Non-Equilibrium Master Equations

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Contents

This lecture aims at providing graduate students in physics and neighboring sciences with a heuristic approach to master equations. Although the focus of the lecture is on rate equations, their derivation will be based on quantum-mechanical principles, such that basic knowledge of quantum theory is mandatory. The lecture will try to be as self-contained as possible and aims at providing rather recipes than proofs.

As successful learning requires practice, a number of exercises will be given during the lecture, the solution to these exercises may be turned in in the next lecture (computer algebra may be used if applicable), for which students may earn points. Students having earned 50 % of the points at the end of the lecture are entitled to three ECTS credit points.

This script will be made available online at

http://wwwitp.physik.tu-berlin.de/~ schaller/.

In any first draft errors are quite likely, such that corrections and suggestions should be addressed to

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literature:

[1] Michael A. Nielsen and Isaac L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press, Cambridge (2000).

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Chapter 1

An introduction to Master Equations

1.1 Master Equations – A 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 evolution equations themselves involve amplitudes rather than observables in the lowest level, such that a stochastic evolution is intrinsic. In order to understand such processes in great detail, a description should include such random events via a probabilistic description. For dynamical systems, probabilities associated with events may evolve in time, and the determining equation for such a process is called **master equation**.

Box 1 (Master Equation) *A master equation is a first order differential equation describing the time evolution of probabilities, e.g. for discrete events*

$$\frac{dP_k}{dt} = \sum_\ell \left[T_{k\ell}P_\ell - T_{\ell k}P_k\right] , \tag{1.1}$$

where the $T_{k\ell}$ are transition rates between events ℓ and k. 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.

When the transition matrix $T_{k\ell}$ is symmetric, all processes are reversible at the level of the master equation description. Mostly, master equations are phenomenologically motivated and not derived from first principles, but in the case of open quantum systems we will also discuss microscopic derivations. Already the Markovian quantum master equation does not only involve probabilities (diagonals of the density matrix) but also coherences (off-diagonals) in the master equation. Here, therefore the term master equation is used in a weaker condition as simply the evolution equation for probabilities.

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

$$\sum_k \frac{dP_k}{dt} = \sum_{k\ell} \left(T_{k\ell}P_\ell - T_{\ell k}P_k\right) = \sum_{k\ell} \left(T_{\ell k}P_k - T_{\ell k}P_k\right) = 0 . \tag{1.2}$$

Beyond this, all probabilities must remain positive, which is also respected by a normal master equation. 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. After some time, the probability P_k may approach zero (but all others are non-negative). Its time-derivative is then given by

$$\left.\frac{dP_k}{dt}\right|_{P_k=0} = +\sum_\ell T_{k\ell} P_\ell \geq 0\,, \tag{1.3}$$

such that $P_k < 0$ is impossible. 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 (1.1) automatically preserves the sum of probabilities and also keeps $0 \leq P_i(t) \leq 1$ – a valid initialization provided. That is, under the evolution of a master equation, probabilities remain probabilities.

1.1.1 Example 1: Fluctuating two-level system

Let us consider a system of two possible events, 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 two states of an excitable atom, etc. To introduce some dynamics, let the transition rate from $0 \to 1$ be denoted by $T_{01} > 0$ and the inverse transition rate $1 \to 0$ be denoted by $T_{10} > 0$. The associated master equation is then given by

$$\frac{d}{dt}\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} -T_{01} & +T_{10} \\ +T_{01} & -T_{10} \end{pmatrix}\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} \tag{1.4}$$

Exercise 1 (Temporal Dynamics of a two-level system) *(1 point)*
Calculate the solution of Eq. (1.4). What is the stationary state?

Exercise 2 (Tunneling mice) *(1 point)*
Two identical mice are put in a box consisting of two (left and right) compartments. Afterwards they randomly change compartments with rate T. Set up the master equation for the probabilities to find both mice in the left (P_L) or right (P_R) compartments or in a balanced configuration (P_B).

1.1.2 Example 2: Diffusion Equation

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

$$\begin{aligned} \dot{P}_i(t) &= TP_{i-1}(t) + TP_{i+1}(t) - 2TP_i(t) \\ &= T\Delta x^2 \frac{P_{i-1}(t) + P_{i+1}(t) - 2P_i(t)}{\Delta x^2}\,, \end{aligned} \tag{1.5}$$

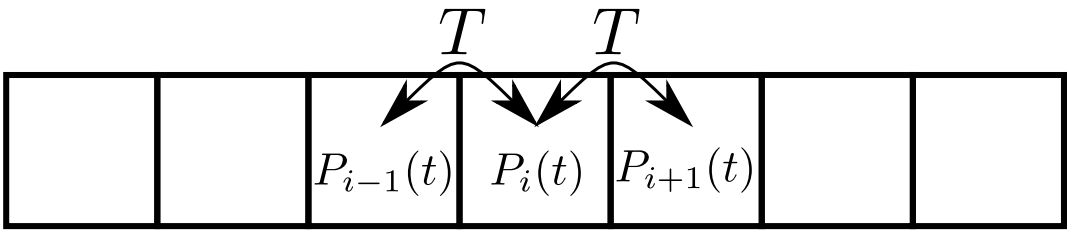

Figure 1.1: Linear chain of compartments coupled with a transition rate T, where only next neighbors are coupled to each other symmetrically.

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

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2} \qquad \text{with} \qquad D = T\Delta x^2 \,. \tag{1.6}$$

Such diffusion equations are used to describe the distribution of chemicals in a soluble 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 (spatially-dependent diffusion coefficient). A corresponding model (in next-neighbor approximation) would be given by

$$\dot{P}_i = T_{i-1,i}P_{i-1}(t) + T_{i+1,i}P_{i+1}(t) - (T_{i,i-1} + T_{i,i+1})P_i(t) \,, \tag{1.7}$$

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

$$\begin{aligned} \frac{\partial P}{\partial t} &= \frac{\partial^2}{\partial x^2}\left[A(x)P(x,t)\right] + \frac{\partial}{\partial x}\left[B(x)P(x,t)\right] \\ &\equiv \frac{A_{i-1}P_{i-1} - 2A_iP_i + A_{i+1}P_{i+1}}{\Delta x^2} + \frac{B_{i+1}P_{i+1} - B_{i-1}P_{i-1}}{2\Delta x} \\ &= \left[\frac{A_{i-1}}{\Delta x^2} - \frac{B_{i-1}}{2\Delta x}\right]P_{i-1} - \frac{2A_i}{\Delta x^2}P_i + \left[\frac{A_{i+1}}{\Delta x^2} + \frac{B_{i+1}}{2\Delta x}\right]P_{i+1} \,, \end{aligned} \tag{1.8}$$

which is equivalent to our master equation when

$$A_i = \frac{\Delta x^2}{2}\left[T_{i,i-1} + T_{i,i+1}\right] \,, \qquad B_i = \Delta x\left[T_{i,i-1} - T_{i,i+1}\right] \,. \tag{1.9}$$

We conclude that the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \frac{\partial^2}{\partial x^2}\left[A(x)P(x,t)\right] + \frac{\partial}{\partial x}\left[B(x)P(x,t)\right] \tag{1.10}$$

with $A(x) \geq 0$ preserves norm and positivity of the probability distribution $P(x,t)$.

Exercise 3 (Reaction-Diffusion Equation) *(1 point)*
Along a linear chain of compartments consider the master equation for two species

$$\begin{aligned}\dot{P}_i &= T\left[P_{i-1}(t) + P_{i+1}(t) - 2P_i(t)\right] - \gamma P_i(t)\,,\\ \dot{p}_i &= \tau\left[p_{i-1}(t) + p_{i+1}(t) - 2p_i(t)\right] + \gamma P_i(t),\end{aligned}$$

where $P_i(t)$ may denote the concentration of a molecule that irreversibly reacts with chemicals in the soluble 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.

1.2 Density Matrix Formalism

1.2.1 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 in which of these states the system is. Such systems can be conveniently described by the density matrix.

Box 2 (Density Matrix) *The density matrix can be written as*

$$\rho = \sum_i p_i \left|\Phi_i\right\rangle \left\langle\Phi_i\right|\,, \tag{1.11}$$

where $0 \leq p_i \leq 1$ denote the probabilities to be in the state $|\Phi_i\rangle$ with $\sum_i p_i = 1$. Note that we do not generally require the states 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:* $\mathrm{Tr}\{\rho\} = 1$
- *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 $\rho = |\Phi_{\bar{i}}\rangle\langle\Phi_{\bar{i}}|$. Evidently, a density matrix is pure if and only if $\rho = \rho^2$.

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

$$\langle A\rangle = \langle\Psi|\,A\,|\Psi\rangle \tag{1.12}$$

can be obtained conveniently from the corresponding pure density matrix $\rho = |\Psi\rangle\langle\Psi|$ by simply computing the trace

$$\begin{aligned}\langle A\rangle &\equiv \mathrm{Tr}\{A\rho\} = \mathrm{Tr}\{\rho A\} = \mathrm{Tr}\{A|\Psi\rangle\langle\Psi|\} \\ &= \sum_n \langle n|A|\Psi\rangle\langle\Psi|n\rangle = \langle\Psi|\left(\sum_n |n\rangle\langle n|\right)A|\Psi\rangle \\ &= \langle\Psi|A|\Psi\rangle\ . \end{aligned} \tag{1.13}$$

When the state is not exactly known but its probability distribution, the expectation value is obtained by computing the weighted average

$$\langle A\rangle = \sum_i P_i \langle\Phi_i|A|\Phi_i\rangle\ , \tag{1.14}$$

where P_i denotes the probability to be 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

$$\begin{aligned}\langle A\rangle &\equiv \mathrm{Tr}\{A\rho\} = \mathrm{Tr}\left\{A\sum_i p_i|\Phi_i\rangle\langle\Phi_i|\right\} = \sum_i p_i \mathrm{Tr}\{A|\Phi_i\rangle\langle\Phi_i|\} \\ &= \sum_i p_i \sum_n \langle n|A|\Phi_i\rangle\langle\Phi_i|n\rangle = \sum_i p_i \langle\Phi_i|\left(\sum_n |n\rangle\langle n|\right)A|\Phi_i\rangle \\ &= \sum_i p_i \langle\Phi_i|A|\Phi_i\rangle\ . \end{aligned} \tag{1.15}$$

Exercise 4 (Superposition vs Localized States) *(1 point)*
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* $p_a = p_b = 1/2$.

1.2.2 Dynamical Evolution in a closed system

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

$$\left|\dot\Psi(t)\right\rangle = -\mathrm{i}H(t)|\Psi(t)\rangle \tag{1.16}$$

the time evolution operator

$$U(t) = \hat\tau \exp\left\{-i\int_0^t H(t')dt'\right\} \tag{1.17}$$

may be defined as the solution to the operator equation

$$\dot U(t) = -\mathrm{i}H(t)U(t)\,. \tag{1.18}$$

For constant $H(0) = H$, 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

$$\dot{\rho} = -\mathrm{i}\,[H(t), \rho(t)] \tag{1.19}$$

with the formal solution $\rho(t) = U(t)\rho(0)U^\dagger(t)$, compare Eq. (1.17).

When we simply apply this evolution equation to a density matrix that is not pure, we obtain

$$\rho(t) = \sum_i p_i U(t)\,|\Phi_i\rangle\langle\Phi_i|\,U^\dagger(t)\,, \tag{1.20}$$

i.e., transitions between the (now time-dependent) state vectors $|\Phi_i(t)\rangle = U(t)\,|\Phi_i\rangle$ are impossible with unitary evolution. This means that the von-Neumann evolution equation does yield the same dynamics as the Schrödinger equation if it is restarted on different initial states.

Exercise 5 (Preservation of density matrix properties by unitary evolution) *(1 point) Show that the von-Neumann (1.19) equation preserves self-adjointness, trace, and positivity of the density matrix.*

Also the Measurement process can 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

$$p_m = \langle\Psi|\,M_m^\dagger M_m\,|\Psi\rangle \tag{1.21}$$

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

$$|\Psi\rangle \overset{m}{\to} \frac{M_m\,|\Psi\rangle}{\sqrt{\langle\Psi|\,M_m^\dagger M_m\,|\Psi\rangle}}\,. \tag{1.22}$$

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

Box 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 to obtain result m is given by*

$$p_m = \mathrm{Tr}\left\{M_m^\dagger M_m \rho\right\} \tag{1.23}$$

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

$$\rho \overset{m}{\to} \rho' = \frac{M_m \rho M_m^\dagger}{\mathrm{Tr}\left\{M_m^\dagger M_m \rho\right\}} \tag{1.24}$$

It is therefore straightforward to see that description by Schrödinger equation or von-Neumann equation with the respective measurement postulates are equivalent. The density matrix formalism conveniently includes statistical mixtures in the description but at the cost of quadratically increasing the number of state variables.

Exercise 6 (Preservation of density matrix properties by measurement) *(1 point)*
Show that the measurement postulate preserves self-adjointness, trace, and positivity of the density matrix.

1.2.3 Most general dynamical Evolution

Any dynamical evolution equation for the density matrix should (at least in some approximate sense) preserve its interpretation as density matrix, i.e., trace, hermiticity, and positivity must be preserved. By construction, the mesurement postulate and unitary evolution preserve these properties. However, more general evolutions are conceivable. 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 [4].

Box 4 (Lindblad form) *A master equation of Lindblad form has the structure*

$$\dot{\rho} = \mathcal{L}\rho = -\mathrm{i}\,[H,\rho] + \sum_{\alpha,\beta=1}^{N^2-1} \gamma_{\alpha\beta}\left(A_\alpha \rho A_\beta^\dagger - \frac{1}{2}\left\{A_\beta^\dagger A_\alpha, \rho\right\}\right), \tag{1.25}$$

where the hermitian operator $H = H^\dagger$ can be interpreted as an effective Hamiltonian and $\gamma_{\alpha\beta} = \gamma_{\beta\alpha}^*$ 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 $\lambda_i \geq 0$).

Exercise 7 (Trace and Hermiticity preservation by Lindblad forms) *(1 points)*
Show that the Lindblad form master equation preserves trace and hermiticity of the density matrix.

The Lindblad type master equation can be written in 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 $A_\alpha = \sum_{\alpha'} U_{\alpha'\alpha} L_{\alpha'}$. Inserting this

decomposition in the master equation, we obtain

$$\begin{aligned}\dot{\rho} &= -\mathrm{i}\,[H,\rho] + \sum_{\alpha,\beta=1}^{N^2-1} \gamma_{\alpha\beta}\left(A_\alpha \rho A_\beta^\dagger - \frac{1}{2}\left\{A_\beta^\dagger A_\alpha, \rho\right\}\right) \\ &= -\mathrm{i}\,[H,\rho] + \sum_{\alpha',\beta'}\left[\sum_{\alpha\beta}\gamma_{\alpha\beta}U_{\alpha'\alpha}U^*_{\beta'\beta}\right]\left(L_{\alpha'}\rho L_{\beta'}^\dagger - \frac{1}{2}\left\{L_{\beta'}^\dagger L_{\alpha'}, \rho\right\}\right) \\ &= -\mathrm{i}\,[H,\rho] + \sum_{\alpha}\gamma_\alpha\left(L_\alpha \rho L_\alpha^\dagger - \frac{1}{2}\left\{L_\alpha^\dagger L_\alpha, \rho\right\}\right)\,, \end{aligned} \tag{1.26}$$

where γ_α denote the N^2-1 non-negative eigenvalues of the dampening matrix. Evidently, the representation of a master equation is not unique. Any other unitary operation would lead to a different non-diagonal 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

$$\begin{aligned} L_\alpha &\to L'_\alpha = L_\alpha + a_\alpha \\ H &\to H' = H + \frac{1}{2\mathrm{i}}\sum_\alpha \gamma_\alpha\left(a_\alpha^* L_\alpha - a_\alpha L_\alpha^\dagger\right) + b\,, \end{aligned} \tag{1.27}$$

with complex numbers a_α and a real number b. The first of the above equations can be exploited to choose the Lindblad operators L_α traceless.

Exercise 8 (Shift invariance) *(1 points)*
Show the invariance of the diagonal representation of a Lindblad form master equation (1.26) with respect to the transformation (1.27).

We would like to demonstrate the preservation of positivity here. Let us get rid of the unitary evolution term by transforming to a comoving frame $\rho = e^{-iHt}\tilde{\rho}e^{+iHt}$, where the master equation assumes the form

$$\dot{\boldsymbol{\rho}} = \sum_\alpha \gamma_\alpha\left(\boldsymbol{L}_\alpha(t)\boldsymbol{\rho}\boldsymbol{L}_\alpha^\dagger(t) - \frac{1}{2}\left\{\boldsymbol{A}_\alpha^\dagger(t)\boldsymbol{A}_\alpha(t), \boldsymbol{\rho}\right\}\right) \tag{1.28}$$

with the transformed time-dependent operators $\boldsymbol{L}_\alpha(t) = e^{+iHt}L_\alpha e^{-iHt}$. 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 $K = N^2-1$

$$\begin{aligned} W_1(t) &= \mathbf{1}\,, \\ W_2(t) &= \frac{1}{2}\sum_\alpha \gamma_\alpha(t)\boldsymbol{L}_\alpha^\dagger(t)\boldsymbol{L}_\alpha(t)\,, \\ W_3(t) &= \boldsymbol{L}_1(t)\,, \\ &\vdots \\ W_{K+2}(t) &= \boldsymbol{L}_K(t)\,. \end{aligned} \tag{1.29}$$

Discretizing the time-derivative in (1.28) one transforms the differential equation for the density matrix into an iteration equation

$$\begin{aligned}\boldsymbol{\rho}(t+\Delta t) &= \boldsymbol{\rho(t)} + \Delta t \sum_\alpha \gamma_\alpha \left[\boldsymbol{L}_\alpha(t)\boldsymbol{\rho}(t)\boldsymbol{L}_\alpha^\dagger(t) - \frac{1}{2}\left\{\boldsymbol{L}_\alpha^\dagger(t)\boldsymbol{L}_\alpha(t), \boldsymbol{\rho}(t)\right\}\right] \\ &= \sum_{\alpha\beta} w_{\alpha\beta}(t) W_\alpha(t)\boldsymbol{\rho}(t)W_\beta^\dagger(t)\,, \end{aligned} \tag{1.30}$$

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

$$w(t) = \left(\begin{array}{cc|ccc} 1 & -\Delta t & 0 & \cdots & 0 \\ -\Delta t & 0 & 0 & \cdots & 0 \\ \hline 0 & 0 & \Delta t\gamma_1(t) & & \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & & & \Delta t\gamma_K(t) \end{array}\right), \tag{1.31}$$

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

$$\rho(t+\Delta t) = \sum_\alpha w_\alpha(t)\tilde{W}_\alpha(t)\rho(t)\tilde{W}_\alpha^\dagger(t) \tag{1.32}$$

with $w_\alpha(t)$ denoting the eigenvalues of the matrix (1.31) and in particular the only negative eigenvalue being given by $w_1(t) = \frac{1}{2}\left(1 - \sqrt{1+4\Delta t^2}\right)$. Now, we use the spectral decomposition of the density matrix at time t – $\rho(t) = \sum_a P_a(t)\left|\Psi_a(t)\right\rangle\left\langle\Psi_a(t)\right|$ – to demonstrate approximate positivity of the density matrix at time $t + \Delta t$

$$\begin{aligned}\left\langle\Phi\right|\rho(t+\Delta t)\left|\Phi\right\rangle &= \sum_{\alpha,a} w_\alpha(t)P_a(t)\left|\left\langle\Phi\right|\tilde{W}_\alpha(t)\left|\Psi_a(t)\right\rangle\right|^2 \\ &\geq \frac{1}{2}\left(1-\sqrt{1+4\Delta t^2}\right)\sum_a P_a(t)\left|\left\langle\Phi\right|\tilde{W}_1(t)\left|\Psi_a(t)\right\rangle\right|^2 \\ &\geq -\Delta t^2 \sum_a P_a(t)\left|\left\langle\Phi\right|\tilde{W}_1(t)\left|\Psi_a(t)\right\rangle\right|^2 \overset{\Delta t\to 0}{\to} 0\,, \end{aligned} \tag{1.33}$$

such that the violation of positivity vanishes faster than the discretization width as Δt goes to zero.

1.2.4 Master Equation for a cavity in a thermal bath

Consider the Lindblad form master equation

$$\begin{aligned}\dot{\rho_{\rm S}} &= -i\left[\Omega a^\dagger a, \rho_{\rm S}\right] + \gamma(1+n_B)\left[a\rho_{\rm S}a^\dagger - \frac{1}{2}a^\dagger a\rho_{\rm S} - \frac{1}{2}\rho_{\rm S}a^\dagger a\right] \\ &\quad +\gamma n_B\left[a^\dagger\rho_{\rm S}a - \frac{1}{2}aa^\dagger\rho_{\rm S} - \frac{1}{2}\rho_{\rm S}aa^\dagger\right], \end{aligned} \tag{1.34}$$

with bosonic operators $\left[a, a^\dagger\right] = \mathbf{1}$ and Bose-Einstein bath occupation $n_B = \left[e^{\beta\Omega} - 1\right]^{-1}$ and cavity frequency Ω. In Fock-space representation, these operators act as $a^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$ (where $0 \leq n < \infty$), such that the above master equation couples only the diagonals of the density matrix $\rho_n = \langle n| \rho_{\rm S} |n\rangle$ to each other

$$\begin{aligned} \dot{\rho_n} &= \gamma(1+n_B)\left[(n+1)\rho_{n+1} - n\rho_n\right] + \gamma n_B\left[n\rho_{n-1} - (n+1)\rho_n\right] \\ &= \gamma n_B n \rho_{n-1} - \gamma\left[n + (2n+1)n_B\right]\rho_n + \gamma(1+n_B)(n+1)\rho_{n+1} \end{aligned} \tag{1.35}$$

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

$$\frac{\bar{\rho}_{n+1}}{\bar{\rho}_n} = \frac{n_B}{1+n_B} = e^{-\beta\Omega}, \tag{1.36}$$

i.e., the stationary state is a thermalized Gibbs state with the reservoir temperature.

Exercise 9 (Moments) *(1 points)*
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 (1.34).

1.2.5 Master Equation for a driven cavity

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

$$\dot{\rho_{\rm S}} = -\mathrm{i}\left[\Omega a^\dagger a + \frac{P}{2}e^{+i\omega t}a + \frac{P^*}{2}e^{-i\omega t}a^\dagger, \rho_{\rm S}\right] + \gamma\left[a\rho_{\rm S}a^\dagger - \frac{1}{2}a^\dagger a\rho_{\rm S} - \frac{1}{2}\rho_{\rm S}a^\dagger a\right] \tag{1.37}$$

with the Laser frequency ω and amplitude P. The transformation $\rho = e^{+\mathrm{i}\omega a^\dagger a t}\rho_{\rm S}e^{-\mathrm{i}\omega a^\dagger a t}$ maps to a time-independent master equation

$$\dot{\rho} = -\mathrm{i}\left[(\Omega-\omega)a^\dagger a + \frac{P}{2}a + \frac{P^*}{2}a^\dagger, \rho\right] + \gamma\left[a\rho a^\dagger - \frac{1}{2}a^\dagger a\rho - \frac{1}{2}\rho a^\dagger a\right]. \tag{1.38}$$

This equation obviously couples coherences and populations in the Fock space representation.

Exercise 10 (Coherent state) *(1 points)*
Using the driven cavity master equation, show that the stationary expectation value of the cavity occupation fulfils

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

1.2.6 Tensor Product

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

Box 5 (Tensor Product) *Let V and W be Hilbert spaces (vector spaces with 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* $\langle a|b\rangle = \sum_{ijk\ell} a^*_{ij} b_{k\ell} \langle v_i|v_k\rangle \langle w_j|w_\ell\rangle = \sum_{ij} a^*_{ij} b_{ij}$

If more than just two vector spaces are combined to form a larger vector space, 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 four-dimensional, of three qubits 8-dimensional, and of n qubits 2^n-dimensional. Eventually, this exponential growth of the Hilbert space dimension for composite quantum systems is at the heart of quantum computing.

Exercise 11 (Tensor Products of Operators) *(1 points)*
Let $\boldsymbol{\sigma}$ denote the Pauli matrices, i.e.,

$$\sigma^1 = \begin{pmatrix} 0 & +1 \\ +1 & 0 \end{pmatrix} \qquad \sigma^2 = \begin{pmatrix} 0 & -\mathrm{i} \\ +\mathrm{i} & 0 \end{pmatrix} \qquad \sigma^3 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$$

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 is inherited, this typically enables a convenient calculation of the trace

in case of a few operator decomposition, e.g., for just two operators

$$\begin{aligned} \mathrm{Tr}\left\{A\otimes B\right\} &= \sum_{n_A,n_B}\left\langle n_A,n_B\right| A\otimes B\left|n_A,n_B\right\rangle \\ &= \left[\sum_{n_A}\left\langle n_A\right| A\left|n_A\right\rangle\right]\left[\sum_{n_B}\left\langle n_B\right| B\left|n_B\right\rangle\right] \\ &= \mathrm{Tr}_A\{A\}\mathrm{Tr}_B\{B\}\,, \end{aligned} \tag{1.39}$$

where $\mathrm{Tr}_{A/B}$ denote the trace in the Hilbert space of A and B, respectively.

1.2.7 The partial trace

For composed 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 $\rho\to\mathrm{Tr_B}\left\{\rho\right\}$ to such a reduced density matrix should leave all expectation values of observables acting on the considered subsystem only invariant, i.e.,

$$\mathrm{Tr}\left\{A\otimes\mathbf{1}\rho\right\}=\mathrm{Tr}\left\{A\mathrm{Tr_B}\left\{\rho\right\}\right\}\,. \tag{1.40}$$

If this basic condition was not fulfilled, there would be no point in defining such a thing as a reduced density matrix: Measurement would yield different results depending on the Hilbert space of the experimenters feeling.

Box 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*

$$\mathrm{Tr_B}\left\{\left|a_1\right\rangle\left\langle a_2\right|\otimes\left|b_1\right\rangle\left\langle b_2\right|\right\}=\left|a_1\right\rangle\left\langle a_2\right|\mathrm{Tr}\left\{\left|b_1\right\rangle\left\langle b_2\right|\right\}\,. \tag{1.41}$$

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

$$\begin{aligned} \mathrm{Tr_B}\left\{C\right\} &= \mathrm{Tr_B}\left\{\sum_{\alpha\beta\gamma\delta}c_{\alpha\beta\gamma\delta}\left|a_\alpha\right\rangle\left\langle a_\beta\right|\otimes\left|b_\gamma\right\rangle\left\langle b_\delta\right|\right\} \\ &= \sum_{\alpha\beta\gamma\delta}c_{\alpha\beta\gamma\delta}\mathrm{Tr_B}\left\{\left|a_\alpha\right\rangle\left\langle a_\beta\right|\otimes\left|b_\gamma\right\rangle\left\langle b_\delta\right|\right\} \\ &= \sum_{\alpha\beta\gamma\delta}c_{\alpha\beta\gamma\delta}\left|a_\alpha\right\rangle\left\langle a_\beta\right|\mathrm{Tr}\left\{\left|b_\gamma\right\rangle\left\langle b_\delta\right|\right\} \\ &= \sum_{\alpha\beta\gamma\delta}c_{\alpha\beta\gamma\delta}\left|a_\alpha\right\rangle\left\langle a_\beta\right|\sum_\epsilon\left\langle b_\epsilon|b_\gamma\right\rangle\left\langle b_\delta|b_\epsilon\right\rangle \\ &= \sum_{\alpha\beta}\left[\sum_\gamma c_{\alpha\beta\gamma\gamma}\right]\left|a_\alpha\right\rangle\left\langle a_\beta\right|\,. \end{aligned} \tag{1.42}$$

The definition 6 is the only linear map that respects the invariance of expectation values.

Exercise 12 (Partial Trace) *(1 points)*
Compute the partial trace of a pure density matrix $\rho = |\Psi\rangle\langle\Psi|$ *in the bipartite state*

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

Chapter 2

Obtaining a Master Equation

2.1 Phenomenologic Derivations (Educated Guesses)

Before discussing rigorous derivations, we give some more examples of phenomenologically motivated master equations.

2.1.1 The single resonant level

Consider a nanostructure (quantum dot) capable of hosting a single electron with on-site energy ϵ. Let $P_0(t)$ denote the probability of finding the dot empty and $P_1(t)$ the opposite probability of finding an electron in the dot. When we do now couple the dot to a junction with tunneling rate Γ, its occupation will fluctuate depending on the Fermi level of the junction, see Fig. 2.1. In

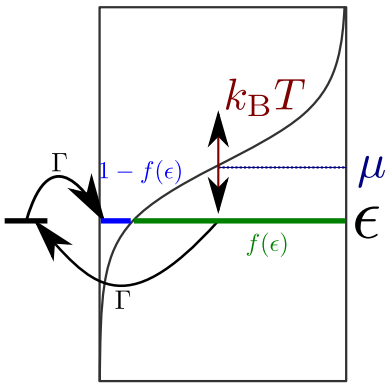

Figure 2.1: A single quantum dot coupled to a single junction, where the electronic occupation of energy levels is well approximated by a Fermi distribution.

particular, if at time t the dot was empty, the probability to find an electron in the dot at time $t + \Delta t$ is roughly given by $\Gamma \Delta t f(\epsilon)$ with the Fermi function defined as

$$f(\omega) = \frac{1}{e^{\beta(\omega-\mu)} + 1}\,, \tag{2.1}$$

where β denotes the inverse temperature and μ the chemical potential of the junction. The transition rate is thus given by the tunneling rate Γ multiplied by the probability to have an electron in the junction at the required energy ϵ ready to jump into the system. The inverse

probability to find an initially filled dot empty reads $\Gamma\Delta t\,[1-f(\epsilon)]$, i.e., here one has to muliply the tunneling probability with the probability to have a free slot in the junction, such that we have

$$\frac{d}{dt}\begin{pmatrix} P_0 \\ P_1 \end{pmatrix} = \begin{pmatrix} -\Gamma f(\epsilon) & +\Gamma(1-f(\epsilon)) \\ +\Gamma f(\epsilon) & -\Gamma(1-f(\epsilon)) \end{pmatrix}\begin{pmatrix} P_0 \\ P_1 \end{pmatrix}, \tag{2.2}$$

where the diagonal elements follow directly from trace conservation. The stationary state fulfils

$$\frac{P_1}{P_0} = \frac{f(\epsilon)}{1-f(\epsilon)} = e^{-\beta(\epsilon-\mu)}, \tag{2.3}$$

i.e., the quantum dot equilibrates with the reservoir. Here we have been able to describe the system only by occupation probabilities (no coherences), which is possible since due to charge conservation one cannot create superpositions of differently charged states. In the corresponding density matrix formalism, the coherences would simply vanish.

2.1.2 Cell culture growth in constrained geometries

Consider a population of cells that divide (proliferate) with a certain rate α. These cells live in a constrained geometry (e.g., a petri dish) that admits at most K cells. Let $P_i(t)$ denote the probability to have i cells in the compartment. Assuming that the proliferation rate α is sufficiently small, we can easily set up a master equation

$$\begin{aligned}
\dot{P}_0 &= 0\,, \\
\dot{P}_1 &= -1\cdot\alpha\cdot P_1\,, \\
\dot{P}_2 &= -2\cdot\alpha\cdot P_2 + 1\cdot\alpha\cdot P_1\,, \\
&\vdots \\
\dot{P}_\ell &= -\ell\cdot\alpha\cdot P_\ell + (\ell-1)\cdot\alpha\cdot P_{\ell-1}\,, \\
&\vdots \\
\dot{P}_{K-1} &= -(K-1)\cdot\alpha\cdot P_{K-1} + (K-2)\cdot\alpha\cdot P_{K-2}\,, \\
\dot{P}_K &= +(K-1)\cdot\alpha P_{K-1}\,.
\end{aligned} \tag{2.4}$$

The prefactors arise since any of the ℓ cells may proliferate. Arranging the probabilities in a single vector, this may also be written as $\dot{\boldsymbol{P}} = L\boldsymbol{P}$, where the matrix L contains the rates. When we have a single cell as initial condition (full knowledge), i.e., $P_1(0)=1$, 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

$$\langle\ell\rangle = e^{+\alpha t}\left[1-\left(1-e^{-\alpha t}\right)^K\right]. \tag{2.5}$$

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

However, one may not be only interested in the evolution by mean values (especially when one wants e.g. to model tumour growth) but also would like to have some idea about the evolution of a single trajectory. In case of a rate equation (where coherences are not included), it is possible to generate single trajectories also from the master equation by Monte-Carlo simulation. Suppose 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 to be in a different state read

$$\boldsymbol{P}(t+\Delta t) \approx [\mathbf{1}+\Delta t L]\,\boldsymbol{P}(t)\,, \tag{2.6}$$

which for our simple example boils down to

$$P_\ell(t+\Delta t) \approx (1-\ell\alpha\Delta t)P_\ell(t)\,, \qquad P_{\ell+1}(t+\Delta t) \approx +\ell\alpha\Delta t P_\ell(t)\,. \tag{2.7}$$

To simulate a single trajectory, one may simply draw a random number and determine whether the transition has occurred ($P_{\text{jump}} = \ell\alpha\Delta t$) or not. If the transition occurs, we do again have complete knowledge and may set $P_\alpha(t+\Delta t) = \delta_{\ell+1,\alpha}$. If the transition does not occur, we also have complete knowledge and remain at $P_\alpha(t+\Delta t) = \delta_{\ell\alpha}$. In any case, this looks effectively like a measurement of the cell number that is performed at intervals of Δt. The simple average of many such trajectories will yield the mean evolution predicted by the master equation, see Fig. 2.2.

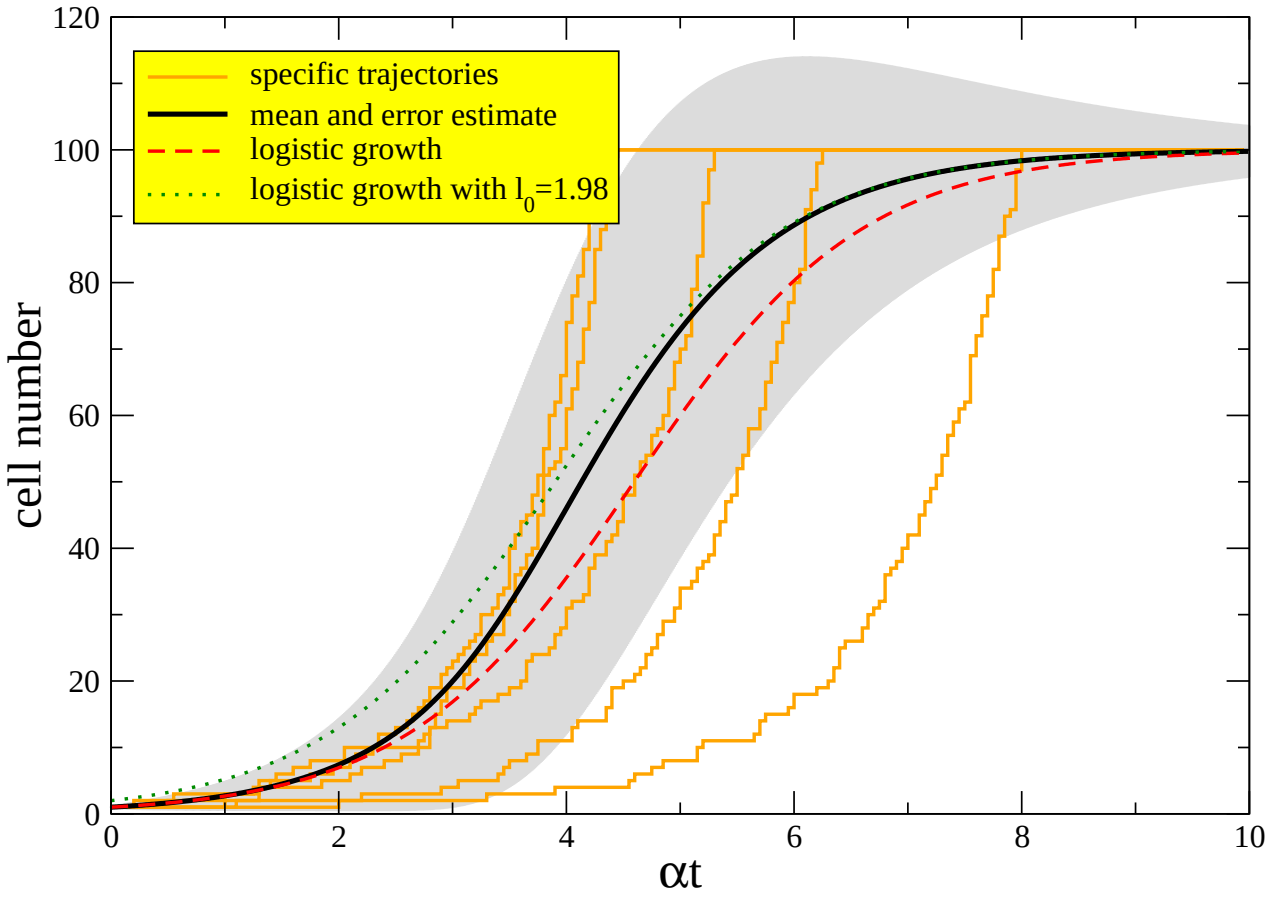

Figure 2.2: Population dynamics for the linear master equation (black curve $\langle\ell\rangle$ and shaded area determined from $\sqrt{\langle\ell^2\rangle - \langle\ell\rangle^2}$) and for the logistic growth equation (dashed red curve) for carrying capacity $K = 100$. For identical initial and final 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 asyptotics. An average of lots of specific trajectories would converge towards the black curve.

2.2 Derivations for Open Quantum Systems

In some cases, it is possible to derive a master equation rigorously based only on a few assumptions. Open quantum systems for example are mostly treated as part of a much larger closed quantum

system (the union of system and bath), where the partial trace is used to eliminate the unwanted (typically many) degrees of freedom of the bath, see Fig. 2.3. Technically speaking, we will consider

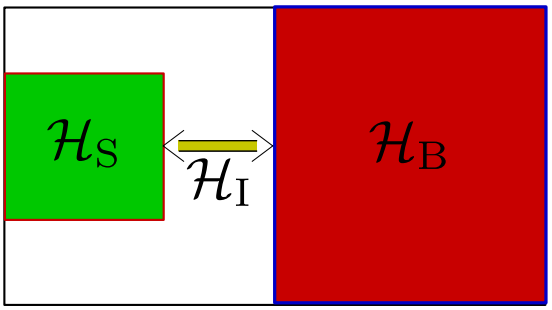

Figure 2.3: An open quantum system can be conceived as being part of a larger closed quantum system, where the system part ($\mathcal{H}_\mathrm{S}$) is coupled to the bath ($\mathcal{H}_\mathrm{B}$) via the interaction Hamiltonian $\mathcal{H}_\mathrm{I}$.

Hamiltonians of the form

$$H = \mathcal{H}_\mathrm{S} \otimes \mathbf{1} + \mathbf{1} \otimes \mathcal{H}_\mathrm{B} + \mathcal{H}_\mathrm{I}\,, \tag{2.8}$$

where the system and bath Hamiltonians act only on the system and bath Hilbert space, respectively. In contrast, the interaction Hamiltonian acts on both Hilbert spaces

$$\mathcal{H}_\mathrm{I} = \sum_\alpha A_\alpha \otimes B_\alpha\,, \tag{2.9}$$

where the summation boundaries are in the worst case limited by the dimension of the system Hilbert space. As we consider physical observables here, it is required that all Hamiltonians are self-adjoint.

Exercise 13 (Hermiticity of Couplings) *(1 points)*
Show that it is always possible to choose hermitian coupling operators $A_\alpha = A_\alpha^\dagger$ and $B_\alpha = B_\alpha^\dagger$ using that $\mathcal{H}_\mathrm{I} = \mathcal{H}_\mathrm{I}^\dagger$.

2.2.1 Weak Coupling Regime

When the interaction $\mathcal{H}_\mathrm{I}$ is small, it is justified to apply perturbation theory. The von-Neumann equation in the joint total quantum system

$$\dot{\rho} = -i\left[\mathcal{H}_\mathrm{S} \otimes \mathbf{1} + \mathbf{1} \otimes \mathcal{H}_\mathrm{B} + \mathcal{H}_\mathrm{I}, \rho\right] \tag{2.10}$$

describes the full evolution of the combined density matrix. This equation can be formally solved by the unitary evolution $\rho(t) = e^{-iHt}\rho_0 e^{+iHt}$, which however is impractical to compute as H involves too many degrees of freedom.

Transforming to the interaction picture

$$\boldsymbol{\rho}(t) = e^{+i(\mathcal{H}_\mathrm{S}+\mathcal{H}_\mathrm{B})t}\rho(t)e^{-i(\mathcal{H}_\mathrm{S}+\mathcal{H}_\mathrm{B})t}\,, \tag{2.11}$$

which will be denoted by bold symbols throughout, the von-Neumann equation transforms into

$$\dot{\boldsymbol{\rho}} = -i\left[\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t), \boldsymbol{\rho}\right] , \tag{2.12}$$

where the in general time-dependent interaction Hamiltonian

$$\begin{aligned} \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t) &= e^{+i(\mathcal{H}_{\mathrm{S}}+\mathcal{H}_{\mathrm{B}})t}\mathcal{H}_{\mathrm{I}}e^{-i(\mathcal{H}_{\mathrm{S}}+\mathcal{H}_{\mathrm{B}})t} = \sum_{\alpha} e^{+i\mathcal{H}_{\mathrm{S}}t}A_{\alpha}e^{-i\mathcal{H}_{\mathrm{S}}t}\otimes e^{+i\mathcal{H}_{\mathrm{B}}t}B_{\alpha}e^{-i\mathcal{H}_{\mathrm{B}}t} \\ &= \sum_{\alpha} \boldsymbol{A}_{\boldsymbol{\alpha}}(t)\otimes \boldsymbol{B}_{\boldsymbol{\alpha}}(t) \end{aligned} \tag{2.13}$$

allows to perform perturbation theory.

Born-Markov-Secular Approximations

Without loss of generality we will assume here the case of hermitian coupling operators $A_\alpha = A_\alpha^\dagger$ and $B_\alpha = B_\alpha^\dagger$. One heuristic way to perform perturbation theory is to formally integrate Eq. (2.13) and to re-insert the result in the r.h.s. of Eq. (2.13). The time-derivative of the system density matrix is obtained by performing the partial trace

$$\dot{\boldsymbol{\rho}}_{\mathbf{S}} = -i\mathrm{Tr}_{\mathrm{B}}\left\{[\boldsymbol{\mathcal{H}}_{\mathbf{I}}(\boldsymbol{t}), \rho_0]\right\} - \int_0^t \mathrm{Tr}_{\mathrm{B}}\left\{[\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t), [\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t'), \boldsymbol{\rho}(t')]]\, dt'\right\} . \tag{2.14}$$

This integro-differential equation is still exact but unfortunately not closed as the r.h.s. does not depend on ρ_{S} but the full density matrix at all previous times.

