

# Introduction to the Theory of Open Quantum Systems

Lecture notes, SoSe 2023

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These notes are still in continual development  
and will be regularly updated in the ISIS course.



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# Chapter 1

## Basics

### 1.1 Motivation: Why Open Quantum Systems?

#### Observation 1:

- *Classical mechanics*: 2nd Newton

$$m\ddot{x} = F$$

describes conservative and dissipative forces. E.g. Harmonic oscillator

$$F_{\text{cons}} = -kx, \quad F_{\text{diss}} = -m\gamma\dot{x},$$

gives equation of motion

$$\ddot{x} + \gamma\dot{x} + \omega^2 x = 0$$

where  $\omega = \sqrt{k/m}$ .

- *Standard quantum mechanics course*: Schrödinger equation (no hats!)

$$i\hbar\partial_t|\psi(t)\rangle = H|\psi(t)\rangle \tag{1.1}$$

can only describe conservative systems. Proof: Time-evolution of expectation values

$$d_t\langle H \rangle = \frac{1}{i\hbar}\langle [H, H] \rangle + \langle \partial_t H \rangle = 0.$$

Schrödinger Equation cannot describe dissipative dynamics.

How to describe dissipation in q.m.? Harmonic oscillator (no dissipation)

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2$$

with canonically conjugated variables  $[x, p] = i\hbar$ . Consider Heisenberg equations of motion

$$\dot{x}(t) = \frac{p(t)}{m}, \quad \dot{p}(t) = -m\omega^2 x(t),$$

where the equation for  $p(t)$  is the “quantized version of 2nd Newton”. Naive idea: Add dissipative force by hand

$$\dot{x}(t) = \frac{p(t)}{m}, \quad \dot{p}(t) = -m\omega^2 x(t) - \gamma p(t).$$

But then:

$$d_t[x(t), p(t)] = [\dot{x}(t), p(t)] + [x(t), \dot{p}(t)] = -\gamma[x(t), p(t)]$$

and therefore the commutator decays

$$[x(t), p(t)] = e^{-\gamma t}[x(0), p(0)] = e^{-\gamma t}i\hbar,$$

for which the Heisenberg uncertainty relation becomes

$$\Delta x \Delta p \geq \frac{\hbar}{2} e^{-\gamma t}.$$

However this is inconsistent since we expect that dissipation leads the dynamics into the ground state of the harmonic oscillator so the standard uncertainty relation still must apply.

**Conclusion 1:** Schrödinger/Heisenberg equations cannot describe dissipative dynamics.

### Observation 2:

- *Statistical mechanics:* System weakly coupled (what does that mean?) to a “heat bath” (what does that mean?) of temperature  $T$  will relax to canonical ensemble

$$\varrho_{th} = \frac{e^{-H/(k_B T)}}{Z} \quad (1.2)$$

Reminder: Density matrix - statistical mixture of pure quantum states

$$\varrho = \sum_n p_n |\phi_n\rangle \langle \phi_n| \quad (1.3)$$

hermitian operator that describes a quantum system that is with classical probability  $p_n$  in state  $|\phi_n\rangle$  (all  $|\phi_n\rangle$  orthogonal).

- *Quantum mechanics:* Time evolution: von-Neumann equation (apply Schrödinger equation to Eq. (1.3))

$$\partial_t \varrho = -\frac{i}{\hbar} [H, \varrho]$$

leaves purity  $\text{tr}(\varrho^2)$  of the density matrix unchanged. Proof:

$$\begin{aligned} \partial_t \text{tr}(\varrho^2) &= \text{tr}(\partial_t \varrho \varrho) + \text{tr}(\varrho \partial_t \varrho) \stackrel{\text{cyc. perm.}}{=} 2\text{tr}(\varrho \partial_t \varrho) \\ &= -\frac{2i}{\hbar} [\text{tr}(\varrho H \varrho) - \text{tr}(\varrho \varrho H)] \stackrel{\text{cyc. perm.}}{=} 0 \end{aligned}$$

If the system is initiated in a pure state  $\varrho(0) = |\psi\rangle\langle\psi|$ ,  $\text{tr}(\varrho(0)^2) = 1$ , how does the state evolve to the thermal state  $\varrho_{\text{th}}$  in Eq. (1.2) which is mixed,  $\text{tr}(\varrho_{\text{th}}^2) < 1$ ?

Von-Neumann equation cannot describe the evolution towards the thermal state.

**Conclusion 2:** Weak coupling and heat bath of stat. mech. remain undefined microscopically. Von-Neumann equation cannot describe thermalization dynamics of density matrix for system in contact with heat bath.

### Observation 3:

- *Quantum mechanics:* Measurement postulate:

Without being “observed”: State  $|\psi(t)\rangle$  of the system evolves according to Schrödinger eq. (1.1).

When “observed” with observable  $O$ : Nature abruptly switches its laws and the state “collapses” into one of the eigenstates  $|\varphi_n\rangle$  of the observable

$$O = \sum_n o_n |\varphi_n\rangle\langle\varphi_n|.$$

- This leaves us with open questions: Who decides what an observer is? Does it have to be a human? cat? insect? bacterium? an atom?

One might answer: as soon as information about the state is extracted. But what if only a little bit of information is extracted? How can this “extraction of information” be described? It must be possible to describe it by a full quantum mechanical theory of the system and its observer.

**Conclusion 3:** The measurement postulate lacks a microscopic justification. Such a theory needs to describe the interaction of a small quantum system with its measurement environment.

**Final conclusion:**

There is a need for a theory that describes the microscopic dynamics of a small quantum system in (weak) contact with its environment. As environment we generally consider a much larger quantum system which can exchange energy, heat, particles, information,... with the system.

This is what we will consider in this course on the **Theory of Open Quantum Systems**. Excellent books that complement this course are Refs. [1, 2, 3, 4, 5, 6].

## 1.2 Classical probability theory and stochastic processes

### 1.2.1 Probability space, random variables

We have already observed that the contact to the environment will create fluctuations such that we can only describe the quantum state of our system statistically. Therefore, let us begin by studying classical probability theory and statistical processes, whose quantum analogs we will then have to define later.

**Probability space:**

- *Space of events:* A  $\sigma$ -Algebra over the sample space  $\Omega$ , e.g.  $\Omega = \mathbb{R}$ ,  $\Omega = [0, 1]$ ,  $\Omega = \{1, 2, 3, 4, 5, 6\}$ .

$\sigma$ -Algebra: system  $\mathcal{A}$  of subsets of  $\Omega$  with following properties:

1.  $\Omega \in \mathcal{A}$  and  $\{\emptyset\} \in \mathcal{A}$ .
2. If  $A_1 \in \mathcal{A}$  and  $A_2 \in \mathcal{A}$ , then also union  $A_1 \cup A_2 \in \mathcal{A}$ , intersection  $A_1 \cap A_2 \in \mathcal{A}$ , and difference  $A_1 \setminus A_2 \in \mathcal{A}$ ,
3. Countable sequence of  $A_n \in \mathcal{A}$ , then also their union  $\cup_{n=1}^{\infty} A_n \in \mathcal{A}$ ,

Example:  $\Omega = \{H, T\}$ ,  $\mathcal{A} = \{\{\emptyset\}, \{H\}, \{T\}, \{H, T\}\}$ . Interpretation: No event, event  $H$ =heads (elementary event), event  $T$ =tails (elementary event), event  $H$  or event  $T$  occurs.

- *Probability measure:* A map  $P : \mathcal{A} \rightarrow \mathbb{R}$  (i.e. each event  $A \in \mathcal{A}$  gets assigned a real number  $P(A) \in \mathbb{R}$ ) is called a probability measure if it satisfies the Kolmogorov axioms:
  1. Non-Negativity:  $P(A) \geq 0$ ,  $\forall A \in \mathcal{A}$ ,
  2. Normalization:  $P(\Omega) = 1$ ,
  3.  $\sigma$ -additivity: For all countable sequence of disjoint events  $A_n \in \mathcal{A}$ ,  $A_i \cap A_j = \{\emptyset\}$   $\forall i \neq j$  we have  $P(\cup_{n=1}^{\infty} A_n) = \sum_{n=1}^{\infty} P(A_n)$ .



These axioms alone are sufficient to build up a consistent probability theory. In direct consequence one for example has

4. Monotonicity:  $A \subseteq B, P(A) \leq P(B)$ ,
5. Probability of empty set:  $P(\{\}) = 0$ ,
6. Complement rule:  $P(A^c) = P(\Omega \setminus A) = 1 - P(A)$
7. Numeric bound:  $0 \leq P(A) \leq 1$
8. Addition law:  $P(A \cup B) = P(A) + P(B) - P(A \cap B)$

*Example:*  $\Omega = \{H, T\}, \mathcal{A} = \{\{\}, \{H\}, \{T\}, \{H, T\}\}$ .

1.  $P_1(\{\}) = 0, P_1(\{H\}) = \frac{1}{2}, P_1(\{T\}) = \frac{1}{2}, P_1(\{H, T\}) = 1$  is a probability measure describing a coin toss.
2.  $P_2(\{\}) = 0, P_2(\{H\}) = \frac{1}{9}, P_2(\{T\}) = \frac{8}{9}, P_2(\{H, T\}) = 1$  is another probability measure on the same event space.

- *Conditional probabilities:* We define

$$P(A_1|A_2) = \frac{P(A_1 \cap A_2)}{P(A_2)}$$

as the conditional probability that event  $A_1$  occurs under the condition that event  $A_2$  has occurred. An immediate consequence of this definition is Bayes's theorem

$$P(A_1|A_2) = P(A_2|A_1) \frac{P(A_1)}{P(A_2)}.$$

These events are called statistically independent if

$$P(A_1|A_2) = P(A_1) \quad \text{or equivalently} \quad P(A_1 \cap A_2) = P(A_1)P(A_2).$$

### Random variables:

Elements  $\omega \in \Omega$  of sample space are abstract objects (like heads and tails on a coin). We want to associate numbers with these events so that we can calculate sums, products... This leads us to the concept of random variables.

- *Random variable:* A measurable function  $X : \Omega \rightarrow \mathbb{R}$  is a random variable. (Measurable function: For all elements  $B \in \mathcal{B}$  where  $\mathcal{B}$  is the  $\sigma$ -algebra of Borel sets of  $\mathbb{R}$ , which includes all open and closed intervals, the pre-image  $A = X^{-1}(B) \in \mathcal{A}$  is in space of events). We can then define the probability distribution of  $X$  as

$$P(X \in B) = P(X^{-1}(B)).$$

A random variable  $X$  therefore gives a probability distribution to all intervals  $B \subseteq \mathbb{R}$  (or more generally all Borel sets  $B$ ) on the real axis.

*Example:*  $\Omega = \{H, T\}$ ,  $\mathcal{A} = \{\{\}, \{H\}, \{T\}, \{H, T\}\}$ , with probability measure  $P_1$  for a coin toss from above.  $X(H) = 1, X(T) = -1$ . Then we have for example

- $P(X \in [-2, 0]) = \frac{1}{2}$
- $P(X \in [-2, 2]) = 1$
- $P(X \in [-5, -2]) = 0$
- $P(X \in \{1\}) = \frac{1}{2}$

A particular Borel set is the interval  $(-\infty, x]$  with  $x \in \mathbb{R}$ . This leads to the cumulative distribution function

$$P(X \leq x) = P(X \in (-\infty, x]).$$

- *Probability density:* The random variable  $X$  is set to have a probability density  $\varrho(x)$  if the cumulative distribution function can be written as

$$P(X \leq x) = \int_{-\infty}^x \varrho(x) dx.$$

This probability density  $\varrho(x)$  and its quantum analog will turn out to be a central object for our studies of the theory of open (quantum) systems.

*Example from above:*

$$P(X \leq x) = \begin{cases} 0, & x < -1, \\ \frac{1}{2}, & -1 \leq x < 1, \\ 1, & 1 \leq x. \end{cases} \quad \varrho(x) = \frac{1}{2}\delta(x+1) + \frac{1}{2}\delta(x-1).$$

- *Multivariate random variable:* We can also consider mappings of the form  $X : \Omega \rightarrow \mathbb{R}^d$ , where  $\omega \mapsto X(\omega) = (X_1(\omega), X_2(\omega), \dots, X_d(\omega))$ . The probability of this multivariate random variable to fall into Borel set  $B \subset \mathbb{R}^d$  is again given by

$$P(X \in B) = P(X^{-1}(B)).$$

and it exists a multivariate probability density if

$$P(X_1 \leq x_1, \dots, X_d \leq x_d) = \int_{-\infty}^{x_1} \dots \int_{-\infty}^{x_d} d^d x \varrho(x_1, \dots, x_d).$$

In accordance with our earlier definition, two random variables are therefore statistically independent if

$$P(X_1 \leq x_1, X_2 \leq x_2) = P(X_1 \leq x_1)P(X_2 \leq x_2)$$

for all  $x_1, x_2$ . On the level of the probability density this is equivalent to a factorizing probability density

$$\varrho(x_1, x_2) = \varrho_1(x_1)\varrho_2(x_2).$$

*Example from statistical mechanics:*  $\Omega$  is the space of states of one particle in 1D,  $\mathcal{A}$  some corresponding space of events,  $P$  the corresponding probability measure at temperature  $T$ .  $X = (Q, P)$  is the random variable of its microstate which is described by its position  $Q$  and momentum  $P$ . Then

$$\varrho_{\text{th}}(q, p) = \frac{e^{-\beta H(q, p)}}{Z(\beta)}$$

is the thermal canonical state, which is described by a probability density over phase space, and  $\beta = 1/(k_B T)$ . From statistical mechanics we know that this state emerges at long times  $t \rightarrow \infty$  when the system is coupled to a bath of temperature  $T$ . However, if we initialize the particle at time  $t = 0$  in the state  $q = 0, p = 0$ , how can we describe this thermalization i.e.

$$\varrho(q, p, t = 0) = \delta(q)\delta(p) \xrightarrow{t \rightarrow \infty} \varrho(q, p, t = \infty) = \varrho_{\text{th}}(q, p).$$

This will lead to the concept of stochastic processes.

- *Expectation value, variance, covariance:* Assume a random variable  $X$  with probability density  $\varrho(x)$ . The expectation value or mean is then defined as

$$\langle X \rangle = \int_{-\infty}^{\infty} x \varrho(x) dx.$$

More generally, the expectation value of some function  $g(X)$  is defined as

$$\langle g(X) \rangle = \int_{-\infty}^{\infty} g(x) \varrho(x) dx,$$

e.g. the  $m$ -th moment of the distribution is given by  $\langle X^m \rangle$ . The variance of the random variable  $X$  is defined by

$$\text{Var}(X) = \langle [X - \langle X \rangle]^2 \rangle = \langle X^2 \rangle - \langle X \rangle^2,$$

and describes the extent that realizations of the random variable  $X$  fluctuate around the expectation value  $\langle X \rangle$ . In particular, if  $\text{Var}(X) = 0$ , then  $X$  will be deterministic, i.e. it takes only one value  $x = \langle X \rangle$  with probability 1.

For a multivariate random variable  $X = (X_1, \dots, X_d)$  we define the covariance matrix by

$$\text{Cov}(X_i, X_j) = \langle [X_i - \langle X_i \rangle][X_j - \langle X_j \rangle] \rangle, \quad (1.4)$$

such that  $\text{Var}(X_i) = \text{Cov}(X_i, X_i)$ . The covariance matrix is symmetric and positive semidefinite. The statistical independence of two random variables  $X_i, X_j$  implies that the two brackets in definition (1.4) can be “averaged individually” and we see that in that case the covariance vanishes,  $\text{Cov}(X_i, X_j) = 0$ . The converse is not necessarily true. One can also define the correlation coefficient

$$\text{Cor}(X_i, X_j) = \frac{\text{Cov}(X_i, X_j)}{\sqrt{\text{Var}(X_i)\text{Var}(X_j)}},$$

which is normalized  $|\text{Cor}(X_i, X_j)| \leq 1$ .

*Example:* A multivariate random variable  $X = (X_1, \dots, X_n)$  is Gaussian if its probability density is of the form

$$\varrho(x_1, \dots, x_d) = \frac{1}{Z_0} e^{-\frac{1}{2} \sum_{ij} x_i A_{ij} x_j} = \frac{1}{Z_0} e^{-\frac{1}{2} x^T \mathbf{A} x}$$

with symmetric and positive definite matrix  $\mathbf{A}$ . The matrix can therefore always be represented as  $\mathbf{A} = \mathbf{T} \mathbf{D} \mathbf{T}^T$  with diagonal matrix  $\mathbf{D} = \text{diag}(\lambda_1, \dots, \lambda_d)$  and orthogonal matrix  $\mathbf{T}$ . With this we can define a variable transformation  $z = \mathbf{T}^T x$ . This allows us to calculate the normalization factor

$$\begin{aligned} Z_0 &= \int d^d x e^{-\frac{1}{2} x^T \mathbf{A} x} = \int d^d z e^{-\frac{1}{2} z^T \mathbf{D} z} \\ &= \prod_i \int dz_i e^{-\frac{1}{2} \lambda_i z_i^2} = \prod_i \sqrt{\frac{2\pi}{\lambda_i}} = \sqrt{\frac{(2\pi)^d}{\det(\mathbf{A})}}. \end{aligned}$$

We want to calculate the expectation values  $\langle X_i \rangle$  and higher moments  $\langle X_i X_j \rangle, \dots$ . For this it is helpful to introduce a source term  $J = (J_1, \dots, J_d)$ .

$$Z(J) = \int d^d x e^{-\frac{1}{2} x^T \mathbf{A} x + J^T x},$$

which is equivalent to the (more traditional) definition of a characteristic function (where  $J = ik$ ). This can be solved by completion of the square  $x = y + \mathbf{A}^{-1} J$

$$Z(J) = \int d^d y e^{-\frac{1}{2} y^T \mathbf{A} y + \frac{1}{2} J^T \mathbf{A}^{-1} J} = Z_0 e^{\frac{1}{2} J^T \mathbf{A}^{-1} J}.$$

From this we find

$$\begin{aligned}\langle X_{k_1} \cdots X_{k_n} \rangle &= \frac{1}{Z_0} \int d^d x \, x_{k_1} \cdots x_{k_n} e^{-\frac{1}{2} x^T \mathbf{A} x + J^T x} \Big|_{J=0} \\ &= \frac{1}{Z_0} \partial_{J_{k_1}} \cdots \partial_{J_{k_n}} Z(J) \Big|_{J=0}.\end{aligned}$$

Expanding the exponential

$$Z(J) = Z_0 \left( 1 + \frac{1}{2} J^T \mathbf{A}^{-1} J + \dots \right)$$

we finally have

$$\langle X_i \rangle = \frac{1}{Z_0} \partial_{J_i} Z(J) \Big|_{J=0} = 0,$$

i.e. the mean (the first momentum) of the distribution vanishes (as all odd momenta),

$$\text{Cov}(X_i, X_j) = \langle X_i X_j \rangle = \frac{1}{Z_0} \partial_{J_i} \partial_{J_j} Z(J) \Big|_{J=0} = \frac{1}{2} [(\mathbf{A}^{-1})_{ij} + (\mathbf{A}^{-1})_{ji}] = (\mathbf{A}^{-1})_{ij},$$

where in the last step we have used that  $\mathbf{A}^{-1}$  is symmetric since  $(\mathbf{A}^{-1})^T = (\mathbf{A}^T)^{-1} = \mathbf{A}^{-1}$ . Hence, the matrix  $\mathbf{A}$  that defines the Gaussian state is given by the inverse covariance matrix, i.e. by knowledge of all second momenta  $\langle X_i X_j \rangle$  of the distribution, the Gaussian state is already completely characterized. By expanding the exponential in  $Z(J)$  to higher order and keeping track of the combinatorics one can prove Wick's theorem, e.g.

$$\begin{aligned}\langle X_i X_j X_k X_l \rangle &= (\mathbf{A}^{-1})_{ij} (\mathbf{A}^{-1})_{kl} + (\mathbf{A}^{-1})_{ik} (\mathbf{A}^{-1})_{jl} + (\mathbf{A}^{-1})_{il} (\mathbf{A}^{-1})_{jk} \\ &= \langle X_i X_j \rangle \langle X_k X_l \rangle + \langle X_i X_k \rangle \langle X_j X_l \rangle + \langle X_i X_l \rangle \langle X_k X_j \rangle,\end{aligned}$$

and analogously all higher order momenta are given by the sum of the permutations of the reduced second order momenta.

*Application 1 (trivial):* Consider  $d = 1$ ,  $\varrho(x) = \frac{1}{Z_0} e^{-\frac{x^2}{2\sigma^2}}$ : Then  $\langle X \rangle = 0$ ,  $\text{Var}(X) = \langle X^2 \rangle = (\frac{1}{\sigma^2})^{-1} = \sigma^2$ ,  $\langle X^3 \rangle = 0$ ,  $\langle X^4 \rangle = 3\sigma^4$ .

