This is a really powerful result: *any trace-preserving Liouvillian must have a zero eigenvalue. Its right eigenvector will be the steady-state of the equation, whereas the left eigenvector will be the identity.* Of course, a more subtle question is whether this steady-state is unique. That is, whether the eigenvalue 0 is degenerate or not. I would say quite often the steady-state is unique, but unfortunately this really depends on the problem in question.

Let us now return to the general solution (4.90). Using the diagonal decomposition (4.95) we get

$$\rho(t) = \sum_{\alpha} e^{\lambda_{\alpha} t} x_{\alpha} \Big[ y_{\alpha}^{\dagger} \operatorname{vec}(\rho(0)) \Big] = \sum_{\alpha} c_{\alpha} e^{\lambda_{\alpha} t} x_{\alpha}, \qquad (4.98)$$

where  $c_{\alpha} = y_{\alpha}^{\dagger} \operatorname{vec}(\rho(0))$  are just coefficients related to the initial conditions (you may see a similarity here with the usual solution of Schrödinger's equation). From this result we also arrive at another important property of Liouvillians: *the eigenvalues must always have a non-positive real part*. That is to say, either  $\lambda_{\alpha} = 0$  or  $\operatorname{Re}(\lambda_{\alpha}) < 0$ . Otherwise, the exponentials would blow up, which would be unphysical.

As an example, the Liouvillian in Eq. (4.89) has eigenvalues

$$\operatorname{eigs}(\hat{\mathcal{D}}) = \left\{-\gamma, -\frac{\gamma}{2}, -\frac{\gamma}{2}, 0\right\}.$$
(4.99)

In this case they turn out to be real. But if we also add a unitary term, then they will in general be complex. Notwithstanding their real part will always be non-positive.

Assume now that the zero eigenstate is unique. Then we can write Eq. (4.98) as

$$\rho(t) = c_0 \boldsymbol{x}_0 + \sum_{\alpha \neq 0} c_\alpha \ e^{\lambda_\alpha t} \ \boldsymbol{x}_\alpha.$$
(4.100)

I really like this result. First, note that in the first term  $c_0 = y_0^{\dagger} \operatorname{vec}(\rho(0)) = 1$  by normalization. Secondly, in the second term all eigenvalues have negative real part so that, in the long-time limit, they will relax to zero. Consequently, we see that

$$\lim_{t \to \infty} \rho(t) = x_0. \tag{4.101}$$

which, as expected, is the steady-state (4.97). Thus, we conclude that if the steadystate is unique, no matter where you start, the system will always eventually relax towards the steady-sate. The real part of the eigenvalues  $\lambda_{\alpha}$  therefore tell you about the *relaxation rate* of the different terms. That is, they give you information on the time-scale with which the relaxation will occur.

## 4.4 Microscopic derivation of the Lindblad equation

In this section we will begin our discussion concerning microscopic derivations of quantum master equations. The idea is quite simple: we start with a system S interacting with an environment E through some coupling Hamiltonian V. We then assume E is enormous, chaotic, filthy and ugly, so that we can try to trace it out and

obtain an equation just for S. Our hope is that despite all the approximations, our final equations will have Lindblad's form [Eq. (4.42)]. But reality is not so kind, so you may get a bit frustrated as we go along.

This is due to two main reasons. First, we will have to do several approximations which are hard to justify. They are hard because they involve assumptions about a macroscopically large and highly chaotic bath, for which it is really hard to do any calculations. Secondly, these derivations are highly model dependent. I will try to give you a general recipe, but we will see examples where this recipe is either insanely hard to implement or, what is worse, leads to unphysical results.

The derivation of microscopic equations for quantum systems is a century old topic. And for many decades this did not advance much. The reason is precisely because these derivations are model dependent. In classical stochastic processes that is not the case and you can write down quite general results. In fact, you can even write them down without microscopic derivations, using only phenomenological ingredients. For instance, Langevin augmented Newton's equation with a random force and then *later* deduced what the properties of this force had to be, using equilibrium statistical mechanics. Langevin's equation works great! It describes a ton of experiments in the most wide variety of situations, from particles in a fluid to noise in electrical circuits. In the quantum realm, unfortunately, that is simply not the case. It is impossible to write down general equations using only phenomenology. And everything *has* to be model-dependent because operators don't commute, so if add a new ingredient to the Hamiltonian, it will not necessarily commute with what was there before.

