

Week 6

PHY 435 / 635 Decoherence and Open Quantum Systems

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4 Markovian Open Quantum Systems

So far we had considered decoherence either via some simplistic state-mappings $|\Psi(0)\rangle \rightarrow |\Psi(t)\rangle$ or via solving the full many-body problem in some simple cases and then taking the partial trace over the environment to reduce dynamics onto the system:

$$\hat{\rho}_S(t) = \text{Tr}_E\{\hat{U}(t)\hat{\rho}_{tot}(0)\hat{U}^\dagger(t)\}, \quad (4.1)$$

where $\hat{\rho}_{tot}(0)$ is the initial system plus environment density matrix and $\hat{U}(t)$ the total time evolution operator.

The approach (4.1) is typically impractical because the environment will be too large or too complex to obtain $\hat{U}(t)$. We thus need to learn some techniques to circumvent having to obtain $\hat{U}(t)$ to know about $\hat{\rho}_S(t)$.

4.1 Master-Equation formulation of open quantum systems

What we are after, is called a

Master equation, which is a dynamical map

$$\hat{\rho}_S(t) = \hat{V}(t)[\hat{\rho}_S(0)]. \quad (4.2)$$

- Here $\hat{V}(t)$ takes the role of the time-evolution operator, only it works on the level of the system density matrix only. Since $\hat{V}(t)$ is mapping an operator (the density matrix at $t = 0$) onto another operator (the density matrix at $t > 0$), it is also called a superoperator.
- If a Master equation is exact, we would have $\hat{V}(t)[\hat{\rho}_S(0)] = \text{Tr}_E\{\hat{U}(t) \underbrace{\hat{\rho}_{tot}(0)}_{=\hat{\rho}_S(0)\otimes\hat{\rho}_E(0)} \hat{U}^\dagger(t)\}$,
however typically this is only approximately the case.

In this section 4, we will first only consider Master equations that are local in time. This means we will write a

Markovian Master equation

$$\frac{d}{dt}\hat{\rho}_S(t) = \hat{\mathcal{L}}[\hat{\rho}_S(t)] = -\frac{i}{\hbar}[\hat{H}'_S, \hat{\rho}_S(t)] + \hat{\mathcal{D}}[\hat{\rho}_S(t)], \quad (4.3)$$

where again $\hat{\mathcal{L}}$ and $\hat{\mathcal{D}}$ are super-operators.

- In (4.3), the evolution of the reduced density matrix depends only on the current state of the density matrix, not on its history ($\hat{\rho}_S(t')$, for $t' < t$). In the language of section 1.5.6, we can classify this evolution as Markovian.
- Note that the first part in (4.3) corresponds to a von Neumann type equation just as in (3.2), as we would have for the unitary evolution of a closed system. Note, however, that the Hamiltonian \hat{H}'_S is not quite the system Hamiltonian \hat{H}_S .
- We shall see that a new non-unitary dissipator $\hat{\mathcal{D}}$ can take care of decoherence.

4.2 Born-Markov Master equation

In the previous section we have only formally introduced how a Master equation would look like. To use this concept, we have to be able to derive it from our open quantum system models, consisting of \hat{H}_S , \hat{H}_E and \hat{H}_{int} as listed in section 2. The derivation is lengthy but so central to this course that we show it in almost full detail.

We assume that the interaction Hamiltonian takes the form

$$\hat{H}_{\text{int}} = \sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha}, \quad (4.4)$$

where the \hat{S}_{α} act on the system only and \hat{E}_{α} on the environment only. This was the case for all examples in section 2. We now move to an interaction picture with $\hat{H}_0 = \hat{H}_S + \hat{H}_E$ and $\hat{V} = \hat{H}_{\text{int}}$. In this section we set $\hbar = 1$ to compress notation.

Using the definitions in section 1.5.5 we then have the interaction operator and density matrix in the interaction-picture as

$$\hat{H}_{\text{int}}^{(I)}(t) = e^{i\hat{H}_0 t} \hat{H}_{\text{int}} e^{-i\hat{H}_0 t}, \quad (4.5)$$

$$\hat{\rho}^{(I)}(t) = e^{i\hat{H}_0 t} \hat{\rho}(t) e^{-i\hat{H}_0 t} = e^{i\hat{H}_0 t} e^{-i\hat{H} t} \hat{\rho}(0) e^{i\hat{H} t} e^{-i\hat{H}_0 t}. \quad (4.6)$$

Using these, we can start from (3.2) and derive the

Interaction-picture Liouville-von Neumann equation

$$\frac{d}{dt}\hat{\rho}^{(I)}(t) = -i[\hat{H}_{\text{int}}^{(I)}(t), \hat{\rho}^{(I)}(t)], \quad (4.7)$$

stating that in the interaction picture, evolution of the density matrix follows directly from the interaction Hamiltonian.

