

6. Master Equation Formalism

Here is the answer to Einstein's question about the moon. Yes, it is there when no one observes it – because the environment is already, and without cease, ‘measuring’ it. All of the photons of sunlight that bounce off the moon are agents of decoherence, and more than adequate to fix its position in space and give it a sharp outline. The universe is always looking.

– Philip Ball, *Beyond Weird*

Open quantum systems occur in a wide range of disciplines. In particular, the dynamics of open quantum systems have been studied extensively in the field of quantum optics. The time evolution of an open quantum system can be described by a continuous-time approach, with a differential equation that properly describes non-unitary behaviour. This is the master equation approach.

The master equation is a differential equation of $\hat{\rho}_S(t)$, the reduced density matrix of the open quantum system S that interacts with an environment E . It conveniently allows us to determine the dynamics of the system without needing to first determine the dynamics of the total system-environment combination and then tracing out the environment degrees of freedom. (See Fig. 6.1).

The master equation approach is motivated by two issues. First, we are usually not interested in the dynamics of the environment or of the global system-environment composite. What we care about is the influence of the environment on the system of interest. Second, it is often impossible to analytically determine the time evolution of the full density matrix. In such cases, one can use approximation schemes that lead to master equations for the approximate evolution of the reduced density matrix.

6.1 Gorini-Kossakowski-Sudarshan-Lindblad Master Equation

The most general Markovian master equation is given by the Gorini-Kossakowski-Sudarshan-Lindblad¹ master equation, or more commonly called the Lindblad master equation.

¹Named after Vittorio Gorini, Andrzej Kossakowski, George Sudarshan and Göran Lindblad.

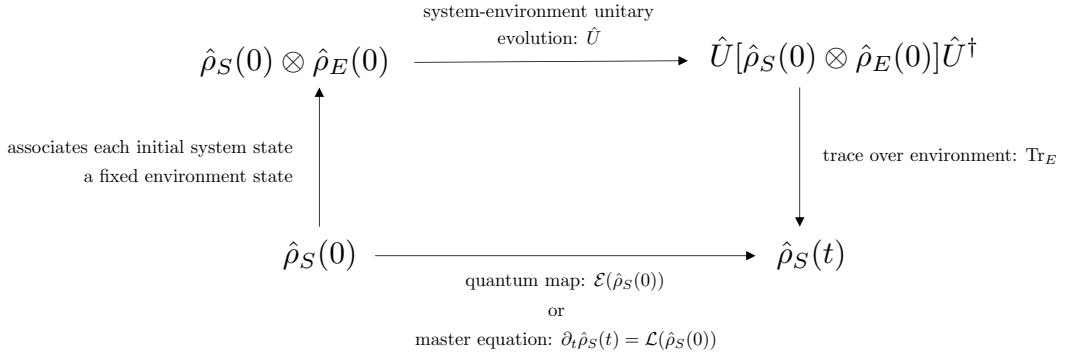


Figure 6.1: The quantum map and the master equation approaches conveniently allow us to determine the dynamics of the system without needing to first determine the dynamics of the total system-environment combination and then tracing out the environment degrees of freedom. The effects of the environment are neatly encapsulated in simple rate parameters and jump operators in the master equation description.

Lindblad Master Equation

$$\frac{d\hat{\rho}_S}{dt} = \underbrace{-\frac{i}{\hbar}[\hat{H}'_S, \hat{\rho}_S]}_{\text{unitary dynamics}} + \sum_j \underbrace{\left(\hat{L}_j \hat{\rho}_S \hat{L}_j^\dagger - \frac{1}{2} \{\hat{L}_j^\dagger \hat{L}_j, \hat{\rho}_S\} \right)}_{\text{non-unitary dynamics, } \mathcal{D}(\hat{\rho}_S)}, \quad (6.1)$$

where $\hat{\rho}_S$ is the system density operator, \hat{L}_j are Lindblad jump operators, $\{a, b\} \equiv ab + ba$ denotes an anticommutator, and \hat{H}'_S is the system Hamiltonian. The prime represents the system Hamiltonian with an energy shift due to the presence of the environment, called the Lamb shift. Note that some texts ignore the Lamb shift and use \hat{H}_S , the system Hamiltonian, since the Lamb shift is a renormalization of the energy levels of the system and does not have to do with the non-unitary evolution.

Göran Lindblad (9 Jul 1940 - 30 Nov 2022) is associated with this equation because he showed in 1976 that terms of the form $\hat{L}_j \hat{\rho}_S \hat{L}_j^\dagger - \frac{1}{2} \{\hat{L}_j^\dagger \hat{L}_j, \hat{\rho}_S\}$ always preserve positivity, provided $\gamma_j \geq 0$, in a paper “*On the generators of quantum dynamical semigroups*”. Also in 1976, Gorini, Kossakowski and Sudarshan derived similar results, in a paper “*Completely positive dynamical semigroups of N-level systems*”. It is therefore also called the GKSL master equation.

The master equation above is expressed in the Schrödinger picture. It is also possible to derive it in the Heisenberg picture, given in terms of a Heisenberg operator \hat{A} :

$$\frac{d\hat{A}}{dt} = -\frac{i}{\hbar}[\hat{H}'_S, \hat{A}] + \sum_j \left(\hat{L}_j \hat{A} \hat{L}_j^\dagger - \frac{1}{2} \{\hat{L}_j^\dagger \hat{L}_j, \hat{A}\} \right). \quad (6.2)$$

The first term on the right represents coherent, unitary dynamics just like the Liouville-von Neumann equation. The second set of terms represent non-unitary dynamics arising from what is called Lindblad jump operators \hat{L}_j , which we will explain shortly. In contrast with the dynamics of a closed system which is unitary, the evolution equation for the reduced density matrix will, in general, be non-unitary. This is because the trace operation used to obtain the reduced density matrix is a non-unitary operation; the master equation must in general also be non-unitary.

The Lindblad master equation is sometimes written more concisely in two ways,

$$\frac{\partial \hat{\rho}_S}{\partial t} = -\frac{i}{\hbar}[\hat{H}'_S, \hat{\rho}_S] + \mathcal{D}(\hat{\rho}_S) \quad (6.3)$$

$$\frac{\partial \hat{\rho}_S}{\partial t} = \mathcal{L}(\hat{\rho}_S), \quad (6.4)$$

where \mathcal{L} and \mathcal{D} are superoperators acting on the reduced density operator. The second form of

the master equation is analogous to a set of differential equations, e.g. $\dot{\vec{x}} = A\vec{x}$ with solution $\vec{x}(t) = e^{At}\vec{x}(0)$, where e^{At} is called the map from $\vec{x}(0)$ to $\vec{x}(t)$ and A is the generator of the map. This allows us to write its formal solution, shown here for the case of time-independent \mathcal{L} , as

$$\hat{\rho}_S(t) = \lim_{n \rightarrow \infty} \left(1 + \frac{\mathcal{L}t}{n} \right)^n (\hat{\rho}_S(0)) = e^{\mathcal{L}t} \hat{\rho}_S(0), \quad (6.5)$$

which is rather similar to the time-evolution propagator for a pure state $|\psi(t)\rangle = e^{-(i/\hbar)\hat{H}t} |\psi(0)\rangle$, except that the evolution of an open quantum system is in general, not unitary. That is, it can be propagated forward in time, but because we have insufficient information about the environment, it cannot be reversed in time.

This equation is also local in time: the change of $\hat{\rho}_S$ depends only on $\hat{\rho}_S$ evaluated at t but not at any earlier times $t' < t$. It is therefore a *Markovian* master equation.

To explain what the Lindblad jump operators \hat{L}_j are, it is instructive to derive the Lindblad master equation from the completely-positive and trace-preserving (CPTP) quantum map formalism.

6.2 Derivation I: Arguments from CPTP map

In this section, we shall derive the Lindblad master equation from an infinitesimal time evolution described by the Kraus operator sum representation, or quantum map.

First, from a Taylor series expansion of the density operator around $t = 0$, we have

$$\hat{\rho}(dt) = \hat{\rho}(0) + \left. \frac{\partial \hat{\rho}}{\partial t} \right|_{t=0} dt + \mathcal{O}(dt^2). \quad (6.6)$$

From the Kraus operator representation, or quantum map, we can also write

$$\hat{\rho}(dt) = \sum_{\alpha} \hat{E}_{\alpha}(dt) \hat{\rho}(0) \hat{E}_{\alpha}^{\dagger}(dt). \quad (6.7)$$

These two equations should agree to the first order in the time interval, dt . In order to get the first term $\hat{\rho}(0)$, one of the Kraus operators must contain an identity operator. So, we write

$$\hat{E}_0 = \hat{\mathbb{I}} + \hat{L}_0 dt, \quad (6.8)$$

so that

$$\begin{aligned} \hat{E}_0 \hat{\rho}(0) \hat{E}_0^{\dagger} &= (\hat{\mathbb{I}} + \hat{L}_0 dt) \hat{\rho}(0) (\hat{\mathbb{I}} + \hat{L}_0 dt)^{\dagger} \\ &= \hat{\rho}(0) + (\hat{L}_0 \hat{\rho}(0) + \hat{\rho}(0) \hat{L}_0^{\dagger}) dt + \mathcal{O}(dt^2). \end{aligned} \quad (6.9)$$

