Quantum Stochastic Thermodynamics

Foundations and Selected Applications

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This book is dedicated to the memory of my PhD supervisor, Tobias Brandes

Preface

Recent decades have seen much progress in our understanding of thermodynamic processes at the nanoscale. But nanoscale systems are very small, in most applications far from equilibrium, often subject to strong fluctuations, and sometimes even characterized by exotic quantum properties—so it seems as if these features rule out any possibility to find a consistent thermodynamic description for them.

It is the primary objective of this book to show that this is not the case. There is a thermodynamic framework, characterized by a remarkable internal consistency, which is able to describe nanoscale systems even under extreme conditions. Moreover, this framework does not only reaffirm the common folklore of thermodynamics (*there is no perpetual motion machine, etc.*), but it provides a wealth of beautiful results beyond the traditional scope of thermodynamics—opening up the possibility to understand a plethora of different physical situations from a unified perspective.

The main title "Quantum Stochastic Thermodynamics" shall suggest that the present book is about a synthesis of two research fields: classical stochastic thermodynamics and quantum thermodynamics. Both have pushed the boundaries of the applicability of the laws of thermodynamics by explaining and supplementing them with microscopic considerations. For a considerable large class of nanoscale systems and processes, I believe that most foundational questions are settled by now. The present book is supposed to fill a gap in the literature by justifying this claim in detail for a large variety of situations. I am also convinced that its content will prove important to explore new territories at the rapidly evolving frontiers of this field.

The subtitle "Foundations and Selected Applications" shall emphasize that the reader can mainly expect explanations about the basic theoretical pillars. These explanations are supposed to be pedagogically accessible. However, the book is also driven by the desire to introduce a general and versatile framework characterized by conceptual clarity—in complete awareness of the fact that this poses additional technical obstacles for the beginner. To remedy for that, a considerable effort is spent to transparently explain common 'jargon' in the community (nonequilibrium entropies, local detailed balance, Landauer's principle, entropy production, time–reversal symmetry, the arrow of time, etc.), which often appears unnecessarily mystified (a problem, which seems to have tradition in thermodynamics and statistical mechanics). The reader will not seldomly find the same (or closely related) results derived in different ways in order to generate confidence and trust in the framework.

The field of quantum stochastic thermodynamics fascinates, however, not only because it allows to addresss foundational questions about the nature of heat, entropy or the second law, but also because it might have direct practical applications in a world with increasing nanotechnological abilities. These applications could come in form of efficient thermoelectric devices, powerful energy harvesters, fast cooling strategies, or energy–efficient computers, among other more exotic applications. To tie a close connection between foundational and practical problems, this book treats a few selected applications in detail.

Unfortunately, due to a lack of time and understanding on the author's side, this book cannot cover all possible directions, which are investigated at the moment. The selected material is obviously biased and I ask for the forbearance of my many colleagues, who feel that the present book misses some important ideas.

How to read this book

This book is written for graduate students, who know the basics of quantum mechanics and equilibrium statistical mechanics and who can't wait to combine these fields to understand nonequilibrium phenomena. As a rule of thumb, you are ready to delve into the book if the following equations do not scare you off:

$$\begin{aligned}
\frac{\partial}{\partial t}\rho(t) &= -\frac{i}{\hbar}[H,\rho(t)], \\
\rho &= \sum_n \lambda_n |n\rangle\langle n|, \\
\mathcal{Z}(\beta) &= \mathrm{tr}\{e^{-\beta H}\}, \\
\mathcal{U}(\beta) &= -\frac{\partial}{\partial\beta}\ln\mathcal{Z}(\beta), \\
S_B &= k_B \ln V, \\
f(\epsilon) &= \frac{1}{e^{\beta(\epsilon-\mu)}+1}.
\end{aligned}$$

Of course, this book is also written for more experienced researchers. I hope that they will have no troubles in jumping between different sections of this book (though it might help to first look at the "Basic Notation" section below). To get further acquainted with the book, I here summarize its most important features.

STRUCTURE OF THE BOOK: To get a complete picture, I believe one should sooner or later read the entire book and then, it is perhaps most beneficial to go through it in linear order. However, I also believe that the impatient reader should not be afraid to skip sections or chapters. For instance, Chapter 1 ("Quantum Stochastic Processes") appears to be the most abstract one, in particular its second half. While I believe that this more abstract point of view helps to view the entire field in a clear and unified way, it is certainly not necessary to reach an understanding of Chapter 2 ("Classical Stochastic Thermodynamics"), which solely requires some basic background knowledge of the theory of classical stochastic processes. Likewise, readers with some familiarity with open quantum system theory can directly start reading Chapter 3 ("Quantum Thermodynamics Without Measurements"). To understand Chapter 4 ("Quantum Fluctuation Theorems"), some background information from previous chapters is required. For some sections of Chapter 5 ("Operational Quantum Stochastic Thermodynamics") it is necessary to have read and understood also the end of Chapter 1. Finally, three appendices complement this book about topics, which appear at various points in the main text, but whose detailed exposition requires a longer detour, which would blur the main narrative.

STRUCTURE OF THE SECTIONS: Typically, I have tried to start each section with a small paragraph motivating its content and to end each section with a small summary or outlook. To facilitate orientation, some sections (in particular longer ones) are divided into subsections using unnumbered subtitles. Furthermore, important statements are distinguished by longer italic text and boxed equations highlight important definitions or results.

INDEX: I have tried to make a long and informative index list. Words or phrases appearing in this list are printed in a **boldface** font in the main text at the point, where they are first introduced or explained. However, as I said above, the book is characterized by presenting similar concepts in different contexts and from different perspectives. Thus, the book is not written as an encyclopaedia, but tries to keep a narrative, which is most beneficial for pedagogical purposes.

EXERCISES: Various exercises are scattered throughout the text. These exercises, sometimes supplemented by (hopefully) helpful hints how to solve them, should be rather simple because I believe there is no benefit from torturing the reader. Exercises fall, however, into two categories. The first category of exercises are the short ones. They are supposed to supply simple crosschecks for the reader or, by asking to derive some equations, to make the reader acquainted with standard mathematical manipulations in the field. Then, there are also various longer exercises, which might even require some simple symbolic programming. These longer exercises are typically meant to introduce ideas, concepts or results, whose detailed exposition would probably bore the more experienced reader in the field. Thus, the exercises help to keep the book more concise, while allowing me at the same time to cover a wider range of topics. I remark that all exercises appear during the text at the point where they fit best the overall narrative.

REFERENCES: In contrast to the exercises, all references are relegated to a special "Further reading" section at the end of each chapter. Having the overall pedagogical purpose of the book in mind, I indeed believe that there is little benefit from mentioning references during the main exposition of the material. Moreover, it ought to be clear that, given the breadth and scope of the present book, it is impossible to give credit to all contributions and, seen again from a pedagogical perspective, I believe there is little benefit from trying to do so here. Hence, this book should not be confused with a conventional 'review article.' Most citations are given to the latest work, where the main concepts or equations I rely on were first introduced or derived. Other citations typically refer to expositions, which go beyond the here presented material in a wider sense (i.e., books, review or introductory articles about fields related to but not part of quantum stochastic thermodynamics). Finally, some citations are added for historical clarity. Thus, the overall idea is that the list of references provides a first *orientation* for the newcomer, not an exhaustive list of contributions to the field.

Basic Notation

I tried to keep abbreviations to a minimum and used only those, which are widely used in the literature. The three most important abbreviations, which appear scattered throughout the text, are CP (completely positive), CPTP (completely positive and trace–preserving) and BMS (Born–Markov–secular). In some equations, I write h.c. to denote the Hermitian conjugate. Also the abbreviation POVM (positive operator–valued measure) is used occasionally.

Below, I further provide a non–exhaustive list of the most important notation used throughout the book.

GENERAL MATHEMATICS: Matrices are denoted by capital letters (such as M). Boldface letters are used for vectors (e.g., a vector of probabilities $\boldsymbol{p}$) and sequences (e.g., a sequence of measurement results $\mathbf{r}$), but their elements are written as, e.g., p_j or r_n. Multiplication of vectors and matrices is written without a dot (e.g., $M\boldsymbol{p}$). $[A,B] = AB - BA$ and $\{A,B\} = AB + BA$ denote the commutator and anticommutator, respectively. A superscript $*$, T or $\dagger$ denotes complex conjugate, transpose or the conjugate transpose, respectively. The imaginary unit is denoted i and the symbol $\mathcal{O}(x)$ denotes that $\lim_{x\to 0} |\mathcal{O}(x)/x| < \infty$. Total and partial derivatives (e.g., with respect to time t) appearing in inline equations are written as d_t and ∂_t, respectively. Often used functions are the Heaviside step function $\Theta(x)$, the Kronecker delta $\delta_{m,n}$ and the Dirac delta function $\delta(x-y)$.

QUANTUM DYNAMICS: I use Dirac notation for states $|\psi\rangle$ and their conjugate transpose $\langle\psi|$, which live in a Hilbert space $\mathcal{H}$ and its dual, respectively. The scalar product is written as $\langle\phi|\psi\rangle$. To avoid unwanted technicalities, I assume Hilbert spaces are (or can be approximated to be) finite dimensional: $d = \dim\mathcal{H} < \infty$. The density matrix is typically denoted by ρ, whereas most other operators are denoted by capital letters such as $H, P, X, \dots$ and I is the identity. Exceptions are the familiar bosonic and fermionic creation and annihilation operators (denoted typically by $a^{(\dagger)}, b^{(\dagger)}, c^{(\dagger)}, d^{(\dagger)}$) and the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The trace of some operator O is denoted $\mathrm{tr}\{O\}$. Superoperators (also simply called maps), which map operators onto operators, are always denoted by calligraphic letters such as $\mathcal{C}, \mathcal{D}, \mathcal{L}, \dots$. The tensor product is denoted $\otimes$ and additional subscripts $A, B, S\dots$ are used to indicate on which subspace some operator is acting (e.g., ρ_S) or to denote the partial trace (e.g., $\mathrm{tr}_B\{\dots\}$).

STATISTICAL MECHANICS: Equilibrium concepts are denoted by calligraphic letters such as the equilibrium internal energy $\mathcal{U}$ or equilibrium entropy $\mathcal{S}$. Exceptions are parameters such as temperature T or chemical potential μ. Out–of–equilibrium quantities are denoted by, e.g., U and S if they refer to some expectation value or ensemble average. Thermodynamic quantities defined along single stochastic trajectories are denoted by small Latin letters (e.g., u and s). The canonical ensemble (or Gibbs state) is denoted by the Greek letter π. For instance, $\pi_S(\beta)$ denotes the Gibbs state of some system S at inverse temperature β.

FINALLY, every process starts at the initial time $t_0 = 0$. Moreover, I do *not* set Boltzmann's and Planck's constant k_B and $\hbar$ to one. I believe that this makes the physical content of many equations more insightful. For practical manipulations, this choice is, of course, not the most convenient one, but since the majority of literature sets $k_B \equiv 1$ and $\hbar \equiv 1$, I thought it is good to keep them here explicit.

Acknowledgements

This book is dedicated to the memory of Tobias Brandes because—already long before I enjoyed being his PhD student—his inspiring and unprecedented lectures were the reason why I actually turned towards theoretical physics. In my opinion, Tobias' approach to physics was dual, tackling deep and conceptual problems while having at the same time an eye on experimentally well–grounded approaches and models, which also work 'in practice.' I view my own research, and in particular this book, in tradition of his philosophy; perhaps with some bias more towards conceptual and general ideas. I hope Tobias would have enjoyed reading it.

Concerning the topics exposed here I further owe much of my detailed knowledge to Massimiliano Esposito and Gernot Schaller. Both never hesitated to share their insights and ideas with me about various topics in statistical mechanics, stochastic thermodynamics, nonequilibrium physics and open quantum systems. Much of their knowledge is reflected here; yet, I believe I succeeded to also add my own twist.

A special thanks goes to Kavan Modi. A short, but in retrospective important discussion at the Kavli Institute in Santa Barbara in 2018 inspired me to look at the problem from a different angle and part of the material presented in Chapter 5, and in some sense the motivation to write this book, is a consequence of that discussion.

Many more colleagues have shared their insights and thoughts with me. Those, on which I could particularly rely on concerning the topics presented in this book, include Robert Alicki, Janet Anders, Felipe Barra, Victor Bastidas, Javier Cerrillo, Luis Correa, María García Díaz, David Gelbwaser–Klimovsky, John Goold, Giacomo Guarnieri, Géraldine Haack, Christopher Jarzynski, Matteo Lostaglio, Mark Mitchison, Kavan Modi, Wolfgang Muschik, Juan Parrondo, Martí Perarnau–Llobet, Matteo Polettini, Andreu Riera-Campeny, Felix Ritort, Àngel Rivas, Dominik Šafránek, Rafael Sánchez, Anna Sanpera, Udo Seifert, Michalis Skotiniotis, Christopher Wächtler and Andreas Winter. It makes me a bit sad to know that I probably forgot to correctly acknowledge all the people, who contributed to my actual understanding of this topic. There were clearly many more people who influenced my thinking.

