Chapter 1
Dynamics of Open Quantum Systems

Abstract This chapter provides a brief introduction to quantum systems that are coupled to large reservoirs. It aims to remind the reader of well-known concepts necessary for the understanding of the book and does not claim to provide a self-contained introduction. It starts with a brief summary of the conventions used in the book and then introduces master equations with some examples. This also requires us to introduce the density matrix: among other things, we discuss its evolution in a closed system and under measurements. To connect to system-reservoir theories, we also review the definition of the tensor product and the partial trace. Finally, we introduce the Lindblad form of a quantum master equation and discuss its properties before closing with some remarks on the superoperator representation of master equations.

With the tremendous advances during the last century in our ability to prepare and control the smallest systems, quantum theory has proven extremely successful. This evolution has not only been driven by mere interest in basic principles. Perfect control of quantum systems would also allow one to build extremely powerful computers that could solve special problems such as number factoring [1], database search [2], or simply simulation of other quantum systems [3, 4] much faster than we can do with classical computers. Unfortunately, the promises of quantum computation have turned out to be hard to keep, since the fragile quantum coherence necessary for quantum computation to work usually rapidly decays. This process—commonly termed decoherence [5–7]—is induced by the presence of reservoirs that can significantly alter the true quantum dynamics. With the sophisticated experimental setups in present-day proof-of-principle implementations of quantum computers [8] or quantum simulators [9–11], these reservoirs usually cannot be assumed to be in thermal equilibrium.

The coupling between a quantum system and a structured non-equilibrium environment can however also be seen as a chance: the smallest quantum systems can also be seen as nanomachines that exchange energy and matter with their surroundings. From a thermodynamic viewpoint, such nanomachines are coupled to an environment that is out of equilibrium and might thus be able to perform useful tasks such as generating electrical current from a heat gradient [12]. Alternatively, they could function as heating or cooling devices [13].

In either case, the effect of non-equilibrium environments on a quantum system is a topic that deserves to be thoroughly understood. This book provides some basic steps towards a description of open quantum systems subject to non-equilibrium environments.

1.1 Conventions

Altogether, we will use the following conventions without further notice in the book.

Planck's constant $\hbar = 1.0546 \times 10^{-34}$ J s will be set to one; i.e., we will absorb it in the Hamiltonian of every considered system. This implies that all energies will have dimensions of inverse time. Similarly, Boltzmann's constant $k_{\rm B} = 1.3806 \times 10^{-23}$ J/K will also not occur in this book; it will be hidden in the inverse temperature $\beta = 1/(k_{\rm B}T)$ with temperature T.

The quantity $[A, B] \equiv AB - BA$ denotes the commutator between two operators A and B, whereas $\{A, B\} = AB + BA$ denotes their anti-commutator.

Operators in the interaction picture will be written by boldface symbols $\boldsymbol{O}(t) = e^{+iH_0t} O e^{-iH_0t}$, with H_0 and t denoting the free Hamiltonian and time, respectively.

We will represent superoperators, i.e., linear operations on operators, by calligraphic symbols. For example, the linear operation $\mathscr{K}[O] = \sum_{ij} K_i O K_j$ on the operator O will—after short notice—be denoted by $\mathscr{K} O$.

Throughout the book, we will denote the Fermi–Dirac distribution (or just the Fermi function) of a particular reservoir α by

$$f_\alpha(\omega) = \frac{1}{e^{\beta_\alpha(\omega - \mu_\alpha)} + 1},\tag{1.1}$$

where β_α and μ_α represent the inverse temperature and chemical potential of the reservoir α, respectively. Similarly, we will denote the Bose–Einstein distribution of bosonic reservoirs by

$$n_\alpha(\omega) = \frac{1}{e^{\beta_\alpha(\omega - \mu_\alpha)} - 1},\tag{1.2}$$

where we will however mostly consider $\mu_\alpha = 0$.

Finally, we mention that only a few abbreviations will be used in the book. The ones to remember are single electron transistor (SET), double quantum dot (DQD), quantum point contact (QPC), Kubo–Martin–Schwinger (KMS), and Baker–Campbell–Hausdorff (BCH).

1.2 Evolution of Closed Systems

Before we start with the non-equilibrium, we will briefly review closed quantum systems. The dynamics of such a closed quantum system can already be complicated

enough, since the evolution of its state vector $|\Psi\rangle$ obeys the Schrödinger equation

$$\left|\dot{\Psi}(t)\right\rangle = -\mathrm{i}H(t)\left|\Psi(t)\right\rangle, \tag{1.3}$$

where we have absorbed the Planck constant $\hbar$ in the Hamiltonian $H(t)$. A time-dependent Hamiltonian in the Schrödinger picture would mean that the system is actually not really closed: changing the parameters of the Hamiltonian normally requires an interaction with the outside world. However, time-dependent Hamiltonians may also arise in transformed pictures, e.g., when a time-dependent unitary transformation $|\tilde{\Psi}(t)\rangle = e^{+\mathrm{i}H_0 t}|\tilde{\Psi}(t)\rangle$ is applied to Eq. (1.3) with an initially time-independent Hamiltonian.

Exercise 1.1 (Transformation to the interaction picture) Assuming a time-independent Hamiltonian $H = H_0 + V$, show that the Schrödinger equation in the interaction picture becomes

$$\left|\dot{\tilde{\Psi}}(t)\right\rangle = -\mathrm{i}V(t)\left|\tilde{\Psi}(t)\right\rangle, \tag{1.4}$$

where $V(t) = e^{+\mathrm{i}H_0 t} V e^{-\mathrm{i}H_0 t}$ denotes the time-dependent Hamiltonian and $|\tilde{\Psi}(t)\rangle = e^{+\mathrm{i}H_0 t}|\Psi(t)\rangle$ the state vector in the interaction picture.

The Schrödinger equation is formally solved by the unitary propagator

$$U(t) = \hat{\tau}\exp\left\{-\mathrm{i}\int_0^t H(t')\,dt'\right\}, \tag{1.5}$$

with the time-ordering operator $\hat{\tau}$. Time ordering sorts time-dependent operators depending on their time argument; i.e., formally it acts as

$$\hat{\tau}\,\boldsymbol{O}(t_1)\boldsymbol{O}(t_2) = \Theta(t_1 - t_2)\boldsymbol{O}(t_1)\boldsymbol{O}(t_2) + \Theta(t_2 - t_1)\boldsymbol{O}(t_2)\boldsymbol{O}(t_1) \tag{1.6}$$

with the Heaviside theta function

$$\Theta(x) = \begin{cases} 1: & x > 0, \\ 1/2: & x = 0, \\ 0: & x < 0. \end{cases} \tag{1.7}$$

Its role in the time evolution operator can however also be defined by the time derivative

$$\dot{U}(t) = -\mathrm{i}H(t)U(t). \tag{1.8}$$

In the case of a time-independent Hamiltonian however, time ordering is not necessary and we simply obtain $U(t) = e^{-\mathrm{i}Ht}$. This neglect of time ordering is possible only when the commutator of the Hamiltonian with itself vanishes at different times $[H(t), H(t')] = 0$. In the general case however, the study of time-dependent Hamiltonians is usually quite difficult and is normally restricted to periodic [14] or

adiabatic [15] time dependencies. Turning the question around, it is simpler to take a time-dependent trajectory of the state vector and to obtain a corresponding time-dependent Hamiltonian [16]. Unfortunately, this is often not the question asked in the experimental setup.

In any case however, unitary evolution ($U^\dagger(t)U(t) = \mathbf{1}$) means that the information about the initial state is conserved in every solution to the Schrödinger equation. A unitarily evolving system cannot evolve towards a single stationary state, since from that state the information about the initial configuration cannot be extracted. For a constant Hamiltonian, we may expand the initial state in the eigenstates $H|n\rangle = E_n|n\rangle$ of the Hamiltonian, and the time-dependent solution to the Schrödinger equation is then simply given by $|\Psi(t)\rangle = \sum_n c_n^0 \exp\{-iE_n t\}|n\rangle$. For a finite number of system energies E_n, this will always evolve periodically and thus return to its initial state after some recurrence time. When the system becomes large however, approximate notions of a stationary state in a closed quantum system exist [17].

Furthermore, realistic quantum systems can usually not be regarded as closed; i.e., they are not perfectly isolated from their environment (composed of thermal reservoirs, detectors, and other things). The naive approach of simply simulating the evolution of both the system and its environment is unfortunately prohibitive. With increasing size, the complexity to simulate a quantum system grows exponentially, and a typical reservoir with $\mathscr{O}\{10^{23}\}$ degrees of freedom would in the simplest case require the storage of $\mathscr{O}\{2^{10^{23}}\}$ bits, which is completely impossible. With our limited abilities one should therefore be content with a theory that describes only a small part of our universe—conventionally called the system. In this restricted subspace, the dynamics may no longer be expected to be unitary. That is, a simple time dependence of external parameters in the Hamiltonian cannot account for the observed dynamics, which the Schrödinger equation (1.3) will fail to predict. In such cases, the system can no longer be described by a pure state $|\Psi\rangle$, and the density matrix formalism is required. This formalism will be introduced in the following sections.