*Application 2:* Consider the Hamiltonian

$$H(q_1, q_2, p_1, p_2) = \sum_{i=1}^2 \left( \frac{p_i^2}{2m} + \frac{m\omega_i^2}{2} q_i^2 \right) + \frac{\kappa}{2} (q_1 - q_2)^2$$

describing two harmonic oscillators that are coupled “linearly” (the force is linear) with strength  $\kappa$ . One corresponding physical system are two masses  $m$  that are each

attached with a spring to a fixed wall and then coupled with another spring. The corresponding thermal canonical ensemble is Gaussian

$$\begin{aligned}\varrho(q_1, q_2, p_1, p_2) &= \frac{e^{-\beta H}}{Z} \\ &= \frac{1}{Z} \exp \left[ -\frac{\beta}{2} (q_1, q_2, p_1, p_2) \begin{pmatrix} m\omega_1^2 + \kappa & -\kappa & 0 & 0 \\ -\kappa & m\omega_2^2 + \kappa & 0 & 0 \\ 0 & 0 & \frac{1}{m} & 0 \\ 0 & 0 & 0 & \frac{1}{m} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix} \right]\end{aligned}$$

We therefore find the thermal means  $\langle Q_i \rangle = \langle P_i \rangle = 0$ , and fluctuations

$$\langle P_i^2 \rangle = m/\beta, \quad \langle P_i Q_j \rangle = 0,$$

$$\begin{aligned}\begin{pmatrix} \langle Q_1^2 \rangle & \langle Q_1 Q_2 \rangle \\ \langle Q_2 Q_1 \rangle & \langle Q_2^2 \rangle \end{pmatrix} &= \beta^{-1} \begin{pmatrix} m\omega_1^2 + \kappa & -\kappa \\ -\kappa & m\omega_2^2 + \kappa \end{pmatrix}^{-1} \\ &= \frac{\beta^{-1}}{m^2 \omega_1^2 \omega_2^2 + \kappa m (\omega_1^2 + \omega_2^2)} \begin{pmatrix} m\omega_2^2 + \kappa & \kappa \\ \kappa & m\omega_1^2 + \kappa \end{pmatrix}.\end{aligned}$$

For uncoupled oscillators,  $\kappa = 0$ , we directly recover our expectation from the equipartition theorem  $\langle P_i^2 \rangle / 2m = k_B T / 2 = m\omega_i^2 \langle Q_i^2 \rangle / 2$ . For finite coupling  $\kappa$ , however, we observe that the fluctuations of  $\langle Q_1^2 \rangle$  get shifted corresponding to an effective frequency shift for the first oscillator. One is tempted to ask for an effective probability distribution for the particle 1 only. By looking at how we calculate expectation values for particle 1

$$\langle Q_1 \rangle = \int_{-\infty}^{\infty} dq_1 \int_{-\infty}^{\infty} dq_2 \int_{-\infty}^{\infty} dp_1 \int_{-\infty}^{\infty} dp_2 \, q_1 \varrho(q_1, q_2, p_1, p_2).$$

we observe that we can define the reduced probability density

$$\varrho_1(q_1, p_1) = \int_{-\infty}^{\infty} dq_2 \int_{-\infty}^{\infty} dp_2 \, \varrho(q_1, q_2, p_1, p_2)$$

that averages over all configurations of particle 2. All expectation values for particle 1 only can then be calculated from this reduced probability density only, e.g.

$$\langle Q_1 \rangle = \int_{-\infty}^{\infty} dq_1 \int_{-\infty}^{\infty} dp_1 \, q_1 \varrho_1(q_1, p_1).$$

Indeed, the reduced density matrix can be written again as an effective Harmonic oscillator Hamiltonian (Homework)

$$\varrho_1(q_1, p_1) = \frac{1}{Z_{\text{eff}}} e^{-\beta H_{\text{eff}}(q_1, p_1)} = \frac{1}{Z_{\text{eff}}} e^{-\beta \left( \frac{p_1^2}{2m} + \frac{m\omega_{\text{eff}}^2}{2} q_1^2 \right)}$$

with an effective frequency such that  $k_B T/2 = m\omega_{\text{eff}}^2 \langle Q_1^2 \rangle / 2$  for all  $\kappa$ .

We conclude that in the presence of a finite coupling ( $\kappa \neq 0$ ) to an environment/other degrees of freedom, the Gibbs state from statistical physics for the reduced subsystem 1 gets redistributed. One can interpret this shift with an effective Hamiltonian (or Hamiltonian of mean force [7] which is a related concept). Only in the utraweak coupling limit of  $\kappa \rightarrow 0$  we recover the Gibbs state also for the reduced subsystem of oscillator 1.

### 1.2.2 Stochastic processes, Markov processes

We now want to turn to the case where the random variable acquires some time dependance. (Think of our particle that is initialized at some point in phase space, so  $(Q(0), P(0))$  is deterministic; How does the corresponding random variable  $(Q(t), P(t))$  evolve over time until it is thermal? This defines a stochastic process).

- *Stochastic process*: A mapping  $X : \Omega \times [t_i, t_f] \rightarrow \mathbb{R}^d$  is called a stochastic process, if  $X(\cdot, t)$  is a (multivariate) random variable for all  $t \in [t_i, t_f] \subseteq \mathbb{R}$ . Keeping the sample  $\omega \in \Omega$  fixed, we call the mapping

$$t \mapsto X(\omega, t)$$

a realization, trajectory or sample path of the stochastic process. In practice, one usually characterizes the stochastic processes by the correlations of the stochastic variables  $X(t_n)$  at a finite set of times  $t_n$  via the joint probability distribution of order  $m$ ,

$$P(B_1, t_1; B_2, t_2; \dots B_m, t_m) = P(X(t_1) \in B_1, X(t_2) \in B_2, \dots, X(t_m) \in B_m), \quad (1.5)$$

which characterizes the probability that the  $X(t_n)$  take a value in  $B_n$  during the evolution of the random variable in the stochastic process.

- *Markov processes* are stochastic processes  $X(t)$  that have a “short memory”. This property makes Markov processes easy to deal with since it means that the  $m$ th order joint probability distributions in Eq. (1.5) can be reconstructed from just two distribution functions.

The condition for rapid decrease of memory can be formulated as the *Markov condition*

$$P(X(t) \in B | X(t_m) = x_m, \dots, X(t_1) = x_1) = P(X(t) \in B | X(t_m) = x_m),$$

for  $t_1 < t_2 < \dots < t_m < t$ . I.e. the conditional probability (remember  $P(A|B) = P(A \cap B)/P(B)$ ) that the event  $X(t) \in B$  after  $X(t_1) = x_1, \dots, X(t_m) = x_m$  occurs

does only depend on the latest event  $X(t_m) = x_m$  instead of the full history of events. The process therefore has no “memory” of its history.

*Example 1:* Let  $X(t) = X_{\text{coin}}(t)$  a stochastic process which is given by the random variable of independent coin tosses at each time  $t$ . Since the probability for a coin toss at time  $t$  is completely independent of the history of the tosses, the process is Markovian.

*Example 2:* Let  $X(t) = (Q(t), P(t))$  a stochastic process that is given by the deterministic evolution  $(q(t), p(t))$  of a classical system according to Hamilton’s equation of motion

$$d_t q = \partial_p H, \quad d_t p = -\partial_q H$$

(i.e.

$$P((Q(t), P(t)) \in B) = \begin{cases} 1 & \text{if } (q(t), p(t)) \in B \\ 0 & \text{else.} \end{cases}$$

The conditional probability to find  $(Q(t), P(t)) \in B$  only depends on the last event  $Q(t_m) = q_m, P(t_m) = p_m$  in the sense that whether the trajectory with this initial condition is such that  $(q(t), p(t)) \in B$ . The evolution is independent of the history at earlier times  $t_1, t_2, \dots$ . Hamiltonian mechanics is therefore Markovian.

Generally, all processes that are generated in this way from a first order differential equation are Markovian and are called *deterministic processes*.

- *Joint probability densities for Markov processes* The Markov property has consequences also on the level of the probability density

$$P(B_m, t_m; \dots B_1, t_1) = \int_{B_m} dx_m \cdots \int_{B_1} dx_1 \varrho(x_m, t_m; \dots x_1, t_1)$$

with the corresponding conditional probability densities

$$\varrho(x, t | x_m, t_m; \dots x_1, t_1) = \frac{\varrho(x, t; x_m, t_m; \dots x_1, t_1)}{\varrho(x_m, t_m; \dots x_1, t_1)} \quad (1.6)$$

in terms of which the Markov condition reads

$$\varrho(x, t | x_m, t_m; \dots x_1, t_1) = \varrho(x, t | x_m, t_m) \quad (1.7)$$

We see that the conditional transition probability or *propagator*

$$T(x, t | x', t') \equiv \varrho(x, t | x', t')$$



that the process takes the value  $x$  at time  $t$  after it has taken the value  $x'$  at time  $t'$  takes an important role for Markov processes. By definition (1.6) we can use the propagator to write

$$\varrho(x, t) = \int dx' T(x, t | x', t') \varrho(x', t'). \quad (1.8)$$

Treating  $x$  like the continuous index of a matrix, the integral over  $x'$  in Eq. (1.8) corresponds to the continuous version of a matrix-vector multiplication so we can represent Eq. (1.8) as the action of a linear operator

$$\varrho(t) = T(t | t') \varrho(t')$$

Let us consider e.g. three times  $t_1 < t_2 < t_3$  and the corresponding joint probability density

$$\begin{aligned} \varrho(x_3, t_3; x_2, t_2; x_1, t_1) &\stackrel{(1.6)}{=} \varrho(x_3, t_3 | x_2, t_2; x_1, t_1) \varrho(x_2, t_2; x_1, t_1) \\ &\stackrel{(1.7), (1.6)}{=} T(x_3, t_3 | x_2, t_2) T(x_2, t_2 | x_1, t_1) \varrho(x_1, t_1) \end{aligned} \quad (1.9)$$

By generalising this to higher orders, we observe that due to the Markov condition the  $m$ th order joint probability distributions can be recreated just from the initial density  $\varrho(x, t_0)$  and the propagator  $T(x, t | x', t')$  alone,

$$\varrho(x_m, t_m; \dots; x_1, t_1) = \prod_{k=1}^m T(x_{k+1}, t_{k+1} | x_k, t_k) \varrho(x_1, t_1), \quad (1.10)$$

i.e. the Markov process is sufficiently described by knowledge of these two functions. Finally, the Markov property also has consequences for the propagator itself. To see this, we integrate Eq. (1.9) over  $x_2$

$$\varrho(x_3, t_3; x_1, t_1) = \int dx_2 T(x_3, t_3 | x_2, t_2) T(x_2, t_2 | x_1, t_1) \varrho(x_1, t_1)$$

After dividing by  $\varrho(x_1, t_1)$ , we find the Chapman-Kolmogorov Equation

$$T(x_3, t_3 | x_1, t_1) = \int dx_2 T(x_3, t_3 | x_2, t_2) T(x_2, t_2 | x_1, t_1) \quad (1.11)$$

Intuitively, the probability to go from  $(x_1, t_1)$  to  $(x_3, t_3)$  can be decomposed into the probability to go from  $(x_1, t_1)$  to some intermediate state  $(x_2, t_2)$  and then from  $(x_2, t_2)$  to  $(x_3, t_3)$  and summing over all possible intermediate states  $x_2$  (since the process has no memory, the  $2 \rightarrow 3$  evolution cannot be influenced by the earlier  $1 \rightarrow 2$  evolution).

Using the notation in terms of linear operators, the Chapman-Kolmogorov equation takes the form

$$T(t_3|t_1) = T(t_3|t_2)T(t_2|t_1).$$

- *Stationary and homogeneous processes* A process is called *stationary* if all joint probability densities are invariant under time translations, i.e.

$$\varrho(x_m, t_m + \tau; \dots x_1, t_1 + \tau) = \varrho(x_m, t_m; \dots x_1, t_1)$$

This means that all joint probabilities only depend on the time differences  $t_m - t_n$  instead of the explicit times  $t_m, t_n$ . In particular the density  $\varrho(x, t)$  for the unconditioned probability is time-independent,  $\varrho(x, t) = \varrho(x)$ . Stationary processes describe for example equilibrium fluctuations in statistical mechanics.

A stochastic process is called *homogeneous* if the propagator only depends on time differences, i.e.

$$T(t|t') = T(t - t'|0) \equiv T(t - t')$$

A stationary process is homogeneous, but there are homogeneous processes that are not stationary (e.g. Wiener process). For homogeneous Markov processes the Chapman-Kolmogorov Eqn. therefore reads

$$T(t + t') = T(t)T(t')$$

which is also known as the semigroup property. The term *semigroup* emphasises that the family  $T(t), t \geq 0$  is, in general, not a full group since the process is not necessarily invertible and  $t$  is restricted to nonnegative values.

In the following let us discuss different kinds of Markov processes that we want to classify by the behaviour of their specific realizations: There are processes with continuous (see Fig. 1.1(a)) and discontinuous (Fig. 1.1(b)) sample paths  $x(t)$ . It can be shown that realizations of a Markov process are continuous with probability one if

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int_{|x-x'| > \varepsilon} dx T(x, t + \Delta t | x', t) = 0$$

for all  $\varepsilon > 0$ , i.e. the propagator to transition outside of an  $\varepsilon$ -neighbourhood vanishes faster than  $\Delta t$ .

- *Class 1: Jump processes and (classical) master equation* We first consider one class of processes with discontinuous paths, so called jump processes. They are described by the transition rates

$$W(x|x', t),$$

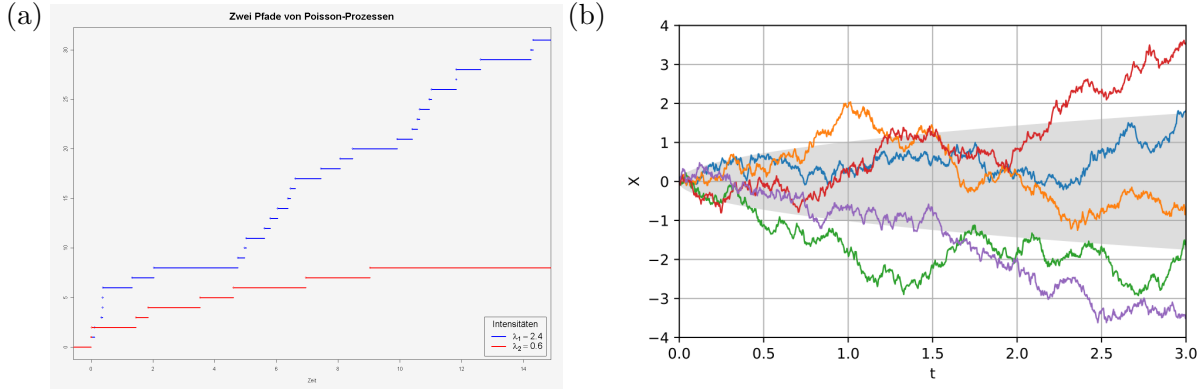


Figure 1.1: Sample paths  $x(t)$  of different kind of Markov processes. (a) Poisson process [8], which is a jump process with discontinuous sample paths. (b) Wiener process [9], whose sample paths are continuous. Different colors represent different sample paths and the grey background is the expected standard deviation.

for which  $W(x|x', t)\Delta t$  is the probability density for an instantaneous jump from state  $x'$  to state  $x$  within the infinitesimal time interval  $[t, t + \Delta t]$ . The total rate for any jump out of state  $x'$  to occur is therefore given by

$$\int dx W(x|x', t).$$

The propagator  $T(x, t + \Delta t|x', t)$  for this short time interval is hence given by either a jump occurring or no jump occurring

$$T(x, t + \Delta t|x', t) = W(x|x', t)\Delta t + \left(1 - \Delta t \int dx'' W(x''|x', t)\right) \delta(x - x') + \mathcal{O}(\Delta t^2).$$

As it should, for  $\Delta t \rightarrow 0$  the propagator approaches the delta function  $\delta(x - x') = T(x, t|x', t)$ . We can now bring the Chapman-Kolmogorov equation to a differential form,

$$\begin{aligned} \partial_t T(x, t|x', t') &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} [T(x, t + \Delta t|x', t') - T(x, t|x', t')] \\ &\stackrel{\text{CK}}{=} \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[ \int dx'' T(x, t + \Delta t|x'', t) T(x'', t|x', t') - T(x, t|x', t') \right] \\ &= \int dx'' [W(x|x'', t) T(x'', t|x', t') - W(x''|x, t) T(x, t|x', t')] \end{aligned}$$

This is the differential Chapman-Kolmogorov equation for jump processes. It is also called the *master equation*. To emphasize the difference to quantum master equations

that we will encounter later we will also call it *classical master equation*. It also holds for the unconditioned probability density  $\varrho(x, t)$ ,

$$\partial_t \varrho(x, t) = \int dx' [W(x|x', t)\varrho(x', t) - W(x'|x, t)\varrho(x, t)] \quad (1.12)$$

but of course only the solution in terms of the full propagator  $T$  is sufficient to fully describe the Markov process. The master equation has an easy physical interpretation: The rate of change of the probability density  $\varrho(x, t)$  of state  $x$  is given by the probability density  $\varrho(x', t)$  of all other states  $x'$  and the rate  $W(x|x', t)$  to jump from  $x'$  to  $x$ , minus the probability to jump from state  $x$  into all other states  $x'$ . The process is homogeneous if the rate is time-independent  $W(x|x', t) = W(x|x')$ .

If a process is integer-valued, the probability densities can be understood as a sum of delta-functions

$$\varrho(x, t) = \sum_{n \in \mathbb{N}_0} P(n, t) \delta(x - n),$$

and the above discussed properties take similar form but with sums replacing the integrals. E.g. the master equation for the probability distribution reads

$$\partial_t P(n, t) = \sum_{n'} [W(n|n', t)P(n', t) - W(n'|n, t)P(n, t)], \quad (1.13)$$

and the action of the propagator is according to

$$P(n, t) = \sum_{n'} T(n, t|n', t') P(n', t').$$

*Example 1: Fermi's golden rule* Consider a quantum system with Hamiltonian  $H = H_0 + V$  and eigenstates  $|i\rangle$  of the unperturbed Hamiltonian  $H_0$  with continuous spectrum. Time-dependent perturbation theory yields the jump rate

$$W(f|i) = \frac{2\pi}{\hbar} |\langle f|V|i\rangle|^2 D(E_f)$$

for the state  $|i\rangle$  to jump under the dynamics with perturbation  $V$  into final state  $|f\rangle$  which lies in an energy continuum with density of states  $D(E_f)$ . The corresponding master equation (1.12) hence describes the dynamics of the *populations*  $\varrho(i, t)$  of the unperturbed eigenstates  $|i\rangle$ .

*Example 2: Poisson process* The poisson process is an important example for the class of jump processes. One example where it occurs is photon emission. Think of some classical current density  $\vec{j}(\vec{x}, t)$  that is coupled to a quantized radiation field  $\vec{A}(\vec{x})$ .

From QED and Fermi's golden rule [1] one finds that for a steadily oscillating current, the rate for single-photon emission  $W(n+1|n) = \gamma$  is constant and independent from previous processes. The number  $N(t)$  of photons in the field  $\vec{A}(\vec{x})$  becomes a stochastic Markov process known as (homogeneous) Poisson process.

The poisson process is therefore governed by the master equation

$$\partial_t T(n, t|n', t') = \gamma T(n-1, t|n', t') - \gamma T(n, t|n', t')$$

with initial condition  $T(n, t|n', t) = \delta_{nn'}$ . It is solved by the propagator (show by plugging in)

$$T(n, t|n', t') = \frac{[\gamma(t-t')]^{n-n'}}{(n-n')!} e^{-\gamma(t-t')}$$

for  $n \geq n'$  (since jumps can occur to higher photon number only). The master equation (1.13) for the Poisson process with  $P(n, 0) = \delta_{n,0}$  is solved by

$$P(n, t) = \frac{(\gamma t)^n}{n!} e^{-\gamma t}$$

Hence, the distribution of statistically independent jump processes that occur with a constant rate  $\gamma$  is given by a Poisson distribution with mean and variance

$$\langle N(t) \rangle = \text{Var}(N(t)) = \gamma t,$$

which explains its importance since such processes occur in many systems in nature. A sample path for the Poisson process is shown in Fig. 1.1(a).