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Finally and almost needless to say, all mistakes and opinions expressed here are entirely my own. I am always grateful to receive further comments, questions and feedback (to get in contact with me I suggest you type in my name in your preferred search engine and look up my up–to–date email address). Errata will be announced on my homepage.

Contents

1

Quantum Stochastic Processes

Summary. This chapter describes the basic features of open quantum systems, i.e., quantum systems that are affected by noise due to uncontrollable degrees of freedom of an environment or bath. This noise is responsible for effects such as dissipation, decoherence and irreversibility. We study the equilibrium states of open quantum systems and review tools from quantum measurement theory, which describe how to extract information from an (open) quantum system. We generalize these tools to multi–time statistics and define the notion of a quantum stochastic process and a quantum Markov process. Finally, we study in which cases a quantum stochastic process looks classical.

1.1 Isolated Quantum Systems

Time–independent case

A quantum system is described by a Hilbert space $\mathcal{H}$ and a state ρ called the density matrix, which acts on that space. The density matrix is characterized by the facts that it is Hermitian, $\rho^\dagger = \rho$ (with $\dagger$ denoting the Hermitian conjugate), has unit trace, $\mathrm{tr}\{\rho\} = 1$, and is positive, $\rho \geq 0$. Here, the notation $\rho \geq 0$ is shorthand for $\langle\psi|\rho|\psi\rangle \geq 0$ for all $|\psi\rangle \in \mathcal{H}$.

The state of an isolated quantum system, i.e., a quantum system which is not in contact with any other part of the world, obeys the Liouville–von Neumann equation

$$\frac{\partial}{\partial t}\rho(t) = -\frac{i}{\hbar}[H, \rho(t)]. \tag{1.1}$$

Here, H is the Hamiltonian operator characterizing the total energy of the system and $[A, B] \equiv AB - BA$ is the commutator. Furthermore, i and $\hbar$ are the familiar imaginary unit and Planck's constant. Note that we will also use the notation $\partial_t \rho(t)$ to denote a partial derivative with respect to time.

Isolated quantum systems have some important characteristics:

(i) There exists a unitary time evolution operator $U(t) \equiv \exp(-iHt/\hbar)$, which means that $U(t)U(t)^\dagger = U(t)^\dagger U(t) = I$, where I denotes the identity matrix. This time evolution operator propagates the system state according to

$$\rho(t) = U(t)\rho(0)U(t)^\dagger, \tag{1.2}$$

where $\rho(0)$ denotes the initial state of the quantum system.

(ii) The spectrum of the state $\rho(t)$, i.e., its eigenvalues λ_k, do not change in time:

$$\rho(t) = \sum_k \lambda_k |\psi_k(t)\rangle\langle\psi_k(t)|. \tag{1.3}$$

Here, λ_k is time–independent and $|\psi_k(t)\rangle$ belongs to an orthonormal basis of wave functions, i.e., $\langle\psi_k(t)|\psi_\ell(t)\rangle = \delta_{k,\ell}$ with the Kronecker delta $\delta_{k,\ell}$. Note that the spectrum can be degenerate, i.e., it is possible that $\lambda_k = \lambda_\ell$ for some $k \neq \ell$. Equation (1.3) follows from the fact that any unitary transformation of the form (1.2) leaves the spectrum invariant since the characteristic polynomial does not change:

$$\det\{\rho(t) - \lambda I\} = \det\{U(t)[\rho(0) - \lambda I]U(t)^\dagger\} = \det\{\rho(0) - \lambda I\}. \tag{1.4}$$

Here, $\det\{\dots\}$ denotes the determinant of a matrix.

(iii) The purity of $\rho(t)$, which measures the 'mixedness' of a state and is defined as $\mathrm{tr}\{\rho^2\}$, is conserved. This follows immediately from point (ii) above or, alternatively, from eqn (1.1) and the fact that the trace is cyclic, i.e., $\mathrm{tr}\{ABC\} = \mathrm{tr}\{CAB\}$. In particular, if the initial state is pure, i.e., $\mathrm{tr}\{\rho(0)^2\} = 1$, we have $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ for some wave function $|\psi(t)\rangle$. This wave function evolves in time according to the familiar Schrödinger equation:

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -\frac{i}{\hbar}H|\psi(t)\rangle. \tag{1.5}$$

Since the Schrödinger equation can be applied to compute the time evolution of any of the $|\psi_k(t)\rangle$ in eqn (1.3), it is equivalent to the Liouville–von Neumann equation (1.1).

(iv) The **von Neumann entropy** of the system, which is defined as

$$S_{\mathrm{vN}}(\rho) \equiv -\mathrm{tr}\{\rho \ln \rho\}, \tag{1.6}$$

is constant in time. This follows again from point (ii) above because $S_{\mathrm{vN}}[\rho(t)] = -\sum_k \lambda_k \ln \lambda_k$, which implies that the von Neumann entropy quantifies the classical uncertainty about the state of the system. Alternatively, the conservation of von Neumann entropy follows by using

$$\frac{d}{dt}S_{\mathrm{vN}}[\rho(t)] = -\mathrm{tr}\left\{\frac{d\rho(t)}{dt}\ln\rho(t)\right\} \tag{1.7}$$

and eqn (1.1). Note that eqn (1.7) holds only if the rank of the density operator does not change during the evolution, which is guaranteed by point (ii) above. If the rank changes in time, the von Neumann entropy is not differentiable. Note that we use a subscript 'vN' for the von Neumann entropy throughout the book because we want to distinguish it from the notion of *thermodynamic* entropy introduced later on. Readers unfamiliar with information theoretic concepts of entropy can find an overview in Appendix A.

Time–dependent case

Quantum systems are often subjected to time–dependent fields in a lab, which can be treated semiclassically (e.g., laser light). In this case, the Hamiltonian becomes time–dependent and is denoted by $H(\lambda_t)$, where the time–dependent parameter λ_t specifies the external fields. We prefer the notation $H(\lambda_t)$ instead of $H(t)$ to avoid any possible confusion with the Heisenberg picture. In the following, λ_t is called a *driving* or *control protocol* and the state of such a *driven system* evolves in time according to the Liouville–von Neumann equation (1.1) with H replaced by $H(\lambda_t)$.

The evolution $\rho(t) = U(t,0)\rho(0)U^\dagger(t,0)$ is still described by a unitary operator $U(t,0)$, but its explicit computation is now more complicated. Formally, we have

$$\begin{aligned} U(t,0) &= \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1 H(\lambda_1)\int_0^{t_1} dt_2 H(\lambda_2)\cdots\int_0^{t_{n-1}} dt_n H(\lambda_n) \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1\cdots\int_0^t dt_n [H(\lambda_1)\ldots H(\lambda_n)]_+ \\ &\equiv \exp_+\left[-\frac{i}{\hbar}\int_0^t ds H(\lambda_s)\right], \end{aligned} \tag{1.8}$$

where we abbreviated $\lambda_{t_j} \equiv \lambda_j$ and the subscript $+$ denotes time–ordering. By dividing the time interval $[0,t]$ into $n = t/\delta t$ small steps δt, we can also write

$$U(t,0) \approx \prod_{j=0}^{n-1} e^{-iH(\lambda_j)\delta t/\hbar}, \tag{1.9}$$

which becomes exact in the limit $n \to \infty$.

Strictly speaking, a driven quantum system is not isolated as it is in contact with the external driving field. However, it is easy to check that the points (i) to (iv) above are still satisfied for such a driven system. In contrast, the time evolution of a quantum system, which interacts with another quantum system, is markedly different as we will see in the rest of this chapter. Therefore, it seems wise to call a quantum system 'isolated' as long as it evolves in time according to the Liouville–von Neumann equation (1.1), whether the Hamiltonian is time–independent or not.

1.2 System–Bath Theories and the Origin of Noise

In reality, nobody has ever observed an isolated quantum system, at the very end because the mere act of 'observing' a quantum system requires to couple it with an external detector. We will, however, postpone the discussion of quantum measurement theory to Section 1.4 and are here rather concerned with the fact that many quantum systems interact with *uncontrollable* degrees of freedom of a so–called *environment* or *bath*. One example is an atom (the 'system') interacting with the many electromagnetic modes of the surrounding space (the 'environment'). Another example is a single spin, e.g., an impurity in a metal or crystal, interacting with many remaining spins and phonons (lattice vibrations) of the surroundings. Finally, the historical origin of the

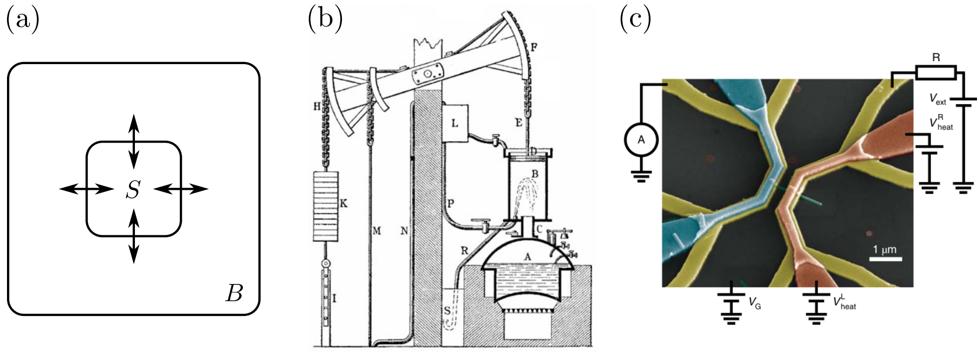

Fig. 1.1 Open quantum systems. (a) Rough sketch of a system S in contact with a bath B with which it can exchange energies, particles, entropy, etc. (b) Diagram of the Newcomen atmospheric steam engine as an example of an ancient 'open quantum system:' Already thermodynamics divided the universe into a system part and reservoirs. (c) (False–coloured) scanning electron microscope image of a modern open quantum system: a quantum dot formed by a nanowire (thin green line) in contact with electron reservoirs (yellow) and heaters (blue and red). The picture is taken from Josefsson *et al.* (2018) and such setups will be treated in further detail in Sec. 3.10.

theory of thermodynamics is rooted in the desire to understand, e.g., steam of water in a container in contact with hot air produced by burning coal on the one side and cold water on the other side. Here, the system is defined by the container, which contains the so–called working medium or working fluid, whereas the outside hot air and cold water are called a *heat bath* or *reservoir*. We will also use these words from Chapter 2 on. In this chapter, however, we use the broader term 'environment' or 'bath' to refer to any external, uncontrollable part of the world, not necessarily described by a thermodynamic variable such as temperature. It will become clear throughout this book that the predictive power of the second law comes from an efficient description of these uncontrollable degrees of freedom about which we have only very little information.

Quantum systems which are not isolated but in contact with a bath or environment are called *open* quantum systems, see Fig. 1.1 for sketches. Conceptually, many different approaches exist to describe them theoretically and a very powerful one is to model the bath itself as another quantum system such that the system *and* the bath (which we sometimes also call the *universe*) constitute one big isolated quantum system. This is the origin of system–bath theory and we will see below that this is indeed not an assumption: any open quantum system can be seen as being part of a larger isolated quantum system.

Mathematically, the system–bath composite is a *bipartite* quantum system described by the tensor product of the system and bath Hilbert space: $\mathcal{H}_S \otimes \mathcal{H}_B$. The dimension of that space is $\dim(\mathcal{H}_S \otimes \mathcal{H}_B) = \dim \mathcal{H}_S \cdot \dim \mathcal{H}_B$. For many applications the dimension of $\mathcal{H}_S$ is very small, e.g., $\dim \mathcal{H}_S = 2$ for a single spin, whereas the dimension of $\mathcal{H}_B$ often very large, e.g., $\dim \mathcal{H}_B = 2^{N_A}$ where the Avogadro number N_A is of the order 10^{23}. The dynamics of the system and the bath is governed by the Hamiltonian $H_{SB} = H_S \otimes I_B + I_S \otimes H_B + V_{SB}$. Here, H_S and H_B denote the Hamiltonian of the isolated system or bath, respectively, and V_{SB} denotes their interaction. They sum up to the total Hamiltonian H_{SB}. Whereas the system and bath Hamiltonian commute (since they live on different Hilbert spaces) we have in general $[V_{SB}, H_S] \neq 0$ and $[V_{SB}, H_B] \neq 0$. In the following, we suppress tensor products with the identity for notational simplicity and write the system–bath Hamiltonian as

$$H_{SB} = H_S + H_B + V_{SB}. \tag{1.10}$$

For simplicity, we assumed no driving λ_t here, but this will change in later chapters. We remark that the tensor product structure of the system–bath composite assumes the system and bath to be distinguishable objects and implies a particular choice of gauge made when identifying what is the 'system' and what is the 'bath.'