- Proof: Assignment.
- Note, this differs from (1.41), since the density matrix is a special kind of operator.

We can now formally integrate the differential equation (4.7) over time from 0 to t and find

$$\hat{\rho}^{(I)}(t) = \hat{\rho}^{(I)}(0) - i \int_0^t dt' [\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}^{(I)}(t')]. \quad (4.8)$$

We now insert (4.8) back into (4.7) and reach

$$\frac{d}{dt} \hat{\rho}^{(I)}(t) = -i [\hat{H}_{\text{int}}^{(I)}(t), \hat{\rho}^{(I)}(0)] - \int_0^t dt' [\hat{H}_{\text{int}}^{(I)}(t), [\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}^{(I)}(t')]]. \quad (4.9)$$

We could repeat this step over and over, but stop here. This perturbative expansion makes sense if \hat{H}_{int} is "small", see below. Next, using $\hat{\rho}_S^{(I)}(t) = \text{Tr}_{\mathcal{E}} \{ \hat{\rho}^{(I)}(t) \}$ (proof: assignment), we find

$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) = -i \text{Tr}_{\mathcal{E}} [\hat{H}_{\text{int}}^{(I)}(t), \hat{\rho}^{(I)}(0)] - \int_0^t dt' \text{Tr}_{\mathcal{E}} [\hat{H}_{\text{int}}^{(I)}(t), [\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}^{(I)}(t')]]. \quad (4.10)$$

In the literature, the first term in (4.10) is set to zero, stating that if that was not the case, we can redefine \hat{H}_0 and \hat{H}_{int} to make it so.

So far we have mainly complicated things without gain, the rhs of (4.10) still depends on $\hat{\rho}^{(I)}(t')$, the entire density matrix (including the environment) at all earlier times $t' < t$.

Let us address the first problem by invoking the

Born approximation, that the system environment coupling is "weak", and the environment so large that the system does not significantly affect it. Mathematically we express the latter by

$$\hat{\rho}(t) \approx \hat{\rho}_S(t) \otimes \hat{\rho}_{\mathcal{E}}(0), \quad (4.11)$$

with $\hat{\rho}_{\mathcal{E}}(0) \approx \text{const.}$ the environmental initial state.

- We define "weak" operationally, as "the lines (4.9) and (4.11) are valid".
- The " \approx " instead of " $=$ " is important. We cannot have " $=$ " since this would imply a pure reduced system state and we want to describe decoherence. We will thus only use (4.11) to simplify (4.10) and not assume that it actually implies a separable system-environment state.

We have thus now reached:

$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) = - \int_0^t dt' \text{Tr}_{\mathcal{E}} [\hat{H}_{\text{int}}^{(I)}(t), [\hat{H}_{\text{int}}^{(I)}(t'), \hat{\rho}_S^{(I)}(t') \otimes \hat{\rho}_{\mathcal{E}}(0)]], \quad (4.12)$$

which no longer depends on the full environmental dynamics.

Now note that

$$\begin{aligned}\hat{H}_{\text{int}}^{(I)}(t') &= e^{i\hat{H}_0 t'} \hat{H}_{\text{int}} e^{-i\hat{H}_0 t'} = \sum_{\alpha} (e^{i\hat{H}_S t'} \hat{S}_{\alpha} e^{-i\hat{H}_S t'}) \otimes (e^{i\hat{H}_{\mathcal{E}} t'} \hat{E}_{\alpha} e^{-i\hat{H}_{\mathcal{E}} t'}) \\ &= \sum_{\alpha} \hat{S}_{\alpha}^{(I)}(t') \otimes \hat{E}_{\alpha}^{(I)}(t'),\end{aligned}\quad (4.13)$$

which allows us to write

$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) = - \int_0^t dt' \sum_{\alpha\beta} \text{Tr}_{\mathcal{E}} [\hat{S}_{\alpha}^{(I)}(t) \otimes \hat{E}_{\alpha}^{(I)}(t), [\hat{S}_{\beta}^{(I)}(t') \otimes \hat{E}_{\beta}^{(I)}(t'), \hat{\rho}_S^{(I)}(t') \otimes \hat{\rho}_{\mathcal{E}}(0)]] \quad (4.14)$$

