Quantum Langevin Equation

Throughout this course we have assumed that thermal equilibrium could always be reached by placing the system in contact with an environment. However, we have never really discussed how this relaxation may actually take place.

The reason is that relaxation is problem specific, whereas the equilibrium state is universal.

But in order for you to have some idea of how this relaxation takes place, in these notes I want to discuss one concrete model of system environment interaction.

In our model the system is described by a single bosonic mode a, whereas the environment are described by an infinite number of bosonic modes b_k. The total S+E Hamiltonian is assumed to have the form

$$H = \omega a^\dagger a + \sum_k \Omega_k b_k^\dagger b_k + \sum_k g_k (a^\dagger b_k + b_k^\dagger a) \qquad (1)$$

The bath modes b_k do not interact directly, but they all interact with the system, with an interaction strength g_k. Moreover, Ω_k is the frequency of mode b_k. Although we represent them as a discrete set of frequencies, in the end we will assume the Ω_k vary quasi-continuously.

In these notes we shall work in the Heisenberg picture. So here is a quick review. the state ρ in the Schrödinger picture obeys the von Neumann Eq

$$\frac{d\rho}{dt} = -i[H, \rho] \tag{2}$$

whose solution is

$$\rho(t) = e^{-iHt} \rho(0) e^{iHt} \tag{3}$$

Expectation values of observables then become

$$\langle A \rangle_t = \mathrm{tr}\{A\rho(t)\} = \mathrm{tr}\{A e^{-iHt} \rho(0) e^{iHt}\} \tag{4}$$

But using the cyclic property of the trace we can also write this as

$$\langle A \rangle_t = \mathrm{tr}\{A(t)\rho(0)\} \tag{5}$$

where I defined the Heisenberg picture operator

$$\boxed{A(t) = e^{iHt} A e^{-iHt}} \tag{6}$$

Some people write this as $A_H(t)$, to remember in which picture we are in. I always put the (t), so that A is in the Schrödinger picture and $A(t)$ in Heisenberg's

Differentiating (6) with respect to t, we find that $A(t)$ obeys

$$\boxed{\frac{dA(t)}{dt} = i\,[H, A(t)]} \tag{7}$$

with the initial condition

$$A(0) = A = \text{Schrödinger picture operator} \tag{8}$$

In the Heisenberg picture the operators evolve in time and the state remains fixed. This can be seen in Eq (5), where the trace is over the initial state $\rho(0)$.

Another comment: because of (6), the commutator in (7) may be written as

$$[H, A(t)] = e^{iHt}\,[H, A]\,e^{-iHt} \tag{9}$$

so to compute $[H, A(t)]$, we can just compute $[H, A]$ and then put (t) everywhere.

Heisenberg equations for the operators a and b_n

Let us now apply Eq (7) to the operators a and b_n, with H given by Eq (1). We find

$$\frac{da(t)}{dt} = -i\omega a(t) - i\sum_n g_n b_n(t) \tag{10a}$$

$$\frac{db_n(t)}{dt} = -i\Omega_n b_n(t) - i g_n a(t) \tag{10b}$$

These are a system of coupled ordinary differential equations for $a(t)$ and $b_n(t)$. Once we solve them, we can compute expectation values using Eq (5).

For concreteness, we shall assume that S and E were initially uncorrelated and the bath modes were in equilibrium at a temperature T. Thus

$$\rho(0) = \rho_S(0) \otimes \rho_E(0) \tag{11}$$

$$\rho_E(0) = \prod_n (1 - e^{-\beta\Omega_n})\, e^{-\beta\Omega_n b_n^\dagger b_n} \tag{12}$$

[the state $\rho_S(0)$ of the system is arbitrary.].

Before we continue, one thing that is important to realize is that the Heisenberg picture may mess up the commutation relations.

Recall that, from (6)

$$a(t) := e^{iHt} a e^{-iHt}$$
$$b_u(t) := e^{iHt} b_u e^{-iHt} \qquad (13)$$

commutation relations at equal times remain fine

$$[a(t), a^\dagger(t)] = [e^{iHt} a e^{-iHt}, e^{iHt} a^\dagger e^{-iHt}]$$
$$= e^{iHt}[a, a^\dagger] e^{-iHt}$$
$$= 1 \qquad (14)$$

or

$$[a(t), b_u(t)] = e^{iHt}[a, b_u] e^{-iHt} = 0 \qquad (15)$$

and so on. However, commutation relations at different times become non-trivial. For instance,

$$[a(t), a^\dagger(t')] = [e^{iHt} a e^{-iHt}, e^{iHt'} a^\dagger e^{-iHt'}]$$
$$= e^{iHt} a e^{-iH(t-t')} a^\dagger e^{-iHt'}$$
$$- e^{iHt'} a^\dagger e^{-iH(t'-t)} a e^{-iHt}$$

$$= ? \qquad (16)$$

the result of this commutation relation will depend on H and is in general non-trivial.