Since the system–bath composite is isolated, its global state described by the density operator $\rho_{SB}(t)$ evolves according to the Liouville–von Neumann equation (1.1) with H replaced by H_{SB}. The system evolution is obtained by taking the partial trace:

$$\rho_S(t) = \mathrm{tr}_B\{\rho_{SB}(t)\}. \tag{1.11}$$

In contrast to the isolated case, the evolution of an open quantum system is significantly different. None of the four points mentioned in Section 1.1 remain true:

(i') The time evolution of $\rho_S(t)$ is not described by a unitary operator.

(ii') The eigenvalues of the system state change in time, i.e., eqn (1.3) is replaced by

$$\rho_S(t) = \sum_k \lambda_k(t) |\psi_k(t)\rangle_S \langle \psi_k(t)|. \tag{1.12}$$

(iii') Since the eigenvalues of $\rho_S(t)$ change, the purity of the state can change too. In particular, an initially pure state becomes mixed in general.

(iv') The von Neumann entropy is no longer conserved. Note that the von Neumann entropy of the system can become larger or smaller during the evolution, without violating the second law of thermodynamics. The second law states only that the thermodynamic entropy of the universe, i.e., the system and the bath, cannot become smaller in time. It does not imply that the von Neumann entropy of the system state cannot decrease.

Illustrative example

We illustrate the above arguments by considering an assembly of n interacting spins. Readers unfamiliar with open quantum systems are invited to explicitly follow this example by doing their own numerics for it. We assume that the spins are described by the following global Hamiltonian

$$H_{SB} = \frac{\hbar\Omega}{2} \sum_{i=1}^{n} \sigma_z^{(i)} + \frac{\hbar}{2} \sum_{i=1}^{n} \sum_{j>i} g_{ij} \sigma_x^{(i)} \sigma_x^{(j)}, \tag{1.13}$$

where $\sigma_\alpha^{(i)}$ $(\alpha = x, y, z)$ are the familiar Pauli matrices acting on spin i. The first term describes n isolated spins with energy gap $\hbar\Omega$. The second term describes the interaction between two spins with coupling strength g_{ij}. As our system we now choose one of the spins, say the first, such that $H_S = \hbar\Omega\sigma_z^{(1)}/2$. The bath Hamiltonian consequently becomes $H_B = \hbar\Omega\sum_{i=2}^n \sigma_z^{(i)}/2 + \hbar\sum_{i=2}^n\sum_{j>i} g_{ij}\sigma_x^{(i)}\sigma_x^{(j)}/2$ and the remaining part defines the interaction Hamiltonian V_{SB}. The initial state of the system and bath is assumed to be decorrelated:

$$\rho_{SB}(0) = \rho_S(0) \otimes \rho_B(0), \tag{1.14}$$

In the simulations, we take $\rho_S(0) = |+\rangle\langle+|_S$ to be a pure state. Here, $|+\rangle \equiv (|0\rangle + |1\rangle)/\sqrt{2}$ denotes a coherent superposition of the eigenstates of σ_z (with $\sigma_z|0\rangle = -|0\rangle$ and $\sigma_z|1\rangle = +|1\rangle$), which coincide with the energy eigenstates of H_S. The bath instead is taken to be a canonical equilibrium (Gibbs) ensemble with respect to the inverse temperature β, denoted by

$$\rho_B(0) = \pi_B \equiv \frac{e^{-\beta H_B}}{\mathcal{Z}_B}, \quad \mathcal{Z}_B \equiv \mathrm{tr}_B\{e^{-\beta H_B}\}, \tag{1.15}$$

where $\mathcal{Z}_B$ is the partition function of the bath. Therefore, we assume the following situation: previous to the initial time the first spin is decoupled from the others and prepared in a superposition of energy eigenstates. Then, at time $t = 0$ we suddenly switch on the interaction with the bath, which is assumed to be thermalized.

We aim at a numerical exact simulation of the system–bath dynamics based on the Liouville–von Neumann equation (1.1). For n spins the total density matrix as well as the unitary time evolution operator are $2^n \times 2^n$ matrices. This exponential growth in size necessarily limits us to consider only a few spins, precisely we consider 7 spins in total (i.e., the bath consists of 6 spins). Note that one is often interested in a bath, which is *much* larger in size. Computing the exact dynamics of an open quantum system then quickly becomes impossible, which motivates the need for efficient and reliable approximation schemes. For the moment, however, a small bath suffices to illustrate our points above. To continue with the discussion of our model, let us choose the spin–spin interactions g_{ij} random from a uniform distribution over $[0, 1]$. We do not explicitly write down the values for g_{ij} here because the dynamics are qualitatively similar for most choices.

Numerical results for an initial (dimensionless) bath temperature of $\beta\hbar\Omega = 10$ are shown in Fig. 1.2. Note that this bath temperature is relatively cold, i.e., the energy gap $\hbar\Omega$ of each single spin is 10 times larger than the typical energy $k_BT = \beta^{-1}$ of a thermal excitation. Figure 1.2 (a) shows the time evolution of the expectation value $\langle\sigma_x^{(1)}\rangle(t) = \mathrm{tr}_1\{\sigma_x^{(1)}\rho_S(t)\}$. For better comparison we also plot its time evolution in case that the spin was isolated, i.e., for $V_{SB} = 0$ (thin grey line). Their difference is quite striking, in particular it is difficult to recognize any structure or pattern for the open quantum system case. Figure 1.2 (b) shows the purity, which decreases as expected. Note that the minimal value of the purity for a two–level system is 1/2. Figure 1.2 (c) shows the evolution of the von Neumann entropy, which is no longer conserved. Note that the maximum value for the von Neumann entropy of a two–level system is $\ln 2 \approx 0.7$. Figure 1.2 (d) shows the time evolution of a quantity, which plays an important role throughout the book. It is known as the **quantum relative entropy** defined in general as

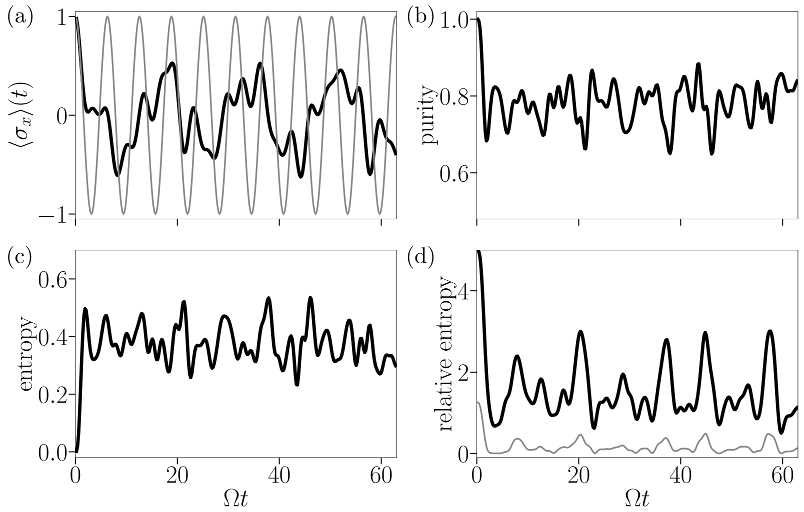

Fig. 1.2 Exemplary time evolution of an open quantum system for a 'cold' bath. The thin grey line in the upper left picture shows the time evolution of an isolated system with identical system Hamiltonian. The thin grey line in the lower right picture shows the time evolution of the quantum relative entropy with respect to a reference state, which describes a refined equilibrium state introduced in Section 1.3.

$$D(\rho|\sigma) \equiv \mathrm{tr}\{\rho(\ln\rho - \ln\sigma)\} \geq 0 \tag{1.16}$$

for two arbitrary density matrices ρ and σ. The relative entropy is non–negative and only zero if $\rho = \sigma$. It can be regarded as a measure of statistical 'distance' between ρ and σ and further information is provided in Appendix A. In particular, we plot

$$D\left[\rho_S(t)\left|\frac{e^{-\beta H_S}}{\mathcal{Z}_S}\right.\right], \tag{1.17}$$

i.e., the distance between the reduced system state and its associated Gibbs state at the inverse temperature of the bath. One could naively expect that this difference should become very small for long times in accordance with equilibrium statistical mechanics. This is not the case for two important reasons. First, a bath of only 6 spins is still too small to induce equilibration of a small quantum system. Second, even if the bath were larger, equilibrium statistical mechanics in fact predicts a state *different* from the Gibbs state as we will explain in detail in the next section. The time evolution of the relative entropy with respect to this different state is shown by the thin grey line, which is much closer to zero than eqn (1.17).

Finally, Fig. 1.3 shows the same plots as before, but for a different initial temperature of the bath. This time we chose $\beta\hbar\Omega = 1$ such that the thermal excitation energies are comparable with the energy gap of each single spin. Equivalently, one could say that we have more 'noise' in the bath. The difference compared with the cold case $\beta\hbar\Omega = 10$ is quite striking. Oscillations are much less pronounced and eqn (1.17) becomes quite small after some transient time. This means that the standard equilibrium

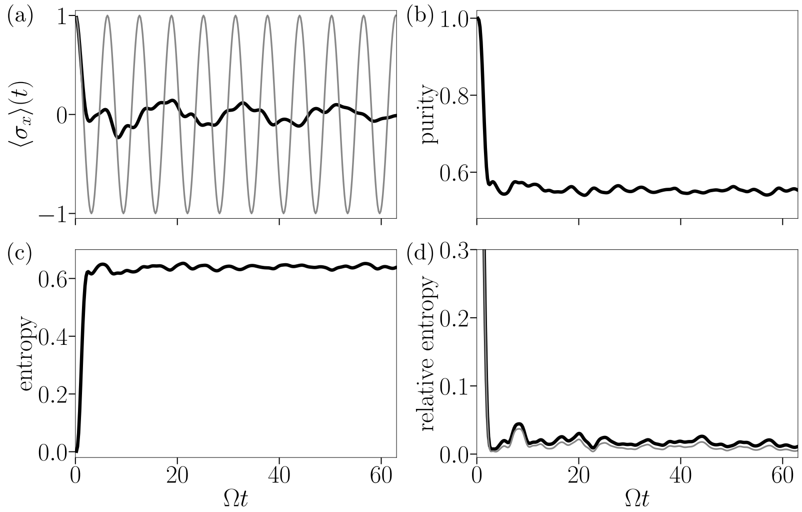

Fig. 1.3 Exemplary time evolution of an open quantum system for a 'hot' bath.

Gibbs ensemble describes the system state quite well. In fact, the system is well described by a completely mixed state $\rho_S(t) \approx I_S/2$, which follows by considering the time evolution of the purity.

To conclude, an open quantum system behaves very different from an isolated quantum system. Even for a very small bath of only 6 spins effects such as equilibration and thermalization start to become visible. Next, we consider equilibrium states of open quantum systems in case that the bath is much larger.

1.3 Equilibrium States of Open Quantum Systems

Before we analyse equilibrium states of open quantum systems, it might be worth to ask the question whether an open quantum system can actually reach an equilibrium state. In fact, we have introduced open quantum systems via the system–bath paradigm, i.e., a composite system that evolves unitarily in time. This implies that, as long as the system–bath composite can be described by a finite dimensional Hilbert space, the dynamics is **quasi–periodic**. By this we mean the following. Let $|\psi(0)\rangle$ denote the initial state of an arbitrary isolated system, which is here assumed to be pure for simplicity. We denote the eigenvalues and eigenstates of its Hamiltonian H by E_n and $|n\rangle$, respectively. Then, if we expand the initial state as $|\psi(0)\rangle = \sum_n c_n|n\rangle$ with complex coefficients c_n obeying $\sum_n |c_n|^2 = 1$, we can write the state at time t as

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar}|n\rangle, \tag{1.18}$$

i.e., it is a sum of periodic functions with frequencies $\omega_n \equiv E_n/\hbar$. If we wait long enough, we might wonder whether there exists some time t and a set of natural numbers $\{k_n\}$ such that $\omega_n t = 2\pi k_n$ for all n. This would then imply that $\langle\psi(0)|\psi(t)\rangle = 1$, i.e., the system returned back to its initial state. If all frequencies are rational numbers, we can straightforwardly find such a time t. By assumption we can then write $\omega_n = q_n/r_n$ for some $q_n \in \mathbb{N}$ and $r_n \in \mathbb{N}$. In particular, if we define $N \equiv \prod_n r_n$, we can write $\omega_n = m_n/N$ for all n and some $m_n \in \mathbb{N}$. Thus, by choosing $t = 2\pi k N$, we obtain $\langle\psi(0)|\psi(t)\rangle = 1$ for all $k \in \mathbb{N}$, i.e., the quantum system returns infinitely often to its initial state.

