

## Lecture 15: Decoherence - master equations

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## I. MASTER EQUATIONS

We follow the derivation of master equations that can be found in *eg*[1] . Let us start with the system-bath model Hamiltonian.

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_{SB} + \mathcal{H}_{bath}, \quad (1)$$

$$\mathcal{H}_S = \hbar \sum_i \omega_i |i\rangle \langle i|, \quad (2)$$

$$\mathcal{H}_{SB} = \hat{A} \hat{f}. \quad (3)$$

The system is assumed to be a multilevel system with energy eigenstates  $|i\rangle$  and energy levels  $\hbar\omega_i$ . In the interaction Hamiltonian,  $\hat{A}$  consists of only system variables and  $\hat{f}$  is a bath operator. In Schrodinger picture, the density matrix  $\rho_{SR}$  for the system+bath varies according to

$$i\hbar\dot{\rho}_{SR} = [\mathcal{H}, \rho_{SR}]. \quad (4)$$

Then we move into the interaction picture, where

$$\rho_I = e^{\frac{i}{\hbar}(\mathcal{H}_S + \mathcal{H}_{bath})t} \rho e^{-\frac{i}{\hbar}(\mathcal{H}_S + \mathcal{H}_{bath})t} \quad (5)$$

$$\mathcal{H}_I = e^{\frac{i}{\hbar}(\mathcal{H}_S + \mathcal{H}_{bath})t} \mathcal{H}_{SB} e^{-\frac{i}{\hbar}(\mathcal{H}_S + \mathcal{H}_{bath})t}. \quad (6)$$

We have

$$\mathcal{H}_I = e^{i\sum_j \omega_j |j\rangle \langle j| t} \hat{A} \hat{f}(t) e^{-i\sum_k \omega_k |k\rangle \langle k| t} \quad (7)$$

$$= \sum_{j,k} e^{i(\omega_j - \omega_k)t} |j\rangle \langle j| \hat{A} \hat{f}(t) |k\rangle \langle k| \quad (8)$$

$$= \sum_{j,k} e^{i(\omega_j - \omega_k)t} \langle j| \hat{A} |k\rangle |j\rangle \langle k| \hat{f}(t) \quad (9)$$

$$= \sum_{j,k} |j\rangle \langle k| A_{jk} e^{i(\omega_j - \omega_k)t} \hat{f}(t) \quad (10)$$

where

$$\hat{f}(t) = e^{\frac{i}{\hbar}\mathcal{H}_{bath}t} \hat{f} e^{-\frac{i}{\hbar}\mathcal{H}_{bath}t} \quad (11)$$

and we used the fact that  $e^{i\sum_j \omega_j |j\rangle \langle j| t} = \sum_j e^{i\omega_j t} |j\rangle \langle j|$  ( $\mathcal{H}_S$  is diagonal in the  $\{|j\rangle\}$  basis) and  $[\hat{f}(t), |j\rangle \langle j|] = 0$ .

Equation 4 for the time evolution of the density matrix can be rewritten in the interaction picture:

$$\dot{\rho}_I = -\frac{i}{\hbar}[\mathcal{H}_I, \rho_I]. \quad (12)$$

We can derive

$$\rho_I(t) = -\frac{i}{\hbar} \int_0^t [\mathcal{H}_I(t'), \rho_I(t')] dt' + \rho_I(0) \quad (13)$$

$$\dot{\rho}_I(t) = -\frac{i}{\hbar}[\mathcal{H}_I(t), \rho_I(0)] - \frac{1}{\hbar^2} \int_0^t [\mathcal{H}_I(t), [\mathcal{H}_I(t'), \rho_I(t')]] dt'. \quad (14)$$

At this point, we apply:

1. Born approximation (weak coupling assumption):  $\rho_I(t) = \rho_{bath} \otimes \rho(t)$ , assuming that  $H_{SB}$  is much less than either  $\mathcal{H}_{bath}$  or  $\mathcal{H}_s$  and the bath density matrix is not significantly affected by the interaction;
2. Markov approximation:  $\rho_I(t') = \rho_I(t)$ , assuming that the rate of change of the interaction picture system density operator is low compared to that of the bath operator.

