Lecture 7

Learning goals

- To remind yourself (or just learn) about the concepts of density matrix, pure state, mixed state, and decoherence.
- To understand how the system-reservoir formalism is used for describing the behaviour of a quantum system coupled to environment (i.e., an open quantum system); phenomena such as decoherence and decay.
- To be able to derive the corresponding master equation and to solve it for the case of harmonic oscillators.
- To understand how spontanous emission is predicted by the master equation technique, and how the quantum nature of the reservoir (the quantized electromagnetic vacuum) plays a role there.

12 Open quantum systems and decoherence

Literature: P. Meystre and M. Sargent III, Elements of quantum optics (Springer), Chapters 13.3, 14.1; S.M. Barnett and P.M. Radmore, Methods in Theoretical Quantum Optics (Oxford University Press), Chapter 5.6

12.1 Density-matrix (recap)

The need for a density matrix can be motivated in the following way. One can have a system (say, of two levels e and g) in several different states.
Case 1: A quantum superposition state:

$$\frac{1}{\sqrt{2}}(|g\rangle + |e\rangle).$$

This has 50% probability of being in the ground and in the excited states. In addition, it is a coherent superposition, i.e. quantum interference effects etc. are possible.
Case 2: The system might be in a state that is probablistic, but totally classical: we just have 50% of probability of being in the ground and excited states, but no quantum coherence.
Case 3: The system has one more option, of being "in between" Case 1 and Case 2.
How to describe all the Cases 1, 2 and 3? Wavefunctions only describe the Case 1. Density matrices, instead, can describe all of them.

As an example, let us consider the system studied in previous lectures: a two-level atom and a quantized field. The basis states used were $|\sigma\rangle|n\rangle \equiv |\sigma n\rangle$ where $\sigma \in \{e, g\}$ and $n \in \mathcal{N}$ is the photon number. The general form of the wavefunction is

$$|\Psi(t)\rangle = \sum_{\sigma n} \alpha_{\sigma n}(t)|\sigma n\rangle. \tag{12.1}$$

The expectation value of an operator A is

$$\langle A(t)\rangle = \sum_{\sigma,\sigma',n,m} \alpha^*_{\sigma' m}(t)\alpha_{n\sigma}(t)\langle \sigma' m|A|\sigma n\rangle. \tag{12.2}$$

The density matrix of the state $|\Psi(t)\rangle$ is

$$\begin{aligned}\rho(t) =&|\Psi(t)\rangle\langle\Psi(t)| \\ =& \sum_{\sigma,\sigma',n,m} \alpha^*_{\sigma' m}(t)\alpha_{\sigma n}(t)|\sigma n\rangle\langle\sigma' m| \\ =& \sum_{\sigma,\sigma',n,m} \rho_{\sigma,n,\sigma',m}(t)|\sigma n\rangle\langle\sigma' m|.\end{aligned} \tag{12.3}$$

The density matrix is clearly an operator. Comparing Equations (12.2) and (12.3), the expectation value of an operator A can now be written in terms of the elements of the density matrix and becomes

$$\langle A(t)\rangle = \sum_{\sigma,\sigma',n,m} \rho_{\sigma,n,\sigma',m}(t)\langle\sigma' m|A|\sigma n\rangle = \sum_{\sigma,\sigma',n,m} \rho_{\sigma,n,\sigma',m}A_{\sigma',m,\sigma,n} = Tr\left[A\rho(t)\right]. \tag{12.4}$$

That is, finding the expectation value of A is equal to calculating the trace of the operator (or matrix) $A\rho(t)$. Reminder: the trace of a matrix M is $Tr[M] = \sum_n M_{nn}$, and the trace of an operator $\hat{O}$ is $Tr[\hat{O}] = \sum_n \langle n|\hat{O}|n\rangle$ where the states $|n\rangle$ form a complete basis.

The density matrix has several useful properties. It is Hermitian, normalized and also the trace operation has convenient properties such as cyclicity and invariance to unitarity transformations.