*Increments of the Poisson process* We define the increment of the Poisson process via

$$dN(t) = N(t+dt) - N(t)$$

By using that

$$P(dN(t) = dn) = \sum_n T(n+dn, t+dt|n, t) P(n, t) = \frac{(\gamma dt)^{dn}}{dn!} e^{-\gamma dt}, \quad (1.14)$$

where in the last step we have plugged in the explicit expressions for the Poisson process from above, we find that

$$\langle dN(t) \rangle = \text{Var}(dN(t)) = \gamma dt,$$

or equivalently

$$\langle dN(t)^2 \rangle = \text{Var}(dN(t)) + \langle dN(t) \rangle^2 = \gamma dt + (\gamma dt)^2.$$

Taking  $dt$  to be infinitesimally small we have

$$\langle dN(t)^2 \rangle = \langle dN(t) \rangle = \gamma dt.$$

We observe that even though the first order of the increment  $dN(t)$  is linear in  $dt$  already, also the second order increment  $dN(t)^2$  is linear in  $dt$  which is different from our standard differential calculus for deterministic processes. Since, by looking at Eq. (1.14), we see that a jump with  $dn \geq 2$  only occurs on the order of  $dt^2$  or higher, for infinitesimal  $dt$  we therefore also have

$$dN(t)^2 = dN(t).$$

- *Class 2: Diffusion processes and Fokker-Planck equation* Remember that we wanted to characterize Markov processes by the property whether their realizations are continuous or not.

*Deterministic processes* Trivially, one class of realizations with continuous sample paths are deterministic processes  $X(t) = (X_1(t), \dots, X_d(t))$ , which are given by the solution of a first-order differential equation

$$d_t X(t) = g(X(t), t). \quad (1.15)$$

On the level of the propagator, we therefore have

$$T(x, t + \Delta t | x', t) = \delta(x - (x' + g(x', t)\Delta t))$$

since at time  $t + \Delta t$  the particle has to go from  $x'$  to  $x' + g(x')\Delta t$ . Using the fundamental property (1.8) of the propagator, we find

$$\begin{aligned} \partial_t \varrho(x, t) &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[ \int dx' T(x, t + \Delta t | x', t) \varrho(x', t) - \varrho(x, t) \right] \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \left[ \int dx' \delta(x - (x' + g(x', t)\Delta t)) \varrho(x', t) - \varrho(x, t) \right]. \end{aligned}$$

By expanding the delta function in a Taylor series around  $x = x'$  we have

$$\partial_t \varrho(x, t) = - \int dx' \sum_{i=1}^d \partial_{x_i} \delta(x - x') g_i(x', t) \varrho(x', t) = - \sum_{i=1}^d \partial_{x_i} [g_i(x, t) \varrho(x, t)], \quad (1.16)$$

where in the last step first we have transformed  $\partial_{x_i}$  to  $\partial_{x'_i}$  (and a factor of  $-1$ ) and then performed partial integration (again a factor of  $-1$ ). This is the differential Chapman-Kolmogorov equation for deterministic processes, or also called Liouville equation.

*Diffusion processes* There is however another class with continuous sample paths, diffusion processes. They can be derived as a certain limit of jump processes, which we obtain by writing the transition rates as

$$W(x|x', t) = f(x', y = x - x', t)$$

i.e. we rewrite the rates as a function  $f$  with starting point  $x'$  and jump distance  $y = x - x'$ . Note that for generality we assume a multivariate diffusion process, so that  $x = (x_1, \dots, x_d)$  and  $y$  analogously. The assumption will then be that  $f$  is sharply peaked around  $y = 0$  only. Plugging this form into the master eq. (1.12), we have

$$\partial_t \varrho(x, t) = \int dy f(x - y, y, t) \varrho(x - y, t) - \varrho(x, t) \int dy f(x, y, t).$$

Since  $f$  is sharply peaked around  $y = 0$  only, we can expand the gain term up to second order in  $y$  to find

$$\begin{aligned} \partial_t \varrho(x, t) &= \int dy f(x, y, t) \varrho(x, t) - \int dy \sum_i y_i \partial_{x_i} [f(x, y, t) \varrho(x, t)] \\ &\quad + \frac{1}{2} \int dy \sum_{i,j} y_i y_j \partial_{x_i} \partial_{x_j} [f(x, y, t) \varrho(x, t)] - \varrho(x, t) \int dy f(x, y, t). \end{aligned}$$

Finally by introducing the first and second moment of  $f$  with respect to its second argument,

$$g_i(x, t) = \int dy y_i f(x, y, t), \quad D_{ij}(x, t) = \int dy y_i y_j f(x, y, t),$$

we arrive at the differential Chapman-Kolmogorov equation for diffusion processes,

$$\partial_t \varrho(x, t) = - \sum_i \partial_{x_i} [g_i(x, t) \varrho(x, t)] + \frac{1}{2} \sum_{i,j} \partial_{x_i} \partial_{x_j} [D_{ij}(x, t) \varrho(x, t)]. \quad (1.17)$$

This is the famous *Fokker-Planck equation*. A formally identical equation holds for the propagator of the process. We observe that the first term in Eq. (1.17) is identical to the Liouville Eq. (1.16). The first term therefore describes a deterministic drift according to Eq. (1.15), while the second term describes the diffusion of the stochastic variable  $X(t)$  with diffusion matrix  $D(x, t)$  which is symmetric and positive semidefinite.

The fact that the Fokker-Planck Eq. (1.17) preserves the total probability can be seen since it can also be written as a continuity equation

$$\partial_t \varrho(x, t) + \sum_i \partial_{x_i} J_i(x, t) = 0$$

with probability current density

$$J_i(x, t) = g_i(x, t)\varrho(x, t) - \frac{1}{2} \sum_j \partial_{x_j} [D_{ij}(x, t)\varrho(x, t)].$$

*Example: Brownian motion, Wiener process* The most prominent example of a diffusion process is obtained by setting  $g(x, t) = 0, D(x, t) = 1$ . This leads to the propagator of the *Brownian motion* process

$$T(x, t|x', t') = \frac{1}{\sqrt{2\pi(t-t')}} \exp\left(-\frac{(x-x')^2}{2(t-t')}\right).$$

which is gaussian in space. Since it only depends on temporal and spatial differences, the process is homogenous in time and space. If we further take the initial density

$$\varrho(x, t=0) = \delta(x)$$

we obtain the famous *Wiener process*  $W(t) = X(t)$ . A sample path of the process is shown in Fig. 1.1(b). Its time-dependent probability density follows from

$$\varrho(x, t) = \int dx' T(x, t|x', 0)\varrho(x', 0) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right),$$

which is gaussian with

$$\langle W(t) \rangle = 0, \quad \text{Var}(W(t)) = \langle W(t)^2 \rangle = t.$$

The corresponding standard deviation is plotted in Fig. 1.1(b). As discussed earlier, we observe that even though the process is homogenous, it is not stationary. The two-time correlations follow for  $t \geq s$

$$\begin{aligned} \langle W(t)W(s) \rangle &= \int dx_2 \int dx_1 x_1 x_2 \varrho(x_2, t, x_1, s) \\ &\stackrel{t \geq s, (1.10)}{=} \int dx_2 \int dx_1 x_1 x_2 T(x_2, t|x_1, s) \varrho(x_1, s) \\ &\stackrel{x_2 \rightarrow x_2 + x_1}{=} \int dx_2 \int dx_1 x_1 (x_2 + x_1) \frac{e^{-\frac{x_2^2}{2(t-s)}}}{\sqrt{2\pi(t-s)}} \frac{e^{-\frac{x_1^2}{2s}}}{\sqrt{2\pi s}} = s \end{aligned}$$

where the last integral follows from our knowledge about Gaussian states from Sec. 1.2.1. For the case  $t < s$  the roles of  $t$  and  $s$  are interchanged giving

$$\langle W(t)W(s) \rangle = \min(t, s)$$



which is valid for all  $t, s$ .

*Increments of the Wiener process* We again define the increment of the process as

$$dW(t) = W(t + dt) - W(t).$$

With this we directly obtain

$$\begin{aligned}\langle dW(t) \rangle &= \langle W(t + dt) \rangle - \langle W(t) \rangle = 0, \\ \langle dW(t)^2 \rangle &= \langle W(t + dt)^2 \rangle - 2\langle W(t + dt)W(t) \rangle + \langle W(t)^2 \rangle = t + dt - 2t + t = dt.\end{aligned}$$

Similar to the Poisson increments, the differentials  $dW(t)$  are therefore behaving very differently to what we know from deterministic differential calculus, where when we want to take into account all terms up to  $dt$  we have to include terms up to second order in  $dW(t)$ . At two different times  $t > s$ , however, we find

$$\begin{aligned}\langle dW(t)dW(s) \rangle &= \langle W(t + dt)W(s + dt) \rangle - \langle W(t + dt)W(s) \rangle - \langle W(t)W(s + dt) \rangle + \langle W(t)W(s) \rangle \\ &= (s + dt) - s - (s + dt) + s = 0,\end{aligned}$$

and hence that Wiener increments at different times are uncorrelated.

Note that the above can also be understood from the infinitesimal propagator

$$T(x + dx, t + dt | x, t) = \frac{1}{\sqrt{2\pi dt}} \exp\left(-\frac{dx^2}{2dt}\right)$$

which is gaussian with respect to  $dx$  with variance  $dt$ . This also tells us immediately how to simulate the Wiener process numerically: We fix a small but finite  $\Delta t$ . Then the increments  $\Delta W$  are obtained by generating random numbers with Gaussian distribution with Variance  $\Delta t$ . Then the process follows by adding this increment in each timestep  $W(t + \Delta t) = W(t) + \Delta W$ . An example python code that does this is

```
import numpy as np

# Process parameter
dt = 0.05
# Initial condition.
x = 0.0
# Number of time-iterations to compute.
n = 20

# Iterate to compute the steps of the Brownian motion.
for k in range(n):
    x = x + np.sqrt(dt)*np.random.randn()
    print(x)
```

For a multivariate random variable of statistically independent Wiener processes  $W(t) = (W_1(t), \dots, W_d(t))$  this generalizes to

$$\langle dW_i(t) \rangle = 0, \quad \langle dW_i(t) dW_j(t) \rangle = \delta_{ij} dt. \quad (1.18)$$

### 1.2.3 Stochastic calculus for diffusion processes

Up to now we have formulated the dynamics of the stochastic process  $X(t)$  in terms of its probability density with the help of the propagator. Alternatively, one can also describe the dynamics in terms of a differential equation for the random variable  $X(t)$ . Of course, in this differential equation there cannot only enter deterministic terms, but there will occur a fluctuating term.

*Itô calculus for diffusion processes* Consider a multivariate diffusion process  $X(t) = (X_1(t), \dots, X_d(t))$ , which is governed by the Fokker-Planck eqn. (1.17). By using the increment of the process  $dX(t) = X(t + dt) - X(t)$ , the expectation value of an arbitray function  $f(X(t))$  is evolving according to

$$\begin{aligned} \langle df(t) \rangle &= \langle f(X(t) + dX(t)) - f(X(t)) \rangle = dt \partial_t \langle f(X(t)) \rangle = dt \int dx f(x) \partial_t \varrho(x, t) \\ &\stackrel{(1.17)}{=} dt \int dx f(x) \left\{ - \sum_k \partial_{x_k} [g_k(x) \varrho(x, t)] + \frac{1}{2} \sum_{k,l} \partial_{x_k} \partial_{x_l} [D_{kl}(x) \varrho(x, t)] \right\} \\ &\stackrel{\text{Partial int.}}{=} \left\langle \sum_k g_k(X(t)) \partial_k f(X(t)) + \frac{1}{2} \sum_{k,l} D_{kl}(X(t)) \partial_k \partial_l f(X(t)) \right\rangle dt. \end{aligned} \quad (1.19)$$

Let us first take  $f(x) = x_i$ . We find

$$\langle dX_i(t) \rangle = \langle g_i(X(t)) \rangle dt \quad (1.20)$$

As we have already seen, the first term in this evolution is generated by a deterministic drift according to  $dX_i = g_i(X(t))dt$ . For the second term, let us use  $f(x) = x_i x_j$

$$\langle dX_i(t) dX_j(t) \rangle = \langle D_{ij}(X(t)) \rangle dt. \quad (1.21)$$

By comparing this to Eq. (1.18), we suspect that the process can be generated by an appropriate combination of independent Wiener increments  $dW_i(t)$ . The Ansatz therefore is that the increments  $dX_i$  obey the *stochastic differential equation (in the Itô sense)*

$$dX_i = g_i(X(t))dt + \sum_j B_{ij}(X(t))dW_j(t). \quad (1.22)$$

Since the Wiener increments average to zero  $\langle dW_j(t) \rangle = 0$  we directly reproduce Eq. (1.20). For the covariances we find

$$\langle dX_i(t)dX_j(t) \rangle = \left\langle \sum_{k,l} B_{ik}(X(t))B_{jl}(X(t)) dW_k(t)dW_l(t) \right\rangle + \mathcal{O}(dt^2).$$

Using Eq. (1.18), and comparing to Eq. (1.21) we observe that the coefficients  $B_{ij}(x)$  have to fulfill the condition

$$\sum_k B_{ik}(x)B_{jk}(x) = D_{ij}(x).$$

It can be shown that the diffusion process  $X(t)$  that is generated from the stochastic differential equation (1.22) with this choice of the coefficients indeed is giving rise to a Markov process that is governed by the Fokker-Planck equation. Since we know how to create the finite Wiener increments  $\Delta W_i$ , it also allows us to solve Eq. (1.22) numerically.

Note that a rigorous treatment of stochastic differential equation requires an introduction of stochastic integrals, where the corresponding one to our notation is the *Itô integral*. Equation (1.22) can be interpreted as stochastic differential equation in Itô form (as opposed to the other prominent Stratonovich form).

In order to see that indeed the expectation value of a function  $f$  of the process is identical to the one of the Fokker-Planck equation we expand the function in a Taylor expansion up to second order

$$\begin{aligned} \langle f(X(t) + dX(t)) - f(X(t)) \rangle &= \\ &= \left\langle \sum_k \left[ g_k dt + \sum_i B_{ki} dW_i(t) \right] \partial_k f + \frac{1}{2} \sum_{kl} \left[ \sum_{ij} B_{ki} B_{lj} dW_i(t) dW_j(t) \right] \partial_k \partial_l f \right\rangle + \mathcal{O}(dt^2) \\ &= \left\langle \sum_k g_k \partial_k f + \frac{1}{2} \sum_{kl} D_{kl} \partial_k \partial_l f \right\rangle dt, \end{aligned}$$

which reproduces Eq. (1.19) (we have suppressed the dependences on  $X(t)$  for notational simplicity). Note that similar calculations lead to the *Itô formula* which holds directly on the level of the differential  $df(X(t)) = f(X(t) + dX(t)) - f(X(t))$ ,

$$df(X(t)) = \sum_k \left[ g_k dt + \sum_i B_{ki} dW_i(t) \right] \partial_k f + \frac{1}{2} \sum_{kl} D_{kl} \partial_k \partial_l f dt.$$

This can be summarized into new rules for the Itô differential calculus

$$\begin{aligned} dW_i(t)dW_j(t) &= \delta_{ij}dt \\ dW_i(t)dt &= 0 \\ [dW_i(t)]^k &= 0 \quad \text{for } k > 2. \end{aligned}$$

We can therefore intuitively understand  $dW_j(t) \sim dt^{1/2}$ , and hence have to pick up all orders  $dt^{1/2}$ ,  $dt$  and disregard terms of order  $dt^{3/2}$  and higher.

*Example: Langevin equation* Consider a particle that is immersed in a fluid of temperature  $T$ . Newton's equation of motion can help us describe the dampening

$$m dv = -m\gamma v$$

due to the viscosity of the fluid, but since  $v(t \rightarrow \infty) = 0$  it is clear that it cannot describe our naive expectation that the particle thermalizes with temperature  $T$  of the fluid. From experimental observations we know that the particle undergoes a fluctuating dynamics that is referred to as Brownian motion (note that unfortunately even though the name is identical, it is not the same as the Brownian motion process). This has motivated Langevin to propose an additional fluctuating force  $\eta(t)$  leading to the Langevin equation

$$m dv = -m\gamma v + \eta(t) \tag{1.23}$$

with vanishing average  $\langle \eta(t) \rangle = 0$  and correlation function

$$\langle \eta(t)\eta(t') \rangle = \lambda \delta(t - t')$$

that is instantaneous time, and where the force-autocorrelation strength  $\lambda$  is at this point seemingly a free parameter. Comparing this to our results for the Wiener increments

$$\langle dW(t)dW(t') \rangle = \begin{cases} dt & t = t' \\ 0 & t \neq t' \end{cases}$$

it becomes clear that we can relate this fluctuating force to the Wiener increments. We make the Ansatz

$$\eta(t)dt = \sqrt{\lambda} dW(t)$$

which we see that it is correct since on the one hand

$$\int \langle \eta(t)\eta(t') \rangle dt' = \int \lambda \delta(t - t') dt' = \lambda$$

and on the other hand

$$\int \langle \eta(t) \eta(t') \rangle dt' = \int \lambda \left\langle \frac{dW(t)}{dt} dW(t') \right\rangle = \lambda.$$

Multiplying the Langevin eq. (1.23) with  $dt$ , it therefore becomes the stochastic differential equation

$$dv = -\gamma v dt + \frac{\sqrt{\lambda}}{m} dW(t).$$

The solution of this s.d.e. is given by the *Ornstein-Uhlenbeck process*. In our language from above with  $X(t) = v(t)$  being our random variable, we therefore have

$$g(v) = -\gamma v, \quad B(v) = \frac{\sqrt{\lambda}}{m}, \quad D(v) = B(v)^2 = \frac{\lambda}{m^2}.$$

Hence, we know that  $v(t)$  is distributed according to the probability density  $\varrho(v, t)$  that follows from the Fokker-Planck eqn. (1.17)

$$\begin{aligned} \partial_t \varrho(v, t) &= -\partial_v [g(v) \varrho(v, t)] + \frac{1}{2} \partial_v^2 [D(v) \varrho(v, t)] \\ &= \gamma \partial_v [v \varrho(v, t)] + \frac{1}{2} \frac{\lambda}{m^2} \partial_v^2 \varrho(v, t). \end{aligned}$$

In the steady state, we have  $\partial_t \varrho(v, t_{ss}) = 0$ , so on the r.h.s. we therefore must have

$$\gamma v \varrho(v, t_{ss}) + \frac{1}{2} \frac{\lambda}{m^2} \partial_v^2 \varrho(v, t_{ss}) = C,$$

with a constant  $C$  so that after acting upon it with  $\partial_v$  it becomes 0. Since the solution must be invariant under transforming  $v$  to  $-v$  we find that  $C = 0$ . We observe that for  $C = 0$  this equation is solved by the ansatz

$$\varrho(v, t_{ss}) = N \exp \left( -\frac{\gamma m^2}{\lambda} v^2 \right),$$

which is consistent with our expectation of a thermal steady state

$$\varrho_{th}(v) = N \exp \left( -\frac{mv^2}{2k_B T} \right),$$

With this we find that the parameter  $\lambda$  related to the of the fluctuating force is therefore given by

$$\lambda = \gamma 2k_B T m$$

and therefore the diffusion constant is

$$D = \frac{\gamma 2k_{\text{B}}T}{m}.$$

This is the Einstein-Smoluchowski relation. We observe that the strength of the Diffusion constant, that characterizes the *fluctuations*, is proportional to the damping constant  $\gamma$  describing the *dissipation*. The reason is that both stem microscopically from interactions with the thermal environment. It is an early example of the fluctuation-dissipation theorem.

## Chapter 2

# Quantum Probability, Quantum Dynamical semigroups

### 2.1 Quantum probability

First let us remember from standard quantum mechanics, that the first postulate of q.m. is that the *state* of a system is given by a vector in Hilbert space  $|\psi\rangle \in \mathcal{H}$ . The state however cannot be observed itself, but only its properties through *observables*

$$R : \mathcal{H} \rightarrow \mathcal{H}$$

which are linear, self-adjoint operators,  $R = R^\dagger$ , on the Hilbert space. For determining measurement outcomes, we need to characterize their spectrum (assume discrete spectrum)

$$R = \sum_{n,k} r_n |\psi_{n,k}\rangle \langle \psi_{n,k}| = \sum_n r_n \Pi_n \quad (2.1)$$

with eigenvalues  $r_n \in \mathbb{R}$  that are real and the index  $k$  running over all eigenstates  $|\psi_{n,k}\rangle$  spanning the corresponding (degenerate) subspace with spectral projector  $\Pi_n = \sum_k |\psi_{n,k}\rangle \langle \psi_{n,k}|$ . The second postulate is that the measurement outcomes of a (projective) measurement of observable  $R$  for a system in state  $|\psi\rangle$  are given by the eigenvalues  $r_n$  with corresponding probabilities

$$P_n = P(R = r_n) = \langle \psi | \Pi_n | \psi \rangle = \langle \Pi_n \rangle \quad (2.2)$$

where we have used the definition of expectation value for a system in state  $|\psi\rangle$  according to

$$\langle B \rangle = \langle \psi | B | \psi \rangle. \quad (2.3)$$

After the measurement of value  $r_n$ , the system is in state  $\Pi_n|\psi\rangle/\sqrt{P_n}$ . It is apparent that at any fixed time, the observable  $R$  can therefore be regarded somehow as a random variable. However, since we are free to choose different observables  $R_1, R_2$ , that do not necessarily commute,  $[R_1, R_2] \neq 0$ , the measurement probabilities will depend on which of the observables is measured first, and therefore cannot be described by a classical probability distribution  $P(R_1 = r_{1,n}, R_2 = r_{2,n})$ . Hence, we need to develop a generalized theory of *quantum probability*.