Tracing out the part of  $\rho_I$  that is related with the bath, which is  $\rho(t) = \text{Tr}_{bath}[\rho_I(t)]$ , gives

$$\begin{aligned} \dot{\rho}(t) &= -\frac{i}{\hbar} \text{Tr}_{bath}[\mathcal{H}_I(t), \rho_I(0)] - \frac{1}{\hbar^2} \int_0^t \text{Tr}_{bath}[\mathcal{H}_I(t), [\mathcal{H}_I(t'), \rho_{bath} \otimes \rho(t)]] dt' \\ &= -\frac{i}{\hbar} \text{Tr}_{bath}[\mathcal{H}_I(t), \rho_I(0)] - \frac{1}{\hbar^2} \int_0^t \text{Tr}_{bath}[\mathcal{H}_I(t) \mathcal{H}_I(t') \rho_I(t) - \mathcal{H}_I(t) \rho_I(t) \mathcal{H}_I(t') \\ &\quad - \mathcal{H}_I(t') \rho_I(t) \mathcal{H}_I(t) + \rho_I(t) \mathcal{H}_I(t') \mathcal{H}_I(t)] dt'. \end{aligned} \quad (15)$$

. We assume  $\text{Tr}_{bath}[\mathcal{H}_I(t), \rho_I(0)] = 0$ . This holds if the bath part  $f$  of the interaction Hamiltonian has zero expectation value over the density matrix of the environment at the initial time. If this is not the case, this component can be introduced as an additional component to the system Hamiltonian.

We calculate next the first term in the second integral of Eq. (16).

$$\frac{1}{\hbar^2} \int_0^t \text{Tr}_{\text{bath}}[\mathcal{H}_I(t)\mathcal{H}_I(t')\rho_I(t)] \quad (17)$$

$$= \frac{1}{\hbar^2} \int_0^t \text{Tr}_{\text{bath}} \left[ \sum_{jk} |j\rangle\langle k| A_{jk} e^{i\omega_{jk}t} \hat{f}(t) \sum_{j'k'} |j'\rangle\langle k'| A_{j'k'} e^{i\omega_{j'k'}t'} \hat{f}(t') \rho_{\text{bath}} \otimes \rho(t) \right] dt' \quad (18)$$

$$= \frac{1}{\hbar^2} \int_0^t \sum_{jkk'} |j\rangle\langle k'| \rho(t) A_{jk} A_{kk'} e^{i\omega_{jk}t - i\omega_{k'k}t'} \text{Tr}_{\text{bath}}[\hat{f}(t)\hat{f}(t')\rho_{\text{bath}}] \quad (19)$$

$$= \frac{1}{\hbar^2} \sum_{jkk'} A_{jk} A_{kk'} |j\rangle\langle k'| \rho(t) \int_0^t e^{i\omega_{jk}t - i\omega_{k'k}t'} \langle \hat{f}(t)\hat{f}(t') \rangle dt'. \quad (20)$$

We defined  $\omega_{jk} = \omega_j - \omega_k$ . We assume stationary noise, that is

$$\langle \hat{f}(t)\hat{f}(t') \rangle = \langle \hat{f}(t-t')\hat{f}(0) \rangle. \quad (21)$$

(This is the case when the expectation value is defined over a thermal state of the environment, or in general any density matrix which commutes with the environment Hamiltonian). We can define the power spectrum of the noise as the Fourier transform of its time correlation<sup>1</sup>:

$$S(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle \hat{f}(\tau)\hat{f}(0) \rangle \quad (22)$$

$$\langle \hat{f}(\tau)\hat{f}(0) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\tau} S(\omega) \quad (23)$$

Assuming that the noise has a short correlation time, we can replace the lower limit of the