Things start to become more subtle if the ratio $\omega_n/\omega_{n'}$ of some pair of frequencies becomes *irrational*. Indeed, it then never happens that $\langle\psi(0)|\psi(t)\rangle = 1$. However, irrational numbers can be approximated arbitrarily well by rational numbers. Hence, it seems reasonable to expect from the foregoing argument that the system returns after a sufficiently long time to its initial state up to a *very small error*. Indeed, one can prove that an isolated finite dimensional quantum system returns arbitrarily close to its initial state infinitely often, i.e., for any $\epsilon > 0$ there exist infinitely many times t such that $|\langle\psi(0)|\psi(t)\rangle| = 1-\epsilon$. This is known as quasi-periodicity. This result is also known from classical mechanics as **Poincaré's recurrence theorem**. Obviously, since an open quantum system is a part of a larger isolated system, this also implies that any open quantum system state returns infinitely often arbitrarily close to its initial state. This seems to imply that we should not expect an open quantum system to equilibrate at all and Poincaré's recurrence theorem has played an important historical role in the debate whether it is possible to derive the laws of thermodynamics from an underlying microscopic perspective: If all states return arbitrarily close to their initial state, why do we observe any irreversibility?

The key insight to resolve this question lies in the fact that the next time t for which $|\langle\psi(0)|\psi(t)\rangle| = 1-\epsilon$ happens grows incredibly fast with the number of coefficients c_n in eqn (1.18). This number is expected to scale with the number of particles in the system because it is experimentally extremely unlikely to prepare a many–body system in a state $|\psi(0)\rangle$, which contains only a few energy eigenstates $|n\rangle$. Then, if the isolated system is composed out of N particles, e.g., the N spins in the previous example, one generically expects the average recurrence time to scale *double exponentially* with N, i.e., $t = \mathcal{O}\{\exp[\exp(N)]\}$. If one assumes that the number of particles is typically of the order of 10^{23}, the problem of Poincaré recurrences becomes irrelevant for all human time scales.

Therefore, we assume for now that the system equilibrates and reaches a stationary state $\lim_{t\to\infty}\rho_S(t)$, where the notation $t \to \infty$ means that we consider times much larger than typical time scales of the open system evolution, but still, of course, smaller than the Poincaré recurrence time. The next question is then: to which state will the open quantum system equilibrate? Finding a complete answer to that question turns out to be hard and is still subject of intense research. Since this is not the topic of the book, we here restrict ourselves to invoking arguments from equilibrium statistical mechanics, which work well in many cases.

For this purpose, we consider the familiar **Gibbs state** or **canonical ensemble**, defined for any system with Hamiltonian H by

$$\pi \equiv \frac{e^{-\beta H}}{\mathcal{Z}}, \quad \mathcal{Z} \equiv \mathrm{tr}\{e^{-\beta H}\}. \tag{1.19}$$

Here, $\beta = (k_B T)^{-1}$ is the inverse temperature and $\mathcal{Z}$ the partition function. If the internal energy $\mathcal{U} = \mathrm{tr}\{H\pi\}$ is fixed, the Gibbs state is characterized by the fact that it maximizes the von Neumann entropy with the inverse temperature implicitly defined through the relation $\mathcal{U} = -\partial_\beta \ln \mathcal{Z}$. Vice versa, for a fixed von Neumann entropy $S_{\mathrm{vN}}(\pi)$, the Gibbs state minimizes the energy with the inverse temperature implicitly defined through the relation $S_{\mathrm{vN}}(\pi) = -\beta^2\partial_\beta(\beta^{-1}\ln \mathcal{Z})$.

Now, suppose that the system–bath composite is well described by a global Gibbs state $\pi_{SB} = e^{-\beta H_{SB}}/\mathcal{Z}_{SB}$ with $\mathcal{Z}_{SB} \equiv \mathrm{tr}_{SB}\{e^{-\beta H_{SB}}\}$. How does the reduced system state $\mathrm{tr}_B\{\pi_{SB}\}$ look like? Perhaps surprisingly, it turns out that in general $\mathrm{tr}_B\{\pi_{SB}\} \neq \pi_S = e^{-\beta H_S}/\mathcal{Z}_S$. Only in case of very weak coupling between the system and the bath, i.e., if V_{SB} is negligible compared to H_S and H_B, the reduced system state equals the conventional canonical ensemble. For non–negligible coupling V_{SB}, however, we define $\pi_S^* \equiv \mathrm{tr}_B\{\pi_{SB}\}$ and we have $\pi_S^* \neq \pi_S$.

Nevertheless, it is still possible to write π_S^* in an *apparent* Gibbs form with respect to an *effective* Hamiltonian $\tilde{H}_S$:

$$\pi_S^* = \mathrm{tr}_B\{\pi_{SB}\} = \frac{e^{-\beta\tilde{H}_S}}{\tilde{Z}_S}. \tag{1.20}$$

In fact, this is possible for every density matrix ρ_S by defining $\tilde{H}_S \equiv -\beta^{-1}\ln(\tilde{Z}_S\rho_S)$, and not only for π_S^*. Notice that $\tilde{H}_S$ is only fixed up to an arbitrary choice of the positive normalization constant $\tilde{Z}_S$. For the reduced state π_S^* of a canonical equilibrium ensemble there is one convenient choice for the effective partition function, which we denote by $\mathcal{Z}_S^* = \tilde{Z}_S$ and which is obtained by setting

$$\boxed{\mathcal{Z}_S^* \equiv \frac{\mathcal{Z}_{SB}}{\mathcal{Z}_B} = \frac{\mathrm{tr}_{SB}\{e^{-\beta H_{SB}}\}}{\mathrm{tr}_B\{e^{-\beta H_B}\}}.} \tag{1.21}$$

That is, the effective partition function $\mathcal{Z}_S^*$ is the ratio of the partition functions of the system–bath composite and of the bath *alone*. The corresponding effective Hamiltonian is known as the **Hamiltonian of mean force** and reads explicitly

$$\boxed{H_S^* = -\frac{1}{\beta}\ln(\mathcal{Z}_S^*\pi_S^*) = -\frac{1}{\beta}\ln\frac{\mathrm{tr}_B\{e^{-\beta H_{SB}}\}}{\mathcal{Z}_B}.} \tag{1.22}$$

One quickly verifies that $\mathrm{tr}_B\{\pi_{SB}\} = e^{-\beta H_S^*}/\mathcal{Z}_S^*$. The Hamiltonian of mean force provides a neat concept used various times in the following chapters. Physically speaking, it can be seen as an effective free energy landscape for the system, a claim that becomes clearer in Chapter 2. Notice that the Hamiltonian of mean force depends explicitly on the inverse temperature β. For weak coupling V_{SB}, H_S^* reduces to H_S. Thus, the familiar canonical ensemble only emerges in the weak coupling regime.

It is natural to ask: Does the effective Gibbs state (1.20) represent a good approximation to the equilibrated open quantum system state, i.e., is $\pi_S^* \approx \lim_{t\to\infty}\rho_S(t)$? If that is the case, we say that the system *thermalizes*, which is a stronger requirement than equilibration alone, which only assumes the system state to become time–independent for long times. Paralleling the objections raised by Poincaré's recurrence theorem above that equilibration can never strictly happen, similar doubts may rise for the case of thermalization. In particular, no initial system–bath state $\rho_{SB}(0)$ different from π_{SB} will ever reach the latter state during the evolution.

Exercise 1.1 Show that, if $\rho_{SB}(0) \neq \pi_{SB}$ and if H_{SB} is time–independent, then $\rho_{SB}(t) \neq \pi_{SB}$ for all t.

However, similar to the case of equilibration, also thermalization should be regarded as a convenient *illusion* by recalling that our experimental capabilities are limited. For a bath with its prosaic 10^{23} degrees of freedom, the full system–bath state $\rho_{SB}(t)$, which is defined on a Hilbert space of dimension of the order of $10^{10^{23}}$, remains experimentally inaccessible. Instead, one typically has access only to a restricted set of observables, for instance, those determined by looking at the open quantum system. Thermalization to eqn (1.20) is then very likely to happen as long as one can meaningfully associate some macroscopic temperature T to the bath. Exceptions are, for instance, a bath consisting of two parts kept at different temperatures (a scenario, which becomes relevant for later chapters to study transport processes) or a bath prepared in a giant Schödinger cat state as a superposition of two very different energies (an unlikely scenario). Furthermore, also in presence of additional conservation laws, i.e., if some observables commute with the global Hamiltonian, thermalization to eqn (1.20) will typically not happen. However, if these scenarios can be excluded, many open quantum systems thermalize to eqn (1.20), regardless of the initial state $\rho_S(0)$. In fact, this observation is confirmed by our example at the end of Section 1.2. The grey lines in Figs. 1.2 (d) and 1.3 (d) shows the time evolution of $D[\rho_S(t)|\pi_S^*]$. We see that even for a bath of only six spins, π_S^* can represent a good approximation to the open system state, even at low temperatures, i.e., in the regime where quantum fluctuations dominate thermal fluctuations.

The last observation raises the question whether the deviation of π_S^* from the standard Gibbs state π_S is mainly caused by quantum effects. In general, this does not need to be the case, but we will return to this question more rigorously in Section 3.6 when we discuss the zeroth law of thermodynamics. For now, we conclude this section by studying an important class of models for which there is a clear difference between π_S^* and π_S in the quantum and classical regime.

Exercise 1.2 Consider a harmonic oscillator with frequency ω and Hamiltonian (in mass-weighted coordinates) $H_S = \frac{1}{2}(p_S^2 + \omega^2 x_S^2)$ coupled to a 'bath' of one other harmonic oscillator with the same frequency ω. The global Hamiltonian is

$$H_{SB} = H_S + \frac{1}{2}\left[p_B^2 + \omega^2\left(x_B - \frac{c}{\omega^2}x_S\right)^2\right]. \tag{1.23}$$

Here, the coupling strength is c and we have written the Hamiltonian in a manifestly positive form such that $H_{SB} \geq 0$ for any choice of ω and c. Now, show first that, if treated as a classical system, there is no correction to the thermal state of the system: $\pi_S^* = \pi_S = e^{-\beta H_S}/\mathcal{Z}_S$. *Hint:* Remember that the trace over the bath degrees of freedom becomes classically an integral over the phase space coordinates (x_B, p_B) of the bath.

Then, show that quantum mechanically this is no longer true. *Hint:* You are not asked to directly compute H_S^*, but only to show that $\pi_S^* \neq \pi_S$. This can be done in various ways.

One way is to compute the equilibrium variance of the system coordinate $\mathrm{tr}\{x_S^2\pi_{SB}\}$ by changing to normal modes. Denote the (squared) eigenfrequencies of H_{SB} by $\Omega_\pm^2 \equiv [c^2 + 2\omega^4 \pm \sqrt{c^4 + 4c^2\omega^4}]/2\omega^2$ and show that

$$\mathrm{tr}\{x_S^2\pi_{SB}\} = \hbar\frac{e^{\beta\hbar(\Omega_+ + \Omega_-)} - 1}{(\Omega_+ + \Omega_-)(e^{\beta\hbar\Omega_+} - 1)(e^{\beta\hbar\Omega_-} - 1)}. \tag{1.24}$$

Confirm that in the classical limit ($\hbar \to 0$) this result is independent of the coupling strength c. Also confirm that for $c \to 0$ you recover the result $\mathrm{tr}_S\{x_S^2\pi_S\} = \hbar\coth(\beta\hbar\omega/2)/2\omega$ showing that even at zero temperature quantum fluctuations give rise to a non-zero variance.

The above result can be generalized to a system–bath Hamiltonian of the form

$$H_{SB} = H_S + \frac{1}{2}\sum_k \left[p_k^2 + \omega_k^2\left(x_k - \frac{c_k}{\omega_k^2}S\right)^2\right]. \tag{1.25}$$

This describes a system with arbitrary Hamiltonian H_S coupled via an arbitrary system coupling operator S to a bunch of harmonic oscillators. Such system–bath models, which are well justified whenever the statistics of the bath are (approximately) Gaussian, are known as **Caldeira–Leggett models** and they play an important role in the theory of open quantum systems. Convince yourself of the fact that for a classical system the Hamiltonian of mean force is identical to the system Hamiltonian: $H_S^* = H_S$. Obviously, this does no longer hold for quantum systems. Computing the exact reduced equilibrium state of the open quantum system is possible, but it is no longer a triviality.