A single Kraus operator is equivalent to unitary evolution, so there must be other Kraus operators in general. Since the $\alpha = 0$ operator gives the $\hat{\rho}(0)$ term already, we write the other Kraus operators without the identity, as

$$\hat{E}_{\alpha} = \sqrt{dt} \hat{L}_{\alpha}, \quad \text{for } \alpha \geq 1, \dots, K-1, \quad (6.10)$$

so that these Kraus operators also produce terms that are first order in the time interval,

$$\hat{E}_{\alpha} \hat{\rho}(0) \hat{E}_{\alpha}^{\dagger} = \hat{L}_{\alpha} \hat{\rho}(0) \hat{L}_{\alpha}^{\dagger} dt, \quad \text{for } \alpha \geq 1, \dots, K-1, \quad (6.11)$$

where $K \leq d^2$, and d is the dimension of the system. Since these operators have to respect the Kraus sum normalization condition², at least up to $\mathcal{O}(dt)$, we have

$$\hat{\mathbb{I}} = \sum_{\alpha} \hat{E}_{\alpha}^{\dagger} \hat{E}_{\alpha} = \hat{\mathbb{I}} + dt \left(\hat{L}_0 + \hat{L}_0^{\dagger} + \sum_{\alpha \geq 1} \hat{L}_{\alpha}^{\dagger} \hat{L}_{\alpha} \right) + \mathcal{O}(dt^2), \quad (6.12)$$

²Recall Eq. (5.15) and Ex. 5.2, that this comes from unitarity, i.e. trace-preserving, consideration.

which implies that the terms in brackets add up to zero. We can decompose \hat{L}_0 into a Hermitian \hat{A} and an anti-Hermitian $-i\hat{H}$ part, with $\hat{A}^\dagger = \hat{A}$ and $\hat{H}^\dagger = -\hat{H}$. In this way, $\hat{L}_0 = \hat{A} - i\hat{H}$, and $\hat{L}_0 + \hat{L}_0^\dagger = 2\hat{A}$. Putting this into Eq. (6.12), we get

$$\hat{A} = -\frac{1}{2} \sum_{\alpha \geq 1} \hat{L}_\alpha^\dagger \hat{L}_\alpha. \quad (6.13)$$

Putting all these together in the Kraus OSR,

$$\begin{aligned} \hat{\rho}(dt) &= \hat{E}_0 \hat{\rho}(0) \hat{E}_0^\dagger + \sum_{\alpha \geq 1} \hat{E}_\alpha \hat{\rho}(0) \hat{E}_\alpha^\dagger \\ &= \hat{\rho}(0) + dt \left((\hat{A} - i\hat{H}) \hat{\rho}(0) + \hat{\rho}(0) (\hat{A} + i\hat{H}) \right) + dt \sum_{\alpha \geq 1} \hat{L}_\alpha \hat{\rho}(0) \hat{L}_\alpha^\dagger + \mathcal{O}(dt^2) \\ &= \hat{\rho}(0) - i[\hat{H}, \hat{\rho}(0)]dt + \{\hat{A}, \hat{\rho}(0)\}dt + dt \sum_{\alpha \geq 1} \hat{L}_\alpha \hat{\rho}(0) \hat{L}_\alpha^\dagger + \mathcal{O}(dt^2) \\ &= \hat{\rho}(0) - i[\hat{H}, \hat{\rho}(0)]dt + \sum_{\alpha \geq 1} \left(\hat{L}_\alpha \hat{\rho}(0) \hat{L}_\alpha^\dagger - \frac{1}{2} \{\hat{L}_\alpha^\dagger \hat{L}_\alpha, \hat{\rho}(0)\} \right) dt + \mathcal{O}(dt^2) \\ \therefore \frac{\partial \hat{\rho}(t)}{\partial t} \Big|_{t=0} &= \lim_{dt \rightarrow 0} \frac{\hat{\rho}(dt) - \hat{\rho}(0)}{dt} = -i[\hat{H}, \hat{\rho}(0)] + \sum_{\alpha \geq 1} \hat{L}_\alpha \hat{\rho}(0) \hat{L}_\alpha^\dagger - \frac{1}{2} \{\hat{L}_\alpha^\dagger \hat{L}_\alpha, \hat{\rho}(0)\}. \end{aligned} \quad (6.14)$$

Now, in order that this equation reduces to the Liouville-von Neumann equation in the case when all $\hat{L}_\alpha = 0$ for $\alpha \geq 1$, we need to identify the operator \hat{H} as the system Hamiltonian and replace it: $\hat{H} \rightarrow \frac{1}{\hbar} \hat{H}_S$. Next, we recognize that the units of this equation is 1/time, so all the \hat{L}_α operators have units of $\sqrt{\text{rate}}$. Sometimes they are written in a dimensionless way by replacing them as such: $\hat{L}_\alpha \rightarrow \sqrt{\gamma_\alpha} \hat{L}_\alpha$ where γ_α are non-negative rates.

6.2.1 Markovian assumption

This result is valid as a short time expansion near $t = 0$. If we now assume that this equation is valid for all times $t > 0$, then we have essentially assumed the Markovian limit, which states (informally) that there is no memory in the evolution, as manifested by the fact that the evolution “resets” every Δt_{coarse} (which is dt in the above derivation). This Markovian approximation will be useful if $\Delta t_{\text{coarse}} \gg \Delta t_{\text{env}}$, where the latter is the time scale for the quantum correlations between the system and the environment to decay, so that the environment has no memory of the information that it acquired from the system. In such a case, we can neglect the possibility that the information may feed back from the environment into the system again to influence the subsequent evolution of the system. Therefore, the time scale over which we wish to observe the system’s evolution, which we call Δt_{obs} , should follow the hierarchy

$$\Delta t_{\text{obs}} \gg \Delta t_{\text{coarse}} \gg \Delta t_{\text{env}}. \quad (6.15)$$

Therefore, we derive the Lindblad master equation:

$$\frac{d\hat{\rho}_S}{dt} = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S] + \sum_j \underbrace{\hat{L}_j \hat{\rho}_S \hat{L}_j^\dagger}_{\text{quantum jumps}} - \underbrace{\frac{1}{2} \{\hat{L}_j^\dagger \hat{L}_j, \hat{\rho}_S\}}_{\text{trace renormalization}}. \quad (6.16)$$

With this approach, the Lamb shift is not derived. We shall see another physically motivated derivation that will be able to derive this.

6.3 Stochastic Processes and the Wiener-Khinchin-Einstein theorem

In this section, we present concepts of noise and basic methods of characterizing noise processes. This will be important in understanding the second way of deriving the Lindblad master equation later.

Noise is a stochastic or random process. It can only be statistically characterized. We can only discuss the averaged quantity of a single system over a certain time interval, or the averaged

quantity of many identical systems at a certain time instance. The former is called a time average and the latter, an ensemble average. An ensemble average is a convenient theoretical concept because it is directly related to probability density functions, which can be generally obtained by the theoretical analysis of a given physical system. On the other hand, a time average is more directly related to real experiments. It is not possible to prepare an infinite number of identical systems in reality.

Ergodicity

If a stochastic process is *ergodic*, then ensemble averages (which are usually from theoretical predictions) are equivalent to time averages (which are usually from experimental data).

Ergodicity becomes useful if we have only one sample time-series of a stochastic process, instead of the entire ensemble. A single sample function will often provide little information about the statistics of the process. However, if the process is ergodic, i.e. time averages equal ensemble averages, then all statistical information can be derived from just one sample function.

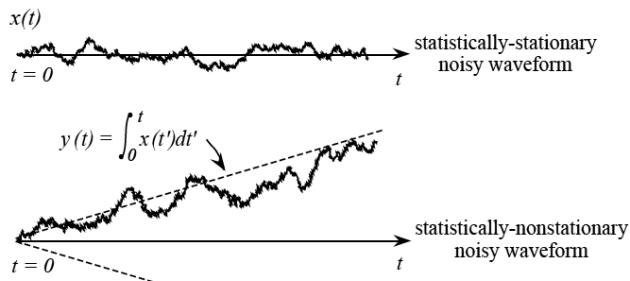


Figure 6.2: Stationary (top) vs non-stationary (bottom) time signals. Figure from Yamamoto's lecture notes.

Stationarity

A stationary stochastic process is one where its statistics do not change with time.

This implies that statistics of a stochastic process $x(t)$ such as its mean $\langle x(t) \rangle$ is independent of the time t so that it does not matter at what absolute time the average is taken. Also, its autocorrelation $\langle x(t_2)x(t_1) \rangle$ depends only on the time difference $\tau = t_2 - t_1$.

1. **Wide-sense (or weak) stationarity.** When only the first moment (mean) and the second moment (autocorrelation) are constant. This condition is sufficient to analyze a given stochastic process with the Wiener-Khinchin-Einstein theorem.
2. **Strict-sense stationarity.** If N -th order moments are constant for any given N .