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<sup>1</sup> The proof for the fact that the Fourier transform of the autocorrelation is equal to the power spectral density of the noise can be found in [2], section 1.3

time integral in Eq. (20) with  $-\infty$ . Eq. (20) can be rewritten as

$$\frac{1}{\hbar^2} \int_0^t \text{Tr}_{\text{bath}}[\mathcal{H}_I(t)\mathcal{H}_I(t')\rho_I(t)] \quad (24)$$

$$= \frac{1}{2\pi\hbar^2} \sum_{jkk'} A_{jk} A_{kk'} |j\rangle\langle k'| \rho(t) \int_{-\infty}^t e^{i\omega_{jk}t - i\omega_{k'k}t'} \int_{-\infty}^{\infty} e^{-i\omega(t-t')} S(\omega) d\omega dt' \quad (25)$$

$$= \frac{1}{2\pi\hbar^2} \sum_{jkk'} A_{jk} A_{kk'} |j\rangle\langle k'| \rho(t) \int_{-\infty}^{\infty} d\omega S(\omega) e^{i(\omega_{jk} - \omega_{k'k})t} \int_{-\infty}^t e^{i(\omega - \omega_{k'k})(t' - t)} dt' \quad (26)$$

$$= \frac{1}{2\hbar^2} \sum_{jkk'} A_{jk} A_{kk'} |j\rangle\langle k'| \rho(t) e^{i(\omega_{jk} - \omega_{k'k})t} \int_{-\infty}^{\infty} d\omega S(\omega) \delta(\omega - \omega_{k'k}) \quad (27)$$

$$= \frac{1}{2\hbar^2} \sum_{jkk'} A_{jk} A_{kk'} |j\rangle\langle k'| \rho(t) e^{i(\omega_{jk} - \omega_{k'k})t} S(\omega_{k'k}) \quad (28)$$

$$\approx \frac{1}{2\hbar^2} \sum_{jk} |A_{jk}|^2 |j\rangle\langle j| \rho(t) S(\omega_{jk}) \quad (29)$$

where

$$\frac{1}{2\pi} \int_{-\infty}^t e^{i(\omega - \omega_{k'k})(t' - t)} dt' = -\frac{1}{2\pi} \int_{\infty}^0 e^{-i(\omega - \omega_{k'k})(t - t')} d(t - t') = \frac{1}{2} \delta(\omega - \omega_{k'k}) \quad (30)$$

In the case of  $k' \neq j$ , all the terms with  $e^{i(\omega_{jk} - \omega_{k'k})t}$  in Eq. (28) will be average out by the rotating wave approximation.

The other terms in the integral of Eq. (16) can be calculated in a similar way. The second term

$$\frac{1}{\hbar^2} \int_0^t \text{Tr}_{\text{bath}}[\mathcal{H}_I(t)\rho_I(t)\mathcal{H}_I(t')] \quad (31)$$

$$= \frac{1}{\hbar^2} \int_0^t \sum_{jkj'k'} |j\rangle\langle k| \rho(t) |j'\rangle\langle k'| A_{jk} A_{j'k'} e^{i\omega_{jk}t} e^{i\omega_{j'k'}t'} \langle \hat{f}(t') \hat{f}(t) \rangle dt' \quad (32)$$

$$= \frac{1}{2\pi\hbar^2} \sum_{jkj'k'} |j\rangle\langle k| \rho(t) |j'\rangle\langle k'| A_{jk} A_{j'k'} e^{i(\omega_{jk} + \omega_{j'k'})t} \int_{-\infty}^{\infty} d\omega S(\omega) \int_0^t e^{-i(\omega - \omega_{j'k'})(t' - t)} dt' \quad (33)$$

$$= \frac{1}{2\hbar^2} \sum_{jkj'k'} |j\rangle\langle k| \rho(t) |j'\rangle\langle k'| A_{jk} A_{j'k'} e^{i(\omega_{jk} + \omega_{j'k'})t} S(\omega_{j'k'}) \quad (34)$$

$$\approx \frac{1}{2\hbar^2} \sum_{jk} |j\rangle\langle k| \rho(t) |k\rangle\langle j| |A_{jk}|^2 S(-\omega_{jk}) \quad (35)$$

The third term  $\frac{1}{\hbar^2} \int_0^t \text{Tr}_{\text{bath}}[\mathcal{H}_I(t')\rho_I(t)\mathcal{H}_I(t)]$  has the same expression as Eq. (35).