$$\begin{aligned}&= -i \int_0^t dt' \sum_{\alpha\beta} \left\{ \right. \\ &\hat{S}_{\alpha}^{(I)}(t) \hat{S}_{\beta}^{(I)}(t') \hat{\rho}_S^{(I)}(t') \text{Tr}_{\mathcal{E}} \left\{ \hat{E}_{\alpha}^{(I)}(t) \hat{E}_{\beta}^{(I)}(t') \hat{\rho}_{\mathcal{E}}(0) \right\} - \hat{S}_{\beta}^{(I)}(t') \hat{\rho}_S^{(I)}(t') \hat{S}_{\alpha}^{(I)}(t) \text{Tr}_{\mathcal{E}} \left\{ \hat{E}_{\beta}^{(I)}(t') \hat{\rho}_{\mathcal{E}}(0) \hat{E}_{\alpha}^{(I)}(t) \right\} \\ &\left. - \hat{S}_{\alpha}^{(I)}(t) \hat{\rho}_S^{(I)}(t') \hat{S}_{\beta}^{(I)}(t') \text{Tr}_{\mathcal{E}} \left\{ \hat{E}_{\alpha}^{(I)}(t) \hat{\rho}_{\mathcal{E}}(0) \hat{E}_{\beta}^{(I)}(t') \right\} + \hat{\rho}_S^{(I)}(t') \hat{S}_{\beta}^{(I)}(t') \hat{S}_{\alpha}^{(I)}(t) \text{Tr}_{\mathcal{E}} \left\{ \hat{\rho}_{\mathcal{E}}(0) \hat{E}_{\beta}^{(I)}(t') \hat{E}_{\alpha}^{(I)}(t) \right\} \right\}.\end{aligned}$$

After the equality we have only expanded the two nested commutators and split everything into the system versus environment part of the tensor product.

Since it occurs repeatedly in (4.14), we now define the

Environment self-correlation functions,

$$\mathcal{C}_{\alpha,\beta}(t, t') \equiv \text{Tr}_{\mathcal{E}} \left\{ \hat{E}_{\alpha}^{(I)}(t) \hat{E}_{\beta}^{(I)}(t') \hat{\rho}_{\mathcal{E}}(0) \right\} = \text{Tr}_{\mathcal{E}} \left\{ \hat{E}_{\alpha}^{(I)}(t - t') \hat{E}_{\beta}^{(I)}(0) \hat{\rho}_{\mathcal{E}}(0) \right\} \equiv \mathcal{C}_{\alpha,\beta}(t - t') \quad (4.15)$$

- We can also write $\mathcal{C}_{\alpha,\beta}(t, t') = \langle \hat{E}_{\alpha}^{(I)}(t) \hat{E}_{\beta}^{(I)}(t') \rangle$, see Eq. (3.6).
- The $\mathcal{C}_{\alpha,\beta}(t, t')$ quantify to what extent the environmental operator $\hat{E}_{\alpha}^{(I)}(t)$ at time t is correlated with another such operator β at another time t' , given the environmental state $\hat{\rho}_{\mathcal{E}}(0)$.
- This can be viewed as "memory" of the environment: Does the environment still know at time $t - t'$, what the system did to it at time 0? The time range $t - t'$ over which (4.15) significantly differs from 0 is called memory time or correlation time τ_{corr} of the environment.
- For the middle equality we assume that the environment is always in a stationary state and hence $[\hat{H}_{\mathcal{E}}, \hat{\rho}_{\mathcal{E}}] = 0$.⁵ Since it is stationary, correlations cannot depend on the absolute time, only on time differences.

With (4.15) we can write (4.14) a bit more nicely as

⁵This implies a stationary state due to (3.2), taking into account that the system does not significantly affect the environment.

Quantum master equation in the second Born approximation,

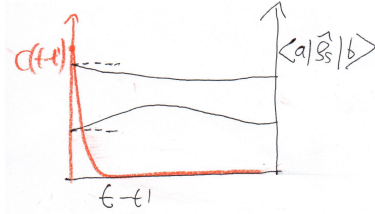
$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) = - \int_0^t dt' \sum_{\alpha\beta} \left\{ \mathcal{C}_{\alpha,\beta}(t-t') [\hat{S}_\alpha^{(I)}(t), \hat{S}_\beta^{(I)}(t') \hat{\rho}_S^{(I)}(t')] + \mathcal{C}_{\beta,\alpha}(t'-t) [\hat{\rho}_S^{(I)}(t') \hat{S}_\beta^{(I)}(t'), \hat{S}_\alpha^{(I)}(t)] \right\} \quad (4.16)$$