As another interesting example, consider

$$[a, b_u(t)] = [a, e^{iHt} b_u e^{-iHt}] = ? \tag{17}$$

At $t=0$, $b_u(0) = b_u$ commutes with a. But for $t>0$ this is no longer true. So even though a and b_u live in separate Hilbert spaces ($a = a \otimes I_E$ and $b_u = I_S \otimes b_u$), the same is not true for a and $b_u(t)$. We say that $b_u(t)$ will have a finite support on the Hilbert space of a

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Returning now to Eq (10), we shall solve them formally using the following naughty trick. Instead of trying to find an actual solution, we will assume that $a(t)$ is some known function, so that we can formally write down a solution to (10b). Recall that the ODE

$$\frac{dx}{dt} = \lambda x + g(t) \tag{18}$$

has the solution

$$x(t) = e^{\lambda t} x(0) + \int_0^t dt' \, e^{\lambda(t-t')} g(t') \tag{19}$$

Thus, the solution of (10b) will be

$$b_n(t) = e^{-i\Omega_n t} b_n(0) - i g_n \int_0^t dt' \, e^{-i\Omega_n(t-t')} a(t') \qquad (20)$$

This solution is exact, although at first it may not seem very useful since we don't know what $a(t)$ is.

Next we plug this into (10a), which gives

$$\frac{da(t)}{dt} = -i\omega \, a(t) - i \sum_n g_n e^{-i\Omega_n t} b_n + \\ - \sum_n g_n^2 \int_0^t dt' \, e^{-i\Omega_n(t-t')} a(t') \qquad (21)$$

where I already used the fact that $b_n(0) = b_n$, is the Schrödinger picture operator.

Next it is convenient to define

$$\tilde{a}(t) = e^{i\omega t} a(t) \qquad (22)$$

then

$$\frac{d\tilde{a}(t)}{dt} = i\omega \tilde{a}(t) + e^{i\omega t} \frac{da(t)}{dt}$$

$$= i\omega \tilde{a}(t) - i\omega \tilde{a}(t) - i \sum_n g_n e^{i(\omega-\Omega_n)t} b_n \\ - \sum_n g_n^2 \int_0^t dt' \, e^{i(\omega-\Omega_n)(t-t')} \tilde{a}(t')$$

Thus $\tilde{a}(t)$ obeys

$$\frac{d\tilde{a}}{dt} = -i\sum_n \gamma_n e^{i(\omega-\Omega_n)t} b_n + - \sum_n \gamma_n^2 \int_0^t dt' \, e^{i(\omega-\Omega_n)(t-t')} \tilde{a}(t') \tag{23}$$

we can make this equation clearer by defining the <u>noise operator</u>

$$\boxed{f(t) = -i\sum_n \gamma_n e^{i(\omega-\Omega_n)t} b_n} \tag{24}$$

and the <u>memory Kernel</u>

$$\boxed{M(t-t') = \sum_n \gamma_n^2 \, e^{i(\omega-\Omega_n)(t-t')}} \tag{25}$$

Eq (23) then finally becomes

$$\boxed{\frac{d\tilde{a}(t)}{dt} = f(t) - \int_0^t dt' \, M(t-t')\tilde{a}(t')} \tag{26}$$

This is the <u>quantum Langevin equation</u>. The operator $f(t)$ is a noise because it depends only on the Schrödinger operators b_n of the bath. Hence, it is affected by the initial fluctuations in $\rho_B(0)$.

The last term in (26), on the other hand, is like a damping term $-\gamma a(t)$. The difference is that a term like $-\gamma a(t)$ damps based on the current value of the operator at time t. The term in (26), on the other hand, damps based on the entire history $a(t')$, with $t' < t$, weighted by a kernel $M(t-t')$, which reflects the influence of $a(t')$ in damping at time t. For this reason, Eq (26) is said to describe a non-Markovian evolution (Markovian evolutions are memoryless, like fish!)

The Wigner - Weisskopf approximation

Let's talk a bit more about the memory kernel in Eq (25). Recall that even though the Ω_k are discrete, the number of modes in the bath is so dense that the Ω_k will form a quasi-continuum of frequencies from 0 to ∞. We can describe this mathematically by introducing the spectral density

$$J(\Omega) = \pi \sum_k g_k^2 \, \delta(\Omega - \Omega_k) \tag{27}$$

where the factor of π is introduced by convenience. The idea is that $J(\Omega)$ will be a bunch of δ peaks at the frequencies Ω_k. If the Ω_k are far apart, then $J(\Omega)$ will be quite irregular. But if they form a dense and smooth quasi-continuum, then $J(\Omega)$ will be a smooth function.