The fourth term:

$$\frac{1}{\hbar^2} \int_0^t \text{Tr}_{\text{bath}}[\rho_I(t) \mathcal{H}_I(t') \mathcal{H}_I(t)] \quad (36)$$

$$= \frac{1}{2\hbar^2} \sum_{jkk'} \rho(t) |j\rangle \langle k'| A_{jk} A_{kk'} e^{i(\omega_{jk} + \omega_{kk'})t} S(\omega_{jk}) \quad (37)$$

$$\approx \frac{1}{2\hbar^2} \sum_{jk} \rho(t) |j\rangle \langle j| |A_{jk}|^2 S(\omega_{jk}) \quad (38)$$

Altogether, the master equation Eq. (16) in the Born-Markov approximation is

$$\dot{\rho}(t) = \frac{1}{2\hbar^2} \sum_{jk} |A_{jk}|^2 S(\omega_{jk}) [2|k\rangle \langle j| \rho(t) |j\rangle \langle k| - \rho(t) |j\rangle \langle j| - |j\rangle \langle j| \rho(t)]. \quad (39)$$

For a qubit, we consider the sum above with  $j, k = 0, 1$ . In the following we consider the difference in the effect of the qubit for high-frequency noise (around the qubit frequency) and low-frequency noise.

### A. High-frequency noise

We take a two level system with a transition frequency  $\omega_{10} = \omega_1 - \omega_0 \neq 0$ . We assume the environmental noise to be such that the low frequency noise is negligible, that is we take  $S(0) = 0$ . This is for example the case for coupling to the free electromagnetic field. The density of states vanishes around zero frequency which results in this contribution being negligible. In 39 only the terms for which  $j \neq k$  in the expression for the spectral density are kept. We find

$$\dot{\rho}(t) = \Gamma_{1 \rightarrow 0} [\hat{\sigma}_- \rho(t) \hat{\sigma}_+ - \frac{1}{2} \hat{\sigma}_+ \hat{\sigma}_- \rho(t) - \frac{1}{2} \rho(t) \hat{\sigma}_+ \hat{\sigma}_-] + \Gamma_{0 \rightarrow 1} [\hat{\sigma}_+ \rho(t) \hat{\sigma}_- - \frac{1}{2} \hat{\sigma}_- \hat{\sigma}_+ \rho(t) - \frac{1}{2} \rho(t) \hat{\sigma}_- \hat{\sigma}_+] \quad (40)$$

In the superoperator form,

$$\dot{\rho}(t) = \Gamma_{1 \rightarrow 0} \mathcal{D}[\hat{\sigma}_-] \rho(t) + \Gamma_{0 \rightarrow 1} \mathcal{D}[\hat{\sigma}_+] \rho(t) \quad (41)$$

where  $\mathcal{D}[\hat{\sigma}] \rho(t) \rightarrow \hat{\sigma} \rho(t) \hat{\sigma}^\dagger - \frac{1}{2} \hat{\sigma}^\dagger \hat{\sigma} \rho(t) - \frac{1}{2} \rho(t) \hat{\sigma}^\dagger \hat{\sigma}$  is the damping operator. So, the relaxation rate:

$$\Gamma_{1 \rightarrow 0} = \frac{1}{\hbar^2} |A_{10}|^2 S(\omega_{10}) \quad (42)$$

$$\Gamma_{0 \rightarrow 1} = \frac{1}{\hbar^2} |A_{10}|^2 S(\omega_{01}). \quad (43)$$

The two rates in equations 42 and 43 are different due to the difference between  $S(\omega_{10})$  and  $S(\omega_{01}) = S(-\omega_{10})$ . This difference stems from the difference between the expectation values  $\langle \hat{f}(t')\hat{f}(t) \rangle$  and  $\langle \hat{f}(t)\hat{f}(t') \rangle$ . If  $f$  was a classical variable, we would have  $\langle f(t')f(t) \rangle = \langle f(t)f(t') \rangle$ ; however, commutation of operators defined at different times do not commute in general. We have the following important result:

$$S(-\omega) = e^{-\beta\omega} S(\omega). \quad (44)$$

This result holds quite generally for any physical system which is in equilibrium at temperature  $T = 1/k_B\beta$ .