We used the cyclic property of the trace $\text{Tr}_\mathcal{E} \{ \hat{E}_\alpha \hat{E}_\beta \hat{\rho}_\mathcal{E} \} = \text{Tr}_\mathcal{E} \{ \hat{E}_\beta \hat{\rho}_\mathcal{E} \hat{E}_\alpha \} = \text{Tr}_\mathcal{E} \{ \hat{\rho}_\mathcal{E} \hat{E}_\alpha \hat{E}_\beta \}$

Warning: A partial trace is only cyclic as long as operators within act in the space being traced over. Thus e.g. $\text{Tr}_\mathcal{E} \{ \hat{S}_\alpha \hat{E}_\alpha \hat{\rho} \} \neq \text{Tr}_\mathcal{E} \{ \hat{\rho} \hat{S}_\alpha \hat{E}_\alpha \}$, with full density matrix $(\mathcal{S} + \mathcal{E}) \hat{\rho}$.

Finally let us also invoke the

Markov approximation, under which the environmental memory time τ_{corr} is much shorter than the characteristic time-scale for changes in the system τ_S , thus $\tau_{\text{corr}} \ll \tau_S$. τ_S is typically set by \hat{H}_S , for example by the differences of energy eigenvalues of \hat{H}_S , e.g. $\tau_S \sim |E_n - E_m|/\hbar$. However τ_S may also be affected by relaxation due to the environment.



left: Sketch of the scenario where the Markov approximation is valid. The environment correlations decay substantially faster than $\hat{\rho}_S$ evolves.

The Markov approximation has two consequences:

- (i) It allows us to replace $\hat{\rho}_S^{(I)}(t') \rightarrow \hat{\rho}_S^{(I)}(t)$ in the time integrals occurring in (4.16), corresponding to the dashed approximation in the figure above.
- (ii) We now can extend the integral $\int_0^t \rightarrow \int_{-\infty}^t$ (since $\mathcal{C}_{\alpha,\beta}(t-t') = 0$ for large $|t-t'|$ anyway).f

Let us implement consequence (i) only for now, we then obtain the

Redfield equations,

$$\frac{d}{dt} \hat{\rho}_S^{(I)}(t) = - \sum_{\alpha} \left\{ [\hat{S}_\alpha^{(I)}(t), \hat{\Gamma}_\alpha(t) \hat{\rho}_S^{(I)}(t)] + [\hat{\rho}_S^{(I)}(t) \hat{\Gamma}_\alpha^\dagger(t), \hat{S}_\alpha^{(I)}(t)] \right\} \quad (4.17)$$

With $\hat{\Gamma}_\alpha(t) = \int_0^t dt' \sum_{\beta} \mathcal{C}_{\alpha,\beta}(t-t') \hat{S}_\beta^{(I)}(t')$, and assuming Hermitian \hat{S} and \hat{E} .

- The Redfield equation is on first sight already local in time, but it still depends "on the past" in a hidden way, since the definition of $\Gamma_\alpha(t)$ refers to an initialisation (start of dynamics) at $t = 0$. Thus (4.17) it is not yet Markovian (BP).

After consequence (ii) following from the Markov approximation and the substitution $\tau = t - t'$, we have

$$\frac{d}{dt}\hat{\rho}_S^{(I)}(t) = - \int_0^\infty \tau \sum_{\alpha\beta} \left\{ \mathcal{C}_{\alpha,\beta}(\tau) [\hat{S}_\alpha^{(I)}(t), \hat{S}_\beta^{(I)}(t-\tau)\hat{\rho}_S^{(I)}(t)] + \mathcal{C}_{\beta,\alpha}(-\tau) [\hat{\rho}_S^{(I)}(t)\hat{S}_\beta^{(I)}(t-\tau), \hat{S}_\alpha^{(I)}(t)] \right\} \quad (4.18)$$

Now we can transform (4.18) back into the Schrödinger picture for the density matrix. The steps are technical and can be found in SD. We see

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] - \int_0^\infty d\tau \sum_{\alpha\beta} \left\{ \mathcal{C}_{\alpha,\beta}(\tau) [\hat{S}_\alpha^{(I)}(0), \hat{S}_\beta^{(I)}(-\tau)\hat{\rho}_S(t)] + \mathcal{C}_{\beta,\alpha}(-\tau) [\hat{\rho}_S(t)\hat{S}_\beta^{(I)}(-\tau), \hat{S}_\alpha^{(I)}(0)] \right\} \quad (4.19)$$