### Setting up the problem

Ok. Sorry about the bla-bla. Let's get down to business. Here is the deal: we have a composite S+E system evolving according to a Hamiltonian

$$H = H_S + H_E + V, (4.102)$$

where  $H_S$  and  $H_E$  live on the separate Hilbert spaces of S and E, whereas V connects the two. We now consider their unitary evolution according to von Neumann's equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho],\tag{4.103}$$

where  $\rho$  is the total density matrix of S+E. What we want is to take the partial trace of Eq. (4.103) and try to write down an equation involving only  $\rho_S = \text{tr}_E \rho$ .

Everything is done in the interaction picture with respect to  $H_0 = H_S + H_E$  [see Sec. 3.3]: That is, we define  $\tilde{\rho} = e^{iH_0t}\rho e^{-iH_0t}$ . Then  $\tilde{\rho}$  will also satisfy a von Neumann equation, but with an effective Hamiltonian  $\tilde{V}(t) = e^{iH_0t}Ve^{-iH_0t}$ . In order not to clutter the notation I will henceforth drop the tilde and write this equation simply as

$$\frac{d\rho}{dt} = -i[V(t),\rho], \qquad V(t) = e^{iH_0 t} V e^{-iH_0 t}.$$
(4.104)

I know this seems sloppy, but you will thank me later, as these tilde's make everything so much uglier. Just please remember that this  $\rho$  is not the same as the  $\rho$  appearing in

Eq. (4.103). In considering the evolution of Eq. (4.104), we will also assume that at t = 0 the system and the environment were uncorrelated, so that

$$\rho(0) = \rho_S(0) \otimes \rho_E(0) = \rho_S(0)\rho_E(0). \tag{4.105}$$

The initial state of S can be anything, whereas the initial state of  $\rho_E(0)$  is usually assumed to be a thermal state,

$$\rho_E(0) = \frac{e^{-\beta H_E}}{Z}, \qquad Z = \text{tr}(e^{-\beta H_E}),$$
(4.106)

although other variations may also be used.

f

The result I want to derive does not depend on the model we choose for the environment. However, in 99.99% of the cases, one chooses the bath to be composed of a (usually infinite) set of harmonic oscillators. That is, the Hamiltonian  $H_E$  in Eq. (4.102) is usually chosen to be

$$H_E = \sum_k \Omega_k b_k^{\dagger} b_k, \tag{4.107}$$

where the  $b_k$  are a set of independent bosonic operators<sup>7</sup> and  $\Omega_k$  are some frequencies. Usually it is assumed that the  $\Omega_k$  varies almost continuously with k. The logic behind the assumption (4.107) is based on the fact that the two most widely used baths in practice are the electromagnetic field and the phonons in a crystal, both of which are bosonic in nature.

As for the system-environment interaction, it is usually assumed that this is linear in the bosonic operators  $b_k$ . So V would look something like

$$V = \sum_{\alpha,k} \left\{ g_{\alpha k} M_{\alpha} b_k^{\dagger} + g_{\alpha k}^* A_{\alpha}^{\dagger} b_k \right\},$$
(4.108)

where  $M_{\alpha}$  are system operators and  $g_{\alpha k}$  are numbers. The justification for this kind of coupling is two-fold. First, it turns out there are many system in the literature where this type of coupling naturally appears; and second because this is one of the few types of couplings for which we can actually do the calculations! An important property of the a coupling such as (4.108) and a thermal state such as (4.106) is that, since  $\langle b_k \rangle_{\text{th}} = 0$ , it follows that r

$$\operatorname{tr}_{E} \left[ V \rho_{E}(0) \right] = 0.$$
 (4.109)

This property will greatly simplify the calculations we shall do next.<sup>8</sup>

<sup>7</sup>Whenever we say "independent set" we mean they all commute. Thus, the bosonic algebra may be written as [b

$$b_k, b_q^{\dagger}] = \delta_{k,q}, \qquad [b_k, b_q] = 0.$$

<sup>8</sup> Pro-tip: If you ever encounter a model where for which (4.109) is not true, redefine the system Hamiltonian and the interaction potential to read

$$V' = V - \text{tr}_E(V\rho_E(0)), \qquad H_S = H_S + \text{tr}_E(V\rho_E(0)).$$

This of course doesn't change the total Hamiltonian. But now  $tr_E(V'\rho_E(0)) = 0$ . But please note that this only works when  $[\rho_E(0), H_E] = 0$ .