To close the above equation, we employ factorization of the initial density matrix

$$\rho_0 = \rho_{\mathrm{S}}^0 \otimes \bar{\rho}_{\mathrm{B}} \tag{2.15}$$

together with perturbative considerations: Assuming that $\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t) = \mathcal{O}\{\lambda\}$ with λ beeing a small dimensionless perturbation parameter (solely used for bookkeeping purposes here) and that the environment is so large such that it is hardly affected by the presence of the system, we may formally expand the full density matrix

$$\boldsymbol{\rho}(t) = \boldsymbol{\rho}_{\mathbf{S}}(t)\otimes\bar{\rho}_{\mathrm{B}} + \mathcal{O}\{\lambda\} , \tag{2.16}$$

where the neglect of all higher orders is known as **Born approximation**. Eq. (2.14) demonstrates that the Born approximation is equivalent to a perturbation theory in the interaction Hamiltonian

$$\dot{\boldsymbol{\rho}}_{\mathbf{S}} = -i\mathrm{Tr}_{\mathrm{B}}\left\{[\boldsymbol{\mathcal{H}}_{\mathbf{I}}(\boldsymbol{t}), \rho_0]\right\} - \int_0^t \mathrm{Tr}_{\mathrm{B}}\left\{[\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t), [\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t'), \boldsymbol{\rho}_{\mathbf{S}}(t')\otimes\bar{\rho}_{\mathrm{B}}]]\, dt'\right\} + \mathcal{O}\{\lambda^3\} . \tag{2.17}$$

Using the decomposition of the interaction Hamiltonian (2.9), this obviously yields a closed equation for the system density matrix

$$\begin{aligned} \dot{\boldsymbol{\rho}}_{\mathbf{S}} &= -i\sum_{\alpha}\left[\boldsymbol{A}_{\boldsymbol{\alpha}}(t)\rho_{\mathrm{S}}^0\mathrm{Tr}\left\{\boldsymbol{B}_{\boldsymbol{\alpha}}(t)\bar{\rho}_{\mathrm{B}}\right\} - \rho_{\mathrm{S}}^0\boldsymbol{A}_{\boldsymbol{\alpha}}(t)\mathrm{Tr}\left\{\bar{\rho}_{\mathrm{B}}\boldsymbol{B}_{\boldsymbol{\alpha}}(t)\right\}\right] - \sum_{\alpha\beta}\int_0^t\Big[\\ &+\boldsymbol{A}_{\boldsymbol{\alpha}}(t)\boldsymbol{A}_{\boldsymbol{\beta}}(t')\boldsymbol{\rho}_{\mathbf{S}}(t')\mathrm{Tr}\left\{\boldsymbol{B}_{\boldsymbol{\alpha}}(t)\boldsymbol{B}_{\boldsymbol{\beta}}(t')\bar{\rho}_{\mathrm{B}}\right\} \\ &-\boldsymbol{A}_{\boldsymbol{\alpha}}(t)\boldsymbol{\rho}_{\mathbf{S}}(t')\boldsymbol{A}_{\boldsymbol{\beta}}(t')\mathrm{Tr}\left\{\boldsymbol{B}_{\boldsymbol{\alpha}}(t)\bar{\rho}_{\mathrm{B}}\boldsymbol{B}_{\boldsymbol{\beta}}(t')\right\} \\ &-\boldsymbol{A}_{\boldsymbol{\beta}}(t')\boldsymbol{\rho}_{\mathbf{S}}(t')\boldsymbol{A}_{\boldsymbol{\alpha}}(t)\mathrm{Tr}\left\{\boldsymbol{B}_{\boldsymbol{\beta}}(t')\bar{\rho}_{\mathrm{B}}\boldsymbol{B}_{\boldsymbol{\alpha}}(t)\right\} \\ &+\boldsymbol{\rho}_{\mathbf{S}}(t')\boldsymbol{A}_{\boldsymbol{\beta}}(t')\boldsymbol{A}_{\boldsymbol{\alpha}}(t)\mathrm{Tr}\left\{\bar{\rho}_{\mathrm{B}}\boldsymbol{B}_{\boldsymbol{\beta}}(t')\boldsymbol{B}_{\boldsymbol{\alpha}}(t)\right\}\Big]\, dt' . \end{aligned} \tag{2.18}$$

Without loss of generality, we proceed by assuming that the single coupling operator expectation value vanishes

$$\mathrm{Tr}\left\{\boldsymbol{B_\alpha}(t)\bar{\rho}_\mathrm{B}\right\} = 0\,. \tag{2.19}$$

This situation can always be constructed by simultaneously modifying system Hamiltonian $\mathcal{H}_\mathrm{S}$ and coupling operators A_α, see exercise 14.

Exercise 14 (Vanishing single-operator expectation values) *(1 points)*
Show that by modifying system and interaction Hamiltonian

$$\mathcal{H}_\mathrm{S} \to \mathcal{H}_\mathrm{S} + \sum_\alpha g_\alpha A_\alpha\,, \qquad B_\alpha \to B_\alpha - g_\alpha \mathbf{1} \tag{2.20}$$

one can construct a situation where $\mathrm{Tr}\left\{\boldsymbol{B_\alpha}(t)\bar{\rho}_\mathrm{B}\right\} = 0$. *Determine* g_α.

Using the cyclic property of the trace, we obtain

$$\begin{aligned}\dot{\boldsymbol{\rho}}_\mathbf{S} \;=\; -\sum_{\alpha\beta}\int_0^t dt' \Big[& C_{\alpha\beta}(t,t')\left[\boldsymbol{A_\alpha}(t), \boldsymbol{A_\beta}(t')\boldsymbol{\rho_\mathrm{S}}(t')\right] \\ & + C_{\beta\alpha}(t',t)\left[\boldsymbol{\rho_\mathrm{S}}(t')\boldsymbol{A_\beta}(t'), \boldsymbol{A_\alpha}(t)\right]\Big]\end{aligned} \tag{2.21}$$

with the bath correlation function

$$C_{\alpha\beta}(t_1,t_2) = \mathrm{Tr}\left\{\boldsymbol{B_\alpha}(t_1)\boldsymbol{B_\beta}(t_2)\bar{\rho}_\mathrm{B}\right\}\,. \tag{2.22}$$

The integro-differential equation (2.21) is a **non-Markovian master equation**, as the r.h.s. depends on the value of the dynamical variable (the density matrix) at all previous times – weighted by the bath correlation functions. It does preserve trace and hermiticity of the system density matrix, but not necessarily its positivity. Such integro-differential equations can only be solved in very specific cases. Therefore, we motivate further approximations, for which we need to discuss the analytic properties of the bath correlation functions.

It is quite straightforward to see that when the bath Hamiltonian commutes with the bath density matrix $[\mathcal{H}_\mathrm{B}, \bar{\rho}_\mathrm{B}] = 0$, the bath correlation functions actually only depend on the difference of their time arguments $C_{\alpha\beta}(t_1,t_2) = C_{\alpha\beta}(t_1 - t_2)$ with

$$C_{\alpha\beta}(t_1 - t_2) = \mathrm{Tr}\left\{e^{+i\mathcal{H}_\mathrm{B}(t_1-t_2)}B_\alpha e^{-i\mathcal{H}_\mathrm{B}(t_1-t_2)}B_\beta\bar{\rho}_\mathrm{B}\right\}\,. \tag{2.23}$$

Since we chose our coupling operators hermitian, we have the additional symmetry that $C_{\alpha\beta}(\tau) = C^*_{\beta\alpha}(-\tau)$. One can now evaluate several system-bath models and when the bath has a dense spectrum, the bath correlation functions are typically found to be strongly peaked around zero, see exercise 15.

Exercise 15 (Bath Correlation Function) *(1 points)*
Evaluate the Fourier transform $\gamma_{\alpha\beta}(\omega) = \int C_{\alpha\beta}(\tau)e^{+\mathrm{i}\omega\tau}d\tau$ *of the bath correlation functions for the coupling operators* $B_1 = \sum_k h_k b_k$ *and* $B_2 = \sum_k h_k^* b_k^\dagger$ *for a bosonic bath* $\mathcal{H}_\mathrm{B} = \sum_k \omega_k b_k^\dagger b_k$ *in the thermal equilibrium state* $\bar{\rho}_\mathrm{B}^0 = \frac{e^{-\beta\mathcal{H}_\mathrm{B}}}{\mathrm{Tr}\{e^{-\beta\mathcal{H}_\mathrm{B}}\}}$. *You may use the continous representation* $\Gamma(\omega) = 2\pi\sum_k |h_k|^2\delta(\omega-\omega_k)$ *for the tunneling rates.*

This implies that the integro-differential equation (2.21) can also be written as $\dot{\rho}_\mathrm{S} = \int_0^t \mathcal{W}(t-t')\rho_\mathrm{S}(t')dt'$, where the kernel $\mathcal{W}(\tau)$ assigns a much smaller weight to density matrices far in the past than to the density matrix just an instant ago. In the most extreme case, we would approximate $C_{\alpha\beta}(t_1,t_2) \approx \Gamma_{\alpha\beta}\delta(t_1-t_2)$, but we will be cautious here and assume that only the density matrix varies slower than the decay time of the bath correlation functions. Therefore, we replace in the r.h.s. $\boldsymbol{\rho}_\mathbf{S}(t') \to \boldsymbol{\rho}_\mathbf{S}(t)$ (**first Markov approximation**), which yields in Eq. (2.17)

$$\dot{\boldsymbol{\rho}}_\mathbf{S} = -\int_0^t \mathrm{Tr}_\mathrm{B}\left\{[\boldsymbol{\mathcal{H}}_\mathbf{I}(t),[\boldsymbol{\mathcal{H}}_\mathbf{I}(t'),\boldsymbol{\rho}_\mathbf{S}(t)\otimes\bar{\rho}_\mathrm{B}]]\right\}dt' \tag{2.24}$$

This equation is often called **Born-Redfield** equation. It is time-local and preserves trace and hermiticity, but still has time-dependent coefficients (also when transforming back from the interaction picture). We substitute $\tau = t - t'$

$$\begin{aligned}\dot{\boldsymbol{\rho}}_\mathbf{S} &= -\int_0^t \mathrm{Tr}_\mathrm{B}\left\{[\boldsymbol{\mathcal{H}}_\mathbf{I}(t),[\boldsymbol{\mathcal{H}}_\mathbf{I}(t-\tau),\boldsymbol{\rho}_\mathbf{S}(t)\otimes\bar{\rho}_\mathrm{B}]]\right\}d\tau \qquad (2.25)\\ &= -\sum_{\alpha\beta}\int_0^t \left\{C_{\alpha\beta}(\tau)\left[\boldsymbol{A}_{\boldsymbol{\alpha}}(t),\boldsymbol{A}_{\boldsymbol{\beta}}(t-\tau)\boldsymbol{\rho}_\mathbf{S}(t)\right] + C_{\beta\alpha}(-\tau)\left[\boldsymbol{\rho}_\mathbf{S}(t)\boldsymbol{A}_{\boldsymbol{\beta}}(t-\tau),\boldsymbol{A}_{\boldsymbol{\alpha}}(t)\right]\right\}d\tau\end{aligned}$$

The problem that the r.h.s. still depends on time is removed by extending the integration bounds to infinity (**second Markov approximation**) – by the same reasoning that the bath correlation functions decay rapidly

$$\dot{\boldsymbol{\rho}}_\mathbf{S} = -\int_0^\infty \mathrm{Tr}_\mathrm{B}\left\{[\boldsymbol{\mathcal{H}}_\mathbf{I}(t),[\boldsymbol{\mathcal{H}}_\mathbf{I}(t-\tau),\boldsymbol{\rho}_\mathbf{S}(t)\otimes\bar{\rho}_\mathrm{B}]]\right\}d\tau\,. \tag{2.26}$$

This equation is called the **Markovian master equation**, which in the original Schrödinger picture

$$\begin{aligned}\dot{\rho}_\mathrm{S} &= -i\left[\mathcal{H}_\mathrm{S},\rho_\mathrm{S}(t)\right] - \sum_{\alpha\beta}\int_0^\infty C_{\alpha\beta}(\tau)\left[A_\alpha, e^{-\mathrm{i}\mathcal{H}_\mathrm{S}\tau}A_\beta e^{+\mathrm{i}\mathcal{H}_\mathrm{S}\tau}\rho_\mathrm{S}(t)\right]d\tau\\ &\quad -\sum_{\alpha\beta}\int_0^\infty C_{\beta\alpha}(-\tau)\left[\rho_\mathrm{S}(t)e^{-\mathrm{i}\mathcal{H}_\mathrm{S}\tau}A_\beta e^{+\mathrm{i}\mathcal{H}_\mathrm{S}\tau}, A_\alpha\right]d\tau \qquad (2.27)\end{aligned}$$

is time-local, preserves trace and hermiticity, and has constant coefficients – best prerequisites for treatment with established solution methods.

Exercise 16 (Properties of the Markovian Master Equation) *(1 points)*
Show that the Markovian Master equation (2.27) preserves trace and hermiticity of the density matrix.

In addition, it can be obtained easily from the coupling Hamiltonian, since we have not even used that the coupling operators should be hermitian.

There is just one problem left: In the general case, it is not of Lindblad form. Note that there are specific cases where the Markovian master equation is of Lindblad form, but these rather include simple limits. Though this is sometimes considered a rather cosmetic drawback, it may lead to unphysical results such as negative probabilities.

To obtain a Lindblad type master equation, a further approximation is required. The **secular approximation** involves an averaging over fast oscillating terms, but in order to identify the oscillating terms, it is necessary to at least formally calculate the interaction picture dynamics of the system coupling operators. We begin by writing Eq. (2.27) in the interaction picture again explicitly – now using the hermiticity of the coupling operators

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= -\int_0^\infty \sum_{\alpha\beta} \left\{ C_{\alpha\beta}(\tau) \left[\boldsymbol{A}_{\boldsymbol{\alpha}}(t), \boldsymbol{A}_{\boldsymbol{\beta}}(t-\tau)\boldsymbol{\rho}_{\mathbf{S}}(t) \right] + \text{h.c.} \right\} d\tau \\
&= +\int_0^\infty \sum_{\alpha\beta} C_{\alpha\beta}(\tau) \sum_{a,b,c,d} \Big\{ |a\rangle \langle a| \boldsymbol{A}_{\boldsymbol{\beta}}(t-\tau) |b\rangle \langle b| \boldsymbol{\rho}_{\mathbf{S}}(t) |d\rangle \langle d| \boldsymbol{A}_{\boldsymbol{\alpha}}(t) |c\rangle \langle c| \\
&\quad - |d\rangle \langle d| \boldsymbol{A}_{\boldsymbol{\alpha}}(t) |c\rangle \langle c| |a\rangle \langle a| \boldsymbol{A}_{\boldsymbol{\beta}}(t-\tau) |b\rangle \langle b| \boldsymbol{\rho}_{\mathbf{S}}(t) \Big\} d\tau + \text{h.c.}\,, \qquad (2.28)
\end{aligned}$$

where we have introduced the system energy eigenbasis

$$\mathcal{H}_{\mathrm{S}} |a\rangle = E_a |a\rangle \ . \qquad (2.29)$$

We can use this eigenbasis to make the time-dependence of the coupling operators in the interaction picture explicit

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= +\int_0^\infty \sum_{\alpha\beta} C_{\alpha\beta}(\tau) \sum_{a,b,c,d} \Big\{ e^{+\mathrm{i}(E_a-E_b)(t-\tau)} e^{+\mathrm{i}(E_d-E_c)t} \langle a| A_\beta |b\rangle \langle d| A_\alpha |c\rangle |a\rangle \langle b| \boldsymbol{\rho}_{\mathbf{S}}(t) |d\rangle \langle c| \\
&\quad - e^{+\mathrm{i}(E_a-E_b)(t-\tau)} e^{+\mathrm{i}(E_d-E_c)t} \langle a| A_\beta |b\rangle \langle d| A_\alpha |c\rangle |d\rangle \langle c| |a\rangle \langle b| \boldsymbol{\rho}_{\mathbf{S}}(t) \Big\} d\tau + \text{h.c.}\,, \\
&= \sum_{\alpha\beta} \sum_{a,b,c,d} \int_0^\infty C_{\alpha\beta}(\tau) e^{+\mathrm{i}(E_b-E_a)\tau} d\tau e^{-\mathrm{i}(E_b-E_a-(E_d-E_c))t} \langle a| A_\beta |b\rangle \langle c| A_\alpha |d\rangle^* \Big\{ \\
&\quad + |a\rangle \langle b| \boldsymbol{\rho}_{\mathbf{S}}(t) (|c\rangle \langle d|)^\dagger - (|c\rangle \langle d|)^\dagger |a\rangle \langle b| \boldsymbol{\rho}_{\mathbf{S}}(t) \Big\} + \text{h.c.} \qquad (2.30)
\end{aligned}$$

The **secular approximation** now involves neglecting all terms that are oscillatory in time t

(long-time average), i.e., we have

$$\begin{aligned}\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= \sum_{\alpha\beta}\sum_{a,b,c,d}\Gamma_{\alpha\beta}(E_b-E_a)\delta_{E_b-E_a,E_d-E_c}\langle a|A_\beta|b\rangle\langle c|A_\alpha|d\rangle^*\times\\ &\times\Big\{+|a\rangle\langle b|\boldsymbol{\rho}_{\mathbf{S}}(t)(|c\rangle\langle d|)^\dagger-(|c\rangle\langle d|)^\dagger|a\rangle\langle b|\boldsymbol{\rho}_{\mathbf{S}}(t)\Big\}\\ &+\sum_{\alpha\beta}\sum_{a,b,c,d}\Gamma^*_{\alpha\beta}(E_b-E_a)\delta_{E_b-E_a,E_d-E_c}\langle a|A_\beta|b\rangle^*\langle c|A_\alpha|d\rangle\times\\ &\times\Big\{+|c\rangle\langle d|\boldsymbol{\rho}_{\mathbf{S}}(t)(|a\rangle\langle b|)^\dagger-\boldsymbol{\rho}_{\mathbf{S}}(t)(|a\rangle\langle b|)^\dagger|c\rangle\langle d|\Big\}\,, \end{aligned}\tag{2.31}$$

where we have introduced the half-sided Fourier transform of the bath correlation functions

$$\Gamma_{\alpha\beta}(\omega)=\int_0^\infty C_{\alpha\beta}(\tau)e^{+i\omega\tau}d\tau\,.\tag{2.32}$$

This equation preserves trace, hermiticity, and positivity of the density matrix and hence all desired properties, since it is of Lindblad form (which will be shown later). Unfortunately, it is typically not so easy to obtain as it requires diagonalization of the system Hamiltonian first. By using the transformations $\alpha\leftrightarrow\beta$, $a\leftrightarrow c$, and $b\leftrightarrow d$ in the second line and also using that the δ-function is symmetric, we may rewrite the master equation as

$$\begin{aligned}\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= \sum_{\alpha\beta}\sum_{a,b,c,d}\left[\Gamma_{\alpha\beta}(E_b-E_a)+\Gamma^*_{\beta\alpha}(E_b-E_a)\right]\delta_{E_b-E_a,E_d-E_c}\times\\ &\times\langle a|A_\beta|b\rangle\langle c|A_\alpha|d\rangle^*|a\rangle\langle b|\boldsymbol{\rho}_{\mathbf{S}}(t)(|c\rangle\langle d|)^\dagger\\ &-\sum_{\alpha\beta}\sum_{a,b,c,d}\Gamma_{\alpha\beta}(E_b-E_a)\delta_{E_b-E_a,E_d-E_c}\times\\ &\times\langle a|A_\beta|b\rangle\langle c|A_\alpha|d\rangle^*(|c\rangle\langle d|)^\dagger|a\rangle\langle b|\boldsymbol{\rho}_{\mathbf{S}}(t)\\ &-\sum_{\alpha\beta}\sum_{a,b,c,d}\Gamma^*_{\beta\alpha}(E_b-E_a)\delta_{E_b-E_a,E_d-E_c}\times\\ &\times\langle a|A_\beta|b\rangle\langle c|A_\alpha|d\rangle^*\boldsymbol{\rho}_{\mathbf{S}}(t)(|c\rangle\langle d|)^\dagger|a\rangle\langle b|\,. \end{aligned}\tag{2.33}$$

We split the matrix-valued function $\Gamma_{\alpha\beta}(\omega)$ into hermitian and anti-hermitian parts

$$\begin{aligned}\Gamma_{\alpha\beta}(\omega) &= \frac{1}{2}\gamma_{\alpha\beta}(\omega)+\frac{1}{2}\sigma_{\alpha\beta}(\omega)\,,\\ \Gamma^*_{\beta\alpha}(\omega) &= \frac{1}{2}\gamma_{\alpha\beta}(\omega)-\frac{1}{2}\sigma_{\alpha\beta}(\omega)\,,\end{aligned}\tag{2.34}$$

with hermitian $\gamma_{\alpha\beta}(\omega)=\gamma^*_{\beta\alpha}(\omega)$ and anti-hermitian $\sigma_{\alpha\beta}(\omega)=-\sigma^*_{\beta\alpha}(\omega)$. These new functions can be interpreted as full even and odd Fourier transforms of the bath correlation functions

$$\begin{aligned}\gamma_{\alpha\beta}(\omega) &= \Gamma_{\alpha\beta}(\omega)+\Gamma^*_{\beta\alpha}(\omega)=\int_{-\infty}^{+\infty}C_{\alpha\beta}(\tau)e^{+\mathrm{i}\omega\tau}d\tau\,,\\ \sigma_{\alpha\beta}(\omega) &= \Gamma_{\alpha\beta}(\omega)-\Gamma^*_{\beta\alpha}(\omega)=\int_{-\infty}^{+\infty}C_{\alpha\beta}(\tau)\mathrm{sgn}(\tau)\mathrm{e}^{+\mathrm{i}\omega\tau}\mathrm{d}\tau\,.\end{aligned}\tag{2.35}$$

Exercise 17 (Odd Fourier Transform) *(1 points)*
Show that the odd Fourier transform $\sigma_{\alpha\beta}(\omega)$ may be obtained from the even Fourier transform $\gamma_{\alpha\beta}(\omega)$ by a Cauchy principal value integral

$$\sigma_{\alpha\beta}(\omega) = \frac{\mathrm{i}}{\pi}\mathcal{P}\int_{-\infty}^{+\infty}\frac{\gamma_{\alpha\beta}(\Omega)}{\omega-\Omega}d\Omega\,.$$

In the master equation, these replacements lead to

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= \sum_{\alpha\beta}\sum_{a,b,c,d}\gamma_{\alpha\beta}(E_b-E_a)\delta_{E_b-E_a,E_d-E_c}\langle a|A_\beta|b\rangle\langle c|A_\alpha|d\rangle^* \times \\
&\quad\times\left[|a\rangle\langle b|\boldsymbol{\rho}_{\mathbf{S}}(t)(|c\rangle\langle d|)^\dagger - \frac{1}{2}\left\{(|c\rangle\langle d|)^\dagger|a\rangle\langle b|,\boldsymbol{\rho}_{\mathbf{S}}(t)\right\}\right] \\
&\quad -i\sum_{\alpha\beta}\sum_{a,b,c,d}\frac{1}{2\mathrm{i}}\sigma_{\alpha\beta}(E_b-E_a)\delta_{E_b-E_a,E_d-E_c}\langle a|A_\beta|b\rangle\langle c|A_\alpha|d\rangle^* \times \\
&\quad\times\left[(|c\rangle\langle d|)^\dagger|a\rangle\langle b|,\boldsymbol{\rho}_{\mathbf{S}}(t)\right] \\
&= \sum_{\alpha\beta}\sum_{a,b,c,d}\gamma_{\alpha\beta}(E_b-E_a)\delta_{E_b-E_a,E_d-E_c}\langle a|A_\beta|b\rangle\langle c|A_\alpha|d\rangle^* \times \\
&\quad\times\left[|a\rangle\langle b|\boldsymbol{\rho}_{\mathbf{S}}(t)(|c\rangle\langle d|)^\dagger - \frac{1}{2}\left\{(|c\rangle\langle d|)^\dagger|a\rangle\langle b|,\boldsymbol{\rho}_{\mathbf{S}}(t)\right\}\right] \\
&\quad -i\left[\sum_{\alpha\beta}\sum_{a,b,c}\frac{1}{2\mathrm{i}}\sigma_{\alpha\beta}(E_b-E_c)\delta_{E_b,E_a}\langle c|A_\beta|b\rangle\langle c|A_\alpha|a\rangle^*|a\rangle\langle b|,\boldsymbol{\rho}_{\mathbf{S}}(t)\right]\,.
\end{aligned} \tag{2.36}$$

To prove that we have a Lindblad form, it is easy to see first that the term in the commutator

$$H_{\mathrm{LS}} = \sum_{\alpha\beta}\sum_{a,b,c}\frac{1}{2\mathrm{i}}\sigma_{\alpha\beta}(E_b-E_c)\delta_{E_b,E_a}\langle c|A_\beta|b\rangle\langle c|A_\alpha|a\rangle^*|a\rangle\langle b| \tag{2.37}$$

is an effective Hamiltonian. This Hamiltonian is often called Lamb-shift Hamiltonian, since it renormalizes the system Hamiltonian due to the interaction with the reservoir. Note that we have $[\mathcal{H}_{\mathrm{S}}, H_{\mathrm{LS}}] = 0$.

Exercise 18 (Lamb-shift) *(1 points)*
Show that $H_{\mathrm{LS}} = H_{\mathrm{LS}}^\dagger$ and $[H_{\mathrm{LS}}, \mathcal{H}_{\mathrm{S}}] = 0$.

To show the Lindblad-form of the non-unitary evolution, we identify the Lindblad jump operator $L_\alpha = |a\rangle\langle b| = L_{(a,b)}$. For an N-dimensional system Hilbert space with N eigenvectors of $\mathcal{H}_{\mathrm{S}}$ we would have N^2 such jump operators, but in a rotated basis, we may leave out the identity matrix $\mathbf{1} = \sum_a |a\rangle\langle a|$ (which has trivial action). It remains to be shown that the matrix

$$\gamma_{(ab),(cd)} = \sum_{\alpha\beta}\gamma_{\alpha\beta}(E_b-E_a)\delta_{E_b-E_a,E_d-E_c}\langle a|A_\beta|b\rangle\langle c|A_\alpha|d\rangle^* \tag{2.38}$$

is non-negative, i.e., $\sum_{a,b,c,d} x^*_{ab}\gamma_{(ab),(cd)}x_{cd} \geq 0$ for all x_{ab}. We first note that for hermitian coupling operators the Fourier transform matrix at fixed ω is positive (recall that $B_\alpha = B^\dagger_\alpha$ and $[\bar{\rho}_{\rm B}, \mathcal{H}_{\rm B}] = 0$)

$$\begin{aligned}
\Gamma &= \sum_{\alpha\beta} x^*_\alpha \gamma_{\alpha\beta}(\omega) x_\beta \\
&= \int_{-\infty}^{+\infty} d\tau e^{+{\rm i}\omega\tau} {\rm Tr}\left\{ e^{{\rm i}\mathcal{H}_{\rm S}\tau}\left[\sum_\alpha x^*_\alpha B_\alpha\right] e^{-{\rm i}\mathcal{H}_{\rm S}\tau}\left[\sum_\beta x_\beta B_\beta\right]\bar{\rho}_{\rm B}\right\} \\
&= \int_{-\infty}^{+\infty} d\tau e^{+{\rm i}\omega\tau} \sum_{nm} e^{+{\rm i}(E_n - E_m)\tau} \langle n| B^\dagger |m\rangle \langle m| B\bar{\rho}_{\rm B} |n\rangle \\
&= \sum_{nm} 2\pi\delta(\omega + E_n - E_m) |\langle m| B |n\rangle|^2 \rho_n \\
&\geq 0\,. \qquad (2.39)
\end{aligned}$$

Now, we replace the Kronecker symbol in the dampening coefficients by two via the introduction of an auxiliary summation

$$\begin{aligned}
\tilde{\Gamma} &= \sum_{abcd} x^*_{ab}\gamma_{(ab),(cd)}x_{cd} \\
&= \sum_\omega \sum_{\alpha\beta} \sum_{abcd} \gamma_{\alpha\beta}(\omega)\delta_{E_b-E_a,\omega}\delta_{E_d-E_c,\omega} x^*_{ab} \langle a| A_\beta |b\rangle x_{cd} \langle c| A_\alpha |d\rangle^* \\
&= \sum_\omega \sum_{\alpha\beta} \left[\sum_{cd} x_{cd} \langle c| A_\alpha |d\rangle^* \delta_{E_d-E_c,\omega}\right] \gamma_{\alpha\beta}(\omega) \left[\sum_{ab} x^*_{ab} \langle a| A_\beta |b\rangle \delta_{E_b-E_a,\omega}\right] \\
&= \sum_\omega \sum_{\alpha\beta} y^*_\alpha(\omega)\gamma_{\alpha\beta}(\omega) y_\beta(\omega) \geq 0\,. \qquad (2.40)
\end{aligned}$$

Transforming Eq. (2.36) back to the Schrödinger picture (note that the δ-functions prohibit the occurrence of oscillatory factors), we finally obtain the Born-Markov-secular master equation.

Box 7 (BMS master equation) *In the weak coupling limit, an interaction Hamiltonian of the form $\mathcal{H}_{\rm I} = \sum_\alpha A_\alpha \otimes B_\alpha$ with hermitian coupling operators ($A_\alpha = A^\dagger_\alpha$ and $B_\alpha = B^\dagger_\alpha$) and $[\mathcal{H}_{\rm B}, \bar{\rho}_{\rm B}] = 0$ and ${\rm Tr}\{B_\alpha\bar{\rho}_{\rm B}\} = 0$ leads in the system energy eigenbasis $\mathcal{H}_{\rm S}|a\rangle = E_a|a\rangle$ to the Lindblad-form master equation*

$$\begin{aligned}
\dot{\rho}_{\rm S} &= -i\left[\mathcal{H}_{\rm S} + \sum_{ab}\sigma_{ab}|a\rangle\langle b|, \rho_{\rm S}(t)\right] \\
&\quad + \sum_{a,b,c,d}\gamma_{ab,cd}\left[|a\rangle\langle b|\boldsymbol{\rho}_{\rm S}(t)(|c\rangle\langle d|)^\dagger - \frac{1}{2}\left\{(|c\rangle\langle d|)^\dagger|a\rangle\langle b|, \boldsymbol{\rho}_{\rm S}(t)\right\}\right], \\
\gamma_{ab,cd} &= \sum_{\alpha\beta}\gamma_{\alpha\beta}(E_b - E_a)\delta_{E_b-E_a,E_d-E_c}\langle a| A_\beta |b\rangle\langle c| A_\alpha |d\rangle^*\,, \qquad (2.41)
\end{aligned}$$

where the Lamb-shift Hamiltonian $H_{\rm LS} = \sum_{ab}\sigma_{ab}|a\rangle\langle b|$ matrix elements read

$$\sigma_{ab} = \sum_{\alpha\beta}\sum_c \frac{1}{2{\rm i}}\sigma_{\alpha\beta}(E_b - E_c)\delta_{E_b,E_a}\langle c| A_\beta |b\rangle\langle c| A_\alpha |a\rangle^* \qquad (2.42)$$

and the constants are given by even and odd Fourier transforms

$$\begin{aligned}\gamma_{\alpha\beta}(\omega) &= \int_{-\infty}^{+\infty} C_{\alpha\beta}(\tau) e^{+\mathrm{i}\omega\tau} d\tau \,, \\ \sigma_{\alpha\beta}(\omega) &= \int_{-\infty}^{+\infty} C_{\alpha\beta}(\tau)\mathrm{sgn}(\tau)\mathrm{e}^{+\mathrm{i}\omega\tau}\mathrm{d}\tau = \frac{\mathrm{i}}{\pi}\mathcal{P}\int_{-\infty}^{+\infty}\frac{\gamma_{\alpha\beta}(\omega')}{\omega-\omega'}\mathrm{d}\omega'\end{aligned} \tag{2.43}$$

of the bath correlation functions

$$C_{\alpha\beta}(\tau) = \mathrm{Tr}\left\{e^{+\mathrm{i}\mathcal{H}_\mathrm{B}\tau} B_\alpha e^{-\mathrm{i}\mathcal{H}_\mathrm{B}\tau} B_\beta \bar{\rho}_\mathrm{B}\right\} . \tag{2.44}$$

The above definition may serve as a recipe to derive a Lindblad type master equation in the weak-coupling limit. It is expected to yield good results in the weak coupling and Markovian limit (continuous and nearly flat bath spectral density) and when $[\bar{\rho}_\mathrm{B}, \mathcal{H}_\mathrm{B}] = 0$. It requires to rewrite the coupling operators in hermitian form, the calculation of the bath correlation function Fourier transforms, and the diagonalization of the system Hamiltonian.

In the case that the spectrum of the system Hamiltonian is non-degenerate, we have a further simplification, since the δ-functions simplify further, e.g. $\delta_{E_b,E_a} \to \delta_{ab}$. By taking matrix elements of Eq. (2.41) in the energy eigenbasis $\rho_{aa} = \langle a| \rho_\mathrm{S} |a\rangle$, we obtain an effective rate equation for the populations only

$$\dot{\rho}_{aa} = +\sum_b \gamma_{ab,ab}\rho_{bb} - \left[\sum_b \gamma_{ba,ba}\right]\rho_{aa} \,, \tag{2.45}$$

i.e., the coherences decouple from the evolution of the populations. The transition rates from state b to state a reduce in this case to

$$\gamma_{ab,ab} = \sum_{\alpha\beta} \gamma_{\alpha\beta}(E_b - E_a) \langle a| A_\beta |b\rangle \langle a| A_\alpha |b\rangle^* \,, \tag{2.46}$$

which – after inserting all definitions condenses basically to Fermis Golden Rule. A description of open quantum systems is in this limit possible with the same complexity as for closed quantum systems, since only N dynamical variables have to be evolved. Also, this may serve to demonstrate the correspondence between quantum and classical mechanics: If only diagonals of the density matrix remain in the (orthogonal) energy system eigenbasis, this implies that the quantum master equation boils down to a classical rate equation. Even more, if coupled to a single thermal bath, the quantum system simply relaxes to the Gibbs equilibrium, i.e., we obtain simply equilibration of the system temperature with the temperature of the bath.

Coarse-Graining

Although the BMS approximation respects of course the exact initial condition, we have in the derivation made several long-term approximations. For example, the Markov approximation implied that we consider timescales much larger than the decay time of the bath correlation functions. Similarly, the secular approximation implied timescales larger than the inverse minimal splitting

of the system energy eigenvalues. Therefore, we can only expect the solution originating from the BMS master equation to be an asympotically valid long-term approximation.

Coarse-graining in contrast provides a possibility to obtain valid short-time approximations of the density matrix with a generator that is of Lindblad form, see Fig. 2.4. We start with the

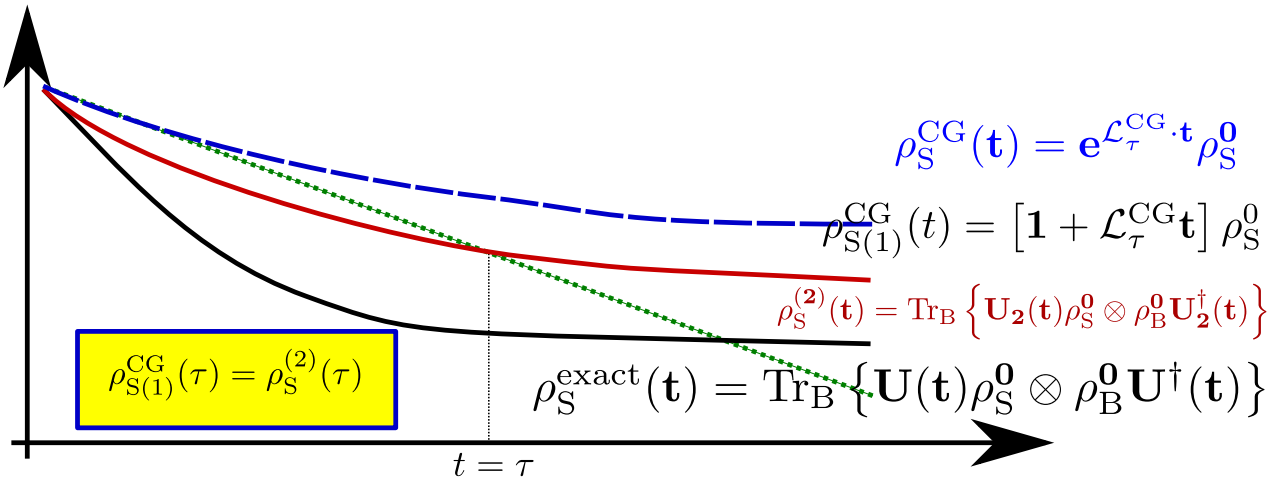

Figure 2.4: Sketch of the coarse-graining perturbation theory. Calculating the exact time evolution operator $\boldsymbol{U}(t) = \tau \exp\left\{-\mathrm{i}\int_0^t \mathcal{H}_{\mathrm{I}}(t')dt'\right\}$ in a closed form is usually prohibitive, which renders the calculation of the exact solution an impossible task (black curve). It is however possible to expand the evolution operator $\mathbf{U_2}(t) = \mathbf{1} - i\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t')dt' - \int_0^t dt_1 dt_2 \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_2)\Theta(t_1 - t_2)$ to second order in $\boldsymbol{\mathcal{H}}_{\mathbf{I}}$ and to obtain the corresponding reduced approximate density matrix. Calculating the matrix exponential of a constant Lindblad-type generator $\mathcal{L}_\tau^{\mathrm{CG}}$ is also usually prohibitive, but the first order approximation may be matched with $\mathbf{U_2}(t)$ at time $t = \tau$ to obtain a defining equation for $\mathcal{L}_\tau^{\mathrm{CG}}$.

von-Neumann equation in the interaction picture (2.12). For factorizing initial density matrices, it is formally solved by $\boldsymbol{U}(t)\rho_{\mathrm{S}}^0 \otimes \bar{\rho}_{\mathrm{B}}\boldsymbol{U}^\dagger(t)$, where the time evolution operator

$$\boldsymbol{U}(t) = \hat{\tau}\exp\left\{-\mathrm{i}\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t')dt'\right\} \tag{2.47}$$

obeys the evolution equation

$$\dot{\boldsymbol{U}} = -i\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t)\boldsymbol{U}(t)\,, \tag{2.48}$$

which defines the time-ordering operator $\hat{\tau}$. Formally integrating this equation with the evident

initial condition $\boldsymbol{U}(0) = \mathbf{1}$ yields

$$\begin{aligned}
\boldsymbol{U}(t) &= \mathbf{1} - \mathrm{i}\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t')\boldsymbol{U}(t')dt' \\
&= \mathbf{1} - \mathrm{i}\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t')dt' - \int_0^t dt'\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t')\left[\int_0^{t'} dt''\boldsymbol{\mathcal{H}}_{\mathbf{I}}(\boldsymbol{t''})\boldsymbol{U}(t'')\right] \\
&\approx \mathbf{1} - \mathrm{i}\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t')dt' - \int_0^t dt_1 dt_2 \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_2)\Theta(t_1 - t_2)\,, \qquad (2.49)
\end{aligned}$$

where the occurrence of the Heaviside function is a consequence of time-ordering. For the hermitian conjugate operator we obtain

$$\boldsymbol{U}^{\dagger}(t) \approx \mathbf{1} + \mathrm{i}\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t')dt' - \int_0^t dt_1 dt_2 \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_2)\Theta(t_2 - t_1)\,. \qquad (2.50)$$

To keep the discussion at a moderate level, we assume $\mathrm{Tr}\{B_\alpha \bar{\rho}_{\mathrm{B}}\} = 0$ from the beginning. The exact solution is approximated by

$$\begin{aligned}
\boldsymbol{\rho}_{\mathbf{S}}^{(\mathbf{2})}(t) &\approx \mathrm{Tr}_{\mathrm{B}}\Big\{\left[\mathbf{1} - \mathrm{i}\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)dt_1 - \int_0^t dt_1 dt_2 \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_2)\Theta(t_1 - t_2)\right]\rho_{\mathrm{S}}^0 \otimes \bar{\rho}_{\mathrm{B}} \times \\
&\quad \times \left[\mathbf{1} + \mathrm{i}\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)dt_1 - \int_0^t dt_1 dt_2 \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_2)\Theta(t_2 - t_1)\right]\Big\} \\
&= \rho_{\mathrm{S}}^0 - \mathrm{i}\mathrm{Tr}_{\mathrm{B}}\left\{\left[\int_0^t \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)dt_1, \rho_{\mathrm{S}}^0 \otimes \bar{\rho}_{\mathrm{B}}\right]\right\} \\
&\quad + \mathrm{Tr}_{\mathrm{B}}\left\{\int_0^t dt_1 \int_0^t dt_2 \boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)\rho_{\mathrm{S}}^0 \otimes \bar{\rho}_{\mathrm{B}}\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_2)\right\} \\
&\quad - \int_0^t dt_1 dt_2 \left[\Theta(t_1 - t_2)\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_2)\rho_{\mathrm{S}}^0 \otimes \bar{\rho}_{\mathrm{B}} + \Theta(t_2 - t_1)\rho_{\mathrm{S}}^0 \otimes \bar{\rho}_{\mathrm{B}}\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_1)\boldsymbol{\mathcal{H}}_{\mathbf{I}}(t_2)\right]\,.
\end{aligned} \qquad (2.51)$$

Again, we introduce the bath correlation functions with two time arguments as in Eq. (2.22)

$$C_{\alpha\beta}(t_1, t_2) = \mathrm{Tr}\left\{\boldsymbol{B}_{\boldsymbol{\alpha}}(t_1)\boldsymbol{B}_{\boldsymbol{\beta}}(t_2)\bar{\rho}_{\mathrm{B}}\right\}\,, \qquad (2.52)$$

such that we have

$$\begin{aligned}
\boldsymbol{\rho}_{\mathbf{S}}^{(\mathbf{2})}(t) &= \rho_{\mathrm{S}}^0 + \sum_{\alpha\beta}\int_0^t dt_1 \int_0^t dt_2 C_{\alpha\beta}(t_1, t_2)\Big[\boldsymbol{A}_{\boldsymbol{\beta}}(t_2)\rho_{\mathrm{S}}^0\boldsymbol{A}_{\boldsymbol{\alpha}}(t_1) \\
&\quad - \Theta(t_1 - t_2)\boldsymbol{A}_{\boldsymbol{\alpha}}(t_1)\boldsymbol{A}_{\boldsymbol{\beta}}(t_2)\rho_{\mathrm{S}}^0 - \Theta(t_2 - t_1)\rho_{\mathrm{S}}^0\boldsymbol{A}_{\boldsymbol{\alpha}}(t_1)\boldsymbol{A}_{\boldsymbol{\beta}}(t_2)\Big]\,. \qquad (2.53)
\end{aligned}$$

At time t, this should for weak-coupling match the evolution by a Markovian generator

$$\boldsymbol{\rho_{\mathrm{S}}}^{\mathrm{CG}}(\tau) \;=\; e^{\mathcal{L}_\tau^{\mathrm{CG}}\cdot\tau}\rho_{\mathrm{S}}^0 \approx \left[\mathbf{1}+\mathcal{L}_\tau^{\mathrm{CG}}\cdot\tau\right]\rho_{\mathrm{S}}^0\,, \tag{2.54}$$

such that we can infer the action of the generator on an arbitrary density matrix

$$\begin{aligned}
\mathcal{L}_\tau^{\mathrm{CG}}\boldsymbol{\rho_{\mathrm{S}}} &= \frac{1}{\tau}\sum_{\alpha\beta}\int_0^\tau dt_1\int_0^\tau dt_2 C_{\alpha\beta}(t_1,t_2)\Big[\boldsymbol{A_\beta}(t_2)\boldsymbol{\rho_{\mathrm{S}}}\boldsymbol{A_\alpha}(t_1)\\
&\quad -\Theta(t_1-t_2)\boldsymbol{A_\alpha}(t_1)\boldsymbol{A_\beta}(t_2)\boldsymbol{\rho_{\mathrm{S}}}-\Theta(t_2-t_1)\boldsymbol{\rho_{\mathrm{S}}}\boldsymbol{A_\alpha}(t_1)\boldsymbol{A_\beta}(t_2)\Big]\\
&= -\mathrm{i}\left[\frac{1}{2\mathrm{i}\tau}\int_0^\tau dt_1\int_0^\tau dt_2\sum_{\alpha\beta}C_{\alpha\beta}(t_1,t_2)\mathrm{sgn}(\mathrm{t}_1-\mathrm{t}_2)\boldsymbol{A_\alpha}(\mathrm{t}_1)\boldsymbol{A_\beta}(\mathrm{t}_2),\boldsymbol{\rho_{\mathrm{S}}}\right]\\
&\quad +\frac{1}{\tau}\int_0^\tau dt_1\int_0^\tau dt_2\sum_{\alpha\beta}C_{\alpha\beta}(t_1,t_2)\left[\boldsymbol{A_\beta}(t_2)\boldsymbol{\rho_{\mathrm{S}}}\boldsymbol{A_\alpha}(t_1)-\frac{1}{2}\left\{\boldsymbol{A_\alpha}(t_1)\boldsymbol{A_\beta}(t_2),\boldsymbol{\rho_{\mathrm{S}}}\right\}\right]
\end{aligned} \tag{2.55}$$

where we have inserted $\Theta(x)=\frac{1}{2}\left[1+\mathrm{sgn(x)}\right]$.