1.3 Master Equations

1.3.1 Definition

Many processes in nature are stochastic. In classical physics, this may be due to our incomplete knowledge of the system. Due to the unknown microstate of, e.g., a gas in a box, the collisions of gas particles with the domain wall will appear random. In quantum theory, the Schrödinger equation (1.3) itself involves amplitudes rather than observables in the lowest level, and measurement of observables will yield a stochastic outcome. In order to understand such processes in great detail, such random events must be included via a probabilistic description. For dynamical systems, probabilities associated with measurement outcomes may evolve in time, and the determining equation for such a process is called a master equation.

Definition 1.1 (Master equation)   A master equation is a first-order differential equation describing the time evolution of probabilities, e.g., for discrete events $k \in \{1, \ldots, N\}$

$$\frac{dP_k}{dt} = \sum_\ell [T_{k\ell} P_\ell - T_{\ell k} P_k],\tag{1.9}$$

where the $T_{k\ell} \geq 0$ are transition rates from state (measurement event) ℓ to state (measurement event) k. Since it is completely defined by the transition rates, it is also termed the rate equation.

The master equation is said to satisfy detailed balance when for the stationary state $\bar{P}_i$ the equality $T_{k\ell} \bar{P}_\ell = T_{\ell k} \bar{P}_k$ holds for all terms separately.

The transition rates must be positive and may in principle also depend on time. When the transition matrix $T_{k\ell}$ is symmetric, all processes are reversible at the level of the master equation description.

Often, master equations are phenomenologically motivated and not derived from first principles. However, in most examples discussed in this book we will use master equations that can be derived from a microscopic underlying model. We will see later that, in its standard form, the Markovian quantum master equation may not only involve probabilities (diagonals of the density matrix, termed populations) but also further auxiliary values (off-diagonal entries, termed coherences). However, it is possible to transform such master equations to a rate equation representation in a suitable basis. Therefore, we will use the term master equation in this book in a somewhat wider sense as an equation that provides the time equation of probabilities.

It is straightforward to show that the master equation conserves the total probability

$$\sum_k \frac{dP_k}{dt} = \sum_{k\ell} (T_{k\ell} P_\ell - T_{\ell k} P_k) = \sum_{k\ell} (T_{\ell k} P_k - T_{\ell k} P_k) = 0.\tag{1.10}$$

Beyond this, all probabilities must remain positive, which is also respected by a rate equation with positive rates: evidently, the solution of the master equation is continuous, such that when initialized with valid probabilities $0 \leq P_i(0) \leq 1$ all probabilities are non-negative initially. Let P_k be the first probability that approaches zero at some time t (when all other probabilities are non-negative). Its time derivative is then given by

$$\left.\frac{dP_k}{dt}\right|_{P_k=0} = +\sum_\ell T_{k\ell} P_\ell \geq 0,\tag{1.11}$$

which simply implies that $P_k(t)$ will increase. In effect, any probability will be repelled from zero, such that negative probabilities are impossible with positive rates.

Finally, the probabilities must remain smaller than one throughout the evolution. This however follows immediately from $\sum_k P_k = 1$ and $P_k \geq 0$ by contradiction.

In conclusion, a master equation of the form (1.9) automatically preserves the sum of probabilities and also keeps $0 \leq P_i(t) \leq 1$—with a valid initialization provided. That is, under the evolution of a rate equation, probabilities remain probabilities.

1.3.2 Examples

1.3.2.1 Fluctuating Two-Level System

Let us consider a system of two possible states, to which we associate the time-dependent probabilities $P_0(t)$ and $P_1(t)$. These events could for example be the two conformations of a molecule, the configurations of a spin, the ground and excited states of an atom, etc. To introduce some dynamics, let the transition rate from $0 \to 1$ be denoted by $T_{10} > 0$ and the inverse transition rate $1 \to 0$ be denoted by $T_{01} > 0$. This implies that the conditional probability to end up in the state 1 at time $(t + \Delta t)$ provided that at time t one is in the state 0, is for sufficiently small time intervals Δt given by $T_{10} \Delta t$. The associated master equation is then a first-order differential equation given by

$$\frac{d}{dt} \begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} -T_{10} & +T_{01} \\ +T_{10} & -T_{01} \end{pmatrix} \begin{pmatrix} P_0 \\ P_1 \end{pmatrix}. \tag{1.12}$$

We note that in the matrix representation, conservation of the trace is fulfilled when the entries in all columns of the rate matrix add up to zero. This can easily be shown to hold more generally.

Exercise 1.2 (Temporal dynamics of a two-level system) Calculate the solution of Eq. (1.12). What is the stationary state? Show that detailed balance is satisfied.

1.3.2.2 Diffusion Equation

Consider an infinite chain of coupled compartments. Now suppose that, along the chain, molecules may move from one compartment to another with a transition rate $T > 0$ that is unbiased, i.e., symmetric in all directions as depicted in Fig. 1.1. The evolution of probabilities obeys the infinite-size master equation

$$\dot{P}_i(t) = T P_{i-1}(t) + T P_{i+1}(t) - 2T P_i(t)$$
$$= T \Delta x^2 \frac{P_{i-1}(t) + P_{i+1}(t) - 2P_i(t)}{\Delta x^2}, \tag{1.13}$$

which converges as $\Delta x \to 0$ and $T \to \infty$ such that $D = T \Delta x^2$ remains constant to the partial differential equation

$$\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P(x,t)}{\partial x^2} \quad \text{with } D = T \Delta x^2, \tag{1.14}$$
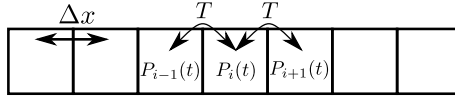
Fig. 1.1 Sketch of a chain of compartments, between which a transition is possible with isotropic and uniform rate $T > 0$. In the limit when the compartment size $\Delta x \to 0$ and $T \to \infty$ such that $\Delta x^2 T = D$ remains constant, the dynamics of the probabilities is described by the diffusion equation

where D is the diffusion constant. Such diffusion equations are used to describe the distribution of chemicals in a solution in the highly diluted limit, the kinetic dynamics of bacteria, and further undirected transport processes. From our analysis of master equations, we can immediately conclude that the diffusion equation preserves positivity and total norm, i.e., $P(x, t) \geq 0$ and $\int_{-\infty}^{+\infty} P(x, t)\, dx = 1$. Note that it is straightforward to generalize to the higher dimensional case.

One can now think of microscopic models where the hopping rates in different directions are not equal (drift) and may also depend on the position (a spatially dependent diffusion coefficient). A position-dependent hopping rate may, e.g., result from a heterogeneous medium through which transport occurs, whereas a difference in the directionality may result from an applied external potential (e.g., in the case of electrons) or some intrinsic preference of the considered species (e.g., in the case of chemotactically active bacteria sensing a present chemical gradient). A corresponding model (in a next-neighbor approximation) would be given by

$$\dot{P}_i = T_{i,i-1} P_{i-1}(t) + T_{i,i+1} P_{i+1}(t) - (T_{i-1,i} + T_{i+1,i}) P_i(t), \qquad (1.15)$$

where $T_{a,b}$ denotes the rate of jumping from b to a; see also Fig. 1.2. An educated guess is given by the ansatz

$$\begin{aligned}
\frac{\partial P}{\partial t} &= \frac{\partial^2}{\partial x^2}\big[A(x)P(x,t)\big] + \frac{\partial}{\partial x}\big[B(x)P(x,t)\big] \\
&\equiv \frac{A_{i-1}P_{i-1} - 2A_i P_i + A_{i+1}P_{i+1}}{\Delta x^2} + \frac{B_{i+1}P_{i+1} - B_{i-1}P_{i-1}}{2\Delta x} \\
&= \left[\frac{A_{i-1}}{\Delta x^2} - \frac{B_{i-1}}{2\Delta x}\right]P_{i-1} - \frac{2A_i}{\Delta x^2}P_i + \left[\frac{A_{i+1}}{\Delta x^2} + \frac{B_{i+1}}{2\Delta x}\right]P_{i+1}, \quad (1.16)
\end{aligned}$$

which is equivalent to our master equation when

$$A_i = \frac{\Delta x^2}{2}[T_{i-1,i} + T_{i+1,i}], \qquad B_i = \Delta x[T_{i-1,i} - T_{i+1,i}]. \qquad (1.17)$$

We conclude that the Fokker–Planck equation

$$\frac{\partial P}{\partial t} = \frac{\partial^2}{\partial x^2}\big[A(x)P(x,t)\big] + \frac{\partial}{\partial x}\big[B(x)P(x,t)\big] \qquad (1.18)$$

with $A(x) \geq 0$ preserves norm and positivity of the probability distribution $P(x, t)$.
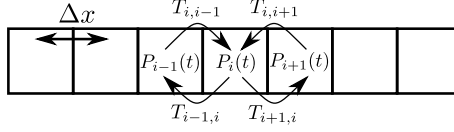
Fig. 1.2 Sketch of a chain of compartments, between which a transition is possible with differing rates $T_{ij} \geq 0$. In contrast to Fig. 1.1, the hopping rates are not uniform, $T_{ij} \neq T$, and may be anisotropic, $T_{ij} \neq T_{ji}$

Exercise 1.3 (Reaction-diffusion equation) Along a linear chain of compartments, consider the master equation for two species

$$\dot{P}_i = T\big[P_{i-1}(t) + P_{i+1}(t) - 2P_i(t)\big] - \gamma\, P_i(t),$$
$$\dot{p}_i = \tau\big[p_{i-1}(t) + p_{i+1}(t) - 2p_i(t)\big] + \gamma\, P_i(t),$$

where $P_i(t)$ may denote the concentration of a molecule that irreversibly reacts with chemicals in the solution to an inert form characterized by $p_i(t)$. To which partial differential equation does the master equation map?