#### The Nakajima-Zwanzig method

We are now ready to introduce the main method that we will use to trace out the environment. There are many ways to do this. I will use here one introduced by Nakajima and Zwanzig<sup>9</sup> because, even though it is not the easiest one, it is (i) the one with the highest degree of control and (ii) useful in other contexts. The method is based on a *projection superoperator* defined as

$$\mathcal{P}\rho(t) = \rho_S(t)\rho_E(0) = \operatorname{tr}_E(\rho(t))\rho_E(0). \tag{4.110}$$

Yeah, I know: this looks weird. The idea is that  $\mathcal{P}$  almost looks like a *marginalizator* (I just came up with that name!): that is, if in the right-hand side we had  $\rho_E(t)$  instead of  $\rho_E(0)$ , this  $\mathcal{P}$  would be projecting a general (possibly entangled) state  $\rho(t)$  into its marginal states  $\rho_S(t) \otimes \rho_E(t)$ . This is like projecting onto a uncorrelated subspace of the full Hilbert space. But  $\mathcal{P}$  does a bit more than that. It projects onto a state where E didn't really move. This is motivated by the idea that the bath is insanely large so that as the system evolves, it practically doesn't change.

For the purpose of simplicity, I will henceforth write  $\rho_E(0)$  as simply  $\rho_E$ . So let us then check that  $\mathcal{P}$  is indeed a projection operator. To do that we project twice:

$$\mathcal{P}^{2}\rho(t) = \mathcal{P}\left[\rho_{S}(t)\rho_{E}\right] = \operatorname{tr}_{E}(\rho_{S}(t)\rho_{E})\rho_{E} = \rho_{S}(t)\rho_{E},$$

which is the same as just projecting once. Since this is a projection operator, we are naturally led to define its complement Q = 1 - P, which projects onto the remaining subspace. It then follows that  $Q^2 = Q$  and QP = PQ = 0. To summarize, P and Q are projection superoperators satisfying

$$\mathcal{P}^2 = \mathcal{P}, \qquad Q^2 = Q, \qquad Q\mathcal{P} = \mathcal{P}Q = 0.$$
 (4.111)

If you ever want to write down a specific formula for this  $\mathcal{P}$  operator, it is actually a quantum operation defined as

$$\mathcal{P}(\rho) = \sum_{k,q} p_k(I_S \otimes |k\rangle \langle q|) \rho(I_S \otimes |q\rangle \langle k|), \qquad (4.112)$$

where  $|q\rangle$  is an arbitrary basis of the environment, whereas  $|k\rangle$  is the eigenbasis of  $\rho_E = \rho_E(0)$  with eigenvalue  $p_k$  [i.e.,  $\rho_E |k\rangle = p_k |k\rangle$ ]. I don't think this formula is very useful, but it is nice to know that you can write down a more concrete expression for it. If we happen to know  $\mathcal{P}\rho$ , then it is easy to compute  $\rho_S(t)$  because, due to Eq. (4.110),

$$\rho_S(t) = \operatorname{tr}_E \left\{ \mathcal{P}\rho(t) \right\}. \tag{4.113}$$

We will also need one last silly change of notation. We define a superoperator

$$\mathcal{V}_t(\rho) = -i[V(t), \rho], \qquad (4.114)$$

<sup>&</sup>lt;sup>9</sup> S. Nakajima, Progr. Theor. Phys. 20, 984 (1958) and R. Zwanzig, J. Chem. Phys. 33, 1338 (1960).

so that Eq. (4.104) becomes

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathcal{V}_t \rho. \tag{4.115}$$

We are now ready for applying the Nakajima-Zwanzig projection method. We begin by multiplying Eq. (4.114) by  $\mathcal{P}$  and then Q on both sides, to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho = \mathcal{P}V_t\rho,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}Q\rho = QV_t\rho.$$

Next we insert a  $1 = \mathcal{P} + Q$  on the right-hand side, leading to

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho = \mathcal{P}\mathcal{V}_{t}\mathcal{P}\rho + \mathcal{P}\mathcal{V}_{t}\mathcal{Q}\rho, \qquad (4.116)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}Q\rho = Q\mathcal{V}_t\mathcal{P}\rho + Q\mathcal{V}_tQ\rho. \tag{4.117}$$

The main point is that now this looks like a system of equations of the form

$$\frac{\mathrm{d}x}{\mathrm{d}t} = A(t)x + A(t)y,\tag{4.118}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = B(t)x + B(t)y, \tag{4.119}$$

where  $x = \mathcal{P}\rho$  and  $y = \mathcal{Q}\rho$  are just "vectors", whereas  $A(t) = \mathcal{P}V_t$  and  $B(t) = \mathcal{Q}V_t$  are just "matrices" (superoperators). What we want in the end is x(t), whereas y(t) is the guy we want to eliminate.