- *Spectral theorem* We begin by generalizing Eq. (2.1) also to observables with a continuous spectrum, which is given by the *spectral theorem for self-adjoint operators*: It states that for any self-adjoint operator  $R$  exists a unique spectral family  $E_r$  such that

$$R = \int_{-\infty}^{\infty} r \, dE_r.$$

The spectral family  $E_r$  is a one-parameter family of commuting orthogonal projection operators which is

1. monotonically increasing i.e.  $E_{r'} \geq E_r$  (i.e.  $E_{r'} - E_r$  is positive semidefinite) for  $r' > r$ ,
2. continuous from the right i.e.  $\lim_{\varepsilon \rightarrow 0^+} E_{r+\varepsilon} = E_r$ ,
3. has limits  $\lim_{r \rightarrow -\infty} E_r = 0$ , and  $\lim_{r \rightarrow \infty} E_r = I$ , where  $I$  denotes the identity.

We can understand this spectral family  $E_r$  as a joint projection on all eigenspaces with eigenvalues  $r' \leq r$ . The differential  $dE_r$  can be vaguely understood as the differential projector on all eigenspaces in the interval  $[r, r + dr]$ .

Note that in the discrete case we have

$$E_r = \sum_{r_n \leq r} \Pi_n = \sum_n \Theta(r - r_n) \Pi_n,$$

hence we find

$$dE_r = \sum_n \delta(r - r_n) \Pi_n \, dr$$

and with this directly recover Eq. (2.1).

Also note that an intuitive (but imprecise) notation that is often used in quantum mechanics is

$$dE_r = |\psi_r\rangle\langle\psi_r| \, dr,$$



which can be helpful to understand the integrals.

Using the representation due to the spectral theorem we can define operator functions

$$f(R) = \int_{-\infty}^{\infty} f(r) \, dE_r.$$

- *Statistical interpretation of quantum mechanics* Let us now axiomatically develop a concept of quantum probability. Consider the set  $\mathcal{R}$  of self-adjoint operators on the Hilbert space  $\mathcal{H}$ . Instead of our definition for pure states, Eq. (2.3) we want to axiomatically find the most general form of an expectation value  $\langle R \rangle$ . An expectation value  $\langle \cdot \rangle$  is a functional on  $\mathcal{R}$ , i.e. it maps each observable  $R \in \mathcal{R}$  to a real number  $\langle R \rangle$ , with the following properties

1. Non-Negativity:  $\langle \Pi \rangle \geq 0$ , for all projectors  $\Pi^2 = \Pi$ ,
2. Normalization:  $\langle I \rangle = 1$ ,
3. Linearity:  $\langle \sum_i c_i R_i \rangle = \sum_i c_i \langle R_i \rangle$ ,  $\forall c_i \in \mathbb{R}$ .

Note that these properties are motivated by the Kolmogorov axioms since in accordance with Eq. (2.2) we want to interpret

$$P(R \leq r) = \langle E_r \rangle$$

as the corresponding cumulative probability distribution for the measurement of observable  $R$ . Even more, with the spectral theorem we find the probability for a measurement outcome in Borel set  $B$  as

$$P(R \in B) = \langle \int_B dE_r \rangle = \int_B \langle dE_r \rangle \quad (2.4)$$

where the last step follows due to the linearity of the functional. We observe that with the requirements 1-3 for the expectation value these definitions satisfy the Kolmogorov axioms leading to a valid statistical interpretation of quantum mechanics. One can then show that the functional  $\langle \cdot \rangle$  can always be written as

$$\langle R \rangle = \text{tr}(R\rho)$$

with the trace operation

$$\text{tr}(\cdot) = \sum_i \langle \varphi_i | \cdot | \varphi_i \rangle \quad \text{with some orthonormal basis (ONB) } \{|\varphi_i\rangle\}_i \text{ of } \mathcal{H},$$

and an operator  $\rho$  with properties

$$\rho^\dagger = \rho \quad (\text{Hermitian}), \quad \rho \geq 0 \quad (\text{pos. semd.}), \quad \text{tr} \rho = 1 \quad (\text{normed}).$$

This operator is called density matrix (or statistical operator) and is the most general form that characterizes the state of a quantum system. From this form of the expectation value we directly find the corresponding variance of observable  $R$ ,

$$\text{Var}(R) = \langle R^2 \rangle - \langle R \rangle^2 = \text{tr}(R^2 \varrho) - \text{tr}(R \varrho)^2.$$

An intuitive interpretation of the density matrix can be found after diagonalizing it,

$$\varrho = \sum_{\alpha} p_{\alpha} |\psi_{\alpha}\rangle \langle \psi_{\alpha}|, \quad (2.5)$$

with eigenvalues  $p_{\alpha} \geq 0$  (since  $\varrho \geq 0$ ) and an ONB  $\{|\psi_{\alpha}\rangle\}_{\alpha}$ . The normalization condition additionally gives

$$1 = \text{tr} \varrho = \sum_{\alpha} p_{\alpha}.$$

Calculating the expectation value  $\langle R \rangle$  therefore yields

$$\langle R \rangle = \text{tr}(R \varrho) = \sum_{\alpha} p_{\alpha} \langle \psi_{\alpha} | R | \psi_{\alpha} \rangle. \quad (2.6)$$

Comparing this to the expectation value for pure states, Eq. (2.3), yields an obvious interpretation: Consider ensembles  $\mathcal{E}_{\alpha}$  of quantum systems that are each prepared in pure state  $|\psi_{\alpha}\rangle$ . If we now consider a total ensemble  $\mathcal{E}$  that is composed by taking states from  $\mathcal{E}_{\alpha}$  with relative frequency  $N_{\alpha}/N$  approaching  $p_{\alpha}$  in the limit of large numbers, it is then described by the state  $\varrho$ . The expectation value in Eq. (2.6) therefore contains two uncertainties: First the quantum uncertainty of the measurement of  $R$  in pure state  $|\psi_{\alpha}\rangle$ , and secondly our classical uncertainty  $p_{\alpha}$  in which pure state  $|\psi_{\alpha}\rangle$  the concrete realization of the quantum system was actually prepared.

It is clear that if  $p_{\alpha} = \delta_{\alpha\alpha_0}$ , this classical uncertainty does not exist and we have

$$\varrho = |\psi_{\alpha_0}\rangle \langle \psi_{\alpha_0}|.$$

We call such states *pure states* and all other states *mixed states*. Since

$$\text{tr}(\varrho^2) = \text{tr} \left( \sum_{\alpha} p_{\alpha}^2 |\psi_{\alpha}\rangle \langle \psi_{\alpha}| \right) = \sum_{\alpha} p_{\alpha}^2$$

we observe that the purity  $\text{tr}(\varrho^2) = 1$  for pure states and  $\text{tr}(\varrho^2) < 1$  for mixed states.

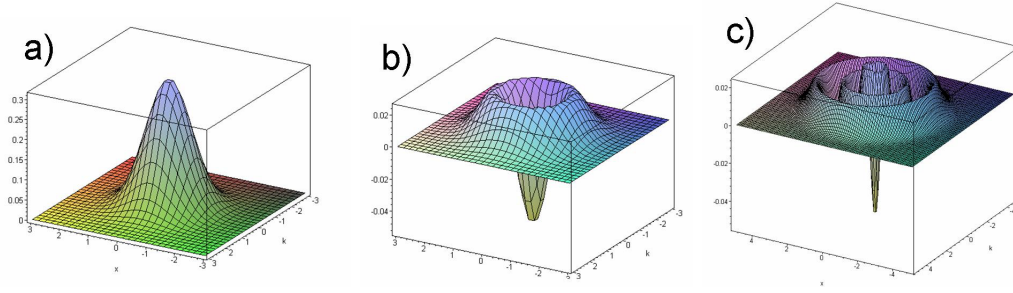


Figure 2.1: Wigner functions [10] for the pure eigenstates of the harmonic oscillator: a)  $n = 0$  ground state b)  $n = 1$  first excited state, c)  $n = 5$ .

- *Connection to classical probability density* Comparing Eq. (2.4) to the definition of the classical probability density

$$P(R \in B) = \int_B \langle dE_r \rangle = \int_B \varrho(r) dr$$

yields the probability density for the measurement outcome  $r$

$$\varrho(r) = \frac{\langle dE_r \rangle}{dr} = \text{tr} \left( \frac{dE_r}{dr} \varrho \right).$$

Take for example  $R = Q$  to be the position operator in one dimension with differential spectral projector

$$dE_q = |q\rangle\langle q|dq.$$

We directly observe

$$\varrho(q) = \langle q|\varrho|q\rangle,$$

i.e. the classical probability density for a measurement outcome  $q$  is given by the *diagonal elements* of the density matrix with respect to the corresponding measurement basis  $|q\rangle$ . The diagonals with respect to the energy eigenbasis (i.e.  $R = H$ ) are therefore sometimes called *populations*. Nevertheless, the full description of the state  $\varrho$  of the system is only given by knowledge of also its offdiagonal elements

$$\langle q|\varrho|q'\rangle, \quad q' \neq q \tag{2.7}$$

which are called *coherences*.

Contrast this to classical mechanics: From Hamiltonian mechanics we remember that the state of the classical system is fully characterized by its phase space density

$$\varrho(q, p),$$

which is a classical probability density. For the quantum system, however, since  $Q$  and  $P$  do not commute we cannot find a common eigenbasis  $|q, p\rangle$  so a direct analog of the classical probability distribution in phase space does not exist (the reason is again that there cannot be a classical joint probability distribution for  $Q$  and  $P$ ). Nevertheless we can introduce center of mass and relative coordinates in Eq. (2.7) according to  $(q, q') \rightarrow (q + \frac{1}{2}q', q - \frac{1}{2}q')$ . Then transforming to the momentum basis with respect to the relative coordinate  $q'$  yields the *Wigner transform* of the density matrix

$$W(q, p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dq' \langle q + \frac{1}{2}q' | \varrho | q - \frac{1}{2}q' \rangle e^{-iq'p/\hbar}.$$

This Wigner function describes a phase space density that tends to the classical phase space density  $\varrho(q, p)$  in the semiclassical limit. For quantum states it is only a quasi-probability distribution since it typically takes also negative values on small scales on the order of a few Planck cells (as we observe in Fig. 2.1 for some harmonic oscillator eigenstates). Nevertheless it is normed

$$1 = \int dq \int dp W(q, p),$$

and we can find the position and momentum distribution by integrating over the other variable,

$$\varrho(q) = \int dp W(q, p), \quad \varrho(p) = \int dq W(q, p).$$

## 2.2 Composite quantum systems

The notion of system and environment is essential for the theory of open quantum systems and makes it necessary for us to study composite quantum systems.

The combined system of system 1 and 2 with Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  is described by the Hilbert space of the tensor product

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2.$$

If we take ONBs  $\{|\varphi_i^{(n)}\rangle\}_i$  of  $\mathcal{H}_n$  a general pure state  $|\psi\rangle$  in the tensor product Hilbert space can be written as

$$|\psi\rangle = \sum_{ij} \alpha_{ij} |\varphi_i^{(1)}\rangle \otimes |\varphi_j^{(2)}\rangle. \quad (2.8)$$

This means that the product basis  $\{|\varphi_i^{(1)}\rangle \otimes |\varphi_j^{(2)}\rangle\}_{ij}$  is a basis for  $\mathcal{H}$  and  $\dim(\mathcal{H}) = \dim(\mathcal{H}_1)\dim(\mathcal{H}_2)$ . If  $A^{(n)}$  is a linear operator acting on  $\mathcal{H}_n$ , the tensor product  $A^{(1)} \otimes A^{(2)}$  is given by

$$A^{(1)} \otimes A^{(2)}(|\varphi^{(1)}\rangle \otimes |\varphi^{(2)}\rangle) = (A^{(1)}|\varphi^{(1)}\rangle) \otimes (A^{(2)}|\varphi^{(2)}\rangle).$$

Any linear operator  $A$  on  $\mathcal{H}$  can be represented as a sum of tensor products

$$A = \sum_{\alpha} A_{\alpha}^{(1)} \otimes A_{\alpha}^{(2)}.$$

The observables of system 1 take the form  $A^{(1)} \otimes I^{(2)}$ , and observables of system 2 take the form  $I^{(1)} \otimes A^{(2)}$ .

In analogy to the classical case, for uncorrelated system 1 and 2 the density matrix factorizes

$$\varrho = \varrho^{(1)} \otimes \varrho^{(2)}.$$

We observe that for such states indeed joint probabilities for observables  $A^{(n)}$  of system 1 and 2 are simply given by their product, since

$$\begin{aligned} \langle A^{(1)} \otimes A^{(2)} \rangle &= \text{tr} \left[ (A^{(1)} \otimes A^{(2)}) (\varrho^{(1)} \otimes \varrho^{(2)}) \right] = \sum_{ij} \langle \varphi_i^{(1)} | \langle \varphi_j^{(2)} | A^{(1)} A^{(2)} \varrho^{(1)} \varrho^{(2)} | \varphi_i^{(1)} \rangle | \varphi_j^{(2)} \rangle \\ &= \text{tr}^{(1)}(A^{(1)} \varrho^{(1)}) \text{tr}^{(2)}(A^{(2)} \varrho^{(2)}) = \langle A^{(1)} \rangle \langle A^{(2)} \rangle \end{aligned}$$

where  $\text{tr}^{(n)}$  denotes the *partial trace* over Hilbert space  $\mathcal{H}_n$ .

If we are only interested in observables in subsystem 1, it is convenient to introduce the *reduced density matrix*

$$\varrho^{(1)} = \text{tr}^{(2)} \varrho$$

which allows us to calculate all observables for subsystem 1,  $A^{(1)} \otimes I^{(2)}$ , via

$$\langle A^{(1)} \rangle = \text{tr}^{(1)}(A^{(1)} \varrho^{(1)}).$$

An important representation of a general state  $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$  of the combined system, Eq. (2.8), follows from the *Schmidt decomposition theorem*: It states that there exist ONBs, the Schmidt bases  $\{|\chi_i^{(n)}\rangle\}_i$  of  $\mathcal{H}_n$ , and Schmidt coefficients  $\alpha_i \in \mathbb{C}$  such that

$$|\psi\rangle = \sum_i \alpha_i |\chi_i^{(1)}\rangle \otimes |\chi_i^{(2)}\rangle.$$

It is important to note that the Schmidt bases depend on the specific state  $|\psi\rangle$ . The number of nonzero Schmidt coefficients  $\alpha_i \neq 0$  is called the *Schmidt rank* or *Schmidt number*. Even though the choice of Schmidt basis is not unique, the Schmidt rank is unique for a given state  $|\psi\rangle$ .

A pure state  $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$  is called *entangled* if it cannot be written as a tensor product  $|\psi\rangle \neq |\varphi^{(1)}\rangle \otimes |\varphi^{(2)}\rangle$ , otherwise we call it *separable*. This means that a state is entangled if its Schmidt rank is larger than one. If all Schmidt coefficients are nonzero and have equal absolute values  $|\alpha_i| = |\alpha_j|$  we call the state *maximally entangled*.

The Schmidt decomposition can be used to prove interesting statements: For example if the combined system is in a pure state  $\varrho = |\psi\rangle\langle\psi|$ , the reduced density matrices  $\varrho^{(1)} = \text{tr}^{(2)}\varrho$  and  $\varrho^{(2)} = \text{tr}^{(1)}\varrho$  have the same eigenvalues

$$\begin{aligned}\varrho^{(1)} &= \text{tr}^{(2)}|\psi\rangle\langle\psi| = \sum_i |\alpha_i|^2 |\chi_i^{(1)}\rangle\langle\chi_i^{(1)}|, \\ \varrho^{(2)} &= \text{tr}^{(1)}|\psi\rangle\langle\psi| = \sum_i |\alpha_i|^2 |\chi_i^{(2)}\rangle\langle\chi_i^{(2)}|.\end{aligned}$$

We observe that after performing the partial trace on an overall pure state  $|\psi\rangle$  of the combined state, the reduced density matrices are only again pure states if  $|\psi\rangle$  is a separable state. If  $|\psi\rangle$  is entangled, the reduced density matrix will be mixed. This also yields another interpretation for the appearance of mixed states in quantum mechanics: Even if we suppose that the dynamics of the “universe” is governed by a pure state, since in any experiment we only have access to a finite degrees of freedom, after tracing over all other degrees of freedom, this state can then occur as a mixed state.

## 2.3 Quantum measurements, quantum operations

- *Projective measurements/ideal quantum measurements* First we want to reformulate the measurement postulate, that we have formulated initially for pure states  $|\psi\rangle$ , on the level of the density matrix  $\varrho$ . Recall that if we have some observable  $R$  with spectral representation

$$R = \int_{-\infty}^{\infty} r \, dE_r,$$

we find the probability of the measurement outcome  $r$  falling in Borel set  $B$  by first integrating the corresponding spectral projector for Borel set  $B$

$$E(B) = \int_B dE_r,$$

by

$$P(R \in B) = \langle E(B) \rangle = \text{tr}(E(B)\varrho) \stackrel{\substack{E(B)^2=E(B) \\ \text{cyc. perm.}}}{=} \text{tr}(E(B)\varrho E(B)).$$

For a pure state we generalize the projection postulate to the projector  $E(B)$ , so that the state after the measurement is

$$|\psi'\rangle = \frac{E(B)|\psi\rangle}{\sqrt{P(R \in B)}}.$$

By writing the density matrix in its diagonal form, Eq. (2.5), and applying this rule to all the  $|\psi_\alpha\rangle$  and using that  $E(B)^\dagger = E(B)$ , we find that the density matrix after measurement of  $r \in B$  is given by

$$\varrho' = \frac{E(B)\varrho E(B)}{\text{tr}(E(B)\varrho E(B))}.$$

This is the von-Neumann-Lüders projection postulate for the density matrix. We note that due to the presence of the denominator the state after the measurement is normalized. Also note that it gives rise to probabilities that are normalized to 1: If we imagine we divide the real axis into disjunct intervals  $\Delta r_\alpha$ , with corresponding projectors  $\Delta E_\alpha$  the states after the measurement are

$$\varrho'_\alpha = \frac{\Delta E_\alpha \varrho \Delta E_\alpha}{P(\Delta r_\alpha)}.$$

with corresponding probabilities  $P(\Delta r_\alpha) = \text{tr}(\Delta E_\alpha \varrho)$  with

$$\sum_\alpha P(\Delta r_\alpha) = \text{tr}\left(\sum_\alpha \Delta E_\alpha \varrho\right) = 1$$

Such a measurement is called *selective measurement* where we keep track of the measurement outcome and divide our original ensemble  $\mathcal{E}$  into sub-ensembles  $\mathcal{E}_\alpha$  that are then described by  $\varrho'_\alpha$ .

We can also think of keeping all states in the ensemble  $\mathcal{E}$  no matter the outcome, i.e. with probability  $P(\Delta r_\alpha)$  the state is given by  $\varrho'_\alpha$  so that the state after the measurement is

$$\varrho' = \sum_\alpha P(\Delta r_\alpha) \varrho'_\alpha = \sum_\alpha \Delta E_\alpha \varrho \Delta E_\alpha.$$

This is called *non-selective measurement*.

*Example:* Position operator  $Q$ : Suppose the system is in pure state  $|\psi\rangle$ . The probability for measuring  $Q \in \Delta = [a, b]$  is given by

$$P(\Delta) = \text{tr}(E(\Delta)|\psi\rangle\langle\psi|) = \text{tr}\left(\int_a^b dq |q\rangle\langle q| |\psi\rangle\langle\psi|\right) = \int_a^b dq |\psi(q)|^2$$

the state after the measurement of  $q$  in interval  $\Delta$  is given by

$$\psi'(q) = \begin{cases} \psi(q)/\sqrt{P(\Delta)} & a \leq q \leq b, \\ 0 & \text{else.} \end{cases}$$

We imagine that in any real world experiment, however, we will never have a measurement device which can exactly resolve the interval  $[a, b]$  but maybe has some Gaussian envelope. It is apparent that such a measurement cannot be described by a projective measurement. This is why we want to develop a generalized measurement theory that also describes such cases.

