuming that $C_{j,k}(t, t')$ decays sufficiently fast when $t \neq t'$. Mathematically this approximation can be expressed by extending $t - t_0 \rightarrow \infty$ which allows one to write

$$\frac{d}{dt} \tilde{\rho}_{\text{S}}(t) = -\frac{1}{\hbar^2} \int_0^\infty d\tau \text{Tr}_{\text{B}} \left\{ [\tilde{V}(t), [\tilde{V}(t - \tau), \tilde{\rho}_{\text{S}}(t) \otimes \rho_{\text{B}}]] \right\}. \quad (76)$$

The time integral contributes a small shift to the natural frequency of the oscillator which is usually neglected.

Exercise: Perform steps 1-3 above. You may want to consult a textbook on quantum optics.

At the end of all this we find

$$\boxed{\frac{d}{dt} \rho_{\text{S}}(t) = \mathcal{L}_{\text{S}} \rho_{\text{S}}(t) \equiv -i\omega_0 [\hat{a}^\dagger \hat{a}, \rho_{\text{S}}(t)] + \gamma (\bar{n} + 1) \mathcal{D}[\hat{a}] \rho_{\text{S}}(t) + \gamma \bar{n} \mathcal{D}[\hat{a}^\dagger] \rho_{\text{S}}(t)} \quad , \quad (77)$$

where the master equation is now parametrised by two real and positive numbers γ and \bar{n} . We have also defined for any \hat{A} and \hat{B} ,

$$\mathcal{D}[\hat{A}] \hat{B} \equiv \hat{A} \hat{B} \hat{A}^\dagger - \frac{1}{2} \hat{A}^\dagger \hat{A} \hat{B} - \frac{1}{2} \hat{B} \hat{A}^\dagger \hat{A}. \quad (78)$$

The parameter \bar{n} is simply the average photon number of the bath at temperature T and frequency ω_0 :

$$\bar{n} = \frac{e^{-\beta \hbar \omega_0}}{1 - e^{-\beta \hbar \omega_0}}. \quad (79)$$

The parameter γ is determined by the coupling constants g_k in \hat{V} . Clearly we can see that if

$$\gamma = 0, \quad (80)$$

then we obtain the Schrödinger equation for a free oscillator

$$\frac{d}{dt} \rho_S(t) = -i \omega_0 [\hat{a}^\dagger \hat{a}, \rho_S(t)]. \quad (81)$$

Thus only for γ nonzero do we couple the system with the bath. Loosely speaking, it will suffice to think of \bar{n} as the energy of the environment at temperature T , and γ as the strength of coupling between the system and bath, and just remember that \bar{n} is given by (79) and

$$\gamma \geq 0. \quad (82)$$

4 Understanding the damped harmonic oscillator

4.1 Zero-temperature environment

To understand the master equation let us first consider the simpler case of a zero-temperature environment:

$$T = 0 \implies \bar{n} = 0. \quad (83)$$

Note that this is the same as saying the bath is in the vacuum state. The master equation is then

$$\frac{d}{dt} \rho_S(t) = -i \omega_0 [\hat{a}^\dagger \hat{a}, \rho_S(t)] + \gamma \left[\hat{a} \rho_S(t) \hat{a}^\dagger - \frac{1}{2} \hat{a}^\dagger \hat{a} \rho_S(t) - \frac{1}{2} \rho_S(t) \hat{a}^\dagger \hat{a} \right]. \quad (84)$$

Equation (84) now requires us to interpret $\mathcal{D}[\hat{a}]$. We can get a rough idea of $\mathcal{D}[\hat{a}]$ if we note that $\hat{a} \rho_S \hat{a}^\dagger$ is proportional to a photon subtracted state in quantum optics. In particular, if ρ_S is a Fock state then $\hat{a} \rho_S \hat{a}^\dagger$ is again a Fock state with one photon less while ‘nothing happens’ in the remaining two terms in (84) (since a Fock state is an eigenstate of $\hat{a}^\dagger \hat{a}$). This hints that $\mathcal{D}[\hat{a}]$ is associated with the loss of energy. By the same token we might associate $\mathcal{D}[\hat{a}^\dagger]$ with a gain in energy for the system. We already know that \bar{n} measures how much energy the bath has and we expect some of this energy to enter the system since it is coupled to the system. At the same time we expect the system to dissipate energy to the bath. If however we set $\bar{n} = 0$ then no energy can enter the system and the exchange of energy between the system and bath becomes unidirectional. In other words, we can interpret the effect of $\mathcal{D}[\hat{a}]$ on the system in (84) to be dissipative. If we interpret $\mathcal{D}[\hat{a}^\dagger]$ as argued, i.e. its effect is to raise the system’s energy, then we would not expect it to appear in the master equation when $\bar{n} = 0$ since in this case there is no energy in the bath to excite the system. This is indeed what we see in (77). This way of thinking about the master equation is rather hand-waving so we will spend more time to make sense of the dissipative terms in Sec. 4.2. Hopefully then, it will become much clearer what these terms mean.