The mean and autocorrelation of a stochastic process are defined as

$$\langle x(t) \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T/2}^{T/2} x(t) dt. \quad (6.17)$$

$$\langle x(t_2)x(t_1) \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x(t_2)x(t_1)p(x(t_1), x(t_2))dt_1 dt_2. \quad (6.18)$$

Note that most texts use a overbar $\bar{\cdot}$ to denote time-averaged quantities and sharp brackets $\langle \cdot \rangle$ to denote ensemble averages. We do not make this important distinction in our notation because we will assume ergodicity holds for what we will be discussing. When the process is stationary, the mean is independent of time and the autocorrelation only depends on the time-interval

$$\tau = t_2 - t_1,$$

$$\langle x(t) \rangle = \langle x \rangle, \quad (6.19)$$

$$\langle x(t_2)x(t_1) \rangle = \langle x(t+\tau)x(t) \rangle = \langle x(\tau)x(0) \rangle. \quad (6.20)$$

The autocorrelation $\langle x(t+\tau)x(t) \rangle$ and variance σ^2 of a stochastic process are related. They are given, for stationary processes, by

$$\sigma^2 \equiv \langle x^2 \rangle - \langle x \rangle^2, \quad (6.21)$$

$$\langle x^2 \rangle \equiv \lim_{\tau \rightarrow 0} \langle x(\tau)x(0) \rangle. \quad (6.22)$$

■ **Example 6.1 — Stationarity vs Ergodicity.** Consider a basket full of batteries. There are some flashlight batteries, some car batteries, and several other kinds of batteries. Suppose that a battery is selected at random and its voltage is measured. This battery voltage $V(t)$ is a member function selected from a certain sub-group of constant battery voltages. This process is stationary but not ergodic in the mean or correlation. The time average is equal to the particular battery voltage selected (say, 1.5V). The statistical average is some other number, depending on what is in the basket. ■

The power spectral density (PSD) $S(\omega)$ of a noisy signal $x(t)$ is a useful quantity that provides information about the “strength” of the noise, i.e. noise power, for each frequency interval. It has units of $[x^2]/\text{Hz}$. If the power of the signal is related to the absolute value square of the signal³, then the units of $S(\omega)$ is W/Hz. Because the PSD may range over several decades of interest, it is commonly converted to dB(W/Hz).

The Wiener-Khinchin-Einstein theorem⁴ is a useful theorem that states that the power spectral density and the noise autocorrelation are Fourier Transform pairs. Note that there are alternate forms of the Fourier Transform in different texts. Different forms of the Fourier Transform result in slightly different transform pairs so make sure that the same set of definitions of forward and inverse transforms are used, to be consistent.

Wiener-Khinchin-Einstein Theorem

Wiener–Khinchin–Einstein theorem states that the autocorrelation function of a wide-sense-stationary stochastic process has a spectral decomposition given by the power spectrum of that process. Each of these two quantities contain the same information about the process and are Fourier Transform pairs.

$$\text{autocorrelation function : } C(\tau) \equiv \langle x(t+\tau)x(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} S(\omega) e^{i\omega\tau} d\omega \quad (6.23)$$

$$\text{power spectral density : } S(\omega) = \int_{-\infty}^{\infty} \langle x(t+\tau)x(t) \rangle e^{-i\omega\tau} d\tau \quad (6.24)$$

The integral of the PSD over a given frequency band computes the total power in the signal over that frequency band. PSD can be specified as one-sided functions of only positive frequencies, or as two-sided functions of positive and negative frequencies, with the latter being half of the former, in order to give the same total power: $S_{\text{one-sided}}(\omega) = 2S_{\text{two-sided}}(\omega)$. One-sided noise PSD are used for real-valued processes because the negative frequencies are redundant.

For a stationary process $\langle x(t+\tau)x(t) \rangle$ is an even function and the PSD is real and even. Therefore, we have for a two-sided PSD,

$$S(\omega) = 2 \int_0^{\infty} \langle x(t+\tau)x(t) \rangle \cos(\omega t) d\tau \quad (6.25)$$

³i.e. $P = \lim_{T \rightarrow 0} \frac{1}{T} \int_{-T/2}^{T/2} |x(t)|^2 dt$.

⁴Albert Einstein explained without proof, the idea in a brief two-page memo in 1914; Norbert Wiener proved this theorem for the case of a deterministic function in 1930; Aleksandr Khinchin formulated an analogous result for stationary stochastic processes in 1934.

Note that some texts use a factor of 4 instead of 2. This is when they use the one-sided PSD. Either definition can be used in our course.

- **Example 6.2** Suppose a noisy waveform $x(t)$ is a statistically-stationary process, with an exponentially decaying autocorrelation function

$$\mathcal{C}_x(\tau) = \mathcal{C}_x(0)e^{-|\tau|/\tau_1}, \quad (6.26)$$

where τ_1 is a relaxation time constant associated with the system's memory time. Using the Wiener-Khinchin-Einstein theorem, show that the unilateral (one-sided) power spectral density is a Lorentzian function

$$S_x(\omega) = 4\mathcal{C}_x(0) \frac{\tau_1}{1 + \omega^2\tau_1^2}. \quad (6.27)$$

These are shown in Fig. 6.3.

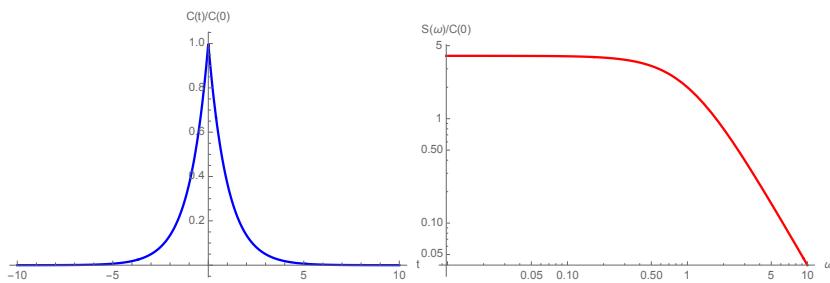


Figure 6.3: Example 6.2.

- **Example 6.3** Suppose a noisy waveform $x(t)$ experiences white (uniform) noise from a stationary stochastic process. The unilateral (one-sided) power spectral density is a constant,

$$S_x(\omega) = S_0. \quad (6.28)$$

Determine the autocorrelation function $\mathcal{C}(\tau)$.

6.4 Derivation II: Physically motivated arguments

In this section, we derive the Lindblad master equation using physically motivated arguments. Central to the arguments are the Born and Markov approximations.

Born approximation

The Born approximation assumes that the system-environment coupling is sufficiently weak, and the environment is reasonably large, such that changes of the density operator of the environment are negligible and the system-environment state remains in an approximate product state at all times, i.e.

$$\hat{\rho}(t) \approx \hat{\rho}_S(t) \otimes \hat{\rho}_E, \quad (6.29)$$

with $\hat{\rho}_E$ approximately constant at all times. Note that this does not imply that there are no excitations in the environment; we are simply only interested in sufficiently long time scales over which environmental excitations have already decayed (the Markovian approximation, below).

Markov approximation

The Markov approximation assumes that memory effects of the environment are negligible, in the sense that any self-correlations within the environment created by the coupling to the system decay rapidly compared to the characteristic timescale over which the state of the system varies noticeably.

We begin by writing the system-environment interaction in diagonal form as

$$\hat{H}_{\text{int}} = \hbar \sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha}, \quad (6.30)$$

where \hat{S}_{α} and \hat{E}_{α} are system and environment operators respectively. Here the system and environment operators are unitary but not necessarily Hermitian, e.g. in the Jaynes-Cummings interaction Hamiltonian of Eq. (3.53), σ_{\pm} , \hat{a} , \hat{a}^{\dagger} are not Hermitian but are unitary. If, however, \hat{S}_{α} are Hermitian, they correspond to physical observables of the system that are continuously monitored by the environment, and give rise to a preferred basis.

It will be shown next that the evolution of the reduced system density operator is given by the *Born-Markov* master equation,

$$\frac{d}{dt} \hat{\rho}_S(t) = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S] - \sum_{\alpha} \left([\hat{S}_{\alpha}, \hat{B}_{\alpha} \hat{\rho}_S(t)] + [\hat{\rho}_S(t) \hat{F}_{\alpha}, \hat{S}_{\alpha}] \right). \quad (6.31)$$

The system operators \hat{B}_{α} and \hat{C}_{α} are given by

$$\hat{B}_{\alpha} \equiv \int_0^{\infty} d\tau \sum_{\beta} \mathcal{C}_{\alpha\beta}(\tau) \hat{S}_{\beta}^{(I)}(-\tau), \quad (6.32)$$

$$\hat{F}_{\alpha} \equiv \int_0^{\infty} d\tau \sum_{\beta} \mathcal{C}_{\beta\alpha}(-\tau) \hat{S}_{\beta}^{(I)}(-\tau), \quad (6.33)$$

Here, the superscript (I) denotes the interaction picture version of the operator, and

$$\mathcal{C}_{\alpha\beta}(\tau) \equiv \langle \hat{E}_{\alpha}(\tau) \hat{E}_{\beta}(0) \rangle_{\hat{\rho}_E} \quad (6.34)$$

are the environment self-correlation functions. If the operators \hat{E}_{α} are Hermitian, they can also be thought of as observables “measured” on the environment by the interaction between the system and the environment. The environment self-correlation functions then tell us to what extent the result of such a “measurement” of a particular \hat{E}_{α} is correlated with the result of a “measurement” of the same observable carried out a time interval τ later.

Therefore, these environment self-correlation functions $\mathcal{C}_{\alpha\beta}(\tau)$ quantify to what degree the environment retains information over time about its interaction with the system. The Markov approximation corresponds to the assumption of a rapid decay of these environment self-correlation functions relative to the timescale set by the evolution of the system.

When, in addition to the Born and Markov assumptions, the *rotating wave approximation* (RWA) is also applied to Eq. (6.31), the Born-Markov master equation can be brought into the Lindblad master equation form. The RWA is justified whenever the typical timescale for the evolution of the system is short in comparison with the relaxation timescale of the system. We shall go through the details of these procedures next.⁵

⁵We make a note here that the details are unnecessary for the course assessment, but are helpful to the student in understanding the master equation in depth.