- *Positive operator valued measurements (POVM)* We observe that for a general definition of a measurement, we need a set of possible outcomes  $m \in \mathcal{M}$  with corresponding probabilities  $P(m)$  and states after measurement  $\varrho'_m$ . However, as we will see, these probabilities and states do not necessarily have to stem from the action of a projector as in the projective measurements.

1. We observe that in order to have a valid probability distribution  $P(m)$  we can also allow for probabilities following from

$$P(m) = \langle F_m \rangle = \text{tr}(F_m \varrho)$$

where  $F_m$  are positive (semidef.) operators (which is less strict than projectors), called *effects*, since then still  $P(m) \geq 0$ . In order for the  $P(m)$  to be interpreted as probabilities we need additionally

$$1 = \sum_{m \in \mathcal{M}} P(m) = \text{tr} \left( \sum_{m \in \mathcal{M}} F_m \varrho \right)$$

implying the condition

$$\sum_{m \in \mathcal{M}} F_m = I.$$

2. For the state after a selective measurement, the most general form is

$$\varrho'_m = \frac{\Phi_m(\varrho)}{P(m)} \tag{2.9}$$



where  $\Phi_m(\varrho)$  is a *quantum operation*, an operation that preserves the properties of the density matrix. In particular, we observe that for  $1 = \text{tr} \varrho'_m$  we need to fulfill the consistency condition

$$P(m) = \text{tr}(F_m \varrho) = \text{tr}(\Phi_m(\varrho)).$$

In analogy to above, the state after a non-selective measurement is given by  $\varrho' = \sum_{m \in \mathcal{M}} \Phi_m(\varrho)$ . In order to further understand this generalized measurement we now want to characterize the possible quantum operations  $\Phi_m(\varrho)$ .

- *Quantum operations, quantum channels* We want to further characterize all possible *quantum operations*  $\Phi(\varrho)$  which are *compatible with quantum mechanics*, i.e. they should be such that they map density matrices  $\varrho$  onto valid density matrices  $\varrho'$  according to Eq. (2.9). This leads to the following requirements: A map  $\Phi(\varrho)$  is a *quantum operation* if

1. As required by postulates of quantum mechanics the map should be linear, i.e.

$$\Phi \left( \sum_i p_i \varrho_i \right) = \sum_i p_i \Phi(\varrho_i).$$

This is intuitively clear if we assume that the  $\varrho_i$  are pure states. Then the mixture  $\sum_i p_i \varrho_i$  corresponds to an experimental procedure where the system is prepared in pure state  $\varrho_i$  with probability  $p_i$ . The operation should then also be understood as individually acting on these pure states and then putting it back into a mixture with the corresponding probabilities.

2. Since  $\varrho' \geq 0$  it is clear that the quantum operation needs to preserve positivity, i.e.  $\Phi(\varrho) \geq 0$  for all  $\varrho \geq 0$ . Nevertheless, since in quantum mechanics there can also exist entangled states between the system and an arbitrary second system with Hilbert space  $\tilde{\mathcal{H}}_n$  with dimension  $n$  (we call it ancilla), this requirement of positivity is not enough: We have to require *complete positivity*, which means that for all  $n \in \mathbb{N}_0$  the map  $\Phi \otimes I_n$  preserves positivity, i.e.

$$(\Phi \otimes I_n)[\varrho_{\text{SA}}] \geq 0 \quad \text{for all } \varrho_{\text{SA}} \geq 0 \text{ on } \mathcal{H} \otimes \tilde{\mathcal{H}}_n$$

here the map acts only on the system and trivially with identity on the ancilla.

3. Since we want to interpret  $\text{tr}(\Phi_m(\varrho))$  as probability for the POVM to return the measurement result  $m$ , we demand

$$0 \leq \text{tr}(\Phi(\varrho)) \leq 1.$$

If  $\text{tr}(\Phi(\varrho)) = 1$  the quantum operation is trace preserving and also called a *quantum channel* or *CPTP (completely positive trace preserving) map*.

Note that this map  $\Phi$  maps operators onto operators and is therefore sometimes called a superoperator. Also note that the quantum channels are the quantum analogon to the classical propagator

$$\varrho(t) = T(t, t')\varrho(t')$$

which also maps classical probability densities onto valid probability densities. Nevertheless, here we have not introduced the notion of time which we will do later.

- *Kraus representation theorem* The representation theorem states that a map is a quantum operation  $\Phi$  if and only if there exists a set of operators  $\Omega_k$  such that

$$\Phi(\varrho) = \sum_k \Omega_k \varrho \Omega_k^\dagger \quad (2.10)$$

with

$$\sum_k \Omega_k^\dagger \Omega_k \leq I. \quad (2.11)$$

The quantum operation is trace preserving (and therefore a quantum channel) if  $\sum_k \Omega_k^\dagger \Omega_k = I$ .

*Proof:* We sketch the proof for finite-dimensional Hilbert spaces. If  $\Phi$  has the representation Eq. (2.10) we see that it is a quantum operation: It is linear and  $\text{tr}(\Phi(\varrho)) = \text{tr}(\sum_k \Omega_k \varrho \Omega_k^\dagger) = \text{tr}(\sum_k \Omega_k^\dagger \Omega_k \varrho) \leq 1$ . Complete positivity follows since

$$\langle \varphi | (\Phi \otimes I)(\varrho) | \varphi \rangle = \sum_k \langle \varphi | (\Omega_k \otimes I) \varrho (\Omega_k^\dagger \otimes I) | \varphi \rangle = \sum_k \langle \varphi_k | \varrho | \varphi_k \rangle \geq 0$$

where in the last step we have used the positivity of the system+ancilla state.

Proving the reverse is a bit more cumbersome: Assume that  $\Phi$  is any quantum operation satisfying conditions 1-3. First we assume that  $\varrho = |\psi\rangle\langle\psi|$ . We introduce an arbitrary orthonormal basis  $\{|\chi_i\rangle\}_i$  of the system's Hilbert space  $\mathcal{H}$  and an ONB  $\{|\tilde{\chi}_i\rangle\}_i$  of the ancilla Hilbert space  $\tilde{\mathcal{H}}$  with the same dimension as the original Hilbert space  $\mathcal{H}$ . We represent the state  $|\psi\rangle$  in this basis

$$|\psi\rangle = \sum_i \alpha_i |\chi_i\rangle.$$

Then we have

$$\Phi(|\psi\rangle\langle\psi|) = \sum_{i,j} \alpha_i \alpha_j^* \Phi(|\chi_i\rangle\langle\chi_j|) = \sum_{ijnm} \alpha_n \alpha_m^* \langle \tilde{\chi}_n | \Phi(|\chi_i\rangle\langle\chi_j|) \otimes (|\tilde{\chi}_i\rangle\langle\tilde{\chi}_j|) | \tilde{\chi}_m \rangle.$$

Let us introduce the maximally entangled state (not normalized)

$$|\Sigma\rangle = \sum_i |\chi_i\rangle \otimes |\tilde{\chi}_i\rangle$$

Hence,

$$\Phi(|\psi\rangle\langle\psi|) = \sum_{nm} \alpha_n \alpha_m^* \langle\tilde{\chi}_n| (\Phi \otimes I)[|\Sigma\rangle\langle\Sigma|] |\tilde{\chi}_m\rangle.$$

Since  $\Phi$  is completely positive, we can diagonalize the positive operator

$$(\Phi \otimes I)[|\Sigma\rangle\langle\Sigma|] = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$$

with  $\lambda_k \geq 0$ . With this we introduce the operators

$$\Omega_k = \sum_n \sqrt{\lambda_k} \langle\tilde{\chi}_n|\phi_k\rangle\langle\chi_n|$$

and finally find

$$\Phi(|\psi\rangle\langle\psi|) = \sum_{nm} \alpha_n \alpha_m^* \langle\tilde{\chi}_n| \sum_k \lambda_k |\phi_k\rangle\langle\phi_k| |\tilde{\chi}_m\rangle = \sum_k \Omega_k |\psi\rangle\langle\psi| \Omega_k^\dagger.$$

This proof can be generalized also to mixed states  $\varrho$  by using the linearity of  $\Phi$ . Eq. (2.11) follows from property 3, the trace property, of the quantum operation.

The Kraus representation theorem is important since it tells us that all “actions” that we perform on a quantum system have to be of this form.

*Example 1: Coherent time evolution* In case of no dissipation the states of the system evolve with unitary time-evolution operator  $U(t, t')$ . The density matrix then follows the evolution

$$\varrho(t) = U(t, t') \varrho(t') U(t, t')^\dagger$$

this is a quantum channel in Kraus form since

$$U(t, t')^\dagger U(t, t') = I.$$

*Example 2: POVM* With our knowledge about quantum operations we now observe that the state after a selective measurement of outcome  $m$  can always be written as

$$\varrho'_m = \frac{\Phi_m(\varrho)}{P(m)} = \frac{\sum_k \Omega_{mk} \varrho \Omega_{mk}^\dagger}{\text{tr}(\sum_k \Omega_{mk} \varrho \Omega_{mk}^\dagger)}.$$

The numerator is a quantum operation and the denominator is due to the renormalization of the ensemble. With this we can identify the effects  $F_m = \sum_k \Omega_{mk}^\dagger \Omega_{mk}$  which are positive operators and fulfill the consistency condition

$$P(m) = \text{tr}(F_m \varrho) = \text{tr}\left(\sum_k \Omega_{mk}^\dagger \Omega_{mk} \varrho\right) = \text{tr}\left(\sum_k \Omega_{mk} \varrho \Omega_{mk}^\dagger\right) = \text{tr}(\Phi_m(\varrho)).$$

Note that in case of the effects being projectors  $F_m = \Pi_m = \Pi_m^2$  this simplifies to the projective measurement

$$\varrho'_m = \frac{\Pi_m \varrho \Pi_m}{\text{tr}(\Pi_m \varrho \Pi_m)}.$$

Since we have  $\sum_m F_m = I$  the non-selective measurement

$$\varrho' = \sum_{m,k} \Omega_{mk} \varrho \Omega_{mk}^\dagger$$

describes a quantum channel.

## 2.4 Quantum dynamical semigroup, Markovian quantum master equation

- *Dynamical map* We can now generalize the notion of stochastic processes to quantum systems: A family  $\{V(t, t')\}_{t \geq t'}$  of maps, that we identify via

$$\varrho(t) = V(t, t') \varrho(t'),$$

with the quantum dynamics, is called *quantum dynamical map* if

1.  $V(t, t')$  is a CPTP map, or a quantum channel, for all times  $t \geq t'$ ,
2.  $V(t, t) = I$ ,

such that it yields a sensible quantum dynamics.

In analogy with the classical processes we call  $V(t, t')$  time-homogeneous if the dynamical map only depends on time differences

$$V(t, t') = V(t - t').$$

Using the Kraus representation theorem, Eq. (2.10), CPTP implies that at all times  $t$ , the dynamical map can be brought into Kraus form

$$\varrho(t) = V(t, t') \varrho(t') = \sum_{\alpha} \Omega_{\alpha}(t, t') \varrho(t') \Omega_{\alpha}(t, t')^\dagger$$

with  $\sum_{\alpha} \Omega_{\alpha}(t, t')^{\dagger} \Omega_{\alpha}(t, t') = I$ . Interestingly, a Kraus form can also be explicitly derived from a global unitary dynamics of the system embedded in a bath environment if the initial state of system and bath is an uncorrelated product state

$$\varrho_{\text{tot}}(0) = \varrho(0) \otimes \varrho_{\text{B}}.$$

Then, since the total system is isolated it evolves with unitary dynamics of system and bath, so we have

$$\varrho(t) = V(t, 0)\varrho(0) = \text{tr}_{\text{B}} \left( U(t, 0)[\varrho(0) \otimes \varrho_{\text{B}}]U(t, 0)^{\dagger} \right). \quad (2.12)$$

We can diagonalize the bath density matrix

$$\varrho_{\text{B}} = \sum_{\alpha} \lambda_{\alpha} |\varphi_{\alpha}\rangle \langle \varphi_{\alpha}|$$

with  $\lambda_{\alpha} \geq 0$  and  $\sum_{\alpha} \lambda_{\alpha} = 1$ . Inserting this in Eq. (2.12) and taking the bath trace with the same basis  $\{|\varphi_{\alpha}\rangle\}_{\alpha}$ , we find the explicit Kraus form

$$V(t, 0)\varrho(0) = \sum_{\alpha, \beta} W_{\alpha\beta}(t)\varrho(0)W_{\alpha\beta}(t)^{\dagger} \quad \text{with} \quad W_{\alpha\beta}(t) = \sqrt{\lambda_{\beta}} \langle \varphi_{\alpha} | U(t, 0) | \varphi_{\beta} \rangle$$

and

$$\sum_{\alpha, \beta} W_{\alpha\beta}(t)^{\dagger} W_{\alpha\beta}(t) = \sum_{\alpha, \beta} \lambda_{\beta} \langle \varphi_{\beta} | U(t, 0)^{\dagger} | \varphi_{\alpha} \rangle \langle \varphi_{\alpha} | U(t, 0) | \varphi_{\beta} \rangle = I.$$

- *Time-homogeneous quantum Markov processes/quantum dynamical semigroups* We now want to generalize the notion of Markovianity also to the quantum dynamics. For time-homogeneous dynamical maps  $V(t)$  there is an accepted definition of Markovianity: Namely if  $V(t)$  forms a *quantum dynamical semigroup* fulfilling the additional properties

3.  $V(t)$  has to be continuous with respect to  $t$ .
4.  $V(t)$  has the semigroup property  $V(t+s) = V(t)V(s)$ ,  $\forall t, s \geq 0$ .

Note that the semigroup property is the straight-forward generalization of the Chapman-Kolmogorov Eq. (1.11) which for time-homogeneous systems we also brought into the form of the semigroup for the propagator  $T(t+s) = T(t)T(s)$ . Remember that, intuitively, it means that there is no memory of the history of the process since we can evolve the system until time  $s$ , and then evolve again until time  $t$  only with the information about the state at time  $s$  and not its history. Further note that due to the semigroup property it actually suffices to require continuity at  $t = 0$  only.

Also note that for *time-inhomogeneous* processes  $V(t, t')$  the definition of Markovianity is still under debate. One possible definition is CP-divisibility, i.e. for all  $s$  we must have  $V(t, t') = V(t, s)V(s, t')$  with all maps being CPTP, which is a natural generalization of the semigroup property. Nevertheless there exist other definitions of Markovianity based on information backflow between system and bath and there are examples that show that they are not equivalent [11] (which in the time-homogeneous case they are).

- *Lindblad master equation* Since the dynamical semigroup is a continuous semigroup, there exists a superoperator  $\mathcal{L}$ , the *generator* of the semigroup, such that we can always write

$$V(t) = \exp(\mathcal{L}t). \quad (2.13)$$

Then, conversely, we may extract the generator  $\mathcal{L}$ , which we call the *Lindblad superoperator*, *Lindbladian* or *GKSL (Gorini-Kossakowski-Sudarshan-Lindblad) superoperator*, from

$$\mathcal{L} = \lim_{\Delta t \rightarrow 0+} \frac{V(\Delta t) - I}{\Delta t}. \quad (2.14)$$

On the level of the density matrix, one finds

$$\partial_t \varrho(t) = \partial_t V(t) \varrho(0) = \mathcal{L}V(t) \varrho(0) = \mathcal{L}\varrho(t), \quad (2.15)$$

which we want to refer to as the *Markovian quantum master equation* for time-homogeneous quantum systems. It is now left to find out how the other properties of the dynamical semigroup, trace preservation and complete positivity, restrict the shape of the superoperator  $\mathcal{L}$ .

Using the Kraus representation, Eq. (2.10), of the dynamical semigroup we are able to find the desired master equation. It is clear that for all  $t$  there exist Kraus operators  $\Omega_i(t)$  such that the dynamical map can be represented as

$$V(t)\varrho = \sum_{i=1}^M \Omega_i(t)\varrho\Omega_i(t)^\dagger \text{ with } I = \sum_{i=1}^M \Omega_i(t)^\dagger\Omega_i(t). \quad (2.16)$$

Here  $M$  represents some number counting the total number of Kraus operators of the channel. If we suppose that  $\dim(\mathcal{H}) = N$  and use that the Kraus operators can be chosen to be linearly independent, making them an operator basis of the Hilbert space  $\mathcal{H}$  which has  $N^2$  elements, we have  $M \leq N^2$ . Since  $V(t)$  is differentiable (because of Eq. (2.14)), for infinitesimal  $dt$  we may write

$$V(0 + dt)\varrho = \varrho + dt\mathcal{L}\varrho \equiv \sum_{i=1}^M \Omega_i(0 + dt)\varrho\Omega_i(0 + dt)^\dagger. \quad (2.17)$$

As a result, the Kraus operators have to obey the form

$$\Omega_i(0 + dt) = \Omega_i^{(0)} + \sqrt{dt}\Omega_i^{(1)} + dt\Omega_i^{(2)} \quad (2.18)$$

where in order to have no term  $\propto \sqrt{dt}$  in Eq. (2.17), it either holds that  $\Omega_i^{(0)} \neq 0$  and  $\Omega_i^{(1)} = 0$  or it holds  $\Omega_i^{(0)} = 0$  and then we may disregard the term  $\Omega_i^{(2)}$ . Since  $V(0)$  is the identity channel, there can be only one Kraus operator with  $\Omega_i^{(0)} \neq 0$ , namely

$$\Omega_1(0 + dt) = I + (K - iH) \cdot dt \quad (2.19)$$

with  $K = K^\dagger$ ,  $H = H^\dagger$ , where we have used that any operator can be written as the sum of its hermitian and its antihermitian part. We represent all other operators as

$$\Omega_{i \neq 1}(0 + dt) = L_{i-1}\sqrt{dt}. \quad (2.20)$$

Plugging this in Eq. (2.17) we find

$$\mathcal{L}\varrho = -i[H, \varrho] + (K\varrho + \varrho K) + \sum_{i=1}^{M-1} L_i\varrho L_i^\dagger. \quad (2.21)$$

From the Kraus sum normalization condition in Eq. (2.16), it follows

$$I = I + dt \underbrace{\left( i(H - H) + 2K + \sum_{i=1}^{M-1} L_i^\dagger L_i \right)}_{=0}. \quad (2.22)$$

Solving for  $K$  we finally find the Lindblad master equation

$$\partial_t \varrho(t) = \mathcal{L}\varrho(t) = -i[H, \varrho(t)] + \sum_{i=1}^{M-1} \left( L_i \varrho(t) L_i^\dagger - \frac{1}{2} \{ L_i^\dagger L_i, \varrho(t) \} \right), \quad (2.23)$$

where  $\{\cdot, \cdot\}$  is the anticommutator,  $\{A, B\} = AB + BA$ . The first part is of the form of the *Liouville-von-Neumann equation* giving rise to the reversible, coherent evolution. Nevertheless,  $H$  is not necessarily the system Hamiltonian  $H_S$ , but may also include contributions stemming from the system-bath interaction (we absorb  $\hbar$  into the Hamiltonian). The second part describes the irreversible, dissipative evolution. It is governed by the *Lindblad operators* (or *jump operators*)  $L_i$ . The first term in the bracket describes how the interaction with the environment transfers populations in the reduced state  $\varrho$ , while the second term is there to conserve the norm of  $\varrho$ . The fact that the first term corresponds to a “jump” is easiest seen by considering a pure state  $\varrho = |\psi\rangle\langle\psi|$  the action of a single jump term then gives

$$L_i |\psi\rangle\langle\psi| L_i^\dagger$$

so we observe that this term leads to an increase in population in state  $|\psi'_i\rangle = L_i|\psi\rangle$ .

Note that this is the most general form that a time-homogeneous Markovian quantum dynamics has to obey and can therefore be regarded as the “analogue of the Schrödinger eq. for the open system”. Also note that when building the concepts of quantum probability axiomatically, we never had to postulate the Schrödinger equation and it comes out here as a byproduct.

Note that we will always choose the Lindblad operators as traceless operators,  $\text{Tr}(L_i) = 0$ . This is because if we would choose operators with a finite trace,  $\tilde{L}_i = c_i I + L_i$ , in Eq. (2.23) (with some complex number  $c_i$ ) it is straight forward to prove that this only leads to a redefinition of the Hamiltonian  $H \rightarrow H + i \sum_{i=1}^{M-1} (c_i^* L_i - c_i L_i^\dagger)$ . The convention of traceless jump operators gets rid of this freedom.