In some cases, the probabilities may not only depend on the probabilities themselves, but also on external parameters, which appear then in the master equation. Here, we will use the term master equation for any equation describing the time evolution of probabilities; i.e., auxiliary variables may appear in the master equation.

1.3.2.3 Cell Culture Growth

Consider a population of identical cells, where each cell may divide (proliferate) with a rate α. These cells live in a constrained geometry (e.g., a Petri dish) that admits at most K cells due to some limitations (space, nutrient supply, etc.). Let $P_i(t)$ denote the probability of having i cells in the Petri dish. Assuming that the proliferation rate α is sufficiently small, we can easily set up a master equation:

$$\dot{P}_0 = 0,$$
$$\dot{P}_1 = -1 \cdot \alpha \cdot P_1,$$
$$\dot{P}_2 = -2 \cdot \alpha \cdot P_2 + 1 \cdot \alpha \cdot P_1,$$
$$\vdots$$
$$\dot{P}_\ell = -\ell \cdot \alpha \cdot P_\ell + (\ell - 1) \cdot \alpha \cdot P_{\ell-1},$$
$$\vdots$$

(1.19)

$$\dot{P}_{K-1} = -(K-1) \cdot \alpha \cdot P_{K-1} + (K-2) \cdot \alpha \cdot P_{K-2},$$

$$\dot{P}_K = +(K-1) \cdot \alpha P_{K-1}.$$

The prefactors in front of the bare rates arise since any of the ℓ cells may proliferate. Arranging the probabilities in a single vector, this may also be written as $\dot{\boldsymbol{P}} = \mathscr{L}\boldsymbol{P}$, where the band-diagonal matrix $\mathscr{L}$ contains the rates. When we have a single cell as the initial condition (full knowledge), i.e., $P_1(0) = 1$ and $P_{\ell \neq 1}(0) = 0$, one can change the carrying capacity $K = \{1, 2, 3, 4, \ldots\}$ and solve for each K the resulting system of differential equations for the expectation value of $\langle \ell \rangle = \sum_{\ell=1}^{K} \ell P_\ell(t)$. These solutions may then be generalized to

$$\langle \ell \rangle = e^{+\alpha t}\left[1 - \left(1 - e^{-\alpha t}\right)^K\right]. \tag{1.20}$$

Similarly, one can compute the expectation value of $\langle \ell^2 \rangle$.

Exercise 1.4 (Cell culture growth) Confirm the validity of Eq. (1.20).

    This result can be compared with the logistic growth equation, obtained from the solution of the differential equation

$$\dot{N} = \alpha \left(1 - \frac{N}{K}\right)N, \tag{1.21}$$

which means that initially cell growth is just given by the bare proliferation rate α and then smoothly reduced when the population approaches the carrying capacity K.

Exercise 1.5 (Logistic growth equation) Solve Eq. (1.21).

    However, one may not only be interested in the evolution by mean values. Sometimes, rare events become quite important (e.g., a benign tumor cell turning malignant), in particular when they are strengthened in the following dynamics. Then it is also useful to obtain some information about the spread of single trajectories from the mean. In the case of a rate equation only involving the probabilities, as in Eq. (1.19), it is possible to also generate single trajectories from the master equation by using Monte Carlo simulation. Suppose that, at time t, the system is in the state ℓ, i.e., $P_\alpha(t) = \delta_{\ell\alpha}$. After a sufficiently short time Δt, the probabilities of being in a different state read as

$$\boldsymbol{P}(t + \Delta t) \approx [\boldsymbol{1} + \Delta t \mathscr{L}]\boldsymbol{P}(t) + \mathscr{O}\{\Delta t\}^2, \tag{1.22}$$

which for our simple example boils down to

$$P_\ell(t + \Delta t) \approx (1 - \ell \alpha \Delta t) P_\ell(t), \qquad P_{\ell+1}(t + \Delta t) \approx +\ell \alpha \Delta t P_\ell(t). \tag{1.23}$$

To simulate a single trajectory, one may now simply draw a random number $\sigma \in [0, 1]$: the probability that a cell divides during this small time interval is given
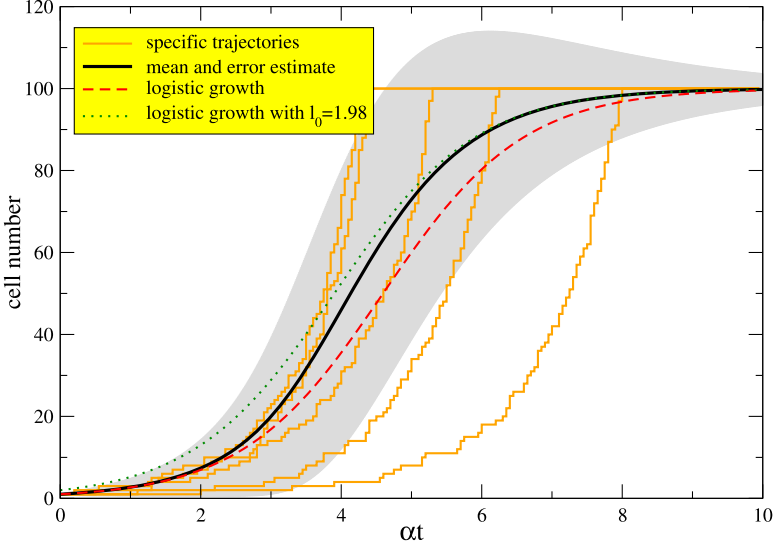
Fig. 1.3 Population dynamics for the linear master equation (*black curve* $\langle \ell \rangle$ and *shaded area* determined from $\sqrt{\langle \ell^2 \rangle - \langle \ell \rangle^2}$) and for the logistic growth equation (*dashed red curve*) for carrying capacity $K = 100$. For identical initial and final states, the master equation solution overshoots the logistic growth curve. A slight modification (*dotted green curve*) of the initial condition in the logistic growth curve yields the same long-term asymptotics. An average of many specific trajectories would converge towards the *black curve*

by $P_{\text{jump}} = \ell \alpha \Delta t \ll 1$. If the random number $\sigma \leq P_{\text{jump}}$, we assume that the transition $P_\ell \to P_{\ell+1}$ has occurred, and we may set $P_\alpha(t + \Delta t) = \delta_{\ell+1,\alpha}$. In contrast, when $\alpha > P_{\text{jump}}$, we assume that no transition has occurred and therefore remain at $P_\alpha(t + \Delta t) = \delta_{\ell\alpha}$. In any case, the simulation keeps track of the actual state of the system as if the cell number were regularly measured at intervals Δt. The ensemble average of many such trajectories will yield the mean evolution predicted by the master equation; see Fig. 1.3. The figure demonstrates that single trajectories may look quite different from the solution of the master equation. Furthermore, the mean and standard deviation (shaded area) may hide important information about single trajectories: in this case, single trajectories must always be bounded by the carrying capacity K. The ensemble averages of trajectories must however coincide with the rate equation solution.

1.4 Density Matrix Formalism

1.4.1 Density Matrix

Suppose one wants to describe a quantum system, where the system state is not exactly known. That is, there is an ensemble of known states $\{|\Phi_i\rangle\}$, but there is

uncertainty regarding in which of these states the system resides. Such systems can be conveniently described by a density matrix.

Definition 1.2 (Density matrix) Any density matrix can be written as

$$\rho = \sum_i p_i |\Phi_i\rangle\langle\Phi_i|, \tag{1.24}$$

where $0 \leq p_i \leq 1$ denote the probabilities of being in the state $|\Phi_i\rangle$ with $\sum_i p_i = 1$. In general, the states are not required to be orthogonal, i.e., $\langle\Phi_i|\Phi_j\rangle \neq \delta_{ij}$. Formally, any matrix fulfilling the properties

- self-adjointness: $\rho^\dagger = \rho$
- normalization: $\text{Tr}\{\rho\} = 1$
- positivity: $\langle\Psi|\rho|\Psi\rangle \geq 0$ for all vectors Ψ

can be interpreted as a valid density matrix.