1.4 Quantum Measurement Theory

We now start to focus on the question how to obtain information about a quantum system by considering measurements at a *single* point in time. For that purpose it is sufficient to simply consider an arbitrary system state ρ_S, neglecting for a moment the possible presence of a bath. We will come back to the question how to treat multi–time measurements under the influence of a bath in Section 1.6 onwards.

Projective measurements

In quantum mechanics the measurement of a system observable X_S is described by the projection postulate. Let $X_S = \sum_{x=1}^n \lambda(x)\Pi_S(x)$ be the spectral decomposition of the observable with n different eigenvalues $\lambda(x)$, which are labeled by the index x. Furthermore, $\{\Pi_S(x)\}$ is a set of projection operators satisfying $\Pi_S(x)\Pi_S(x') = \delta_{x,x'}\Pi_S(x)$ and $\sum_{x=1}^n \Pi_S(x) = I_S$. If the state of the system is ρ_S, then the probability to observe result x is $p(x) = \mathrm{tr}_S\{\Pi_S(x)\rho_S\}$. The *post*–measurement state $\rho_S'(x)$ *conditional* on observing x becomes

$$\rho_S'(x) = \frac{\Pi_S(x)\rho_S\Pi_S(x)}{p(x)}. \tag{1.26}$$

The *average* or *unconditional* post–measurement state ρ_S' of the system follows as

$$\rho_S' = \sum_{x=1}^n p(x)\rho_S'(x) = \sum_{x=1}^n \Pi_S(x)\rho_S\Pi_S(x). \tag{1.27}$$

Notice that this state is in general different from the pre–measurement state, $\rho_S' \neq \rho_S$, which reflects the well–known fact that quantum measurements are disturbing.

This measurement backaction is only absent if the initial state commutes with the observable: $[\rho_S, X_S] = 0$. Even in this case, however, the conditional state (1.26) is in general different from the pre–measurement state, i.e., $\rho'_S(x) \neq \rho_S$. This is not a quantum effect, but a consequence of the fact that the observer updates its state of knowledge about the system. Readers, who feel unfamiliar with this description, are advised to do the following exercise.

Exercise 1.3 Consider the case where all projectors $\Pi_S(x) = |x\rangle\langle x|_S$ are of rank 1 and the system state is pure: $\rho_S = |\psi\rangle\langle\psi|_S$. Convince yourself of the fact that the above framework then reduces to the conventional picture known from introductory textbooks in quantum mechanics. What corresponds to the Born rule? Which equation describes the 'collapse' of the wave function? When does the measurement reveal no information, i.e., when do we have $\rho'_S(x) = \rho_S$? Can you think about physical examples where the projectors are not of rank 1?

Remarkably, it is possible to derive eqn (1.27), which describes the average effect of a quantum measurement, using only unitary dynamics and *no* projection postulate. This works as follows. Consider a second n–dimensional 'auxiliary' quantum system A, called the *ancilla* in the following, which interacts with our system S of interest. Imagine that the initial system–ancilla state is decorrelated, $\rho_{SA} = \rho_S \otimes \rho_A$, and the ancilla is prepared in some fixed pure state $\rho_A = |1\rangle\langle 1|_A$. Furthermore, assume that the overall system–ancilla interaction is described by the following unitary operator

$$V = \sum_{x=1}^{n} \Pi_S(x) \otimes \sum_{r=1}^{n} |r + x - 1\rangle\langle r|_A, \tag{1.28}$$

where we interpret $r + x - 1$ modulo n whenever $r + x - 1 > n$. It is easy to verify that V is unitary satisfying $VV^\dagger = V^\dagger V = I_{SA}$. The joint system–ancilla state after the interaction consequently reads

$$\rho'_{SA} = V\rho_S \otimes \rho_A V^\dagger. \tag{1.29}$$

The reduced state of the system is obtained by tracing out the ancilla,

$$\rho'_S = \mathrm{tr}_A\{V\rho_S \otimes \rho_A V^\dagger\} = \sum_{x=1}^{n} \Pi_S(x)\rho_S\Pi_S(x), \tag{1.30}$$

which is identical to eqn (1.27). Thus, the average effect of a system measurement arises in this picture from interactions of the system with an outside ancilla. By tracing out the ancilla, we loose information and the reduced dynamics is no longer unitary.

To derive the conditional post–measurement state (1.26) in this picture, assume that we subject the ancilla to a projective measurement of the observable $R_A = \sum_{r=1}^{n} r|r\rangle\langle r|_A$. Suppose this projective measurement of R_A reveals outcome r, then the conditional post–measurement reads $\rho'_{SA}(r) = |r\rangle\langle r|_A V\rho_S \otimes \rho_A V^\dagger |r\rangle\langle r|_A$. Keeping the information about r, but tracing out the ancilla degrees of freedom, reveals

$$\tilde{\rho}'_S(r) \equiv \mathrm{tr}_A\{|r\rangle\langle r|_A V\rho_S \otimes \rho_A V^\dagger\} = \Pi_S(r)\rho_S\Pi_S(r). \tag{1.31}$$

After identifying $x \equiv r$, we obtain eqn (1.26) up to normalization. In fact, the trace of the non–normalized state $\tilde{\rho}'_S(r)$ equals the probability to obtain measurement result

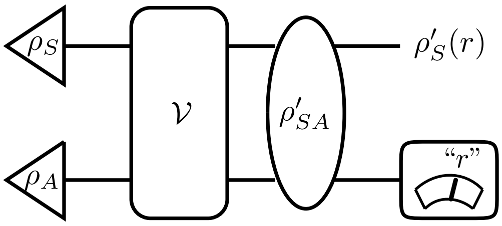

Fig. 1.4 Circuit representation of an ancilla–assisted measurement with time running from left to right. The input states to the process (left triangles) are a system and ancilla state ρ_S and ρ_A. Both interact via a unitary transformation, denoted here with a calligraphic symbol $\mathcal{V}$. The joint state ρ'_{SA} after the interaction is in general correlated. To finally infer something about the system, the experimentalist measures the state of the ancilla, here with projector $|r\rangle\langle r|_A$. The conditional post–measurement state of the system is denoted $\rho'_S(r)$.

r: $p(r) = \text{tr}_S\{\tilde{\rho}'_S(r)\} = \text{tr}_S\{\Pi_S(r)\rho_S\}$. Hence, the normalized state reads $\rho'_S(r) = \tilde{\rho}'_S(r)/p(r)$ in agreement with eqn (1.26).

As we will see throughout the remainder of this book, ancillas provide us with a flexible mathematical tool to think about quantum measurements and much more. They can be seen as comprising the essential features of an environment in an abstract and minimal way. Physically, the use of ancillas can be motivated as follows. In order to find out something about a system, an experimentalist prepares an external *probe* and puts it into contact with the system. Then, both start to interact and, depending on the state of the system, the system imprints some information onto the probe. Finally, the experimentalist reads out the state of the probe in order to infer something about the system. This picture is often justified by recognizing that an experimentalist has precise control about the detectors in the lab—how they are prepared, how they intervene with the system, and how they are read off—whereas the system itself is given by nature and can be only indirectly accessed via the detectors found in the lab. An experiment, in which this picture becomes particularly transparent, will be treated in detail at the end of this book in Section 5.7. A pictorial representation of this process is provided in Fig. 1.4. For the rest of this section we focus on investigating the process in Fig. 1.4 in greater detail, finding that it can describe *generalized* quantum measurements beyond the projection postulate.

Generalized measurements

We generalize the picture above by starting with an arbitary initial ancilla state, written in its eigenbasis as $\rho_A = \sum_j p_j|j\rangle\langle j|_A$, an arbitrary unitary V, not necessarily the one specified in eqn (1.28), and a final projective measurement of some ancilla observable $R_A = \sum_{r=1}^n r|r\rangle\langle r|_A$. As above, we now take a look at the conditional state of the system given the measurement result r of R_A. Tracing out the ancilla, we get the non–normalized system state

$$\tilde{\rho}'_S(r) = \text{tr}_A\{|r\rangle\langle r|_A V\rho_S \otimes \rho_A V^\dagger\} = \sum_j p_j \langle r|_A\big(V|j\rangle_A\big)\rho_S\langle j|_A\big(V^\dagger|r\rangle_A\big). \tag{1.32}$$

Next, we introduce the operators

$$K_j(r) \equiv \sqrt{p_j}\langle r|_A \left(V|j\rangle_A\right). \tag{1.33}$$

Notice that the $K_j(r)$ are still operators acting on the *system* Hilbert space. Using them, we can express eqn (1.32) more compactly as

$$\tilde{\rho}'_S(r) = \sum_j K_j(r)\rho_S K_j^\dagger(r). \tag{1.34}$$

This equation makes it more transparent how the system state gets actually transformed by computing the operators $K_j(r)$ via eqn (1.33). In terms of them, we can also express the probability to obtain measurement result r as

$$p(r) = \text{tr}_S\{\tilde{\rho}'_S(r)\} = \sum_j \text{tr}_S\left\{K_j^\dagger(r)K_j(r)\rho_S\right\}. \tag{1.35}$$

This equation suggests to introduce the following *probability operators*

$$M(r) \equiv \sum_j K_j^\dagger(r)K_j(r), \tag{1.36}$$

which are always positive, $M(r) \geq 0$, which follows from the fact that any operator of the form $A^\dagger A$ is positive. Furthermore, they satisfy the *completeness relation*

$$\sum_r M(r) = I_S. \tag{1.37}$$

Moreover, the set of operators $\{M(r)\}$ completely fixes the measurement *statistics* and therefore plays an important role in quantum measurement theory, where they are known as a **positive operator–valued measure** or, in short, a **POVM**.

Exercise 1.4 Show that any set of operators $\{M(r)\}_r$ satisfying the completeness relation and $M(r) \geq 0$ for all r gives rise to a set of well–defined probabilities $p(r) = \text{tr}_S\{M(r)\rho_S\}$ for any state ρ_S. *Hint:* By 'well–defined' we mean probabilities that are positive and sum up to one.

We now study two examples to illustrate how the projection postulate can be generalized. The first example describes projective measurement of the initially studied observable $X_S = \sum_{x=1}^n \lambda(x)\Pi_S(x)$, but it includes classical measurements errors. For this purpose we relabel $j \equiv x$ in eqn (1.33) and model the measurement with operators $K_x(r) = \sqrt{p(r|x)}\Pi_S(x)$ giving rise to the probability operator

$$M(r) = \sum_x p(r|x)\Pi_S(x). \tag{1.38}$$

For $\{M(r)\}$ to be a POVM, we demand that the $p(r|x)$ are non–negative numbers normalized according to $\sum_r p(r|x) = 1$. Using eqn (1.34), the non–normalized post–measurement state of the system becomes

$$\tilde{\rho}'_S(r) = \sum_x p(r|x)\Pi_S(x)\rho_S\Pi_S(x). \tag{1.39}$$

Its norm equals the probablity to obtain result r, $p(r) = \sum_x p(r|x)\text{tr}_S\{\Pi_S(x)\rho_S\}$, which has a transparent interpretation: Since $\text{tr}_S\{\Pi_S(x)\rho_S\}$ equals the probability to obtain result x in an error–free projective measurement, $p(r|x)$ is the conditional probability to obtain result r given that an error–free measurement had given result x. Thus, due to some errors in the classical data processing, erroneous detection events of $r \neq x$ can occur. The case of error–free measurements is recovered if $p(r|x) = \delta_{r,x}$, where eqn (1.39), after normalization, reduces to eqn (1.26).

The second example also describes a measurement of X_S with errors, but this time the errors cannot be explained classically. For this purpose, let us consider operators $K(r) = \sum_x \sqrt{p(r|x)}\Pi_S(x)$ (without any label j), which gives rise to

$$M(r) = \sum_x p(r|x)\Pi_S(x), \tag{1.40}$$

which *coincides* with eqn (1.38). Thus, they give rise to the same measurement statistics. However, the post–measurement state looks very different:

$$\tilde{\rho}'_S(r) = K(r)\rho_S K(r) = \sum_x \sqrt{p(r|x)}\Pi_S(x)\rho_S \sum_{x'} \sqrt{p(r|x')}\Pi_S(x'). \tag{1.41}$$

This teaches us an important lesson, namely that the probablity operators $M(r)$ do not uniquely fix how the state changes due to the measurement. The next exercise elucidates the difference between eqns (1.39) and (1.41) further.