Exercise: Think about what happens to the photons leaked to the environment. Can they re-enter the system?

4.2 Nonzero-temperature environment

The superoperators $\mathcal{D}[\hat{a}]$ and $\mathcal{D}[\hat{a}^\dagger]$ have somewhat complicated forms. In the above we have made a little bit of sense of them by considering different limiting values of γ and \bar{n} but can we do more? In particular,

- What roles do γ and \bar{n} play in the system evolution?
- Can we get a more precise understanding of the superoperators $\mathcal{D}[\hat{a}]$ and $\mathcal{D}[\hat{a}^\dagger]$?

To answer these questions we consider the effects of $\mathcal{D}[\hat{a}]$ and $\mathcal{D}[\hat{a}^\dagger]$ on system observables. This will translate their action on the system into something tangible.

4.2.1 Damping and thermalisation

Let us consider how the average amplitude of the oscillator evolves first. Using the master equation (77) we find

$$\frac{d}{dt} \langle \hat{a} \rangle_t = -i\omega_0 \langle \hat{a} \rangle_t - \frac{1}{2} \gamma (\bar{n} + 1) \langle \hat{a} \rangle_t + \frac{1}{2} \cancel{\gamma \bar{n} \langle \hat{a} \rangle_t} \quad (85)$$

$$= -\left(\frac{\gamma}{2} + i\omega_0\right) \langle \hat{a} \rangle_t. \quad (86)$$

The solution of this equation is

$$\boxed{\langle \hat{a} \rangle_t = \langle \hat{a} \rangle_0 e^{-i\omega_0 t} e^{-\gamma t/2}}. \quad (87)$$

It is clear from (87) that γ is to be interpreted as a damping coefficient. At time $t = 0$, the oscillator's amplitude starts somewhere on the complex plane at $\langle \hat{a} \rangle_0$ and then revolves around the origin as time goes by. If $\gamma = 0$ then the oscillator would circle the origin at a period of $T_0 = 2\pi/\omega_0$ indefinitely. For $\gamma \neq 0$, the amplitude spirals a little bit towards the origin on each cycle until it eventually gets to the origin and stays there forever.

Next we consider the average energy of the oscillator. Its equation of motion is

$$\frac{d}{dt} \langle \hat{n} \rangle_t = -\gamma \langle \hat{n} \rangle_t + \gamma \bar{n}. \quad (88)$$

Again, we see that γ is a damping coefficient but now \bar{n} also appears which is replenishing the oscillator's energy. Solving (88) gives

$$\boxed{\langle \hat{n} \rangle_t = \langle \hat{n} \rangle_0 e^{-\gamma t} + \bar{n}(1 - e^{-\gamma t})} \quad (89)$$

Unlike the average amplitude, the system's average energy does not decay to zero but is lower bounded:

$$\langle \hat{n} \rangle_{ss} \equiv \lim_{t \rightarrow \infty} \langle \hat{n} \rangle_t = \bar{n}. \quad (90)$$

Physically this is because thermal energy from the bath is entering the system. Note that $\langle \hat{n} \rangle_{ss}$ can also be obtained directly from (88). Recall that this is exactly the average energy of an oscillator with frequency ω_0 and temperature T :

$$\bar{n} = \frac{e^{-\hbar\omega_0/k_B T}}{1 - e^{-\hbar\omega_0/k_B T}}, \quad (91)$$

where we have also written out $\beta = 1/k_B T$ to make the temperature dependence explicit. However, we did not specify the temperature of the system, T is actually the temperature of the environment, so (90) tells us that the system will eventually thermalise to the temperature of the environment. The master equation that we have derived seems to capture the process of thermalisation!

Exercise: Derive (85) and (88) from the master equation (77).

4.2.2 Pauli master equation

We can get an even more detailed understanding of the master equation by thinking about it in the energy basis. More specifically we consider the probability for the system oscillator to be in its n th energy eigenstate at time t . That is to say we will just focus on

$$\wp(n, t) \equiv \langle n | \rho_S(t) | n \rangle. \quad (92)$$

The equation of motion for $\wp(n, t)$ is called the Pauli master equation and $\wp(n, t)$ is often referred to as the population of the n th state. The evolution of $\wp(n, t)$ can thus be calculated directly as the diagonal elements of the master equation (77). The result is

$$\boxed{\frac{\partial}{\partial t} \wp(n, t) = \gamma(\bar{n} + 1)(n + 1)\wp(n + 1, t) - \gamma(\bar{n} + 1)n\wp(n, t) + \gamma\bar{n}n\wp(n - 1, t) - \gamma\bar{n}(n + 1)\wp(n, t)}. \quad (93)$$