For a pure state, one has $p_{\bar{i}} = 1$ and thereby $\rho = |\Phi_{\bar{i}}\rangle\langle\Phi_{\bar{i}}|$ for some particular $\bar{i}$.

Thus, a density matrix is pure if and only if $\rho = \rho^2$.

The expectation value of an operator for a known state $|\Psi\rangle$

$$\langle A \rangle = \langle\Psi|A|\Psi\rangle \tag{1.25}$$

can be obtained conveniently from the corresponding pure density matrix $\rho = |\Psi\rangle\langle\Psi|$ by simply computing the trace (sum of diagonal elements) of $A\rho$:

$$\langle A \rangle \equiv \text{Tr}\{A\rho\} = \text{Tr}\{\rho A\} = \text{Tr}\{A|\Psi\rangle\langle\Psi|\}$$

$$= \sum_n \langle n|A|\Psi\rangle\langle\Psi|n\rangle = \langle\Psi|\left(\sum_n |n\rangle\langle n|\right)A|\Psi\rangle$$

$$= \langle\Psi|A|\Psi\rangle. \tag{1.26}$$

In the first line above, we simply stated an important property of the trace: its invariance under cyclic permutations of its arguments. When the state is not exactly known, but its probability distribution is, the expectation value is obtained by computing the weighted average

$$\langle A \rangle = \sum_i P_i \langle\Phi_i|A|\Phi_i\rangle, \tag{1.27}$$

where P_i denotes the probability of being in state $|\Phi_i\rangle$. The definition of obtaining expectation values by calculating traces of operators with the density matrix is also consistent with mixed states

$$\langle A \rangle \equiv \text{Tr}\{A\rho\} = \text{Tr}\left\{A \sum_i p_i |\Phi_i\rangle\langle\Phi_i|\right\} = \sum_i p_i \,\text{Tr}\{A|\Phi_i\rangle\langle\Phi_i|\}$$

$$= \sum_i p_i \sum_n \langle n|A|\Phi_i\rangle\langle\Phi_i|n\rangle = \sum_i p_i \langle\Phi_i|\left(\sum_n |n\rangle\langle n|\right)A|\Phi_i\rangle$$

$$= \sum_i p_i \langle\Phi_i|A|\Phi_i\rangle. \tag{1.28}$$

Exercise 1.6 (Superposition versus localized states) Calculate the density matrix for a statistical mixture in the states $|0\rangle$ and $|1\rangle$ with probability $p_0 = 3/4$ and $p_1 = 1/4$. What is the density matrix for a statistical mixture of the superposition states $|\Psi_a\rangle = \sqrt{3/4}|0\rangle + \sqrt{1/4}|1\rangle$ and $|\Psi_b\rangle = \sqrt{3/4}|0\rangle - \sqrt{1/4}|1\rangle$ with probabilities $p_a = p_b = 1/2$?

1.4.2 Dynamical Evolution of a Density Matrix

1.4.2.1 Continuous Evolution

The evolution of a pure state vector in a closed quantum system is described by the evolution operator $U(t)$, as, e.g., for the Schrödinger equation (1.3) the time evolution operator (1.5) may be defined as the solution to the operator equation $\dot{U}(t) = -\mathrm{i}H(t)U(t)$. For constant $H(t) = H$, we simply have the solution $U(t) = e^{-\mathrm{i}Ht}$. Similarly, a pure state density matrix $\rho = |\Psi\rangle\langle\Psi|$ would evolve according to the von Neumann equation

$$\dot{\rho} = -\mathrm{i}\big[H(t), \rho(t)\big] \tag{1.29}$$

with the formal solution $\rho(t) = U(t)\rho(0)U^\dagger(t)$; compare Eq. (1.5). This simply means that for pure states, the von Neumann equation yields the same dynamics as the Schrödinger equation, and pure states remain pure under unitary evolution.

When we apply the very same evolution equation (1.29) to a density matrix that is not pure, we obtain

$$\rho(t) = \sum_i p_i U(t)|\Phi_i\rangle\langle\Phi_i|U^\dagger(t). \tag{1.30}$$

This equation implies that transitions between the (now time-dependent) state vectors $|\Phi_i(t)\rangle = U(t)|\Phi_i\rangle$ are impossible with unitary evolution. These are exactly the state vectors that one would have obtained from the Schrödinger equation by initializing with the initial state $|\Phi_i\rangle$. Therefore, the von Neumann evolution equation yields the same dynamics as an ensemble average of the Schrödinger equation solutions corresponding to the different initial states.

Exercise 1.7 (Preservation of density matrix properties by unitary evolution) Show that the von Neumann equation (1.29) preserves self-adjointness, trace, and positivity of the density matrix.

1.4.2.2 Measurement

The measurement process can also be generalized similarly. For a quantum state $|\Psi\rangle$, measurements are described by a set of measurement operators $\{M_m\}$, each corresponding to a certain measurement outcome, and with the completeness relation $\sum_m M_m^\dagger M_m = \mathbf{1}$. The probability of obtaining result m is given by

$$P_m = \langle\Psi|M_m^\dagger M_m|\Psi\rangle \tag{1.31}$$

and after the measurement with outcome m, the quantum state is collapsed:

$$|\Psi\rangle \overset{m}{\to} \frac{M_m|\Psi\rangle}{\sqrt{\langle\Psi|M_m^\dagger M_m|\Psi\rangle}}. \tag{1.32}$$

The projective measurement is just a special case of that with $M_m = |m\rangle\langle m|$.

Definition 1.3 (Measurements with density matrix) For a set of measurement operators $\{M_m\}$ corresponding to different outcomes m and obeying the completeness relation $\sum_m M_m^\dagger M_m = \mathbf{1}$, the probability of obtaining result m is given by

$$P_m = \text{Tr}\{M_m^\dagger M_m \rho\}, \tag{1.33}$$

and the action of measurement on the density matrix—provided that result m was obtained—can be summarized as

$$\rho \overset{m}{\to} \rho' = \frac{M_m \rho M_m^\dagger}{\text{Tr}\{M_m^\dagger M_m \rho\}}. \tag{1.34}$$

The set of measurement operators is also the called positive operator-valued measure (POVM).

It is therefore straightforward to see that the descriptions using the Schrödinger equation and the von Neumann equation with the respective measurement postulates are equivalent. The density matrix formalism conveniently includes statistical mixtures in the description, since it automatically performs the averaging over different initial conditions. Unfortunately, this comes at the cost of quadratically increasing the number of state variables.

Exercise 1.8 (Preservation of density matrix properties by measurement) Show that the measurement postulate preserves self-adjointness, trace, and positivity of the density matrix.

1.4.2.3 Most General Evolution

Finally, we mention here that the most general evolution preserving all the nice properties of a density matrix is called a Kraus map [18]. A density matrix ρ (hermitian, positive definite, and with trace one) can be mapped to another density matrix ρ' via

$$\rho' = \sum_{\alpha\beta} \gamma_{\alpha\beta} A_\alpha \rho A_\beta^\dagger, \quad \text{with} \sum_{\alpha\beta} \gamma_{\alpha\beta} A_\beta^\dagger A_\alpha = \mathbf{1}, \tag{1.35}$$

where the prefactors $\gamma_{\alpha\beta}$ form a hermitian ($\gamma_{\alpha\beta} = \gamma_{\beta\alpha}^*$) and positive definite ($\sum_{\alpha\beta} x_\alpha^* \gamma_{\alpha\beta} x_\beta \geq 0$ or equivalently all eigenvalues of ($\gamma_{\alpha\beta}$) are non-negative) matrix. It is straightforward to see that the above map preserves trace and hermiticity of the density matrix. In addition, ρ' also inherits the positivity from $\rho = \sum_n P_n |n\rangle\langle n|$

$$\langle\Psi|\rho'|\Psi\rangle = \sum_{\alpha\beta} \gamma_{\alpha\beta} \langle\Psi|A_\alpha \rho A_\beta^\dagger|\Psi\rangle = \sum_n P_n \sum_{\alpha\beta} \gamma_{\alpha\beta} \langle\Psi|A_\alpha|n\rangle\langle n|A_\beta^\dagger|\Psi\rangle$$

$$= \sum_n \underbrace{P_n}_{\geq 0} \underbrace{\sum_{\alpha\beta} \left(\langle n|A_\alpha^\dagger|\Psi\rangle\right)^* \gamma_{\alpha\beta} \langle n|A_\beta^\dagger|\Psi\rangle}_{\geq 0} \geq 0. \tag{1.36}$$

Since the matrix $\gamma_{\alpha\beta}$ is hermitian, it can be diagonalized by a suitable unitary transformation, and we introduce the new operators $A_\alpha = \sum_{\alpha'} U_{\alpha\alpha'} \bar{K}_{\alpha'}$:

$$\rho' = \sum_{\alpha\beta} \sum_{\alpha'\beta'} \gamma_{\alpha\beta} U_{\alpha\alpha'} \bar{K}_{\alpha'} \rho U_{\beta\beta'}^* K_{\beta'}^\dagger = \sum_{\alpha'\beta'} \bar{K}_{\alpha'} \rho \bar{K}_{\beta'}^\dagger \underbrace{\sum_{\alpha\beta} U_{\alpha\alpha'} \gamma_{\alpha\beta} U_{\beta\beta'}^*}_{\gamma_{\alpha'} \delta_{\alpha'\beta'}}$$

$$= \sum_\alpha \gamma_\alpha \bar{K}_\alpha \rho \bar{K}_\alpha^\dagger, \tag{1.37}$$

where $\gamma_\alpha \geq 0$ represent the eigenvalues of the matrix ($\gamma_{\alpha\beta}$). Since these are by construction positive, we introduce further new operators $K_\alpha = \sqrt{\gamma_\alpha} \bar{K}_\alpha$ to obtain the simplest representation of a Kraus map.