Finally, let us reformulate the dissipative term in Eq. (2.23) in terms of an arbitrary traceless basis  $\{A_i\}$  of the operators over  $\mathcal{H}$ . That means, we find a transformation  $T$  such that

$$L_i = \sum_{j=1}^{N^2-1} T_{ij} A_j. \quad (2.24)$$

Plugging this in Eq. (2.23), we obtain

$$\partial_t \varrho(t) = -i[H, \varrho(t)] + \sum_{i,j=1}^{N^2-1} d_{ij} \left( A_i \varrho(t) A_j^\dagger - \frac{1}{2} \{A_j^\dagger A_i, \varrho(t)\} \right), \quad (2.25)$$

with coefficient matrix, also called *Kossakowski matrix*,

$$d_{ij} = \sum_{k=1}^{M-1} T_{ki} T_{kj}^*. \quad (2.26)$$

Then, we immediately see that  $d$  is hermitian,  $d_{ij} = d_{ji}^*$ , and for all vectors  $x \in \mathbb{C}^{N^2-1}$  we have

$$x^\dagger d x \geq 0. \quad (2.27)$$

Thus,  $d$  is *positive semidefinite*,  $d \geq 0$ . Conversely, a general superoperator  $\mathcal{L}$  that is brought to the form of Eq. (2.25) (which it can always as long as it preserves the trace) is only a proper Lindbladian, if the matrix  $d$  is positive semidefinite. This requirement is the manifestation of complete positivity.

*Example: Two-level system with decay into the ground state* Consider the Hamiltonian of a two-level system

$$H = \frac{\Delta}{2} \sigma_z$$



with eigenstates  $H|\pm\rangle = \pm\Delta/2|\pm\rangle$ , i.e. energy splitting  $\Delta$ . We suspect that the decay into the ground state is captured by the jump operator

$$L = \sqrt{\gamma}\sigma_-$$

with decay rate  $\gamma$  and

$$\sigma_- = \sigma_x - i\sigma_y = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}.$$

Representing

$$\varrho = \begin{pmatrix} p_+ & c \\ c^* & 1 - p_+ \end{pmatrix}$$

with excited state populations  $p_+$  and ground state population  $p_- = 1 - p_+$  (we already use that  $\text{tr}\varrho = 1$ ) and coherence  $c$ . We find

$$\partial_t \varrho = -i\frac{\Delta}{2}[\sigma_z, \varrho] + \gamma \left( \sigma_- \varrho \sigma_-^\dagger - \frac{1}{2} \{ \sigma_-^\dagger \sigma_-, \varrho \} \right), \quad (2.28)$$

$$\begin{pmatrix} \partial_t p_+ & \partial_t c \\ \partial_t c^* & -\partial_t p_+ \end{pmatrix} = -i\Delta \begin{pmatrix} 0 & c \\ -c^* & 0 \end{pmatrix} + 4\gamma \left[ \begin{pmatrix} 0 & 0 \\ 0 & p_+ \end{pmatrix} - \frac{1}{2} \begin{pmatrix} p_+ & c \\ 0 & 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} p_+ & 0 \\ c^* & 0 \end{pmatrix} \right]$$

This yields the (uncoupled) differential equations

$$\partial_t p_+ = -4\gamma p_+, \quad \partial_t c = -i\Delta c - 2\gamma c,$$

which are solved by

$$p_+(t) = e^{-4\gamma t} p_+(0), \quad c(t) = e^{(-i\Delta - 2\gamma)t} c(0).$$

We observe that without dissipation  $\gamma = 0$ , the population in the eigenstates is conserved and the coherences oscillate with a frequency that is set by the energy difference  $\Delta$ . Note that such coherences can for example be created by taking an initial state

$$|\psi(0)\rangle = \sqrt{\frac{1}{2}}(|+\rangle + |-\rangle) \rightarrow \varrho(0) = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

For finite  $\gamma > 0$  both the coherences and the excited state population decay such that the steady state is given by

$$\varrho(t \rightarrow \infty) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

i.e. all the population is in the ground state. Intuitively, we therefore suspect that the Lindblad equation that we wrote down by hand could therefore describe the dynamics of the two-level system in presence of a bath of temperature  $T = 0$ .

Nevertheless, in order to show that this is actually the case, we are missing a complete microscopic derivation of such a Lindblad equation where we start only from the total Hamiltonian of system and bath. This is what we will discuss in the next chapter.



## Chapter 3

# Microscopic approach: Born-Markov approximation

### 3.1 Born-Markov approximation, Quantum-Optical master equation

Our considerations in Chapter 2 are motivated from a more mathematical point of view, namely from the question what the most general equation of motion for a memoryless (Markovian) evolution of the reduced density matrix is. However, the question remains open what this equation will look like in a concrete physical system. We focus on situations where there is a sensible partition of the total physical Hilbert space  $\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{S}} \oplus \mathcal{H}_{\text{B}}$  into a *system*, with Hamiltonian  $H_{\text{S}}$ , whose dynamics we want to keep track of, and its *environment* or *bath* or *reservoir*, with Hamiltonian  $H_{\text{B}}$  and some interaction  $H_{\text{int}}$  between both. The total Hamiltonian therefore reads ( $I_{\alpha}$  is the identity operator on  $\mathcal{H}_{\alpha}$ ,  $\alpha = \text{S, B}$ )

$$H_{\text{tot}} = H_{\text{S}} \otimes I_{\text{B}} + I_{\text{S}} \otimes H_{\text{B}} + H_{\text{int}}. \quad (3.1)$$

Let  $\varrho_{\text{tot}}(t)$  be the evolution of the total density matrix given by the Liouville-von-Neumann equation

$$\partial_t \varrho_{\text{tot}}(t) = -\frac{i}{\hbar} [H_{\text{tot}}, \varrho_{\text{tot}}(t)], \quad (3.2)$$

which is solved formally by

$$\varrho_{\text{tot}}(t) = U(t) \varrho_{\text{tot}}(0) U^{\dagger}(t)$$

with unitary time-evolution operator  $U(t) = \exp(-\frac{i}{\hbar} H_{\text{tot}} t)$ . Let us consider the reduced density matrix of the system

$$\varrho_{\text{S}}(t) = \text{tr}_{\text{B}} \varrho_{\text{tot}}(t),$$

where  $\text{tr}_B$  is the partial trace over the environmental degrees of freedom.

Starting from the total Hamiltonian, Eq. (3.1), we will perform the Born, Markov and the rotating-wave approximation, which are basically motivated by a separation of time scales of the dynamics, to arrive at a master equation which is of Lindblad form. We illustrate the situation for a phononic heat bath.

### 3.1.1 Born approximation

Let us start by transforming the von-Neumann equation (3.2) into the interaction picture. For any operator  $A(t)$  on  $\mathcal{H}_S \otimes \mathcal{H}_B$ , it is defined via

$$\tilde{A}(t) = [U_S^\dagger(t) \otimes U_B^\dagger(t)] A(t) [U_S(t) \otimes U_B(t)],$$

with  $U_{S/B}(t) = \exp(-\frac{i}{\hbar} H_{S/B} t)$ . Then, Eq. (3.2) takes the form

$$\partial_t \tilde{\varrho}_{\text{tot}}(t) = -\frac{i}{\hbar} [\tilde{H}_{\text{int}}(t), \tilde{\varrho}_{\text{tot}}(t)]. \quad (3.3)$$

We may formally integrate this equation to find

$$\tilde{\varrho}_{\text{tot}}(t) = \tilde{\varrho}_{\text{tot}}(0) - \frac{i}{\hbar} \int_0^t d\tau [\tilde{H}_{\text{int}}(\tau), \tilde{\varrho}_{\text{tot}}(\tau)]. \quad (3.4)$$

If we plug this back into the right hand side of Eq. (3.3) we obtain

$$\partial_t \tilde{\varrho}_{\text{tot}}(t) = -\frac{i}{\hbar} [\tilde{H}_{\text{int}}(t), \tilde{\varrho}_{\text{tot}}(0)] - \frac{1}{\hbar^2} \int_0^t d\tau [\tilde{H}_{\text{int}}(t), [\tilde{H}_{\text{int}}(\tau), \tilde{\varrho}_{\text{tot}}(\tau)]]. \quad (3.5)$$

This equation is equivalent to Eq. (3.3), however it includes the interaction Hamiltonian  $\tilde{H}_{\text{int}}$  on second order, which will be useful for the following considerations.

Throughout the whole derivation we want to assume that the system–bath coupling is ‘weak’ when compared to the energy scales of  $H_S$  and  $H_B$ . We will specify what we mean by ‘weak’ at multiple instances in the derivation. The first instance is now, when we want to discuss correlations between the system and its environment. We require that at  $t = 0$  there are no correlations between the system and its environment. The Hamiltonian  $\tilde{H}_{\text{int}}$  shall be weak such that there is no significant buildup of correlations during the evolution, and we may approximate

$$\tilde{\varrho}_{\text{tot}}(t) \approx \tilde{\varrho}(t) \otimes \tilde{\varrho}_B. \quad (3.6)$$

Here, we have additionally assumed that the environment is ‘large’ in the sense that it has many degrees of freedom. As a result, the state of the reservoir  $\tilde{\varrho}_B$  is unaltered by the weak contact to the ‘smaller’ system. These approximations that lead to Eq. (3.6) are known as *Born approximation*.

Plugging Eq. (3.6) into Eq. (3.5) and performing the trace over the reservoir degrees of freedom we find

$$\partial_t \tilde{\varrho}(t) = -\frac{i}{\hbar} \left[ \text{tr}_B(\tilde{H}_{\text{int}}(t) \tilde{\varrho}_B), \tilde{\varrho}(0) \right] - \frac{1}{\hbar^2} \int_0^t d\tau \text{tr}_B \left[ \tilde{H}_{\text{int}}(t), \left[ \tilde{H}_{\text{int}}(\tau), \tilde{\varrho}(\tau) \otimes \tilde{\varrho}_B \right] \right]. \quad (3.7)$$

Let us discuss the first term of the right hand side of this equation. Note that we may assume that  $H_{\text{shift}} = \text{tr}_B(H_{\text{int}} \varrho_B) = 0$ . Because if it was nonzero, we simply may absorb its contribution in the system Hamiltonian,  $H_{\text{int}} \rightarrow H_{\text{int}} - H_{\text{shift}} \otimes I_B$  and  $H_S \rightarrow H_S + H_{\text{shift}}$  in Eq. (3.1).

Thus (and we assume that the bath is stationary  $[H_B, \varrho_B] = 0$ ), the first term in Eq. (3.7) drops out and we are left with the second term. Using a Schmidt decomposition of the interaction Hamiltonian we find

$$H_{\text{int}} = \sum_{\alpha} s_{\alpha} \otimes B_{\alpha},$$

where we require that the system- and bath coupling operators are Hermitian,  $s_{\alpha} = s_{\alpha}^{\dagger}$ ,  $B_{\alpha} = B_{\alpha}^{\dagger}$ . Transforming this into the interaction picture, we may rewrite Eq. (3.7) as

$$\partial_t \tilde{\varrho}(t) = -\frac{1}{\hbar^2} \sum_{\alpha, \beta} \int_0^t d\tau \left( [\tilde{s}_{\alpha}(t) \tilde{s}_{\beta}(\tau) \tilde{\varrho}(\tau) - \tilde{s}_{\beta}(\tau) \tilde{\varrho}(\tau) \tilde{s}_{\alpha}(t)] \left\langle \tilde{B}_{\alpha}(t) \tilde{B}_{\beta}(\tau) \right\rangle_B + \text{h.c.} \right). \quad (3.8)$$

with  $\langle \cdot \rangle_B = \text{tr}_B(\varrho_B \cdot)$ . This is the master equation in Born approximation. Note that the right-hand side still depends on  $\tilde{\varrho}(\tau)$ , i.e. the evolution is non-Markovian as it will, in general, depend on the history of the reduced state.

### 3.1.2 Markov approximation

In many physical situations, one can get rid of this cumbersome dependence on the history of the state. This will lead us to a discussion of the time scales of the dynamics.

Let us investigate the bath correlation functions  $C_{\alpha\beta}(t, \tau) = \left\langle \tilde{B}_{\alpha}(t) \tilde{B}_{\beta}(\tau) \right\rangle_B$ . We assume that the state of the bath is stationary, so they may only depend on the temporal distance  $t - \tau$ , i.e.

$$C_{\alpha\beta}(t, \tau) \equiv C_{\alpha\beta}(t - \tau) = \left\langle \tilde{B}_{\alpha}(t - \tau) \tilde{B}_{\beta}(0) \right\rangle_B.$$

In most physical reservoirs, these correlation functions will decay on a time scale  $\tau_B$ . Since the reservoir is large, typically, the information gets scrambled on time scales  $\tau_B$  that are much faster than the time scale  $\tau_R$  of the relaxation dynamics of the system,  $\tau_B \ll \tau_R$ . Note that this is especially compatible with our requirement of ‘weak’ system–bath coupling  $H_{\text{int}}$ ,

because the time scale  $\tau_R$  is inversely proportional to the small energy scale of  $H_{\text{int}}$  (to be precise, from Eq. (3.8) we see  $\tau_R$  is scaling as  $\tau_R \propto \hbar^2 \kappa^{-2}$  if  $H_{\text{int}} \propto \kappa$ ). Therefore, on the relevant time scales of the integral in Eq. (3.8), the reduced density matrix is approximately constant. Consequently, we may perform the first step of the *Markov approximation* and replace  $\tilde{\varrho}(\tau)$  with  $\tilde{\varrho}(t)$  to obtain

$$\partial_t \tilde{\varrho}(t) = \frac{1}{\hbar^2} \sum_{\alpha, \beta} \int_0^t d\tau ([\tilde{s}_\beta(\tau) \tilde{\varrho}(t), \tilde{s}_\alpha(t)] C_{\alpha\beta}(t - \tau) + \text{h.c.}). \quad (3.9)$$

This is the *time-dependent Redfield master equation* in the interaction picture.

Now it is convenient to replace the integration variable  $\tau \rightarrow t - \tau$ , such that in the integral it occurs the factor  $C_{\alpha\beta}(\tau)$ . Then, since  $C_{\alpha\beta}(\tau)$  decays rapidly, we may extend the upper bound of the integral to infinity, which is the second part of the Markov approximation,

$$\partial_t \tilde{\varrho}(t) = \frac{1}{\hbar^2} \sum_{\alpha, \beta} \int_0^\infty d\tau ([\tilde{s}_\beta(t - \tau) \tilde{\varrho}(t), \tilde{s}_\alpha(t)] C_{\alpha\beta}(\tau) + \text{h.c.}). \quad (3.10)$$

We can transform back into the Schrödinger picture to find

$$\partial_t \varrho(t) = -\frac{i}{\hbar} [H_S, \varrho(t)] + \frac{1}{\hbar^2} \sum_{\alpha} \left( [u_{\alpha} \varrho(t), s_{\alpha}] + \text{h.c.} \right), \quad (3.11)$$

This is the stationary *Redfield master equation* with operators

$$u_{\alpha} = \sum_{\beta} \int_0^\infty d\tau \tilde{s}_{\beta}(-\tau) C_{\alpha\beta}(\tau),$$

which are a convolution of the interaction-picture system coupling operators with the bath-correlation function. Practically, we can calculate these operators by introducing the eigenbasis of the system Hamiltonian  $H_S |n\rangle = E_n |n\rangle$ . Then we plug in an identity twice

$$u_{\alpha} = \sum_{\beta, nm} \int_0^\infty d\tau |n\rangle \langle n| \tilde{s}_{\beta}(-\tau) |m\rangle \langle m| C_{\alpha\beta}(\tau) = \pi \hbar \sum_{\beta, nm} s_{nm}^{\beta} W_{\alpha\beta}(\Delta_{nm}) |n\rangle \langle m|$$

where we have used energy differences  $\Delta_{nm} = E_n - E_m$  and  $\langle n| \tilde{s}_{\alpha}(-\tau) |m\rangle = e^{-\frac{i}{\hbar} \Delta_{nm} \tau} s_{nm}^{\alpha}$ , with matrix elements  $s_{nm}^{\alpha} = \langle n| s_{\alpha} |m\rangle$  and the (imaginary) Laplace transform of the bath-correlation function

$$W_{\alpha\beta}(E) = \frac{1}{\pi \hbar} \int_0^\infty d\tau e^{-\frac{i}{\hbar} E \tau} C_{\alpha\beta}(\tau). \quad (3.12)$$

Note that Eq. (3.11) is generally not of Lindblad form, which we would wish to hold such that a physical evolution of the density matrix is guaranteed, leading to the somewhat confusing fact that the evolution is not Markovian (in the mathematical sense of Sec. 2.4) even though we have applied the so called Markov approximation. Hence, complete positivity (or even positivity) may be violated during the evolution with the Redfield master equation.

### 3.1.3 Rotating wave approximation

In the ultraweak coupling limit  $H_{\text{int}} \rightarrow 0$ , however, complete positivity is guaranteed. This is because in this limit we may perform the rotating wave approximation (or secular approximation) to find a master equation that is of Lindblad form.

This approximation is again justified from a discussion of time scales of the dynamics. Here, we assume that the time scale of relaxation  $\tau_R$  is slow when compared to a typical time scale of the system dynamics  $\tau_S$ . Therefore, the dynamics may be thought of obeying the form

$$\varrho_{nm}(t) \approx e^{-\frac{i}{\hbar}(E_n - E_m)t} \varrho_{nm}(0) + \mathcal{O}(\kappa^2 t / \hbar^2), \quad (3.13)$$

with fast coherent oscillations on time scale  $\tau_S = \max_{n \neq m} \hbar / (E_n - E_m)$  and slow dissipative dynamics on time scale  $\tau_R \propto \hbar^2 / \kappa^2$  where  $\kappa$  is the order of magnitude of the system–bath coupling,  $H_{\text{int}} \sim \kappa$ . If  $\tau_S \ll \tau_R$  the first term will dephase much faster than the time scale  $\tau_R$  where contributions of the second term start to play a role, so in the dissipative dynamics we may assume that  $\varrho_{nm}(t)$  is asymptotically diagonal.

More formally, this can be seen from transforming (3.11) back into the interaction picture

$$\partial_t \tilde{\varrho}(t) = \frac{\pi}{\hbar} \sum_{\alpha\beta, nmkl} \left( e^{\frac{i}{\hbar}(\Delta_{nm} + \Delta_{kl})t} \left[ s_{nm}^\beta W_{\alpha\beta}(\Delta_{nm}) |n\rangle\langle m| \tilde{\varrho}(t), s_{kl}^\alpha |k\rangle\langle l| \right] + \text{h.c.} \right),$$

where we have additionally spectrally decomposed the coupling operators  $s_\alpha$ . The *rotating wave approximation* (or *secular approximation*) is now to average over a typical time scale of the system time scales  $\tau_S = \max_{n \neq m} \hbar / (E_n - E_m)$  and since  $\tau_S \ll \tau_R$  the density matrix  $\tilde{\varrho}(t)$  is approximately constant on this time scale  $\tau_S$ , so the exponential factor averages out if  $\Delta_{nm} + \Delta_{kl} \neq 0$ . Hence we only keep the terms with  $\Delta_{nm} + \Delta_{kl} = 0$  giving

$$\partial_t \tilde{\varrho}(t) = \frac{\pi}{\hbar} \sum_{\alpha\beta, nm} \left( s_{nm}^\beta s_{mn}^\alpha W_{\alpha\beta}(\Delta_{nm}) \left[ |n\rangle\langle m| \tilde{\varrho}(t), |m\rangle\langle n| \right] + \text{h.c.} \right),$$

which is of Lindblad form since we can define  $L_{nm} = |n\rangle\langle m|$  and

$$R_{nm} + iS_{nm} = \frac{2\pi}{\hbar} \sum_{\alpha\beta} s_{mn}^\alpha s_{nm}^\beta W_{\alpha\beta}(\Delta_{nm}),$$

with real and imaginary part  $R_{nm}$  and  $S_{nm}$  of the rates. Transforming back into the Schrödinger picture and using these definitions, we have

$$\begin{aligned}\partial_t \varrho(t) &= -\frac{i}{\hbar} [H_S, \varrho(t)] + \frac{1}{2} \sum_{nm} \left[ (R_{nm} + iS_{nm}) \left( L_{nm} \varrho(t) L_{nm}^\dagger - L_{nm}^\dagger L_{nm} \varrho(t) \right) \right. \\ &\quad \left. + (R_{nm} - iS_{nm}) \left( L_{nm} \varrho(t) L_{nm}^\dagger - \varrho(t) L_{nm}^\dagger L_{nm} \right) \right] \\ &= -\frac{i}{\hbar} [H_S + H_{LS}, \varrho(t)] + \sum_{nm} R_{nm} \left( L_{nm} \varrho(t) L_{nm}^\dagger - \frac{1}{2} \{ L_{nm}^\dagger L_{nm}, \varrho(t) \} \right). \quad (3.14)\end{aligned}$$

with Lamb-shift Hamiltonian  $H_{LS} = \frac{\hbar}{2} \sum_{nm} S_{nm} L_{nm}^\dagger L_{nm} = \frac{\hbar}{2} \sum_{nm} S_{nm} |m\rangle\langle m|$ . Eq. (3.14) is the *quantum optical master equation*. Since one can show that all rates are positive,  $R_{nm} \geq 0$ , it is apparent that Eq. (3.14) is of Lindblad form and hence the Markovian quantum master equation that we were aiming for. The effect of the environment in the ultraweak coupling limit is hence twofold: Firstly it introduces an energy shift

$$E_m \rightarrow E'_m = E_m + \frac{\hbar}{2} \sum_n S_{nm}$$

which slightly changes the frequencies that occur in the coherent evolution of the system. Secondly, through the jump operators  $L_{nm} = |n\rangle\langle m|$  the dissipative environment introduces quantum jumps between those eigenstates  $|m\rangle$  and  $|n\rangle$  which occur at corresponding jump rate  $R_{nm}$ . These jumps can change the purity of a given initial density matrix and can also describe the evolution of the density matrix towards a thermal state as we will see later, which is the thermalization dynamics that we were searching for in Sec. 1.1.