6.4.1 Interaction Picture Evolution

First, we write the total system-environment Hamiltonian in the usual form as

$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{H}_{\text{int}}, \quad (6.35)$$

$$\hat{H}_{\text{int}} = \hbar \sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha}. \quad (6.36)$$

Taking $\hat{H}_0 \equiv \hat{H}_S + \hat{H}_E$, we switch to the interaction picture, where the full system-environment density matrix evolves according to the von Neumann equation

$$\frac{d\hat{\rho}^{(I)}(t)}{dt} = -\frac{i}{\hbar} [\hat{H}_{\text{int}}^{(I)}(t), \hat{\rho}^{(I)}(t)], \quad (6.37)$$

with $\hat{\rho}^{(I)} = \hat{U}_0^{\dagger} \hat{\rho} \hat{U}_0$ and $\hat{H}_{\text{int}}^{(I)} = \hat{U}_0^{\dagger} \hat{H}_{\text{int}} \hat{U}_0$, where $\hat{U}_0 \equiv e^{-i\hat{H}_0 t/\hbar}$. (See Sections 1.4.3 and 3.5.2.) If we now formally integrate Eq. (6.37), we get

$$\hat{\rho}^{(I)}(t) = \hat{\rho}^{(I)}(0) - \frac{i}{\hbar} \int_0^t dt' [\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}^{(I)}(t')]. \quad (6.38)$$

Inserting this expression for $\hat{\rho}^{(I)}(t)$ back into the RHS of Eq. (6.37), we get

$$\begin{aligned} \frac{d\hat{\rho}^{(I)}(t)}{dt} &= -\frac{i}{\hbar} \left[\hat{H}_{\text{int}}^{(I)}(t), \left(\hat{\rho}^{(I)}(0) - \frac{i}{\hbar} \int_0^t dt' [\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}^{(I)}(t')] \right) \right] \\ &= -\frac{i}{\hbar} [\hat{H}_{\text{int}}^{(I)}(t), \hat{\rho}^{(I)}(0)] - \frac{1}{\hbar^2} \int_0^t dt' [\hat{H}_{\text{int}}^{(I)}(t), [\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}^{(I)}(t')]]. \end{aligned} \quad (6.39)$$

Now we can transform this equation into one involving the reduced density operator of the system by taking the trace over the environment.

$$\frac{d\hat{\rho}_S^{(I)}(t)}{dt} = -\frac{i}{\hbar} \text{Tr}_E [\hat{H}_{\text{int}}^{(I)}(t), \hat{\rho}^{(I)}(0)] - \frac{1}{\hbar^2} \int_0^t dt' \text{Tr}_E [\hat{H}_{\text{int}}^{(I)}(t), [\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}^{(I)}(t')]]. \quad (6.40)$$

Without loss of generality, one can assume that

$$\text{Tr}_E [\hat{H}_{\text{int}}^{(I)}(t), \hat{\rho}^{(I)}(0)] = 0. \quad (6.41)$$

This can always be achieved by a formal redefinition of the Hamiltonians \hat{H}_0 and \hat{H}_{int} . Let us assume the absence of initial correlations between the system and the environment,

$$\hat{\rho}(0) = \hat{\rho}^{(I)}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0). \quad (6.42)$$

Then,

$$\begin{aligned} \text{Tr}_E [\hat{H}_{\text{int}}^{(I)}(t), \hat{\rho}^{(I)}(0)] &= \hbar \sum_{\alpha} \hat{S}_{\alpha}^{(I)}(t) \hat{\rho}_S(0) \underbrace{\text{Tr}_E (\hat{E}_{\alpha}^{(I)}(t) \hat{\rho}_E(0))}_{\langle \hat{E}_{\alpha}(t) \rangle} - \hat{\rho}_S(0) \hat{S}_{\alpha}^{(I)}(t) \underbrace{\text{Tr}_E (\hat{\rho}_E(0) \hat{E}_{\alpha}^{(I)}(t))}_{\langle \hat{E}_{\alpha}(t) \rangle} \\ &= \hbar \sum_{\alpha} \langle \hat{E}_{\alpha}(t) \rangle [\hat{S}_{\alpha}^{(I)}(t), \hat{\rho}_S(0)]. \end{aligned} \quad (6.43)$$

This implies that if our total Hamiltonian does not fulfill the condition in Eq. (6.41), we can rewrite it in the following way so that $\langle \hat{E}_{\alpha}(t) \rangle = 0$, thus satisfying the condition.

$$\hat{H} = \underbrace{\left(\hat{H}_S + \sum_{\alpha} \langle \hat{E}_{\alpha} \rangle \hat{S}_{\alpha} \right)}_{\hat{H}'_S} + \hat{H}_E + \underbrace{\hbar \sum_{\alpha} \hat{S}_{\alpha} \otimes (\hat{E}_{\alpha} - \langle \hat{E}_{\alpha} \rangle)}_{\hat{H}'_{\text{int}}}. \quad (6.44)$$

This is a constant ‘shift’ in the interaction Hamiltonian, $\hat{E}_\alpha \rightarrow \hat{E}_\alpha - \langle \hat{E}_\alpha \rangle$, which manifests itself only through the bath correlation function. The system Hamiltonian is assumed to be changed by just the addition of an energy shift that does not affect the system dynamics.

Having shown that Eq. (6.41) can hold, Eq. (6.40) then simplifies into

$$\frac{d\hat{\rho}_S^{(I)}(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t dt' \text{Tr}_E \left[\hat{H}_{\text{int}}^{(I)}(t), \left[\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}^{(I)}(t') \right] \right]. \quad (6.45)$$

All calculations leading up to this equation have been exact and no approximations have been made. We note that the RHS of Eq. (6.45) depends on the total system-environment density operator $\hat{\rho}^{(I)}(t)$ to be evaluated at all times between 0 and t . Therefore, Eq. (6.45) is not yet a time-local differential equation that would determine the change of $\hat{\rho}_S^{(I)}$ at time t solely in terms of $\hat{\rho}_S^{(I)}(t)$ and a set of known quantities. We would like these desirable properties:

- (i) We would like to express our master equation entirely in terms of the reduced density operator $\hat{\rho}_S^{(I)}(t)$ and the initial state of the environment, i.e., we would like to eliminate any terms pertaining to a time-dependent state of the environment.
- (ii) We would like to eliminate any dependences of the change of $\hat{\rho}_S^{(I)}$ at time t on $\hat{\rho}_S^{(I)}$ evaluated at times $t' < t$.

To achieve these goals, we will need to apply the Born and Markov approximations. Imposing the Born approximation will eliminate the dependence on the full density operator on the RHS of Eq. (6.45), meeting the goal of point (i). The Markov approximation will transform the equation into a time-local differential equation, meeting the goal of point (ii).

6.4.2 Imposing the Born approximation

The Born approximation assumes that the system-environment interaction is weak. The physical intuition behind the Born approximation is that the interaction between the system and the environment is sufficiently weak (the so-called “weak-coupling limit”), and that the environment is large in comparison with the size of the system, such that (i) the density operator for the environment does not change significantly as a consequence of the interaction with the system, and that (ii) the system and the environment remain in a separable state at all times. Therefore, if the system and environment are uncorrelated initially, $\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0)$, we can say that

$$\hat{\rho}(t) \approx \hat{\rho}_S(t) \otimes \hat{\rho}_E(0), \quad \forall t \geq 0. \quad (6.46)$$

It turns out that the Born approximation is a reasonable assumption in many cases of physical interest. Usually, the system is coupled to a very large environment which, viewed as a whole, undergoes only negligibly small changes in the course of the system–environment interaction compared to the change of the state of the system. Of course, due to the interaction Hamiltonian, some correlations between system and environment are expected to appear. On the other hand, we may assume that the time scales of correlation and relaxation of the environment are much smaller than the typical system time scale, as the coupling strength is very small. Therefore, under this strong assumption, we can assume that the environment state is always in equilibrium and decoupled from the system state, for the timescale of interest to us – the system timescale.

Using the Born approximation Eq. (6.46), the master equation Eq. (6.45) becomes

$$\frac{d\hat{\rho}_S^{(I)}(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t dt' \text{Tr}_E \left[\hat{H}_{\text{int}}^{(I)}(t), \left[\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}_S^{(I)}(t') \otimes \hat{\rho}_E(0) \right] \right]. \quad (6.47)$$

6.4.3 Transforming into the frequency domain

To facilitate the application of the rotating wave approximation later, it is necessary to first go into the frequency domain. Expanding \hat{H}_S in its eigenbasis as $\hat{H}_S = \sum_a \varepsilon_a |\varepsilon_a\rangle \langle \varepsilon_a|$, we can write $\hat{U}_0(t) = e^{-i\hat{H}_S t/\hbar} = e^{-i\omega_a t} |\varepsilon_a\rangle \langle \varepsilon_a|$, where $\omega_a = \varepsilon_a/\hbar$. We can write the system operators in the interaction picture as

$$\hat{S}_\alpha^{(I)}(t) = \hat{U}_0^\dagger(t) \hat{S}_\alpha \hat{U}_0(t) = \sum_{a,b} e^{i(\omega_a - \omega_b)t} |\varepsilon_a\rangle \langle \varepsilon_a| \hat{S}_\alpha |\varepsilon_b\rangle \langle \varepsilon_b| = \sum_\omega \hat{S}_\alpha(\omega) e^{-i\omega t}, \quad (6.48)$$

where $\omega \equiv \omega_b - \omega_a$ and

$$\hat{S}_\alpha(\omega) \equiv \sum_{\omega_b - \omega_a = \omega} \langle \varepsilon_a | \hat{S}_\alpha | \varepsilon_b \rangle | \varepsilon_a \rangle \langle \varepsilon_b | = \hat{S}_\alpha^\dagger(-\omega), \quad (6.49)$$

where the last equality follows since Hermitian conjugation interchanges ε_a and ε_b . Also, since $\hat{S}_\alpha(t)$ is Hermitian,

$$\sum_\omega e^{-i\omega t} \hat{S}_\alpha(\omega) = \sum_\omega e^{i\omega t} \hat{S}_\alpha^\dagger(\omega). \quad (6.50)$$