Definition 1.4 (Kraus map) The map

$$\rho(t + \Delta t) = \sum_\alpha K_\alpha(t, \Delta t) \rho(t) K_\alpha^\dagger(t, \Delta t) \tag{1.38}$$

with Kraus operators $K_\alpha(t, \Delta t)$ obeying the relation $\sum_\alpha K_\alpha^\dagger(t, \Delta t) K_\alpha(t, \Delta t) = \mathbf{1}$ preserves hermiticity, trace, and positivity of the density matrix.

Obviously, both unitary evolution and evolution under measurement are just special cases of a Kraus map. Though Kraus maps are heavily used in quantum information [5], they are not often very easy to interpret. For example, it is not straightforward to identify the unitary and the nonunitary part induced by the Kraus map.

1.4.3 Tensor Product

The greatest advantage of the density matrix formalism is visible when quantum systems composed of several subsystems are considered. Then, a tensor product is required to construct the Hilbert space of the combined system. Roughly speaking, it represents a way to construct a larger vector space from two (or more) smaller vector spaces.

Definition 1.5 (Tensor product) Let V and W be Hilbert spaces (vector spaces with a scalar product) of dimension m and n with basis vectors $\{|v\rangle\}$ and $\{|w\rangle\}$, respectively. Then $V \otimes W$ is a Hilbert space of dimension $m \cdot n$, and a basis is spanned by $\{|v\rangle \otimes |w\rangle\}$, which is a set combining every basis vector of V with every basis vector of W.

  Mathematical properties

- bilinearity $(z_1|v_1\rangle + z_2|v_2\rangle) \otimes |w\rangle = z_1|v_1\rangle \otimes |w\rangle + z_2|v_2\rangle \otimes |w\rangle$
- operators acting on the combined Hilbert space $A \otimes B$ act on the basis states as $(A \otimes B)(|v\rangle \otimes |w\rangle) = (A|v\rangle) \otimes (B|w\rangle)$
- any linear operator on $V \otimes W$ can be decomposed as $C = \sum_i c_i A_i \otimes B_i$
- the scalar product is inherited in the natural way; i.e., one has for $|a\rangle = \sum_{ij} a_{ij}|v_i\rangle \otimes |w_j\rangle$ and $|b\rangle = \sum_{k\ell} b_{k\ell}|v_k\rangle \otimes |w_\ell\rangle$ the scalar product $\langle a|b\rangle = \sum_{ijk\ell} a_{ij}^* b_{k\ell} \langle v_i|v_k\rangle \langle w_j|w_\ell\rangle = \sum_{ij} a_{ij}^* b_{ij}$

  We note here that the basis vectors of the joint system are also often written as $|v\rangle \otimes |w\rangle = |vw\rangle$, where the order of v and w determines the subspace to which the quantum numbers are associated.

  If more than just two vector spaces are combined to form a larger vector space, the definition of the tensor product may be applied recursively. As a consequence, the dimension of the joint vector space grows rapidly, as, e.g., exemplified by the case of a qubit: its Hilbert space is just spanned by two vectors $|0\rangle$ and $|1\rangle$. The joint Hilbert space of two qubits is spanned by the vectors $|0\rangle \otimes |0\rangle = |00\rangle$, $|0\rangle \otimes |1\rangle = |01\rangle$, $|1\rangle \otimes |0\rangle = |10\rangle$, and $|1\rangle \otimes |1\rangle = |11\rangle$, and is thus four dimensional. This can be readily scaled up: the dimension of the Hilbert space for three qubits is eight dimensional, and that for n qubits is 2^n dimensional. Eventually, this exponential growth of the Hilbert space dimension for composite quantum systems is at the heart of quantum computing.

Exercise 1.9 (Tensor products of operators) Let σ denote the Pauli matrices, i.e.,

$$\sigma^1 = \begin{pmatrix} 0 & +1 \\ +1 & 0 \end{pmatrix}, \qquad \sigma^2 = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \qquad \sigma^3 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.39)$$

Compute the trace of the operator

$$\Sigma = a\mathbf{1} \otimes \mathbf{1} + \sum_{i=1}^{3} \alpha_i \sigma^i \otimes \mathbf{1} + \sum_{j=1}^{3} \beta_j \mathbf{1} \otimes \sigma^j + \sum_{i,j=1}^{3} a_{ij} \sigma^i \otimes \sigma^j.$$

Since the scalar product in the subsystems is inherited by the scalar product of the composite system, this typically enables a convenient calculation of the trace—given a decomposition into only few tensor products. For example, one has for a single tensor product of two operators

$$
\mathrm{Tr}\{A \otimes B\} = \sum_{n_A, n_B} \langle n_A, n_B | A \otimes B | n_A, n_B \rangle
$$

$$
= \left[\sum_{n_A} \langle n_A | A | n_A \rangle \right] \left[\sum_{n_B} \langle n_B | B | n_B \rangle \right]
$$

$$
= \mathrm{Tr_A}\{A\} \mathrm{Tr_B}\{B\}, \tag{1.40}
$$

where $\mathrm{Tr}_{A/B}$ denote the trace in the Hilbert space of A and B, respectively. Since these traces only involve the summation over the degrees of freedom of a subsystem, they are also called partial traces. Such partial traces are of tremendous importance and will be discussed in the next section.

1.4.4 The Partial Trace

For composite systems, it is usually not necessary to keep all information of the complete system in the density matrix. Rather, one would like to have a density matrix that encodes all the information on a particular subsystem only. Obviously, the map $\rho \to \mathrm{Tr_B}\{\rho\}$ to such a reduced density matrix should leave all expectation values of observables acting on the considered subsystem only invariant, i.e.,

$$
\mathrm{Tr}\{A \otimes \mathbf{1}\rho\} = \mathrm{Tr}\{A \, \mathrm{Tr_B}\{\rho\}\}. \tag{1.41}
$$

If this basic condition were not fulfilled, there would be no point in defining such a thing as a reduced density matrix: measurements would yield different results depending on the Hilbert space of the experimenter's choice.

Definition 1.6 (Partial trace)   Let $|a_1\rangle$ and $|a_2\rangle$ be vectors of state space A and $|b_1\rangle$ and $|b_2\rangle$ vectors of state space B. Then, the partial trace over state space B is defined via

$$
\mathrm{Tr_B}\{|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|\} = |a_1\rangle\langle a_2| \, \mathrm{Tr}\{|b_1\rangle\langle b_2|\}. \tag{1.42}
$$

We note that whereas the trace mapped an operator to a number, the partial trace reduces operators to lower dimensional operators. The partial trace is linear, such that the partial trace of arbitrary operators is calculated similarly. By choosing the $|a_\alpha\rangle$ and $|b_\gamma\rangle$ as an orthonormal basis in the respective Hilbert space, one may therefore calculate the most general partial trace via

$$\mathrm{Tr_B}\{C\} = \mathrm{Tr_B}\left\{\sum_{\alpha\beta\gamma\delta} c_{\alpha\beta\gamma\delta}|a_\alpha\rangle\langle a_\beta| \otimes |b_\gamma\rangle\langle b_\delta|\right\}$$

$$= \sum_{\alpha\beta\gamma\delta} c_{\alpha\beta\gamma\delta}\,\mathrm{Tr_B}\{|a_\alpha\rangle\langle a_\beta| \otimes |b_\gamma\rangle\langle b_\delta|\}$$

$$= \sum_{\alpha\beta\gamma\delta} c_{\alpha\beta\gamma\delta}|a_\alpha\rangle\langle a_\beta|\,\mathrm{Tr}\{|b_\gamma\rangle\langle b_\delta|\}$$

$$= \sum_{\alpha\beta\gamma\delta} c_{\alpha\beta\gamma\delta}|a_\alpha\rangle\langle a_\beta|\sum_\epsilon \langle b_\epsilon|b_\gamma\rangle\langle b_\delta|b_\epsilon\rangle$$

$$= \sum_{\alpha\beta}\left[\sum_\gamma c_{\alpha\beta\gamma\gamma}\right]|a_\alpha\rangle\langle a_\beta|. \qquad (1.43)$$

Definition 1.6 is the only linear map that respects the invariance of expectation values [5].