Exercise 1.5 Consider an initially pure state $\rho_S = |\psi\rangle\langle\psi|_S$. Then, show that the post–measurement state given by eqn (1.41) is always pure, i.e., $[\rho'_S(r)]^2 = \rho'_S(r)$, whereas this is in general not the case for eqn (1.39). Thus, eqn (1.41) preserves the 'quantum character' of the state, whereas eqn (1.39) inevitably introduces classical noise.

Summary

We summarize what we found out in this chapter. By shifting the description of the projective measurement from the system itself to an external ancilla, with which the system interacts in a unitary way, we obtained a more general description of quantum measurements expressed by system state changes of the form (1.34). It includes the case of projective measurements, but as eqns (1.39) and (1.41) have shown also more general transformations. The generalization of the average unconditional system state after a projective measurement, eqn (1.27), follows from eqn (1.34) as

$$\rho'_S = \sum_r p(r)\rho'_S(r) = \sum_r \tilde{\rho}'_S(r) = \sum_r \sum_j K_j(r)\rho_S K_j^\dagger(r). \tag{1.42}$$

To simplify the notation, we introduce the multi–index $\alpha = (r, j)$ and write

$$\rho'_S = \sum_\alpha K_\alpha \rho_S K_\alpha^\dagger. \tag{1.43}$$

Due to trace conservation, we know that the operators K_α must satisfy the completeness relation

$$\sum_{\alpha} K_{\alpha}^{\dagger} K_{\alpha} = 1. \tag{1.44}$$

Apart from this relation, it turns out that the operators K_α are indeed arbitrary. We will learn more about them from an abstract perspective, which is not necessarily related to quantum measurements, in the next section.

It is instructive to point out the similarities and differences between the system–ancilla picture and the system–bath picture of Section 1.2. In both cases the system is *open* due to its coupling to some external degrees of freedom. However, we did not call the ancilla a 'bath' here because its interpretation is quite different in the present context. Whereas the bath was introduced in Section 1.2 as an uncontrollable and typically large object, the small and controllable ancilla of this section was introduced to probe the state of a quantum system. The physical interpretation of this situation is different, but—as the next sections will show in greater detail—the mathematical description is essentially the same. Before proceeding, we conclude this section with a final exercise to elucidate the difference between classical and quantum measurements.

Exercise 1.6 Construct the classical counterpart of the theory above. To this end, replace the notion of the density matrix ρ_S by a vector $\boldsymbol{p}$ with elements $p(x)$ denoting the probability to find the classical system in state x. Let $p(r|x)$ be the conditional probability to obtain the measurement result r given that the system is in state x and define the matrix $M(r)$ with elements $M_{xx'}(r) = \delta_{x,x'} p(r|x)$. What do $\{M(r)\}$ and a POVM have in common? What is the quantum counterpart of the classical expression $M(r)\boldsymbol{p}$? Relate the probability $p(r) = \sum_x p(r|x)p(x)$ to obtain outcome r to the expression $M(r)\boldsymbol{p}$. Show that the (normalized) post–measurement state of the system given result r obeys **Bayes' rule** $p'(x|r) = p(r|x)p(x)/p(r)$. Finally, verify that the average post–measurement state does not change: $\boldsymbol{p}' = \boldsymbol{p}$. Thus, Bayes' rule describes the most general *non–disturbing* classical measurement.

1.5 Operations, Interventions and Instruments

The goal of this section is to review the formalism of quantum measurement theory from an abstract perspective and to introduce some terminology and powerful mathematical results. From now on, we call the map (1.43) in general a (*control*) *operation* or *intervention.* These notions emphasize that an experimentalist has a large amount of freedom to manipulate a quantum system and the intention might not always be to 'measure' the system in a literal sense. We further abbreviate eqn (1.43) as

$$\boxed{\rho_S' = \mathcal{C}\rho_S \equiv \sum_{\alpha} K_{\alpha} \rho_S K_{\alpha}^{\dagger}.} \tag{1.45}$$

The map $\mathcal{C}$, which takes an operator and maps it to another operator, is also known as a **superoperator** to distinguish it from the notion of a 'usual' operator, which 'only' maps vectors onto vectors. Mathematically speaking, this distinction is superfluous: the space of matrices forms itself a vector space and therefore, one can represent any superoperator $\mathcal{C}$ also by a (large) matrix. For physics applications it is, however, advantageous to use a terminology and notation, which distinguishes whether an operator acts on states $|\psi\rangle$ or density matrices ρ. From now on, we frequently use superoperators as an efficient bookkeeping tool. By convention, superoperators are always written with a calligraphic letter such as $\mathcal{C}$ and they act on all operators to their right, i.e., $\mathcal{C}_2\mathcal{C}_1\rho = \mathcal{C}_2[\mathcal{C}_1(\rho)]$. Note that the action of different superoperators does not commute in general, i.e., $\mathcal{C}_2\mathcal{C}_1\rho \neq \mathcal{C}_1\mathcal{C}_2\rho$. Readers, who are exposed to this for the first time, are advised to consult Appendix B before proceeding.

We also introduce the superoperator $\mathcal{C}(r)$ corresponding to eqn (1.34):

$$\boxed{\tilde{\rho}'_S(r) = \mathcal{C}(r)\rho_S \equiv \sum_{\alpha_r} K_{\alpha_r}\rho_S K^\dagger_{\alpha_r},} \tag{1.46}$$

which is obtained from eqn (1.45) by using only a subset of the operators K_α. The subsets of indices $\{\alpha_r\}$ are obtained from the total set $\{\alpha\}$ by a disjoint decomposition such that $\sum_r \mathcal{C}(r) = \mathcal{C}$. In the following we call a set of maps $\{\mathcal{C}(r)\}$ that decomposes an operation $\mathcal{C}$ of the form (1.45) such that $\sum_r \mathcal{C}(r) = \mathcal{C}$ an **instrument**. Notice that, given only eqn (1.45), there are many instruments that decompose $\mathcal{C}$.

Now, our claim is that eqn (1.45) describes the *most general* control operation or intervention we can implement in a laboratory on a quantum system at a single time. To verify this, let us find the minimial conditions we would like to have satisfied by an instrument $\{\mathcal{C}(r)\}$ such that it describes a physically allowed control operation in a lab. Clearly, if the state of the system was previously described by a valid density matrix ρ_S, the minimal requirement is that also the final set of states $\{\tilde{\rho}'_S(r) = \mathcal{C}(r)\rho_S\}$ can be interpreted in a legitimate way as the state of a physical system. Recall that any density matrix ρ is positive, has unit trace, and, if ρ_1 and ρ_2 are two valid density matrices, then their *convex combination* $\lambda\rho_1 + (1-\lambda)\rho_2$ for any $\lambda \in [0,1]$ is another valid density matrix. Therefore, we postulate that any physically legitimate instrument $\{\mathcal{C}(r)\}_r$ should at least satisfy the following:

(i) $\mathcal{C}(r)$ is positive: If $\rho_S \geq 0$, then also $\mathcal{C}(r)\rho_S \geq 0$.

(ii) $\mathcal{C}(r)$ is trace non–increasing: If $\mathrm{tr}\{\rho_S\} = 1$, then $p(r) = \mathrm{tr}\{\mathcal{C}(r)\rho_S\}$ is the probability to apply the map $\mathcal{C}(r)$ (in view of a quantum measurement, it is the probability to obtain result r). If $p(r) = 1$, $\mathcal{C}(r) = \mathcal{C}$ is called trace–preserving.

(iii) $\mathcal{C}(r)$ is convex linear: If $\sum_i \lambda_i \rho_S^{(i)}$ is a statistical mixture of quantum states with $\lambda_i \geq 0$ satisfying $\sum_i \lambda_i = 1$, then

$$\mathcal{C}(r)\sum_i \lambda_i \rho_S^{(i)} = \sum_i \lambda_i \mathcal{C}(r)\rho_S^{(i)}. \tag{1.47}$$

Now, to make things even a little more complicated, it turns out that desideratum (i) is not enough. Remember that $\mathcal{C}(r)$ could describe, for instance, a measurement of a system S coupled to a bath B. Prior to the measurement the system–bath state ρ_{SB} can be arbitrary and we would like to ensure that the post–measurement state also describes a legitimate quantum state. This means that we actually want the global state $\tilde{\rho}'_{SB}(r) = [\mathcal{C}(r) \otimes \mathcal{I}_B]\rho_{SB} \geq 0$ to be positive, where $\mathcal{I}_B$ denotes the identity operation acting on the bath defined via $\mathcal{I}_B\rho_B \equiv \rho_B$ for any state ρ_B. This is *not* necessarily guaranteed by the notion of a positive map. Therefore, we replace (i) by the stronger condition:

(i') $\mathcal{C}(r)$ is **completely positive**: Consider the composite system $\mathcal{H}_S \otimes \mathcal{H}_B$ with $\mathcal{H}_B$ an arbitrary Hilbert space. If $\rho_{SB} \geq 0$ is an arbitrary positive state of the composite system, then also $[\mathcal{C}(r) \otimes \mathcal{I}_B]\rho_{SB} \geq 0$ is positive.

Exercise 1.7 An example for a positive but not completely positive map is the transpose operation $\mathcal{T}$. Let $\rho = \rho_{00}|0\rangle\langle 0| + \rho_{01}|0\rangle\langle 1| + \rho_{10}|1\rangle\langle 0| + \rho_{11}|1\rangle\langle 1|$ be an arbitrary density matrix of a qubit, then the transpose operation with respect to the basis $\{|0\rangle, |1\rangle\}$ is defined via $\mathcal{T}\rho \equiv \rho_{00}|0\rangle\langle 0| + \rho_{10}|0\rangle\langle 1| + \rho_{01}|1\rangle\langle 0| + \rho_{11}|1\rangle\langle 1|$. Show that this map is positive, but not completely positive. *Hint:* As a counterexample consider the transpose operation acting on the first qubit of the pure and maximally entangled bipartite state $(|00\rangle + |11\rangle)/\sqrt{2}$.

We remark that the distinction between positivity and complete positivity is a quantum phenomenon: classically, all postive maps are also completely positive. Furthermore, the next exercise shows that any convex linear map acting on density matrices can be extended to a linear map acting on arbitrary matrices. We therefore use the notions convex linearity and linearity in the following synonymously.

Exercise 1.8 Let $\mathcal{C}$ be a convex linear map acting on density matrices ρ of a Hilbert space with dimension $\dim \mathcal{H} = d$. Show that every complex $d \times d$ matrix A can be written as a linear combination of density matrices ρ_i with complex coefficients $c_i \in \mathbb{C}$, i.e., $A = \sum_i c_i \rho_i$. *Hint:* To do so, you can use the two fundamental results that, first, every A can be written as $A = A_1 + iA_2$ with $A_1 = A_1^\dagger$ and $A_2 = A_2^\dagger$ being Hermitian and, second, every Hermitian A can be decomposed as $A = A_+ - A_-$ with $A_\pm \geq 0$ being positive.

The extension $\tilde{\mathcal{C}}$ of $\mathcal{C}$ is then defined via $\tilde{\mathcal{C}}A \equiv \sum_i c_i \mathcal{C}\rho_i$ and in the following, tacitly assuming this extension, we identify $\mathcal{C} \equiv \tilde{\mathcal{C}}$.

To conclude, physically legitimate operations are mathematically described by an instrument, which is a collection of completely positive, trace non–increasing and linear maps, which we call **CP maps**. All CP maps of an instrument have to add up to a completely positive and trace–preserving map, which we call a **CPTP map**. There are two important theorems to characterize CP(TP) maps mathematically.

Operator–sum representation. *A map $\mathcal{C}(r)$ satisfies desiderata (i'), (ii) and (iii) if and only if it can be written as in eqn (1.46) for some operators K_{α_r} satisfying $\sum_{\alpha_r} K_{\alpha_r}^\dagger K_{\alpha_r} \leq I_S$. If $\sum_{\alpha_r} K_{\alpha_r}^\dagger K_{\alpha_r} = I_S$, then $\mathcal{C}(r) = \mathcal{C}$ is trace–preserving. Equations (1.45) or (1.46) are called the operator–sum representation of a CP(TP) map.*

It is not too hard to show that a map of the form (1.46) with $\sum_{\alpha_r} K_{\alpha_r}^\dagger K_{\alpha_r} \leq I_S$ satisfies points (i'), (ii) and (iii). The other direction is harder to show and not done here. Instead, we only note that the operator–sum representation (1.46) is *not* unique as explicitly shown by the next exercise.