One way to do that is to formally solve for y treating B(t)x(t) as just some timedependent function, and then insert the result in the equation for x. The formal solution for y is

$$y(t) = G(t,0)y(0) + \int_{0}^{t} G(t,t')B(t')x(t'), \qquad (4.120)$$

where G(t, t') is the Green's function for the y equation,

$$G(t,t') = \mathcal{T} \exp\left\{\int_{t'}^{t} \mathrm{d}s B(s)\right\} = \mathcal{T} \exp\left\{\int_{t'}^{t} \mathrm{d}s \mathcal{Q} \mathcal{V}_{s}\right\}$$
(4.121)

Here I had to use the time-ordering operator  $\mathcal{T}$  to write down the solution, exactly as we did when we had to deal with time-dependent Hamiltonians [c.f. Eq. (3.62)].

One lucky simplification we get is that the first term in Eq. (4.120) turns out to be zero. The reason is that  $y = Q\rho$  so  $y(0) = Q\rho(0)$ . But initially the system and the bath start uncorrelated so  $\mathcal{P}\rho(0) = \rho(0)$ . Consequently,  $Q\rho(0) = 0$  since  $Q = 1 - \mathcal{P}$ . Inserting Eq. (4.120) into Eq. (4.118) then yields

$$\frac{\mathrm{d}x}{\mathrm{d}t} = A(t)x + A(t) \int_{0}^{t} \mathrm{d}t' \ G(t,t')B(t')x(t'). \tag{4.122}$$

This is not bad! We have succeed in eliminating completely y(t) and write down an equation for x(t) only. The downside is that this equation is not local in time, with the derivative of x depending on its entire history from time 0 to time t.

Here Eq. (4.109) starts to become useful. To see why, let us rewrite the first term A(t)x:

$$A(t)x = \mathcal{P}\mathcal{V}_t\mathcal{P}\rho = \mathcal{P}\mathcal{V}_t\rho_S\rho_E$$

We further expand this recalling Eq. (4.114):

$$A(t)x = -i\mathcal{P}[V(t), \rho_S \rho_E] = -i\operatorname{tr}_E \left\{ [V(t), \rho_S \rho_E] \right\} \rho_E.$$

But the guy inside is zero because of Eq. (4.109) and this must be true for any  $\rho_s$ . Hence, we conclude that

$$\operatorname{tr}_{E}\left\{V(t)\rho_{E}\right\} = 0 \quad \to \quad \mathcal{P}V_{t}\mathcal{P} = 0. \tag{4.123}$$

This, in turn, implies that A(t)x = 0, so only the last term in Eq. (4.124) survives:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \int_{0}^{t} \mathrm{d}t' A(t)G(t,t')B(t')x(t'). \tag{4.124}$$

Going back to our original notation we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho = \int_{0}^{t} \mathrm{d}t' \,\mathcal{P}\mathcal{V}_{t}G(t,t')\mathcal{Q}\mathcal{V}_{t'}\mathcal{P}\rho(t').$$

A final naughty trick is to write Q = 1 - P. Then there will be a term which is again  $PV_tP = 0$ . Hence we finally get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho = \int_{0}^{t} \mathrm{d}t' \,\mathcal{P}\mathcal{V}_{t}G(t,t')\mathcal{V}_{t'}\mathcal{P}\rho(t'). \tag{4.125}$$

This is the Nakajima-Zwanzig equation. It is a reduced equation for  $\mathcal{P}\rho(t)$  after integrating out the environment. And, what is coolest, this equation is *exact*. Think about it: we didn't do a single approximation so far. We did use some assumptions, in particular Eqs. (4.105) and (4.109). But these are not really restrictive. This is what I like about this Nakajima-Zwanzig method: it gives us, as a starting point, an exact equation for the reduced dynamics of the system. The fact that this equation is non-local in time is then rather obvious. After all, our environment could very well be a single qubit.

The next step is then to start doing a bunch of approximations on top of it, which will be true when the environment is large and nasty.

#### **Approximations!** Approximations everywhere!

Now we have to start doing some approximations in order to get an equation of the Lindblad form. Justifying these approximations will not be easy and, unfortunately, their validity is usually just verified *a posteriori*. But essentially they are usually related to the fact that the bath is macroscopically large and usually, highly complex. Here is a quick dictionary of all the approximations that are usually done:

- Born (or weak-coupling) approximation: assume that the system-environment interaction is weak so that the state of the bath is barely affected.
- Markov approximation: assume bath correlation functions decay quickly. That is, bath-related stuff are fast, whereas system stuff are slow. This is similar in spirit to classical Brownian motion, where your big grain of pollen moves slowly through a bunch of rapidly moving and highly chaotic molecules (chaos helps the excitations die out fast).
- **Rotating-wave (secular) approximation:** like when the CIA tries to kill Jason Bourne to clean up the mess they created.