Box 8 (CG Master Equation) *In the weak coupling limit, an interaction Hamiltonian of the form $\mathcal{H}_{\mathrm{I}}=\sum_\alpha A_\alpha\otimes B_\alpha$ leads to the Lindblad-form master equation in the interaction picture*

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= -\mathrm{i}\left[\frac{1}{2\mathrm{i}\tau}\int_0^\tau dt_1\int_0^\tau dt_2\sum_{\alpha\beta}C_{\alpha\beta}(t_1,t_2)\mathrm{sgn}(\mathrm{t}_1-\mathrm{t}_2)\boldsymbol{A_\alpha}(\mathrm{t}_1)\boldsymbol{A_\beta}(\mathrm{t}_2),\boldsymbol{\rho_{\mathrm{S}}}\right]\\
&\quad +\frac{1}{\tau}\int_0^\tau dt_1\int_0^\tau dt_2\sum_{\alpha\beta}C_{\alpha\beta}(t_1,t_2)\left[\boldsymbol{A_\beta}(t_2)\boldsymbol{\rho_{\mathrm{S}}}\boldsymbol{A_\alpha}(t_1)-\frac{1}{2}\left\{\boldsymbol{A_\alpha}(t_1)\boldsymbol{A_\beta}(t_2),\boldsymbol{\rho_{\mathrm{S}}}\right\}\right],
\end{aligned}$$

where the bath correlation functions are given by

$$C_{\alpha\beta}(t_t,t_2) \;=\; \mathrm{Tr}\left\{e^{+\mathrm{i}\mathcal{H}_{\mathrm{B}}t_1}B_\alpha e^{-\mathrm{i}\mathcal{H}_{\mathrm{B}}t_1}e^{+\mathrm{i}\mathcal{H}_{\mathrm{B}}t_2}B_\beta e^{-\mathrm{i}\mathcal{H}_{\mathrm{B}}t_2}\bar{\rho}_{\mathrm{B}}\right\}. \tag{2.56}$$

We have not used hermiticity of the coupling operators nor that the bath correlation functions do typically only depend on a single argument. However, if the coupling operators were chosen hermitian, it is easy to show the Lindblad form. Obtaining the master equation requires the calculation of bath correlation functions and the evolution of the coupling operators in the interaction picture.

Exercise 19 (Lindblad form) *(1 point)*
By assuming hermitian coupling operators $A_\alpha = A_\alpha^\dagger$, show that the CG master equation is of Lindblad form for all coarse-graining times τ.

Let us make once more the time-dependence of the coupling operators explicit, which is most conveniently done in the system energy eigenbasis. Now, we also assume that the bath correlation functions only depend on the difference of their time arguments $C_{\alpha\beta}(t_1,t_2)=C_{\alpha\beta}(t_1-t_2)$, such that we may use the Fourier transform definitions in Eq. (2.35) to obtain

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= -\mathrm{i}\left[\frac{1}{2\mathrm{i}\tau}\sum_{abc}\int_0^\tau dt_1\int_0^\tau dt_2\sum_{\alpha\beta}C_{\alpha\beta}(t_1-t_2)\mathrm{sgn}(\mathrm{t_1-t_2})\left|\mathrm{a}\right\rangle\left\langle\mathrm{a}\right|\boldsymbol{A_\alpha}(\mathrm{t_1})\left|\mathrm{c}\right\rangle\left\langle\mathrm{c}\right|\boldsymbol{A_\beta}(\mathrm{t_2})\left|\mathrm{b}\right\rangle\left\langle\mathrm{b}\right|,\boldsymbol{\rho}_{\mathbf{S}}\right]\\
&\quad+\frac{1}{\tau}\int_0^\tau dt_1\int_0^\tau dt_2\sum_{\alpha\beta}\sum_{abcd}C_{\alpha\beta}(t_1-t_2)\Big[\left|a\right\rangle\left\langle a\right|\boldsymbol{A_\beta}(t_2)\left|b\right\rangle\left\langle b\right|\boldsymbol{\rho}_{\mathbf{S}}\left|d\right\rangle\left\langle d\right|\boldsymbol{A_\alpha}(t_1)\left|c\right\rangle\left\langle c\right|\\
&\quad-\frac{1}{2}\left\{\left|d\right\rangle\left\langle d\right|\boldsymbol{A_\alpha}(t_1)\left|c\right\rangle\left\langle c\right|\cdot\left|a\right\rangle\left\langle a\right|\boldsymbol{A_\beta}(t_2)\left|b\right\rangle\left\langle b\right|,\boldsymbol{\rho}_{\mathbf{S}}\right\}\Big]\\
&= -\mathrm{i}\frac{1}{4\mathrm{i}\pi\tau}\int d\omega\sum_{abc}\int_0^\tau dt_1\int_0^\tau dt_2\sum_{\alpha\beta}\sigma_{\alpha\beta}(\omega)e^{-\mathrm{i}\omega(t_1-t_2)}e^{+\mathrm{i}(E_a-E_c)t_1}e^{+\mathrm{i}(E_c-E_b)t_2}\times\\
&\quad\times\left\langle c\right|A_\beta\left|b\right\rangle\left\langle c\right|A_\alpha^\dagger\left|a\right\rangle^*\left[\left|a\right\rangle\left\langle b\right|,\boldsymbol{\rho}_{\mathbf{S}}\right]\\
&\quad+\frac{1}{2\pi\tau}\int d\omega\int_0^\tau dt_1\int_0^\tau dt_2\sum_{\alpha\beta}\sum_{abcd}\gamma_{\alpha\beta}(\omega)e^{-\mathrm{i}\omega(t_1-t_2)}e^{+\mathrm{i}(E_a-E_b)t_2}e^{+\mathrm{i}(E_d-E_c)t_1}\left\langle a\right|A_\beta\left|b\right\rangle\left\langle c\right|A_\alpha^\dagger\left|d\right\rangle^*\times\\
&\quad\times\left[\left|a\right\rangle\left\langle b\right|\boldsymbol{\rho}_{\mathbf{S}}\left(\left|c\right\rangle\left\langle d\right|\right)^\dagger-\frac{1}{2}\left\{\left(\left|c\right\rangle\left\langle d\right|\right)^\dagger\left|a\right\rangle\left\langle b\right|,\boldsymbol{\rho}_{\mathbf{S}}\right\}\right].
\end{aligned}\tag{2.57}$$

We perform the temporal integrations by invoking

$$\int_0^\tau e^{\mathrm{i}\alpha_k t_k}dt_k=\tau e^{\mathrm{i}\alpha_k\tau/2}\mathrm{sinc}\left[\frac{\alpha_\mathrm{k}\tau}{2}\right]\tag{2.58}$$

with $\mathrm{sinc(x)}=\mathrm{sin(x)/x}$ to obtain

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= -\mathrm{i}\frac{\tau}{4\mathrm{i}\pi}\int d\omega\sum_{abc}\sum_{\alpha\beta}\sigma_{\alpha\beta}(\omega)e^{\mathrm{i}\tau(E_a-E_b)/2}\mathrm{sinc}\left[\frac{\tau}{2}(\mathrm{E_a-E_c}-\omega)\right]\mathrm{sinc}\left[\frac{\tau}{2}(\mathrm{E_c-E_b}+\omega)\right]\times\\
&\quad\times\left\langle c\right|A_\beta\left|b\right\rangle\left\langle c\right|A_\alpha^\dagger\left|a\right\rangle^*\left[\left|a\right\rangle\left\langle b\right|,\boldsymbol{\rho}_{\mathbf{S}}\right]\\
&\quad+\frac{\tau}{2\pi}\int d\omega\sum_{\alpha\beta}\sum_{abcd}\gamma_{\alpha\beta}(\omega)e^{\mathrm{i}\tau(E_a-E_b+E_d-E_c)/2}\mathrm{sinc}\left[\frac{\tau}{2}(\mathrm{E_d-E_c}-\omega)\right]\mathrm{sinc}\left[\frac{\tau}{2}(\omega+\mathrm{E_a-E_b})\right]\times\\
&\quad\times\left\langle a\right|A_\beta\left|b\right\rangle\left\langle c\right|A_\alpha^\dagger\left|d\right\rangle^*\left[\left|a\right\rangle\left\langle b\right|\boldsymbol{\rho}_{\mathbf{S}}\left(\left|c\right\rangle\left\langle d\right|\right)^\dagger-\frac{1}{2}\left\{\left(\left|c\right\rangle\left\langle d\right|\right)^\dagger\left|a\right\rangle\left\langle b\right|,\boldsymbol{\rho}_{\mathbf{S}}\right\}\right].
\end{aligned}\tag{2.59}$$

Therefore, we have the same structure as before, but now with coarse-graining time dependent dampening coefficients

$$\begin{aligned}
\dot{\boldsymbol{\rho}}_{\mathbf{S}} &= -\mathrm{i}\left[\sum_{ab}\sigma_{ab}^\tau\left|a\right\rangle\left\langle b\right|,\boldsymbol{\rho}_{\mathbf{S}}\right]\\
&\quad+\sum_{abcd}\gamma_{ab,cd}^\tau\left[\left|a\right\rangle\left\langle b\right|\boldsymbol{\rho}_{\mathbf{S}}\left(\left|c\right\rangle\left\langle d\right|\right)^\dagger-\frac{1}{2}\left\{\left(\left|c\right\rangle\left\langle d\right|\right)^\dagger\left|a\right\rangle\left\langle b\right|,\boldsymbol{\rho}_{\mathbf{S}}\right\}\right]
\end{aligned}\tag{2.60}$$

with the coefficients

$$\begin{aligned}\sigma^{\tau}_{ab} &= \frac{1}{2\mathrm{i}}\int d\omega \sum_{c} e^{\mathrm{i}\tau(E_a-E_b)/2}\frac{\tau}{2\pi}\mathrm{sinc}\left[\frac{\tau}{2}(\mathrm{E_a}-\mathrm{E_c}-\omega)\right]\mathrm{sinc}\left[\frac{\tau}{2}(\mathrm{E_b}-\mathrm{E_c}-\omega)\right]\times \\ &\quad\times\left[\sum_{\alpha\beta}\sigma_{\alpha\beta}(\omega)\left\langle c\right|A_\beta\left|b\right\rangle\left\langle c\right|A^\dagger_\alpha\left|a\right\rangle^*\right], \\ \gamma^{\tau}_{ab,cd} &= \int d\omega e^{\mathrm{i}\tau(E_a-E_b+E_d-E_c)/2}\frac{\tau}{2\pi}\mathrm{sinc}\left[\frac{\tau}{2}(\mathrm{E_d}-\mathrm{E_c}-\omega)\right]\mathrm{sinc}\left[\frac{\tau}{2}(\mathrm{E_b}-\mathrm{E_a}-\omega)\right]\times \\ &\quad\times\left[\sum_{\alpha\beta}\gamma_{\alpha\beta}(\omega)\left\langle a\right|A_\beta\left|b\right\rangle\left\langle c\right|A^\dagger_\alpha\left|d\right\rangle^*\right]. \end{aligned} \tag{2.61}$$

Finally, we note that in the limit of large coarse-graining times $\tau\to\infty$, these dampening coefficients converge to the ones in definition 7, i.e.,

$$\begin{aligned}\lim_{\tau\to\infty}\sigma^{\tau}_{ab} &= \sigma_{ab}\,, \\ \lim_{\tau\to\infty}\gamma^{\tau}_{ab,cd} &= \gamma_{ab,cd}\,. \end{aligned} \tag{2.62}$$

Exercise 20 (CG-BMS correspondence) *(1 points)*
Show for hermitian coupling operators that when $\tau\to\infty$, CG and BMS approximation are equivalent. You may use the identity

$$\lim_{\tau\to\infty}\tau\mathrm{sinc}\left[\frac{\tau}{2}(\Omega_\mathrm{a}-\omega)\right]\mathrm{sinc}\left[\frac{\tau}{2}(\Omega_\mathrm{b}-\omega)\right]=2\pi\delta_{\Omega_\mathrm{a},\Omega_\mathrm{b}}\delta(\Omega_\mathrm{a}-\omega)\,.$$

Thermalization

The BMS limit has beyond its relatively compact Lindblad form further appealing properties in the case of a bath that is in thermal equilibrium

$$\bar{\rho}_\mathrm{B}=\frac{e^{-\beta\mathcal{H}_\mathrm{B}}}{\mathrm{Tr}\left\{e^{-\beta\mathcal{H}_\mathrm{B}}\right\}} \tag{2.63}$$

with inverse temperature β. These root in further analytic properties of the bath correlation functions such as the Kubo-Martin-Schwinger (KMS) condition

$$C_{\alpha\beta}(\tau)=C_{\beta\alpha}(-\tau-\mathrm{i}\beta)\,. \tag{2.64}$$

Exercise 21 (KMS condition) *(1 points)*
Show the validity of the KMS condition for a thermal bath with $\bar{\rho}_\mathrm{B}=\frac{e^{-\beta\mathcal{H}_\mathrm{B}}}{\mathrm{Tr}\left\{e^{-\beta\mathcal{H}_\mathrm{B}}\right\}}$.

For the Fourier transform, this shift property implies

$$\begin{aligned}\gamma_{\alpha\beta}(-\omega) &= \int_{-\infty}^{+\infty} C_{\alpha\beta}(\tau)e^{-\mathrm{i}\omega\tau}d\tau = \int_{-\infty}^{+\infty} C_{\beta\alpha}(-\tau-\mathrm{i}\beta)e^{-\mathrm{i}\omega\tau}d\tau \\ &= \int_{+\infty-\mathrm{i}\beta}^{-\infty-\mathrm{i}\beta} C_{\beta\alpha}(\tau')e^{+\mathrm{i}\omega(\tau'+\mathrm{i}\beta)}(-)d\tau' = \int_{-\infty-\mathrm{i}\beta}^{+\infty-\mathrm{i}\beta} C_{\beta\alpha}(\tau')e^{+\mathrm{i}\omega\tau'}d\tau' e^{-\beta\omega} \\ &= \int_{-\infty}^{+\infty} C_{\beta\alpha}(\tau')e^{+\mathrm{i}\omega\tau'}d\tau' e^{-\beta\omega} = \gamma_{\beta\alpha}(+\omega)e^{-\beta\omega}\,, \end{aligned} \tag{2.65}$$

where in the last line we have used that the bath correlation functions are analytic in τ in the complex plane and vanish at infinity, such that we may safely deform the integration contour. Finally, the KMS condition can thereby be used to prove that for a reservoir with inverse temperature β, the density matrix

$$\bar{\rho_{\mathrm{S}}} = \frac{e^{-\beta\mathcal{H}_{\mathrm{S}}}}{\mathrm{Tr}\left\{e^{-\beta\mathcal{H}_{\mathrm{S}}}\right\}} \tag{2.66}$$

is one stationary state of the BMS master equation (and the $\tau\to\infty$ limit of the CG appraoch).

Exercise 22 (Thermalization) *(1 points)*
Show that $\bar{\rho_{\mathrm{S}}} = \frac{e^{-\beta\mathcal{H}_{\mathrm{S}}}}{\mathrm{Tr}\left\{e^{-\beta\mathcal{H}_{\mathrm{S}}}\right\}}$ *is a stationary state of the BMS master equation, when* $\gamma_{\alpha\beta}(-\omega) = \gamma_{\beta\alpha}(+\omega)e^{-\beta\omega}$.

When the reservoir is in the grand-canonical equilibrium state

$$\bar{\rho}_{\mathrm{B}} = \frac{e^{-\beta(\mathcal{H}_{\mathrm{B}}-\mu N_{\mathrm{B}})}}{\mathrm{Tr}\left\{e^{-\beta(\mathcal{H}_{\mathrm{B}}-\mu N_{\mathrm{B}})}\right\}}\,, \tag{2.67}$$

where $N = N_{\mathrm{S}} + N_{\mathrm{B}}$is a conserved quantity $[\mathcal{H}_{\mathrm{S}}+\mathcal{H}_{\mathrm{B}}+\mathcal{H}_{\mathrm{I}}, N_{\mathrm{S}}+N_{\mathrm{B}}] = 0$, the KMS condition is not fulfilled anymore. However, even in this case one can show that a stationary state of the BMS master equation is given by

$$\bar{\rho_{\mathrm{S}}} = \frac{e^{-\beta(\mathcal{H}_{\mathrm{S}}-\mu N_{\mathrm{S}})}}{\mathrm{Tr}\left\{e^{-\beta(\mathcal{H}_{\mathrm{S}}-\mu N_{\mathrm{S}})}\right\}}\,, \tag{2.68}$$

i.e., both temperature β and chemical potential μ equilibrate.

2.2.2 Strong-coupling regime

So far we have considered the situation where the interaction Hamiltonian was the weakest part. One may easily generalize to a situation where the system Hamiltonian is weakest, i.e., formally we are interested in the limit $\epsilon\to 0$ where $H = \mathcal{H}_{\mathrm{S}} + \epsilon^{-1}\mathcal{H}_{\mathrm{I}} + \epsilon^{-2}\mathcal{H}_{\mathrm{B}}$. The derivation based on the conventional Born, and Markov approximations is performed in complete analogy, except that

the secular approximation is not necessary, since in the considered limit, all system energies are effectively zero.

We start in the same interaction picture and perform Born- and Markov approximations, see Eq. (2.27). Now however, the system density matrix changes much faster even than the system coupling operators, such that we may effectively replace $e^{\pm\mathcal{H}_S\tau} \to \mathbf{1}$

$$\dot{\rho}_S = -i\left[\mathcal{H}_S, \rho_S\right] - \sum_{\alpha\beta}\int_0^\infty C_{\alpha\beta}(\tau)\left[A_\alpha, A_\beta\rho_S(t)\right]d\tau - \sum_{\alpha\beta}\int_0^\infty C_{\beta\alpha}(\tau)\left[A_\alpha, \rho_S(t)A_\beta\right]d\tau\,. \quad (2.69)$$

It is straightforward (for hermitian coupling operators) to show that this expression is of Lindblad form.

Box 9 (Singular Coupling Limit) *In the singular coupling limit, an interaction Hamiltonian of the form* $\mathcal{H}_I = \sum_\alpha A_\alpha \otimes B_\alpha$ *with hermitian coupling operators (*$A_\alpha = A_\alpha^\dagger$ *and* $B_\alpha = B_\alpha^\dagger$*) and* $[\mathcal{H}_B, \bar{\rho}_B] = 0$ *and* $\mathrm{Tr}\{B_\alpha\bar{\rho}_B\} = 0$ *leads to the Lindblad-form master equation*

$$\dot{\rho}_S = -i\left[\mathcal{H}_S + \sum_{\alpha\beta}\frac{1}{2i}\sigma_{\alpha\beta}(0)A_\alpha A_\beta, \rho_S(t)\right] + \sum_{\alpha\beta}\gamma_{\alpha\beta}(0)\left[A_\alpha\boldsymbol{\rho_S}(t)A_\beta - \frac{1}{2}\left\{A_\beta A_\alpha, \boldsymbol{\rho_S}(t)\right\}\right], \quad (2.70)$$

where the constants are given by

$$\begin{aligned}\gamma_{\alpha\beta}(0) &= \int_{-\infty}^{+\infty}\mathrm{Tr}\left\{e^{+i\mathcal{H}_B\tau}B_\alpha e^{-i\mathcal{H}_B\tau}B_\beta\bar{\rho}_B\right\}d\tau\,,\\ \sigma_{\alpha\beta}(0) &= \int_{-\infty}^{+\infty}\mathrm{Tr}\left\{e^{+i\mathcal{H}_B\tau}B_\alpha e^{-i\mathcal{H}_B\tau}B_\beta\bar{\rho}_B\right\}\mathrm{sgn}(\tau)\mathrm{d}\tau\,. \end{aligned} \quad (2.71)$$

Formally, the singular coupling limit may also be obtained from the BMS limit by setting all system energies to zero.

Chapter 3

Solving Master Equations

The wide range of applications of master equations have led to multiple solution methods, many specialized to a specific form of the master equation. We consider the special case of Markovian master equations here, i.e., time-local master equations with constant generators. Lindblad form is not explicitly required, just linearity in the density matrix and constant coefficients. We can thus always map to a matrix vector notation, i.e.,

$$\dot{\rho_{\mathrm{S}}} = \mathcal{L}\rho_{\mathrm{S}}\,, \tag{3.1}$$

where ρ_{S} is a vector (of at most dimension d^2 where d is the dimension of the system Hilbert space) and $\mathcal{L}$ is a square matrix (of at most dimension $d^2 \times d^2$). For example, when only rate equations are considered (as in the BMS approximation for non-degenerate levels), the vector ρ_{S} may only contain the populations and the mapping to the superoperator description becomes trivial. In the general case, we map the density matrix to a density vector, where we have conventionally d populations in the first place, and (at most) $d(d-1)$ coherences afterwards. The Liouvillian acting on the density matrix is then mapped to a Liouville superoperator acting on the density vector by identifying the coefficients in the linear system in an arbitrary basis, e.g.

$$\dot{\rho}_{ij} = -\mathrm{i}\left\langle i\right|\left[H,\rho\right]\left|j\right\rangle + \sum_{\alpha\beta}\gamma_{\alpha\beta}\left[\left\langle i\right|A_\alpha\rho A_\beta^\dagger\left|j\right\rangle - \frac{1}{2}\left\langle i\right|\left\{A_\beta^\dagger A_\alpha,\rho\right\}\left|j\right\rangle\right]\,. \tag{3.2}$$

As an example, we consider the Liouvillian

$$L[\rho] = -\mathrm{i}\left[\Omega\sigma^z,\rho\right] + \gamma\left[\sigma^-\rho\sigma^+ - \frac{1}{2}\left\{\sigma^+\sigma^-,\rho\right\}\right] \tag{3.3}$$

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

$$\begin{aligned}
\dot{\rho}_{ee} &= -\gamma\rho_{ee}\,, \qquad \dot{\rho}_{gg} = +\gamma\rho_{ee}\,, \\
\dot{\rho}_{eg} &= \left(-\frac{\gamma}{2} - 2\mathrm{i}\Omega\right)\rho_{eg}\,, \qquad \dot{\rho}_{ge} = \left(-\frac{\gamma}{2} + 2\mathrm{i}\Omega\right)\rho_{ge}\,,
\end{aligned} \tag{3.4}$$

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

$$\begin{pmatrix} \dot{\rho}_{gg} \\ \dot{\rho}_{ee} \\ \dot{\rho}_{ge} \\ \dot{\rho}_{eg} \end{pmatrix} = \begin{pmatrix} 0 & +\gamma & 0 & 0 \\ 0 & -\gamma & 0 & 0 \\ 0 & 0 & -\frac{\gamma}{2} + 2\mathrm{i}\Omega & 0 \\ 0 & 0 & 0 & -\frac{\gamma}{2} - 2\mathrm{i}\Omega \end{pmatrix} \begin{pmatrix} \rho_{gg} \\ \rho_{ee} \\ \rho_{ge} \\ \rho_{eg} \end{pmatrix}\,, \tag{3.5}$$

such that populations and coherences evolve apparently independently. Note however, that the Lindblad form nevertheless ensures for a positive density matrix – valid initial conditions provided.

Exercise 23 (Preservation of Positivity) *(1 points)*
Show that the superoperator in Eq. (3.5) preserves positivity of the density matrix provided that initial positivity $(-1/4 \leq \left|\rho^0_{ge}\right|^2 - \rho^0_{gg}\rho^0_{ee} \leq 0)$ *is given.*

The expectation value of an operator A is then mapped to a product with the trace vector.

Exercise 24 (Expectation values from superoperators) *(1 points)*
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

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

where the matrix $\mathcal{A}$ is the superoperator corresponding to A.

3.1 Analytic Techniques

3.1.1 Full analytic solution with the Matrix Exponential

Trivially, as we have a linear system with constant coefficients, we may obtain the solution of the master equation via

$$\rho(t) = e^{\mathcal{L}t}\rho_0\,, \tag{3.6}$$

such that one would have to calculate the matrix exponential. This is usually quite difficult and constrained to very small dimensions of $\mathcal{L}$, escpecially since the Liouville superoperator $\mathcal{L}$ is not hermitian such that it is no spectral decomposition.

Exercise 25 (Single Resonant Level) *(1 points)*
Calculate the matrix exponential of the Liouvillian superoperator for a single resonant level tunnel-coupled to a single junction

$$\mathcal{L} = \begin{pmatrix} -\Gamma f & +\Gamma(1-f) \\ +\Gamma f & -\Gamma(1-f) \end{pmatrix}$$

when the dot level is much lower than the Fermi edge ($f \to 1$) and when it is much larger than the Fermi edge $f \to 0$.

3.1.2 Equation of Motion Technique

Instead of solving the master equation for the density matrix, it may be more favorable to derive a related linear set of first oder differential equations for observables $\langle B_i \rangle (t)$ of interest instead. In fact, for infinitely large system Hilbert space dimensions such a procedure might even be necessary

$$\begin{aligned}
\left\langle \dot{B}_i(t) \right\rangle &= \mathrm{Tr}\left\{B_i \mathcal{L}\rho(t)\right\} \\
&= -\mathrm{i}\mathrm{Tr}\left\{B_i\left[H,\rho(t)\right]\right\} + \sum_\alpha \gamma_\alpha \mathrm{Tr}\left\{B_i\left(L_\alpha \rho(t) L_\alpha^\dagger - \frac{1}{2}\left\{L_\alpha^\dagger L_\alpha, \rho(t)\right\}\right)\right\} \\
&= \mathrm{Tr}\left\{\left(+\mathrm{i}\left[H,B_i\right] + \sum_\alpha \gamma_\alpha \left[L_\alpha^\dagger B_i L_\alpha - \frac{1}{2}\left\{L_\alpha^\dagger L_\alpha, B_i\right\}\right]\right)\rho(t)\right\} \\
&= \mathrm{Tr}\left\{\left[\sum_j G_{ij} B_j\right]\rho(t)\right\} = \sum_j G_{ij}\left\langle B_j(t)\right\rangle \,, \qquad (3.7)
\end{aligned}$$

where in the last line we have used that there is for a finite dimensional system Hilbert space only a finite set of linearly independent operators. In practise, one can often hope to end up with a much smaller set of equations.

Exercise 26 (EOM for the harmonic oscillator) *(1 points)*
Calculate the expectation value of $a + a^\dagger$ for a cavity in a vacuum bath i.e., for $n_B = 0$ in Eq. (1.34).

3.1.3 Quantum Regression Theorem

As with the Heisenberg picture for closed quantum systems, it may be favorable to keep the density matrix as constant and to shift the complete time-dependence to the operators. From the previous Equation we can conclude for the operators

$$\begin{aligned}
\dot{B}_i(t) &= \mathcal{L}^\dagger B_i(t) = +\mathrm{i}\left[H,B_i(t)\right] + \sum_\alpha \gamma_\alpha \left[L_\alpha^\dagger B_i(t) L_\alpha - \frac{1}{2}\left\{L_\alpha^\dagger L_\alpha, B_i(t)\right\}\right] \\
&= \sum_j G_{ij} B_j(t)\,, \qquad (3.8)
\end{aligned}$$

where we have introduced adjoint Liouvillian $\mathcal{L}^\dagger$. For open quantum systems, it is however often important to calculate the expectation values of operators at different times, which may be facilitated with the help of the quantum regression theorem. We find directly from properties of the matrix exponential

$$\frac{d}{d\tau} B_i(t+\tau) = \mathcal{L}^\dagger B_i(t+\tau) = \sum_j G_{ij} B_j(t+\tau)\,. \qquad (3.9)$$

Using this relation, we find the quantum regression theorem for two-point correlation functions.

Box 10 (Quantum Regression) *Let single observables follow the closed equation* $\left\langle \dot{B}_i \right\rangle = \sum_j G_{ij} \langle B_j \rangle$. *Then, the two-point correlation functions obey the equations*

$$\frac{d}{d\tau} \langle B_i(t+\tau) B_\ell(t) \rangle = \sum_j G_{ij} \langle B_j(t+\tau) B_\ell(t) \rangle \tag{3.10}$$

with exactly the same coefficient matrix G_{ij}.

The advantage of the Quantum regression theorem is that it enables the calculation of expressions for two-point correlation functions just from the evolution of single-operator correlation functions.

Let us consider the example of an SET at infinite bias ($f_L \to 1$ and $f_R \to 0$). The single-operator expectation values obey

$$\frac{d}{dt} \begin{pmatrix} \langle dd^\dagger(t) \rangle \\ \langle d^\dagger d(t) \rangle \end{pmatrix} = \begin{pmatrix} -\Gamma_L & +\Gamma_R \\ +\Gamma_L & -\Gamma_R \end{pmatrix} \begin{pmatrix} \langle dd^\dagger(t) \rangle \\ \langle d^\dagger d(t) \rangle \end{pmatrix} , \tag{3.11}$$

such that the quantum regression theorem tells us

$$\frac{d}{d\tau} \begin{pmatrix} \langle dd^\dagger(t+\tau) d^\dagger d(t) \rangle \\ \langle d^\dagger d(t+\tau) d^\dagger d(t) \rangle \end{pmatrix} = \begin{pmatrix} -\Gamma_L & +\Gamma_R \\ +\Gamma_L & -\Gamma_R \end{pmatrix} \begin{pmatrix} \langle dd^\dagger(t+\tau) d^\dagger d(t) \rangle \\ \langle d^\dagger d(t+\tau) d^\dagger d(t) \rangle \end{pmatrix} . \tag{3.12}$$

3.2 Numerical Techniques

3.2.1 Numerical Integration

Numerical integration is generally performed by discretizing time into sufficiently small steps. Note that there are different discretization schemes, e.g. explicit ones

$$\frac{\rho(t+\Delta t) - \rho(t)}{\Delta t} = \mathcal{L}\rho(t) , \tag{3.13}$$

where the right hand side depends on time t and implicit ones as e.g.

$$\frac{\rho(t+\Delta t) - \rho(t)}{\Delta t} = \mathcal{L}\frac{1}{2} \left[\rho(t) + \rho(t+\Delta t) \right] , \tag{3.14}$$

which first have to be solved (typically requiring matrix inversion) for $\rho(t+\Delta t)$ to propagate the solution from time t to time $t+\Delta t$. As a rule of thumb, explicit schemes are easy to implement but may be numerically unstable (i.e., an adaptive stepsize may be required to bound the numerical error). In contrast, implicit schemes are usually more stable but require a lot of effort to propagate the solution. Here, we will just discuss a fourth-order Runge-Kutta solver.

In order to propagate a density matrix ρ_n at time t, to the density matrix ρ_{n+1} at time $t+\Delta t$,

the fourth-order Runge-Kutta scheme proceeds requires the evaluation of some intermediate values

$$\begin{aligned}
\sigma_{n,1} &= \Delta t \mathcal{L} \rho_n \,, \\
\sigma_{n,2} &= \Delta t \mathcal{L} \left(\rho_n + \frac{1}{2} \sigma_{n,1} \right) \,, \\
\sigma_{n,3} &= \Delta t \mathcal{L} \left(\rho_n + \frac{1}{2} \sigma_{n,2} \right) \,, \\
\sigma_{n,4} &= \Delta t \mathcal{L} \left(\rho_n + \sigma_{n,3} \right) \,, \\
\rho_{n+1} &= \rho_n + \frac{1}{6} \sigma_{n,1} + \frac{1}{3} \sigma_{n,2} + \frac{1}{3} \sigma_{n,3} + \frac{1}{6} \sigma_{n,4} + \mathcal{O}\{\Delta t^5\} \,.
\end{aligned} \tag{3.15}$$

This explicit scheme requires four matrix-vector multiplications per timestep. It should always be used with an adaptive stepsize, which can be controlled by comparing (e.g. by computing the norm of the difference) the result from two successive propagations with stepsize Δt with the result of a single propagation with stepsize $2\Delta t$. If the difference between solutions is too large, the stepsize must be reduced (and the intermediate result should be discarded). If it is not too large, the result can always be accepted. In case the error estimate is too small, the stepsize can later-on be cautiously increased.

Exercise 27 (Order of the RK scheme) *(1 points)*
Acting with the Liouville superoperator performs the time-derivative of the density matrix. Show that the presented scheme (3.15) is of fourth order in Δt, i.e., that

$$\rho_{n+1} = \left[\mathbf{1} + \mathcal{L}\Delta t + \mathcal{L}^2 \frac{\Delta t^2}{2!} + \mathcal{L}^3 \frac{\Delta t^3}{3!} + \mathcal{L}^4 \frac{\Delta t^4}{4!} \right] \rho_n \,.$$

3.2.2 Simulation as a Piecewise Deterministic Process (PDP)

Suppose we would like to solve the Lindblad form master equation (in diagonal representation)

$$\dot{\rho} = -\mathrm{i} \left[H, \rho \right] + \sum_\alpha \gamma_\alpha \left[L_\alpha \rho L_\alpha^\dagger - \frac{1}{2} \left\{ \rho, L_\alpha^\dagger, L_\alpha \right\} \right] \tag{3.16}$$

numerically but do not have the possibility to store the N^2 matrix elements of the density matrix.

Instead, the master equation can be unravelled to a piecewise deterministic process for a pure quantum state. The advantage here lies in the fact that a pure state requires only N complex observables to be evolved.

Consider the nonlinear but deterministic equation

$$|\dot{\Psi}\rangle = -\mathrm{i} \left[H - \frac{\mathrm{i}}{2} \sum_\alpha \gamma_\alpha L_\alpha^\dagger L_\alpha \right] |\Psi\rangle + \frac{1}{2} \left[\sum_\alpha \gamma_\alpha \langle \Psi | L_\alpha^\dagger L_\alpha | \Psi \rangle \right] |\Psi\rangle \,. \tag{3.17}$$

Although this is nonlinear in $|\Psi(t)\rangle$, one can show that the solution is given by

$$|\Psi\rangle = \frac{e^{-\mathrm{i}Mt} |\Psi_0\rangle}{\langle \Psi_0 | e^{+\mathrm{i}M^\dagger t} e^{-\mathrm{i}Mt} |\Psi_0\rangle^{1/2}} \,, \tag{3.18}$$

where we have used the operator $M = H - \frac{\mathrm{i}}{2}\sum_\alpha \gamma_\alpha L_\alpha^\dagger L_\alpha$, which is also often interpreted as a non-hermitian Hamiltonian.

Exercise 28 (Norm for continuous evolution) *(1 points)*
Calculate the norm of the state vector $\langle\Psi(t)|\Psi(t)\rangle$ from Eq. (3.18).

We show the validity of the solution by differentiation

$$\begin{aligned}
\left|\dot\Psi\right\rangle &= -\mathrm{i}M\left|\Psi\right\rangle - \frac{1}{2}\frac{e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle}{\left\langle\Psi_0\right| e^{+\mathrm{i}M^\dagger t}e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle^{3/2}}\mathrm{i}\left[\left\langle\Psi_0\right| e^{+\mathrm{i}M^\dagger t}M^\dagger e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle - \left\langle\Psi_0\right| e^{+\mathrm{i}M^\dagger t}Me^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle\right] \\
&= -\mathrm{i}M\left|\Psi\right\rangle - \frac{1}{2}\frac{e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle}{\left\langle\Psi_0\right| e^{+\mathrm{i}M^\dagger t}e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle^{3/2}}\mathrm{i}\left\langle\Psi_0\right| e^{+\mathrm{i}M^\dagger t}\left[M^\dagger - M\right]e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle \\
&= -\mathrm{i}M\left|\Psi\right\rangle + \frac{1}{2}\frac{e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle}{\left\langle\Psi_0\right| e^{+\mathrm{i}M^\dagger t}e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle^{3/2}}\sum_\alpha \gamma_\alpha\left\langle\Psi_0\right| e^{+\mathrm{i}M^\dagger t}L_\alpha^\dagger L_\alpha e^{-\mathrm{i}Mt}\left|\Psi_0\right\rangle \\
&= -\mathrm{i}M\left|\Psi\right\rangle + \frac{1}{2}\left|\Psi\right\rangle\sum_\alpha \gamma_\alpha\left\langle\Psi\right| L_\alpha^\dagger L_\alpha\left|\Psi\right\rangle\ . \qquad (3.19)
\end{aligned}$$

However, the name PDP already suggests that the process is only piecewise deterministic. Hence, it will be interruppted by stochastic events. The total probability that a jump of the wave function will occur in the infinitesimal interval $[t, t+\Delta t]$ is given by given by

$$P_{\text{jump}} = \Delta t\sum_\alpha \gamma_\alpha\left\langle\Psi\right| L_\alpha^\dagger L_\alpha\left|\Psi\right\rangle\ . \qquad (3.20)$$

That is, if a jump has occurred, one still has to decide which jump. Choosing a particular jump

$$\left|\Psi\right\rangle \to \frac{L_\alpha\left|\Psi\right\rangle}{\sqrt{\left\langle\Psi\right| L_\alpha^\dagger L_\alpha\left|\Psi\right\rangle}} \qquad (3.21)$$

is performed randomly with conditional probability

$$P_\alpha = \frac{\gamma_\alpha\left\langle\Psi\right| L_\alpha^\dagger L_\alpha\left|\Psi\right\rangle}{\sum_\alpha \gamma_\alpha\left\langle\Psi\right| L_\alpha^\dagger L_\alpha\left|\Psi\right\rangle}\,, \qquad (3.22)$$

where the normalization is obvious. This recipe for deterministic (continuous) and jump evolutions may also be written as a single stochastic differential equation, which is often called stochastic Schrödinger equation.

Box 11 (Stochastic Schrödinger Equation) *A Lindblad type master equation of the form*

$$\dot\rho = -\mathrm{i}\left[H,\rho\right] + \sum_\alpha \gamma_\alpha\left[L_\alpha\rho L_\alpha^\dagger - \frac{1}{2}\left\{\rho, L_\alpha^\dagger, L_\alpha\right\}\right] \qquad (3.23)$$

can be effectively modeled by the stochastic differential equation

$$|d\Psi\rangle = \left[-\mathrm{i}H - \frac{1}{2}\sum_\alpha \gamma_\alpha L_\alpha^\dagger L_\alpha + \frac{1}{2}\sum_\alpha \gamma_\alpha \langle\Psi| L_\alpha^\dagger L_\alpha |\Psi\rangle\right]|\Psi\rangle\, dt + \sum_\alpha \left(\frac{L_\alpha|\Psi\rangle}{\sqrt{\langle\Psi| L_\alpha^\dagger L_\alpha |\Psi\rangle}} - |\Psi\rangle\right) dN_\alpha\,, \tag{3.24}$$

where the Poisson increments dN_α satisfy

$$dN_\alpha dN_\beta = \delta_{\alpha\beta} dN_\alpha\,, \qquad \mathcal{E}\,(dN_\alpha) = \gamma_\alpha \langle\Psi| L_\alpha^\dagger L_\alpha |\Psi\rangle\, dt \tag{3.25}$$

and $\mathcal{E}\,(x)$ denotes the classical expectation value (ensemble average).

The last two equations simply mean that at most a single jump can occur at once (practically we have $dN_\alpha \in \{0,1\}$) and that the probability for a jump at time t is given by $P_\alpha = \gamma_\alpha \langle\Psi| L_\alpha^\dagger L_\alpha |\Psi\rangle\, dt$. Numerically, it constitutes a simple recipe, see Fig. 3.1.