Physically, the density matrix has a simple interpretation. The diagonal elements $\rho_{\sigma,n,\sigma,n}$ give the probabilities (called populations) of being in state $n\sigma$ and the off-diagonal elements describe the quantum coherence, effectively telling how 'quantum' the state really is. For instance, in a simple two-level system example, the density matrix of the state $a|e\rangle + b|g\rangle$ is

$$\rho = \begin{pmatrix} \rho_{ee} & \rho_{eg} \\ \rho_{ge} & \rho_{gg} \end{pmatrix} = \begin{pmatrix} |a|^2 & ab^* \\ ba^* & |b|^2 \end{pmatrix}. \tag{12.5}$$

The diagonal elements ρ_{ee} and ρ_{gg} are the probablities $|a|^2$ and $|b|^2$. They are meaningful also classically. The terms ab^* and ba^* are meaningful only in the quantum case. In the totally classical (probablistic) case the density matrix would be

$$\rho = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}. \tag{12.6}$$

This could describe for instance the system at a finite temperature: the system has the probability $|b|^2$ of being in the ground state, but due to thermal fluctuations, it has also the probability $|a|^2$ of being in the excited state. Note that one can also have "intermediate", "partly quantum coherent" cases, where the density matrix is

$$\rho = \begin{pmatrix} |a|^2 & c \\ c^* & |b|^2 \end{pmatrix} \tag{12.7}$$

and $0 < |c| < |ab^*|$ (also, c can have any phase).

The fully quantum coherent states for which the density matrix is of the form (12.5) are called **pure states**. The condition for being in a pure state is $Tr[\rho\rho] = 1$. One can easily see that, for Equation (12.7), the purity condition $Tr[\rho\rho] = 1$ is valid only for the case $c = ab^*$, and $Tr[\rho\rho] < 1$ for the "not totally quantum coherent"

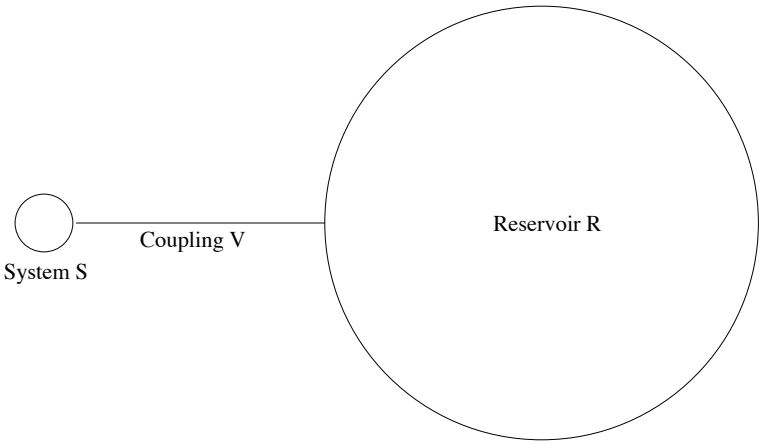

Figure 15: The system - reservoir interaction. The quantum mechanical system of interest (S) is coupled via some coupling (V) to a complicated larger system called the reservoir (R).

case $|c| < |ab^*|$. States of the form (12.6), and (12.7) with $c \neq ab^*$, are called **mixed states**. The process of pure states becoming mixed states, e.g. due to noise or other external disturbance, is called **decoherence**.
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12.2 Open quantum systems

An **open quantum system** refers to a situation where the quantum mechanical system of interest (S) is not completely isolated from the environment. Instead, there is some larger and more complicated system or environment, called a bath or a reservoir (R), to which the system (S) is coupled to, see Fig. 15. Assuming that the coupling (V) is weak, one can use perturbation theory to describe the interaction between S and R.

Notice that this approach is connected to the semi-classical approximation in which the reservoir (R) would be described fully classically and the system (S) quantum mechanically. In the following, the reservoir (R) is also quantized but we assume that its evolution is characterized by a short correlation (or coherence) time, i.e. the reservoir (R) has no memory of past interactions with the system (S). This is called the **Markov approximation** and it is a standard and important approximation. In recent years, many methods that go beyond the Markov approximation have been developed.