We will now go through these approximations step by step, starting with Born/weak coupling. In this case it is useful to rescale the potential by a parameter  $V \rightarrow \epsilon V$  where  $\epsilon$  is assumed to be small (in the end we can reabsorb  $\epsilon$  inside V). In this case the same will be true for the superoperator  $\mathcal{V}_t$  in Eq. (4.114). Hence, Eq. (4.125) is already an equation of order  $\epsilon^2$ . We will then neglect terms of higher order in  $\epsilon$ . These terms actually appear in the Green's function G(t, t'), which we defined in Eq. (4.121). Since now the exponential is of order  $\epsilon$ , if we expand it in a Taylor series we will get

$$G(t,t') = 1 + \epsilon \mathcal{T} \int_{t'}^{t} \mathrm{d} s Q \mathcal{V}_s + O(\epsilon)^2.$$

Thus, if we restrict to an equation of order  $\epsilon^2$ , it suffices to approximate  $G(t, t') \approx 1$  in Eq. (4.125). This is essentially a statement on the fact that the bath state practically does not change. We then get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \int_{0}^{t} \mathrm{d}t' \,\mathcal{P}\mathcal{V}_{t}\mathcal{V}_{t'}\mathcal{P}\rho(t'), \qquad (4.126)$$

where I already reabsorbed  $\epsilon$  inside V, since we won't need it anymore.

Next we talk about the Markov approximation. You should always associate the name Markov with *memory*. A Markovian system is one which has a very poor memory (like fish!). In this case memory is related to how information about the system is dispersed in the environment. The idea is that if the environment is macroscopically large and chaotic, when you shake the system a little bit, the excitations will just diffuse away through the environment and will never come back. So the state of the system at a given time will not really influence it back at some later time by some excitations that bounced back.

To impose this on Eq. (4.126) we do two things. First we assume that  $\rho(t')$  in the right-hand side can be replaced with  $\rho(t)$ . This makes the equation time-local in  $\rho(t)$ . We then get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \int_{0}^{t} \mathrm{d}t' \,\mathcal{P}\mathcal{V}_{t}\mathcal{V}_{t'}\mathcal{P}\rho(t).$$

Next, change integration variables to s = t - t':

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \int_{0}^{t} \mathrm{d}s \,\mathcal{P}\mathcal{V}_{t}\mathcal{V}_{t-s}\mathcal{P}\rho(t).$$

This guy still depends on information occurring at t = 0. To eliminate that we set the upper limit of integration to  $+\infty$  (then then term  $\mathcal{V}_{t-s}$  will sweep all the way from  $-\infty$  to t). We then get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \int_{0}^{\infty} \mathrm{d}s \,\mathcal{P}\mathcal{V}_{t}\mathcal{V}_{t-s}\mathcal{P}\rho(t). \tag{4.127}$$

This equation is now the starting point for writing down actual master equations.

It is convenient to rewrite it in a more human-friendly format. Expanding the superoperators, we get

$$\mathcal{P}V_{t}V_{t-s}\mathcal{P}\rho(t) = \mathcal{P}V_{t}V_{t-s}\rho_{S}(t)\rho_{E}$$
$$= (-i)^{2}\mathcal{P}[V(t), [V(t-s), \rho_{S}(t)\rho_{E}]]$$
$$= -\operatorname{tr}_{E}\left\{ [V(t), [V(t-s), \rho_{S}(t)\rho_{E}]] \right\} \rho_{E}$$

Thus Eq. (4.127) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{S}(t)\rho_{E} = -\int_{0}^{\infty} \mathrm{d}s \ \mathrm{tr}_{E}\left\{\left[V(t),\left[V(t-s),\rho_{S}(t)\rho_{E}\right]\right]\right\}\rho_{E}$$

Taking the trace over E is now trivial and thus gives

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -\int_0^\infty \mathrm{d}s \ \mathrm{tr}_E \left\{ [V(t), [V(t-s), \rho_S(t)\rho_E]] \right\}.$$
(4.128)

This is now starting to look like a recipe. All we need to do is plug in a choice for V(t) and then carry out the commutations, then the E-traces and finally an integral. The result will be an equation for  $\rho_S(t)$ . Once we are done, we just need to remember that we

are still in the interaction picture, so we may want to go back to the Shcrödinger picture. For practical purposes it is also convenient to open the commutators and rearrange this as follows:

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = \int_0^\infty \mathrm{d}s \ \mathrm{tr}_E \left\{ V(t)\rho_S(t)\rho_E V(t-s) - V(t-s)V(t)\rho_S(t)\rho_E \right\} + \mathrm{h.c.}, \tag{4.129}$$

where h.c. stands for Hermitian Conjugate and simply means we should add the dagger of whatever we find in the first term. This is convenient because then out of the four terms, we only need to compute two.