Exercise 1.9 Consider the map $\mathcal{C}\rho = \sum_{\alpha=1}^d K_\alpha \rho K_\alpha^\dagger$ and define $K_\alpha \equiv \sum_\alpha U_{\alpha\beta}\tilde{K}_\beta$ for an arbitrary $d \times d$ unitary matrix U. Show that $\mathcal{C}\rho = \sum_{\alpha=1}^d \tilde{K}_\alpha \rho \tilde{K}_\alpha^\dagger$.

It turns out that there is another important representation theorem for an instrument, which brings us back to our ancilla construction used in the previous section.

Unitary dilation theorem. *A set of maps $\{\mathcal{C}(r)\}$ acting on a d–dimensional system Hilbert space $\mathcal{H}_S$ forms an instrument if and only if there exists a d^2–dimensional 'ancilla' Hilbert space $\mathcal{H}_A$, a unitary U_{SA} acting on $\mathcal{H}_S \otimes \mathcal{H}_A$, a pure ancilla state $|\phi\rangle_A \in \mathcal{H}_S$ and a set of projectors $\{\Pi_A(r)\}$ acting on the ancilla space such that*

$$\boxed{\mathcal{C}(r)\rho_S = \text{tr}_A\{\Pi_A(r)U_{SA}(\rho_S \otimes |\phi\rangle\langle\phi|_A)U_{SA}^\dagger\}} \tag{1.48}$$

for all r. In particular, a map $\mathcal{C}$ is CPTP if and only if it can be written as

$$\boxed{\mathcal{C}\rho_S = \text{tr}_A\{U_{SA}(\rho_S \otimes |\phi\rangle\langle\phi|_A)U_{SA}^\dagger\}.} \tag{1.49}$$

We are not going to prove the unitary dilation theorem here, but only discuss its consequences. For instance, the next exercise shows that the number of operators K_α appearing in the operator–sum representation is at most d^2 with $d = \dim \mathcal{H}_S$.

Exercise 1.10 Use the unitary dilation theorem to derive eqns (1.45) and (1.46) by giving explicit expressions for the operators K_{α_r} and K_α in terms of U_{SA}, $|\phi\rangle_A$ and $\Pi_A(r)$. Confirm that the maximum number of operators K_α is d^2. *Hint:* Remember eqn (1.33).

We remark that it is also possible to use the operator–sum representation to derive the unitary dilation theorem. Hence, both are equivalent statements. The physical significance of the unitary dilation theorem is that it teaches us that every allowed state transformation in quantum mechanics satisfying desiderata (i'), (ii) and (iii) can be constructed by more primitive transformations, namely unitary evolution and projective measurements. We therefore do not need to add any axiom to the standard textbook framework of quantum mechanics in order to describe generalized measurements or other general state transformations.

The unitary dilation theorem also fits well into our system–bath paradigm from Section 1.2 if we regard the ancilla as the bath coupled to the system. From that perspective, it tells us that every state change of a quantum system can be explained through the interaction with an external environment, which we might call an ancilla or a bath depending on the context. Care is, however, required here because the unitary dilation theorem is an *abstract* statement and does not tell us for a given transformation of the system what *is* the actual environment causing this transformation. This is related to the non–uniqueness of the operator–sum representation: there are infinitely many Hilbert spaces $\mathcal{H}_A$, unitary matrices U_{SA}, states $|\phi\rangle_A$ (possibly also mixed states) and projectors $\Pi_A(r)$ satisfying eqns (1.48) and (1.49).

Before concluding this section, we point out a subtle but important observation. What the unitary dilation theorem also teaches us is that satisfying desiderata (i'), (ii) and (iii) is equivalent to representing the interaction of the system with some environment, which is initially *decorrelated* from the system, i.e., of the form $\rho_S \otimes |\phi\rangle\langle\phi|_A$. However, the evolution of an open quantum system (1.11) could also result from a system initially *correlated* with the environment. In this case, the operator–sum representation and the unitary dilation theorem *break down.* The reason is that desideratum (iii) (linearity) is then no longer satisfied. This is exemplified in the next exercise and a way out of this 'dilemma' is presented in Section 1.7.

Exercise 1.11 Consider the interaction of two qubits. The first qubit is called the system and the second the ancilla. We further introduce the maximally entangled states $|\pm\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$, where by convention we set $|ij\rangle \equiv |i\rangle_S \otimes |j\rangle_A$ for $i, j \in \{0, 1\}$. Let the system–ancilla interaction be modeled by the unitary $U_{SA} = |+\rangle\langle+| + |-\rangle\langle 10| + |10\rangle\langle -| + |01\rangle\langle 01|$ (check that this is a unitary matrix). The evolution of the composite system is therefore modeled via $\rho'_{SA} = U_{SA}\rho_{SA}U^\dagger_{SA}$, which is clearly linear with respect to the *joint* input state ρ_{SA} and CPTP.

Next, consider the reduced dynamics of S assuming that the initial system–ancilla state $\rho_{SA} = |+\rangle\langle+|$ is entangled. Verify the following results: (1) the initial reduced system state is $\rho_S = (|0\rangle\langle 0| + |1\rangle\langle 1|)/2$; (2) the final system state is identical to the initial system state, $\rho'_S = \text{tr}_A\{U_{SA}|+\rangle\langle+|U^\dagger_{SA}\} = \rho_S$; (3) if we first perform a measurement of the initial system in its eigenbasis, the initial *system* state does not change on average: $|0\rangle\langle 0|\rho_S|0\rangle\langle 0| + |1\rangle\langle 1|\rho_S|1\rangle\langle 1| = \rho_S$; but (4) the final system state after such an initial measurement

$$\text{tr}_A\{U_{SA}(|0\rangle\langle 0|\rho_{SA}|0\rangle\langle 0| + |1\rangle\langle 1|\rho_{SA}|1\rangle\langle 1|)U^\dagger_{SA}\} = \frac{1}{4}|0\rangle\langle 0| + \frac{3}{4}|1\rangle\langle 1| \tag{1.50}$$

is *different* from ρ_S. Hence, we have a 'paradox' because the same reduced initial system state gives rise to two different final states. Thus, we cannot associate any map $\mathcal{C}$, which only acts on the system part, to this input–output relation.

How can this be resolved? Clearly, from a global point of view there is no paradox: the two initial states $\rho_{SA} = |+\rangle\langle+|$ and $|0\rangle\langle 0|_S\rho_{SA}|0\rangle\langle 0|_S + |1\rangle\langle 1|_S\rho_{SA}|1\rangle\langle 1|_S$ are different (albeit they give rise to the same reduced system state), and hence there can be two different output states. With respect to our construction above, the key insight is to realize that *it is no longer meaningful to speak about different initial system states if the system is initially entangled with its environment* (here, the ancilla). In particular, we assumed that it is possible to mix (or convex combine) different system states without influencing the dynamics, i.e., the definition of the map. This assumption is incompatible with having an initial system state entangled with its environment.

We summarize the content of the last two sections, which play an important role in the following. First, quantum systems can undergo more general state transformations than unitary evolutions and projective measurements. However, even general state transformations can be constructed using only unitary evolutions and projective measurements on a bigger system–ancilla (or system–bath) space. If the desiderata (i'), (ii) and (iii) are satisfied, where point (iii) assumes that the preparation of the initial system state can be disentangled from the effect of the state transformation, then we can either use the operator–sum representation or the unitary dilation theorem. If there is no post–selection (i.e., conditioning on a measurement result r), the state transformation is described by a CPTP map represented either by eqn (1.45) or eqn (1.49). If there is conditioning, the state transformation is described by a CP map represented either by eqn (1.46) or eqn (1.48). On average, all CP maps have to add up to a CPTP map. Vice versa, every CPTP map can be decomposed into a set of CP maps. Such a set is called an instrument.

Finally and for completeness, we mention one extension of the here introduced framework. So far, we have assumed that the dimension d of the system space does not change during the control operation, but for some applications it makes sense to relax this requirement. These applications play a minor role in quantum stochastic thermodynamics and the mathematical modifications we have to add only amount to a correct bookkeeping of the different input and output Hilbert spaces in the notation. Nevertheless, fhe final exercise shows a couple of neat examples of such control operations, which are useful to keep in mind.

Exercise 1.12 Verify that the following maps are CPTP by finding an operator–sum representation for them. *Example 1:* The 'trace map' is defined for any input state ρ by $\mathcal{C}\rho \equiv \mathrm{tr}\{\rho\}$. This map is also often associated with 'discarding a system' as it destroys all the information contained in a system and replaces it by a 'trivial' system living in the Hilbert space $\mathcal{H} = \mathbb{C}$ with the only possible density matrix $\rho_{\mathbb{C}} = 1$. *Example 2:* Consider a bipartite system with Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$. Show that the 'partial trace map' is CPTP: $\mathcal{C}\rho_{12} \equiv \mathrm{tr}_2\{\rho_{12}\} = \rho_1$. *Example 3:* In contrast to Example 1, one can also 'create' a system using a CPTP map, which takes input states from the Hilbert space $\mathcal{H} = \mathbb{C}$, by defining $\mathcal{C}_\rho c \equiv \rho$ for any $c \in \mathbb{C}$ and some fixed density matrix ρ. Note that, according to this example, 'states' in quantum mechanics are CPTP maps. *Example 4:* An extension of Example 3 and in some sense the opposite of Example 2 is the map which 'adds' a fixed state ρ_2 to an input state ρ_1: $\mathcal{C}_{\rho_2}\rho_1 \equiv \rho_1 \otimes \rho_2$.

1.6 Classical Stochastic Processes

In the last sections we have learned about some fundamental aspects of open quantum systems and quantum measurement theory. Before we put these two ingredients together to define a quantum stochastic process, it is worthwhile to recapitulate the definition of a classical stochastic process. Classical stochastic processes have found widespread application in the natural and social sciences. They are commonly used to describe a process in time, which is characterized by a random variable whose observation can be safely assumed not to change the process. It is obvious that this assumption is no longer satisfied for quantum systems. Even classically, this assumption can be violated. This leads to the much richer framework of classical causal models—a topic which we briefly touch at the end of this section.

Let R denote some random variable characterizing the state of a system evolving in time. Simple examples for R with relevance for (quantum) stochastic thermodynamics include the position of a colloidal particle suspended in water (which yields to *Brownian motion*), the number of electrons in a nanostructure such as a quantum dot or the number of photons in a cavity, conformational states of a macromolecule (e.g., folded or unfolded), among many others. In order to infer something about the time evolution of the system, the experimenter measures the value of R at an arbitrary set of times $\{t_\ell\}_{\ell=0}^n$, where here and in the following we assume the order $0 = t_0 < t_1 < \cdots < t_n$. The results of the measurement at time t_ℓ is denoted by r_ℓ. By repeating the experiment many times, the experimenter can gather enough statistics to construct (approximately) the joint probability distribution $p(r_n, t_n; \ldots; r_1, t_1; r_0, t_0)$ to observe r_0 at time t_0, r_1 at time t_1, and so on and so forth up to the last measurement giving result r_n at time t_n. Since the subscript at the measurement result r_ℓ is in one–to–one correspondence with the time t_ℓ of the measurement, we write for brevity

$$p(r_n, \ldots, r_1, r_0) \equiv p(r_n, t_n; \ldots; r_1, t_1; r_0, t_0). \tag{1.51}$$

To be a valid probability distribution, $p(r_n, \ldots, r_1, r_0)$ must satisfy

$$p(r_n, \ldots, r_1, r_0) \geq 0, \qquad \sum_{r_n} \cdots \sum_{r_1} \sum_{r_0} p(r_n, \ldots, r_1, r_0) = 1. \tag{1.52}$$

To save further space in the notation, we write the sequence of measurement results in boldface as $\mathbf{r}_n \equiv (r_n, \dots, r_1, r_0)$. In this notation the content of eqn (1.52) reduces to $p(\mathbf{r}_n) \geq 0$ and $\sum_{\mathbf{r}_n} p(\mathbf{r}_n) = 1$. Note that the sequence $\mathbf{r}_n$ has $n+1$ entries (and not n) since our first measurement happens by convention at time t_0 (and not at t_1).