In general, there can be transfer of energy, momentum, particle number, etc., between the system and the reservoir. Although the combined entity, system (S) + reservoir (R), evolves according to unitary evolution, the evolution of the system (S) can be non-unitary. The system-reservoir interactions can thus, for a large enough reservoir, describe also non-unitary, non-coherent processes such as decay for the system (S). One should thus naturally use the density matrix formalism when describing system-reservoir interactions.

We will now show how this approach can be used to describe system-reservoir interactions in general, and how the method can be used for describing spontaneous emission in particular (the two-level atom is the system, and the many modes of the electro-magnetic vacuum is the reservoir). The Hamiltonian consists of the system, reservoir, and interaction Hamiltonians:

$$H = H_S + H_R + V. \tag{12.8}$$

We work in the interaction picture with

$$H_0 = H_S + H_R. \tag{12.9}$$

The equation of motion of a general density matrix in the interaction picture is (derived in the **Exercise set 7**)

$$\begin{aligned} \frac{d\rho_I}{dt} &= -\frac{i}{\hbar}\left[V_I(t), \rho_I(t)\right] \\ &= -\frac{i}{\hbar}\left[V_I(t), \rho_I(0)\right] - \frac{1}{\hbar^2}\int_0^t dt' \left[V_I(t), \left[V_I(t'), \rho_I(t')\right]\right]. \end{aligned} \tag{12.10}$$

This is called the **master equation** and it is a very important starting point for many calculations, as you will see also below. In our system-reservoir description, this gives the master equation for the total density matrix ρ_{TOT}

$$\frac{d\rho_{TOT}}{dt} = -\frac{i}{\hbar}\left[V_I(t), \rho_{TOT}(t)\right]. \tag{12.11}$$

The initial condition is taken to be

$$\rho_{TOT}(0) = \rho(0) \otimes \rho_R(0), \tag{12.12}$$

where

$$\rho(t) = Tr_R\left(\rho_{TOT}(t)\right) \tag{12.13}$$

is the **reduced density matrix** of the system (S), i.e. the reservoir degrees of freedom have been traced out. Similarly, ρ_R is the reduced density matrix of the reservoir where the system (S) degrees of freedom have been traced out. Note that it is only in the beginning (time zero) that one can assume the direct product form of Equation (12.12); later, due to the interaction, the system and the reservoir become **entangled** and one can no longer assume such a simple decomposition. (Entanglement: for instance, $|\Psi\rangle = a|a\rangle_S|a'\rangle_R + b|b\rangle_S|b'\rangle_R$ cannot be expressed as a direct product of the system and reservoir wavefunctions $|\psi\rangle_S|\phi\rangle_R$. Tracing out R would give $Tr_R[|\Psi\rangle\langle\Psi|] = |a|^2|a\rangle_{SS}\langle a| + |b|^2|b\rangle_{SS}\langle b|$ whereas if the system was in a pure state $a|a\rangle_S + b|b\rangle_S$ the density matrix would contain also the coherence terms ab^*, a^*b, not only $|a|^2$, $|b|^2$. In other words, entanglement (correlations) with the reservoir and then tracing out the reservoir may destroy coherence, partially or completely.)

As usual, one can integrate and iterate Equation (12.11) to obtain

$$\begin{aligned} &\rho_{TOT}(t) = \rho_{TOT}(0) \\ &+ \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \left[V_I(t_1), \left[V_I(t_2), \cdots \left[V_I(t_n), \rho_{TOT}(0)\right]\right]\right]. \end{aligned} \tag{12.14}$$

In the system-reservoir treatment, one is primarily interested in the evolution of the system only. Thus we trace out the reservoir degrees of freedom to obtain the evolution of the reduced density matrix of the system (S):

$$\rho(t) = \rho(0) + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n Tr_R \left([V_I(t_1), [V_I(t_2), \cdots [V_I(t_n), \rho_R(0) \otimes \rho(0)]]]\right). \tag{12.15}$$

One can write this formally as

$$\rho(t) = (1 + U_1(t) + U_2(t) + \cdots)\, \rho(0) \equiv U(t)\rho(0). \tag{12.16}$$