Exercise 1.10 (Partial trace) Compute the partial trace $\rho_A = \mathrm{Tr_B}\{\rho_{AB}\}$ of a pure density matrix $\rho_{AB} = |\Psi\rangle\langle\Psi|$ in the bipartite state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\big(|01\rangle + |10\rangle\big) \equiv \frac{1}{\sqrt{2}}\big(|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle\big).$$

Show that ρ_A is no longer pure.

1.5 Lindblad Quantum Master Equation

Any dynamical evolution equation for the density matrix should preserve its interpretation as a density matrix. This implies that trace, hermiticity, and positivity or the initial condition must be preserved—at least in some approximate sense. By construction, the measurement postulate and unitary evolution preserve these properties. However, more general evolutions are conceivable as, e.g., exemplified by the Kraus map. If we constrain ourselves to master equations that are local in time and have constant coefficients, the most general evolution that preserves trace, self-adjointness, and positivity of the density matrix is given by a Lindblad form [19].

1.5.1 Representations

Definition 1.7 (Lindblad form) A master equation of Lindblad form has the structure

$$\dot\rho = \mathscr{L}\rho = -\mathrm{i}[H, \rho] + \sum_{\alpha,\beta=1}^{N^2-1} \gamma_{\alpha\beta}\left(A_\alpha\rho A_\beta^\dagger - \frac{1}{2}\{A_\beta^\dagger A_\alpha, \rho\}\right), \qquad (1.44)$$

where the hermitian operator $H = H^\dagger$ can be interpreted as an effective Hamiltonian and the dampening matrix $\gamma_{\alpha\beta} = \gamma_{\beta\alpha}^*$ is a positive semidefinite matrix; i.e., it fulfills $\sum_{\alpha\beta} x_\alpha^* \gamma_{\alpha\beta} x_\beta \geq 0$ for all vectors x (or, equivalently, that all eigenvalues of $(\gamma_{\alpha\beta})$ are non-negative, $\lambda_i \geq 0$).

In the above definition, the commutator term with the effective Hamiltonian accounts for the unitary evolution, whereas the remaining terms are responsible for the nonunitary (dissipative) evolution. When derived from a microscopic model, the effective Hamiltonian need not coincide with the system Hamiltonian. This demonstrates that the interaction with a reservoir may also change the unitary part of the evolution.

Exercise 1.11 (Trace and hermiticity preservation by Lindblad forms) Show that the Lindblad form of master equation preserves trace and hermiticity of the density matrix.

The Lindblad-type master equation can be written in a simpler form. As the dampening matrix γ is hermitian, it can be diagonalized by a suitable unitary transformation U, such that $\sum_{\alpha\beta} U_{\alpha'\alpha} \gamma_{\alpha\beta} (U^\dagger)_{\beta\beta'} = \delta_{\alpha'\beta'} \gamma_{\alpha'}$ with $\gamma_\alpha \geq 0$ representing its non-negative eigenvalues. Using this unitary operation, a new set of operators can be defined via $A_\alpha = \sum_{\alpha'} U_{\alpha'\alpha} \bar{L}_{\alpha'}$. Inserting this decomposition in the master equation, we obtain

$$\dot{\rho} = -\mathrm{i}[H, \rho] + \sum_{\alpha,\beta=1}^{N^2-1} \gamma_{\alpha\beta} \left(A_\alpha \rho A_\beta^\dagger - \frac{1}{2} \{ A_\beta^\dagger A_\alpha, \rho \} \right)$$

$$= -\mathrm{i}[H, \rho] + \sum_{\alpha',\beta'} \left[\sum_{\alpha\beta} \gamma_{\alpha\beta} U_{\alpha'\alpha} U_{\beta'\beta}^* \right] \left(\bar{L}_{\alpha'} \rho \bar{L}_{\beta'}^\dagger - \frac{1}{2} \{ \bar{L}_{\beta'}^\dagger \bar{L}_{\alpha'}, \rho \} \right)$$

$$= -\mathrm{i}[H, \rho] + \sum_\alpha \gamma_\alpha \left(\bar{L}_\alpha \rho \bar{L}_\alpha^\dagger - \frac{1}{2} \{ \bar{L}_\alpha^\dagger \bar{L}_\alpha, \rho \} \right), \tag{1.45}$$

where γ_α denote the $N^2 - 1$ non-negative eigenvalues of the dampening matrix. Their positivity also allows us to absorb them into the Lindblad operators $L_\alpha \equiv \sqrt{\gamma_\alpha} \bar{L}_\alpha$ to yield the simplest representation of a Lindblad form,

$$\dot{\rho} = -\mathrm{i}[H, \rho] + \sum_\alpha \left(L_\alpha \rho L_\alpha^\dagger - \frac{1}{2} \{ L_\alpha^\dagger L_\alpha, \rho \} \right). \tag{1.46}$$

Evidently, the representation of a master equation is not unique. Any other unitary operation would lead to a different nondiagonal form which however describes the same master equation. In addition, we note here that the master equation is not

only invariant to unitary transformations of the operators A_α, but in the diagonal representation also to inhomogeneous transformations of the form

$$L_\alpha \to L'_\alpha = L_\alpha + a_\alpha \mathbf{1},$$

$$H \to H' = H + \frac{1}{2\mathrm{i}} \sum_\alpha \left(a_\alpha^* L_\alpha - a_\alpha L_\alpha^\dagger \right) + b\mathbf{1}, \tag{1.47}$$

with complex numbers a_α and a real number b. The first of these equations can be exploited to choose the Lindblad operators L_α traceless, thereby fixing the numbers a_α, whereas b is fixed by gauging the energy of the Hamiltonian.

Exercise 1.12 (Shift invariance) Show the invariance of the diagonal representation of a Lindblad form master equation (1.46) with respect to the transformation (1.47).

1.5.2 Preservation of Positivity

Similar to the transformation into the interaction picture, one can eliminate the unitary evolution term by transforming Eq. (1.45) to a co-moving frame $\rho = e^{-\mathrm{i}Ht}\tilde{\rho}e^{+\mathrm{i}Ht}$. Then, the master equation assumes the form

$$\dot{\rho} = \sum_\alpha \gamma_\alpha \left(L_\alpha(t)\rho L_\alpha^\dagger(t) - \frac{1}{2}\left\{ L_\alpha^\dagger(t)L_\alpha(t), \rho \right\} \right) \tag{1.48}$$

with the transformed time-dependent operators $L_\alpha(t) = e^{+\mathrm{i}Ht}L_\alpha e^{-\mathrm{i}Ht}$. It is also clear that if the differential equation preserves positivity of the density matrix, then it would also do this for time-dependent rates γ_α. Define the operators with $K = N^2 - 1$

$$W_1(t) = \mathbf{1},$$

$$W_2(t) = \frac{1}{2\gamma} \sum_\alpha \gamma_\alpha(t) L_\alpha^\dagger(t)L_\alpha(t),$$

$$W_3(t) = L_1(t), \tag{1.49}$$

$$\vdots$$

$$W_{K+2}(t) = L_K(t),$$

where $\gamma = \sum_\alpha \gamma_\alpha(t)$ has been introduced to render all W_i operators dimensionless. Discretizing the time derivative in Eq. (1.48), one transforms the differential equation for the density matrix into an iteration equation,

$$\boldsymbol{\rho}(t+\Delta t) = \boldsymbol{\rho}(t) + \Delta t \sum_{\alpha} \gamma_{\alpha} \left[\boldsymbol{L}_{\alpha}(t)\boldsymbol{\rho}(t)\boldsymbol{L}_{\alpha}^{\dagger}(t) - \frac{1}{2}\left\{ \boldsymbol{L}_{\alpha}^{\dagger}(t)\boldsymbol{L}_{\alpha}(t), \boldsymbol{\rho}(t) \right\} \right]$$

$$= \sum_{\alpha\beta} w_{\alpha\beta}(t)\, W_{\alpha}(t)\boldsymbol{\rho}(t)\, W_{\beta}^{\dagger}(t), \qquad (1.50)$$

where the dimensionless $w_{\alpha\beta}$ matrix assumes the block form

$$w(t) = \begin{pmatrix} 1 & -\Delta t\gamma & 0 & \cdots & 0 \\ -\Delta t\gamma & 0 & 0 & \cdots & 0 \\ \hline 0 & 0 & \Delta t\gamma_1(t) & & \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & & & \Delta t\gamma_K(t) \end{pmatrix}, \qquad (1.51)$$