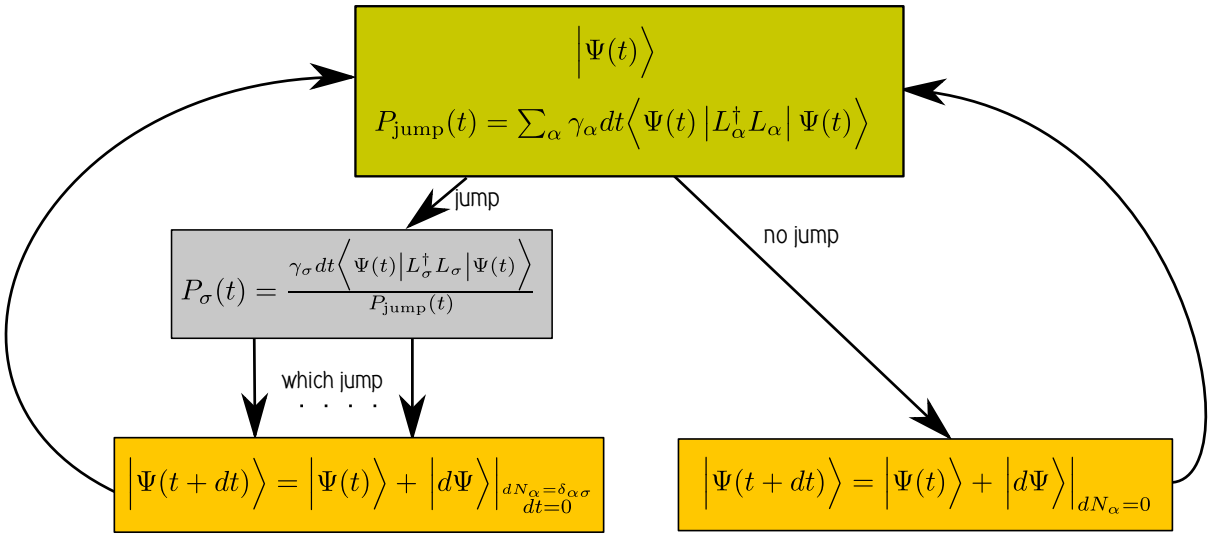

Figure 3.1: Recipe for propagating the stochastic Schrödinger equation in Box 11. At each timestep one can calculate the total probability of a jump occuring during the next timestep. Drawing a random number yields whether a jump should occur or not. Given that a jump occurs, we determine which jump by drawing another random number: Setting the particular $dN_\alpha = 1$ and $dt = 0$ we solve for $|\Psi(t+\Delta t)\rangle = |\Psi(t)\rangle + |d\Psi(t)\rangle$ and proceed with the next timestep. Given that no jump occurs, we simply set $dN_\alpha = 0$ for all α, solve for $|\Psi(t+\Delta t)\rangle = |\Psi(t)\rangle + |d\Psi(t)\rangle$ and proceed with the next timestep.

It remains to be shown that this PDP is actually an unravelling of the master equation, i.e., that the covariance matrix

$$\rho = \mathcal{E}\,(\hat{\pi}) = \mathcal{E}\,(|\Psi\rangle\langle\Psi|) \tag{3.26}$$

fulfils the Lindblad type master equation. To do this we first note that $\langle\Psi| L_\alpha^\dagger L_\alpha |\Psi\rangle = \mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha \hat{\pi}\right\}$. The change of the covariance matrix is given by

$$d\hat{\pi} = |d\Psi\rangle\langle\Psi| + |\Psi\rangle\langle d\Psi| + |d\Psi\rangle\langle d\Psi| \,. \tag{3.27}$$

Note that the last term cannot be neglected completely since the term $\mathcal{E}\left(dN_\alpha dN_\beta\right)$ does not vanish. Making everything explicit we obtain

$$\begin{aligned} d\hat{\pi} &= +dt\left\{-\mathrm{i}\left[H,\hat{\pi}\right] - \frac{1}{2}\sum_\alpha \gamma_\alpha\left\{L_\alpha^\dagger L_\alpha,\hat{\pi}\right\} + \sum_\alpha \gamma_\alpha \hat{\pi}\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}\right\}\right\} \\ &\quad + \sum_\alpha dN_\alpha\left[\frac{L_\alpha\hat{\pi}L_\alpha^\dagger}{\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}\right\}} - \hat{\pi}\right] + \mathcal{O}\{dt^2, dtdN_\alpha\}\,. \end{aligned} \tag{3.28}$$

We now use the general relation

$$\mathcal{E}\left(dN_\alpha g(\hat{\pi})\right) = \gamma_\alpha dt\mathcal{E}\left(\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}\right\} g(\hat{\pi})\right) \tag{3.29}$$

for arbitrary functions $g(\hat{\pi})$ of the projector. This relation can be understood by binning all K values of the actual state $\hat{\pi}^{(k)}(t)$ in the expectation value into L equal-sized compartments where $\hat{\pi}^{(k)} \approx \hat{\pi}^{(\ell)}$. In each compartment, we have N_ℓ realizations of $dN_\alpha^{\ell m}$ with $1 \le m \le N_\ell$ and $\sum_\ell N_\ell = K$, of which we can compute the average first

$$\begin{aligned} \mathcal{E}\left(dN_\alpha g(\hat{\pi})\right) &= \lim_{K\to\infty}\frac{1}{K}\sum_k dN_\alpha^{(k)}(t) g(\hat{\pi}^{(k)}(t)) \\ &= \lim_{L,N_\ell\to\infty}\frac{\sum_\ell N_\ell \frac{1}{N_\ell}\sum_m dN_\alpha^{(\ell m)} g(\hat{\pi}^{(\ell)}(t))}{\sum_\ell N_\ell} \\ &= \lim_{L,N_\ell\to\infty}\frac{\sum_\ell N_\ell \gamma_\alpha dt\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}^{(\ell)}\right\} g(\hat{\pi}^{(\ell)}(t))}{\sum_\ell N_\ell} \\ &= \lim_{L,N_\ell\to\infty}\frac{\sum_\ell N_\ell \gamma_\alpha dt\mathcal{E}\left(\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}^{(\ell)}\right\} g(\hat{\pi}^{(\ell)}(t))\right)}{\sum_\ell N_\ell} \\ &= \gamma_\alpha dt\mathcal{E}\left(\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}^{(\ell)}\right\} g(\hat{\pi}^{(\ell)}(t))\right)\,, \end{aligned} \tag{3.30}$$

where we have used the relation that $\bar{x} = \frac{\sum_i N_i\bar{x}_i}{\sum_i N_i}$ when $\bar{x}_i$ represent averages of disjoint subsets of the complete set. Specifically, we apply it on the expressions

$$\begin{aligned} \mathcal{E}\left(dN_\alpha\frac{\hat{\pi}}{\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}\right\}}\right) &= \gamma_\alpha dt\mathcal{E}\left(\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}\right\}\frac{\hat{\pi}}{\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}\right\}}\right) = \gamma_\alpha dt\rho\,, \\ \mathcal{E}\left(dN_\alpha\hat{\pi}\right) &= \gamma_\alpha dt\mathcal{E}\left(\mathrm{Tr}\left\{L_\alpha^\dagger L_\alpha\hat{\pi}\right\}\hat{\pi}\right) \end{aligned} \tag{3.31}$$

This implies

$$d\rho = dt\left\{-\mathrm{i}\left[H,\rho\right] + \sum_\alpha \gamma_\alpha\left[L_\alpha\rho L_\alpha^\dagger - \frac{1}{2}\left\{L_\alpha^\dagger L_\alpha,\rho\right\}\right]\right\}\,, \tag{3.32}$$

i.e., the average of trajectories from the stochastic Schrödinger equation yields the same solution as the master equation.

This may be of great numerical use: Simulating the full master equation for an N-dimensional system Hilbert space may involve the storage of $\mathcal{O}\{N^4\}$ real variables in the Liouvillian, whereas for the generator of the stochastic Schrödinger equation one requires only $\mathcal{O}\{N^2\}$ real variables. This is of course weakened since in order to get a realistic estimate on the expectation value, one has to compute K different trajectories, but since typically $K \ll N^2$, the stochastic Schrödinger equation is a useful tool in the numeric modelling of a master equation.

As an example, we study the cavity in a thermal bath. We had the Lindblad type master equation describing the interaction of a cavity mode with a thermal bath

$$\begin{aligned}\dot{\rho_{\mathrm{S}}} &= -i\left[\Omega a^\dagger a, \rho_{\mathrm{S}}\right] + \gamma(1+n_B)\left[a\rho_{\mathrm{S}}a^\dagger - \frac{1}{2}a^\dagger a\rho_{\mathrm{S}} - \frac{1}{2}\rho_{\mathrm{S}}a^\dagger a\right] \\ &\quad +\gamma n_B\left[a^\dagger\rho_{\mathrm{S}}a - \frac{1}{2}aa^\dagger\rho_{\mathrm{S}} - \frac{1}{2}\rho_{\mathrm{S}}aa^\dagger\right]. \end{aligned} \tag{3.33}$$

We can immediately identify the jump operators

$$L_1 = a \qquad \text{and} \qquad L_2 = a^\dagger \tag{3.34}$$

and the corresponding rates

$$\gamma_1 = \gamma(1+n_B) \qquad \text{and} \qquad \gamma_2 = \gamma n_B\,. \tag{3.35}$$

From the master equation, we obtain for the occupation number $n = \langle a^\dagger a\rangle$ the evolution equation $\frac{d}{dt}n = -\gamma n + \gamma n_B$, which is solved by

$$n(t) = n_0 e^{-\gamma t} + n_B\left[1 - e^{-\gamma t}\right]. \tag{3.36}$$

The corresponding stochastic differential equation reads

$$\begin{aligned}|d\Psi\rangle &= \left\{-\mathrm{i}\Omega a^\dagger a - \frac{1}{2}\left[\gamma(1+2n_B)a^\dagger a + \gamma n_B\right] + \frac{1}{2}\left[\gamma(1+2n_B)\langle\Psi|a^\dagger a|\Psi\rangle + \gamma n_B\right]\right\}|\Psi\rangle\,dt \\ &\quad + \left(\frac{a|\Psi\rangle}{\sqrt{\langle\Psi|a^\dagger a|\Psi\rangle}} - |\Psi\rangle\right)dN_1 + \left(\frac{a^\dagger|\Psi\rangle}{\sqrt{\langle\Psi|aa^\dagger|\Psi\rangle}} - |\Psi\rangle\right)dN_2\,, \end{aligned} \tag{3.37}$$

which becomes particularly simple when we do not consider superpositions of Fock basis states from the beginning. E.g., for $|\Psi\rangle = |n\rangle$ we obtain

$$\begin{aligned}|dn\rangle &= \left\{-\mathrm{i}\Omega n - \frac{1}{2}\left[\gamma(1+2n_B)n + \gamma n_B\right] + \frac{1}{2}\left[\gamma(1+2n_B)n + \gamma n_B\right]\right\}|n\rangle\,dt \\ &\quad + \left(|n-1\rangle - |n\rangle\right)dN_1 + \left(|n+1\rangle - |n\rangle\right)dN_2 \\ &= -\mathrm{i}\Omega n dt\,|n\rangle + \left(|n-1\rangle - |n\rangle\right)dN_1 + \left(|n+1\rangle - |n\rangle\right)dN_2 \end{aligned} \tag{3.38}$$

such that superpositions are never created during the evolution. The total probability to have a jump in the system during the interval dt is given by

$$P_{\mathrm{jump}} = \gamma dt\left[(1+n_B)\langle n|a^\dagger a|n\rangle + n_B\langle n|aa^\dagger|n\rangle\right] = \gamma\left[(1+n_B)n + n_B(n+1)\right]dt\,. \tag{3.39}$$

If no jump occurs, the system evolves only oscillatory, which has no effect on the expectation value of $a^\dagger a$. However, if a jump occurs, the respective conditional probability to jump out of the system reads

$$P_1 = \frac{(n_B+1)n}{(n_B+1)n + n_B(n+1)} \tag{3.40}$$

and to jump into the system consequently (these must add up to one)

$$P_2 = \frac{n_B(n+1)}{(n_B+1)n + n_B(n+1)}\,. \tag{3.41}$$

Computing trajectories with a suitable random number generator and averaging the trajectories, we find convergence to the master equation result as expected, see Fig. 3.2.

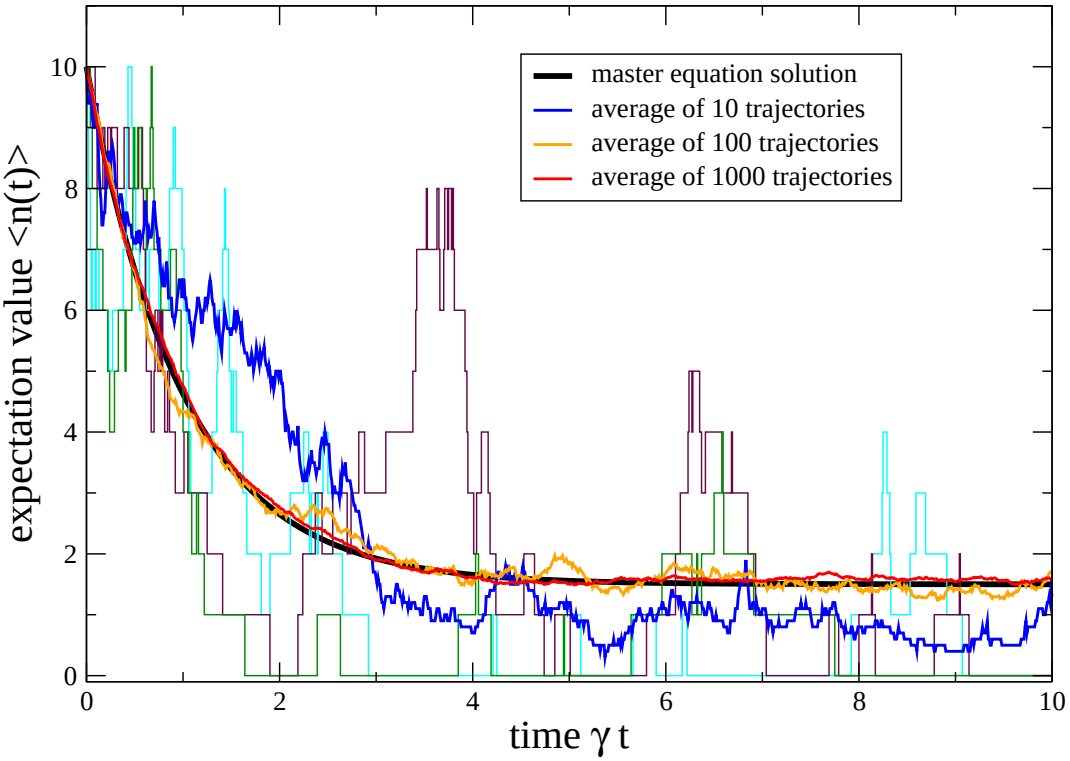

Figure 3.2: Single trajectories of the stochastic Schrödinger equation (curves with integer jumps). The averages of 10, 100, and 1000 trajectories converge to the prediction from the associated master equation. Parameters: $\gamma dt = 0.01$, $n_B = 1.5$.

Chapter 4

Multi-Terminal Coupling : Non-Equilibrium Case I

The most obvious way to achieve non-equilibrium dynamics is to use reservoir states that are non-thermalized, i.e., states that cannot simply be characterized by just temperature and chemical potential. Since the derivation of the master equation only requires $[\bar{\rho}_{\mathrm{B}}, \mathcal{H}_{\mathrm{B}}] = 0$, this would still allow for many nontrivial models, $\langle n| \bar{\rho}_{\mathrm{B}} |n\rangle$ could e.g. follow multi-modal distributions. Alternatively, a non-equilibrium situation may be established when a system is coupled to different thermal equilibrium baths or of course when the system itself is externally driven – either unconditionally (open-loop feedback) or conditioned on the actual state of the system (closed-loop feedback).

First, we will consider the case of multiple reservoirs at different thermal equilibria that are only indirectly coupled via the system: Without the system, they would be completely independent. Since these are chosen at different equilibria, they drag the system towards different thermal states, and the resulting stationary state is in general a non-thermal one. Since the different compartments interact only indirectly via the system, we have the case of a multi-terminal system, where one can most easily derive the corresponding master equation, since each contact may be treated separately. Therefore, we do now consider multiple (K) reservoirs held at different chemical potentials and different temperatures

$$\bar{\rho}_{\mathrm{B}} = \frac{e^{-\beta(\mathcal{H}_{\mathrm{B}}^{(1)} - \mu N_{\mathrm{B}}^{(1)})}}{\mathrm{Tr}\left\{e^{-\beta(\mathcal{H}_{\mathrm{B}}^{(1)} - \mu N_{\mathrm{B}}^{(1)})}\right\}} \otimes \ldots \otimes \frac{e^{-\beta(\mathcal{H}_{\mathrm{B}}^{(K)} - \mu N_{\mathrm{B}}^{(K)})}}{\mathrm{Tr}\left\{e^{-\beta(\mathcal{H}_{\mathrm{B}}^{(K)} - \mu N_{\mathrm{B}}^{(K)})}\right\}} \,. \tag{4.1}$$

To each of the reservoirs, the system is coupled via different coupling operators

$$\mathcal{H}_{\mathrm{I}} = \sum_{\alpha} A_{\alpha} \otimes \sum_{\ell=1}^{k} B_{\alpha}^{(\ell)} \,. \tag{4.2}$$

Since we assume that the first order bath correlation functions vanish $\left\langle B_{\alpha}^{\ell} \bar{\rho}_{\mathrm{B}} \right\rangle = 0$, the tensor product implies that the second-order bath correlation functions may be computed additively

$$C_{\alpha\beta}(\tau) = \sum_{\ell=1}^{K} C_{\alpha\beta}^{(\ell)}(\tau) \,, \tag{4.3}$$

which transfers to their Fourier transforms and thus, also to the final Liouvillian (to second order

in the coupling)

$$\mathcal{L} = \sum_{\ell=1}^{K} \mathcal{L}^{(\ell)} \,. \tag{4.4}$$

The resulting stationary state is in general a non-equilibrium one. Let us however first identify a trivial case where the coupling structure of all Liouvillians is identical

$$\mathcal{L}^{(\ell)} = \Gamma^{(\ell)} \left[\mathcal{L}_0 + \boldsymbol{\beta}^{(\ell)} \mathcal{L}_1 \right] , \tag{4.5}$$

where $\boldsymbol{\beta}^{(\ell)}$ is a parameter encoding the thermal properties of the respective bath (e.g. a Fermi-function evaluated at one of the systems transition frequencies) and $\mathcal{L}_{0/1}$ are superoperators independent of the respective bath and $\Gamma^{(\ell)}$ represent different coupling constants. For coupling to a single reservoir, the stationary state is defined via the equation

$$\mathcal{L}^{(\ell)} \bar{\rho}^{(\ell)} = \Gamma^{(\ell)} \left[\mathcal{L}_0 + \boldsymbol{\beta}^{(\ell)} \mathcal{L}_1 \right] \bar{\rho}^{(\ell)} = 0 \tag{4.6}$$

and thus implicitly depends on the thermal parameter $\bar{\rho}^{(\ell)} = \bar{\rho}(\boldsymbol{\beta}^{(\ell)})$. For the total Liouvillian, it follows that the dependence of the full stationary state on all thermal parameters simply given by the same dependence on an average thermal parameter

$$\sum_{\ell} \mathcal{L}^{(\ell)} \bar{\rho} = \sum_{\ell} \Gamma^{(\ell)} \left[\mathcal{L}_0 + \boldsymbol{\beta}^{(\ell)} \mathcal{L}_1 \right] \bar{\rho} = \left[\sum_{\ell} \Gamma^{(\ell)} \right] \left[\mathcal{L}_0 + \frac{\sum_{\ell} \Gamma^{(\ell)} \boldsymbol{\beta}^{(\ell)}}{\sum_{\ell'} \Gamma^{(\ell')}} \mathcal{L}_1 \right] \bar{\rho} \,, \tag{4.7}$$

such that the dependence is simply $\bar{\rho} = \bar{\rho} \left(\frac{\sum_{\ell} \Gamma^{(\ell)} \boldsymbol{\beta}^{(\ell)}}{\sum_{\ell} \Gamma^{(\ell)}} \right)$

This can be illustrated by upgrading the Liouvillian for a single resonant level coupled to a single junction

$$\mathcal{L} = \begin{pmatrix} -\Gamma f & +\Gamma(1-f) \\ +\Gamma f & -\Gamma(1-f) \end{pmatrix} , \tag{4.8}$$

where the Fermi function $f = \left[e^{\beta(\epsilon-\mu)} + 1 \right]^{-1}$ of the contact is evaluated at the dot level ϵ, to the Liouvillian for a single-electron transistor (SET) coupled to two (left and right) junctions

$$\mathcal{L} = \begin{pmatrix} -\Gamma_L f_L - \Gamma_R f_R & +\Gamma_L(1-f_L) + \Gamma_R(1-f_R) \\ +\Gamma_L f_L + \Gamma_R f_R & -\Gamma_L(1-f_L) - \Gamma_R(1-f_R) \end{pmatrix} . \tag{4.9}$$

Now, the system is coupled to two fermionic reservoirs, and in order to support a current, the dot level ϵ must be within the transport window, see Fig. 4.1. This also explains the name single-electron transistor, since the dot level ϵ may be tuned by a third gate, which thereby controls the current.

Exercise 29 (Pseudo-Nonequilibrium) *(1 points)*
Show that the stationary state of Eq.(4.9) is a thermal one, i.e., that

$$\frac{\bar{\rho}_{11}}{\bar{\rho}_{00}} = \frac{\bar{f}}{1-\bar{f}} \,.$$

Determine $\bar{f}$ in dependence of Γ_α and f_α.

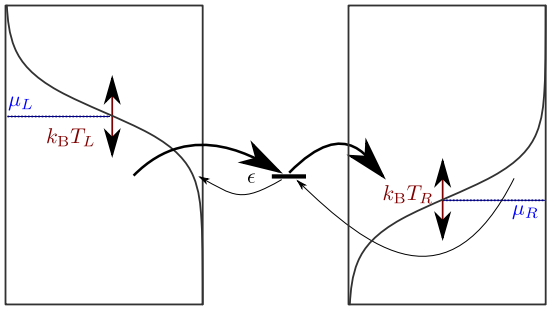

Figure 4.1: Sketch of a single resonant level (QD at energy level ϵ) coupled to two junctions with different Fermi distributions (e.g. with different chemical potentials or different temperatures. If the dot level ϵ is changed with a third gate, the device functions as a transistor, since the current through the system is exponentially suppressed when the the dot level ϵ is not within the transport window.

4.1 Conditional Master equation from conservation laws

Suppose we have derived a QME for an open system, where the combined system obeys the conservation of some conserved quantity (e.g., the total number of particles). Then, it can be directly concluded that a change in the system particle number by e.g. minus one must be directly accompagnied by the corresponding change of the reservoir particle number by plus one. For couplings to multiple reservoirs these terme can also be uniquely identified, since the Liouvillians are additive. Whereas its actual density matrix says little about the number of quanta that have already passed the quantum system, a full trajectory would reveal this information. In such cases, it is reasonable to discretize the master equation in time, where it can most easily be upgraded to an n-resolved (conditional) master equation. In what follows, we just track the particle number in a single attached reservoir and denote by $\rho^{(n)}(t)$ the system density matrix under the condition that n net particles have left into the monitored reservoirs, but the method may easily be generalized. Assuming that at time t, we have n particles transferred to the reservoir, we may discretize the conventional master equation $\dot{\rho} = \mathcal{L}\rho$ in time and identify terms that increase or decrease the particle number (often called jumpers)

$$\dot{\rho^{(n)}} = \mathcal{L}_0\rho^{(n)} + \mathcal{L}^+\rho^{(n-1)} + \mathcal{L}^-\rho^{(n+1)}\,. \tag{4.10}$$

Since the total number of transferred particles is normally not constrained, this immediately yields an infinite set of equations for the system density matrix. Exploiting the translational invariance suggests to use the Fourier transform

$$\rho(\chi,t) = \sum_n \rho^{(n)}(t)e^{+\mathrm{i}n\chi}\,, \tag{4.11}$$

which again reduces the dimension of the master equation

$$\dot{\rho}(\chi,t) = \left[\mathcal{L}_0 + e^{+\mathrm{i}\chi}\mathcal{L}^+ + e^{-\mathrm{i}\chi}\mathcal{L}^-\right]\rho(\chi,t) = \mathcal{L}(\chi)\rho(\chi,t)\,. \tag{4.12}$$

As an example, we convert the SET master equation (4.9) into an n-resolved version, where n should denote the number of particles that have tunneled into the right reservoir

$$\begin{aligned}\dot{\rho}^{(n)} &= \begin{pmatrix} -\Gamma_L f_L - \Gamma_R f_R & +\Gamma_L(1-f_L) \\ +\Gamma_L f_L & -\Gamma_L(1-f_L) - \Gamma_R(1-f_R)\end{pmatrix}\rho^{(n)} \\ &\quad + \begin{pmatrix} 0 & \Gamma_R(1-f_R) \\ 0 & 0\end{pmatrix}\rho^{(n-1)} + \begin{pmatrix} 0 & 0 \\ +\Gamma_R f_R & 0\end{pmatrix}\rho^{(n+1)}\,.\end{aligned} \tag{4.13}$$

Performing the Fourier transformation reduces the dimension (exploiting the shift invariance) at the price of introducing the counting field

$$\dot{\rho}(\chi,t) = \begin{pmatrix} -\Gamma_L f_L - \Gamma_R f_R & +\Gamma_L(1-f_L) + \Gamma_R(1-f_R)e^{+\mathrm{i}\chi} \\ +\Gamma_L f_L + \Gamma_R f_R e^{-\mathrm{i}\chi} & -\Gamma_L(1-f_L) - \Gamma_R(1-f_R) \end{pmatrix} \rho(\chi,t)\,. \tag{4.14}$$

Formally, this just corresponds to the replacement $(1-f_R) \to (1-f_R)e^{+\mathrm{i}\chi}$ and $f_R \to f_R e^{-\mathrm{i}\chi}$ in the off-diagonal matrix elements of the Liouvillian (which correspond to particle jumps).

4.2 Microscopic derivation with a detector model

Unfortunately, we do not always have a conserved quantity that may only change when tunneling across the system-reservoir junction takes place. A counter-example may be the tunneling between two reservoirs, that is merely modified by the presence of the quantum system (e.g. quantum point contact monitoring a charge qubit) and is not connected with a particle change in the system. In such cases, we may not identify a change in the system state with a microcanonical change of the reservoir state. However, such problems can still be handled with a quantum master equation by introducing a virtual detector at the level of the interaction Hamiltonian. Suppose that in the interaction Hamiltonian we can identify terms associated with a change of the tracked obervable in the reservoir

$$\mathcal{H}_\mathrm{I} = A_+ \otimes B_+ + A_- \otimes B_- + \sum_{\alpha\neq\{+,-\}} A_\alpha \otimes B_\alpha\,, \tag{4.15}$$

where B_+ increases and B_- decreases the reservoir particle number. We extend the system Hilbert space by adding a virtual detector

$$\begin{aligned} \mathcal{H}_\mathrm{S} &\to \mathcal{H}_\mathrm{S} \otimes \mathbf{1}\,, \qquad \mathcal{H}_\mathrm{B} \to \mathcal{H}_\mathrm{B} \\ \mathcal{H}_\mathrm{I} &\to + \left[A_+ \otimes D^\dagger\right] \otimes B_+ + [A_- \otimes D] \otimes B_- + \sum_{\alpha\neq\{+,-\}} [A_\alpha \otimes \mathbf{1}] \otimes B_\alpha\,, \end{aligned} \tag{4.16}$$

where $D = \sum_n |n\rangle\langle n+1|$ and $D^\dagger = \sum_n |n+1\rangle\langle n|$. Considering the detector as part of the system and decomposing the system density matrix as

$$\rho(t) = \sum_n \rho^{(n)}(t) \otimes |n\rangle\langle n|\,, \tag{4.17}$$

we can use the method of our choice to obtain the conditional master equation by virtue of

$$\begin{aligned} DD^\dagger = D^\dagger D &= \mathbf{1}\,, \\ \langle n|\, DA_-\rho A_+ D^\dagger\, |n\rangle &= A_-\rho^{(n+1)}A_+\,, \\ \langle n|\, D^\dagger A_+\rho A_- D\, |n\rangle &= A_+\rho^{(n-1)}A_-\,. \end{aligned} \tag{4.18}$$

4.3 Full Counting Statistics

To obtain the probability of having n tunneled particles into a respective reservoir, we have to sum over the different system configurations of the corresponding conditional density matrix

$$P_n(t) = \mathrm{Tr}\left\{\rho^{(n)}(t)\right\}\,. \tag{4.19}$$

In view of the identities

$$\mathrm{Tr}\left\{\rho(\chi,t)\right\} = \mathrm{Tr}\left\{e^{\mathcal{L}(\chi)t}\rho_0\right\} = \sum_n P_n(t)e^{+\mathrm{i}n\chi} \equiv \mathcal{M}(\chi,t)\,, \tag{4.20}$$

we see that in order to evaluate moments $\langle n^k\rangle$, we simply have to take derivatives with respect to the counting field

$$\langle n^k(t)\rangle = \sum_n n^k P_n(t) = (-\mathrm{i}\partial_\chi)^k \sum_n P_n(t)e^{+\mathrm{i}n\chi}\bigg|_{\chi=0} = (-\mathrm{i}\partial_\chi)^k\, \mathcal{M}(\chi,t)|_{\chi=0}\,. \tag{4.21}$$

Based on a conditional master equation, this enables a very convenient calculation of the stationary current. Taking the stationary density matrix $\mathcal{L}(0)\bar\rho = 0$ as initial condition (the stationary current is independent on the initial occupation of the density matrix), we obtain for the current as the time derivative of the first moment

$$\begin{aligned}
I &= \langle \dot n(t)\rangle \\
&= -\mathrm{i}\partial_\chi \frac{d}{dt}\,\mathrm{Tr}\left\{e^{\mathcal{L}(\chi)t}\bar\rho\right\}\big|_{\chi=0} \\
&= -\mathrm{i}\partial_\chi\,\mathrm{Tr}\left\{\mathcal{L}(\chi)e^{\mathcal{L}(\chi)t}\bar\rho\right\}\big|_{\chi=0} \\
&= -\mathrm{i}\mathrm{Tr}\Big\{\mathcal{L}'(0)\bar\rho + \left[\mathcal{L}'(0)\mathcal{L}(0)+\mathcal{L}(0)\mathcal{L}'(0)\right]t\bar\rho \\
&\quad + \left[\mathcal{L}'(0)\mathcal{L}^2(0)+\mathcal{L}(0)\mathcal{L}'(0)\mathcal{L}(0)+\mathcal{L}^2(0)\mathcal{L}'(0)\right]\frac{t^2}{2}\bar\rho + \ldots\Big\} \\
&= -\mathrm{i}\mathrm{Tr}\left\{\mathcal{L}'(0)\bar\rho\right\}\,,
\end{aligned} \tag{4.22}$$

where we have used $\mathcal{L}(0)\bar\rho = 0$ and also $\mathrm{Tr}\left\{\mathcal{L}(0)\sigma\right\} = 0$ for all operators σ (trace conservation).

Exercise 30 (Stationary SET current) *(1 points)*
Calculate the stationary current through the SET (4.14).

Sometimes a description in terms of cumulants is more convenient. The cumulant-generating function is defined as the logarithm of the moment-generating function

$$\mathcal{C}(\chi,t) = \ln \mathcal{M}(\chi,t)\,, \tag{4.23}$$

such that all cumulants may be obtained via simple differentiation

$$\langle\langle n^k\rangle\rangle = (-\mathrm{i}\partial_\chi)^k\, \mathcal{C}(\chi,t)|_{\chi=0}\,. \tag{4.24}$$

Cumulants and Moments are of course related, we just summarize relations for the lowest few cumulants

$$\begin{aligned}
\langle\langle n\rangle\rangle &= \langle n\rangle\,, \qquad \langle\langle n^2\rangle\rangle = \langle n^2\rangle - \langle n\rangle^2\,, \\
\langle\langle n^3\rangle\rangle &= \langle n^3\rangle - 3\langle n\rangle\langle n^2\rangle + 2\langle n\rangle^3\,, \\
\langle\langle n^4\rangle\rangle &= \langle n^4\rangle - 4\langle n\rangle\langle n^3\rangle - 3\langle n^2\rangle^2 + 12\langle n\rangle^2\langle n^2\rangle - 6\langle n\rangle^4\,.
\end{aligned} \tag{4.25}$$

The advantage of this description lies in the fact that the long-term evolution of the cumulant-generating function is usually given by the dominant eigenvalue of the Liouvillian

$$\mathcal{C}(\chi,t) \approx \lambda(\chi)t\,, \tag{4.26}$$

where $\lambda(\chi)$ is the (uniqueness assumed) eigenvalue of the Liouvillian that vanishes at zero counting field $\lambda(0) = 0$. For this reason, the dominant eigenvalue is also interpreted as the cumulant-generating function of the stationary current.

Exercise 31 (current CGF for the SET) *(1 points)*
Calculate the dominant eigenvalue of the SET Liouvillian (4.14) in the infinite bias limit $f_L \to 1$ and $f_R \to 0$. What is the value of the current?

We show this by using the decomposition of the Liouvillian in Jordan Block form

$$\mathcal{L}(\chi) = Q(\chi)\mathcal{L}_J(\chi)Q^{-1}(\chi)\,, \tag{4.27}$$

where $Q(\chi)$ is a (non-unitary) similarity matrix and $\mathcal{L}_J(\chi)$ contains the eigenvalues of the Liouvillian on its diagonal – distributed in blocks with a size corresponding to the eigenvalue multiplicity. We assume that there exists one stationary state $\bar{\rho}$, i.e., one eigenvalue $\lambda(\chi)$ with $\lambda(0) = 0$ and that all other eigenvalues have a larger negative real part near $\chi = 0$. Then, we use this decomposition in the matrix exponential to estimate its long-term evolution

$$\begin{aligned}
\mathcal{M}(\chi,t) &= \mathrm{Tr}\left\{e^{\mathcal{L}(\chi)t}\rho_0\right\} = \mathrm{Tr}\left\{e^{Q(\chi)\mathcal{L}_J(\chi)Q^{-1}(\chi)t}\rho_0\right\} = \mathrm{Tr}\left\{Q(\chi)e^{\mathcal{L}_J(\chi)t}Q^{-1}(\chi)\rho_0\right\} \\
&\to \mathrm{Tr}\left\{Q(\chi)\begin{pmatrix} e^{\lambda(\chi)\cdot t} & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{pmatrix}Q^{-1}(\chi)\rho_0\right\} \\
&= e^{\lambda(\chi)\cdot t}\mathrm{Tr}\left\{Q(\chi)\begin{pmatrix} 1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{pmatrix}Q^{-1}(\chi)\rho_0\right\} = e^{\lambda(\chi)t}c(\chi)
\end{aligned} \tag{4.28}$$

with some polynomial $c(\chi)$ depending on the matrix $Q(\chi)$. This implies that the cumulant-generating function

$$\mathcal{C}(\chi,t) = \ln\mathcal{M}(\chi,t) = \lambda(\chi)t + \ln c(\chi) \approx \lambda(\chi)t \tag{4.29}$$

becomes linear in $\lambda(\chi)$ for large times.

4.4 Fluctuation Theorems

The probability distribution $P_n(t)$ is given by the inverse Fourier transform of the moment-generating function

$$P_n(t) = \frac{1}{2\pi}\int_{-\pi}^{+\pi}\mathcal{M}(\chi,t)e^{-in\chi}d\chi = \frac{1}{2\pi}\int_{-\pi}^{+\pi}e^{\mathcal{C}(\chi,t)-in\chi}d\chi\,. \tag{4.30}$$

Accordingly, a symmetry in the cumulant-generating function (or moment-generating function) of the form

$$\mathcal{C}(-\chi,t)=\mathcal{C}(+\chi+\mathrm{i}\ln(\alpha),t) \tag{4.31}$$

leads to a symmetry of the probabilities

$$\begin{aligned}\frac{P_{+n}(t)}{P_{-n}(t)} &= \frac{\frac{1}{2\pi}\int_{-\pi}^{+\pi}e^{\mathcal{C}(\chi,t)-\mathrm{i}n\chi}d\chi}{\frac{1}{2\pi}\int_{-\pi}^{+\pi}e^{\mathcal{C}(\chi,t)+\mathrm{i}n\chi}d\chi}=\frac{\int_{-\pi}^{+\pi}e^{\mathcal{C}(\chi,t)-\mathrm{i}n\chi}d\chi}{\int_{-\pi}^{+\pi}e^{\mathcal{C}(-\chi,t)-\mathrm{i}n\chi}d\chi}\\ &= \frac{\int_{-\pi}^{+\pi}e^{\mathcal{C}(\chi,t)-\mathrm{i}n\chi}d\chi}{\int_{-\pi}^{+\pi}e^{\mathcal{C}(\chi+\mathrm{i}\ln(\alpha),t)-\mathrm{i}n\chi}d\chi}=\frac{\int_{-\pi}^{+\pi}e^{\mathcal{C}(\chi,t)-\mathrm{i}n\chi}d\chi}{\int_{-\pi+\mathrm{i}\ln(\alpha)}^{+\pi+\mathrm{i}\ln(\alpha)}e^{\mathcal{C}(\chi,t)-\mathrm{i}n[\chi-\mathrm{i}\ln(\alpha)]}d\chi}\\ &= e^{+n\ln(\alpha)}\,,\end{aligned} \tag{4.32}$$

where we have used in the last step that $\mathcal{C}(-\pi+\mathrm{i}\ln(\alpha),t)=\mathcal{C}(+\pi+\mathrm{i}\ln(\alpha),t)$, such that we can add two further integration paths from $-\pi$ to $-\pi+\mathrm{i}\ln(\alpha)$ and from $+\pi+\mathrm{i}\ln(\alpha)$ to $+\pi$. The value of the cumulant-generating function along these paths is the same, such that due to the different integral orientation there is not net change. Note that the system may be very far from thermodynamic equilibrium but still obey a symmetry of the form (4.31), which leads to a fluctuation theorem of the form (4.32) being valid far from equilibrium.

As example, we consider the SET (which is always in thermal equilibrium). The characteristic polynomial $\mathcal{D}(\chi)=|\mathcal{L}(\chi)-\lambda\mathbf{1}|$ of the Liouvillian (4.14) and therefore also all eigenvalues obeys the symmetry

$$\mathcal{D}(-\chi)=\mathcal{D}\left(+\chi+\mathrm{i}\ln\left[\frac{f_L(1-f_R)}{(1-f_L)f_R}\right]\right)=\mathcal{D}\left(\chi+\mathrm{i}\left[(\beta_R-\beta_L)\,\epsilon+\beta_L\mu_L-\beta_R\mu_R\right]\right)\,, \tag{4.33}$$

which leads to the fluctuation theorem

$$\lim_{t\to\infty}\frac{P_{+n}(t)}{P_{-n}(t)}=e^{n[(\beta_R-\beta_L)\epsilon+\beta_L\mu_L-\beta_R\mu_R]}\,. \tag{4.34}$$

For equal temperatures, this becomes

$$\lim_{t\to\infty}\frac{P_{+n}(t)}{P_{-n}(t)}=e^{n\beta V}\,, \tag{4.35}$$

which directly demonstrates that the current

$$I=\frac{d}{dt}\langle n(t)\rangle=\frac{d}{dt}\sum_{n=-\infty}^{+\infty}nP_n(t)=\sum_{n=1}^{\infty}n\left[P_{+n}(t)-P_{-n}(t)\right]=\sum_{n=1}^{\infty}nP_n(t)\left[1-e^{-n\alpha}\right] \tag{4.36}$$

always follows the voltage.

4.5 The double quantum dot

We consider a double quantum dot with internal tunnel coupling T and Coulomb interaction U that is weakly coupled to two fermionic contacts via the rates Γ_L and Γ_R, see Fig. 4.2. The

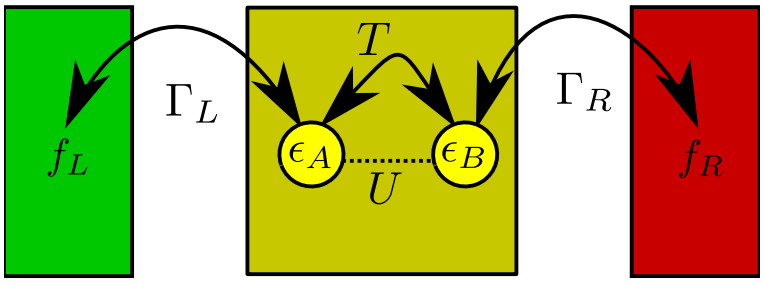

Figure 4.2: A double quantum dot (system) with on-site energies $\epsilon_{A/B}$ and internal tunneling amplitude T and Coulomb interaction U may host at most two electrons. It is weakly tunnel-coupled to two fermionic contacts via the rates $\Gamma_{L/R}$ at different thermal equilibria described by the Fermi distributions $f_{L/R}(\omega)$.

corresponding Hamiltonian reads

$$\begin{aligned}
\mathcal{H}_{\rm S} &= \epsilon_A d_A^\dagger d_A + \epsilon_B d_B^\dagger d_B + T\left(d_A d_B^\dagger + d_B d_A^\dagger\right) + U d_A^\dagger d_A d_B^\dagger d_B\,,\\
\mathcal{H}_{\rm B} &= \sum_k \epsilon_{kL} c_{kL}^\dagger c_{kL} + \sum_k \epsilon_{kR} c_{kR}^\dagger c_{kR}\,,\\
\mathcal{H}_{\rm I} &= \sum_k \left(t_{kL} d_A c_{kL}^\dagger + t_{kL}^* c_{kL} d_A^\dagger\right) + \sum_k \left(t_{kR} d_B c_{kR}^\dagger + t_{kR}^* c_{kR} d_B^\dagger\right)\,.
\end{aligned} \tag{4.37}$$

Note that we do not have a tensor product decomposition in the interaction Hamiltonian, as the coupling operators anti-commute, e.g.,

$$\{d, c_{kR}\} = 0\,. \tag{4.38}$$

We may however use the Jordan Wigner transform, which decomposes the Fermionic operators in terms of Pauli matrices acting on different spins

$$\begin{aligned}
d_A &= \sigma^- \otimes \mathbf{1} \otimes \mathbf{1} \otimes \ldots \otimes \mathbf{1}\,, \qquad d_B = \sigma^z \otimes \sigma^- \otimes \mathbf{1} \otimes \ldots \otimes \mathbf{1}\,,\\
c_{kL} &= \sigma^z \otimes \sigma^z \otimes \underbrace{\sigma^z \otimes \ldots \otimes \sigma^z}_{k-1} \otimes \sigma^- \otimes \mathbf{1} \otimes \ldots \otimes \mathbf{1}\,,\\
c_{kR} &= \sigma^z \otimes \sigma^z \otimes \underbrace{\sigma^z \otimes \ldots \otimes \sigma^z}_{K_L} \otimes \underbrace{\sigma^z \otimes \ldots \otimes \sigma^z}_{k-1} \otimes \sigma^- \otimes \mathbf{1} \otimes \ldots \otimes \mathbf{1}
\end{aligned} \tag{4.39}$$

to map to a tensor-product decomposition of the interaction Hamiltonian, where $\sigma^\pm = \frac{1}{2}\left[\sigma^x \pm \mathrm{i}\sigma^y\right]$. The remaining operators follow from $(\sigma^+)^\dagger = \sigma^-$ and vice versa. This decomposition automatically obeys the fermionic anti-commutation relations such as e.g. $\left\{c_k, d^\dagger\right\} = 0$ and may therefore also be used to create a fermionic operator basis with computer algebra programs (e.g. use `KroneckerProduct` in Mathematica).