With the spectral density (27) the memory kernel (25) is written as

$$\boxed{M(t) = \frac{1}{\pi} \int_0^\infty d\Omega \, J(\Omega) \, e^{i(\omega - \Omega) t}} \tag{28}$$

which you can verify by substituting (27) in (28)

Let us now assume that $J(\Omega)$ is a smooth function and that $\omega t >> 1$. Then $e^{i(\omega-\Omega)t}$ will oscillate really fast as a function of Ω, except when $\Omega \sim \omega$. Thus, in (28) we may approximately set $J(\Omega) \to J(\omega)$, leading to

$$M(t) \simeq \frac{J(\omega)}{\pi} \int_0^\infty e^{i(\omega-\Omega)t} d\Omega \qquad (29)$$

This idea of removing smooth functions from the integral, is called the Wigner-Weisskopf approximation.

The resulting integral in (29) is just the Fourier transform of the Heaviside Θ function

$$\frac{1}{\pi} \int_0^\infty d\Omega\, e^{i(\omega-\Omega)t} = \frac{e^{i\omega t}}{\pi} \int_{-\infty}^\infty d\Omega\, \Theta(\Omega)\, e^{-i\Omega t}$$

$$= e^{i\omega t} \left\{ \delta(t) - \frac{i}{\pi t} \right\}$$

$$= \delta(t) - \frac{i e^{i\omega t}}{\pi t} \qquad (30)$$

where I used the fact that $e^{i\omega t}\delta(t) = \delta(t)$. The last term is highly oscillatory and becomes negligible when $\omega t >> 1$. Thus we conclude that

$$\frac{1}{\pi} \int_0^\infty d\Omega\, e^{i(\omega-\Omega)t} \simeq \delta(t) \qquad (31)$$

Markovian evolution

With the Wigner-Weisskopf approximation and Eq (31), the memory kernel (29) becomes approximately

$$\boxed{M(t) \simeq J(\omega)\,\delta(t)} \qquad (32)$$

This is the Markov limit: for smooth $J(\Omega)$ and $\omega t \gg 1$, the system becomes memoryless. Going back now to the Langevin Eq (26), we get

$$\int_0^t dt'\, M(t-t')\,\tilde{a}(t') = J(\omega)\int_0^t dt'\,\delta(t-t')\,\tilde{a}(t')$$

$$= \frac{J(\omega)}{2}\,\tilde{a}(t)$$

For convenience, let us define

$$\chi = \frac{J(\omega)}{2} \qquad (33)$$

then Eq (26) finally reduces to

$$\boxed{\frac{d\tilde{a}(t)}{dt} = f(t) - \chi\,\tilde{a}(t)} \qquad (34)$$

which is the Markovian version of the quantum Langevin equation.

We can also say a few extra things about the noise operator $f(t)$ [Eq (24)]. First, since the b_k are just the Schrödinger operators, we get $[f(t), f(t')] = 0$. However

$$[f(t), f^\dagger(t')] = \sum_{kq} \gamma_k \gamma_q \, e^{i(\omega - \Omega_k)t} e^{-i(\omega - \Omega_q)t'} \underbrace{[b_k, b_q^\dagger]}_{\delta_{kq}}$$

$$= \sum_k \gamma_k^2 \, e^{i(\omega - \Omega_k)(t - t')}$$

$$= M(t - t')$$

where I used (25). Thus

$$\boxed{[f(t), f^\dagger(t')] = M(t - t')} \tag{35}$$

which is absolutely general. For the Markovian case (32), this then becomes

$$\boxed{[f(t), f^\dagger(t')] = 2\kappa \, \delta(t - t')} \tag{36}$$

Let us also say something about the expectation values of $f(t)$. Recall that since we are in the Heisenberg picture, averages are always taken with respect to $\rho(0)$. Since we are assuming the bath was originally in a thermal state [Eq (12)] we get $\langle b_u \rangle = 0$, so that $\langle f(t) \rangle = 0$. Similarly, since $\langle b_u b_q \rangle = 0$, we also get $\langle f(t) f(t') \rangle = 0$. The interesting guys are of the form

$$\langle f(t) f^\dagger(t') \rangle = \sum_{uq} \gamma_u \gamma_q \, e^{i(\omega - \Omega_u)t} \, e^{-i(\omega - \Omega_q)t'} \langle b_u b_q^\dagger \rangle$$