which makes it particularly easy to diagonalize; the lower right block is already diagonal and the eigenvalues of the upper 2 by 2 block may be directly obtained by solving for the roots of the characteristic polynomial $\lambda^2 - \lambda - (\gamma\Delta t)^2 = 0$. Again, we introduce the corresponding unitary transformation $\tilde{W}_{\alpha}(t) = \sum_{\alpha'} u_{\alpha'\alpha}(t) W_{\alpha'}(t)$ to find that

$$\rho(t+\Delta t) = \sum_{\alpha} w_{\alpha}(t)\,\tilde{W}_{\alpha}(t)\rho(t)\,\tilde{W}_{\alpha}^{\dagger}(t) \qquad (1.52)$$

with $w_{\alpha}(t)$ denoting the eigenvalues of the matrix (1.51) and in particular the only negative eigenvalue being given by $w_1(t) = \frac{1}{2}(1 - \sqrt{1+4(\gamma\Delta t)^2})$. Now, we use the spectral decomposition of the density matrix at time t, $\rho(t) = \sum_a P_a(t)|\Psi_a(t)\rangle\langle\Psi_a(t)|$, to demonstrate approximate positivity of the density matrix at time $t + \Delta t$:

$$\langle\Phi|\rho(t+\Delta t)|\Phi\rangle = \sum_{\alpha,a} w_{\alpha}(t)P_a(t)\big|\langle\Phi|\tilde{W}_{\alpha}(t)\big|\Psi_a(t)\rangle\big|^2$$

$$\geq \frac{1}{2}\left(1 - \sqrt{1+4(\gamma\Delta t)^2}\right)\sum_a P_a(t)\big|\langle\Phi|\tilde{W}_1(t)\big|\Psi_a(t)\rangle\big|^2$$

$$\geq -(\gamma\Delta t)^2 \sum_a P_a(t)\big|\langle\Phi|\tilde{W}_1(t)\big|\Psi_a(t)\rangle\big|^2 \overset{\Delta t\to 0}{\longrightarrow} 0, \qquad (1.53)$$

such that the violation of positivity vanishes faster than the discretization width as Δt goes to zero. This limit just yields the differential equation of the Lindblad form master equation, which shows that the latter preserves positivity. It should be noted however that numerical solutions of the Lindblad master equation using a forward-time discretization may yield negative probabilities if the time step Δt is chosen too large.

1.5.3 Rate Equation Representation

Since Eq. (1.45) at all times preserves hermiticity of the density matrix, it can always be diagonalized by a unitary transformation $\rho_D(t) = U(t)\rho(t)U^\dagger(t)$. Inserting this transformation in the master equation (1.46) yields

$$\dot{\rho}_D = \dot{U}U^\dagger \rho_D + U\dot{\rho}U^\dagger + \rho_D U\dot{U}^\dagger = -\mathrm{i}\big[\mathrm{i}\dot{U}U^\dagger, \rho_D\big] + U\dot{\rho}U^\dagger$$

$$= -\mathrm{i}\big[\boldsymbol{H}(t) + \boldsymbol{H}_{\mathrm{eff}}(t), \rho_D\big]$$

$$+ \sum_\alpha \bigg[\boldsymbol{L}_\alpha(t)\rho_D \boldsymbol{L}_\alpha^\dagger(t) - \frac{1}{2}\big\{\boldsymbol{L}_\alpha^\dagger(t)\boldsymbol{L}_\alpha(t), \rho_D\big\}\bigg], \qquad (1.54)$$

with transformed Lindblad operators $\boldsymbol{L}_\alpha(t) = U(t)L_\alpha U^\dagger(t)$ and the effective Hamiltonian $\boldsymbol{H}_{\mathrm{eff}}(t) = \mathrm{i}\dot{U}(t)U^\dagger(t)$.

Exercise 1.13 (Hermiticity of effective Hamiltonian) Show that the effective Hamiltonian $\boldsymbol{H}_{\mathrm{eff}}(t) = \mathrm{i}\dot{U}(t)U^\dagger(t)$ is hermitian.

Now using the fact that in the time-dependent basis ρ_D is diagonal, $\rho_D = \sum_a \rho_{aa}(t)|a(t)\rangle\langle a(t)|$, we obtain

$$\dot{\rho}_{aa} = \sum_\alpha \sum_b \big|\langle a|\boldsymbol{L}_\alpha(t)|b\rangle\big|^2 \rho_{bb} - \sum_\alpha \langle a|\boldsymbol{L}_\alpha^\dagger(t)\boldsymbol{L}_\alpha(t)|a\rangle \rho_{aa}, \qquad (1.55)$$

which has the structure of a rate equation with positive but time-dependent rates [20]. Unfortunately, to obtain such a rate equation, one first has to diagonalize the time-dependent solution of Eq. (1.46), i.e., to solve the complicated master equation beforehand. It is therefore not very practical in most cases, unless one is given a rate equation from the start. Nevertheless, it shows that rate equations—if set up in the correct basis—can yield a quite general description of master equation dynamics. The basis within which the long-term density matrix becomes diagonal is also called a pointer basis.

1.5.4 Examples

1.5.4.1 Cavity in a Thermal Bath

Consider the Lindblad form master equation

$$\dot{\rho}_S = -\mathrm{i}\big[\Omega a^\dagger a, \rho_S\big] + \gamma(1 + n_B)\bigg[a\rho_S a^\dagger - \frac{1}{2}a^\dagger a\rho_S - \frac{1}{2}\rho_S a^\dagger a\bigg]$$

$$+ \gamma n_B \bigg[a^\dagger \rho_S a - \frac{1}{2}aa^\dagger \rho_S - \frac{1}{2}\rho_S aa^\dagger\bigg]. \qquad (1.56)$$

Here a and $a^\dagger$ are bosonic annihilation and creation operators, respectively, fulfilling the bosonic commutation relations $[a, a^\dagger] = \mathbf{1}$. The dampening matrix is given by the Bose–Einstein bath occupation $n_B = [e^{\beta\Omega} - 1]^{-1}$ evaluated at cavity frequency Ω and a bare emission and absorption rate $\gamma > 0$. In Fock space representation, these operators act as $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $a|n\rangle = \sqrt{n}|n-1\rangle$ (where $0 \le n < \infty$), such that the above master equation couples only the diagonals of the density matrix $\rho_n = \langle n|\rho_S|n\rangle$ to each other,

$$\dot{\rho}_n = \gamma(1 + n_B)\big[(n+1)\rho_{n+1} - n\rho_n\big] + \gamma n_B\big[n\rho_{n-1} - (n+1)\rho_n\big]$$

$$= \gamma n_B n\rho_{n-1} - \gamma\big[n + (2n+1)n_B\big]\rho_n + \gamma(1 + n_B)(n+1)\rho_{n+1}, \quad (1.57)$$

in a tridiagonal form. That makes it particularly easy to calculate the stationary state of the populations recursively, since the boundary solution $n_B\bar{\rho}_0 = (1 + n_B)\bar{\rho}_1$ implies for all n the relation

$$\frac{\bar{\rho}_{n+1}}{\bar{\rho}_n} = \frac{n_B}{1 + n_B} = e^{-\beta\Omega}. \quad (1.58)$$

Consequently, the stationary populations are consistent with a thermalized Gibbs state

$$\bar{\rho} = \frac{e^{-\beta\Omega a^\dagger a}}{\text{Tr}\{e^{-\beta\Omega a^\dagger a}\}} \quad (1.59)$$

with the inverse reservoir temperature β. Such a Gibbs state however does not have coherences in the Fock space basis. To investigate their evolution, we calculate the time derivative of $\rho_{nm} = \langle n|\rho_S|m\rangle$,

$$\dot{\rho}_{nm} = \left[-i\Omega(n - m) - \gamma(1 + n_B)\frac{n + m}{2} - \gamma n_B\frac{n + 1 + m + 1}{2}\right]\rho_{nm}$$

$$+ \gamma(1 + n_B)\sqrt{(n+1)(m+1)}\rho_{n+1,m+1} + \gamma n_B\sqrt{nm}\rho_{n-1,m-1}, \quad (1.60)$$

which, when $n \ne m$, shows that the coherences do not formally depend on the dynamics of the populations. However, they couple strongly to other coherences. In particular, we observe that coherences $\rho_n^\Delta = \rho_{n,n+\Delta}$ with integer $\Delta \ne 0$ and $\Delta \ge -n$ couple only to coherences with the same difference $\rho_{n\pm1}^\Delta$:

$$\dot{\rho}_n^\Delta = \big[+i\Omega\Delta - \gamma(1 + n_B)(n + \Delta/2) - \gamma n_B(n + 1 + \Delta/2)\big]\rho_n^\Delta$$

$$+ \gamma(1 + n_B)\sqrt{(n+1)(n+1+\Delta)}\rho_{n+1}^\Delta + \gamma n_B\sqrt{n(n+\Delta)}\rho_{n-1}^\Delta, \quad (1.61)$$

which also corresponds to a tridiagonal system for each fixed difference Δ. For each Δ it is straightforward to see that $\bar{\rho}_n^\Delta = 0$ is a stationary solution.