The interaction Hamiltonian is Hermitian, and the system and environment operators commute since they act on different Hilbert spaces, so

$$\hat{H}_{\text{int}}^{(I)} = \hbar \sum_\alpha \hat{S}_\alpha^{(I)}(t) \hat{E}_\alpha^{(I)}(t) = \hbar \sum_\alpha \hat{S}_\alpha^{(I)\dagger}(t) \hat{E}_\alpha^{(I)\dagger}(t) \quad (6.51)$$

$$= \hbar \sum_{\alpha, \omega} e^{-i\omega t} \hat{S}_\alpha^{(I)}(\omega) \hat{E}_\alpha^{(I)}(t) = \hbar \sum_{\alpha, \omega} e^{i\omega t} \hat{S}_\alpha^{(I)\dagger}(\omega) \hat{E}_\alpha^{(I)\dagger}(t). \quad (6.52)$$

6.4.4 Imposing the Markov approximation

For notational ease, we now drop the superscripts (I) on the system and environment operators, with the understanding that they are interaction picture operators whenever we see the time or frequency arguments, i.e. (t) , (ω) . We leave the superscript on the density operator intact because we will transform it back to the Schrödinger picture later. Inserting the diagonal form of the interaction Hamiltonian into Eq. (6.47), we get

$$\begin{aligned} & \frac{d\hat{\rho}_S^{(I)}(t)}{dt} \\ &= - \int_0^t dt' \sum_{\alpha, \beta} \text{Tr}_E \left[\hat{S}_\alpha(t) \hat{E}_\alpha(t), \left[\hat{S}_\beta(t') \hat{E}_\beta(t'), \hat{\rho}_S^{(I)}(t') \otimes \hat{\rho}_E(0) \right] \right] \end{aligned} \quad (6.53)$$

$$= - \int_0^t dt' \sum_{\alpha, \beta} \left\{ \hat{S}_\alpha(t) \hat{S}_\beta(t') \hat{\rho}_S^{(I)}(t') \text{Tr}_E \left[\hat{E}_\alpha(t) \hat{E}_\beta(t') \hat{\rho}_E(0) \right] \right. \quad (6.54)$$

$$- \hat{S}_\alpha(t) \hat{\rho}_S^{(I)}(t') \hat{S}_\beta(t') \text{Tr}_E \left[\hat{E}_\alpha(t) \hat{\rho}_E(0) \hat{E}_\beta(t') \right] \quad (6.55)$$

$$+ \hat{\rho}_S^{(I)}(t') \hat{S}_\beta(t') \hat{S}_\alpha(t) \text{Tr}_E \left[\hat{\rho}_E(0) \hat{E}_\beta(t') \hat{E}_\alpha(t) \right] \quad (6.56)$$

$$\left. - \hat{S}_\beta(t') \hat{\rho}_S^{(I)}(t') \hat{S}_\alpha(t) \text{Tr}_E \left[\hat{E}_\beta(t') \hat{\rho}_E(0) \hat{E}_\alpha(t) \right] \right\}. \quad (6.57)$$

Here, we note that lines (6.54) and (6.56) are Hermitian conjugates of each other, as are lines (6.55) and (6.57). Further, the trace over the environment can be defined as

$$\mathcal{C}_{\alpha\beta}(t, t') \equiv \text{Tr}_E \left(\hat{E}_\alpha(t) \hat{E}_\beta(t') \hat{\rho}_E(0) \right) = \langle \hat{E}_\alpha(t) \hat{E}_\beta(t') \rangle_{\hat{\rho}_E}. \quad (6.58)$$

Assuming the environment is stationary (i.e. $\hat{\rho}_E$ commutes with \hat{H}_E),

$$\begin{aligned} \mathcal{C}_{\alpha\beta}(t, t') &= \text{Tr}_E \left(e^{i\hat{H}_E t/\hbar} \hat{E}_\alpha(0) e^{-i\hat{H}_E t/\hbar} e^{i\hat{H}_E t'/\hbar} \hat{E}_\beta(0) \underbrace{e^{-i\hat{H}_E t'/\hbar} \hat{\rho}_E(0)}_{\text{commutes}} \right) \\ &= \text{Tr}_E \left(e^{i\hat{H}_E t/\hbar} \hat{E}_\alpha(0) e^{-i\hat{H}_E t/\hbar} e^{i\hat{H}_E t'/\hbar} \hat{E}_\beta(0) \hat{\rho}_E(0) e^{-i\hat{H}_E t'/\hbar} \right) \\ &= \text{Tr}_E \left(\underbrace{e^{-i\hat{H}_E t'/\hbar} e^{i\hat{H}_E t/\hbar}}_{\text{from cyclic property}} \hat{E}_\alpha(0) e^{-i\hat{H}_E t/\hbar} e^{i\hat{H}_E t'/\hbar} \hat{E}_\beta(0) \hat{\rho}_E(0) \right) \\ &= \langle \hat{E}_\alpha(t - t') \hat{E}_\beta(0) \rangle_{\hat{\rho}_E} \\ &\equiv \mathcal{C}_{\alpha\beta}(\tau). \end{aligned} \quad (6.59)$$

where $\tau \equiv t - t'$, i.e. we implicitly associate time τ with the first index (α), whereas the second index (β) is associated with time = 0. Assuming a stationary bath, only the time difference τ matters, therefore in the last line, only the time difference argument remains. We also have

$$\mathcal{C}_{\beta\alpha}^*(\tau) = \langle \hat{E}_\beta(\tau) \hat{E}_\alpha(0) \rangle_{\hat{\rho}_E}^* = \langle (\hat{E}_\beta(\tau) \hat{E}_\alpha(0))^\dagger \rangle_{\hat{\rho}_E} = \langle \hat{E}_\alpha(0) \hat{E}_\beta(\tau) \rangle_{\hat{\rho}_E} = \mathcal{C}_{\alpha\beta}(-\tau). \quad (6.60)$$

We see that the environment auto-correlation or self-correlation functions depend only on the time interval between the results of the two identical “measurements” on the environment, represented by a particular operator \hat{E}_α . Note that the auto-correlation function $\mathcal{C}_{\alpha\beta}(\tau)$ is complex. You cannot directly measure a quantum correlation function, but observables are often related to the real or imaginary part of correlation functions, or other combinations of correlation functions.

Inserting this into Eq. (6.53), and noting that the second set of terms are Hermitian conjugate pairs with the first set, we get

$$\begin{aligned} \frac{d\hat{\rho}_S^{(I)}(t)}{dt} &= - \int_0^t dt' \sum_{\alpha,\beta} \left\{ \mathcal{C}_{\alpha\beta}(t-t') \left[\hat{S}_\alpha(t) \hat{S}_\beta(t') \hat{\rho}_S^{(I)}(t') - \hat{S}_\beta(t') \hat{\rho}_S^{(I)}(t') \hat{S}_\alpha(t) \right] \right. \\ &\quad \left. + \underbrace{\mathcal{C}_{\beta\alpha}^*(t-t')}_{\mathcal{C}_{\alpha\beta}^*(t-t')} \left[\hat{\rho}_S^{(I)}(t') \hat{S}_\beta(t') \hat{S}_\alpha(t) - \hat{S}_\alpha(t) \hat{\rho}_S^{(I)}(t') \hat{S}_\beta(t') \right] \right\}. \end{aligned} \quad (6.61)$$

$$= - \int_0^t dt' \sum_{\alpha,\beta} \left\{ \mathcal{C}_{\alpha\beta}(t-t') \left[\hat{S}_\alpha(t) \hat{S}_\beta(t') \hat{\rho}_S^{(I)}(t') - \hat{S}_\beta(t') \hat{\rho}_S^{(I)}(t') \hat{S}_\alpha(t) \right] + \text{h.c.} \right\} \quad (6.62)$$

Eq. (6.62) is known as the *Redfield* equation. It is notoriously non-CP, which means that the density matrix can become non-positive. To fix this, we can impose the Markov approximation. It turns out that in many physical situation of interest, the environment can be assumed to very quickly “forget” any internal self-correlations that have been established in the course of the interaction with the system: any dynamically established quantum correlations between parts of the environment are destroyed on a timescale τ_{env} much shorter than the characteristic timescale τ_{sys} over which the reduced interaction-picture density operator $\hat{\rho}_S^{(I)}$ of the system changes noticeably. This assumption $\tau_{\text{sys}} \gg \tau_{\text{env}}$ constitutes the Markov approximation.