Now take the time derivative

$$\frac{d\rho(t)}{dt} = \dot{U}(t)\rho(0) = \dot{U}(t)U^{-1}(t)\rho(t) = \left(\dot{U}_1(t) + \dot{U}_2(t) + \cdots\right) U^{-1}(t)\rho(t). \tag{12.17}$$

The term $\dot{U}_1$ is in usual cases zero. It is proportional to terms of the form $Tr_R(V(t)\rho_R)$, and typically $V(t)$ creates or destroys an excitation in the reservoir, therefore the trace becomes zero if there are no special correlations in the reservoir. Now we assume a reservoir for which $Tr_R(V(t)\rho_R) = 0$ and thus $\dot{U}_1 = 0$. We are aiming at doing perturbation theory with respect to V, so next we observe that $\dot{U}_2 \propto V^2$ and $U^{-1}(t) \propto 1 + V + V^2 + \cdots$. Thus the perturbation theory up to second order gives the result

$$\frac{d\rho(t)}{dt} \simeq \dot{U}_2(t)\rho(t) = \frac{-1}{\hbar^2} \int_0^t dt_1 Tr_R \left([V_I(t), [V_I(t_1), \rho_R \otimes \rho(t)]]\right). \tag{12.18}$$

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12.2.1 Example: the damped harmonic oscillator

Now we will calculate what the second order master equation (12.18) actually gives for a specific example where the system S is a harmonic oscillator of the frequency ω_0 and the reservoir R (also called the bath) is formed by a large number of other oscillators with the frequencies ω_j. This is a basic model that can be easily expanded to describe many physical situations. The interaction Hamiltonian in the interaction picture is

$$V_I(t) = \hbar \left(a^\dagger \Gamma(t) e^{i\omega_0 t} + a\Gamma^\dagger(t) e^{-i\omega_0 t}\right), \tag{12.19}$$

where $\Gamma(t) = \sum_j g_j b_j e^{-i\omega_j t}$, a and b_j are the annihilation operators for the system and the reservoir excitations, respectively, and g_j are the coupling constants between the system and the j^{th} reservoir mode. Here Γ are also sometimes called the noise operators, because the reservoir interaction describes noise from the point of view of the system S. Inserting this V_I into Equation (12.18) one obtains terms with different orderings of the operators a, $a^\dagger$ and $\rho(t)$, due to the commutators, and the terms are multiplied by the integrals I_i given below (c.f. **Exercise Set 7**). Note

the trace over the reservoir degrees of freedom, therefore the noise operators Γ lead simply to some complex numbers after taking the trace. In other words,

$$\frac{d\rho(t)}{dt} = -\frac{1}{\hbar} f(a, a^\dagger, \rho(t), I_i), \tag{12.20}$$

where the form of f is derived in the exercises. The integrals are

$$I_1 = \int_0^t dt_1 \langle \Gamma(t)\Gamma(t_1)\rangle_R e^{i\omega_0(t+t_1)} \tag{12.21}$$

$$I_2 = \int_0^t dt_1 \langle \Gamma^\dagger(t)\Gamma^\dagger(t_1)\rangle_R e^{-i\omega_0(t+t_1)} \tag{12.22}$$

$$I_3 = \int_0^t dt_1 \langle \Gamma(t)\Gamma^\dagger(t_1)\rangle_R e^{i\omega_0(t-t_1)} \tag{12.23}$$

$$I_4 = \int_0^t dt_1 \langle \Gamma^\dagger(t)\Gamma(t_1)\rangle_R e^{-i\omega_0(t-t_1)}. \tag{12.24}$$

One can write explicitly the correlators, e.g.

$$\langle \Gamma^\dagger(t)\Gamma(t_1)\rangle_R = \sum_{i,j} g_i g_j \langle b_i^\dagger b_j\rangle_R e^{i(\omega_i t - \omega_j t_1)}. \tag{12.25}$$