Since in equilibrium

$$\langle b_u b_q^\dagger \rangle = \delta_{uq} \left[\bar{n}(\Omega_u) + 1 \right] \tag{37}$$

where

$$\bar{n}(\Omega_u) = \frac{1}{e^{\beta \Omega_u} - 1} \tag{38}$$

we get

$$\langle f(t) f^\dagger(t') \rangle = \sum_u \gamma_u^2 \, e^{i(\omega - \Omega_u)(t - t')} \left[\bar{n}(\Omega_u) + 1 \right]$$

We now convert this to an integral, as in (28):

$$\langle f(t) f^\dagger(t') \rangle = \int_0^\infty \frac{d\Omega}{\pi} J(\Omega) \, e^{i(\omega - \Omega)(t - t')} \left[\bar{n}(\Omega) + 1 \right]$$

And finally, we use Wigner-Weisskopf [eq (29)] again, to write

$$\langle f(t) f^{\dagger}(t') \rangle \simeq J(\omega)\left[\bar{n}(\omega)+1\right] \int_0^{\infty} \frac{d\Omega}{\pi}\, e^{i(\omega-\Omega)(t-t')}$$

$$= 2\kappa\left[\bar{n}(\omega)+1\right] \delta(t-t')$$

Using also (30), we get $\langle f^{\dagger}(t) f(t') \rangle = 2\kappa\, \bar{n}(\omega)\, \delta(t-t')$. Thus, to summarize, in the Markov limit and assuming a thermal state for the bath, the noise operator satisfies

$$\boxed{\begin{aligned} &\langle f(t) \rangle = \langle f(t) f(t') \rangle = 0 \\ &\langle f^{\dagger}(t) f(t) \rangle = 2\kappa\, \bar{n}(\omega)\, \delta(t-t') \\ &\langle f(t) f^{\dagger}(t') \rangle = 2\kappa\left[\bar{n}(\omega)+1\right] \delta(t-t') \end{aligned}}$$

(39)

(40)

(41)

Relaxation towards equilibrium

We are finally ready to illustrate how Eq (34) leads to a relaxation towards equilibrium. The solution of (34) is

$$\tilde{a}(t) = e^{-\kappa t} a + \int_0^t dt' \, e^{-\kappa(t-t')} f(t') \tag{42}$$

where I used the fact that $\tilde{a}(0) = a(0) = a$. Let's use this to compute, for instance, $\langle a^\dagger a \rangle_t$. Since we are in the Heisenberg picture

$$\langle a^\dagger a \rangle_t = \langle a^\dagger(t) a(t) \rangle_0 = \langle \tilde{a}^\dagger(t) \tilde{a}(t) \rangle_0 \tag{43}$$

where I used the fact that since $\tilde{a}(t) = a(t) e^{i\omega t}$, $a^\dagger(t) a(t) = \tilde{a}^\dagger(t) \tilde{a}(t)$.

Thus, using (42), we get

$$\langle \tilde{a}^\dagger(t) \tilde{a}(t) \rangle = e^{-2\kappa t} \langle a^\dagger a \rangle_0 + \int_0^t dt' \, e^{-\kappa(t-t')} e^{-\kappa t} \left\{ \langle a^\dagger f(t') \rangle_0 + \langle f^\dagger(t') a \rangle_0 \right\}$$

$$+ \int_0^t dt' \int_0^t dt'' \, e^{-\kappa(t-t')} e^{-\kappa(t-t'')} \langle f^\dagger(t') f(t'') \rangle_0$$

But since the averages are over the initial state, $\langle a^\dagger f(t') \rangle = 0$.

Moreover, we don't do anything with $\langle a^\dagger a \rangle_0$, since the initial state of the system is arbitrary.

Using Eq (40) we then get

$$\langle a^\dagger a\rangle_t = e^{-2\kappa t}\langle a^\dagger a\rangle_0 + \int_0^t dt' \int_0^t dt''\, e^{-\kappa(t-t')}\, e^{-\kappa(t-t'')}\, 2\kappa \bar{n}(\omega)\,\delta(t'-t'')$$

$$= e^{-2\kappa t}\langle a^\dagger a\rangle_0 + 2\kappa\,\bar{n}(\omega) \underbrace{\int_0^t dt'\, e^{-2\kappa(t-t')}}_{\frac{1-e^{-2\kappa t}}{2\kappa}}$$

thus

$$\boxed{\langle a^\dagger a\rangle_t = e^{-2\kappa t}\langle a^\dagger a\rangle_0 + (1-e^{-2\kappa t})\,\bar{n}(\omega)} \qquad (44)$$

voilà relaxation! the system starts with an arbitrary occupation $\langle a^\dagger a\rangle_0$. Then, as time passes, this $\langle a^\dagger a\rangle_0$ is suppressed and replaced with the <u>bath-induced</u> <u>occupation</u> $\bar{n}(\omega)$. this is how the system relaxes towards the population imposed by the bath.