In other words, the environment self-correlations functions $\mathcal{C}_{\alpha\beta}(\tau)$ are sharply peaked around $\tau \equiv t - t' = 0$ and decay on a timescale much shorter than the timescale set by τ_{sys} . It allows us to extend the lower limit of the integration on the RHS of Eq. (6.61) to $-\infty$, since the self-correlation functions (and thus the integrand) vanish for $t' \ll t$, i.e. the integrand is effectively zero over the extended integration range. Taking the extended integration range is only valid if the environment self-correlations functions are exponentially decaying, $|\mathcal{C}_{\alpha\beta}(\tau)| \sim e^{-(\tau/\tau_{\text{env}})^k}$ for $k > 0$. Also, the reduced interaction-picture density operator $\hat{\rho}_S^{(I)}$ of the system changes only insignificantly during the typical time interval over which the environment self-correlations functions $\mathcal{C}_{\alpha\beta}(\tau)$ vanish, we can replace the retarded-time density operator by the current-time density operator. Therefore, by performing the following steps

- (i) Replace retarded-time density operator with current-time density operator:
 $\hat{\rho}_S^{(I)}(t') \rightarrow \hat{\rho}_S^{(I)}(t),$
- (ii) Substituting $t' = t - \tau$,
- (iii) Taking $\int_0^t dt' \rightarrow \int_{-\infty}^t dt' = \int_{\infty}^0 d(-\tau) = \int_0^{\infty} d\tau,$

we get

$$\begin{aligned} \frac{d\hat{\rho}_S^{(I)}(t)}{dt} &= \\ &- \int_0^{\infty} d\tau \sum_{\alpha,\beta} \left\{ \mathcal{C}_{\alpha\beta}(\tau) \left[\hat{S}_\alpha(t) \hat{S}_\beta(t-\tau) \hat{\rho}_S^{(I)}(t) - \hat{S}_\beta(t-\tau) \hat{\rho}_S^{(I)}(t) \hat{S}_\alpha(t) \right] + \text{h.c.} \right\} \end{aligned} \quad (6.63)$$

Finally, we have the following properties of this master equation.

- (i) The RHS of this master equation no longer depends on the full time-dependent density operator $\hat{\rho}^{(I)}(t)$, but only on the reduced density operator $\hat{\rho}_S^{(I)}(t)$, of the system and the initial state of the environment $\hat{\rho}_E(0)$.
- (ii) The initial state of the environment enters through the self-correlation functions $\mathcal{C}_{\alpha\beta}(\tau)$.
- (iii) The master equation is local in time.
- (iv) Only completely known quantities, namely the operators $\hat{S}_\alpha(t)$ and $\hat{E}_\alpha(t)$ (which are determined a priori by the form of the Hamiltonian), enter into the master equation with time arguments other than t .

6.4.5 Applying the Rotating Wave Approximation

Now, we consider the terms in the brackets in Eq. (6.63) and write them in terms of the eigendecomposition of Eq. (6.48), (6.50):

$$\hat{S}_\alpha(t)\hat{S}_\beta(t-\tau)\hat{\rho}_S^{(I)}(t) = \sum_{\omega,\omega'} e^{i\omega\tau} e^{i(\omega'-\omega)t} \hat{S}_\alpha^\dagger(\omega') \hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t), \quad (6.64)$$

$$\hat{S}_\beta(t-\tau)\hat{\rho}_S^{(I)}(t)\hat{S}_\alpha(t) = \sum_{\omega,\omega'} e^{i\omega\tau} e^{i(\omega'-\omega)t} \hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t) \hat{S}_\alpha^\dagger(\omega'). \quad (6.65)$$

The entire τ -dependence is thus in the factor $e^{i\omega\tau}$. We collect all τ -dependent terms,

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty d\tau \mathcal{C}_{\alpha\beta}(\tau) e^{i\omega\tau}, \quad (6.66)$$

$$\Gamma_{\beta\alpha}^*(\omega) = \int_0^\infty d\tau \mathcal{C}_{\beta\alpha}^*(\tau) e^{-i\omega\tau} = \int_0^\infty d\tau \mathcal{C}_{\alpha\beta}(-\tau) e^{-i\omega\tau} = \int_{-\infty}^0 d\tau \mathcal{C}_{\alpha\beta}(\tau) e^{i\omega\tau}. \quad (6.67)$$

This is the one-sided Fourier transform of the environment self-correlation functions, which gives us the power spectral density of the environment, by the Wiener-Khinchin-Einstein theorem.⁶ In general, $\Gamma_{\alpha\beta}(\omega)$ is a complex function.

We can write the master equation now as

$$\frac{d\hat{\rho}_S^{(I)}(t)}{dt} = - \sum_{\alpha,\beta} \sum_{\omega,\omega'} \left\{ \Gamma_{\alpha\beta}(\omega) e^{i(\omega-\omega')t} [\hat{S}_\alpha^\dagger(\omega'), \hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t)] \right\} + \text{h.c.} \quad (6.68)$$

Note that \hat{S} and \hat{E} each have units of $\sqrt{\text{frequency}}$, and Γ is dimensionless. The rotating wave approximation, also known as secular approximation, can now be applied. This approximation is based on the idea that the terms with $\omega \neq \omega'$ in Eq. (6.68) are rapidly oscillating if $|\omega - \omega'|t \gg 1$. These fast oscillations average to zero and do not contribute significantly to the evolution of the system. We can then consider that only the resonant terms, $\omega = \omega'$, contribute to the dynamics and remove all the others. Eq. (6.68) then reduces to

$$\frac{d\hat{\rho}_S^{(I)}(t)}{dt} = - \sum_{\alpha,\beta} \sum_{\omega} \left\{ \Gamma_{\alpha\beta}(\omega) [\hat{S}_\alpha^\dagger(\omega), \hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t)] + \Gamma_{\beta\alpha}^*(\omega) [\hat{\rho}_S^{(I)}(t) \hat{S}_\alpha^\dagger(\omega), \hat{S}_\beta(\omega)] \right\}. \quad (6.69)$$

First, we define the *full* Fourier transform of the environment self-correlation function, i.e. the full power spectral density of the environment, as

$$\gamma_{\alpha\beta}(\omega) \equiv \int_{-\infty}^\infty d\tau e^{i\omega\tau} \mathcal{C}_{\alpha\beta}(\tau) = \Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega). \quad (6.70)$$

The inverse transform is then

$$\mathcal{C}_{\alpha\beta}(\tau) = \frac{1}{2\pi} \int_{-\infty}^\infty d\omega e^{-i\omega'\tau} \gamma_{\alpha\beta}(\omega'). \quad (6.71)$$

⁶Note that the difference in the sign of the exponent in Eq. (6.66) vs that in the theorem, Eq. (6.24), is a matter of convention. The physical meaning remains unchanged.

Using Eq. (6.60), we show that $\gamma(\omega)$ is a Hermitian matrix:

$$\gamma_{\alpha\beta}^*(\omega) = \int_{-\infty}^{\infty} d\tau e^{-i\omega\tau} \mathcal{C}_{\alpha\beta}^*(\tau) = \int_{-\infty}^{\infty} d\tau e^{-i\omega\tau} \mathcal{C}_{\beta\alpha}(-\tau) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \mathcal{C}_{\beta\alpha}(\tau) = \gamma_{\beta\alpha}(\omega). \quad (6.72)$$

To divide the dynamics into unitary and non-unitary parts, we now decompose the operators $\Gamma_{\alpha\beta}(\omega)$ into Hermitian and anti-Hermitian parts,

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2} \gamma_{\alpha\beta}(\omega) + i\pi_{\alpha\beta}(\omega), \quad (6.73)$$

where the anti-Hermitian part⁷ is given by

$$\pi_{\alpha\beta}(\omega) \equiv -\frac{i}{2} (\Gamma_{\alpha\beta}(\omega) - \Gamma_{\alpha\beta}^*(\omega)). \quad (6.74)$$

By these definitions, we can separate the Hermitian and non-Hermitian parts of the dynamics and obtain the Lamb shift.

6.4.6 Lamb Shift

Putting Eq. (6.73) into Eq. (6.69),

$$\begin{aligned} \frac{d\hat{\rho}_S^{(I)}(t)}{dt} &= - \sum_{\alpha,\beta} \sum_{\omega} \left\{ \left(\frac{1}{2} \gamma_{\alpha\beta}(\omega) + i\pi_{\alpha\beta}(\omega) \right) [\hat{S}_\alpha^\dagger(\omega), \hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t)] \right. \\ &\quad \left. + \left(\frac{1}{2} \gamma_{\alpha\beta}(\omega) - i\pi_{\alpha\beta}(\omega) \right) [\hat{\rho}_S^{(I)}(t) \hat{S}_\alpha^\dagger(\omega), \hat{S}_\beta(\omega)] \right\} \\ &= -i \sum_{\alpha,\beta} \sum_{\omega} \pi_{\alpha\beta}(\omega) [\hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega), \hat{\rho}_S^{(I)}(t)] \\ &\quad + \sum_{\alpha,\beta} \sum_{\omega} \gamma_{\alpha\beta}(\omega) \left(\hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t) \hat{S}_\alpha^\dagger(\omega) - \frac{1}{2} \left\{ \hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega), \hat{\rho}_S^{(I)}(t) \right\} \right). \end{aligned} \quad (6.75)$$

Defining the Lamb shift Hamiltonian,⁸

$$\hat{H}_{LS} \equiv \hbar \sum_{\alpha,\beta} \sum_{\omega} \pi_{\alpha\beta}(\omega) \hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega), \quad (6.76)$$

we then have the interaction picture master equation

$$\begin{aligned} \frac{d\hat{\rho}_S^{(I)}(t)}{dt} &= -\frac{i}{\hbar} [\hat{H}_{LS}, \hat{\rho}_S^{(I)}(t)] + \sum_{\alpha,\beta} \sum_{\omega} \gamma_{\alpha\beta}(\omega) \left(\hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t) \hat{S}_\alpha^\dagger(\omega) - \frac{1}{2} \left\{ \hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega), \hat{\rho}_S^{(I)}(t) \right\} \right). \end{aligned} \quad (6.77)$$

It can also be shown that

$$[\hat{H}_{LS}, \hat{H}_S] = 0. \quad (6.78)$$

6.4.7 Transforming back to the Schrödinger Picture

To transform back to the Schrödinger picture, we note that $\hat{\rho}_S^{(I)}(t) = e^{i\hat{H}_{ST}/\hbar} \hat{\rho}_S(t) e^{-i\hat{H}_{ST}/\hbar}$, so

$$\begin{aligned} \frac{d}{dt} \hat{\rho}_S^{(I)}(t) &= \frac{d}{dt} (e^{i\hat{H}_{ST}/\hbar} \hat{\rho}_S(t) e^{-i\hat{H}_{ST}/\hbar}) = \frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S^{(I)}(t)] + e^{i\hat{H}_{ST}/\hbar} \left(\frac{d}{dt} \hat{\rho}_S(t) \right) e^{-i\hat{H}_{ST}/\hbar} \\ \implies \frac{d}{dt} \hat{\rho}_S(t) &= -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S(t)] + e^{-i\hat{H}_{ST}/\hbar} \left(\frac{d}{dt} \hat{\rho}_S^{(I)}(t) \right) e^{i\hat{H}_{ST}/\hbar}. \end{aligned} \quad (6.79)$$

⁷We have assumed, but not shown that $\pi(\omega)$ is Hermitian, i.e. $\pi_{\alpha\beta}(\omega) = \pi_{\beta\alpha}^*(\omega)$. Lidar's detailed derivations, specifically Eqs. (530–534) show this result. In that derivation he uses S in place of π .