For a usual thermal reservoir $\langle b_i b_j\rangle_R = Tr_R[b_i b_j \rho_R] = 0$ and $\langle b_i^\dagger b_j^\dagger\rangle_R = 0$, thus $I_1 = I_2 = 0$ (this could be different for some exotic reservoirs with special correlations, e.g. a "squeezed reservoir"). For a thermal reservoir of harmonic oscillators, one has

$$\langle b_i^\dagger b_j\rangle_R = Tr_R[b_i^\dagger b_j \rho_R] = \bar{n}_i \delta_{ij} \tag{12.26}$$

$$\langle b_i b_j^\dagger\rangle_R = Tr_R[b_i b_j^\dagger \rho_R] = (\bar{n}_i + 1)\delta_{ij}. \tag{12.27}$$

Here $\bar{n}$ is the average occupation number. The reservoir is assumed to be large and thus one can replace the discrete summations and quantities by ones that are continuous in frequency, e.g. $\bar{n}_i \to \bar{n}(\omega)$ and $g_i \to g(\omega)$. The integrals become (derivation in **Exercise Set 7**)

$$I_3 = \frac{\gamma}{2}(\bar{n}(\omega_0) + 1) - i\Delta \tag{12.28}$$

$$I_4 = \frac{\gamma}{2}\bar{n}(\omega_0) - i\Delta'. \tag{12.29}$$

Here

$$\gamma = \rho_{dos}(\omega_0) g^2(\omega_0), \tag{12.30}$$

ρ_{dos} is the density of states that enters when changing the summations into integrals (please do not confuse it with some density matrix...), and

$$\Delta = P\left[\int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \frac{1}{\epsilon} \rho_{dos}(\epsilon + \omega_0) g^2(\epsilon + \omega_0)(\bar{n}(\epsilon + \omega_0) + 1)\right], \tag{12.31}$$

where P denotes the principal value (Δ' is similar, but the "1" is missing from $(\bar{n}(\epsilon + \omega_0) + 1)$). The Δ (Δ') is the **Lamb shift** and is usually very small; it will be neglegted in this lecture from now on (it would simply shift the energy levels of the system S slightly due to the reservoir interaction). As said before, $\bar{n}$ is the average

occupation number in a thermal (temperature T) reservoir of harmonic oscillators, that is, $\bar{n}(\omega_0) = 1/(e^{\hbar\omega_0/(kT)} - 1)$.

Combining the above, one obtains the final result for the master equation:

$$\begin{aligned} \frac{d\rho}{dt} &= \frac{\gamma}{2}(\bar{n}(\omega_0)+1)\left(2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a\right) \\ &+ \frac{\gamma}{2}\bar{n}(\omega_0)\left(2a^\dagger\rho a - aa^\dagger\rho - \rho aa^\dagger\right). \end{aligned} \tag{12.32}$$

This is a very important basic result and can be used in various contexts to describe system-reservoir interactions and, e.g., decay processes.

One can now easily calculate the time evolution of various quantities. For instance, the expectation value $\langle a\rangle$ behaves as (derivation in **Exercise Set 7**)

$$\frac{d\langle a\rangle}{dt} = \frac{d}{dt}Tr(a\rho) = Tr\left(a\frac{d\rho}{dt}\right) = -\frac{\gamma}{2}Tr(a\rho), \tag{12.33}$$

which gives

$$\langle a(t)\rangle = \langle a(0)\rangle e^{-\gamma t/2}. \tag{12.34}$$

The quantity $\langle a(t)\rangle$ tells about the phase coherence of the oscillator. Thus, the result given by the master equation says that, due to the coupling to the reservoir, the phase coherence, i.e. the quantum coherence, of the system S decays exponentially with the rate $\gamma/2$ (reminder: γ contains the density of states in the reservoir and the strength of the system-reservoir coupling, so the result is intuitive). This decay describes the process of **decoherence**: when a small quantum system is coupled to a much larger reservoir (in some contexts one can call the reservoir "noise"), the quantum coherence of the system decays, and initial pure states become mixed states. The exponential form of the decay basically follows from assuming that the reservoir is large, i.e. that the system is coupled to a continuum of reservoir states. With some other structure of the reservoir states, the time-dependence of the decay could be non-exponential. Similarly, one can show (**Exercise Set 7**) by considering $\frac{d\langle n(t)\rangle}{dt} = \frac{d}{dt}Tr\left(a^\dagger a\rho\right)$ that the mean occupation number will exponentially approach that of the reservoir:

$$\langle n(t)\rangle = \langle n(0)\rangle e^{-\gamma t} + \bar{n}(1 - e^{-\gamma t}). \tag{12.35}$$