One first important manifestation of this result is the detailed balance condition. We take a qubit in a mixed state (coherence between states  $|0\rangle$  and  $|1\rangle$  always vanishes after a long enough time). With  $P_0$  and  $P_1$  the populations for the two qubit states the condition of stationarity for the population is

$$P_0\Gamma_{0\rightarrow 1} = P_1\Gamma_{1\rightarrow 0}. \quad (45)$$

This is the detailed balance condition. Together with equation 44 it implies

$$\frac{P_1}{P_0} = e^{-\beta\hbar\omega_{10}}. \quad (46)$$

We find that the steady state of the qubit is characterized by a ratio of the populations given by the Boltzmann factor, with the temperature being the environment temperature.

The evolution of the populations is given by the following coupled equation

$$\frac{dP_0}{dt} = -\Gamma_{0\rightarrow 1}P_0 + \Gamma_{1\rightarrow 0}P_1 \quad (47)$$

$$\frac{dP_1}{dt} = -\Gamma_{1\rightarrow 0}P_1 + \Gamma_{0\rightarrow 1}P_0. \quad (48)$$

Starting with an arbitrary population  $P_1(t) - P_0(t)$  the steady state is reached with a decay rate

$$\Gamma_1 = \Gamma_{1\rightarrow 0} + \Gamma_{0\rightarrow 1}. \quad (49)$$

The inverse

$$T_1 = 1/\Gamma_1 \quad (50)$$

of this rate is called the *relaxation time* or the  $T_1$  *time* of the qubit. At low temperatures,  $\hbar\omega_{10} \gg k_B T$ , the dominant component of 49 is  $\Gamma_{1\rightarrow 0}$  so  $T_1 \approx 1/\Gamma_{1\rightarrow 0}$ .

We examine next the decay time of the off-diagonal elements of the density matrix in 40. We have

$$\dot{\rho}_{01} = -\frac{\Gamma_{1 \rightarrow 0} + \Gamma_{1 \rightarrow 0}}{2}\rho_{01}. \quad (51)$$

The coherence decay on a time scale called the *dephasing time* or  $T_2$  *time*. We have

$$T_2 = 2T_1 \quad (52)$$

We stress the point that this relation between the relaxation and dephasing times is a result of the absence of noise at low frequency. The  $T_1/T_2$  terminology comes from the field nuclear magnetic resonance, where the two decay times are associated with physically distinct processes.

## B. Low-frequency noise

We consider the possibility that the environment has noise at zero frequency. The dephasing process of a qubit is characterized by the Eq. 39 when  $j = k$  and also a contribution we left out in 31 (terms with  $j = k$ ,  $j' = k'$ , but excluding  $j = j'$ , which has already been taken into account). This leads to a term on the RHS of (40)

$$\dot{\rho}(t) = \Gamma_{\varphi} \mathcal{D}[\hat{\sigma}_z] \rho(t) \quad (53)$$

where the dephasing rate is

$$\Gamma_{\varphi} = \frac{1}{2\hbar^2}(|A_{11} - A_{00}|^2)S(0). \quad (54)$$

The addition of this term leads to

$$\dot{\rho}_{01} = -\frac{\Gamma_{1 \rightarrow 0} + \Gamma_{1 \rightarrow 0}}{2}\rho_{01} - \Gamma_{\varphi}\rho_{01}. \quad (55)$$

The total dephasing time is therefore given by

$$\frac{1}{T_2} = \frac{1}{2T_1} + \frac{1}{T_{\varphi}} \quad (56)$$

with

$$T_{\varphi} = \frac{1}{\Gamma_{\varphi}}. \quad (57)$$



$T_\varphi$  is called the *pure dephasing time* to distinguish it from the dephasing time  $2T_1$  connected to the relaxation time.  $T_\varphi$  ranges between 0 (when low frequency noise dominates) and  $\infty$  when dephasing is limited by relaxation. In superconducting qubits,  $T_\varphi$  may be significant depending on the type of qubit considered and details of the implementation.

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- [1] H. Carmichael, *An Open Systems Approach to Quantum Optics* (1993).
  - [2] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II*, 2nd ed., edited by H. K. V. Lotsch, Springer Series in Solid-State Sciences, Vol. 2 (Springer Verlag, 1991).