⁸To justify calling \hat{H}_{LS} a Hamiltonian, we should show that it is Hermitian.

Next, we will insert the expression for $\frac{d}{dt}\hat{\rho}_S^{(I)}(t)$ in Eq. (6.77) into Eq. (6.79). The algebraic manipulation can be tedious, so we note here that when terms like the following are encountered, they lead to

$$\begin{aligned} & e^{-i\hat{H}_{ST}/\hbar} \hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t) e^{i\hat{H}_{ST}/\hbar} \\ &= \sum_{\omega_b - \omega_a = \omega} \sum_{\omega_d - \omega_c = \omega} \langle \varepsilon_a | \hat{S}_\alpha^\dagger | \varepsilon_b \rangle \langle \varepsilon_c | \hat{S}_\beta | \varepsilon_d \rangle e^{-i\hat{H}_{ST}/\hbar} |\varepsilon_a\rangle \langle \varepsilon_b | \varepsilon_c \rangle \langle \varepsilon_d | e^{i\hat{H}_{ST}/\hbar} \hat{\rho}_S(t) e^{-i\hat{H}_{ST}/\hbar} e^{i\hat{H}_{ST}/\hbar} \\ &= \sum_{\omega_b - \omega_a = \omega} \sum_{\omega_d - \omega_c = \omega} \langle \varepsilon_b | \hat{S}_\alpha^\dagger | \varepsilon_a \rangle \langle \varepsilon_a | \hat{S}_\beta | \varepsilon_b \rangle e^{-i\omega_a t} |\varepsilon_a\rangle \langle \varepsilon_b | \varepsilon_c \rangle \langle \varepsilon_d | e^{i\omega_d t} \hat{\rho}_S(t) \\ &= \sum_{\omega_b - \omega_a = \omega} \sum_{\omega_d - \omega_c = \omega} \langle \varepsilon_b | \hat{S}_\alpha^\dagger | \varepsilon_a \rangle \langle \varepsilon_a | \hat{S}_\beta | \varepsilon_b \rangle e^{-i\omega_a t} |\varepsilon_a\rangle e^{i\omega_b t} \delta_{bc} e^{-i\omega_c t} \langle \varepsilon_d | e^{i\omega_d t} \hat{\rho}_S(t) \\ &= \hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega) \hat{\rho}_S(t). \end{aligned} \quad (6.80)$$

Similarly,

$$e^{-i\hat{H}_{ST}/\hbar} \hat{S}_\alpha^\dagger(\omega) \hat{\rho}_S^{(I)}(t) \hat{S}_\beta(\omega) e^{i\hat{H}_{ST}/\hbar} = \hat{S}_\alpha^\dagger(\omega) \hat{\rho}_S(t) \hat{S}_\beta(\omega), \quad (6.81)$$

This gives us

$$\begin{aligned} & e^{-i\hat{H}_{ST}/\hbar} \left(\hat{S}_\beta(\omega) \hat{\rho}_S^{(I)}(t) \hat{S}_\alpha^\dagger(\omega) - \frac{1}{2} \left\{ \hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega), \hat{\rho}_S^{(I)}(t) \right\} \right) e^{i\hat{H}_{ST}/\hbar} \\ &= \hat{S}_\beta(\omega) \hat{\rho}_S(t) \hat{S}_\alpha^\dagger(\omega) - \frac{1}{2} \left\{ \hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega), \hat{\rho}_S(t) \right\}. \end{aligned} \quad (6.82)$$

Since \hat{H}_S and \hat{H}_{LS} commute (Eq. (6.78)),

$$e^{-i\hat{H}_{ST}/\hbar} [\hat{H}_{LS}, \hat{\rho}_S^{(I)}(t)] e^{i\hat{H}_{ST}/\hbar} = [\hat{H}_{LS}, \hat{\rho}_S(t)]. \quad (6.83)$$

6.4.8 The Lindblad Master Equation in Schrödinger Picture

Thus, after much hard work, we obtain the master equation in Schrödinger Picture,

$$\begin{aligned} & \frac{d\hat{\rho}_S(t)}{dt} \\ &= -\frac{i}{\hbar} [\hat{H}_S + \hat{H}_{LS}, \hat{\rho}_S(t)] + \sum_{\alpha, \beta} \sum_{\omega} \gamma_{\alpha\beta}(\omega) \left(\hat{S}_\beta(\omega) \hat{\rho}_S(t) \hat{S}_\alpha^\dagger(\omega) - \frac{1}{2} \left\{ \hat{S}_\alpha^\dagger(\omega) \hat{S}_\beta(\omega), \hat{\rho}_S(t) \right\} \right). \end{aligned} \quad (6.84)$$

We note that for complete positivity, $\gamma(\omega) > 0$, i.e. all its eigenvalues γ_j are greater than zero. This also means that it can be diagonalized, and we can write the Lindblad master equation in the Schrödinger Picture, in diagonal form,

$$\begin{aligned} & \frac{d\hat{\rho}_S(t)}{dt} \\ &= -\frac{i}{\hbar} [\underbrace{\hat{H}_S + \hat{H}_{LS}}_{\equiv \hat{H}'_S}, \hat{\rho}_S(t)] + \sum_j \gamma_j(\omega) \left(\hat{L}'_j(\omega) \hat{\rho}_S(t) \hat{L}'_j^\dagger(\omega) - \frac{1}{2} \left\{ \hat{L}'_j^\dagger(\omega) \hat{L}'_j(\omega), \hat{\rho}_S(t) \right\} \right). \end{aligned} \quad (6.85)$$

Subsuming $\sqrt{\gamma_j}$ into each Lindblad jump operator \hat{L}'_j , i.e. $\hat{L}_j \equiv \sqrt{\gamma_j} \hat{L}'_j$, and dropping the ω arguments, we finally have the master equation as we had written right at the start of the chapter, in Eq. (6.1):

$$\frac{d\hat{\rho}_S(t)}{dt} = -\frac{i}{\hbar} [\hat{H}'_S, \hat{\rho}_S(t)] + \sum_j \left(\hat{L}_j \hat{\rho}_S(t) \hat{L}_j^\dagger - \frac{1}{2} \left\{ \hat{L}_j^\dagger \hat{L}_j, \hat{\rho}_S(t) \right\} \right). \quad (6.86)$$

We summarise this derivation with a chart in Fig. 6.4.

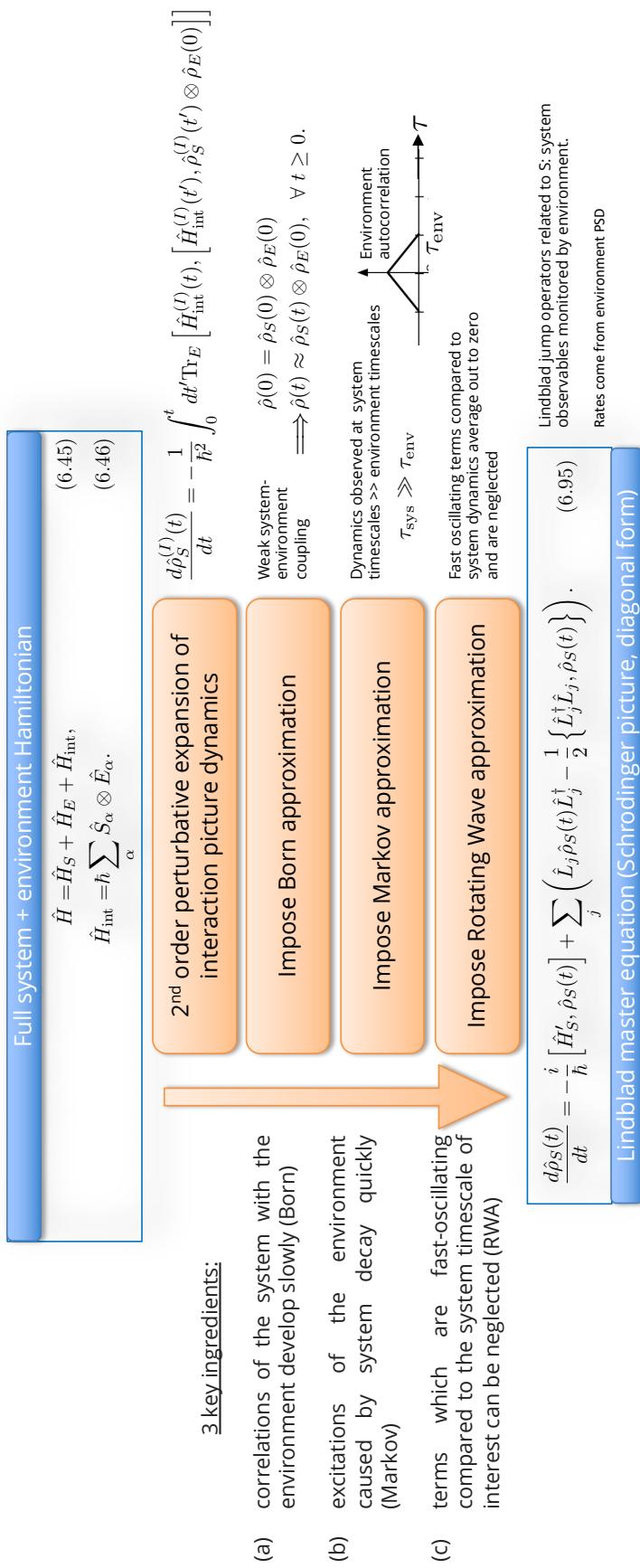


Figure 6.4: Overview of key ingredients in the derivation of the Lindblad master equation, from physically motivated arguments.