Interestingly, if we introduce the energy eigenbasis for the density matrix

$$\varrho(t) = \sum_n p_n(t) |n\rangle\langle n| + \sum_{n \neq m} \varrho_{nm}(t) |n\rangle\langle m|$$

the dynamics of the populations  $p_n(t)$  and the coherences  $\varrho_{nm}(t)$ ,  $n \neq m$ , in Eq. (3.14) decouple,

$$\begin{aligned}\partial_t \varrho_{nm}(t) &= -\frac{i}{\hbar} (E'_n - E'_m) \varrho_{nm}(t) - \frac{1}{2} \sum_k (R_{kn} + R_{km}) \varrho_{nm}(t) \equiv -\Gamma_{nm} \varrho_{nm}(t) \\ \partial_t p_n(t) &= \sum_m (R_{nm} p_m(t) - R_{mn} p_n(t))\end{aligned} \quad (3.15)$$

which is usually referred to as *dynamical decoupling*. We directly observe that the coherences decay  $\varrho_{nm}(t) = \varrho_{nm}(0) \exp(-\Gamma_{nm} t)$  such that the state is asymptotically diagonal in the energy eigenbasis. The dynamics of the populations  $p_n(t)$  is given by a classical master equation with jump rates  $R_{nm}$  from state  $m$  to  $n$ , which is also called *Pauli rate equation*.



### 3.1.4 Rates for coupling to thermal phonon reservoir

We want to find the Born-Markov rates for a typical heat bath. Let us specify the environmental degrees of freedom and the system–environment coupling in Eq. (3.1). A common choice for a bath environment is a collection of harmonic oscillators

$$H_B = \sum_{\alpha} \hbar \omega_{\alpha} b_{\alpha}^{\dagger} b_{\alpha}$$

It describes the quantized oscillatory (phononic) degrees of freedom in a heat bath, with bosonic annihilation operator  $b_{\alpha}$  and frequency  $\omega_{\alpha}$ . We want to focus on the *diffusive regime*, where the system couples to the displacement  $x_{\alpha} \propto (b_{\alpha}^{\dagger} + b_{\alpha})$  of the oscillators. Let us assume that the oscillators couple to some system coupling operator  $s$ . Then, the system–bath coupling takes the form

$$H_{\text{int}} = \kappa s \otimes \sum_{\alpha} c_{\alpha} (b_{\alpha}^{\dagger} + b_{\alpha}),$$

with (real) coupling coefficients  $c_{\alpha}$  to each mode  $\alpha$ . We have extracted the overall strength  $\kappa$  of the interaction, while  $s$  and  $c_{\alpha}$  are assumed on the order of unity. Note that the Hamiltonian  $H_{\text{int}}$  already has the form of a direct product. Thus, we have only one bath coupling operator  $B = \sum_{\alpha} c_{\alpha} (b_{\alpha}^{\dagger} + b_{\alpha})$ .

Finally, let us fix the state  $\varrho_B$  of the reservoir. We want to assume that it is in a thermal state with temperature  $T$  (phonons have chemical potential  $\mu = 0$ ),

$$\varrho_B = \frac{1}{\text{tr}_B(e^{-H_B/k_B T})} e^{-H_B/k_B T} = \prod_{\alpha} \left(1 - e^{-\hbar \omega_{\alpha}/k_B T}\right) e^{-\hbar \omega_{\alpha} b_{\alpha}^{\dagger} b_{\alpha}/k_B T}.$$

Note that indeed we have  $\text{tr}_B(H_{\text{int}} \varrho_B) = 0$ . Let us compute the bath-correlation function

$$C(t) = \left\langle \tilde{B}(t) \tilde{B}(0) \right\rangle_B.$$

First, we transform the bath-coupling operator to the interaction picture,

$$\tilde{B}(t) = \sum_{\alpha} c_{\alpha} \left( e^{i\omega_{\alpha} t} b_{\alpha}^{\dagger} + e^{-i\omega_{\alpha} t} b_{\alpha} \right).$$

This yields

$$C(t) = \sum_{\alpha} c_{\alpha}^2 \left[ e^{i\omega_{\alpha} t} n(\hbar \omega_{\alpha}) + e^{-i\omega_{\alpha} t} (n(\hbar \omega_{\alpha}) + 1) \right],$$

where we have defined the Planck occupation function  $n(E) = (\exp(E/k_B T) - 1)^{-1}$ .

Let us define the spectral density of the bath,

$$\bar{J}(E) = \sum_{\alpha} c_{\alpha}^2 \delta(E - \hbar\omega_{\alpha}),$$

which counts how many bath modes there are at energy  $E$  and how strong the system is coupled to them. Typically, Markovian baths have a continuum of modes  $\alpha$  such that  $\bar{J}(E)$  is a continuous function. A very prominent choice is  $\bar{J}(E) = E$ , the *ohmic bath*. This is because in the classical limit of the kinetic Hamiltonian  $H = p^2/2m + V(q)$ , this choice (together with system coupling operator  $s = -q$  and  $\gamma = \kappa^2$ ) gives rise to a Langevin equation with a linear friction term  $-\gamma\dot{q}$ . Other common choices are  $\bar{J}(E) = E^d$ , where for  $d > 1$  the bath is called *superohmic*, and for  $d < 1$  *subohmic*. Also, to avoid divergences it is often needed to add a cutoff scale to  $\bar{J}(E)$ , for example by using an exponential cutoff at energy  $E_c$ ,  $\bar{J}(E) = E \exp(-E/E_c)$ .

With this choice, we write

$$W(E) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dE' \int_0^{\infty} d\tau e^{-\frac{i}{\hbar}E\tau} \bar{J}(E') \left[ e^{\frac{i}{\hbar}E'\tau} n(E') + e^{-\frac{i}{\hbar}E'\tau} (n(E') + 1) \right], \quad (3.16)$$

where we have used that  $\bar{J}(E) = 0$  for  $E < 0$  and exchanged the two integrals. First, let us split the complex function  $W$  into its real and imaginary part

$$W(E) = g(E) + iw(E).$$

Then, the integrals can be evaluated using the Sokhotski–Plemelj formula ( $\mathcal{P}$  is the Cauchy principle value),

$$\lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} d\omega \int_0^{\infty} d\tau e^{-i\omega\tau - \varepsilon\tau} f(\omega) = \pi f(0) - i\mathcal{P} \int_{-\infty}^{\infty} d\omega \frac{f(\omega)}{\omega}, \quad (3.17)$$

since we can rewrite Eq. (3.16) by transforming  $E' \rightarrow E - E'$  in the first term and  $E' \rightarrow -E + E'$  in the second term

$$W(E) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dE' \int_0^{\infty} d\tau e^{-\frac{i}{\hbar}E'\tau} \left[ \bar{J}(E - E') n(E - E') + \bar{J}(-E + E') (n(-E + E') + 1) \right].$$

Hence we directly obtain the real part of the bath-correlation function

$$g(E) = \begin{cases} \bar{J}(E)n(E) & \text{for } E \geq 0, \\ \bar{J}(-E)(n(-E) + 1) & \text{for } E < 0. \end{cases} \quad (3.18)$$

Note that for the Planck distribution it holds that

$$n(-E) + 1 = \frac{1}{e^{-E/k_B T} - 1} + 1 = \frac{e^{-E/k_B T}}{e^{-E/k_B T} - 1} = -n(E)$$

such that it is convenient to define the antisymmetrized spectral density

$$J(E) = \bar{J}(E) - \bar{J}(-E),$$

which allows for a compact form which is valid for all  $E$ ,

$$g(E) = J(E)n(E) = \frac{J(E)}{e^{E/k_B T} - 1}. \quad (3.19)$$

From this we find the Pauli rates for the phonon bath

$$R_{nm} = \frac{2\pi\kappa^2}{\hbar} |\langle n|s|m\rangle|^2 g(E_n - E_m). \quad (3.20)$$

This is the main result of this section. This rate is of Fermi's golden rule type as it depends on the matrix element of the coupling operator squared multiplied by some function which counts the density of states in the bath. However, it differs from Fermi's golden rule because we additionally have to take into account the thermal occupation of the bath at the given energy difference that occurs in the process.

Note that since the state  $\varrho_B$  of the bath is thermal, it holds that

$$g(-E) = e^{E/k_B T} g(E). \quad (3.21)$$

As a result, the rates  $R_{nm}$  fulfill  $R_{nm}/R_{mn} = e^{(E_m - E_n)/k_B T}$  and hence the following condition: there exist probabilities  $p_n$  such that

$$R_{nm}p_m = R_{mn}p_n \quad \text{for all } n, m. \quad (3.22)$$

It means that in the steady state of the Pauli rate equation (3.15),  $\partial_t p_n(t) = 0$ , all terms in the sum on the r.h.s. vanish *individually*. This condition is known as *detailed balance*, because there is no net probability flow between state  $n$  and  $m$ . This condition is only fulfilled in *thermal equilibrium*. In our case, it immediately follows that the probabilities  $p_n$  are given by the Boltzmann factors

$$p_n \propto \exp(-E_n/k_B T).$$

Combined with the fact that the state is diagonal in the energy eigenbasis it is clear that for coupling to a thermal bath the quantum optical master equation correctly predicts thermalization towards the canonical ensemble

$$\varrho(t \rightarrow \infty) = \frac{1}{Z} e^{-H/k_B T}.$$

As soon as we choose rates  $R_{nm}$  that do not fulfill a detailed balance condition, the system will relax to a *nonequilibrium steady state*. Possibly the easiest way of breaking detailed balance is by coupling the system to two heat baths of different temperature  $T_1$  and  $T_2$ . Then the total rates  $R_{nm}$  will be the sum of the individual rates of when the system is coupled to one of the baths only.

## 3.2 Examples

### 3.2.1 Decay of a two-level system, Spin-Boson model

We are now in the position that we can derive Eq. (2.28) describing the decay of a two-level system also microscopically. For this we consider the Hamiltonian of the *Spin-Boson model*

$$H_{\text{tot}} = \frac{\Delta}{2} \sigma_z + \kappa \sigma_x \sum_{\alpha} c_{\alpha} (b_{\alpha}^{\dagger} + b_{\alpha}) + \sum_{\alpha} \hbar \omega_{\alpha} b_{\alpha}^{\dagger} b_{\alpha}$$

(in the original Spin-Boson model the role of  $\sigma_x$  and  $\sigma_z$  is interchanged). The model is versatile since it describes universally the dynamics of a two-level system in the environment of harmonic oscillators. This might be for example an atom interacting with its surrounding electromagnetic field or two computational levels of a superconducting circuit (used for quantum computation) interacting with its environment.

We can now directly write down the quantum optical master equation that describes the dynamics of this model in the ultraweak coupling limit  $\kappa \rightarrow 0$ ,

$$\partial_t \varrho(t) = -\frac{i}{\hbar} \left[ \frac{\Delta}{2} \sigma_z, \varrho(t) \right] + \sum_{nm} R_{nm} \left( L_{nm} \varrho(t) L_{nm}^{\dagger} - \frac{1}{2} \left\{ L_{nm}^{\dagger} L_{nm}, \varrho(t) \right\} \right),$$

where we have ignored the Lamb-shift contribution. The dissipator drives transitions between the energy eigenstates,  $L_{nm} = |n\rangle\langle m|$ , where for the two-level system there are only two states  $|n\rangle = |+\rangle, |-\rangle$ . Plugging in  $s = \sigma_x$  into the rates, Eq. (3.20), we find

$$\begin{aligned} R_{nm} &= \frac{2\pi\kappa^2}{\hbar} |\langle n|\sigma_x|m\rangle|^2 g(E_n - E_m) \\ &= \frac{2\pi\kappa^2}{\hbar} \times \begin{cases} g(-\Delta) = J(\Delta)[1 + n(\Delta)] & n = -, m = + \\ g(\Delta) = J(\Delta)n(\Delta) & n = +, m = - \\ 0 & n = m \end{cases}. \end{aligned}$$

Defining the overall rate  $\gamma = J(\Delta)\pi\kappa^2/(2\hbar)$  and using that  $\sigma_+ = 2|+\rangle\langle -|$ ,  $\sigma_- = 2|-\rangle\langle +|$ , we finally find that the quantum optical master equation takes the form

$$\partial_t \varrho(t) = -\frac{i}{\hbar} \left[ \frac{\Delta}{2} \sigma_z, \varrho(t) \right] + \gamma [1 + n(\Delta)] D(\sigma_-)[\varrho(t)] + \gamma n(\Delta) D(\sigma_+)[\varrho(t)] \quad (3.23)$$

with  $D(L)[\cdot] = L \cdot L^{\dagger} - \frac{1}{2} \{L^{\dagger} L, \cdot\}$ . We observe three different dissipative processes: The first one is the *spontaneous decay* into the ground state that we postulated in Eq. (2.28), which also occurs at bath temperature  $T = 0$ , where the bath modes are empty  $n(\Delta) = 0$ . The other terms correspond to *thermally induced emission* and *absorption*.

*Resonance fluorescence.* We imagine that the two-level atom is additionally driven time-periodically with an external laser field. In dipole approximation,  $H_d = -\vec{E}(t)\vec{d}(t)$  the field couples to the dipole operator  $\vec{d}(t) \propto \sigma_x$  of the atom. Hence in the Schrödinger picture, the Hamiltonian of the system takes the form

$$H_S = \frac{\Delta}{2}\sigma_z + E \cos(\omega_0 t)\sigma_x = \frac{\Delta}{2}\sigma_z + \frac{E}{4}(e^{i\omega_0 t} + e^{-i\omega_0 t})(\sigma_+ + \sigma_-).$$

This is the *Rabi model*. Transforming into the rotating frame with regards to the undriven Hamiltonian,

$$\tilde{\varrho}(t) = e^{\frac{i}{\hbar}\frac{\Delta}{2}\sigma_z t} \varrho(t) e^{-\frac{i}{\hbar}\frac{\Delta}{2}\sigma_z t}$$

we find for the coherent evolution in the rotating frame we have

$$\partial_t \tilde{\varrho}(t) = -\frac{i}{\hbar} \left[ \frac{E}{4} (e^{i\omega_0 t} + e^{-i\omega_0 t}) \left( e^{i\frac{\Delta}{\hbar}t} \sigma_+ + e^{-i\frac{\Delta}{\hbar}t} \sigma_- \right), \tilde{\varrho}(t) \right]$$

We assume that the atom is driven on resonance with the transition energy,  $\hbar\omega_0 = \Delta$ . Hence, after factoring out all terms we observe that there are secular terms  $\exp(\pm i(\omega_0 - \Delta/\hbar)t) = 1$  and nonsecular terms  $\exp(\pm i(\omega_0 + \Delta/\hbar)t) = \exp(\pm i2\omega_0 t)$  which rotate fast and can again be neglected in a rotating wave approximation. Hence, in the co-rotating frame the resonantly driven atom can again be described by a static problem. If this system is now additionally coupled to an environment, we can make the rough approximation that the dissipator is still given by the one of the undriven system in Eq. (3.23).

$$\partial_t \tilde{\varrho}(t) = -\frac{i}{\hbar} \left[ \frac{E}{2} \sigma_x, \tilde{\varrho}(t) \right] + \gamma[1 + n(\Delta)]D(\sigma_-)[\tilde{\varrho}(t)] + \gamma n(\Delta)D(\sigma_+)[\tilde{\varrho}(t)]. \quad (3.24)$$

Let us introduce the Bloch vector  $\langle \vec{\sigma} \rangle = \text{tr}(\varrho \vec{\sigma})$  with  $\vec{\sigma} = \sum_i \sigma_i \vec{e}_i$ . It follows from the most general form of the density matrix of the two-level system

$$\varrho = \begin{pmatrix} p_+ & c \\ c^* & 1 - p_+ \end{pmatrix} = \frac{I}{2} + \frac{1}{2} [2\text{Re}(c)\sigma_x - 2\text{Im}(c)\sigma_y + (-1 + 2p_+)\sigma_z]$$

that

$$\langle \vec{\sigma} \rangle = \begin{pmatrix} 2\text{Re}(c) \\ -2\text{Im}(c) \\ -1 + 2p_+ \end{pmatrix}$$

is a vector inside (for mixed states) or on (for pure states) the unit sphere (the Bloch sphere). Since it is also characterized by three real numbers it provides a unique representation of the state of the two-level system. All states on the  $z$ -axis correspond to classical

mixtures between the ground state  $|-\rangle$  and the excited state  $|+\rangle$ . States with a finite  $x$  and  $y$  components are coherent superpositions between ground and excited state.

Plugging this into Eq. (3.24), we find that the equation of motion for the Bloch vector therefore reads

$$d_t \langle \vec{\sigma}(t) \rangle = G \langle \vec{\sigma}(t) \rangle + \vec{b}$$

with

$$G = \begin{pmatrix} -2\Gamma & 0 & 0 \\ 0 & -2\Gamma & -E \\ 0 & E & -4\Gamma \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} 0 \\ 0 \\ -4\gamma \end{pmatrix},$$

where  $\Gamma = \gamma(1 + 2n(\Delta))$ . This is the optical Bloch equation describing the dynamics of the Bloch vector resonantly driven two-level system in contact with a thermal environment. The stationary state  $d_t \langle \vec{\sigma}(t) \rangle = 0$  follows directly from

$$\langle \vec{\sigma} \rangle_{\text{ss}} = -G^{-1} \vec{b} = \frac{1}{8\Gamma^2 + E^2} \begin{pmatrix} -\frac{8\Gamma^2 + E^2}{2\Gamma} & 0 & 0 \\ 0 & -4\Gamma & E \\ 0 & -E & -2\Gamma \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 4\gamma \end{pmatrix} = \frac{1}{8\Gamma^2 + E^2} \begin{pmatrix} 0 \\ 4\gamma E \\ -8\gamma\Gamma \end{pmatrix},$$

We observe that without the driving  $E = 0$ , the Bloch vector follows from the thermal average

$$\langle \vec{\sigma} \rangle_{\text{ss}} = \begin{pmatrix} 0 \\ 0 \\ -\frac{\gamma}{\Gamma} = -\frac{e^{\Delta/(k_B T)} - 1}{e^{\Delta/(k_B T)} + 1} \end{pmatrix},$$

which lies on the  $z$ -Axis and for  $\langle \vec{\sigma} \rangle_{\text{ss}}(T \rightarrow 0) = -\vec{e}_z$  as well as  $\langle \vec{\sigma} \rangle_{\text{ss}}(T \rightarrow \infty) = 0$  as expected. If the driving is switched on,  $E \neq 0$ , the Bloch vector becomes polarized in the  $y$ -direction, which corresponds to coherent oscillations with the driving frequency in the Schrödinger picture.

### 3.2.2 Caldeira-Legett model, damped harmonic oscillator

Another seminal model of open quantum systems is the Caldeira-Legett model: Consider a Brownian particle of mass  $m$  with coordinate  $x$  in a potential  $V(x)$ . The particle is assumed to be coupled to a bath consisting of a large number of harmonic oscillators with masses  $m_n$  and frequencies  $\omega_n$ . System and bath are coupled via position-position coupling.

The total Hamiltonian is then given by the *Caldeira-Leggett model*, which reads

$$H = \frac{p^2}{2m} + V_c(x) + \sum_n \left( \frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 x_n^2 \right) - x \sum_n C_n x_n \quad (3.25)$$

with total potential

$$V_c(x) = V(x) + \underbrace{x^2 \sum_n \frac{C_n^2}{2m_n\omega_n^2}}_{H_c},$$

with system potential  $V(x)$  and the second term being a counter term that is added since the system-bath interaction would otherwise lead to an effective potential on the system (which is exactly canceled by this counter term). This can be seen since we can rewrite

$$H = \frac{p^2}{2m} + V(x) + \sum_n \left[ \frac{p_n^2}{2m_n} + \frac{1}{2}m_n\omega_n^2 \left( x_n - \frac{C_n}{m_n\omega_n^2}x \right)^2 \right]$$

and if we imagine to redefine  $x'_n = \frac{m_n\omega_n^2}{C_n}x_n$  we observe that the model corresponds to coupled harmonic oscillators where in the potential we only couple the position differences  $(x'_n - x)^2$  as required by translational invariance.