Exercise 32 (Jordan-Wigner transform) *(1 points)*
Show that for fermions distributed on N sites, the decomposition

$$c_i = \underbrace{\sigma^z \otimes \ldots \otimes \sigma^z}_{i-1} \otimes \sigma^- \otimes \underbrace{\mathbf{1} \otimes \ldots \otimes \mathbf{1}}_{N-i}$$

preserves the fermionic anti-commutation relations

$$\{c_i, c_j\} = \mathbf{0} = \left\{c_i^\dagger, c_j^\dagger\right\}, \qquad \left\{c_i, c_j^\dagger\right\} = \delta_{ij}\mathbf{1}.$$

Show also that the fermionic Fock space basis $c_i^\dagger c_i \left|n_1, \ldots, n_N\right\rangle = n_i \left|n_1, \ldots, n_N\right\rangle$ *obeys* $\sigma_i^z \left|n_1, \ldots, n_N\right\rangle = (-1)^{n_i+1} \left|n_1, \ldots, n_N\right\rangle$.

Inserting the decomposition (4.39) in the Hamiltonian, we may simply use the relations

$$\begin{aligned}
(\sigma^x)^2 &= (\sigma^y)^2 = (\sigma^z)^2 = \mathbf{1}, \qquad \sigma^+\sigma^- = \frac{1}{2}\left[\mathbf{1} + \sigma^z\right], \qquad \sigma^-\sigma^+ = \frac{1}{2}\left[\mathbf{1} - \sigma^z\right], \\
\sigma^z\sigma^- &= -\sigma^-, \qquad \sigma^-\sigma^z = +\sigma^-, \qquad \sigma^z\sigma^+ = +\sigma^+, \qquad \sigma^+\sigma^z = -\sigma^+
\end{aligned} \tag{4.40}$$

to obtain a system of interacting spins

$$\begin{aligned}
\mathcal{H}_{\mathrm{S}} &= \epsilon_A \frac{1}{2}\left[\mathbf{1} + \sigma_A^z\right] + \epsilon_B \frac{1}{2}\left[\mathbf{1} + \sigma_B^z\right] + T\left[\sigma_A^- \sigma_B^+ + \sigma_A^+ \sigma_B^-\right] + U \frac{1}{2}\left[\mathbf{1} + \sigma_A^z\right] \frac{1}{2}\left[\mathbf{1} + \sigma_B^z\right] \\
\mathcal{H}_{\mathrm{B}} &= \sum_k \epsilon_{kL} \frac{1}{2}\left[\mathbf{1} + \sigma_{kL}^z\right] + \sum_k \epsilon_{kR} \frac{1}{2}\left[\mathbf{1} + \sigma_{kR}^z\right] \\
\mathcal{H}_{\mathrm{I}} &= \sigma_A^- \sigma_B^z \otimes \sum_k t_{kL} \left[\prod_{k'<k} \sigma_{k'L}^z\right] \sigma_{kL}^+ + \sigma_A^+ \sigma_B^z \otimes \sum_k t_{kL}^* \left[\prod_{k'<k} \sigma_{k'L}^z\right] \sigma_{kL}^- \\
&\quad + \sigma_B^- \otimes \sum_k t_{kR} \left[\prod_{k'} \sigma_{k'L}^z\right] \left[\prod_{k''<k} \sigma_{k''R}^z\right] \sigma_{kR}^+ + \sigma_B^+ \otimes \sum_k t_{kR}^* \left[\prod_{k'} \sigma_{k'L}^z\right] \left[\prod_{k''<k} \sigma_{k''R}^z\right] \sigma_{kR}^-
\end{aligned} \tag{4.41}$$

.

With this, we could proceed by simply viewing the Hamiltonian as a complicated total system of non-locally interacting spins. However, the order of operators in the nonlocal Jordan-Wigner transformation may be chosen as convenient without destroying the fermionic anticommutation relations. We may therefore also define new fermionic operators on the subspace of the system (first two sites, with reversed order) and the baths (all remaining sites with original order), respectively

$$\begin{aligned}
\tilde{d}_A &= \sigma^- \otimes \sigma^z, \qquad \tilde{d}_B = \mathbf{1} \otimes \sigma^-, \\
\tilde{c}_{kL} &= \underbrace{\sigma^z \otimes \ldots \otimes \sigma^z}_{k-1} \otimes \sigma^- \otimes \mathbf{1} \otimes \ldots \otimes \mathbf{1}, \\
\tilde{c}_{kR} &= \underbrace{\sigma^z \otimes \ldots \otimes \sigma^z}_{K_L} \otimes \underbrace{\sigma^z \otimes \ldots \otimes \sigma^z}_{k-1} \otimes \sigma^- \otimes \mathbf{1} \otimes \ldots \otimes \mathbf{1}.
\end{aligned} \tag{4.42}$$

These new operators obey fermionic anti-commutation relations in system and bath separately (e.g. $\{\tilde{d}_A, \tilde{d}_B\} = \mathbf{0}$ and $\{\tilde{c}_{kL}, \tilde{c}_{k'L}\} = \mathbf{0}$), but act on different Hilbert spaces, such that system and bath operators do commute by construction (e.g. $[\tilde{d}_A, \tilde{c}_{kL}] = 0$). In the new operator basis, the Hamiltonian appears as

$$\begin{aligned}
\mathcal{H}_{\mathrm{S}} &= \left[\epsilon_A \tilde{d}_A^\dagger \tilde{d}_A + \epsilon_B \tilde{d}_B^\dagger \tilde{d}_B + T\left(\tilde{d}_A \tilde{d}_B^\dagger + \tilde{d}_B \tilde{d}_A^\dagger\right) + U \tilde{d}_A^\dagger \tilde{d}_A \tilde{d}_B^\dagger \tilde{d}_B\right] \otimes \mathbf{1}, \\
\mathcal{H}_{\mathrm{B}} &= \mathbf{1} \otimes \left[\sum_k \epsilon_{kL} \tilde{c}_{kL}^\dagger \tilde{c}_{kL} + \sum_k \epsilon_{kR} \tilde{c}_{kR}^\dagger \tilde{c}_{kR}\right], \\
\mathcal{H}_{\mathrm{I}} &= \tilde{d}_A \otimes \sum_k t_{kL} \tilde{c}_{kL}^\dagger + \tilde{d}_A^\dagger \otimes \sum_k t_{kL}^* \tilde{c}_{kL} + \tilde{d}_B \otimes \sum_k t_{kR} \tilde{c}_{kR}^\dagger + \tilde{d}_B^\dagger \otimes \sum_k t_{kR}^* \tilde{c}_{kR},
\end{aligned} \tag{4.43}$$

which is the same (for this and some more special cases) as if we had ignored the fermionic nature of the annihilation operators from the beginning. We do now proceed by calculating the Fourier transforms of the bath correlation functions

$$\begin{aligned} \gamma_{12}(\omega) &= \Gamma_L(-\omega) f_L(-\omega)\,, \qquad \gamma_{21}(\omega) = \Gamma_L(+\omega)[1 - f_L(+\omega)]\,, \\ \gamma_{34}(\omega) &= \Gamma_R(-\omega) f_R(-\omega)\,, \qquad \gamma_{43}(\omega) = \Gamma_R(+\omega)[1 - f_R(+\omega)] \end{aligned} \tag{4.44}$$

with the continuum tunneling rates $\Gamma_\alpha(\omega) = 2\pi \sum_k |t_{k\alpha}|^2 \delta(\omega - \epsilon_{k\alpha})$ and Fermi functions $f_\alpha(\epsilon_{k\alpha}) = \left\langle c^\dagger_{k\alpha} c_{k\alpha} \right\rangle$.

Exercise 33 (DQD bath correlation functions) *(1 points)*
Calculate the Fourier transforms (4.44) of the bath correlation functions for the double quantum dot.

Next, we diagonalize the system Hamiltonian (in the Fock space basis)

$$\begin{aligned} E_0 &= 0\,, \qquad |v_0\rangle = |00\rangle\,, \\ E_- &= \epsilon - \sqrt{\Delta^2 + T^2}\,, \qquad |v_-\rangle \propto \left[\left(\Delta + \sqrt{\Delta^2 + T^2} \right) |10\rangle + T\,|01\rangle \right]\,, \\ E_+ &= \epsilon + \sqrt{\Delta^2 + T^2}\,, \qquad |v_+\rangle \propto \left[\left(\Delta - \sqrt{\Delta^2 + T^2} \right) |10\rangle + T\,|01\rangle \right]\,, \\ E_2 &= 2\epsilon + U\,, \qquad |v_2\rangle = |11\rangle\,, \end{aligned} \tag{4.45}$$

where $\Delta = (\epsilon_B - \epsilon_A)/2$ and $\epsilon = (\epsilon_A + \epsilon_B)/2$ and $|01\rangle = -\tilde{d}^\dagger_B |00\rangle$, $|10\rangle = \tilde{d}^\dagger_A |00\rangle$, and $|11\rangle = \tilde{d}^\dagger_B \tilde{d}^\dagger_A |00\rangle$. We have not symmetrized the coupling operators but to obtain the BMS limit, we may alternatively use Eqns. (2.60) and (2.61) when $\tau \to \infty$. Specifically, when we have no degeneracies in the system Hamiltonian ($\Delta^2 + T^2 > 0$), the master equation in the energy eigenbasis (where $a, b \in \{0, -, +, 2\}$) becomes a rate equation $\dot{\rho}_{aa} = +\sum_b \gamma_{ab,ab} \rho_{bb} - \left[\sum_b \gamma_{ba,ba}\right] \rho_{aa}$ with the rate coefficients

$$\gamma_{ab,ab} = \sum_{\alpha\beta} \gamma_{\alpha\beta}(E_b - E_a) \langle a| A_\beta |b\rangle \langle a| A^\dagger_\alpha |b\rangle^* \,. \tag{4.46}$$

We may calculate the Liouvillians for the interaction with the left and right contact separately

$$\gamma_{ab,ab} = \gamma^L_{ab,ab} + \gamma^R_{ab,ab}\,, \tag{4.47}$$

since we are constrained to second order perturbation theory in the tunneling amplitudes. Since we have $\tilde{d}_A = A^\dagger_2 = A_1 = \tilde{d}_A$ and $\tilde{d}_B = A^\dagger_4 = A_2 = \tilde{d}_B$, we obtain for the left-associated dampening coefficients

$$\begin{aligned} \gamma^L_{ab,ab} &= \gamma_{12}(E_b - E_a) |\langle a| A_2 |b\rangle|^2 + \gamma_{21}(E_b - E_a) |\langle a| A_1 |b\rangle|^2\,, \\ \gamma^R_{ab,ab} &= \gamma_{34}(E_b - E_a) |\langle a| A_4 |b\rangle|^2 + \gamma_{43}(E_b - E_a) |\langle a| A_3 |b\rangle|^2\,. \end{aligned} \tag{4.48}$$

In the wideband (flatband) limit $\Gamma_{L/R}(\omega) = \Gamma_{L/R}$, we obtain for the nonvanishing transition rates

in the energy eigenbasis

$$
\begin{aligned}
\gamma^L_{0-,0-} &= \Gamma_L\gamma_+[1-f_L(\epsilon-\sqrt{\Delta^2+T^2})]\,, \qquad \gamma^R_{0-,0-} = \Gamma_R\gamma_-[1-f_R(\epsilon-\sqrt{\Delta^2+T^2})]\,,\\
\gamma^L_{0+,0+} &= \Gamma_L\gamma_-[1-f_L(\epsilon+\sqrt{\Delta^2+T^2})]\,, \qquad \gamma^R_{0+,0+} = \Gamma_R\gamma_+[1-f_R(\epsilon+\sqrt{\Delta^2+T^2})]\,,\\
\gamma^L_{-2,-2} &= \Gamma_L\gamma_-[1-f_L(\epsilon+U+\sqrt{\Delta^2+T^2})]\,, \qquad \gamma^R_{-2,-2} = \Gamma_R\gamma_+[1-f_R(\epsilon+U+\sqrt{\Delta^2+T^2})]\,,\\
\gamma^L_{+2,+2} &= \Gamma_L\gamma_+[1-f_L(\epsilon+U-\sqrt{\Delta^2+T^2})]\,, \qquad \gamma^R_{+2,+2} = \Gamma_R\gamma_-[1-f_R(\epsilon+U-\sqrt{\Delta^2+T^2})]\,,\\
\gamma^L_{-0,-0} &= \Gamma_L\gamma_+ f_L(\epsilon-\sqrt{\Delta^2+T^2})\,, \qquad \gamma^R_{-0,-0} = \Gamma_R\gamma_- f_R(\epsilon-\sqrt{\Delta^2+T^2})\,,\\
\gamma^L_{+0,+0} &= \Gamma_L\gamma_- f_L(\epsilon+\sqrt{\Delta^2+T^2})\,, \qquad \gamma^R_{+0,+0} = \Gamma_R\gamma_+ f_R(\epsilon+\sqrt{\Delta^2+T^2})\,,\\
\gamma^L_{2-,2-} &= \Gamma_L\gamma_- f_L(\epsilon+U+\sqrt{\Delta^2+T^2})\,, \qquad \gamma^R_{2-,2-} = \Gamma_R\gamma_+ f_R(\epsilon+U+\sqrt{\Delta^2+T^2})\,,\\
\gamma^L_{2+,2+} &= \Gamma_L\gamma_+ f_L(\epsilon+U-\sqrt{\Delta^2+T^2})\,, \qquad \gamma^R_{2+,2+} = \Gamma_R\gamma_- f_R(\epsilon+U-\sqrt{\Delta^2+T^2})\,,
\end{aligned}
\tag{4.49}
$$

with the dimensionless coefficients

$$
\gamma_\pm = \frac{1}{2}\left[1 \pm \frac{\Delta}{\sqrt{\Delta^2+T^2}}\right] \tag{4.50}
$$

arising from the matrix elements of the system coupling operators. This rate equation can also be visualized with a network, see Fig. 4.3.

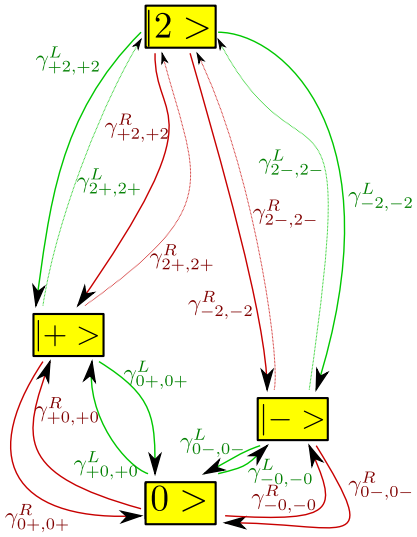

Figure 4.3: Configuration space of a serial double quantum dot coupled to two leads. Due to the hybridization of the two levels, electrons may jump directly from the left contact to right-localized modes and vice versa, such that in principle all transitios are driven by both contacts. However, the relative strength of the couplings is different, such that the two Liouillians have a different structure. In the Coulomb-blockade limit, transitions to the doubly occupied state are forbidden (dotted lines), such that the system dimension can be reduced.

As the simplest example of the resulting rate equation, we study the high-bias and Coulomb-blockade limit $f_{L/R}(\epsilon+U\pm\sqrt{\Delta^2+T^2}) \to 0$ and $f_L(\epsilon\pm\sqrt{\Delta^2+T^2}) \to 1$ and $f_R(\epsilon\pm\sqrt{\Delta^2+T^2}) \to 0$ when $\Delta \to 0$ (such that $\gamma_\pm \to 1/2$). This removes any dependence on T and therefore, a current will be predicted even when $T \to 0$ (where we have a disconnected structure). However, precisely in this limit, the two levels E_- and E_+ become energetically degenerate, such that we cannot neglect the couplings to the coherences anymore and the BMS limit is not applicable. The resulting Liouvillian reads

$$
\mathcal{L} = \frac{1}{2}\begin{pmatrix} -2\Gamma_L & \Gamma_R & \Gamma_R & 0 \\ \Gamma_L & -\Gamma_R & 0 & \Gamma_L+\Gamma_R \\ \Gamma_L & 0 & -\Gamma_R & \Gamma_L+\Gamma_R \\ 0 & 0 & 0 & -2(\Gamma_L+\Gamma_R) \end{pmatrix}, \tag{4.51}
$$

where it becomes visible that the doubly occupied state will simply decay and may therefore – since we are interested in the long-term dynamics – be eliminated completely

$$\mathcal{L}_{\mathrm{CBHB}} = \frac{1}{2}\begin{pmatrix} -2\Gamma_L & \Gamma_R & \Gamma_R \\ \Gamma_L & -\Gamma_R & 0 \\ \Gamma_L & 0 & -\Gamma_R \end{pmatrix}. \tag{4.52}$$

Switching to a conditional Master equation by counting all electrons in the right junction and performing the Fourier summation corresponds formally to the replacement $\Gamma_R \to \Gamma_R e^{+\mathrm{i}\chi}$ in all off-diagonal matrix elements (corresponding to single-electron jumps), such that we have

$$\mathcal{L}_{\mathrm{CBHB}}(\chi) = \frac{1}{2}\begin{pmatrix} -2\Gamma_L & \Gamma_R e^{+\mathrm{i}\chi} & \Gamma_R e^{+\mathrm{i}\chi} \\ \Gamma_L & -\Gamma_R & 0 \\ \Gamma_L & 0 & -\Gamma_R \end{pmatrix}. \tag{4.53}$$

Exercise 34 (Stationary Current) *(1 points)*
Calculate the stationary current of Eq.(4.53).

Exercise 35 (Nonequilibrium Stationary State) *(1 points)*
Show that the stationary state of Eq. (4.52) cannot be written as a grand-canonical equilibrium state by disproving the equations $\bar{\rho}_{--}/\bar{\rho}_{00} = e^{-\beta(E_- - E_0 - \mu)}$, $\bar{\rho}_{++}/\bar{\rho}_{00} = e^{-\beta(E_+ - E_0 - \mu)}$ *and* $\bar{\rho}_{++}/\bar{\rho}_{--} = e^{-\beta(E_+ - E_-)}$

Chapter 5

Direct bath coupling : Non-Equilibrium Case II

Another nonequilibrium situation may be generated by a multi-component bath with components interacting directly (i.e., even without the presence of the system) via a small interface. However, the interaction may be modified by the presence of the quantum system. A prototypical example for such a bath is a quantum point contact: The two leads are held at different potentials and through a tiny contact charges may tunnel. The tunneling process is however highly sensitive to the presence of nearby charges, in the Hamiltonian this is modeled by a capacitive change of the tunneling amplitudes. When already the baseline tunneling amplitudes (in a low transparency QPC) are small, we may apply the master equation formalism without great efforts, as will be demonstrated at two examples.

5.1 Monitored SET

High-precision tests of counting statistics have been performed with a quantum point contact that is capacitively coupled to a single-electron transistor. The Hamiltonian of the system depicted in Fig. 5.1 reads

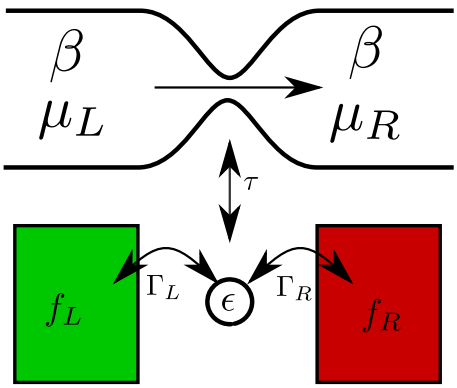

Figure 5.1: Sketch of a quantum point contact (in fact, a two component bath with the components held at different chemical potential) monitoring a single electron transistor. The tunneling through the quantum point contact is modified when the SET is occupied.

$$\begin{aligned}
\mathcal{H}_{\rm S} &= \epsilon d^\dagger d\,, \\
\mathcal{H}_{\rm B} &= \sum_k \epsilon_{kL} c_{kL}^\dagger c_{kL} + \sum_k \epsilon_{kL} c_{kR}^\dagger c_{kR} + \sum_k \varepsilon_{kL} \gamma_{kL}^\dagger \gamma_{kL} + \sum_k \varepsilon_{kL} \gamma_{kR}^\dagger \gamma_{kR}\,, \\
\mathcal{H}_{\rm I} &= \left[\sum_k t_{kL} d c_{kL}^\dagger + \sum_k t_{kR} d c_{kR}^\dagger + \text{h.c.}\right] + \left[\sum_{kk'} \left(t_{kk'} + d^\dagger d \tau_{kk'}\right) \gamma_{kL} \gamma_{k'R}^\dagger + \text{h.c.}\right], \quad (5.1)
\end{aligned}$$

where ϵ denotes the dot level, $c_{k\alpha}$ annihilate electrons on SET lead α and $\gamma_{k\alpha}$ are the annihilation operators for the QPC lead α. The QPC baseline tunneling amplitude is given by $t_{kk'}$ and describes the scattering of and electron from mode k in the left lead to mode k' in the right QPC contact. When the nearby SET is occupied it is modified to $t_{kk'} + \tau_{kk'}$, where $\tau_{kk'}$ represents the change of the tunneling amplitude.

We will derive a master equation for the dynamics of the SET due to the interaction with the QPC and the two SET contacts. In addition, we are interested not only in the charge counting statistics of the SET but also the QPC. The Liouvillian for the SET-contact interaction is well known and has been stated previously (we insert counting fields at the right lead)

$$\mathcal{L}_{\rm SET}(\chi) = \begin{pmatrix} -\Gamma_L f_L - \Gamma_R f_R & +\Gamma_L(1-f_L) + \Gamma_R(1-f_R) e^{+{\rm i}\chi} \\ +\Gamma_L f_L + \Gamma_R f_R e^{-{\rm i}\chi} & -\Gamma_L(1-f_L) - \Gamma_R(1-f_R) \end{pmatrix}. \quad (5.2)$$

We will therefore derive the dissipator for the SET-QPC interaction separately. To keep track of the tunneled QPC electrons, we insert a virtual detector operator in the respective tunneling Hamiltonian

$$\begin{aligned}
\mathcal{H}_{\rm I}^{\rm QPC} &= \sum_{kk'} \left(t_{kk'}\mathbf{1} + d^\dagger d \tau_{kk'}\right) B^\dagger \gamma_{kL} \gamma_{k'R}^\dagger + \sum_{kk'} \left(t_{kk'}^*\mathbf{1} + d^\dagger d \tau_{kk'}^*\right) B \gamma_{k'R} \gamma_{kL}^\dagger \\
&= \mathbf{1} \otimes B^\dagger \otimes \sum_{kk'} t_{kk'} \gamma_{kL} \gamma_{k'R}^\dagger + \mathbf{1} \otimes B \otimes \sum_{kk'} t_{kk'}^* \gamma_{k'R} \gamma_{kL}^\dagger \\
&\quad + d^\dagger d \otimes B^\dagger \otimes \sum_{kk'} \tau_{kk'} \gamma_{kL} \gamma_{k'R}^\dagger + d^\dagger d \otimes B \otimes \sum_{kk'} \tau_{kk'}^* \gamma_{k'R} \gamma_{kL}^\dagger\,. \quad (5.3)
\end{aligned}$$

Note that we have implicitly performed the mapping to a tensor product representation of the fermionic operators, which is unproblematic here as between SET and QPC no particle exchange takes place and the electrons in the QPC and the SET may be treated as different particle types. To simplify the system, we assume that the change of tunneling amplitudes affects all modes in the same manner, i.e., $\tau_{kk'} = \tilde{\tau} t_{kk'}$, which enables us to combine some coupling operators

$$\mathcal{H}_{\rm I}^{\rm QPC} = \left[\mathbf{1} + \tilde{\tau} d^\dagger d\right] \otimes B^\dagger \otimes \sum_{kk'} t_{kk'} \gamma_{kL} \gamma_{k'R}^\dagger + \left[\mathbf{1} + \tilde{\tau}^* d^\dagger d\right] \otimes B \otimes \sum_{kk'} t_{kk'}^* \gamma_{k'R} \gamma_{kL}^\dagger\,. \quad (5.4)$$

The evident advantage of this approximation is that only two correlation functions have to be computed. We can now straightforwardly (since the baseline tunneling term is not included in the bath Hamiltonian) map to the interaction picture

$$B_1(\tau) = \sum_{kk'} t_{kk'} \gamma_{kL} \gamma_{k'R}^\dagger e^{-{\rm i}(\varepsilon_{kL} - \varepsilon_{k'R})\tau}\,, \qquad B_2(\tau) = \sum_{kk'} t_{kk'}^* \gamma_{k'R} \gamma_{kL}^\dagger e^{+{\rm i}(\varepsilon_{kL} - \varepsilon_{k'R})\tau}\,. \quad (5.5)$$

For the first bath correlation function we obtain

$$\begin{aligned} C_{12}(\tau) &= \sum_{kk'}\sum_{\ell\ell'} t_{kk'}t^*_{\ell\ell'}e^{-\mathrm{i}(\varepsilon_{kL}-\varepsilon_{k'R})\tau}\left\langle \gamma_{kL}\gamma^\dagger_{k'R}\gamma_{\ell'R}\gamma^\dagger_{\ell L}\right\rangle \\ &= \sum_{kk'}|t_{kk'}|^2 e^{-\mathrm{i}(\varepsilon_{kL}-\varepsilon_{k'R})\tau}\left[1-f_L(\varepsilon_{kL})\right]f_R(\varepsilon_{k'R}) \\ &= \frac{1}{2\pi}\int\int T(\omega,\omega')\left[1-f_L(\omega)\right]f_R(\omega')e^{-\mathrm{i}(\omega-\omega')\tau}d\omega d\omega' , \end{aligned} \tag{5.6}$$

where we have introduced $T(\omega,\omega') = 2\pi\sum_{kk'}|t_{kk'}|^2\delta(\omega-\varepsilon_{kL})\delta(\omega-\varepsilon_{k'R})$. Note that in contrast to previous tunneling rates, this quantity is dimensionless. The integral factorizes when $T(\omega,\omega')$ factorizes (or when it is flat $T(\omega,\omega')=t$). In this case, the correlation function $C_{12}(\tau)$ is expressed as a product in the time domain, such that its Fourier transform will be given by a convolution integral

$$\begin{aligned} \gamma_{12}(\Omega) &= \int C_{12}(\tau)e^{+\mathrm{i}\Omega\tau}d\tau \\ &= t\int d\omega d\omega'\left[1-f_L(\omega)\right]f_R(\omega')\delta(\omega-\omega'-\Omega) \\ &= t\int\left[1-f_L(\omega)\right]f_R(\omega-\Omega)d\omega . \end{aligned} \tag{5.7}$$

For the other correlation function, we have

$$\gamma_{21}(\Omega) = t\int f_L(\omega)\left[1-f_R(\omega+\Omega)\right]d\omega . \tag{5.8}$$

Exercise 36 (Correlation functions for the QPC) *(1 points)*
Show the validity of Eqns. (5.8).

The structure of the Fermi functions demonstrates that the shift Ω can be included in the chemical potentials. Therefore, we consider integrals of the type

$$I = \int f_1(\omega)\left[1-f_2(\omega)\right]d\omega . \tag{5.9}$$

At zero temperature, these should behave as $I \approx (\mu_1-\mu_2)\Theta(\mu_1-\mu_2)$, where $\Theta(x)$ denotes the Heaviside-Θ function, which follows from the structure of the integrand, see Fig. 5.2. For finite temperatures, the value of the integral can also be calculated, for simplicity we constrain ourselves to the (experimentally relevant) case of equal temperatures ($\beta_1=\beta_2=\beta$), for which we obtain

$$\begin{aligned} I &= \int\frac{1}{\left(e^{\beta(\mu_2-\omega)}+1\right)\left(e^{-\beta(\mu_1-\omega)}+1\right)}d\omega \\ &= \lim_{\delta\to\infty}\int\frac{1}{\left(e^{\beta(\mu_2-\omega)}+1\right)\left(e^{-\beta(\mu_1-\omega)}+1\right)}\frac{\delta^2}{\delta^2+\omega^2}d\omega , \end{aligned} \tag{5.10}$$

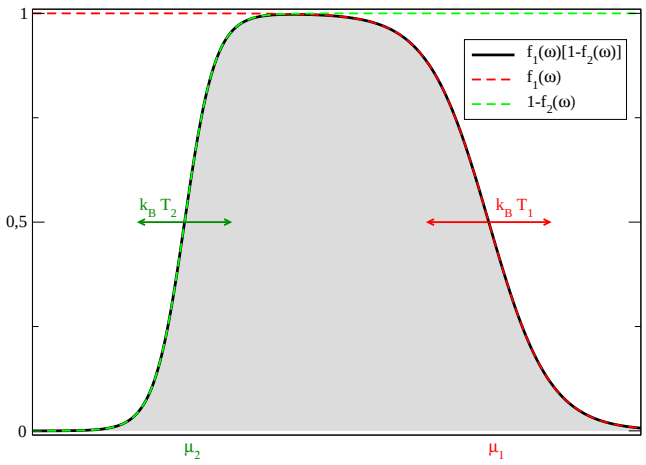

Figure 5.2: Integrand in Eq. (5.9). At zero temperature at both contacts, we obtain a product of two step functions and the area under the curve is given by the difference $\mu_1 - \mu_2$ as soon as $\mu_1 > \mu_2$ (and zero otherwise).

where we have introduced the Lorentzian-shaped regulator to enforce convergence. By identifying the poles of the integrand

$$\begin{aligned} \omega^*_{\pm} &= \pm \mathrm{i}\delta\,, \\ \omega^*_{1,n} &= \mu_1 + \frac{\pi}{\beta}(2n+1) \\ \omega^*_{2,n} &= \mu_2 + \frac{\pi}{\beta}(2n+1) \end{aligned} \tag{5.11}$$

where $n \in \{0, \pm 1, \pm 2, \pm 3, \ldots$ we can solve the integral by using the residue theorem, see also Fig. 5.3 for the integration contour. Finally, we obtain for the integral

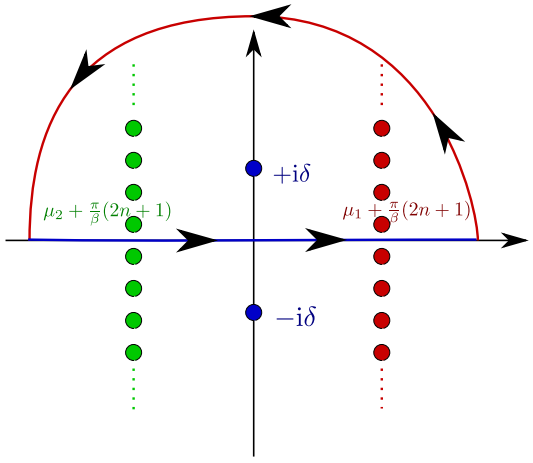

Figure 5.3: Poles and integration contour for Eq. (5.9) in the complex plane. The integral along the real axis (blue line) closed by an arc (red curve) in the upper complex plane, along which (due to the regulator) the integrand vanishes sufficiently fast.

$$\begin{aligned} I &= 2\pi \mathrm{i} \lim_{\delta\to\infty} \Big\{ \mathrm{Res}\, f_1(\omega)\,[1-f_2(\omega)]\, \frac{\delta^2}{\delta^2+\omega^2}\Big|_{\omega=+\mathrm{i}\delta} + \sum_{n=0}^{\infty} \mathrm{Res}\, f_1(\omega)\,[1-f_2(\omega)]\, \frac{\delta^2}{\delta^2+\omega^2}\Big|_{\omega=\mu_1+\frac{\pi}{\beta}(2n+1)} \\ &\quad + \sum_{n=0}^{\infty} \mathrm{Res}\, f_1(\omega)\,[1-f_2(\omega)]\, \frac{\delta^2}{\delta^2+\omega^2}\Big|_{\omega=\mu_2+\frac{\pi}{\beta}(2n+1)} \Big\} \\ &= \frac{\mu_1-\mu_2}{1-e^{-\beta(\mu_1-\mu_2)}}\,, \end{aligned} \tag{5.12}$$

which automatically obeys the simple zero-temperature ($\beta \to \infty$) limit. With the replacements

$\mu_1 \to \mu_R + \Omega$ and $\mu_2 \to \mu_L$, we obtain for the first bath correlation function

$$\gamma_{12}(\Omega) = t\frac{\Omega - V}{1 - e^{-\beta(\Omega - V)}}\,, \tag{5.13}$$

where $V = \mu_L - \mu_R$ is the QPC bias voltage. Likewise, with the replacements $\mu_1 \to \mu_L$ and $\mu_2 \to \mu_R - \Omega$, the second bath correlation function becomes

$$\gamma_{21}(\Omega) = t\frac{\Omega + V}{1 - e^{-\beta(\Omega + V)}}\,. \tag{5.14}$$

Now we can calculate the transition rates in our system (containing the virtual detector and the quantum dot) for a non-degenerate system spectrum. However, now the detector is part of our system. Therefore, the system state is not only characterized by the number of charges on the SET dot $a \in \{0, 1\}$ but also by the number of charges n that have tunneled through the QPC and have thereby changed the detector state

$$\dot{\rho}_{(a,n)(a,n)} = \sum_{b,m} \gamma_{(a,n)(b,m),(a,n)(b,m)} \rho_{(b,m)(b,m)} - \left[\sum_{b,m} \gamma_{(b,m)(a,n),(b,m)(a,n)}\right] \rho_{(a,n)(a,n)}\,. \tag{5.15}$$

Shortening the notation by omitting the double-indices we may also write

$$\dot{\rho}^{(n)}_{aa} = \sum_{b,m} \gamma_{(a,n),(b,m)} \rho^{(m)}_{bb} - \left[\sum_{b,m} \gamma_{(b,m),(a,n)}\right] \rho^{(n)}_{aa}\,, \tag{5.16}$$

where $\rho^{(n)}_{aa} = \rho_{(a,n),(a,n)}$ and $\gamma_{(a,n),(b,m)} = \gamma_{(a,n)(a,n),(b,m)(b,m)}$. It is evident that the coupling operators $A_1 = (\mathbf{1} + \tilde{\tau} d^\dagger d) \otimes B^\dagger$ and $A_2 = (\mathbf{1} + \tilde{\tau}^* d^\dagger d) \otimes B$ only allow for sequential tunneling through the QPC at lowest order (i.e., $m = n \pm 1$) and do not induce transitions between different dot states (i.e., $a = b$), such that the only non-vanishing contributions may arise for

$$\begin{aligned}
\gamma_{(0,n)(0,n+1)} &= \gamma_{12}(0) \langle 0, n| A_2 |0, n+1\rangle \langle 0, n| A_1^\dagger |0, n+1\rangle^* = \gamma_{12}(0)\,,\\
\gamma_{(0,n)(0,n-1)} &= \gamma_{21}(0) \langle 0, n| A_1 |0, n-1\rangle \langle 0, n| A_2^\dagger |0, n-1\rangle^* = \gamma_{21}(0)\,,\\
\gamma_{(1,n)(1,n+1)} &= \gamma_{12}(0) \langle 1, n| A_2 |1, n+1\rangle \langle 1, n| A_1^\dagger |1, n+1\rangle^* = \gamma_{12}(0)|1 + \tilde{\tau}|^2\,,\\
\gamma_{(1,n)(1,n-1)} &= \gamma_{21}(0) \langle 1, n| A_1 |1, n-1\rangle \langle 1, n| A_2^\dagger |1, n-1\rangle^* = \gamma_{21}(0)|1 + \tilde{\tau}|^2\,.
\end{aligned} \tag{5.17}$$

The remaining terms just account for the normalization.

Exercise 37 (Normalization terms) *(1 points)*
Compute the remaining rates

$$\sum_m \gamma_{(0,m)(0,m),(0,n)(0,n)}\,, \qquad \text{and} \qquad \sum_m \gamma_{(1,m)(1,m),(1,n)(1,n)}$$

explicitly.

Adopting the notation of conditional master equations, this leads to the connected system

$$\begin{aligned}\dot{\rho}_{00}^{(n)} &= \gamma_{12}(0)\rho_{00}^{(n+1)} + \gamma_{21}(0)\rho_{00}^{(n-1)} - \left[\gamma_{12}(0)+\gamma_{21}(0)\right]\rho_{00}^{(n)} \\ \dot{\rho}_{11}^{(n)} &= |1+\tilde{\tau}|^2\gamma_{12}(0)\rho_{11}^{(n+1)} + |1+\tilde{\tau}|^2\gamma_{21}(0)\rho_{11}^{(n-1)} - |1+\tilde{\tau}|^2\left[\gamma_{12}(0)+\gamma_{21}(0)\right]\rho_{11}^{(n)}\,, \end{aligned} \quad (5.18)$$

such that after Fourier transformation with the counting field ξ for the QPC, we obtain the following dissipator

$$\mathcal{L}_{\rm QPC}(\xi) = \begin{pmatrix} \left[\gamma_{21}\left(e^{+i\chi}-1\right)+\gamma_{12}\left(e^{-i\chi}-1\right)\right] & 0 \\ 0 & |1+\tilde{\tau}|^2\left[\gamma_{21}\left(e^{+i\chi}-1\right)+\gamma_{12}\left(e^{-i\chi}-1\right)\right] \end{pmatrix}, \quad (5.19)$$

which could not have been deduced directly from a Liouvillian for the SET alone. More closely analyzing the Fourier transforms of the bath correlation functions

$$\begin{aligned}\gamma_{21} &= \gamma_{21}(0) = t\frac{V}{1-e^{-\beta V}}\,, \\ \gamma_{12} &= \gamma_{12}(0) = t\frac{V}{e^{+\beta V}-1} \end{aligned} \quad (5.20)$$

we see that for sufficiently large QPC bias voltages, transport becomes unidirectional and only one contribution remains and the other one is exponentially suppressed. The sum of both Liouvillians (5.2) and (5.19) constitutes the total dissipator

$$\mathcal{L}(\chi,\xi) = \mathcal{L}_{\rm SET}(\chi) + \mathcal{L}_{\rm QPC}(\xi)\,, \quad (5.21)$$

which can be used to calculate the probability distributions for tunneling through both transport channels (QPC and SET).

Exercise 38 (QPC current) *(1 points)*
Show that the stationary state of the SET is unaffected by the additional QPC dissipator and calculate the stationary current through the QPC for Liouvillian (5.21).

When we consider the case $\{\Gamma_L,\Gamma_R\} \ll \{tV, |1+\tilde{\tau}|tV\}$, we approach a bistable system, and the counting statistics approaches the case of telegraph noise. When the dot is empty or filled throughout respectively, the current can easily be determined as

$$I_0 = \left[\gamma_{21}(0)-\gamma_{12}(0)\right]\,, \qquad I_1 = |1+\tilde{\tau}|^2\left[\gamma_{21}(0)-\gamma_{12}(0)\right]\,. \quad (5.22)$$

For finite time intervals Δt, the number of electrons tunneling through the QPC Δn is determined by the probability distribution

$$P_{\Delta n}(\Delta t) = \frac{1}{2\pi}\int_{-\pi}^{+\pi} {\rm Tr}\left\{e^{\mathcal{L}(0,\xi)\Delta t - i\Delta n\xi}\rho(t)\right\} d\xi\,, \quad (5.23)$$

where $\rho(t)$ represents the initial density matrix. This quantity can e.g. be evaluated numerically. When Δt is not too large (such that the stationary state is not really reached) and not too small

(such that there are sufficiently many particles tunneling through the QPC to meaningfully define a current), a continuous measurement of the QPC current maps to a fixed-point iteration as follows: Measuring a certain particle number corresponds to a projection, i.e., the system-detector density matrix is projected to a certain measurement outcome which occurs with the probability $P_{\Delta n}(\Delta t)$

$$\rho = \sum_n \rho^{(n)} \otimes |n\rangle \langle n| \overset{m}{\to} \frac{\rho^{(m)}}{\mathrm{Tr}\,\{\rho^{(m)}\}} \,. \tag{5.24}$$

The density matrix after the measurement is then used as initial state for the next iteration, and the ratio of measured particles divided by measurement time gives a current estimate $I(t) \approx \frac{\Delta n}{\Delta t}$. Such current trajectories are used to track the full counting statistics through quantum point contacts, see Fig. 5.4

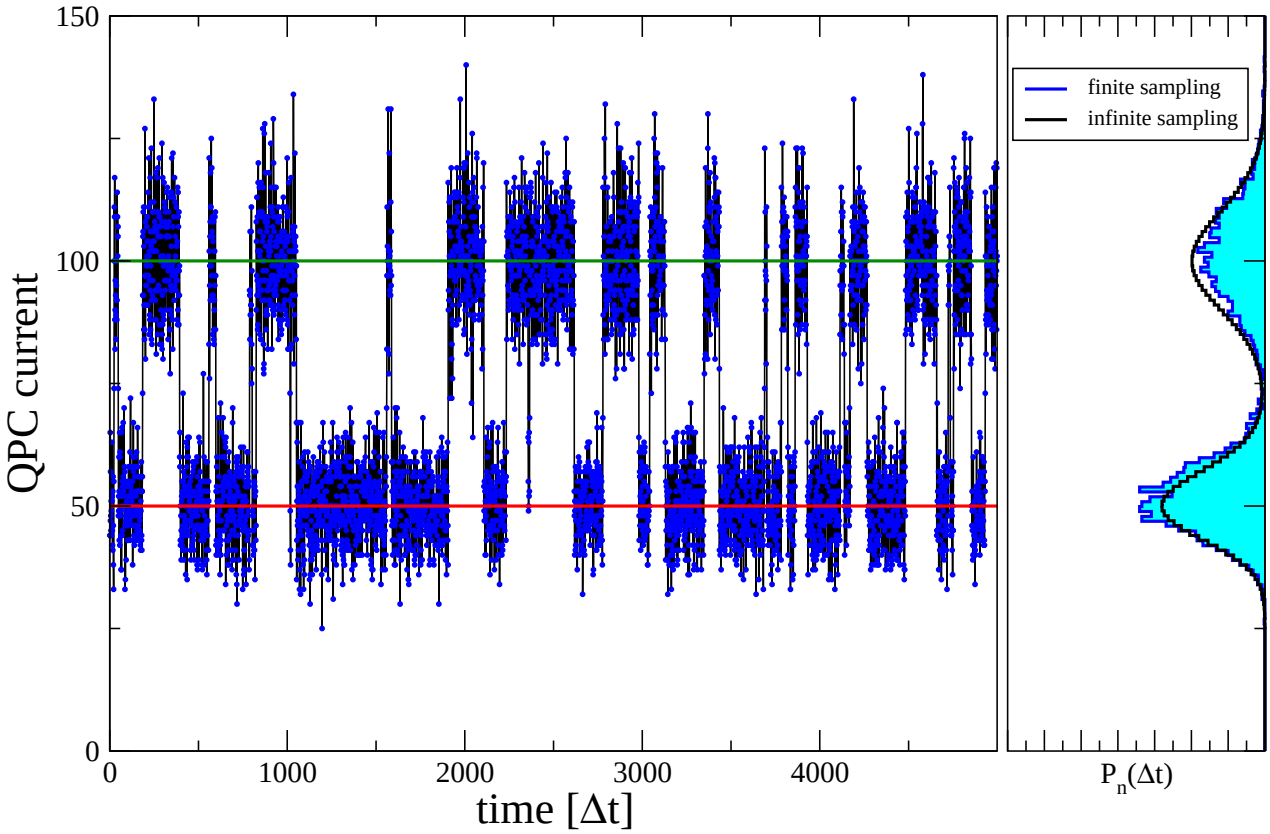

Figure 5.4: Numerical simulation of the time-resolved QPC current for a fluctuating dot occupation. At infinite SET bias, the QPC current allows to reconstruct the full counting statistics of the SET, since each current blip from low (red line) to high (green line) current corresponds to an electron leaving the SET to its right junction. Parameters: $\Gamma_L \Delta t = \Gamma_R \Delta t = 0.01$, $\gamma_{12}(0) = |1+\tilde{\tau}|^2 \gamma_{12}(0) = 0$, $\gamma_{21}(0) = 100.0$, $|1+\tilde{\tau}|^2 \gamma_{21}(0) = 50.0$, $f_L = 1.0$, $f_R = 0.0$. The right panel shows the corresponding probability distribution $P_n(\Delta t)$ versus $n = I\Delta t$, where the blue curve is sampled from the left panel and the black curve is the theoretical limit for infinitely long times.