As we will see below, it turns out that sometimes Eq. (4.129) is still not in Lindblad form. In these cases we will have to make a third approximation, which is the rotatingwave approximation (RWA) we discussed in the context of the Rabi model (Sec. 3.3). That is, *every now and then we will have to throw away some rapidly oscillatory terms*. The reason why this may be necessary is related to an argument about *time-scales and coarse graining*. The point worth remembering is that **bath-stuff are fast and system-stuff are slow**. This is again similar to classical Brownian motion: if the bath is a bear, trying to score some honey, then the bath is a swarm of bees desperately fighting to save their home.<sup>10</sup> During the time scale over which the bear takes a few steps, the bees have already lived half their lifetime. Due to this reason, a master equation is only *resolved* over time-scales much larger than the bath scales. If we ever encounter rapidly oscillatory terms, then they mean we are trying to model something in a time scale which we are not resolved. That is why it is justified to throw them away. So, in a sense, the RWA here is us trying to fix up the mess we ourselves created.

# 4.5 Microscopic derivation for the quantum harmonic oscillator

Now that we have a general recipe for finding Lindblad equations, we need to learn how to apply it. Let's do that in the context of a quantum harmonic oscillator coupled to a bath of harmonic oscillators. The three Hamiltonians in Eq. (4.102) will be taken to be

$$H = \omega a^{\dagger} a + \sum_{k} \Omega_{k} b_{k}^{\dagger} b_{k} + \sum_{k} \lambda_{k} (a^{\dagger} b_{k} + b_{k}^{\dagger} a).$$
(4.130)

This is the simplest model possible of an open quantum system. And, it turns out, this model can actually be solved exactly, as we will in fact do in the next chapter. It also turns out that for this model the RWA is not necessary (we will see a variation of it in the next section).

The first step is to compute the interaction picture potential V(t). Using Eq. (3.32)

<sup>&</sup>lt;sup>10</sup>A. A. Milne, Winnie-the-Pooh. New York, NY: Penguin Group, 1954.

we get

$$V(t) = e^{iH_0 t} V e^{-iH_0 t} = \sum_k \lambda_k \Big\{ e^{i\Delta_k t} a^{\dagger} b_k + e^{-i\Delta_k t} b_k^{\dagger} a \Big\},$$
(4.131)

where  $\Delta_k = \omega - \Omega_k$  is the detuning between the system oscillator and each bath mode. Now we plug this into the first term in Eq. (4.129). This gives a messy combination of four term:

$$V(t)\rho_{S}\rho_{E}V(t-s) = \sum_{k,q} \lambda_{k}\lambda_{q} \Big\{ e^{i(\Delta_{k}+\Delta_{q})t} e^{-i\Delta_{q}s} a^{\dagger}b_{k}\rho_{S}\rho_{E}a^{\dagger}b_{q} \\ + e^{i(\Delta_{k}-\Delta_{q})t} e^{i\Delta_{q}s} a^{\dagger}b_{k}\rho_{S}\rho_{E}ab_{q}^{\dagger} \\ + e^{-i(\Delta_{k}-\Delta_{q})t} e^{-i\Delta_{q}s} ab_{k}^{\dagger}\rho_{S}\rho_{E}a^{\dagger}b_{q} \\ + e^{-i(\Delta_{k}+\Delta_{q})t} e^{i\Delta_{q}s} ab_{k}^{\dagger}\rho_{S}\rho_{E}ab_{q}^{\dagger} \Big\}.$$

We will continue to work with this guy, which is only one of the terms in Eq. (4.129). However, once we learn how to deal with it, it will be easy to repeat the procedure for the other terms.

Next we take the trace over the environment. This is a nice exercise on how to move things around. For instance,

$$\operatorname{tr}_{E}\left\{a^{\dagger}b_{k}\rho_{S}\rho_{E}ab_{q}^{\dagger}\right\}=a^{\dagger}\rho_{S}a\operatorname{tr}_{E}\left\{b_{k}\rho_{E}b_{q}^{\dagger}\right\}=a^{\dagger}\rho_{S}a\langle b_{q}^{\dagger}b_{k}\rangle.$$