*Damped harmonic oscillator.* If we assume a quadratic potential  $V(x) = \frac{m\omega^2}{2}x^2$  we can rewrite the Caldeira-Leggett model Eq. (3.25) with bosonic creation and annihilation operators as

$$H = \underbrace{\hbar\omega \left( a^\dagger a + \frac{1}{2} \right)}_{H_S} + H_c + \underbrace{\sum_n \hbar\omega_n \left( b_n^\dagger b_n + \frac{1}{2} \right)}_{H_B} \underbrace{-x}_s \sum_n \underbrace{C_n \sqrt{\frac{\hbar}{2m_n\omega_n}}}_{\kappa C_n} (b_n^\dagger + b_n)$$

This Hamiltonian is exactly of the form that we assumed in Sec. 3.1.4. We immediately observe that the eigenenergies and eigenstates of the system are given by the harmonic oscillator eigenstates

$$H_S |n\rangle = \hbar\omega \left( n + \frac{1}{2} \right) |n\rangle.$$

In analogy to the Spin-Boson model in the ultraweak coupling limit  $\kappa \ll \hbar\omega$  we can perform the Born-, Markov and rotating-wave approximation with system coupling operator  $s = -x = -\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)$  to find the quantum-optical master equation

$$\partial_t \varrho(t) = -\frac{i}{\hbar} \left[ \hbar\omega \left( a^\dagger a + \frac{1}{2} \right), \varrho(t) \right] + \gamma [1 + n(\hbar\omega)] D(a)[\varrho(t)] + \gamma n(\hbar\omega) D(a^\dagger)[\varrho(t)] \quad (3.26)$$

again with  $D(L)[\cdot] = L \cdot L^\dagger - \frac{1}{2}\{L^\dagger L, \cdot\}$  and rate  $\gamma = \frac{\pi\kappa^2}{m\omega}J(\hbar\omega)$ . Here we have additionally neglected  $H_{LS}, H_c \propto \kappa^2$  since their contribution is much smaller than the system Hamiltonian. The first dissipative term corresponds to the annihilation of a phonon/photon in the

system and the emission of a phonon into the bath. The second term corresponds to the annihilation of a phonon in the bath and a creation of a phonon in the system. Eq. (3.26) can describe, for example, the state of the field inside a cavity. The environment is provided by the modes outside of the cavity into which the cavity field can decay with rate  $\gamma$ .

*Adjoint master equation.* Similar to the isolated systems, when can also define a Heisenberg picture where the state  $\varrho_H$  is time-independent and all time dependance is in the operators  $A_H(t)$ , and both pictures coincide at  $t = 0$ ,  $A_H(0) = A$ ,  $\varrho_H = \varrho(0)$ . We can identify this by looking at the expectation value that must be independent of the picture we are in,

$$\langle A \rangle(t) = \text{tr}(A\varrho(t)) \equiv \text{tr}(A_H(t)\varrho_H).$$

Hence if  $\varrho(t)$  evolves with the general Lindblad master equation

$$\partial_t \varrho(t) = -\frac{i}{\hbar} [H, \varrho(t)] + L\varrho(t)L^\dagger - \frac{1}{2} \{L^\dagger L, \varrho(t)\}$$

we require

$$\begin{aligned} \partial_t \langle A \rangle(t)|_{t=0} &= \text{tr}(A\partial_t \varrho(t))|_{t=0} = \text{tr} \left[ A \left( -\frac{i}{\hbar} [H, \varrho(0)] + L\varrho(0)L^\dagger - \frac{1}{2} \{L^\dagger L, \varrho(0)\} \right) \right] \\ &\equiv \text{tr}(\partial_t A_H(t)\varrho_H)|_{t=0}. \end{aligned}$$

By performing cyclic permutations in the trace to get  $\varrho(0) = \varrho_H$  to the right position we observe that this is fulfilled if

$$\partial_t A_H(t) = \frac{i}{\hbar} [H, A_H(t)] + L^\dagger A_H(t)L - \frac{1}{2} \{L^\dagger L, A_H(t)\}.$$

This is the *adjoint master equation* for the evolution of the operators in the Heisenberg picture. Note that in our reasoning we focused on  $t = 0$ , but since the master equation is time-homogeneous, this has to hold also for all times  $t$ .

According to this, we find that for the damped harmonic oscillator in Eq. (3.26) the adjoint master equation reads

$$\partial_t A_H(t) = \frac{i}{\hbar} \left[ \hbar\omega \left( a^\dagger a + \frac{1}{2} \right), A_H(t) \right] + \gamma [1 + n(\hbar\omega)] D^\dagger(a)[A_H(t)] + \gamma n(\hbar\omega) D^\dagger(a^\dagger)[A_H(t)] \quad (3.27)$$

with adjoint dissipator  $D^\dagger(L)[\cdot] = L^\dagger \cdot L - \frac{1}{2} \{L^\dagger L, \cdot\}$ . Solving this equation for the annihilation, creation and number operator  $A_H(0) = a, a^\dagger, a^\dagger a$  we find

$$\begin{aligned} a_H(t) &= e^{(-i\omega - \gamma/2)t} a, \\ a_H^\dagger(t) &= e^{(i\omega - \gamma/2)t} a^\dagger, \\ (a^\dagger a)_H(t) &= e^{-\gamma t} a^\dagger a + n(\hbar\omega)(1 - e^{-\gamma t}). \end{aligned}$$



From this we directly infer the mean amplitude of the oscillator

$$\langle a \rangle(t) = \text{tr}(a_H(t)\varrho_H) = e^{(-i\omega - \gamma/2)t} \langle a \rangle(0), \quad (3.28)$$

and the mean number of quanta

$$\langle a^\dagger a \rangle(t) = \text{tr}((a^\dagger a)_H(t)\varrho_H) = e^{-\gamma t} \langle a^\dagger a \rangle(0) + n(\hbar\omega)(1 - e^{-\gamma t}) \quad (3.29)$$

The mean oscillator amplitude thus follows an exponential spiral in the complex plane, decaying for  $\gamma t \gg 1$  to the origin. The mean number of quanta turns from the initial  $\langle a^\dagger a \rangle(0)$  to the thermal value  $n(\hbar\omega)$  which is independent of the initial condition.

*Coherent state representation (P-representation).* In quantum optical applications one often studies the master equation in phase space representation. To this end we introduce the *coherent states* from standard quantum mechanics

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle = e^{\alpha a^\dagger - \alpha^* a} |0\rangle, \quad (3.30)$$

with  $\alpha \in \mathbb{C}$ . The states are normalized to 1 but not orthogonal to each other, i.e.  $\langle \beta | \alpha \rangle \neq 0$  for  $\alpha \neq \beta$ . The coherent states are eigenstates of the non-hermitian annihilation operator  $a$ ,

$$a|\alpha\rangle = \alpha|\alpha\rangle.$$

Remember that

$$\begin{aligned} \langle \alpha | x | \alpha \rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle \alpha | (a^\dagger + a) | \alpha \rangle = \sqrt{\frac{2\hbar}{m\omega}} \text{Re}(\alpha), \\ \langle \alpha | p | \alpha \rangle &= i\sqrt{\frac{\hbar m\omega}{2}} \langle \alpha | (a^\dagger - a) | \alpha \rangle = \sqrt{2\hbar m\omega} \text{Im}(\alpha), \end{aligned}$$

so that the real part of  $\alpha$  is associated with the position and the imaginary part with the momentum of the oscillator in a coherent pure state, and since it has minimal uncertainty in  $x$  and  $p$  it corresponds to a state that is localized in phase space.

The coherent states form an overcomplete set of states satisfying

$$I = \frac{1}{\pi} \int d^2\alpha |\alpha\rangle \langle \alpha| \quad (3.31)$$

with  $d^2\alpha = d\text{Re}(\alpha)d\text{Im}(\alpha)$  representing the integral over the complex plane. We can use this identity to find a different representation of the density matrix of the harmonic oscillator. Since all operators on the Hilbert space of the harmonic oscillator can be represented as a combination of powers of creation and annihilation operators  $a^j (a^\dagger)^k$ , we can write

$$\varrho = \sum_{j,k} c_{jk} a^j (a^\dagger)^k.$$

Inserting the over-completeness relation, Eq. (3.31), between  $a^j$  and  $(a^\dagger)^k$ , we have

$$\varrho = \frac{1}{\pi} \int d^2\alpha \sum_{jk} c_{jk} \alpha^j |\alpha\rangle\langle\alpha| (\alpha^*)^k = \int d^2\alpha P(\alpha, \alpha^*) |\alpha\rangle\langle\alpha|.$$

This is the *Glauber-Sudarshan P-representation* of the state of the harmonic oscillator. It is an alternative quasiprobability distribution in phase space to the Wigner function. We can interpret that  $P(\alpha, \alpha^*)$  assigns a (quasi)-probability to each point  $\alpha$  in phase space.  $P(\alpha, \alpha^*)$  however can also take negative values. Nevertheless it is normed due to the normalization of the trace

$$1 = \text{tr} \varrho = \int d^2\alpha P(\alpha, \alpha^*).$$

The dynamics under the quantum optical master equation (3.26) can therefore be recast into the dynamics of the P-representation using

$$\varrho(t) = \int d^2\alpha P(\alpha, \alpha^*, t) |\alpha\rangle\langle\alpha|. \quad (3.32)$$

A product of creation and annihilation operators is said to be normal ordered if all powers  $a^\dagger$  stand left to all powers of  $a$ . For such normal ordered products we find

$$\langle (a^\dagger)^p a^q \rangle(t) = \text{tr} \left[ (a^\dagger)^p a^q \varrho(t) \right] = \int d^2\alpha (\alpha^*)^p \alpha^q P(\alpha, \alpha^*, t).$$

This is an important property of the P-distribution that expectation values of normal ordered products of creation and annihilation operators turn into a corresponding moment of the distribution  $P(\alpha, \alpha^*, t)$ .

We can derive an evolution equation for the distribution by plugging Eq. (3.32) into the master equation (3.26) and using the properties

$$\begin{aligned} a|\alpha\rangle\langle\alpha| &= \alpha|\alpha\rangle\langle\alpha|, & |\alpha\rangle\langle\alpha|a^\dagger &= \alpha^*|\alpha\rangle\langle\alpha|, \\ a^\dagger|\alpha\rangle\langle\alpha| &= (\partial_\alpha + \alpha^*)|\alpha\rangle\langle\alpha|, & |\alpha\rangle\langle\alpha|a &= (\partial_{\alpha^*} + \alpha)|\alpha\rangle\langle\alpha|, \end{aligned}$$

which can be proved by using the definition of the coherent state, Eq. (3.30). For example

$$\begin{aligned} (\partial_\alpha + \alpha^*) \underbrace{e^{-\frac{1}{2}|\alpha|^2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle}_{|\alpha\rangle} &= (-\alpha^* + \alpha^*)|\alpha\rangle + e^{-\frac{1}{2}|\alpha|^2} \sum_n n \frac{\alpha^{n-1}}{\sqrt{n!}} |n\rangle \\ &= e^{-\frac{1}{2}|\alpha|^2} \sum_n \sqrt{n+1} \frac{\alpha^n}{\sqrt{n!}} |n+1\rangle = a^\dagger |\alpha\rangle \end{aligned}$$

where in the first step we use the product rule and in the second step we shift the summation index.

When acting with those operators on Eq. (3.32) for the we perform integration by parts and find a minus sign so we find the following correspondence rules

$$a\rho \leftrightarrow \alpha P, \quad \rho a^\dagger \leftrightarrow \alpha^* P, \quad a^\dagger \rho \leftrightarrow (-\partial_\alpha + \alpha^*) P, \quad \rho a \leftrightarrow (-\partial_{\alpha^*} + \alpha) P.$$

With these relations we find a equation of motion for the P-representation

$$\partial_t P(\alpha, \alpha^*, t) = - \left[ \left( -i\omega - \frac{\gamma}{2} \right) \partial_\alpha \alpha + \left( i\omega - \frac{\gamma}{2} \right) \partial_{\alpha^*} \alpha^* \right] P(\alpha, \alpha^*, t) + \gamma n(\hbar\omega) \partial_\alpha \partial_{\alpha^*} P(\alpha, \alpha^*, t), \quad (3.33)$$

which describes the evolution of the quasiprobability distribution in phase space. The equation is similar to the classical Fokker-Planck equation (1.17), however here for a complex stochastic variable and for the quasiprobability  $P$ . The first term corresponds to a deterministic drift and the second term to a diffusion that is absent at  $T = 0$ .

Let us solve this equation for initial value

$$P(\alpha, \alpha^*, 0) = \delta^2(\alpha - \alpha_0)$$

which means that the initial state is a coherent state  $|\alpha_0\rangle$ . This can be solved by plugging in a (two-dimensional) Gaussian ansatz

$$P(\alpha, \alpha^*, t) = \frac{1}{\pi \sigma^2(t)} e^{-|\alpha - \beta(t)|^2 / \sigma^2(t)}$$

into Eq. (3.33) and derive differential equations for  $\beta(t)$  and  $\sigma^2(t)$ . An easier way is to realize that  $\beta(t)$  is given by the mean amplitude

$$\beta(t) = \int d^2\alpha \alpha P(\alpha, \alpha^*, t) = \langle a \rangle(t) \stackrel{(3.28)}{=} \alpha_0 e^{(-i\omega - \gamma/2)t}$$

and similarly

$$\sigma^2(t) = \text{Var}(|\alpha|) = \langle a^\dagger a \rangle(t) - \langle a^\dagger \rangle(t) \langle a \rangle(t) \stackrel{(3.29), (3.28)}{=} n(\hbar\omega)(1 - e^{-\gamma t})$$

The P-representation is therefore given by a Gaussian wave packet which spirals around the origin. The width  $\sigma^2(t)$  increases from the zero to the thermal average. Note that at  $T = 0$  the initial coherent state remains coherent under time evolution.

In analogy with Sec. 1.2.3 we can associate the complex Fokker-Planck eq. (3.33) with a stochastic processes generated from the complex stochastic Itô differential equation

$$d\alpha(t) = \left( -i\omega + \frac{\gamma}{2} \right) \alpha(t) dt + \sqrt{\gamma n(\hbar\omega)} dW(t)$$

giving rise to a complex Ornstein-Uhlenbeck process. Here  $dW(t)$  is the increment of a complex Wiener process satisfying

$$\langle dW(t) \rangle = 0, \quad dW(t)dW(t) = 0, \quad dW(t)dW(t)^* = dt,$$

which can be generated from two statistically independent real Wiener process

$$dW(t) = \frac{1}{\sqrt{2}} (dW_1(t) + idW_2(t)).$$

### 3.3 Quantum Brownian Motion

Let us again turn to the Caldeira-Leggett model

$$H = \frac{p^2}{2m} + V(x) + H_c + \sum_n \left( \frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 x_n^2 \right) \underbrace{-x}_s \underbrace{\sum_n C_n x_n}_B$$

with counter-term

$$H_c = x^2 \sum_n \frac{C_n^2}{2m_n \omega_n^2},$$

but now we will also allow for arbitrary potentials  $V(x)$  and situations where the system time scale is not necessarily fast when compared to the relaxation timescale anymore, so we cannot perform the rotating wave approximation. This is natural in the limit where is no system potential  $V(x)$ , which we can imagine as harmonic confinement frequency  $\omega \rightarrow 0$  since then the level spacing gets smaller and smaller leading to a divergence of the system time scales.

Nevertheless, if the bath-correlation times are short (which is true at high temperature  $T$ ) a different master equation can be found. To this end let us begin with the Redfield master equation in the Schrödinger picture

$$\partial_t \varrho(t) = -\frac{i}{\hbar} [H_S + H_c, \varrho(t)] + \underbrace{\frac{1}{\hbar^2} \left( [u\varrho(t), s] + \text{h.c.} \right)}_{\mathcal{K}[\varrho(t)]},$$

with

$$u = \int_0^\infty d\tau \tilde{s}(-\tau) \langle \tilde{B}(\tau) \tilde{B}(0) \rangle.$$

Note that since  $H_c \propto \kappa^2$  is second order in the coupling strength  $\kappa$  while  $H_{\text{int}} \propto \kappa$  is first order, it is consistent on second order to include the counter term on the level of the Hamiltonian only and not in the dissipator. To proceed, it is convenient to rewrite the bath correlation function in terms of real and imaginary part

$$\langle \tilde{B}(\tau) \tilde{B}(0) \rangle = \frac{1}{2} D_1(\tau) - \frac{i}{2} D(\tau)$$

by introducing the correlation functions

$$\begin{aligned} D(\tau) &= i \langle [\tilde{B}(\tau), \tilde{B}(0)] \rangle = i [\tilde{B}(\tau), \tilde{B}(0)], \\ D_1(\tau) &= \langle \{ \tilde{B}(\tau), \tilde{B}(0) \} \rangle, \end{aligned}$$

which are often referred to as dissipation and noise kernel. In  $D(\tau)$  we have used that for the noninteracting bath and linear coupling  $B$  in the Caldeira-Leggett model, the commutator is a complex number, so we can omit the average. Using that

$$B = \sum_n C_n \sqrt{\frac{\hbar}{2m_n \omega_n}} (b_n^\dagger + b_n) = \sum_n c_n (b_n^\dagger + b_n),$$

we can directly apply our results for the coupling to a thermal phonon bath, Sec. 3.1.4, giving

$$\tilde{B}(t) = \sum_n c_n (e^{i\omega_n t} b_n^\dagger + e^{-i\omega_n t} b_n).$$

Again using the definition of the spectral density of the bath

$$\bar{J}(E) = \sum_n c_n^2 \delta(E - \hbar\omega_n),$$

we have

$$\begin{aligned} D(\tau) &= i [\tilde{B}(\tau), \tilde{B}(0)] = \sum_n c_n^2 i (-e^{i\omega_n \tau} + e^{-i\omega_n \tau}) = 2 \int_0^\infty \bar{J}(E) \sin(E\tau/\hbar) dE, \\ D_1(\tau) &= \langle \{ \tilde{B}(\tau), \tilde{B}(0) \} \rangle = \sum_n c_n^2 (e^{i\omega_n \tau} + e^{-i\omega_n \tau}) [2n(\hbar\omega_n) + 1] \\ &= 2 \int_0^\infty \bar{J}(E) \coth\left(\frac{E}{2k_B T}\right) \cos(E\tau/\hbar) dE. \end{aligned}$$

With this we can rewrite the Redfield dissipator

$$\begin{aligned} \mathcal{K}[\varrho(t)] &= \frac{1}{\hbar^2} \int_0^\infty d\tau \left\{ [\tilde{s}(-\tau) \varrho(t), s] \left( \frac{D_1(\tau)}{2} - \frac{iD(\tau)}{2} \right) + [s, \varrho(t) \tilde{s}(-\tau)] \left( \frac{D_1(\tau)}{2} + \frac{iD(\tau)}{2} \right) \right\} \\ &= \frac{1}{\hbar^2} \int_0^\infty d\tau \left\{ \frac{iD(\tau)}{2} [s, \{\tilde{s}(-\tau), \varrho(t)\}] - \frac{D_1(\tau)}{2} [s, [\tilde{s}(-\tau), \varrho(t)]] \right\}. \end{aligned}$$

Now to arrive at the master equation for quantum brownian motion, instead of performing the rotating wave approximation in the system, we now assume that the time scale of the bath (on which  $D_1$  and  $D$  decay) is much than the typical time scales of the system,  $\tau_B \ll \tau_S$ . Note that this is an additional approximation to the one that we made when performing the Markov approximation, where we assumed  $\tau_B \ll \tau_R$ . Under this assumption we can approximate that for short time scales

$$\tilde{s}(-\tau) = e^{-iH_S\tau/\hbar} s e^{iH_S\tau/\hbar} \approx s - \frac{i}{\hbar} [H_S, s] \tau = -x + \frac{p}{m} \tau.$$

Under this approximation, the dissipator can be written as

$$\begin{aligned} \mathcal{K}[\varrho(t)] = & \frac{i}{2\hbar^2} \int_0^\infty d\tau D(\tau) [x, \{x, \varrho(t)\}] - \frac{i}{2\hbar^2 m} \int_0^\infty d\tau \tau D(\tau) [x, \{p, \varrho(t)\}] \\ & - \frac{1}{2\hbar^2} \int_0^\infty d\tau D_1(\tau) [x, [x, \varrho(t)]] + \frac{1}{2\hbar^2} \int_0^\infty d\tau \tau D_1(\tau) [x, [p, \varrho(t)]] . \end{aligned}$$

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