5.2 Monitored charge qubit

A quantum point contact may also be used to monitor a nearby charge qubit, see Fig. 5.5. The

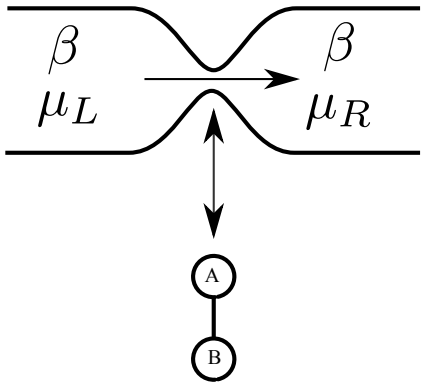

Figure 5.5: Sketch of a quantum point contact monitoring a double quantum dot with a single electron loaded (charge qubit). The current through the quantum point contact is modified by the position of the charge qubit electron, i.e., a measurement in the σ^z basis is performed.

QPC performs a measurement of the electronic position, since its current is highly sensitive on it. This corresponds to a σ^x measurement performed on the qubit. However, the presence of a detector does of course also lead to a back-action on the probed system. Here, we will derive a master equation for the system to quantify this back-action.

The Hamiltonian of the charge qubit is given by

$$H_{\rm CQB} = \epsilon_A d_A^\dagger d_A + \epsilon_B d_B^\dagger d_B + T\left(d_A d_B^\dagger + d_B d_A^\dagger\right) , \tag{5.25}$$

where we can safely neglect Coulomb interaction, since to form a charge qubit, the number of electrons on this double quantum dot is fixed to one. The matrix representation is therefore just two-dimensional in the $|n_A, n_B\rangle \in \{|10\rangle, |01\rangle\}$ basis and can be expressed by Pauli matrices

$$H_{\rm CQB} = \begin{pmatrix} \epsilon_A & T \\ T & \epsilon_B \end{pmatrix} = \frac{\epsilon_A + \epsilon_B}{2}\mathbf{1} + \frac{\epsilon_A - \epsilon_B}{2}\sigma^z + T\sigma^x \equiv \epsilon\mathbf{1} + \Delta\sigma^z + T\sigma^x , \tag{5.26}$$

i.e., we may identify $d_A^\dagger d_A = \frac{1}{2}(\mathbf{1} + \sigma^z)$ and $d_B^\dagger d_B = \frac{1}{2}(\mathbf{1} - \sigma^z)$. The tunneling part of the QPC Hamiltonian reads

$$\mathcal{H}_{\rm I} \;=\; d_A^\dagger d_A \otimes \sum_{kk'} t^A_{kk'}\gamma_{kL}\gamma^\dagger_{k'R} + d_B^\dagger d_B \otimes \sum_{kk'} t^B_{kk'}\gamma_{kL}\gamma^\dagger_{k'R} + \text{h.c.} , \tag{5.27}$$

where $t^{A/B}_{kk'}$ represents the tunneling amplitudes when the electron is localized on dots A and B, respectively. After representing the charge qubit in terms of Pauli matrices, the full Hamiltonian

reads

$$\begin{aligned} H &= \epsilon\mathbf{1} + \Delta\sigma^z + T\sigma^x \\ &\quad + \frac{1}{2}\left[\mathbf{1}+\sigma^z\right] \otimes \left[\sum_{kk'} t^A_{kk'}\gamma_{kL}\gamma^\dagger_{k'R} + \sum_{kk'} t^{A*}_{kk'}\gamma_{k'R}\gamma^\dagger_{kL}\right] \\ &\quad + \frac{1}{2}\left[\mathbf{1}-\sigma^z\right] \otimes \left[\sum_{kk'} t^B_{kk'}\gamma_{kL}\gamma^\dagger_{k'R} + \sum_{kk'} t^{B*}_{kk'}\gamma_{k'R}\gamma^\dagger_{kL}\right] \\ &\quad + \sum_k \varepsilon_{kL}\gamma^\dagger_{kL}\gamma_{kL} + \sum_k \varepsilon_{kR}\gamma^\dagger_{kR}\gamma_{kR}\,. \end{aligned} \tag{5.28}$$

To reduce the number of correlation functions we again assume that all tunneling amplitudes are modified equally $t^A_{kk'} = \tilde{\tau}_A t_{kk'}$ and $t^B_{kk'} = \tilde{\tau}_B t_{kk'}$ with baseline tunneling amplitudes $t_{kk'}$ and real constants τ_A and τ_B. Then, only a single correlation function needs to be calculated

$$\mathcal{H}_{\rm I} = \left[\frac{\tilde{\tau}_A}{2}\left(\mathbf{1}+\sigma^z\right) + \frac{\tilde{\tau}_B}{2}\left(\mathbf{1}-\sigma^z\right)\right] \otimes \left[\sum_{kk'} t_{kk'}\gamma_{kL}\gamma^\dagger_{k'R} + \sum_{kk'} t^*_{kk'}\gamma_{k'R}\gamma^\dagger_{kL}\right], \tag{5.29}$$

which becomes explicitly

$$\begin{aligned} C(\tau) &= \left\langle \sum_{kk'\ell\ell'} \left[t_{kk'}\gamma_{kL}\gamma^\dagger_{k'R}e^{-{\rm i}(\varepsilon_{kL}-\varepsilon_{k'R})\tau} + t^*_{kk'}\gamma_{k'R}\gamma^\dagger_{kL}e^{+{\rm i}(\varepsilon_{kL}-\varepsilon_{k'R})\tau}\right]\left[t_{\ell\ell'}\gamma_{\ell L}\gamma^\dagger_{\ell' R} + t^*_{\ell\ell'}\gamma_{\ell' R}\gamma^\dagger_{\ell L}\right]\right\rangle \\ &= \sum_{kk'}|t_{kk'}|^2\left[e^{-{\rm i}(\varepsilon_{kL}-\varepsilon_{k'R})\tau}\left\langle\gamma_{kL}\gamma^\dagger_{k'R}\gamma_{k'R}\gamma^\dagger_{kL}\right\rangle + e^{+{\rm i}(\varepsilon_{kL}-\varepsilon_{k'R})\tau}\left\langle\gamma_{k'R}\gamma^\dagger_{kL}\gamma_{kL}\gamma^\dagger_{k'R}\right\rangle\right] \\ &= \frac{1}{2\pi}\int d\omega d\omega' T(\omega,\omega')\left[e^{-{\rm i}(\omega-\omega')\tau}[1-f_L(\omega)]f_R(\omega') + e^{+{\rm i}(\omega-\omega')\tau}f_L(\omega)[1-f_R(\omega')]\right] \end{aligned} \tag{5.30}$$

where we have in the last step replaced the summation by a continuous integration with $T(\omega,\omega') = 2\pi\sum_{kk'}|t_{kk'}|^2\delta(\omega-\varepsilon_{kL})\delta(\omega'-\varepsilon_{k'R})$. We directly conclude for the Fourier transform of the bath correlation function

$$\begin{aligned} \gamma(\Omega) &= \int d\omega d\omega' T(\omega,\omega')\left[\delta(\Omega-\omega+\omega')[1-f_L(\omega)]f_R(\omega') + \delta(\Omega+\omega-\omega')f_L(\omega)[1-f_R(\omega')]\right] \\ &= \int d\omega\left[T(\omega,\omega-\Omega)[1-f_L(\omega)]f_R(\omega-\Omega) + T(\omega,\omega+\Omega)f_L(\omega)[1-f_R(\omega+\Omega)]\right]. \end{aligned} \tag{5.31}$$

In what follows, we will consider the wideband limit $T(\omega,\omega') = 1$ (the weak-coupling limit enters the $\tilde{\tau}_{A/B}$ parameters), such that we may directly use the result from the previous section

$$\gamma(\Omega) = \frac{\Omega+V}{1-e^{-\beta(\Omega+V)}} + \frac{\Omega-V}{1-e^{-\beta(\Omega-V)}}, \tag{5.32}$$

where $V = \mu_L - \mu_R$ denotes the bias voltage of the quantum point contact. Since we are not interested in its counting statistics here, we need not introduce any counting fields. The derivation of the master equation in the system energy eigenbasis requires diagonalization of the system Hamiltonian first

$$\begin{aligned} E_- &= \epsilon - \sqrt{\Delta^2+T^2}, \qquad |-\rangle = \frac{\Delta-\sqrt{\Delta^2+T^2}\,|0\rangle + T\,|1\rangle}{\sqrt{T^2+\left(\Delta-\sqrt{\Delta^2+T^2}\right)^2}} \\ E_+ &= \epsilon + \sqrt{\Delta^2+T^2}, \qquad |+\rangle = \frac{\Delta+\sqrt{\Delta^2+T^2}\,|0\rangle + T\,|1\rangle}{\sqrt{T^2+\left(\Delta+\sqrt{\Delta^2+T^2}\right)^2}}. \end{aligned} \tag{5.33}$$

Exercise 39 (Diagonalization of a single-qubit Hamiltonian) *(1 points)*
Calculate eigenvalues and eigenvectors of the system Hamiltonian.

Following the Born-, Markov-, and secular approximations – compare definition 7 – we obtain a Lindblad Master equation for the qubit

$$\dot{\rho} = -\mathrm{i}\left[\mathcal{H}_{\mathrm{S}} + H_{\mathrm{LS}}, \rho\right] + \sum_{abcd} \gamma_{ab,cd} \left[|a\rangle\langle b| \, \rho \, (|c\rangle\langle d|)^{\dagger} - \frac{1}{2}\left\{ (|c\rangle\langle d|)^{\dagger} |a\rangle\langle b| \, , \rho \right\} \right] , \tag{5.34}$$

where the summation only goes over the two energy eigenstates and H_{LS} denotes the frequency renormalization. Since the two eigenvalues of our system are non-degenerate, the Lamb-shift Hamiltonian is diagonal in the system energy eigenbasis and does not affect the dynamics of the populations, which decouples according to the rate equation

$$\dot{\rho}_{aa} = \sum_{b} \gamma_{ab,ab}\rho_{bb} - \left[\sum_{b} \gamma_{ba,ba} \right] \rho_{aa} \tag{5.35}$$

completely from the coherences. In particular, we have

$$\begin{aligned} \dot{\rho}_{--} &= \gamma_{--,--}\rho_{--} + \gamma_{-+,-+}\rho_{++} - \gamma_{--,--}\rho_{--} - \gamma_{+-,+-}\rho_{--} \\ &= \gamma_{-+,-+}\rho_{++} - \gamma_{+-,+-}\rho_{--} \, , \\ \dot{\rho}_{++} &= \gamma_{+-,+-}\rho_{--} - \gamma_{-+.-+}\rho_{++} \, , \end{aligned} \tag{5.36}$$

which when written as a matrix becomes

$$\begin{pmatrix} \dot{\rho}_{--} \\ \dot{\rho}_{++} \end{pmatrix} = \begin{pmatrix} -\gamma_{+-,+-} & +\gamma_{-+,-+} \\ +\gamma_{+-,+-} & -\gamma_{-+,-+} \end{pmatrix} \begin{pmatrix} \rho_{--} \\ \rho_{++} \end{pmatrix} . \tag{5.37}$$

The required dampening coefficients read

$$\begin{aligned} \gamma_{-+,-+} &= \gamma(E_+ - E_-)|\langle -| \, A \, |+\rangle|^2 = \gamma(+2\sqrt{\Delta^2 + T^2}) \frac{T^2}{4(\Delta^2 + T^2)} \left(\tilde{\tau}_A - \tilde{\tau}_B\right)^2 \, , \\ \gamma_{+-,+-} &= \gamma(E_- - E_+)|\langle +| \, A \, |-\rangle|^2 = \gamma(-2\sqrt{\Delta^2 + T^2}) \frac{T^2}{4(\Delta^2 + T^2)} \left(\tilde{\tau}_A - \tilde{\tau}_B\right)^2 . \end{aligned} \tag{5.38}$$

Exercise 40 (Qubit Dissipation) *(1 points)*
Show the validity of Eqns. (5.38).

This shows that when the QPC current is not dependent on the qubit state $\tilde{\tau}_A = \tilde{\tau}_B$, the dissipation on the qubit vanishes completely, which is consistent with our initial interaction Hamiltonian. In addition, in the pure dephasing limit $T \to 0$, we do not have any dissipative back-action of the measurement device on the qubit. Equation (5.37) obviously also preserves the trace of the density matrix. The stationary density matrix is therefore defined by

$$\frac{\bar{\rho}_{++}}{\bar{\rho}_{--}} = \frac{\gamma_{+-,+-}}{\gamma_{-+,-+}} = \frac{\gamma(-2\sqrt{\Delta^2 + T^2})}{\gamma(+2\sqrt{\Delta^2 + T^2})} . \tag{5.39}$$

When the QPC bias voltage vanishes (at equilibrium), we have

$$\frac{\gamma(-2\sqrt{\Delta^2+T^2})}{\gamma(+2\sqrt{\Delta^2+T^2})} \to e^{-\beta 2\sqrt{\Delta^2+T^2}} = e^{-\beta(E_+-E_-)}\,, \tag{5.40}$$

i.e., the qubit thermalizes with the temperature of the QPC. When the QPC bias voltage is large, the qubit is driven away from this thermal state.

Exercise 41 (Strongly monitored qubit) *(1 points)*
Calculate the stationary qubit state in the infinite bias regimes $V \to \pm\infty$.

The evolution of coherences decouples from the diagonal elements of the density matrix. The hermiticity of the density matrix allows to consider only one coherence

$$\begin{aligned}\dot\rho_{-+} &= -\mathrm{i}\left(E_- + \Delta E_- - E_+ - \Delta E_+\right)\rho_{-+} \\ &\quad + \left[\gamma_{--,++} - \frac{1}{2}\left(\gamma_{--,--}+\gamma_{++,++}+\gamma_{-+,-+}+\gamma_{+-,+-}\right)\right]\rho_{-+}\,,\end{aligned} \tag{5.41}$$

where $\Delta E_\pm$ corresponds to the energy renormalization due to the Lamb-shift, which induces a frequency renormalization of the qubit. The real part of the above equation is responsible for the dampening of the coherence, its calculation requires the evaluation of all remaining nonvanishing dampening coefficients

$$\begin{aligned}\gamma_{-+,-+}+\gamma_{+-,+-} &= \left[\gamma(+2\sqrt{\Delta^2+T^2})+\gamma(-2\sqrt{\Delta^2+T^2})\right]\frac{T^2}{4(T^2+\Delta^2)}\left(\tilde\tau_A-\tilde\tau_B\right)^2\,, \\ \gamma_{--,--}+\gamma_{++,++}-2\gamma_{--,++} &= \gamma(0)\frac{\Delta^2}{T^2+\Delta^2}\left(\tilde\tau_A-\tilde\tau_B\right)^2\,.\end{aligned} \tag{5.42}$$

Using the decomposition of the dampening, we may now calculate the decoherence rate

$$\begin{aligned}\gamma &= \frac{1}{2}\left(\gamma_{-+,-+}+\gamma_{+-,+-}\right)+\frac{1}{2}\left(\gamma_{--,--}+\gamma_{++,++}-2\gamma_{--,++}\right) \\ &= \frac{\left(\tilde\tau_A-\tilde\tau_B\right)^2}{8}\frac{T^2}{\Delta^2+T^2}\Big\{\left(V+2\sqrt{\Delta^2+T^2}\right)\coth\left[\frac{\beta}{2}\left(V+2\sqrt{\Delta^2+T^2}\right)\right] \\ &\quad +\left(V-2\sqrt{\Delta^2+T^2}\right)\coth\left[\frac{\beta}{2}\left(V-2\sqrt{\Delta^2+T^2}\right)\right]\Big\} \\ &\quad +\frac{\left(\tilde\tau_A-\tilde\tau_B\right)^2}{2}\frac{\Delta^2}{\Delta^2+T^2}V\coth\left[\frac{\beta V}{2}\right]\,,\end{aligned} \tag{5.43}$$

which vanishes as reasonably expected when we set $\tilde\tau_A=\tilde\tau_B$. Noting that $x\coth(x)\geq 1$ does not only prove its positivity (i.e., the coherences always decay) but also enables one to obtain a rough lower bound

$$\gamma \geq \frac{\left(\tilde\tau_A-\tilde\tau_B\right)^2}{2\beta}\frac{T^2+2\Delta^2}{T^2+\Delta^2} \tag{5.44}$$

on the dephasing rate. This lower bound is valid when the QPC voltage is rather small. For large voltages $|V|\gg\sqrt{\Delta^2+T^2}$, the dephasing rate is given by

$$\gamma \approx \frac{\left(\tilde\tau_A-\tilde\tau_B\right)^2}{2}\frac{T^2+2\Delta^2}{T^2+\Delta^2}|V| \tag{5.45}$$

and thus is limited by the voltage rather than the temperature.

Chapter 6

Open-loop control: Non-Equilibrium Case III

Time-dependent equations of the form

$$\dot{\rho} = \mathcal{L}(t)\rho(t) \tag{6.1}$$

are notoriously difficult to solve unless $\mathcal{L}(t)$ fulfills special properties. One such special case is e.g. the case of commuting superoperators, where the solution can be obtained from the exponential of an integral

$$[\mathcal{L}(t), \mathcal{L}(t')] = \mathbf{0} \qquad \Longrightarrow \qquad \rho(t) = \exp\left(-\mathrm{i}\int_0^t \mathcal{L}(t')dt'\right)\rho_0\,. \tag{6.2}$$

Another special case is one with a very slow time-dependence and a unique stationary state $\mathcal{L}(t)\bar{\rho}_t = 0$, where the time-dependent density matrix can be assumed to adiabatically follow the stationary state $\rho(t) \approx \bar{\rho}_t$. For fast time-dependencies, there exists the analytically solvable case of a train of δ-kicks

$$\mathcal{L}(t) = \mathcal{L}_0 + \sum_{i=1}^{\infty} \ell_i \delta(t - t_i)\,, \tag{6.3}$$

where the solution reads $(t_n < t < t_{n+1})$

$$\rho(t) = e^{\mathcal{L}_0(t-t_n)}\left[e^{\ell_n} e^{\mathcal{L}_0(t_n - t_{n-1})}\right] \times \ldots \times \left[e^{\ell_2} e^{\mathcal{L}_0(t_2-t_1)}\right]\left[e^{\ell_1} e^{\mathcal{L}_0(t_1)}\right]\rho_0\,, \tag{6.4}$$

which can be considerably simplified using e.g. Baker-Campbell-Haussdorff relations when the kicks are identical $\ell_i = \ell$.

Here, we will be concerned with piecewise-constant time-dependencies, such that the problem can be mapped to ordinary differential equations with constant coefficients, which are evolved a certain amount of time. After an instantaneous switch of the coefficients, one simply has initial conditions taken from the final state of the last evolution period, which can be evolved further and so on.

6.1 Single junction

The simplest model to study counting statistics is that of a single junction. Not making the microscopic model explicit, it will in the small tunneling limit obey the equations

$$\dot{P}_n = +\gamma P_{n-1}(t) + \bar{\gamma} P_{n+1} - \left[\gamma + \bar{\gamma}\right] P_n(t)\,, \tag{6.5}$$

where $P_n(t)$ denotes the probability to have n particles passed the junction after time t. Accordingly, γ represents the tunneling rate from left to right and $\bar{\gamma}$ the opposite tunneling rate, see Fig. 6.1. Depending on the microscopic underlying model, these parameters may depend on parti-

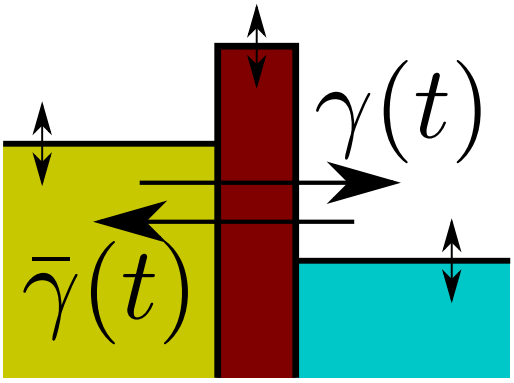

Figure 6.1: Sketch of a single junction with left-to-right and right-to-left tunneling rates γ and $\bar{\gamma}$, respectively. These parameters can be changed in a time-dependent manner by modifying the microscopic model (double-headed arrows).

cle concentrations on left and right side of the tunneling barrier and on the height of the barrier etc and may thus be modified in time. First let us consider the time-independent case. After Fourier transformation $P(\chi,t)=\sum_n P_n(t)e^{+in\chi}$, the n-resolved equation becomes

$$\dot{P}(\chi,t)=\left[\gamma(e^{+i\chi}-1)+\bar{\gamma}(e^{-i\chi}-1)\right]P(\chi,t)\,. \tag{6.6}$$

This is thus in perfect agreement with what we had for the quantum point contact statistics in Eq. (5.19). With the initial condition $P(\chi,0)=1$ it is solved by

$$P(\chi,t)=\exp\left\{\left[\gamma(e^{+i\chi}-1)+\bar{\gamma}(e^{-i\chi}-1)\right]t\right\}\,. \tag{6.7}$$

Exercise 42 (Cumulants) *(1 points)*
Show that the cumulants of the probability distribution $P_n(t)$ are given by

$$\left\langle\left\langle n^k\right\rangle\right\rangle=\left[\gamma+(-1)^k\bar{\gamma}\right]t\,.$$

This initial condition is chosen because we assume that at time $t=0$, no particle has crossed the junction $P_n(0)=\delta_{n,0}$. The probability to count n particles after time t can be obtained from the inverse Fourier transform

$$P_n(t)=\frac{1}{2\pi}\int_{-\pi}^{+\pi}\exp\left\{\left[\gamma(e^{+i\chi}-1)+\bar{\gamma}(e^{-i\chi}-1)\right]t\right\}e^{-in\chi}d\chi\,. \tag{6.8}$$

This probability can for this onedimensional model be calculated analytically even in the case of

bidirectional transport

$$\begin{aligned} P_n(t) &= e^{-(\gamma+\bar{\gamma})t} \sum_{a,b=0}^{\infty} \frac{(\gamma t)^a}{a!} \frac{(\bar{\gamma} t)^b}{b!} \frac{1}{2\pi} \int_{-\pi}^{+\pi} e^{+\mathrm{i}(a-b-n)\chi} d\chi \\ &= e^{-(\gamma+\bar{\gamma})t} \sum_{a,b=0}^{\infty} \frac{(\gamma t)^a}{a!} \frac{(\bar{\gamma} t)^b}{b!} \delta_{a-b,n} \\ &= e^{-(\gamma+\bar{\gamma})t} \begin{cases} \sum_{a=n}^{\infty} \frac{(\gamma t)^a}{a!} \frac{(\bar{\gamma} t)^{a-n}}{(a-n)!} & : \quad n \geq 0 \\ \sum_{a=0}^{\infty} \frac{(\gamma t)^a}{a!} \frac{(\bar{\gamma} t)^{a-n}}{(a-n)!} & : \quad n < 0 \end{cases} \\ &= e^{-(\gamma+\bar{\gamma})t} \left(\frac{\gamma}{\bar{\gamma}}\right)^{n/2} \mathcal{J}_n(2\sqrt{\gamma\bar{\gamma}}t)\,, \end{aligned} \tag{6.9}$$

where $\mathcal{J}_n(x)$ denotes a modified Bessel function of the first kind – defined as the solution of

$$z^2 \mathcal{J}_n''(z) + z\mathcal{J}_n'(z) - (z^2 + n^2)\mathcal{J}_n(z) = 0\,. \tag{6.10}$$

In the unidirectional transport limit, this reduces to a normal Poissonian distribution

$$\lim_{\bar{\gamma}\to 0} P_n(t) = \begin{cases} e^{-\gamma t} \frac{(\gamma t)^n}{n!} & : \quad n \geq 0 \\ 0 & : \quad n < 0 \end{cases}\,. \tag{6.11}$$

Exercise 43 (Poissonian limit) *(1 points)*
Show the Poissonian distribution in the unidirectional transport limit.

Now we consider the case of a time-dependent rate $\gamma \to \gamma(t)$ with a piecewise-constant time dependence and for simplicity constrain ourselves to unidirectional transport as shown in Fig. 6.2. The fact that the model is scalar (has no internal structure) implies that the probability distribution

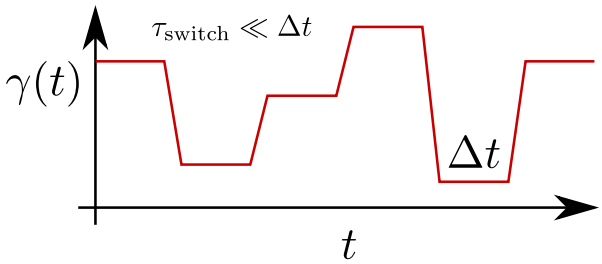

Figure 6.2: Time-dependent tunneling rate which is (nearly) piecewise constant during the intervals Δt. In the model, we neglect the switching time τ_{switch} completely.

of measuring particles in the αth time interval is completely independent from the outcome of the interval $\alpha - 1$. If we denote the cumulant during the interval Δt in the α-th interval by $\langle\langle n^k \rangle\rangle_\alpha$, we find for the average

$$\langle\langle \bar{n^k} \rangle\rangle = \frac{1}{N} \sum_{\alpha=1}^{N} \langle\langle n^k \rangle\rangle_\alpha = \frac{1}{N} \sum_{\alpha=1}^{N} \gamma_\alpha \Delta t = \langle\gamma\rangle\, \Delta t\,, \tag{6.12}$$

i.e., the average cumulant is simply described by an average tunneling rate – regardless of the actual form of the protocol.

6.2 Electronic pump

We consider a system with the simplest possible internal structure, which has just the two states empty and filled. A representative of such a system is the single-electron transistor. The tunneling of electrons through such a transistor is stochastic and thereby in some sense uncontrolled. This implies that e.g. the current fluctuations through such a device (noise) can not be suppressed completely.

6.2.1 Time-dependent tunneling rates

We consider piecewise-constant time-dependencies of the tunneling rates $\Gamma_L(t)$ and $\Gamma_R(t)$ with an otherwise arbitrary protocol

$$\mathcal{L}(\chi,t)=\begin{pmatrix} -\Gamma_L(t)f_L-\Gamma_R(t)f_R & +\Gamma_L(t)(1-f_L)+\Gamma_R(t)(1-f_R)e^{+\mathrm{i}\chi} \\ +\Gamma_L(t)f_L+\Gamma_R(t)f_R e^{-\mathrm{i}\chi} & -\Gamma_L(t)(1-f_L)-\Gamma_R(t)(1-f_R)\end{pmatrix}. \tag{6.13}$$

The situation is also depicted in Fig. 6.3.

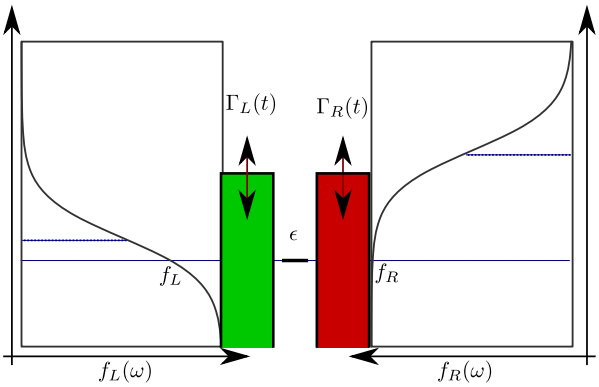

Figure 6.3: Time-dependent tunneling rates which follow a piecewise constant protocol. Dot level and left and right Fermi functions are assumed constant.

Let the tunneling rates during the i-th time interval be denoted by Γ_L^i and Γ_R^i and the corresponding constant Liouvillian during this time interval by $\mathcal{L}_i(\chi)$. The density matrix after the time interval Δt is now given by

$$\rho_{i+1}=e^{\mathcal{L}_i(0)\Delta t}\rho_i\,, \tag{6.14}$$

such that it has no longer the form of a master equation but becomes a fixed-point iteration. In what follows, we will without loss of generality assume $f_L\leq f_R$, such that the source lead is right and the drain lead is left. Utilizing previous results, the stationary state of the Liouvillian $\mathcal{L}_i$ is given by

$$\bar{f}_i=\frac{\Gamma_L^i f_L+\Gamma_R^i f_R}{\Gamma_L^i+\Gamma_R^i} \tag{6.15}$$

and thereby ($\Gamma_{L/R}^i\geq 0$) obeys $f_L\leq\bar{f}_i\leq f_R$. This implies that after a few transient iterations, the density vector will hover around within the transport window

$$f_L\leq n_i=\left\langle d^\dagger d\right\rangle_i\leq f_R\qquad\forall\qquad i\geq i^*\,. \tag{6.16}$$

The occupations will therefore follow the iteration equation

$$\begin{pmatrix}1-n_{i+1}\\ n_{i+1}\end{pmatrix}=e^{\mathcal{L}_i(0)\Delta t}\begin{pmatrix}1-n_i\\ n_i\end{pmatrix}. \tag{6.17}$$

To calculate the number of particles tunneling into the source reservoir, we consider the moment-generating function

$$\mathcal{M}_i(\chi,\Delta t)=\mathrm{Tr}\left\{e^{\mathcal{L}_i(\chi)\Delta t}\begin{pmatrix}1-n_i\\ n_i\end{pmatrix}\right\} \tag{6.18}$$

and calculate the first moment

$$\begin{aligned}\langle n\rangle_i &= (-\mathrm{i})\partial_\chi\,\mathcal{M}_i(\chi,\Delta t)|_{\chi=0}\\ &= \frac{1}{(\Gamma_L^i+\Gamma_R^i)^2}\Big[-\Gamma_R^2(f_R-n_i)\left(1-e^{-(\Gamma_L^i+\Gamma_R^i)\Delta t}\right)\\ &\quad+\Gamma_L^i\Gamma_R^i\left((n_i-f_L)\left(1-e^{-(\Gamma_L^i+\Gamma_R^i)\Delta t}\right)-(f_R-f_L)(\Gamma_L^i+\Gamma_R^i)\Delta t\right)\Big]\le 0\,.\end{aligned} \tag{6.19}$$

The first term is evidently negative when n_i is within the transport window $f_L\le n_i\le f_R$, and that the second term is also negative follows from its upper bound $n_i\to f_R$, where we can use that $1-e^{-x}\le x$ for all $x\ge 0$ which is the case for $x=(\Gamma_L^i+\Gamma_R^i)\Delta t$.

It follows that the average current always points from right (source for constant rates) to left (drain for constant rates) regardless of the actual protocol $\Gamma_{L/R}^\alpha$ chosen. In other words: With simply modifying the tunneling rates (not taking into account whether the dot is occupied or not) it is not possible to revert the direction of the current.

6.2.2 With performing work

To obtain transport against the bias, it is therefore necessary to modify the Fermi functions e.g. by changing the chemical potentials or temperatures in the contacts. However, this first possibility may for fast driving destroy the thermal equilibrium in the contacts, such that we consider changing the dot level $\epsilon(t)$. Intuitively, it is quite straightforward to arrive at a protocol that should lift electrons from left to right and thereby pumps electrons from low to high chemical potentials, see Fig. 6.4. The propagators for the first and second half cycles read

$$\begin{aligned}\mathcal{L}_1(\chi) &= \begin{pmatrix}-\Gamma_L^{\max}f_L(\epsilon^{\min})-\Gamma_R^{\min}f_R(\epsilon^{\min}) & +\Gamma_L^{\max}[1-f_L(\epsilon^{\min})]+\Gamma_R^{\min}[1-f_R(\epsilon^{\min})]e^{+\mathrm{i}\chi}\\ +\Gamma_L^{\max}f_L(\epsilon^{\min})+\Gamma_R^{\min}f_R(\epsilon^{\min})e^{-\mathrm{i}\chi} & -\Gamma_L^{\max}[1-f_L(\epsilon^{\min})]-\Gamma_R^{\min}[1-f_R(\epsilon^{\min})]\end{pmatrix},\\ \mathcal{L}_2(\chi) &= \begin{pmatrix}-\Gamma_L^{\min}f_L(\epsilon^{\max})-\Gamma_R^{\max}f_R(\epsilon^{\max}) & +\Gamma_L^{\min}[1-f_L(\epsilon^{\max})]+\Gamma_R^{\max}[1-f_R(\epsilon^{\max})]e^{+\mathrm{i}\chi}\\ +\Gamma_L^{\min}f_L(\epsilon^{\max})+\Gamma_R^{\max}f_R(\epsilon^{\max})e^{-\mathrm{i}\chi} & -\Gamma_L^{\min}[1-f_L(\epsilon^{\max})]-\Gamma_R^{\max}[1-f_R(\epsilon^{\max})]\end{pmatrix},\end{aligned} \tag{6.20}$$

respectively. The evolution of the density vector now follows the fixed point iteration scheme

$$\rho(t+T)=\mathcal{P}_2\mathcal{P}_1\rho(t)=e^{\mathcal{L}_2(0)T/2}e^{\mathcal{L}_1(0)T/2}\rho(t)\,. \tag{6.21}$$

After a period of transient evolution, the density vector at the end of the pump cycle will approach a value where $\rho(t+T)\approx\rho(t)=\bar\rho$. This value is the stationary density matrix in a stroboscopic sense and is defined by the eigenvalue equation

$$e^{\mathcal{L}_2(0)T/2}e^{\mathcal{L}_1(0)T/2}\bar\rho=\bar\rho \tag{6.22}$$

with $\mathrm{Tr}\{\bar\rho\}=1$. Once this stationary state has been determined, we can easily define the moment-generating functions for the pumping period in the (stroboscopically) stationary regime

$$\mathcal{M}_1(\chi,T/2)=\mathrm{Tr}\left\{e^{\mathcal{L}_1(\chi)T/2}\bar\rho\right\}\,,\qquad \mathcal{M}_2(\chi,T/2)=\mathrm{Tr}\left\{e^{\mathcal{L}_2(\chi)T/2}e^{\mathcal{L}_1(0)T/2}\bar\rho\right\}\,, \tag{6.23}$$

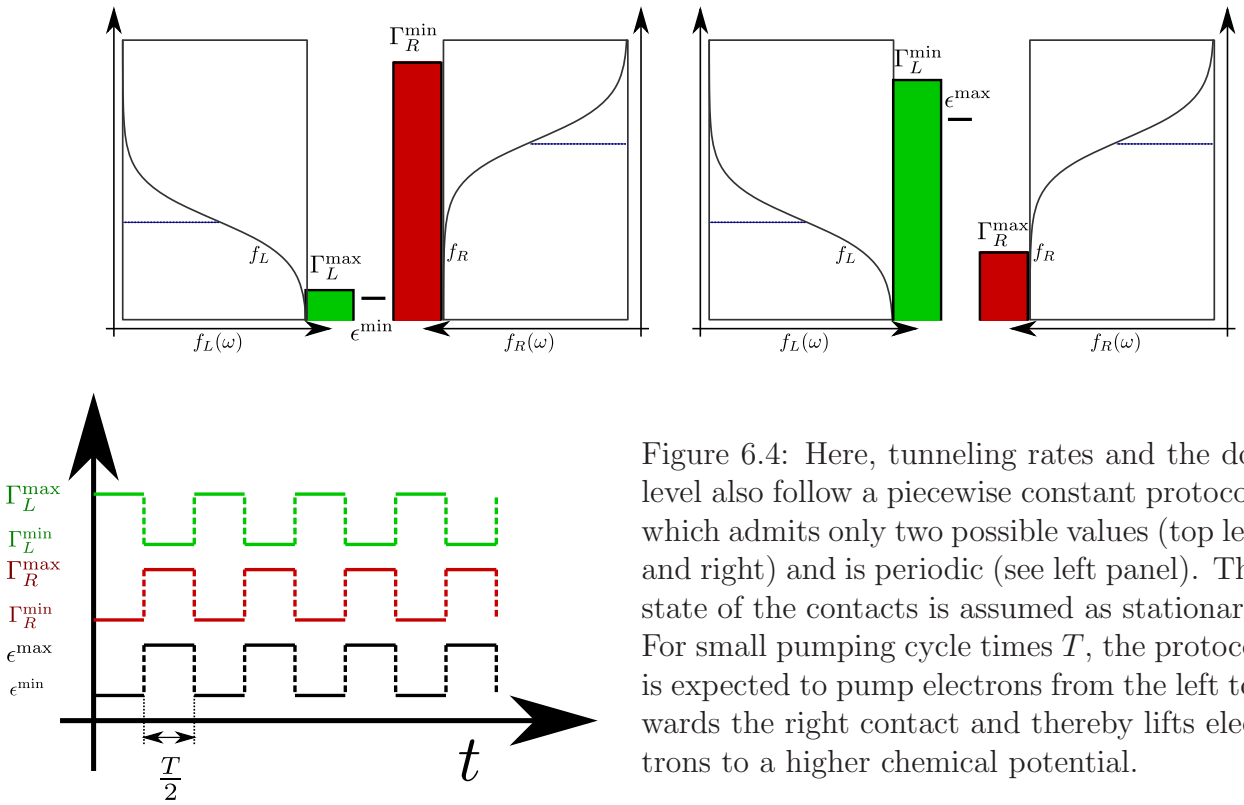

Figure 6.4: Here, tunneling rates and the dot level also follow a piecewise constant protocol, which admits only two possible values (top left and right) and is periodic (see left panel). The state of the contacts is assumed as stationary. For small pumping cycle times T, the protocol is expected to pump electrons from the left towards the right contact and thereby lifts electrons to a higher chemical potential.

where $\mathcal{M}_1$ describes the statistics in the first half cycle and $\mathcal{M}_2$ in the second half cycle and the moments can be extracted in the usual way. The distribution for the total number of particles tunneling during the complete pumping cycle $n = n_1 + n_2$ is given by

$$P_n(T) = \sum_{n_1,n_2\,:\,n_1+n_2=n} P_{n_1}(T/2)P_{n_2}(T/2) = \sum_{n_1,n_2} \delta_{n,n_1+n_2} P_{n_1}(T/2)P_{n_2}(T/2)\,. \tag{6.24}$$

Then, the first moment may be calculated by simply adding the first moments of the particles tunneling through both half-cycles

$$\begin{aligned}\langle n\rangle &= \sum_n nP_n = \sum_n n \sum_{n_1,n_2} \delta_{n,n_1+n_2} P_{n_1}(T/2)P_{n_2}(T/2) = \sum_{n_1,n_2} (n_1+n_2)P_{n_1}(T/2)P_{n_2}(T/2) \\ &= \langle n_1\rangle + \langle n_2\rangle\ .\end{aligned} \tag{6.25}$$

In the following, we will constrain ourselves for simplicity to symmetric tunneling rates $\Gamma_L^{\min} = \Gamma_R^{\min} = \Gamma^{\min}$ and $\Gamma_L^{\max} = \Gamma_R^{\max} = \Gamma^{\max}$. In this case, we obtain the simple expression for the average number of particles during one pumping cycle

$$\begin{aligned}\langle n\rangle &= \frac{\Gamma^{\max}\Gamma^{\min}}{\Gamma^{\max}+\Gamma^{\min}}\frac{T}{2}\left[f_L(\epsilon^{\max}) - f_R(\epsilon^{\max}) + f_L(\epsilon^{\min}) - f_R(\epsilon^{\min})\right] \\ &\quad + \frac{\Gamma^{\max}-\Gamma^{\min}}{\left(\Gamma^{\max}+\Gamma^{\min}\right)^2}\left[\Gamma^{\max}\left(f_L(\epsilon^{\min}) - f_R(\epsilon^{\max})\right) + \Gamma^{\min}\left(f_R(\epsilon^{\min}) - f_L(\epsilon^{\max})\right)\right] \times \\ &\quad \times \tanh\left[\frac{T}{4}\left(\Gamma^{\min}+\Gamma^{\max}\right)\right]\ .\end{aligned} \tag{6.26}$$

The first term (which dominates for slow pumping, i.e., large T) is negative when $f_L(\omega) < f_R(\omega)$. It is simply given by the average of the two SET currents one would obtain for the two half cycles.