In a final step we define

$$\begin{aligned} \hat{B}_\alpha &= \int_0^\infty d\tau \sum_\beta \mathcal{C}_{\alpha,\beta}(\tau) \hat{S}_\beta^{(I)}(-\tau), \\ \hat{C}_\alpha &= \int_0^\infty d\tau \sum_\beta \mathcal{C}_{\beta,\alpha}(-\tau) \hat{S}_\beta^{(I)}(-\tau), \end{aligned} \quad (4.20)$$

and write the

Born-Markov Masterequation as

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] - \sum_\alpha \left\{ [\hat{S}_\alpha, \hat{B}_\alpha \hat{\rho}_S(t)] + [\hat{\rho}_S(t) \hat{C}_\alpha, \hat{S}_\alpha] \right\} \quad (4.21)$$

- The essential difference between (4.17) and (4.21) is that we integrate over all of delays in (4.20). Thus the operators \hat{B}_α and \hat{C}_α are time-independent and we have finally reached a Markovian Master equation.

4.3 Lindblad Master equation

One of the shortcomings of the Born-Markov equation (4.21), is that it does not guarantee the positivity (positive definite-ness) of the evolving reduced density matrix:

$$\langle \Psi(t) | \hat{\rho}_S(t) | \Psi(t) \rangle \geq 0, \quad (4.22)$$

for any pure state $|\Psi(t)\rangle$ of the system. We need this so that when we diagonalize it, $\hat{\rho}_S(t) = \sum_k p_k |\varphi_k\rangle\langle\varphi_k|$, all eigenvalues $p_k \geq 0$ and can be interpreted as a probability.

It can be shown that the most general Master equation that guarantees (4.22) must take the form

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] + \frac{1}{2} \sum_{\alpha\beta} \gamma_{\alpha\beta} \left\{ [\hat{S}_\alpha, \hat{\rho}_S(t)\hat{S}_\beta^\dagger] + [\hat{S}_\alpha\hat{\rho}_S(t), \hat{S}_\beta^\dagger] \right\} \quad (4.23)$$

Here the coefficients $\gamma_{\alpha\beta}$ control all processes to do with the environmental coupling.

- This is a special case of a Born-Markov ME (4.21), but not equivalent.
- We can frequently derive such a form from (4.21) under the additional secular (or rotating wave-approximation), which neglects all terms in the Master equation that rotate fastest (i.e. contain a $e^{i\omega t}$ with the largest ω).

We can simplify (4.23) somewhat by diagonalising the coefficient matrix $\gamma_{\alpha\beta}$ and then reach the

Lindblad Masterequation in the standard form

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}'_S, \hat{\rho}_S(t)] - \frac{1}{2} \sum_{\mu} \kappa_{\mu} \left\{ \hat{L}_{\mu}^{\dagger}\hat{L}_{\mu}\hat{\rho}_S(t) + \hat{\rho}_S(t)\hat{L}_{\mu}^{\dagger}\hat{L}_{\mu} - 2\hat{L}_{\mu}\hat{\rho}_S(t)\hat{L}_{\mu}^{\dagger} \right\} \quad (4.24)$$

- Already (4.23) is also called "Lindblad Masterequation".
- \hat{H}'_S is called the Lamb shifted Hamiltonian, and contains the original \hat{H}_S plus some energy shifts arising due to the coupling to the environment.
- The \hat{L}_{μ} are called Lindblad operators and encapsulate any decoherence process. They are obtained as linear combinations of the original \hat{S}_{α} operators.
- Comparing (4.24) with (4.3), this now defines the dissipator $\hat{D}[\hat{\rho}]$ we set out to find.
- The Eq. (4.24) only contains the density matrix at time $t = 0$ and time-independent operators, so is manifestly Markovian.
- If the \hat{L}_{μ} are Hermitian (observables), which does not have to be the case, we can write (4.24) as

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}'_S, \hat{\rho}_S(t)] - \frac{1}{2} \sum_{\mu} \kappa_{\mu} [\hat{L}_{\mu}, [\hat{L}_{\mu}, \hat{\rho}_S(t)]]. \quad (4.25)$$

We have now achieved a central goal of this course, all the equations (4.16), (4.17), (4.21) and (4.24) allow us to deal with the evolution of the system in $\hat{\rho}_S$ only, without having to explicitly model the environment. This only enters indirectly, through its correlation functions $\mathcal{C}(\tau)$, see (4.15).

We will devote the entire chapter 4 later, to non-Markovian techniques, based on (4.15).