Thus, we get

$$\operatorname{tr}_{E}\left\{V(t)\rho_{S}\rho_{E}V(t-s)\right\} = \sum_{k,q} \lambda_{k}\lambda_{q}\left\{e^{i(\Delta_{k}+\Delta_{q})t}e^{-i\Delta_{q}s} a^{\dagger}\rho_{S}a^{\dagger}\langle b_{q}b_{k}\rangle + e^{i(\Delta_{k}-\Delta_{q})t}e^{i\Delta_{q}s} a^{\dagger}\rho_{S}a\langle b_{q}^{\dagger}b_{k}\rangle + e^{-i(\Delta_{k}-\Delta_{q})t}e^{-i\Delta_{q}s} a\rho_{S}a^{\dagger}\langle b_{q}b_{k}^{\dagger}\rangle + e^{-i(\Delta_{k}+\Delta_{q})t}e^{i\Delta_{q}s} a\rho_{S}a\langle b_{q}^{\dagger}b_{k}^{\dagger}\rangle\right\}.$$

$$(4.132)$$

We are finally ready to use the initial state of the bath. If we assume that the bath is in the thermal Gibbs state (4.106), then we get

$$\langle b_q b_k \rangle = 0, \tag{4.133}$$

$$\langle b_q^{\dagger} b_k \rangle = \delta_{q,k} \bar{n}(\Omega_k), \tag{4.134}$$

$$\langle b_k b_q^{\dagger} \rangle = \langle b_q^{\dagger} b_k \rangle + \delta_{k,q} = \delta_{k,q} (\bar{n}(\Omega_k) + 1), \qquad (4.135)$$

where

$$\bar{n}(x) = \frac{1}{e^{\beta x} - 1}.$$
(4.136)

Plugging everything we then get

$$\operatorname{tr}_{E}\left\{V(t)\rho_{S}\rho_{E}V(t-s)\right\} = \sum_{k}\lambda_{k}^{2}\left\{e^{i(\omega-\Omega_{k})s}\,\bar{n}(\Omega_{k})\,a^{\dagger}\rho_{S}a + e^{-i(\omega-\Omega_{k})s}[\bar{n}(\Omega_{k})+1]\,a\rho_{S}a^{\dagger}\right\}.$$

$$(4.137)$$

This is now a good point to introduce an important concept known as the **spectral density of the bath**. It is defined as

$$J(\Omega) = 2\pi \sum_{k} \lambda_k^2 \delta(\Omega - \Omega_k).$$
(4.138)

This is defined to be a function of a continuous variable  $\Omega$  and, in general, this function will look like a series of delta-peaks whenever  $\Omega$  equals one of the  $\Omega_k$ . However, for a macroscopically large bath, the frequencies  $\Omega_k$  will change smoothly with *k* and therefore  $J(\Omega)$  will become a smooth function. In terms of Eq. (4.138), Eq. (4.137) can be written as an integral

$$\operatorname{tr}_{E}\left\{V(t)\rho_{S}\rho_{E}V(t-s)\right\} = \int_{0}^{\infty} \frac{\mathrm{d}\Omega}{2\pi} J(\Omega)\left\{e^{i(\omega-\Omega)s}\bar{n}(\Omega)a^{\dagger}\rho_{S}a + e^{-i(\omega-\Omega)s}(\bar{n}(\Omega)+1)a\rho_{S}a^{\dagger}\right\},$$
(4.139)

where we used the fact that  $\Omega$  cannot be negative, since it is a frequency. It is really nice to notice that all properties of the system-bath interaction are summarized in the spectral density  $J(\Omega)$ . This means that the tiny details of  $\lambda_k$  do not matter. All that matter is their combined effect.

Finally, still with Eq. (4.129) in mind, we compute the integral in s.

$$\int_{0}^{\infty} \mathrm{d}s \operatorname{tr}_{E} \left\{ V(t)\rho_{S}\rho_{E}V(t-s) \right\} = \int_{0}^{\infty} \mathrm{d}s \int_{0}^{\infty} \frac{\mathrm{d}\Omega}{2\pi} J(\Omega) \left\{ e^{i(\omega-\Omega)s}\bar{n}(\Omega)a^{\dagger}\rho_{S}a + e^{-i(\omega-\Omega)s}(\bar{n}(\Omega)+1)a\rho_{S}a^{\dagger} \right\}$$

$$(4.140)$$

To continue, the best thing to do is to take the s integral first. And, of course, what we would love to do is use the delta-function identity

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}s}{2\pi} e^{i(\omega-\Omega)s} = \delta(\omega-\Omega). \tag{4.141}$$

There is one tiny problem: in Eq. (4.140) the lower limit of integration is 0 instead of  $-\infty$ . The correct identity is then

$$\int_{0}^{\infty} \frac{\mathrm{d}s}{2\pi} e^{i(\omega-\Omega)s} = \frac{1}{2}\delta(\omega-\Omega) - \frac{i}{2}P\frac{1}{\omega-\Omega},\tag{4.142}$$

where *P* denotes the Cauchy principal value. It can be shown that this last term only causes a tiny rescaling of the oscillator frequency  $\omega$  (i.e., it leads to a unitary contribution, instead of a dissipative one). For this reason, it is usually called a **Lamb shift**.