The second term however is present when $\Gamma^{\max} > \Gamma^{\min}$ and may be positive when the dot level is changed strongly enough souch that $f_L(\epsilon^{\min}) > f_R(\epsilon^{\max})$ and $f_R(\epsilon^{\min}) > f_L(\epsilon^{\max})$. For large differences in the tunneling rates and small pumping times T it may even dominate the first term, such that the net particle number may be positive even though the bias would favor the opposite current direction, see Fig. 6.5. The second cumulant can be similarly calculated

$$\langle n^2 \rangle - \langle n \rangle^2 = \langle n_1^2 \rangle - \langle n_1 \rangle^2 + \langle n_2^2 \rangle - \langle n_2 \rangle^2 \ . \tag{6.27}$$

Exercise 44 (Second Cumulant for joint distributions) *(1 points)*
Show the validity of the above equation.

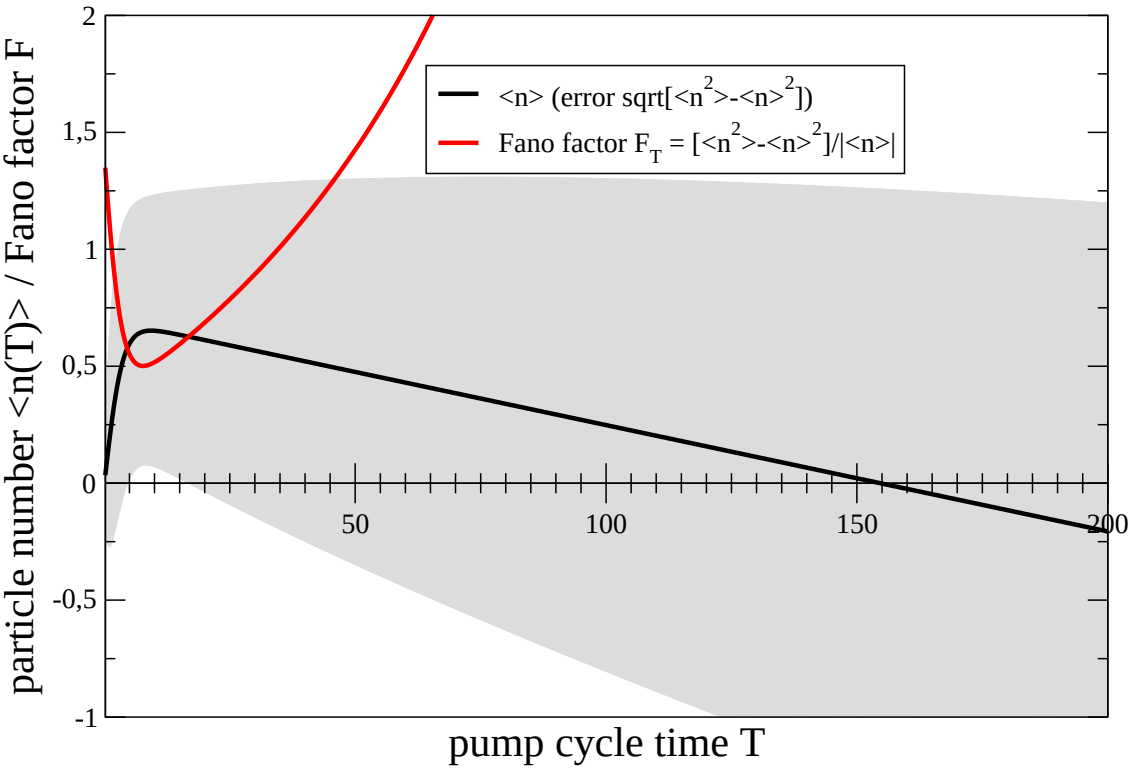

Figure 6.5: Average number of tunneled particles during one pump cycle. Parameters have been chosen as $\Gamma^{\max} = 1$, $\Gamma^{\min} = 0.1$, $f_L(\epsilon^{\min}) = 0.9$, $f_R(\epsilon^{\min}) = 0.95$, $f_L(\epsilon^{\max}) = 0$, $f_R(\epsilon^{\max}) = 0.05$, such that for slow pumping (large T), the current $I = \langle n \rangle / T$ must become negative. The shaded region characterizes the width of the distribution, and the Fano factor demonstrates that around the maximum pump current, the signal-to-noise ratio is most favorable.

When the dot level is shifted to very low and very large values (large pumping power), the bias is negligible (alternatively, we may also consider an unbiased situation from the beginning). In this case, we can assume $f_L(\epsilon^{\min}) = f_R(\epsilon^{\min}) = f(\epsilon^{\min})$ and $f_L(\epsilon^{\max}) = f_R(\epsilon^{\max}) = f(\epsilon^{\max})$. Then, the second term dominates always and the particle number simplifies to

$$\langle n \rangle = \left[f(\epsilon^{\min}) - f(\epsilon^{\max}) \right] \frac{\Gamma^{\max} - \Gamma^{\min}}{\Gamma^{\max} + \Gamma^{\min}} \tanh \left[\frac{T}{4} \left(\Gamma^{\min} + \Gamma^{\max} \right) \right] \ . \tag{6.28}$$

This becomes maximal for large pumping time and large power consumption ($f(\epsilon^{\min}) - f(\epsilon^{\max}) = 1$). In this idealized limit, we easily obtain for the Fano factor for large cycle times T

$$F_T = \frac{\langle n^2 \rangle - \langle n \rangle^2}{|\langle n \rangle|} \overset{T\to\infty}{\to} \frac{2\Gamma^{\max}\Gamma^{\min}}{\left(\Gamma^{\max} + \Gamma^{\min}\right)^2}\,, \tag{6.29}$$

which demonstrates that the pump works efficient and noiseless when $\Gamma^{\max} \gg \Gamma^{\min}$.

At infinite bias $f_L(\omega) =$ and $f_R(\omega) = 0$, the pump does not transport electrons against any potential or thermal gradient but can still be used to control the statistics of the tunneled electrons. For example, it is possible to reduce the noise to zero also in this limit when $\Gamma^{\min} \to 0$.

Chapter 7

Closed-loop control: Non-Equilibrium Case IV

Closed-loop (or feedback) control means that the system is monitored (either continuously or at certain times) and that the result of these measurements is fed back by changing some parameter of the system. Under measurement with outcome m (an index characterizing the possible outcomes), the density matrix transforms as

$$\rho \xrightarrow{m} \frac{M_m \rho M_m^\dagger}{\mathrm{Tr}\left\{M_m^\dagger M_m \rho\right\}}\,, \tag{7.1}$$

and the probability at which this outcome occurs is given by $\mathrm{Tr}\left\{M_m^\dagger M_m\right\}$. This can also be written in superoperator notation

$$\rho \xrightarrow{m} \frac{\mathcal{P}_m \rho}{\mathrm{Tr}\left\{\mathcal{P}_m \rho\right\}}\,. \tag{7.2}$$

Let us assume that conditioned on the measurement result m at time t, we apply a propagator for the time interval Δt. Then, a measurement result m at time t provided, the density matrix at time $t + \Delta t$ will be given by

$$\rho^{(m)}(t + \Delta t) = e^{\mathcal{L}^{(m)}\Delta t} \frac{\mathcal{P}_m \rho}{\mathrm{Tr}\left\{\mathcal{P}_m \rho\right\}}\,. \tag{7.3}$$

However, to obtain an effective description of the density matrix evolution, we have to average over all measurement outcomes – where we have to weight each outcome by the corresponding probability

$$\rho(t + \Delta t) = \sum_m \mathrm{Tr}\left\{\mathcal{P}_m \rho(t)\right\} e^{\mathcal{L}^{(m)}\Delta t} \frac{\mathcal{P}_m \rho}{\mathrm{Tr}\left\{\mathcal{P}_m \rho\right\}} = \sum_m e^{\mathcal{L}^{(m)}\Delta t} \mathcal{P}_m \rho(t)\,. \tag{7.4}$$

Note that this is an iteration scheme, the conditioned Liouvillian $\mathcal{L}^{(m)}$ may well depend on the time t (at which the measurement is performed) as long as it is constant during the interval $[t, t + \Delta t]$.

7.1 Single junction

To start with the simplest possible system, we reconsider here the case of a single junction in the unidirectional transport limit, which is described by

$$\dot{\rho}_n = \gamma \rho_{n-1} - \gamma \rho_n\,, \tag{7.5}$$

where the parameter γ describes the speed at which the resulting Poissonian distribution

$$\rho_n(\Delta t) = \begin{cases} e^{-\gamma\Delta t}\frac{(\gamma\Delta t)^n}{n!} & : \quad n \geq 0 \\ 0 & : \quad n < 0 \end{cases} \tag{7.6}$$

moves towards larger n. When we arrange the probabilities in an infinite-dimensional vector, the master equation becomes

$$\frac{d}{dt}\begin{pmatrix} \vdots \\ \rho_{n-1} \\ \rho_n \\ \vdots \end{pmatrix} = \begin{pmatrix} \ddots & & & \\ \ddots & -\gamma & & \\ & +\gamma & -\gamma & \\ & & \ddots & \ddots \end{pmatrix}\begin{pmatrix} \vdots \\ \rho_{n-1} \\ \rho_n \\ \vdots \end{pmatrix}. \tag{7.7}$$

For the initial state $\rho_n(0) = \delta_{n,0}$ we have written the solution explicitly. Using the translational invariance in n and the superposition principle, we can therefore write the general solution explicitly as

$$\begin{pmatrix} \rho_0(t+\Delta t) \\ \rho_1(t+\Delta t) \\ \rho_2(t+\Delta t) \\ \vdots \\ \rho_n(t+\Delta t) \\ \vdots \end{pmatrix} = e^{-\gamma\Delta t}\begin{pmatrix} 1 & & & \\ \gamma\Delta t & 1 & & \\ \frac{(\gamma\Delta t)^2}{2} & \gamma\Delta t & 1 & \\ \vdots & \vdots & \ddots & \ddots \\ \frac{(\gamma\Delta t)^n}{n!} & \frac{(\gamma\Delta t)^{n-1}}{(n-1)!} & \cdots & \cdots \\ \vdots & \vdots & & \end{pmatrix}\begin{pmatrix} \rho_0(t) \\ \rho_1(t) \\ \rho_2(t) \\ \vdots \\ \rho_n(t) \\ \vdots \end{pmatrix} \tag{7.8}$$

which takes the form $\boldsymbol{\rho}(t+\Delta t) = \mathcal{W}(\Delta t)\boldsymbol{\rho}(t)$ with the infinite-dimensional propagation matrix $\mathcal{W}(\Delta t)$.

Exercise 45 (Probability conservation) *(1 points)*
Show that the above introduced propagator $\mathcal{W}(\Delta t)$preserves the sum of all probabilities, i.e., that $\sum_n \rho_n(t+\Delta t) = \sum_n \rho_n(t)$.

We have found previously that an open-loop control scheme does not drastically modify the picture. We do now consider regular measurements of the number of tunneled particles being performed at time intervals Δt. The major difference to our previous considerations is now that we modify the tunneling rate γ in dependence on the initial state $\boldsymbol{\rho}(t)$ and on the time t, i.e., we have $\gamma \to \gamma_m(t)$, where m denotes the total number of particles measured at time t. Then, the propagation matrix becomes (omitting for brevity the dependence on t in the rates)

$$\mathcal{W}(t,\Delta t) = \begin{pmatrix} e^{-\gamma_0\Delta t} & & & \\ e^{-\gamma_0\Delta t}(\gamma_0\Delta t) & e^{-\gamma_1\Delta t} & & \\ e^{-\gamma_0\Delta t}\frac{(\gamma_0\Delta t)^2}{2} & e^{-\gamma_1\Delta t}(\gamma_1\Delta t) & e^{-\gamma_2\Delta t} & \\ \vdots & \vdots & \vdots & \ddots \\ e^{-\gamma_0\Delta t}\frac{(\gamma_0\Delta t)^n}{n!} & e^{-\gamma_1\Delta t}\frac{(\gamma_1\Delta t)^{n-1}}{(n-1)!} & e^{-\gamma_2\Delta t}\frac{(\gamma_2\Delta t)^{n-2}}{(n-2)!} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{7.9}$$

When we would denote the normal propagator in Eq. (7.8) with an index i as $\mathcal{W}^{(i)} = \mathcal{W}|_{\gamma=\gamma_i}$, the full effective feedback propagator can also be written as

$$\mathcal{W}(t,\Delta t) = \sum_n \mathcal{W}^{(n)}(t,\Delta t)\mathcal{P}^{(n)}\,, \tag{7.10}$$

where the matrix elements of the projection superoperator $\mathcal{P}^{(n)}_{ij} = \delta_{in}\delta_{jn}$ vanish except at position n on the diagonal.

Exercise 46 (Effective Feedback Propagator) *(1 points)*
Show the validity of Eq. (7.10).

This naturally includes the measurement process into the description of feedback: Measuring n tunneled particles at time t projects the density vector as

$$\rho(t) \to \frac{\mathcal{P}^{(n)}\rho(t)}{\mathrm{Tr}\left\{\mathcal{P}^{(n)}\rho(t)\right\}}\,, \tag{7.11}$$

which occurs with probability $\mathrm{Tr}\left\{\mathcal{P}^{(n)}\rho(t)\right\}$. When we compute the average outcome of such a measurement but do not perform any feedback, we have to multiply with the corresponding probability to obtain the average density matrix at time $t+\Delta t$

$$\bar{\rho}(t+\Delta t) = \sum_n \mathcal{W}(t,\Delta t)\mathcal{P}^{(n)}\rho(t) = \mathcal{W}(t,\Delta t)\rho(t)\,. \tag{7.12}$$

With feedback however, a propagator that is conditioned on the measurement result has to be applied

$$\bar{\rho}(t+\Delta t) = \sum_n \mathcal{W}^{(n)}(t,\Delta t)\mathcal{P}^{(n)}\rho(t)\,, \tag{7.13}$$

which corresponds to Eq. (7.10).

The matrix elements of the effective feedback propagatoor read

$$\mathcal{W}_{nm}(t,\Delta t) = \begin{cases} e^{-\gamma_m \Delta t}\frac{(\gamma_m\Delta t)^{(n-m)}}{(n-m)!} & : \quad n \geq m \\ 0 & : \quad n < m \end{cases}\,, \tag{7.14}$$

where e.g. one simple feedback protocol would be given by

$$\gamma_m(t) = \begin{cases} \gamma + \alpha\left(\gamma - \frac{m}{t}\right) & : \quad m \leq \gamma t\left[1+\frac{1}{\alpha}\right] \\ 0 & : \quad \text{else} \end{cases}\,. \tag{7.15}$$

Such a feedback protocol would aim to stabilize a mean of $m = \gamma t$ and should also keep the width of the distribution at a finite value. For general feedback protocols, we obtain for the first moment at time $t+\Delta t$

$$\begin{aligned} \langle n\rangle_{t+\Delta t} &= \sum_n n\rho_n(t+\Delta t) = \sum_n n\sum_m \mathcal{W}_{nm}(t,\Delta t)\rho_m(t) = \sum_m\left[\sum_n n\mathcal{W}_{nm}(t,\Delta t)\right]\rho_m(t) \\ &= \sum_m\left[\sum_{n=m}^{\infty} n e^{-\gamma_m\Delta t}\frac{(\gamma_m\Delta t)^{(n-m)}}{(n-m)!}\right]\rho_m(t) = \sum_m\left[\sum_{n=0}^{\infty}(n+m)e^{-\gamma_m\Delta t}\frac{(\gamma_m\Delta t)^n}{n!}\right]\rho_m(t) \\ &= \sum_m\left(\gamma_m\Delta t + m\right)\rho_m(t) = \langle\gamma_n\rangle_t\,\Delta t + \langle n\rangle_t\,, \end{aligned} \tag{7.16}$$

such that the change of the first moment during time interval Δt is determined by the average tunneling rate. Similarly, we obtain for the second moment

$$\begin{aligned}\left\langle n^2\right\rangle_{t+\Delta t} &= \sum_n n^2\rho_n(t+\Delta t) = \sum_m \left[\sum_{n=0}^{\infty}(n+m)^2 e^{-\gamma_m\Delta t}\frac{(\gamma_m\Delta t)^n}{n!}\right]\rho_m(t)\\ &= \sum_m \left[\gamma_m\Delta t\,(1+\gamma_m\Delta t)+2\gamma_m\Delta t m+m^2\right]\rho_m(t)\\ &= \left\langle\gamma_n^2\right\rangle_t\Delta t^2+\left\langle\gamma_n(1+2n)\right\rangle_t\Delta t+\left\langle n^2\right\rangle_t . \end{aligned} \tag{7.17}$$

This implies for the variance under feedback

$$\begin{aligned}\left\langle n^2\right\rangle_{t+\Delta t}-\left\langle n\right\rangle^2_{t+\Delta t} &= \Delta t^2\left[\left\langle\gamma_n^2\right\rangle_t-\left\langle\gamma_n\right\rangle_t^2\right]+\Delta t\left[\left\langle\gamma_n\right\rangle_t+2\left\langle\gamma_n n\right\rangle_t-2\left\langle\gamma_n\right\rangle_t\left\langle n\right\rangle_t\right]\\ &\quad+\left\langle n^2\right\rangle_t-\left\langle n\right\rangle_t^2 .\end{aligned} \tag{7.18}$$

For large Δt, the first term on the r.h.s. will dominate, such that due to $\left\langle\gamma_n^2\right\rangle_t-\left\langle\gamma_n\right\rangle_t^2=\left\langle\left(\gamma_n-\left\langle\gamma_n\right\rangle\right)^2\right\rangle\geq 0$ the variance will always increase. For small Δt however, the second term may dominate, such that for adapted feedback protocols, the variance of the distribution may decrease during Δt.

Exercise 47 (Variance evolution without feedback) *(1 points)*
Show that without feedback $\gamma_m(t)=\gamma$, the variance during the iteration will for arbitrary distributions always increase as $\left(\left\langle n^2\right\rangle_{t+\Delta t}-\left\langle n\right\rangle^2_{t+\Delta t}\right)-\left(\left\langle n^2\right\rangle_t-\left\langle n\right\rangle_t^2\right)=\gamma\Delta t$.

It is however clear that the resulting distribution cannot have a completely vanishing width, as for this case one would also obtain a growing variance in time.

Exercise 48 (Variance evolution of a localized distribution) *(1 points)*
Show that for arbitrary feedback, the variance of a localized distribution $\rho_m(t)=\delta_{m\bar{m}}$ the variance will always increase unless $\gamma_{\bar{m}}=0$.

Therefore, the resulting time-dependent distribution may be expected to have a finite width if the iteration scheme is performed in a range where the feedback is negative. This can be illustrated at the example of a continuous ($n\to x$) Gaussian distribution

$$\rho_x(t)=\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(x-\gamma t)^2}{2\sigma^2}} \tag{7.19}$$

with mean $\mu=\gamma t=\left\langle x\right\rangle_t$ and width σ. The control scheme

$$\gamma_x(t)=\gamma e^{\alpha}e^{-\frac{\alpha x}{\gamma t}} \tag{7.20}$$

leads to the following expectation values (replacing sums by integrals and extending the integration range over the complete real axis)

$$\left\langle\gamma_x\right\rangle = \gamma e^{\frac{\alpha^2\sigma^2}{2\gamma^2t^2}}, \qquad \left\langle\gamma_x^2\right\rangle=\gamma^2e^{2\frac{\alpha^2\sigma^2}{\gamma^2t^2}}, \qquad \left\langle x\gamma_x\right\rangle=e^{\frac{\alpha^2\sigma^2}{2\gamma^2t^2}}\left[\gamma^2t-\frac{\alpha\sigma^2}{t}\right], \tag{7.21}$$

which leads to a change of the variance of

$$\begin{aligned}\Delta\sigma^2 &= \Delta t^2\left[\langle\gamma_x^2\rangle_t - \langle\gamma_x\rangle_t^2\right] + \Delta t\left[\langle\gamma_x\rangle_t + 2\langle x\gamma_x\rangle_t - 2\langle x\rangle_t\langle\gamma_x\rangle_t\right] \\ &= \Delta t^2\gamma^2 e^{\frac{\alpha^2\sigma^2}{\gamma^2t^2}}\left[e^{\frac{\alpha^2\sigma^2}{\gamma^2t^2}} - 1\right] + \frac{\Delta t}{t}e^{\frac{\alpha^2\sigma^2}{2\gamma^2t^2}}\left[\gamma t - 2\alpha\sigma^2\right] . \end{aligned} \tag{7.22}$$

Neglecting the quadratic contribution (small Δt) the variance is stabilized when the feedback strength is adapted with time and width of the distribution $\alpha \geq \frac{\gamma t}{2\sigma^2}$. This is also confirmed by the numerical propagation of an initially localized probability distribution with the iteration scheme (7.12) in Fig. 7.1. Without feedback (thin lines), the distribution propagates, but also

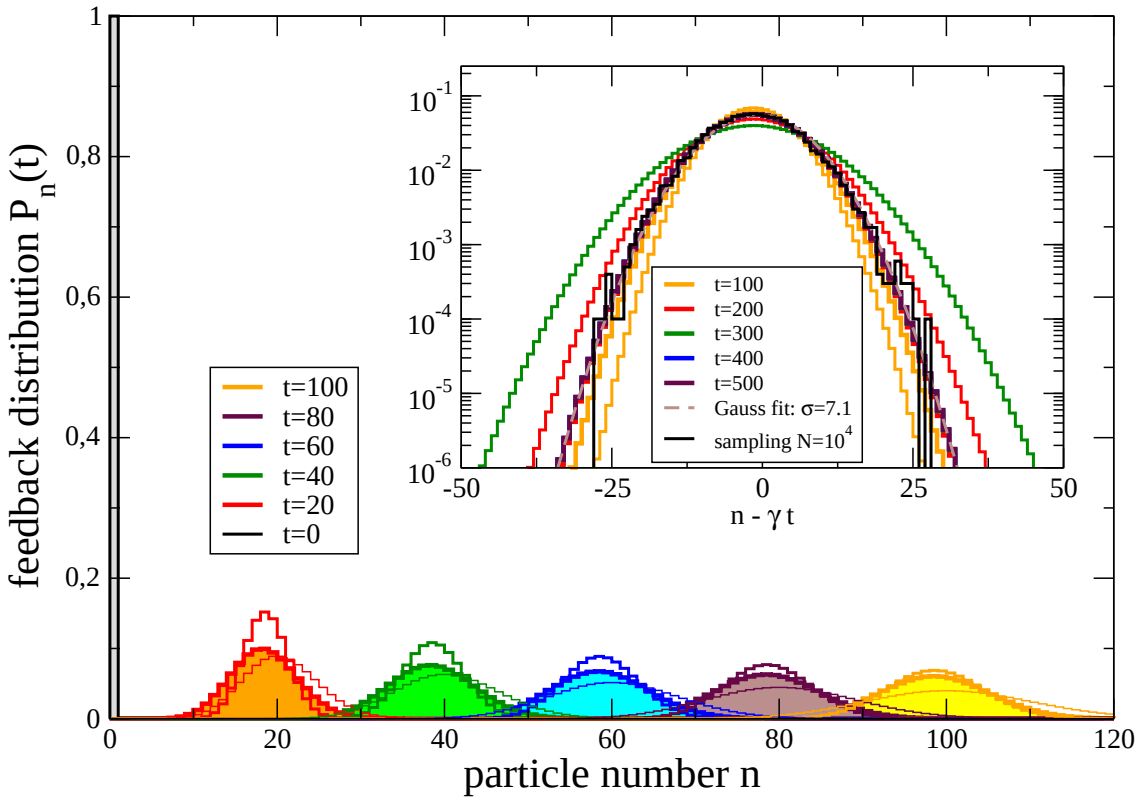

Figure 7.1: Plot of probability distributions $P_n(t)$ without feedback (Poissonian evolution, thin lines), with constant feedback strength (medium thickness) and with time-proportional feedback strength (thick curves). The inset shows the long-time evolution for constant feedback strength (increasing width) and time-proportional feedback strength (stationary width). The fit (dashed curve) demonstrates that the stationary distribution is Gaussian. In addition, a direct sampling of the feedback protocol yields the same distribution. Parameters: $\gamma = 1$, $\Delta t = 1$, $\alpha = 1$ for constant feedback and $\alpha = 0.01t$ for time-proportional feedback.

increases its width in time. With constant feedback strength, the distribution propagates at the same speed and its width is reduced but still increases with time for sufficiently large times. Only when the feedback strength is chosen to scale linarly in time, the shape of the distribution becomes stabilized. This in turn allows to determine the stationary width in dependence of the feedback strength $\alpha = \alpha_0 t$ as follows: Inserting this dependence in Eq. (7.22) leads to a condition under

which the variance of a Gaussian distribution remains constant

$$0 = (\gamma\Delta t)e^{y/2}\left[e^{y}-1\right]+1-2\frac{\gamma}{\alpha_0}y \tag{7.23}$$

with the variable

$$y = \frac{\alpha_0^2\sigma^2}{\gamma^2}\,. \tag{7.24}$$

This transcendental equation can for given Δt, γ and α_0 be solved numerically for y, which in turn enables one to determine the stationary width σ. For example, for $\gamma\Delta t = 1$ and $\gamma/\alpha_0 = 100$ we find a numerical solution $y \approx 0.005025$, which corresponds to a width of $\sigma \approx 7.1$. This width is exactly found in the Gaussian fit of the numerical solution (compare the inset of Fig. 7.1). The validity of this effective description under feedback is further underlined by a direct sampling of the feedback protocol (also compare the inset): Here, the feedback parameter is adjusted at finite time intervals Δt, and dependent on the previous measurement result. Therefore, under the chosen feedback protocol

$$\gamma_n(t) = \gamma e^{\alpha_0 t}e^{-\frac{\alpha_0 n}{\gamma}} \tag{7.25}$$

the long-term limit leads to a frozen distribution which propagates with a constant shape.

These findings can be made more explicit for linear feedback of the form

$$\gamma_n(t) = \gamma\left[1-g(n-\gamma t)\right] \tag{7.26}$$

with the dimensionless feedback parameter $g > 0$. It can be thought of an approximation of scheme (7.25) for small $g = \alpha_0/\gamma \ll 1$. Of course, the above scheme formally allows for negative rates when $n \gg \gamma_0 t$. In reality however, the probability for such a process is exponentially suppressed for sufficiently large times, since for large times the width of a Poissonian process is sufficiently smaller than its mean value $\sigma/\mu = 1/\sqrt{\gamma t}$. The linear feedback scheme has the advantage that Eqns. (7.16) and (7.18) only couple to themselves and can thus be solved

$$\begin{aligned} C_1(t+\Delta t) - C_1(t) &= \gamma\Delta t\left[1-gC_1(t)+g\gamma t\right]\,, \\ C_2(t+\Delta t) - C_2(t) &= \gamma^2\Delta t^2 g^2 C_2(t) + \gamma\Delta t\left[1+\gamma g t - gC_1(t) - 2gC_2(t)\right]\,. \end{aligned} \tag{7.27}$$

In the limit of small Δt, the differential version of these equations read

$$\begin{aligned} \dot{C}_1 &= \gamma\left[1-gC_1(t)+g\gamma t\right]\,, \\ \dot{C}_2 &= \gamma\left[1+\gamma g t - gC_1(t) - 2gC_2(t)\right] \end{aligned} \tag{7.28}$$

and admit for the initial conditions $C_1(0) = 0$ and $C_2(0) = 0$ the simple solution

$$C_1(t) = \gamma t\,, \qquad C_2(t) = \frac{1-e^{-2g\gamma t}}{2g}\,, \tag{7.29}$$

which shows a continuous evolution towards a constant width of $\bar{\sigma} = \sqrt{\lim_{t\to\infty} C_2(t)} = \frac{1}{\sqrt{2g}}$.

7.2 Maxwell's demon

Maxwell invented his famous demon as a thought experiment to demonstrate that thermodynamics is a macroscopic effective theory: An intelligent being (the demon) living in a box is measuring the speed of molecules of some gas in the box. An initial thermal distribution of molecules implies that the molecules have different velocities. The demon measures the velocities and inserts an impermeable wall whenever the the molecule is too fast or lets it pass into another part of the box when it is slow. As time progresses, this would lead to a sorting of hot and cold molecules, and the temperature difference could be exploited to perform work.

This is nothing but a feedback (closed-loop) control scheme: The demon performs a measurement (is the molecule slow or fast) and then uses the information to perform an appropriate control action on the system (inserting a wall or not). Classically, the insertion of a wall requires in the idealized case no work, such that only information is used to create a temperature gradient. However, the Landauer principle states that with each bit of information erased, heat of at least $k_B T \ln(2)$ is dissipated into the environment. To remain functionable, the demon must at some point start to delete the information, which leads to the dissipation of heat. The dissipated heat will exceed the energy obtainable from the thermal gradient.

An analog of a Maxwell demon may be implemented in an electronic context: There, an experimentalist takes the role of the demon. The box is replaced by the SET (including the contacts), on which by a nearby QPC a measurement of the dot state (simply empty or filled) is performed. Depending on the measurement outcome, the tunneling rates are modified in time in a piecewise constant manner: When there is no electron on the dot, the left tunneling rate Γ_L is increased (low barrier) and the right tunneling rate Γ_R is decreased (high barrier). The opposite is done when there is an electron on the dot, see Fig. 7.2. Thus, the only difference in comparison

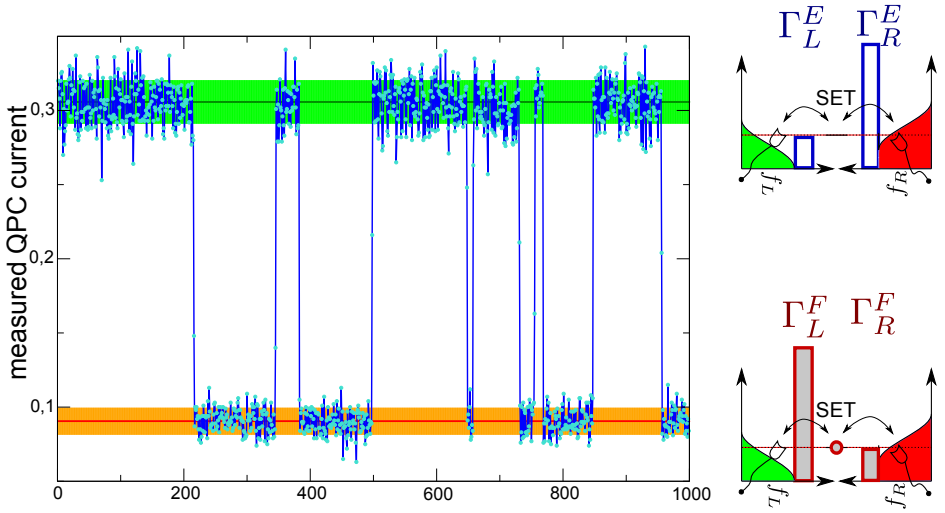

Figure 7.2: Sketch of the feedback scheme: For a filled dot (low QPC current), the left tunneling rate is minimal and the right tunneling rate is maximal and vice-versa for an empty dot. The dot level itself is not changed.

to Sec. 6.2.1 is that now information of the system is used to modify the tunneling rates. Very simple considerations already demonstrate that with this scheme, it will be possible to transport electrons against an existing bias only with time-dependent tunneling rates. When one junction is

completely decoupled $\Gamma^{\rm min}_{L/R} \to 0$, this will completely rectify the transport from left to right also against the bias (if the bias is finite). In the following, we will address the statistics of this device.

The first step is to identify an effective evolution equation for the density matrix accounting for measurement and control. In this case, both processes occur continuously, which enables us to consider infinitesimally small time intervals Δt. For an empty dot at time t, i.e., for $\rho_E(t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, the density vector at time $t + \Delta t$ will be given by

$$\rho_E(t + \Delta t) = \left[\mathbf{1} + \Delta t \mathcal{L}^{(E)}\right] \rho_E(t)\,. \tag{7.30}$$

Similarly, we have for a filled dot $\rho_E(t) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\rho_F(t + \Delta t) = \left[\mathbf{1} + \Delta t \mathcal{L}^{(F)}\right] \rho_F(t)\,. \tag{7.31}$$

Both equations can be combined using a projection superoperator

$$\rho(t + \Delta t) = \left\{\left[\mathbf{1} + \Delta t \mathcal{L}^{(E)}\right] \mathcal{P}_E + \left[\mathbf{1} + \Delta t \mathcal{L}^{(F)}\right] \mathcal{P}_F\right\} \rho(t) \tag{7.32}$$

with the operators

$$\mathcal{P}_E = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \mathcal{P}_F = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{7.33}$$

Since we have $\mathcal{P}_E + \mathcal{P}_F = \mathbf{1}$, this defines when $\Delta t \to 0$ (continous control limit) an effective Liouvillian

$$\mathcal{L}_{\rm eff} = \mathcal{L}^{(E)}\mathcal{P}_E + \mathcal{L}^{(F)}\mathcal{P}_F\,, \tag{7.34}$$

which is in complete equivalence with Eq. (7.10) when $\Delta t \to 0$. Note that this can be performed with and without counting fields. Taking into account the diagonal structure of the projection superoperators, this simply implies that the effective Liouvillian under feedback has the first column from the Liouvillian conditioned on an empty dot and the second column from the Liouvillian conditioned on the filled dot

$$\mathcal{L}_{\rm eff}(\chi_L, \chi_R) = \begin{pmatrix} -\Gamma^E_L f_L - \Gamma^E_R f_R & +\Gamma^F_L (1-f_L) e^{+{\rm i}\chi_L} + \Gamma^F_R (1-f_R) e^{+{\rm i}\chi_R} \\ +\Gamma^E_L f_L e^{-{\rm i}\chi_L} + \Gamma^E_R f_R e^{-{\rm i}\chi_R} & -\Gamma^F_L (1-f_L) - \Gamma^F_R (1-f_R) \end{pmatrix}. \tag{7.35}$$

Evidently, it still obeys trace conservation but now the tunneling rates in the two columns are different ones.

Exercise 49 (Current at zero bias) *(1 points)*
Calculate the feedback-current at zero bias $f_L = f_R = f$ in dependence on f. What happens at zero temperatures, where $f \to \{0, 1\}$?

The effective Liouvillian describes the average evolution of trajectories under continuous monitoring and feedback. The validity of the effective description can be easily checked by calculating Monte-Carlo solutions as follows:

Starting e.g. with a filled dot, the probability to jump out e.g. to the right lead during the small time interval Δt reads $P^{(F)}_{\text{out,R}} = \Gamma^F_R(1-f_R)\Delta t$. Similarly, we can write down the probabilities to jump out to the left lead and also the probabilities to jump onto an empty dot from either the left or right contact

$$\begin{aligned} P^{(F)}_{\text{out,R}} &= \Gamma^F_R(1-f_R)\Delta t\,, \qquad P^{(F)}_{\text{out,L}} = \Gamma^F_L(1-f_L)\Delta t\,, \\ P^{(E)}_{\text{in,R}} &= \Gamma^E_R f_R \Delta t\,, \qquad P^{(E)}_{\text{in,L}} = \Gamma^E_L f_L \Delta t\,. \end{aligned} \tag{7.36}$$

Naturally, these jump probabilities also uniquely determine the change of the particle number on either contact. The remaining probability is simply the one that no jump occurs during Δt. A Monte-Carlo simulation is obtained by drawing a random number and choosing one out of three possible outcomes for empty (jumping in from left contact, from right contact, or remaining empty) and for a filled (jumping out to left contact, to right contact, or remaining filled) dot. Repeating the procedure several times yields a single trajectory for $n(t)$, $n_L(t)$, and $n_R(t)$. The ensemble average of many such trajectories agree perfectly with the solution

$$\begin{aligned} \langle n\rangle_t &= \text{Tr}\left\{d^\dagger d e^{\mathcal{L}_{\text{eff}}(0,0)t}\rho_0\right\}\,, \\ \langle n_L\rangle_t &= (-\mathrm{i}\partial_\chi)\,\text{Tr}\left\{e^{\mathcal{L}_{\text{eff}}(\chi,0)t}\rho_0\right\}\big|_{\chi=0}\,, \\ \langle n_R\rangle_t &= (-\mathrm{i}\partial_\chi)\,\text{Tr}\left\{e^{\mathcal{L}_{\text{eff}}(0,\chi)t}\rho_0\right\}\big|_{\chi=0} \end{aligned} \tag{7.37}$$

of the effective feedback master equation, see Fig. 7.3. To compare with the case without feedback, we parametrize the change of tunneling rates by dimensionless constants

$$\Gamma^E_L = e^{\delta^E_L}\Gamma_L\,, \qquad \Gamma^E_R = e^{\delta^E_R}\Gamma_R\,, \qquad \Gamma^F_L = e^{\delta^F_L}\Gamma_L\,, \qquad \Gamma^F_R = e^{\delta^F_R}\Gamma_R\,, \tag{7.38}$$

where $\delta^\beta_\alpha \to 0$ reproduces the case without feedback and $\delta^\beta_\alpha > 0 (< 0)$ increases (decreases) the tunneling rate to contact α conditioned on dot state β. The general current can directly be calculated as

$$I = \frac{f_L(1-f_R)\Gamma^E_L\Gamma^F_R - (1-f_L)f_R\Gamma^F_L\Gamma^E_R}{\Gamma^E_L f_L + \Gamma^F_L(1-f_L) + \Gamma^E_R f_R + \Gamma^F_R(1-f_R)}\,, \tag{7.39}$$

which reduces to the conventional current without feedback when $\Gamma^\beta_\alpha \to \Gamma_\alpha$. For finite feedback strength however, this will generally induce a non-vanishing current at zero bias, see Fig. 7.4. In our idealized setup, this current is only generated by the information on whether the dot is occupied or empty – hence the interpretation as a Maxwell demon. When the contacts are held at equal temperatures $\beta_L = \beta_R = \beta$, this raises the question for the maximum power

$$P = -IV \tag{7.40}$$

generated by the device.

In what follows, we will consider symmetric feedback characterized by a single parameter

$$\Delta^E_L = \Delta^F_R = -\Delta^F_L = -\Delta^E_R = +\delta\,, \tag{7.41}$$

where $\delta > 0$ favors transport from left to right and $\delta < 0$ transport from right to left and also symmetric tunneling rates $\Gamma = \Gamma_L = \Gamma_R$. With these assumptions, it is easy to see that for large feedback strengths $\delta \gg 1$, the current simply becomes

$$I \to \Gamma e^{\delta}\frac{f_L(1-f_R)}{f_L + (1-f_R)}\,. \tag{7.42}$$

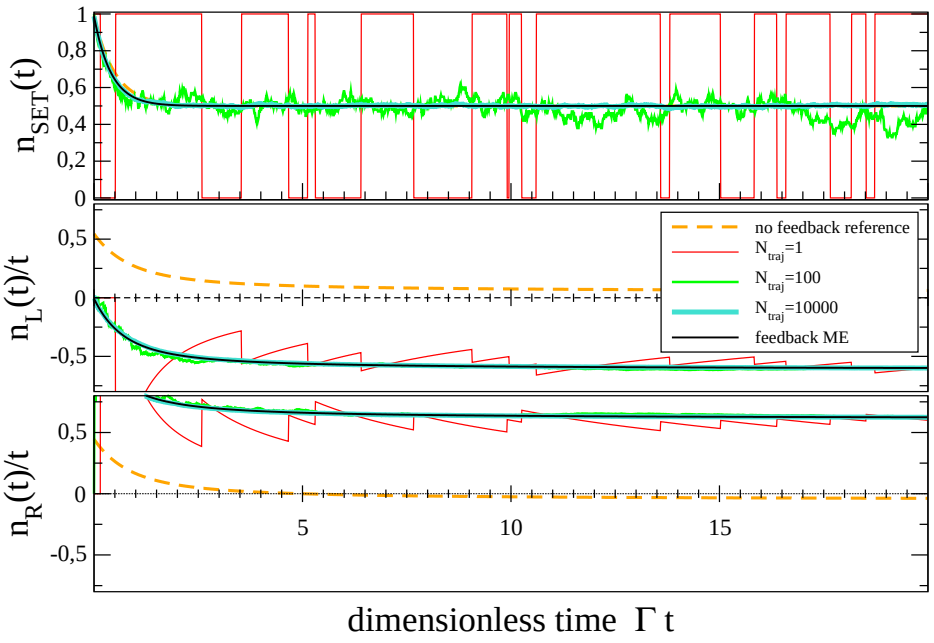

Figure 7.3: Comparison of a single (thin red curve with jumps, same realization in all panels) and the average of 100 (medium thickness, green) and 10000 (bold smooth curve, turquoise) trajectories with the solution from the effective feedback master equation (thin black) for the dot occupation (top), the number of particles on the left (middle), and the number of particles on the right (bottom). The average of the trajectories converges to the effective feedback master equation result. The reference curve without feedback (dashed orange) may be obtained by using vanishing feedback parameters and demonstrates that the direction of the current may actually be reversed via sufficiently strong feedback. Parameters: $\Gamma_L = \Gamma_R \equiv \Gamma$, $f_L = 0.45$, $f_R = 0.55$, $\delta_L^E = \delta_R^F = 1.0$, $\delta_R^E = \delta_L^F = -10.0$, and $\Gamma\Delta t = 0.01$.