Exercise 1.14 (Moments) Calculate the expectation value of the number operator $n = a^\dagger a$ and its square $n^2 = a^\dagger a a^\dagger a$ in the stationary state of the master equation (1.56).

1.5.4.2 Driven Cavity with Losses

When the cavity is driven with a laser and simultaneously coupled to a vacuum bath $n_B = 0$, we obtain the master equation

$$
\dot{\rho}_S = -i\left[\Omega a^\dagger a + \frac{P}{2} e^{+i\omega t} a + \frac{P^*}{2} e^{-i\omega t} a^\dagger, \rho_S \right]
$$

$$
+ \gamma\left[a\rho_S a^\dagger - \frac{1}{2} a^\dagger a \rho_S - \frac{1}{2}\rho_S a^\dagger a \right] \tag{1.62}
$$

with the laser frequency ω and amplitude P. The transformation $\rho = e^{+i\omega a^\dagger a t} \times \rho_S e^{-i\omega a^\dagger a t}$ maps to a time-independent master equation,

$$
\dot{\rho} = -i\left[(\Omega - \omega) a^\dagger a + \frac{P}{2} a + \frac{P^*}{2} a^\dagger, \rho \right] + \gamma\left[a\rho a^\dagger - \frac{1}{2} a^\dagger a \rho - \frac{1}{2}\rho a^\dagger a \right]. \tag{1.63}
$$

This equation obviously couples coherences and populations in the Fock space representation. Therefore, it does not assume a simple rate equation form in this basis. Nevertheless, a solution of the resulting equation of motion can be found for particular operators.

Exercise 1.15 (Coherent state) Using the driven cavity master equation, show that the stationary expectation value of the cavity occupation fulfills

$$
\lim_{t\to\infty} \langle a^\dagger a \rangle = \frac{|P|^2}{\gamma^2 + 4(\Omega - \omega)^2}.
$$

1.6 Superoperator Notation

The Lindblad master equation may be a bit impractical for calculations, as one is often more used to the solution of first-order differential equations that are written as $\dot{v} = Av$, where A is a matrix and v is a vector. Since the Lindblad equation is linear in the density matrix ρ, one can easily convert it into such a form, where one writes $\dot{\rho} = \mathscr{L}\rho$. In this representation, $\mathscr{L}$ is a matrix, and the density matrix becomes a density vector. Conventionally, the mapping to a density vector is performed by first

placing d populations and then the $d(d-1)$ coherences:

$$\rho = \begin{pmatrix} \rho_{11} & \cdots & \rho_{1N} \\ \vdots & & \vdots \\ \rho_{N1} & \cdots & \rho_{NN} \end{pmatrix} \quad \Leftrightarrow \quad \|\rho\rangle\rangle = \begin{pmatrix} \rho_{11} \\ \vdots \\ \rho_{NN} \\ \rho_{12} \\ \rho_{21} \\ \vdots \\ \rho_{N-1,N} \\ \rho_{N,N-1} \end{pmatrix}. \tag{1.64}$$

A master equation can now be written as

$$\dot{\rho} = \mathscr{L}\rho, \tag{1.65}$$

where the superoperator corresponding to the Lindblad form (1.46) acts like an ordinary operator on the density vector. In this representation, the trace of a density matrix corresponds to multiplication with the vector

$$\langle\langle 0\| = (\underbrace{1,\ldots,1}_{N\times}, \underbrace{0,\ldots,0}_{N(N-1)\times}), \tag{1.66}$$

i.e., $\mathrm{Tr}\{\rho\} = \langle\langle 0\|\rho\rangle\rangle$. Thus, when the Hilbert space dimension of the quantum system is d, ρ_S is a vector of dimension d^2, and the superoperator $\mathscr{L}$ is represented by a $d^2 \times d^2$ matrix. At first sight, such a representation does not seem very efficient. However, for many specific cases, the structure of the superoperator $\mathscr{L}$ may directly allow for a simplified treatment. If for example it has block structure—as will be the case in the quantum optical master equation when the system has no degeneracies—one may treat the blocks separately, which is routinely done. To be more specific, the mapping can generally be performed as

$$\dot{\rho}_{ij} = -\mathrm{i}\langle i|\left[H, \sum_{kl} \rho_{kl}|k\rangle\langle l| \right]|j\rangle$$

$$+ \sum_{\alpha\beta} \gamma_{\alpha\beta}\left[\langle i|A_\alpha \sum_{kl} \rho_{kl}|k\rangle\langle l|A_\beta^\dagger|j\rangle - \frac{1}{2}\langle i|\left\{ A_\beta^\dagger A_\alpha, \sum_{kl}\rho_{kl}|k\rangle\langle l| \right\}|j\rangle \right]$$

$$= \sum_{kl} \mathscr{L}_{ij,kl}\rho_{kl}. \tag{1.67}$$

Similarly, we can also transform linear operators into superoperators. However, we must specify on which side of the density matrix the operator is supposed to act.

As an example, we consider the Liouvillian

$$L[\rho] = -\mathrm{i}\left[\Omega\sigma^z, \rho\right] + \gamma\left[\sigma^-\rho\sigma^+ - \frac{1}{2}\{\sigma^+\sigma^-, \rho\} \right] \tag{1.68}$$

with $\sigma^\pm = \frac{1}{2}(\sigma^x \pm i\sigma^y)$ in the eigenbasis of $\sigma^z|e\rangle = |e\rangle$ and $\sigma^z|g\rangle = -|g\rangle$, where we have $\sigma^+|g\rangle = |e\rangle$ and $\sigma^-|e\rangle = |g\rangle$. From the master equation, we obtain

$$\dot{\rho}_{ee} = -\gamma\rho_{ee}, \qquad \dot{\rho}_{gg} = +\gamma\rho_{ee},$$

$$\dot{\rho}_{eg} = \left(-\frac{\gamma}{2} - 2i\Omega\right)\rho_{eg}, \qquad \dot{\rho}_{ge} = \left(-\frac{\gamma}{2} + 2i\Omega\right)\rho_{ge}, \tag{1.69}$$

such that when we arrange the matrix elements in a vector $\rho = (\rho_{gg}, \rho_{ee}, \rho_{ge}, \rho_{eg})^T$, the master equation reads

$$\begin{pmatrix} \dot{\rho}_{gg} \\ \dot{\rho}_{ee} \\ \dot{\rho}_{ge} \\ \dot{\rho}_{eg} \end{pmatrix} = \begin{pmatrix} 0 & +\gamma & 0 & 0 \\ 0 & -\gamma & 0 & 0 \\ 0 & 0 & -\frac{\gamma}{2} + 2i\Omega & 0 \\ 0 & 0 & 0 & -\frac{\gamma}{2} - 2i\Omega \end{pmatrix} \begin{pmatrix} \rho_{gg} \\ \rho_{ee} \\ \rho_{ge} \\ \rho_{eg} \end{pmatrix}. \tag{1.70}$$

We note that populations and coherences evolve apparently independently. Note however that the Lindblad form nevertheless ensures a positive density matrix—with valid initial conditions provided.

Exercise 1.16 (Preservation of Positivity) Show that the superoperator in Eq. (1.70) preserves positivity of the density matrix provided that initial positivity ($-1/4 \leq |\rho_{ge}^0|^2 - \rho_{gg}^0\rho_{ee}^0 \leq 0$) is given.

Furthermore, note that we do not need to exponentiate a matrix to solve Eq. (1.70): its special structure makes it possible to solve for ρ_{eg} and ρ_{ge}, and ρ_{ee} independently. The equation for ρ_{gg} does depend on the result for ρ_{ee}; however, we may readily obtain the solution by exploiting trace conservation $\rho_{gg} = 1 - \rho_{ee}$. It is of course also possible to represent ordinary operators as superoperators. This however requires one to specify on which side the operator is acting; for example, one has

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix} \hat{=} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \rho_{gg} \\ \rho_{ee} \\ \rho_{ge} \\ \rho_{eg} \end{pmatrix},$$

$$\begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \hat{=} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \rho_{gg} \\ \rho_{ee} \\ \rho_{ge} \\ \rho_{eg} \end{pmatrix}. \tag{1.71}$$

Exercise 1.17 (Expectation values from superoperators) Show that for a Liouvillian superoperator connecting N populations (diagonal entries) with M coherences (off-diagonal entries) acting on the density matrix $\rho(t) = (P_1, \ldots, P_N, C_1, \ldots, C_M)^T$,

the trace in the expectation value of an operator can be mapped to the matrix element

$$\langle A(t) \rangle = (\underbrace{1, \ldots, 1}_{N\times}, \underbrace{0, \ldots, 0}_{M\times}) \cdot \mathscr{A} \cdot \rho(t),$$

where the matrix $\mathscr{A}$ is the superoperator corresponding to multiplication with A from the left.

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