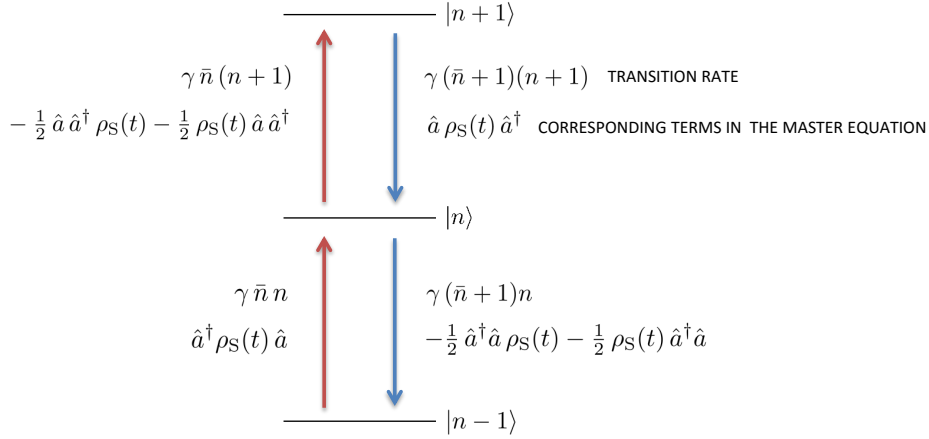


Fig. 1: Interpretation of the population dynamics of the damped harmonic oscillator. Each term in (93) describes a transition indicated by an arrow. The corresponding rate for the transition is shown next to the arrow. Furthermore, the derivation of (93) shows us exactly which terms in the superoperators $\mathcal{D}[\hat{a}]$ and $\mathcal{D}[\hat{a}^\dagger]$ contribute to a given transition which is also shown by the operators appearing to each arrow.

The population of each energy eigenstate can thus be seen to couple only to the population of other energy eigenstates, there is no coupling between populations and coherences. We can interpret the positive contributions in (93) [$\gamma(\bar{n}+1)(n+1)\varphi(n+1, t)$ and $\gamma \bar{n} n \varphi(n-1, t)$] as transitions to state $|n\rangle$ from $|n+1\rangle$ and $|n-1\rangle$, while the negative contributions [$-\gamma(\bar{n}+1)n\varphi(n, t)$ and $-\gamma \bar{n}(n+1)\varphi(n, t)$] can be interpreted as transitions out of state $|n\rangle$ and into states $|n+1\rangle$ and $|n-1\rangle$. We depict the correspondence between each term in (93) and the transition they describe in Fig. 1.

4.2.3 Steady-state photon statistics—thermalisation revisited

We obtained the steady-state average energy of the oscillator in (90). In principle this should be consistent with the steady-state solution of the Pauli master equation. That is, we expect

$$\langle \hat{n} \rangle_{\text{ss}} = \sum_{n=0}^{\infty} n \varphi_{\text{ss}}(n), \quad (94)$$

where $\varphi_{\text{ss}}(n)$ is the steady-state solution of (93), i.e.

$$\varphi_{\text{ss}}(n) = \lim_{t \rightarrow \infty} \varphi(n, t). \quad (95)$$

Solving for the steady state of the Pauli master equation we find

$$\boxed{\varphi_{\text{ss}}(n) = \frac{1}{\bar{n}+1} \left(\frac{\bar{n}}{\bar{n}+1} \right)^n}. \quad (96)$$

This now gives us all the photon statistics of the system oscillator at steady state.

Exercise: Show that (96) gives an average photon number consistent with (90).

We did not obtain

$$(\rho_S)_{\text{ss}} = \lim_{t \rightarrow \infty} \rho_S(t) \quad (97)$$

from the master equation. However, with (96) we can now solve for $(\rho_S)_{\text{ss}}$ directly by noting that it must be the solution to

$$\langle n | (\rho_S)_{\text{ss}} | n \rangle = \varphi_{\text{ss}}(n) = \frac{1}{\bar{n}+1} \left(\frac{\bar{n}}{\bar{n}+1} \right)^n. \quad (98)$$

It is simple to see that the solution to (98) is

$$(\rho_S)_{ss} = \frac{1}{\bar{n} + 1} \left(\frac{\bar{n}}{\bar{n} + 1} \right)^{\hat{a}^\dagger \hat{a}} . \quad (99)$$

We can express (99) in what might be a more familiar form using (91):

$$\boxed{(\rho_S)_{ss} = (1 - e^{-\beta \hbar \omega_0}) e^{-\beta \hbar \omega_0 \hat{a}^\dagger \hat{a}}} , \quad (100)$$

which is a thermal state! If we are to be rigorous then we should show that it really is the long-time solution of the master equation by substituting (100) back into (77) and verify that

$$\mathcal{L}_S (\rho_S)_{ss} = 0 . \quad (101)$$

Exercise: Derive (100) from (99), using (91).