However, in order to actually compute the Lamb shift, we need more details about the bath and the calculations are quite hard. Hence, this is seldom done in practice. Usually, we just remember that  $\omega$  has been renormalized a bit.

Neglecting the lamb-shift we then get

$$\int_{0}^{\infty} \mathrm{d}s \operatorname{tr}_{E} \left\{ V(t)\rho_{S}\rho_{E}V(t-s) \right\} = \int_{0}^{\infty} \mathrm{d}\Omega \, \frac{J(\Omega)}{2} \delta(\omega-\Omega) \left\{ \bar{n}(\Omega)a^{\dagger}\rho_{S}a + (\bar{n}(\Omega)+1)a\rho_{S}a^{\dagger} \right\}$$
$$= \frac{J(\omega)}{2} \left\{ \bar{n}(\omega)a^{\dagger}\rho_{S}a + (\bar{n}(\omega)+1)a\rho_{S}a^{\dagger} \right\}. \tag{4.143}$$

We did it! We started all the way with Eq. (4.129) and computed the first term. Now, I know this seems there is still a long way to go, but computing the other terms is actually quite easy.

Going back to Eq. (4.132), we now compute

$$\operatorname{tr}_{E}\left\{V(t)\rho_{S}\rho_{E}V(t-s)\right\} = \sum_{k,q} \lambda_{k}\lambda_{q}\left\{e^{i(\Delta_{k}+\Delta_{q})t}e^{-i\Delta_{q}s} a^{\dagger}a^{\dagger}\rho_{S}\langle b_{q}b_{k}\rangle\right.$$
$$\left.+e^{i(\Delta_{k}-\Delta_{q})t}e^{i\Delta_{q}s} aa^{\dagger}\rho_{S}\langle b_{q}^{\dagger}b_{k}\rangle\right.$$
$$\left.+e^{-i(\Delta_{k}-\Delta_{q})t}e^{-i\Delta_{q}s} a^{\dagger}a\rho_{S}\langle b_{q}b_{k}^{\dagger}\rangle$$
$$\left.+e^{-i(\Delta_{k}+\Delta_{q})t}e^{i\Delta_{q}s} aa\rho_{S}\langle b_{q}^{\dagger}b_{k}^{\dagger}\rangle\right\}.$$
(4.144)

The work now stops here. If we just think about this for a second we will notice that this has the *exact* same structure as (4.132), except that the order of the operators is exchanged. For instance, in the second line of (4.132) we had  $a^{\dagger}\rho_{S}a^{\dagger}$ . Now we have  $aa^{\dagger}\rho_{S}$ . You can see Lindblad's form  $L\rho L^{\dagger} - \frac{1}{2}L^{\dagger}L\rho - \frac{1}{2}\rho L^{\dagger}L$  is starting to appear.

If we now repeat the same procedure we will get at the same form as (4.143), but with the operators exchanged:

$$\operatorname{tr}_{E}\left\{V(t-s)V(t)\rho_{S}\rho_{E}\right\} = \frac{J(\omega)}{2}\left\{\bar{n}(\omega)aa^{\dagger}\rho_{S} + (\bar{n}(\omega)+1)a^{\dagger}a\rho_{S}\right\}.$$
(4.145)

For simplicity, I will now change notations to

$$J(\omega) := \gamma, \qquad \bar{n}(\omega) := \bar{n} = \frac{1}{e^{\beta\omega} - 1}.$$
(4.146)

Then, combining (4.143) and (4.145) into Eq. (4.129) we get

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = \frac{\gamma}{2}\bar{n}\left\{a^{\dagger}\rho_S a - aa^{\dagger}\rho_S\right\} + \frac{\gamma}{2}(\bar{n}+1)\left\{a\rho_S a^{\dagger} - a^{\dagger}a\rho_S\right\} + \mathrm{h.c.}.$$

We cannot forget the h.c. Plugging it back, we then finally get

$$\frac{d\rho_S}{dt} = \gamma \bar{n} \Big[ a^{\dagger} \rho_S a - \frac{1}{2} \{ a a^{\dagger}, \rho_S \} \Big] + \gamma (\bar{n} + 1) \Big[ a \rho_S a^{\dagger} - \frac{1}{2} \{ a^{\dagger} a, \rho_S \} \Big].$$
(4.147)

Yay! We did it. We derived the master equation for a harmonic oscillator (is anyone still here?).