6.5 References

1. Lecture 8 of MIT OpenCourseWare 22-51 “Quantum theory of radiation interactions” presents a very readable derivation of the Lindblad master equation. http://ocw.mit.edu/courses/nuclear-engineering/22-51-quantum-theory-of-radiation-interactions-fall-2012/lecture-notes/MIT22_51F12_Ch8.pdf
2. Derivation from CPTP map:
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 - Daniel Manzano, *A short introduction to the Lindblad master equation*, AIP Advances 10, 025106 (2020). <https://doi.org/10.1063/1.5115323>
4. Stochastic Processes:
 - Yoshihisa Yamamoto’s lecture notes “*Fundamentals of Noise processes*”.
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6.6 Discussion Set

Lindblad Master Equation

Problem 6.1 — Phase damping for a single qubit. In this problem, you will study a Lindblad equation model that generates the dynamics of the phase damping map. Take $\hat{H}_S = 0$, so that we see purely the effect of the Lindblad operator. In this model, there is only one Lindblad jump operator, $\hat{L} = \sqrt{\gamma}\hat{\sigma}_z$.

- (i) Derive the differential equation that describe the evolution of the density matrix.
- (ii) If the qubit was initially in a state $\hat{\rho}(0) = \frac{1}{2}(\hat{\mathbb{I}} + \vec{v}(0) \cdot \hat{\sigma})$, derive the Bloch vector components $\vec{v}(t)$ as a function of time.
- (iii) Hence, show that the Bloch sphere collapses to the z -axis exponentially fast with rate 2γ .

Problem 6.2 — Amplitude damping for a single qubit. In this problem, you will construct a Lindblad master equation for amplitude damping. Let the single Lindblad operator be $\hat{L} = \sqrt{\gamma}|0\rangle\langle 1| \equiv \sqrt{\gamma}\hat{\sigma}_-$, and take $\hat{H}_S = 0$. Note that $\hat{\sigma}_-^\dagger = \hat{\sigma}_+ = |1\rangle\langle 0|$.

- (i) Derive the differential equation that describe the evolution of the density matrix.
- (ii) If the qubit was initially in a state $\hat{\rho}(0) = \frac{1}{2}(\hat{\mathbb{I}} + \vec{v}(0) \cdot \hat{\sigma})$, derive the Bloch vector components $\vec{v}(t)$ as a function of time.
- (iii) Hence, describe the Bloch sphere evolution in terms of two rates γ and $\gamma/2$.

Problem 6.3 — Damped harmonic oscillator. Consider the case of a harmonic oscillator coupled to the electromagnetic field environment in such a way: (i) the environment is at zero temperature; (ii) the excitation level of the oscillator can cascade down by successive emission of photons, but no absorption of photons will occur.

- (i) When each photon is emitted, at rate Γ , it never interacts again with the oscillator. The evolution is thus Markovian. Write down the single Lindblad jump operator for the system.
- (ii) The harmonic oscillator Hamiltonian is $\hat{H}_S = \hbar\omega(\hat{a}^\dagger\hat{a})$. (It is customary to drop the factor $1/2$ since it corresponds to a redefinition of zero energy.) Write down the Schrödinger-picture master equation in the Lindblad form.
- (iii) If the harmonic oscillator is initially in a Fock state $\hat{\rho}(0) = |N\rangle\langle N|$ where $N = 2$, and $|n\rangle$ is an eigenstate (called Fock state) of the number operator $\hat{n} \equiv \hat{a}^\dagger\hat{a}$, solve the Lindblad equation for the density operator at a later time, $\hat{\rho}(t)$.

Problem 6.4 — Quantum dot transport. Consider a potential well formed in a semiconductor quantum dot. This is the system; it can contain 0 or 1 electron; these states are termed $|0\rangle$ and $|1\rangle$. The environment comprises the left and right leads of the quantum dot. Each lead contains non-interacting electrons in the semiconductor Fermi sea. The Hamiltonian of the quantum dot system in the $\{|0\rangle, |1\rangle\}$ basis is

$$\hat{H} = \begin{pmatrix} 0 & 0 \\ 0 & \Omega \end{pmatrix}. \quad (6.87)$$

Tunneling of an electron between the quantum dot and the leads changes the quantum dot state, and are modelled as Lindblad jump operators. Write down the following Lindblad jump operators in Dirac bra-ket notation.

- (i) \hat{L}_{L1} , corresponding to the tunneling of an electron from the left lead *into* the quantum dot at rate $\Gamma_L f_L(E)$.
- (ii) \hat{L}_{R1} , corresponding to the tunneling of an electron from the quantum dot *out to* the right lead at rate $\Gamma_R(1 - f_R(E))$.
- (iii) \hat{L}_{L2} , corresponding to the tunneling of an electron from the quantum dot *out to* the left lead at rate $\Gamma_L(1 - f_L(E))$.
- (iv) \hat{L}_{R2} , corresponding to the tunneling of an electron from the right lead *into* the quantum dot at rate $\Gamma_R f_R(E)$.

The Fermi-Dirac distributions are $f_L(E) = (1 + e^{(E-\mu_L)/k_B T})^{-1}$ and $f_R(E) = (1 + e^{(E-\mu_R)/k_B T})^{-1}$. For this problem, take $\mu_R < \Omega < \mu_L$.

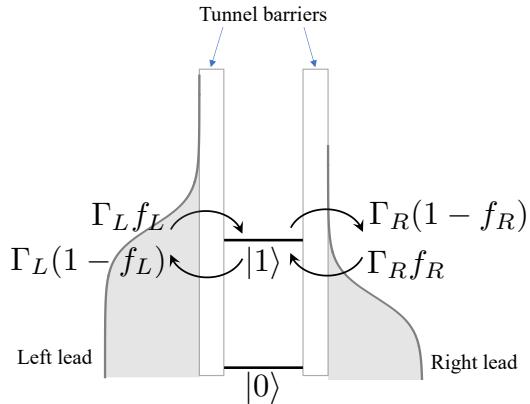


Figure 6.5: Problem 6.4.

- (i) Given that there are no coherences between the $|0\rangle$ and $|1\rangle$ states, i.e. $\rho_{01} = \rho_{10} = 0$, solve the Lindblad master equation for the steady state quantum dot populations, $\bar{\rho}_{00}$ and $\bar{\rho}_{11}$ in the limits of (a) zero temperature, $T = 0$.
- (ii) Does your answer make sense in the limit of $\Gamma_R \gg \Gamma_L$?

Problem 6.5 — Bosonic environment self-correlation. A bosonic environment of quantum harmonic oscillators (e.g. photons or phonons) “monitors” the position of a single particle via the interaction Hamiltonian

$$\hat{H}_{\text{int}} = \hat{x} \otimes \sum_i c_i \hat{q}_i \equiv \hat{x} \otimes \hat{E}, \quad (6.88)$$

where \hat{x} is the position operator for the particle, i is an index running over the environment modes, $\hat{q}_i \equiv \sqrt{\frac{\hbar}{2m_i\omega_i}}(\hat{a}_i + \hat{a}_i^\dagger)$ is the position operator for each bosonic mode, c_i is the coupling strength, and $\hat{E} \equiv \sum_i c_i (\hat{a}_i + \hat{a}_i^\dagger)$. The standard commutation relations hold, $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$. Each mode i of the environment is independent and does not interact with another mode $j \neq i$. The environment is in thermal equilibrium at temperature T and obeys Bose-Einstein statistics such that the mean occupation number of each mode i is given by $\langle \hat{n}_i \rangle_{\hat{\rho}_E} = (e^{\hbar\omega_i/k_B T} - 1)^{-1}$.

- (i) Write down the time evolution of $\hat{q}_i(\tau)$ in the interaction picture, given that the environment Hamiltonian is $\hat{H}_E = \sum_i \hat{a}_i^\dagger \hat{a}_i (\hbar\omega_i + 1/2)$.
- (ii) Show that the environment self-correlation function is

$$\mathcal{C}(\tau) \equiv \langle \hat{E}(\tau) \hat{E} \rangle_{\hat{\rho}_E} = \sum_i \frac{c_i}{2m_i\omega_i} \left(\coth\left(\frac{\hbar\omega_i}{k_B T}\right) \cos(\omega_i \tau) - i \sin(\omega_i \tau) \right). \quad (6.89)$$

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