This is also intuitive: the mean occupation number is related to the energy, and by interacting with the reservoir, the system S becomes thermalized with it and obtains the same average energy.
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12.2.2 Spontaneous emission

To describe spontaneous emission, one can use the above treatment but with certain modifications. First, the system S is now the two-level atom, not a harmonic oscillator. In our treatment of the two-level atom interacting with the quantized field in Lecture 6, we described the interaction between the atom and one mode (one frequency) of the light field. In reality, the atom is often interacting with a continuum of light modes (except when one uses e.g. an optical cavity that restricts

the modes, or monochromatic laser light); in particular, this is the case in spontaneous emission where the atom interacts with the continuum of the available modes in the quantized electromagnetic vacuum field. This continuum of modes is now the reservoir. Now, the reservoir is at zero temperature and its average photon number is zero. The Hamiltonian of the system is (c.f. Lecture 6)

$$H = \frac{1}{2}\hbar\omega_0\sigma_z + \sum_j \hbar\omega_j b_j^\dagger b_j + \hbar(\sigma_+\Gamma + \sigma_-\Gamma^\dagger). \tag{12.36}$$

Here we have denoted $\omega_0 = \omega_{eg}$, $\Gamma = \sum_j g_j b_j$, and ω_j are the frequencies of the quantized vacuum field modes. The Hamiltonian is the same as the starting point of the harmonic oscillator example above, with the replacement $a \to \sigma_-$. Furthermore, we now have zero average photons in the reservoir ($T = 0$), that is, $\bar{n} = 0$. The master equation can thus be directly written based on the harmonic oscillator result (12.32) and using $\bar{n} = 0$:

$$\frac{d\rho}{dt} = \frac{\gamma}{2}\left(2\sigma_-\rho\sigma_+ - \sigma_+\sigma_-\rho - \rho\sigma_+\sigma_-\right). \tag{12.37}$$

Like in the harmonic oscillator example, the coherence term $\rho_{ge} = \langle\sigma_-\rangle$ becomes

$$\langle\sigma_-(t)\rangle = e^{-\frac{\gamma}{2}t}\langle\sigma_-(0)\rangle, \tag{12.38}$$

i.e. there is again decoherence: the coherence term decays exponentially with the rate $\gamma/2$. And the probability of being in the upper state

$$P_{ee}(t) = \rho_{ee}(t) = \langle\sigma_+(t)\sigma_-(t)\rangle = e^{-\gamma t}P_e(0). \tag{12.39}$$

This means that the population of the excited state decays exponentially with the rate γ. Note that this spontaneous emission occurs also at zero temperature and for the vacuum field, i.e. zero average photon number in the reservoir. Remember that the master equation (12.32) has two terms, proportional to $(\bar{n}(\omega_0) + 1)$ and $\bar{n}(\omega_0)$. The "1" in the former comes solely from quantizing the vacuum field, that is, from the orderings of the reservoir operators b and $b^\dagger$ within the integrals (12.23) and (12.24), see Equations (12.26) and (12.27). Since $\bar{n} = 0$ for the zero temperature vacuum, without the "1" there would not be any decay of the excited state population. The quantization of the electromagnetic field is thus required to explain spontaneous emission. Spontaneous emission is the phenomenon on which LEDs are based, and it also gives the fundamental quantum noise limit of lasers and amplifiers. Using the master equation techniques, also the spectrum of spontaneous emission could be calculated. Note that spontaneous emission can be modified (enhanced, suppressed, spectrally changed) by modifying the available reservoir modes, for instance by placing the atom in a cavity supporting only selected modes. For instance, the modification of spontaneous emission rate due to an optical cavity is known under the name Purcell effect.