To determine the maximum power, we would have to maximize with respect to left and right chemical potentials μ_L and μ_R, the lead temperature β and the dot level ϵ. However, as these parameters only enter implicitly in the Fermi functions, it is more favorable to use that for equal temperatures

$$\beta(\mu_L - \mu_R) = \beta V = \ln\left[\frac{f_L(1-f_R)}{(1-f_L)f_R}\right], \tag{7.43}$$

such that we can equally maximize

$$P = -IV = \frac{1}{\beta}(-I\beta V) \to \frac{\Gamma e^{\delta}}{\beta}\left[-\frac{f_L(1-f_R)}{f_L+(1-f_R)}\ln\left(\frac{f_L(1-f_R)}{(1-f_L)f_R}\right)\right]. \tag{7.44}$$

The term in square brackets can now be maximized numerically with respect to the parameters f_L and f_R in the range $0 \le f_{L/R} \le 1$, such that one obtains for the maximum power at strong feedback

$$P \le k_{\mathrm{B}}T\Gamma e^{\delta}0.2785 \qquad \text{at} \qquad f_L = 0.2178 \qquad f_R = 0.7822\,. \tag{7.45}$$

The average work performed between two QPC measurement points at t and $t+\Delta t$ is therefore given by

$$W \le k_{\mathrm{B}}T\Gamma e^{\delta}\Delta t 0.2785\,. \tag{7.46}$$

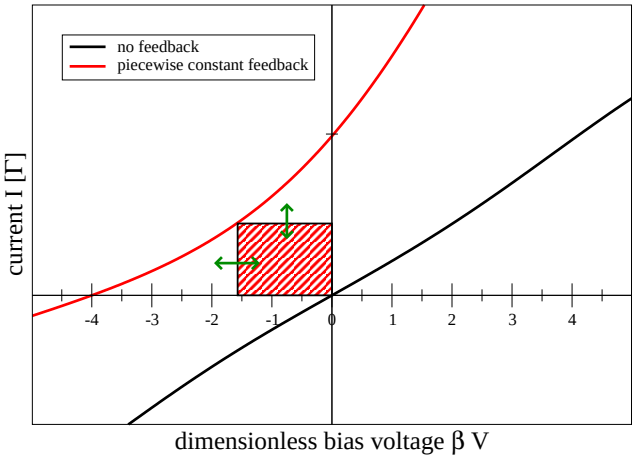

Figure 7.4: Current voltage characteristics for finite feedback strength $\delta = 1$ (red curve) and without feedback $\delta = 0$ (black curve). For finite feedback, the current may point in the other direction than the voltage leading to a positive power $P = -IV$ (shaded region) generated by the device.

However, to perform feedback efficiently, it is required that the QPC sampling rate is fast enough that all state changes of the SET are faithfully detected (no tunneling charges are missed). This requires that $\Gamma e^{\delta} \Delta t < 1$. Therefore, we can refine the upper bound for the average work

$$W \leq k_{\mathrm{B}} T 0.2785\,. \tag{7.47}$$

This has to be contrasted with the Landauer principle, which states that for each deleted bit in the demons brain (each QPC data point enconding high current or low current) heat of

$$Q \geq k_{\mathrm{B}} T \ln(2) \approx k_{\mathrm{B}} T 0.6931 \tag{7.48}$$

is dissipated. The second law is therefore not violated.

The conventional fluctuation theorem for the SET at equal temperatures

$$\frac{P_{+n}(t)}{P_{-n}(t)} = e^{n\beta V} \tag{7.49}$$

is modified in presence of feedback. However, since the Liouvillian still contains the counting fields in the conventional way, simply the factor in the exponential, not the dependence on the number of tunneled electrons n is changed. To evaluate the FT, we identify symmetries in the moment-generating function (or alternatively the eigenvalues of the Liouvillian)

$$\begin{aligned} \lambda(-\chi) &= \lambda\left(+\chi + \mathrm{i}\ln\left[e^{+4\delta}\frac{f_L(1-f_R)}{(1-f_L)f_R}\right]\right) = \lambda\left(+\chi + \mathrm{i}\ln\left[e^{+4\delta}e^{\beta V}\right]\right) \\ &= \lambda(+\chi + \mathrm{i}(4\delta + \beta V))\,. \end{aligned} \tag{7.50}$$

From this symmetry of the cumulant-generating function we obtain for the fluctuation theorem under feedback

$$\lim_{t\to\infty} \frac{P_{+n}(t)}{P_{-n}(t)} = e^{n(\beta V + 4\delta)} = e^{n\beta(V - V^*)}\,, \tag{7.51}$$

where $V^* = -4\delta/\beta$ denotes the voltage at which the current (under feedback) vanishes.

Exercise 50 (Vanishing feedback current) *(1 points)*
Show for equal temperatures that the feedback current vanishes when $V = V^* = -4\delta/\beta$.

However, piecewise constant feedback is not the only relevant scheme. As a further example, let us consider instantaneously applying a fast and short pulse on the tunneling rates whenever the QPC detects a change in the dots occupation, see Fig. 7.5. To change the counting statistics,

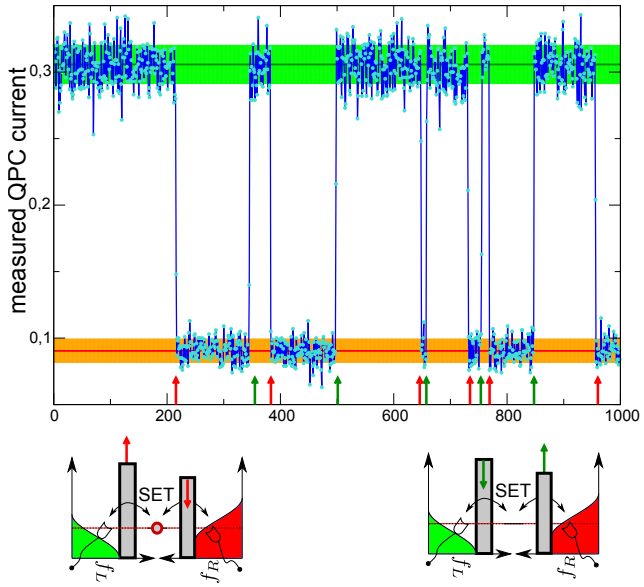

Figure 7.5: Sketch of the modified feedback scheme: This time, feedback control operations are not conditioned on the state of the dot, but on its change. Whenever an electron has jumped into the dot (red arrows), the left tunneling rate is decreased and the right tunneling rate is increases with an instantaneous pulse. The opposite is done when an electron has jumped out of the dot (green arrows). The dot level itself is not changed. To obtain a significant change of the statistics, it is necessary that particles may also tunnel during the pulses. This opens the possibility of setting up feedback schemes with a finite recursion depth: Electrons tunneling during the control operations may trigger further control operations and so on – eventually limited by the finite processing speed of the apparatus and other factors.

the infinitely short pulse of this feedback scheme must be infinitely large and can thus be well represented by a δ function. Since for an SET the QPC does not resolve the direction of the electronic jumps, we can only perform control operations conditioned on particles jumping in and out

$$\mathcal{L}(t) = \mathcal{L}_0 + \sum_{t_{\rm in}} \mathcal{L}^{(I)} + \sum_{t_{\rm out}} \mathcal{L}^{(O)}\,, \tag{7.52}$$

where $t_{\rm in}$ and $t_{\rm out}$ denote the times at which an electron jumps in or out of the dot, respectively. The control Liouvillians have the form

$$\begin{aligned}
\mathcal{L}^{(I)} &= \delta(t-t_{\rm in}) \begin{pmatrix} -\delta_L^I f_L - \delta_R^I f_R & +\delta_L^I (1-f_L) e^{+{\rm i}\chi_L} + \delta_R^I (1-f_R) e^{+{\rm i}\chi_R} \\ +\delta_L^I f_L e^{-{\rm i}\chi_L} + \delta_R^I f_R e^{-{\rm i}\chi_R} & -\delta_L^I (1-f_L) - \delta_R^I (1-f_R) \end{pmatrix}, \\
\mathcal{L}^{(O)} &= \delta(t-t_{\rm out}) \begin{pmatrix} -\delta_L^O f_L - \delta_R^O f_R & +\delta_L^O (1-f_L) e^{+{\rm i}\chi_L} + \delta_R^O (1-f_R) e^{+{\rm i}\chi_R} \\ +\delta_L^O f_L e^{-{\rm i}\chi_L} + \delta_R^O f_R e^{-{\rm i}\chi_R} & -\delta_L^O (1-f_L) - \delta_R^O (1-f_R) \end{pmatrix}
\end{aligned} \tag{7.53}$$

where $\delta_\alpha^\beta > 0$ denote dimensionless feedback parameters and $\delta_\alpha^\beta = 0$ reproduces the case without

feedback. This implies a simple form of the corresponding (dimensionless) propagators

$$\begin{aligned} e^{\kappa^I} &= \exp\begin{pmatrix} -\delta_L^I f_L - \delta_R^I f_R & +\delta_L^I(1-f_L)e^{+\mathrm{i}\chi_L} + \delta_R^I(1-f_R)e^{+\mathrm{i}\chi_R} \\ +\delta_L^I f_L e^{-\mathrm{i}\chi_L} + \delta_R^I f_R e^{-\mathrm{i}\chi_R} & -\delta_L^I(1-f_L) - \delta_R^I(1-f_R) \end{pmatrix}, \\ e^{\kappa^O} &= \exp\begin{pmatrix} -\delta_L^O f_L - \delta_R^O f_R & +\delta_L^O(1-f_L)e^{+\mathrm{i}\chi_L} + \delta_R^O(1-f_R)e^{+\mathrm{i}\chi_R} \\ +\delta_L^O f_L e^{-\mathrm{i}\chi_L} + \delta_R^O f_R e^{-\mathrm{i}\chi_R} & -\delta_L^O(1-f_L) - \delta_R^O(1-f_R) \end{pmatrix} \end{aligned} \tag{7.54}$$

during such an infinitesimally short pulse.

Exercise 51 (δ-kick propagator) *(1 points)*
Calculate the general propagator for a time-dependent Liouvillian of the piecewise-constant form

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_c\Theta(t-t_c)\Theta(t_c+\tau_c-t)\,,$$

where t_c denotes the control time and τ_c the control duration. What is the propagator when $\mathcal{L}_c = \kappa/\tau_c$ in the limit $\tau_c \to 0$?

With these Liouvillians it is still necessary to derive an effective Liouvillian under feedback. For tunneling events during the baseline propagation, we have for the conditional density matrix at time $t+\Delta t$

$$\rho^{(n_L,n_R)}(t+\Delta t) = \left(\frac{1}{2\pi}\right)^2 \int_{-\pi}^{+\pi} \exp\left[\mathcal{L}_0(\chi_L,\chi_R)\Delta t - \mathrm{i}n_L\chi_L - \mathrm{i}n_R\chi_R\right] d\chi_L d\chi_R \rho(t)\,, \tag{7.55}$$

where n_L and n_R denote the number of particles that have tunneled to the left and right junction during Δt, respectively. Since we are interested in continous monitoring, it suffices to expand to first order in Δt. With the splitting of the Liouvillian

$$\mathcal{L}_0(\chi_L,\chi_R) = \mathcal{L}^{(0,0)} + \mathcal{L}^{(1,0)}e^{+\mathrm{i}\chi_L} + \mathcal{L}^{(-1,0)}e^{-\mathrm{i}\chi_L} + \mathcal{L}^{(0,1)}e^{+\mathrm{i}\chi_R} + \mathcal{L}^{(0,-1)}e^{-\mathrm{i}\chi_R} \tag{7.56}$$

it becomes obvious that for small Δt only single-tunneling events need to be considered. The superoperators

$$\begin{aligned} \mathcal{J}^{00}(\Delta t) &= \left(\frac{1}{2\pi}\right)^2 \int_{-\pi}^{+\pi} \exp\left[\mathcal{L}_0(\chi_L,\chi_R)\Delta t\right] d\chi_L d\chi_R \approx \mathbf{1} + \mathcal{L}^{(0,0)}\Delta t\,, \\ \mathcal{J}^{\pm1,0}(\Delta t) &= \left(\frac{1}{2\pi}\right)^2 \int_{-\pi}^{+\pi} \exp\left[\mathcal{L}_0(\chi_L,\chi_R)\Delta t \mp \mathrm{i}\chi_L\right] d\chi_L d\chi_R \approx \mathcal{L}^{\pm1,0}\Delta t\,, \\ \mathcal{J}^{0,\pm1}(\Delta t) &= \left(\frac{1}{2\pi}\right)^2 \int_{-\pi}^{+\pi} \exp\left[\mathcal{L}_0(\chi_L,\chi_R)\Delta t \mp \mathrm{i}\chi_R\right] d\chi_L d\chi_R \approx \mathcal{L}^{0,\pm1}\Delta t \end{aligned} \tag{7.57}$$

now take the role of projection superoperators for a measurement of the particle numbers n_L and n_R during Δt. The effective propagator under feedback from t to $t+\Delta t$ can be written as

$$\rho(t+\Delta t) = \sum_\alpha \mathcal{W}_\alpha(\Delta t)\mathcal{P}_\alpha\rho(t)\,, \tag{7.58}$$

where $\mathcal{W}_\alpha(\Delta t)$ denotes the propagator conditioned on measurement result α and $\mathcal{P}_\alpha$ the corresponding projection superoperator. In the continous measurement limit, this defines an effective Liouvillian via solving

$$\rho(t+\Delta t) = \left[\mathbf{1} + \Delta t \mathcal{L}^{0,0} + e^{\kappa^O}\Delta t\left(\mathcal{L}^{(0,1)} + \mathcal{L}^{(1,0)}\right) + e^{\kappa^I}\Delta t\left(\mathcal{L}^{(0,-1)} + \mathcal{L}^{(-1,0)}\right)\right]\rho(t) \quad (7.59)$$

for the difference quotient $(\rho(t+\Delta t)-\Delta t)/\Delta t$ and letting $\Delta t \to 0$. With counting fields, it reads

$$\mathcal{L}_{\text{eff}} = \mathcal{L}^{(0,0)} + e^{\kappa^O(\chi_L,\chi_R)}\left(e^{+\mathrm{i}\chi_R}\mathcal{L}^{(0,1)} + e^{+\mathrm{i}\chi_L}\mathcal{L}^{(1,0)}\right) + e^{\kappa^I(\chi_L,\chi_R)}\left(e^{-\mathrm{i}\chi_R}\mathcal{L}^{(0,-1)} + e^{-\mathrm{i}\chi_L}\mathcal{L}^{(-1,0)}\right) \quad (7.60)$$

where it becomes quite obvious that the dependence on the counting fields becomes nontrivial. This is valid for a recursion depth zero, i.e., particles tunneling during the control operations do not trigger further control operations. As with the piecewise constant scheme, this may also be compared to a Monte-Carlo simulation of the feedback scheme, see Fig. 7.6 . For some analytic

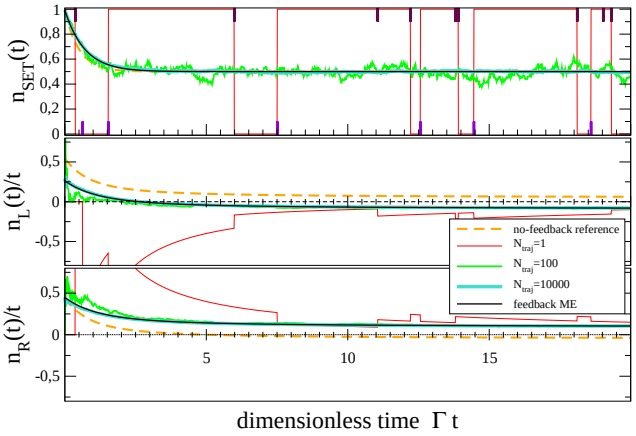

Figure 7.6: The average of the Monte-Carlo trajectories converges to the effective feedback master equation result. Control operations (bold kinks in top graph) are not always correlated with a change in the occupation or the particle number left and right, since only the net particle number after control is displayed. Parameters: $\Gamma_L = \Gamma_R \equiv \Gamma$, $f_L = 0.45$, $f_R = 0.55$, $\delta_L^I = \delta_R^O = 0$, $\delta_R^I = \delta_L^O = 1.0$, and $\Gamma\Delta t = 0.01$.

understanding, let us assume that the control pulses only affect a single junction at a time with a similar feedback strength

$$\begin{aligned} e^{\kappa^I(\chi_R)} &= \exp\begin{pmatrix} -\delta f_R & +\delta(1-f_R)e^{+\mathrm{i}\chi_R} \\ +\delta f_R e^{-\mathrm{i}\chi_R} & -\delta(1-f_R)\end{pmatrix} \overset{\delta\to\infty}{\to} \begin{pmatrix} 1-f_R & e^{+\mathrm{i}\chi_R}(1-f_R) \\ e^{-\mathrm{i}\chi_R}f_R & f_R\end{pmatrix}, \\ e^{\kappa^O(\chi_L)} &= \exp\begin{pmatrix} -\delta f_L & +\delta(1-f_L)e^{+\mathrm{i}\chi_L} \\ +\delta f_L e^{-\mathrm{i}\chi_L} & -\delta(1-f_L)\end{pmatrix} \overset{\delta\to\infty}{\to} \begin{pmatrix} 1-f_L & e^{+\mathrm{i}\chi_L}(1-f_L) \\ e^{-\mathrm{i}\chi_L}f_L & f_L\end{pmatrix}, \end{aligned} \quad (7.61)$$

where the propagators have a finite limit even in the limit of infinite feedback strength.

Exercise 52 (Infinite Feedback Strength) *(1 points)*
Show that for infinite feedback strength coupling to a single junction leads to an immediate equilibration of the density matrix with the contact to which it is coupled during control.

Therefore, the effective Liouvillian for infinite feedback strength is given by

$$\begin{aligned} \mathcal{L}_{\text{eff}}(\chi_L,\chi_R) &= \begin{pmatrix} -\Gamma_L f_L - \Gamma_R f_R & 0 \\ 0 & -\Gamma_L(1-f_L) - \Gamma_R(1-f_R)\end{pmatrix} \\ &+ \begin{pmatrix} 1-f_L & e^{+\mathrm{i}\chi_L}(1-f_L) \\ e^{-\mathrm{i}\chi_L}f_L & f_L\end{pmatrix}\begin{pmatrix} 0 & \Gamma_L(1-f_L)e^{+\mathrm{i}\chi_L} + \Gamma_R(1-f_R)e^{+\mathrm{i}\chi_R} \\ 0 & 0\end{pmatrix} \\ &+ \begin{pmatrix} 1-f_R & e^{+\mathrm{i}\chi_F}(1-f_R) \\ e^{-\mathrm{i}\chi_R}f_R & f_R\end{pmatrix}\begin{pmatrix} 0 & 0 \\ \Gamma_L f_L e^{+\mathrm{i}\chi_L} + \Gamma_R f_R e^{+\mathrm{i}\chi_R} & 0\end{pmatrix}. \end{aligned} \quad (7.62)$$

The non-standard dependence on the counting fields (there are for example counting fields on the diagonal and products of left- and right-associated counting fields) severly disturbs the symmetries, such that the fluctuation theorem is broken

$$\frac{P_{+n}}{P_{-n}} \neq e^{n\alpha} \,. \tag{7.63}$$

7.3 Qubit stabilization

Qubits – any quantum-mechanical two-level system that can be prepared in a superposition of its two states $|0\rangle$ and $|1\rangle$ – are at the heart of quantum computers with great technological promises. The major obstacle to be overcome to build a quantum computer is decoherence: Qubits prepared in pure superposition states (as required for performing quantum computation) tend to decay into a statistical mixture when coupled to a destabilizing reservoir (of which there is an abundance in the real world). Here, we will approach the decoherence with a quantum master equation and use feedback control to act against the decay of coherences.

The system is described by

$$\begin{aligned} \mathcal{H}_{\rm S} &= \frac{\Omega}{2}\sigma^z \,, \qquad \mathcal{H}_{\rm B}^1 = \sum_k \omega_k^1 (b_k^1)^\dagger b_k^1 \,, \qquad \mathcal{H}_{\rm B}^2 = \sum_k \omega_k^2 (b_k^2)^\dagger b_k^2 \\ \mathcal{H}_{\rm I}^1 &= \sigma^z \otimes \sum_k \left[h_k^1 b_k^1 + (h_k^1)^* (b_k^1)^\dagger \right] \,, \qquad \mathcal{H}_{\rm I}^2 = \sigma^x \otimes \sum_k \left[h_k^2 b_k^2 + (h_k^2)^* (b_k^2)^\dagger \right] \,, \end{aligned} \tag{7.64}$$

where σ^α represent the Pauli matrices and b_k bosonic annihilation operators. We assume that the two bosonic baths are independent and at the same temperature, such that we can calculate the dissipators separately. Then, the bath correlation function is also independent on the chosen interaction Hamiltonian (therefore omitting the indices)

$$\begin{aligned} C(\tau) &= \sum_{kk'} \left\langle \left(h_k b_k e^{-{\rm i}\omega_k \tau} + h_k^* b_k^\dagger e^{+{\rm i}\omega_k \tau} \right) \left(h_{k'} b_{k'} + h_{k'}^* b_{k'}^\dagger \right) \right\rangle \\ &= \sum_k |h_k|^2 \left[e^{-{\rm i}\omega_k \tau} (1 + n(\omega_k)) + e^{+{\rm i}\omega_k \tau} n(\omega_k) \right] \\ &= \frac{1}{2\pi} \int_0^\infty J(\omega) \left\{ e^{-{\rm i}\omega\tau} \left[1 + n(\omega) \right] + e^{+{\rm i}\omega\tau} n(\omega) \right\} d\omega \,, \end{aligned} \tag{7.65}$$

where we have introduced the bosonic occupation $n(\omega) = \left[e^{\beta\omega} - 1 \right]^{-1}$ with the inverse bath temperature β and the spectral density $J(\omega) = 2\pi \sum_k |h_k|^2 \delta(\omega - \omega_k)$. We would like to identify the Fourier transform, such that we have to transform the integral to one involving the full real axis. Since all $\omega_k > 0$, the spectral density is defined for positive frequencies but can be analytically continued by defining $J(-\omega) = -J(+\omega)$. Making use of the relation $n(-\omega) = -\left[1 + n(\omega) \right]$, we

rewrite the correlation function as

$$\begin{aligned} C(\tau) &= \frac{1}{2\pi}\int_0^\infty J(\omega)\left[1+n(\omega)\right]e^{-\mathrm{i}\omega\tau}d\omega + \frac{1}{2\pi}\int_{-\infty}^0 J(-\omega)n(-\omega)e^{-\mathrm{i}\omega\tau}d\omega \\ &= \frac{1}{2\pi}\int_0^\infty J(\omega)\left[1+n(\omega)\right]e^{-\mathrm{i}\omega\tau}d\omega + \frac{1}{2\pi}\int_{-\infty}^0 J(\omega)\left[1+n(\omega)\right]e^{-\mathrm{i}\omega\tau}d\omega \\ &= \frac{1}{2\pi}\int_{-\infty}^\infty J(\omega)\left[1+n(\omega)\right]e^{-\mathrm{i}\omega\tau}d\omega\,. \end{aligned} \tag{7.66}$$

We conclude for the Fourier-transform of the bath correlation function

$$\gamma(\omega) = J(\omega)\left[1+n(\omega)\right]\,. \tag{7.67}$$

It is easy to show that it fulfils the KMS condition

$$\gamma(-\omega) = -J(\omega)\left[-n(\omega)\right] = J(\omega)n(\omega) = e^{-\beta\omega}\gamma(+\omega)\,, \tag{7.68}$$

such that we may expect thermalization of the qubits density matrix with the bath temperature. Note that due to the divergence of $n(\omega)$ at $\omega\to 0$, it is favorable to use an Ohmic spectral density such as e.g.

$$J(\omega) = J_0\omega e^{-\omega/\omega_c}\,, \tag{7.69}$$

which grants an existing limit $\gamma(0)$. For a single system coupling operator A, the dampening coefficients in the BMS approximation in Box 7 simplify a bit

$$\begin{aligned} \gamma_{ab,cd} &= \delta(E_b-E_a,E_d-E_c)\gamma(E_b-E_a)\left\langle a\right|A\left|b\right\rangle\left\langle c\right|A\left|d\right\rangle^* \\ \sigma_{ab} &= \delta_{E_a,E_b}\frac{1}{2\mathrm{i}}\sum_c \sigma(E_b-E_c)\left\langle c\right|A\left|b\right\rangle\left\langle c\right|A\left|a\right\rangle^*\,, \end{aligned} \tag{7.70}$$

where the odd Fourier transform $\sigma(\omega)$ of the bath correlation function can be obtained from $\gamma(\omega)$ by a Cauchy-principal value integral and the vectors denote the energy eigenbasis $\sigma^z\left|0\right\rangle = \left|0\right\rangle$ and $\sigma^z\left|1\right\rangle = -\left|1\right\rangle$. The Kronecker symbols automatically imply that many dampening coefficients vanish, such that the action of the full Liouvillian can be written as

$$\begin{aligned} \dot\rho &= -\mathrm{i}\left[\left(\frac{\Omega}{2}+\sigma_{00}\right)\left|0\right\rangle\left\langle 0\right| + \left(-\frac{\Omega}{2}+\sigma_{11}\right)\left|1\right\rangle\left\langle 1\right|,\rho\right] \\ &\quad +\gamma_{00,00}\left[\left|0\right\rangle\left\langle 0\right|\rho\left|0\right\rangle\left\langle 0\right| - \frac{1}{2}\left|0\right\rangle\left\langle 0\right|\rho - \frac{1}{2}\rho\left|0\right\rangle\left\langle 0\right|\right] \\ &\quad +\gamma_{11,11}\left[\left|1\right\rangle\left\langle 1\right|\rho\left|1\right\rangle\left\langle 1\right| - \frac{1}{2}\left|1\right\rangle\left\langle 1\right|\rho - \frac{1}{2}\rho\left|1\right\rangle\left\langle 1\right|\right] \\ &\quad +\gamma_{00,11}\left[\left|0\right\rangle\left\langle 0\right|\rho\left|1\right\rangle\left\langle 1\right|\right] + \gamma_{11,00}\left[\left|1\right\rangle\left\langle 1\right|\rho\left|0\right\rangle\left\langle 0\right|\right] \\ &\quad +\gamma_{01,01}\left[\left|0\right\rangle\left\langle 1\right|\rho\left|1\right\rangle\left\langle 0\right| - \frac{1}{2}\left|1\right\rangle\left\langle 1\right|\rho - \frac{1}{2}\rho\left|1\right\rangle\left\langle 1\right|\right] \\ &\quad +\gamma_{10,10}\left[\left|1\right\rangle\left\langle 0\right|\rho\left|0\right\rangle\left\langle 1\right| - \frac{1}{2}\left|0\right\rangle\left\langle 0\right|\rho - \frac{1}{2}\rho\left|0\right\rangle\left\langle 0\right|\right]\,. \end{aligned} \tag{7.71}$$

It is a general feature of the BMS approximation that for a nondegenerate system Hamiltonian (here $\Omega \neq 0$) the populations and coherences in the energy eigenbasis decouple

$$\begin{aligned}
\dot{\rho}_{00} &= -\gamma_{10,10}\rho_{00} + \gamma_{01,01}\rho_{11}\,, \\
\dot{\rho}_{11} &= +\gamma_{10,10}\rho_{00} - \gamma_{01,01}\rho_{11}\,, \\
\dot{\rho}_{01} &= \left[-\frac{1}{2}\left(\gamma_{00,00} + \gamma_{11,11} - 2\gamma_{00,11} + \gamma_{01,01} + \gamma_{10,10}\right) - \mathrm{i}\left(\Omega + \sigma_{00} - \sigma_{11}\right)\right]\rho_{01}\,, \\
\dot{\rho}_{10} &= \left[-\frac{1}{2}\left(\gamma_{00,00} + \gamma_{11,11} - 2\gamma_{11,00} + \gamma_{01,01} + \gamma_{10,10}\right) + \mathrm{i}\left(\Omega + \sigma_{00} - \sigma_{11}\right)\right]\rho_{10}\,. \qquad (7.72)
\end{aligned}$$

For the two interaction Hamiltonians chosen, we can make the corresponding coefficients explicit

coefficient	A: pure dephasing $A = \sigma^z$	B: dissipation $A = \sigma^x$
$\gamma_{00,00}$	$+\gamma(0)$	0
$\gamma_{00,11}$	$-\gamma(0)$	0
$\gamma_{11,00}$	$-\gamma(0)$	0
$\gamma_{11,11}$	$+\gamma(0)$	0
$\gamma_{01,01}$	0	$\gamma(+\Omega)$
$\gamma_{10,10}$	0	$\gamma(-\Omega)$
σ_{00}	$\frac{\sigma(0)}{2\mathrm{i}}$	$\frac{\sigma(-\Omega)}{2\mathrm{i}}$
σ_{11}	$\frac{\sigma(0)}{2\mathrm{i}}$	$\frac{\sigma(+\Omega)}{2\mathrm{i}}$

and rewrite the corresponding Liouvillian in the ordering $\rho_{00}, \rho_{11}, \rho_{01}, \rho_{10}$ as a superoperator (further abbreviating $\gamma_{0/\pm} = \gamma(0/\pm\Omega)$, $\Sigma = \sigma_{00} - \sigma_{11}$)

$$\begin{aligned}
\mathcal{L}_A &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -2\gamma_0 - \mathrm{i}\Omega & 0 \\ 0 & 0 & 0 & -2\gamma_0 + \mathrm{i}\Omega \end{pmatrix} \\
\mathcal{L}_B &= \begin{pmatrix} -\gamma_- & +\gamma_+ & 0 & 0 \\ +\gamma_- & -\gamma_+ & 0 & 0 \\ 0 & 0 & -\frac{\gamma_- + \gamma_+}{2} - \mathrm{i}(\Omega + \Sigma) & 0 \\ 0 & 0 & 0 & -\frac{\gamma_- + \gamma_+}{2} + \mathrm{i}(\Omega + \Sigma) \end{pmatrix}. \qquad (7.73)
\end{aligned}$$

Both Liouvillians lead to a decay of coherences with a rate (we assume $\Omega > 0$)

$$\begin{aligned}
\gamma_A &= 2\gamma_0 = 2\lim_{\omega\to 0} J(\omega)\left[1 + n(\omega)\right] = 2\frac{J_0}{\beta} = 2J_0 k_{\mathrm{B}} T\,, \\
\gamma_B &= \frac{\gamma_- + \gamma_+}{2} = \frac{1}{2}\left[J(\Omega)[1 + n(\Omega)] + J(-\Omega)[1 + n(-\Omega)]\right] = \frac{1}{2}\left[J(\Omega)[1 + n(\Omega)] + J(\Omega)n(\Omega)\right] \\
&= \frac{1}{2}J(\Omega)\coth\left[\frac{\Omega}{2k_{\mathrm{B}}T}\right], \qquad (7.74)
\end{aligned}$$

which both scale proportional to T for large bath temperatures. Therefore, the application of either Liouvillian or a superposition of both will in the high-temperature limit simply lead to rapid decoherence. The same can be expected from a turnstyle (open-loop control), where the Liouvillians act one at a time following a pre-defined protocol.

The situation changes however, when measurement results are used to determine which Liouvillian is acting. We choose to act with Liouvillian $\mathcal{L}_A$ throughout and to turn on Liouvillian $\mathcal{L}_B$ in

addition – multiplied by a dimensionless feedback parameter $\alpha \geq 0$ – when a certain measurement result is obtained. Given a measurement with just two outcomes, the effective propagator is then given by

$$\mathcal{W}(\Delta t) = e^{\mathcal{L}_A \Delta t}\mathcal{P}_1 + e^{(\mathcal{L}_A + \alpha \mathcal{L}_B)\Delta t}\mathcal{P}_2\,, \tag{7.75}$$

where $\mathcal{P}_i$ are the superoperators corresponding to the action of the measurement operators $M_i \rho M_i^\dagger$ on the density matrix. First, to obtain any nontrivial effect (coupling between coherences and populations), the measurement superoperators should not have the same block structure as the Liouvillians. Therefore, we consider a projective measurement of the σ^x expectation value

$$M_1 = \frac{1}{2}\left[\mathbf{1} + \sigma^x\right]\,, \qquad M_2 = \frac{1}{2}\left[\mathbf{1} - \sigma^x\right]\,. \tag{7.76}$$

These projection operators obviously fulfil the completeness relation $M_1^\dagger M_1 + M_2^\dagger M_2 = \mathbf{1}$. The superoperators corresponding to $M_i \rho M_i^\dagger$ are also orthogonal projectors

$$\mathcal{P}_1 = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}\,, \qquad \mathcal{P}_2 = \frac{1}{4}\begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix}\,. \tag{7.77}$$

Exercise 53 (Measurement superoperators) *(0 points)*
Show the correspondence between M_i and $\mathcal{P}_i$ in the above equations.

In contrast to the previous cases however, they are not complete in this higher-dimensional space $\mathcal{P}_1 + \mathcal{P}_2 \neq \mathbf{1}$. Whereas previously without feedback the average of many measurements led to no effect in the rate equations, this is now different.

Without feedback ($\alpha = 0$), it is easy to see that the measurements still have an effect in contrast to an evolution without measurements

$$\frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & e^{-(2\gamma_0 + \mathrm{i}\Omega)\Delta t} & e^{-(2\gamma_0 + \mathrm{i}\Omega)\Delta t} \\ 0 & 0 & e^{-(2\gamma_0 - \mathrm{i}\Omega)\Delta t} & e^{-(2\gamma_0 - \mathrm{i}\Omega)\Delta t} \end{pmatrix} = e^{\mathcal{L}_A \Delta t}\left(\mathcal{P}_1 + \mathcal{P}_2\right) \neq$$

$$e^{\mathcal{L}_A \Delta t} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{-(2\gamma_0 + \mathrm{i}\Omega)\Delta t} & 0 \\ 0 & 0 & 0 & e^{-(2\gamma_0 - \mathrm{i}\Omega)\Delta t} \end{pmatrix}\,. \tag{7.78}$$

This may have significant consequences – even without dissipation $\gamma_0 = 0$: The repeated application of the propagator for measurement without feedback ($\gamma_0 = 0$ and $\alpha = 0$) yields

$$\left[e^{\mathcal{L}_A \Delta t}\left(\mathcal{P}_1 + \mathcal{P}_2\right)\right]^n = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & e^{-\mathrm{i}\Omega\Delta t}\cos^{n-1}(\Omega\Delta t) & e^{-\mathrm{i}\Omega\Delta t}\cos^{n-1}(\Omega\Delta t) \\ 0 & 0 & e^{+\mathrm{i}\Omega\Delta t}\cos^{n-1}(\Omega\Delta t) & e^{+\mathrm{i}\Omega\Delta t}\cos^{n-1}(\Omega\Delta t) \end{pmatrix}\,. \tag{7.79}$$

Exercise 54 (Repeated measurements) *(0 points)*
Show the validity of the above equation.

In contrast, without the measurements we have for repeated application of the propagator simply

$$\left[e^{\mathcal{L}_A \Delta t}\right]^n = e^{\mathcal{L}_A n \Delta t}\,. \tag{7.80}$$

When we now consider the limit $n \to \infty$ and $\Delta t \to 0$ but $n\Delta t = t$ remaining finite, it becomes obvious that the no-measurement propagator for $\gamma_0 = 0$ simply describes coherent evolution. In contrast, when the measurement frequency becomes large enough, the measurement propagator in Eq. (7.78) approaches

$$\left[e^{\mathcal{L}_A \Delta t}\left(\mathcal{P}_1 + \mathcal{P}_2\right)\right]^n = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix} \tag{7.81}$$

and thereby freezes certain states such as $\bar{\rho} = \frac{1}{2}\left[|0\rangle + |1\rangle\right]\left[\langle 0| + \langle 1|\right]$. This effect is known as Quantum-Zeno effect (a watched pot never boils) and occurs when measurement operators and system Hamiltonian do not commute and the evolution between measurements is unitary (here $\gamma_0 = 0$). When the evolution between measurements is an open one ($\gamma_0 > 0$), the Quantum-Zeno effect cannot be used to stabilize the coherences, which becomes evident from the propagator in Eq. (7.78).

With feedback ($\alpha > 0$) however, the effective propagator $\mathcal{W}(\Delta t)$ does not have the Block structure anymore. It can be used to obtain a fixed-point iteration for the density matrix

$$\rho(t + \Delta t) = \mathcal{W}(\Delta t)\rho(t)\,. \tag{7.82}$$

Here, we cannot even for small Δt approximate the evolution by another effective Liouvillian, since $\lim_{\Delta t \to 0} \mathcal{W}(\Delta t) \neq \mathbf{1}$. Instead, one can analyze the eigenvector of $\mathcal{W}(\Delta t)$ with eigenvalue 1 as the (in a stroboscopic sense) stationary state. It is more convenient however to consider the expectation values of $\langle \sigma^i \rangle_t$ that fully characterize the density matrix via

$$\rho_{00} = \frac{1 + \langle \sigma^z \rangle}{2}\,, \qquad \rho_{11} = \frac{1 - \langle \sigma^z \rangle}{2}\,, \qquad \rho_{01} = \frac{\langle \sigma^x \rangle - \mathrm{i}\,\langle \sigma^y \rangle}{2}\,, \qquad \rho_{10} = \frac{\langle \sigma^x \rangle + \mathrm{i}\,\langle \sigma^y \rangle}{2}\,. \tag{7.83}$$

Note that decoherence therefore implies vanishing expectation values of $\langle \sigma^x \rangle \to 0$ and $\langle \sigma^y \rangle \to 0$ in our setup. Converting the iteration equation for the density matrix into an iteration equation for the expectation values of Pauli matrices we obtain

$$\begin{aligned}
\langle \sigma^x \rangle_{t+\Delta t} &= \frac{e^{-2\gamma_0 \Delta t}}{2}\left\{\left(1 + \langle \sigma^x \rangle_t\right)\cos\left(\Omega \Delta t\right) - \left(1 - \langle \sigma^x \rangle_t\right) e^{-(\gamma_- + \gamma_+)\alpha \Delta t/2}\cos\left[\left(\Omega + \alpha(\Omega + \Sigma)\right)\Delta t\right]\right\} \\
\langle \sigma^y \rangle_{t+\Delta t} &= \frac{e^{-2\gamma_0 \Delta t}}{2}\left\{\left(1 + \langle \sigma^x \rangle_t\right)\sin\left(\Omega \Delta t\right) - \left(1 - \langle \sigma^x \rangle_t\right) e^{-(\gamma_- + \gamma_+)\alpha \Delta t/2}\sin\left[\left(\Omega + \alpha(\Omega + \Sigma)\right)\Delta t\right]\right\} \\
\langle \sigma^z \rangle_{t+\Delta t} &= \frac{(\gamma_+ - \gamma_-)\left(1 - \langle \sigma^x \rangle_t\right)}{2(\gamma_- + \gamma_+)}\left(1 - e^{-(\gamma_- + \gamma_+)\alpha \Delta t}\right)\,,
\end{aligned} \tag{7.84}$$

which (surprisingly) follow just the expectation values $\langle\sigma^x\rangle_t$ on the r.h.s. The first of the above equations can be expanded for small Δt to yield

$$\frac{\langle\sigma^x\rangle_{t+\Delta t} - \langle\sigma^x\rangle_t}{\Delta t} = -\frac{1}{4}\left[8\gamma_0 + \alpha\left(\gamma_- + \gamma_+\right)\right]\langle\sigma^x\rangle_t + \frac{1}{4}\alpha\left(\gamma_- + \gamma_+\right) + \mathcal{O}\{\Delta t\}\,. \tag{7.85}$$

When $\Delta t \to 0$, this becomes a differential equation with the stationary state

$$\langle\bar{\sigma}^x\rangle = \frac{\alpha(\gamma_- + \gamma_+)}{8\gamma_0 + \alpha(\gamma_- + \gamma_+)}\,, \tag{7.86}$$

which approaches 1 for large values of α. Taking into account the large-temperature expansions for the dampening coefficients

$$\gamma_0 = J_0 k_{\rm B} T\,, \qquad \gamma_- + \gamma_+ \approx 2J_0 e^{-\Omega/\omega_c} k_{\rm B} T\,, \tag{7.87}$$

we see that this stabilization effect also holds at large temperatures – a sufficiently strong (and perfect) feedback provided. An initially coherent superposition is thus not only stabilized, but also emerges when the scheme is initialized in a completely mixed state. Also for finite Δt, the fixed-point iteration yields sensible evolution for the expectation values of the Pauli matrices, see Fig. 7.7.

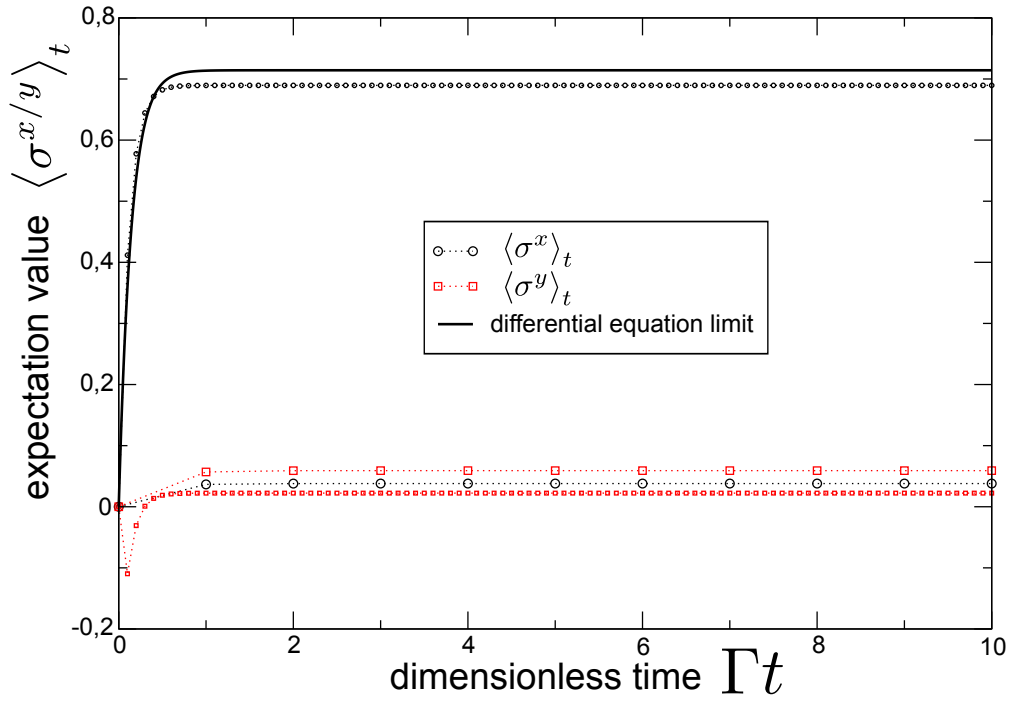

Figure 7.7: Expectation values of the Pauli matrices for finite feedback strength $\alpha = 10$ and finite stepsize Δt (spacing given by symbols). For large Δt, the fixed point is nearly completely mixed. For small Δt, the curve for $\langle\sigma^x\rangle_t$ approaches the differential equation limit (solid line), but the curve for $\langle\sigma^y\rangle_t$ approaches 0. For $\gamma_- = \gamma_+$, the iteration for $\langle\sigma^z\rangle_t$ vanishes throughout. Parameters: $\gamma_- = \gamma_+ = \gamma_0 = \Gamma$, $\Omega\Delta t = \in \{1, 0.1\}$, and $\Sigma\Delta t \in \{0.5, 0.05\}$.