The conditions (1.52) of positivity and normalization have to be satisfied by any probability distribution. Therefore, $p(\mathbf{r}_n)$ does not yet describe a stochastic process, which has one important additional structure. To uncover this additional structure, we need to look at the joint probability distribution $p(r_n, \dots, r_{\ell+1}, r_{\ell-1}, \dots, r_0)$ to obtain the results $r_n, \dots, r_{\ell+1}$, $r_{\ell-1}, \dots, r_0$ by measuring the system at times $t_n, \dots, t_{\ell+1}$, $t_{\ell-1}, \dots, t_0$, i.e., at all times *except* of time t_ℓ, where we perform *no* measurement. To emphasize this fact, we denote this probability by $p(r_n, \dots, \cancel{r_\ell}, \dots, r_0)$. Then, we define a classical stochastic process by the requirement that

$$\boxed{p(r_n, \dots, \cancel{r_\ell}, \dots, r_0) = \sum_{r_\ell} p(r_n, \dots, r_\ell, \dots, r_0)} \tag{1.53}$$

for all $\ell \in \{0, 1, \dots, n\}$. This is known as the **Kolmogorov consistency condition** and it tells us that not measuring the observable R at some point in time is equivalent to measuring it followed by marginalizing about the measurement result. Therefore, the joint probabilities of a classical stochastic process form a *hierarchy*, where the $(n+1)$–time joint probability $p(r_n, \dots, r_1, r_0)$ contains *all* the information about the k–time probabilities (with $k < n+1$) obtained from measuring the system at any subset of the times $\{t_n, \dots, t_1, t_0\}$. Furthermore, an important mathematical result known as the *Daniell–Kolmogorov extension theorem* says that we can also go the reverse way: whenever we have a hierarchy of n–time joint probabilities satisfying the Kolmogorov consistency condition, then they can be constructed as marginals of N–time joint probabilities with $N > n$, which also satisfy the consistency condition. The important point is here that this even holds in the limit of $n \to \infty$. The Daniell–Kolmogorov extension theorem therefore provides a bridge between experimental reality (where any measurement statistics is always finite and described with an $n < \infty$) and its theoretical description (which often uses continuous–time dynamics in form of, e.g., stochastic *differential* equations, which assume $n \to \infty$).

It is clear that the Kolmogorov consistency condition is in general not satisfied for quantum systems. It is, however, noteworthy that even for classical systems eqn (1.53) can be broken. This can happen simply for the reason that the measurement of a classical system can be disturbing as well. Another reason is an experimenter choosing to *actively break* the consistency condition. Examples of the latter kind include the use of feedback control, where an external agent manipulates the dynamics of a system based on the so far available information (say, based on $\mathbf{r}_k$ up to some time t_k). The future probabilities to observe r_n $(n > k)$ are then in general different from the situation where the external agent had not observed the system before (and consequently, had not applied any feedback control). Another example is a clinical trial where the health of patients is monitored at regular intervals and where the process can be actively changed by giving drugs. The health of the patients in the future then depends on the question whether their health was monitored before or not (and consequently, whether they received drugs or not).

These examples show that the theory of classical stochastic processes breaks down if an external agent intervenes the process. The mathematical language appropriate for such kind of situations is the theory of *classical causal models*. Without going into its details, we point out that causal models can *distinguish* between causation and correlation, whereas classical stochastic processes *cannot*. Indeed, classical stochastic processes allow to quantify correlations between two random variables, say X and Y, but the consistency condition forbids us to infer whether X is a *cause* of Y, Y a cause of X, or whether there is no causal relation between X and Y and their correlation is due to another common cause Z. In order to infer causal relationships, it is important that we can change the process and thus violate the consistency condition, for instance, by looking at the behaviour of Y after forcing X to take on a certain value. The following example makes this qualitative reasoning quantitative.

Exercise 1.13 We consider three binary random variables S, B and C with values s, b and c. On a given day S describes whether the sun is shining ($s = 1$) or not ($s = 0$), B describes whether the number of sunburns is high ($b = 1$) or low ($b = 0$) and C describes whether the number of ice cream sales is high ($c = 1$) or low ($c = 0$). We assume the notion of 'high'/'low' to be chosen according to some reasonable treshhold. We further set the conditional probabilities to be $p(b = 1|s = 1) = p(c = 1|s = 1) = p(b = 0|s = 0) = p(c = 0|s = 0) = \lambda$ with $\lambda \in [1/2, 1]$, e.g., $\lambda = 1$ implies that the number of sunburns is always high if the sun is shining. By conservation of probability, $p(b = 0|s = 1) = p(c = 0|s = 1) = p(b = 1|s = 0) = p(c = 1|s = 0) = 1 - \lambda$. Furthermore, we assume the probability for a sunny day to be $p(s = 1) = 1/2$, which implies that the sun is not shining with the same probability $p(s = 0) = 1/2$. Now, first confirm that B and C are correlated unless $\lambda = 1/2$. This can be done in several ways, for instance, by computing the mutual information, which we introduce in Appendix A in detail, between B and C:

$$I_{B:C} \equiv \sum_{b,c} p(b,c) \ln \frac{p(b,c)}{p(b)p(c)} = \ln 2 - S_{\text{Sh}}(2\lambda - 2\lambda^2). \tag{1.54}$$

Here, $S_{\text{Sh}}(p) \equiv -p \ln p - (1-p)\ln(1-p)$ denotes the *binary* Shannon entropy. Verify eqn (1.54) by using $p(b,c) = \sum_s p(b,c,s) = \sum_s p(b|s)p(c|s)p(s)$. Show that $I_{B:C} = 0$ (no correlations) implies $\lambda = 1/2$ and $I_{B:C} = \ln 2$ (maximal correlations) implies $\lambda = 1$. Thus, while B and C are in general correlated, they are not causally related as demonstrated below. Does this sound plausible to you?

Next, we turn to the correlations between S and B. Confirm that $I_{B:S} = \ln 2 - S_{\text{Sh}}(\lambda)$ and find the values of λ for which S and B are maximally correlated/uncorrelated.

Finally, we strongly believe that S is the cause of B (and also of C), i.e., the shining sun triggers sun burns (and ice cream sales). But how can we make this intuition rigorous?

Assume that we have an external mechanism, which can change whether the sun is shining or not (which seems unrealistic at first sight, but we come back to it below). We therefore introduce an additional *intervention variable* I_S (not to be mixed up with the mutual information), which labels the following three actions i: Do nothing, i.e., leave the sun as it is ($i = \text{idle}$), make the sun shining ($i = 1$), or block sun shine ($i = 0$). Now, consider the conditional probability $p(b|s,i)$ for sun burns given sunshine s and intervention i. For $i = \text{idle}$ we set $p(b|s, \text{idle}) = p(b|s)$ as defined above. Furthermore, we assume $p(b|s, i = 1) = \lambda$ and $p(b|s, i = 0) = 1 - \lambda$ *independent* of s because $i \in \{0, 1\}$ overwrites the natural value of s to be identical to i. Next, confirm that the mutual information between B and I_S is

$$I_{B:I_S} = \sum_{b,i} p(b,i) \ln \frac{p(b,i)}{p(b)p(i)} = S_{\text{Sh}}[p(b)] - [1 - p(i = \text{idle})]S_{\text{Sh}}(\lambda) - p(i = \text{idle}) \ln 2, \tag{1.55}$$

where the marginal probability $p(i)$ that we perform a certain intervention is assumed to be controllable in an experiment. We now define that *S is a **cause** of B if there are correlations between I_S and B.* Confirm that there are no correlations between B and I_S, i.e., S is *not* the cause of B, if one of the following two cases happen: either $p(i = \text{idle}) = 1$, which corresponds to the case that we do not perform any intervention and hence, cannot test for causality, or $\lambda = 1/2$, which implies that there are no correlations between B and S at first place. Furthermore, confirm that in general $p(b, s) \neq \sum_i p(b, s, i)$, where $p(b, s) = p(b|s)p(s)$ is the joint probability from the beginning obtained *without* interventions and $p(b, s, i) = p(b|s, i)p(s)p(i)$ is the joint probability with interventions. Thus, the Kolmogorov consistency condition (1.53) is broken in general. Show that the consistency condition is obeyed if and only if $p(i = \text{idle}) = 1$ or $p(i = 0) = p(i = 1)$. Can you see why? Of course, we could also replace B by C above and find that sunshine *causes* a high number of ice cream sales.

Finally, let us return to our assumption that we can change the sunlight by an external intervention. Indeed, such a mechanism is not easy to construct for a human. But to distinguish causation and correlation, it is not necessary that humans perform the intervention: it could be also done by nature, for instance, due to a solar eclipse. Important is only that we can fix the intervention variable independent of the other variables in the model.

1.7 Quantum Stochastic Processes

In this section we introduce the notion of a quantum stochastic process describing the response of an open quantum system to the most general interventions we can perform on it. This generality comes at the price of a high level of abstractness, even though it might help to keep in mind that much of what follows below ‘merely’ presents convenient terminology and notation. We proceed by first applying the notion of a classical stochastic process directly to quantum systems. Afterwards, we show that the idea can be fruitfully generalized to define a quantum stochastic process. Then, we show how to reconstruct a quantum stochastic processes experimentally and we finish by exploring further mathematical consequences of this formalism.

Quantum statistics of a projectively measured system

Even though quantum measurements are in general disturbing, the joint probability $p(\mathbf{r}_n)$ in eqn (1.51) remains a well–defined object in quantum mechanics. Experimentally, it describes the probability to obtain the results $\mathbf{r}_n = (r_n, \dots, r_1, r_0)$ after performing projective measurements of the quantum mechanical observable R with eigenvalues labeled by r at times $0 = t_0 < t_1 < \cdots < t_n$. Theoretically, the probability is computed for an isolated quantum system as

$$\begin{aligned} p(\mathbf{r}_n) = \operatorname{tr}\{&\Pi(r_n)U(t_n, t_{n-1}) \cdots \Pi(r_1)U(t_1, 0)\Pi(r_0)\rho(0) \\ &\times \Pi(r_0)U^\dagger(t_1, 0)\Pi(r_1) \cdots U^\dagger(t_n, t_{n-1})\Pi(r_n)\}. \end{aligned} \tag{1.56}$$

Here, $\rho(0)$ denotes the initial state of the quantum system, followed by a projective measurement $\Pi(r_0)\rho(0)\Pi(r_0)$ with result r_0, followed by a unitary time evolution $U(t_1, 0)\Pi(r_0)\rho(0)\Pi(r_0)U^\dagger(t_1, 0)$ from 0 to t_1, and so on and so forth up to time t_n. Since the expression (1.56) looks quite cumbersome, we introduce the superoperators $\mathcal{P}(r_\ell)$ and $\mathcal{U}(t_\ell, t_k)$ defined via their action $\mathcal{P}(r_\ell)\rho \equiv \Pi(r_\ell)\rho\Pi(r_\ell)$ and

$\mathcal{U}(t_\ell, t_k)\rho = U(t_\ell, t_k)\rho U^\dagger(t_\ell, t_k)$ on an arbitrary state ρ. Then, eqn (1.56) can be expressed more compactly as

$$p(\mathbf{r}_n) = \mathrm{tr}\{\mathcal{P}(r_n)\mathcal{U}(t_n, t_{n-1}) \cdots \mathcal{P}(r_1)\mathcal{U}(t_1, 0)\mathcal{P}(r_0)\rho(0)\}. \tag{1.57}$$

The following exercise shows that these probabilities are well–defined, but in general break the Kolmogorov consistency condition (1.53).

Exercise 1.14 Confirm that $p(\mathbf{r}_n)$ satisfies eqn (1.52) but in general not eqn (1.53).

Next, we return to the system–bath paradigm of Section 1.2. The spirit of system–bath theories was to view the open system S as the *accessible* part of the 'universe,' which can be easily measured and manipulated. In contrast, the bath B represents the *inaccessible* part of the universe about which we have only limited information. Following this spirit, we adapt eqn (1.56) to the case of open quantum systems by restricting R to be a system observable R_S. Then, the joint probability $p(\mathbf{r}_n)$ is

$$\begin{aligned} p(\mathbf{r}_n) = \mathrm{tr}_{SB}\{&[\mathcal{P}_S(r_n) \otimes \mathcal{I}_B]\mathcal{U}_{SB}(t_n, t_{n-1}) \cdots \\ &\times [\mathcal{P}_S(r_1) \otimes \mathcal{I}_B]\mathcal{U}_{SB}(t_1, 0)[\mathcal{P}_S(r_0) \otimes \mathcal{I}_B]\rho_{SB}(0)\}. \end{aligned} \tag{1.58}$$

Here, $\rho_{SB}(0)$ denotes the initial system–bath state, $\mathcal{U}_{SB}(t_\ell, t_k)$ the unitary time evolution from t_k to t_ℓ generated by some system–bath Hamiltonian and $[\mathcal{P}_S(r_\ell) \otimes \mathcal{I}_B]\rho_{SB} = [\Pi_S(r_\ell) \otimes I_B]\rho_{SB}[\Pi_S(r_\ell) \otimes I_B]$ the local projective measurement of the system. To save space, we drop all identity operations in the following. In addition, we understand that all superoperators *without* a subscript act only on the system, e.g., we write $\mathcal{P}(r_\ell)$ instead of $\mathcal{P}_S(r_\ell) \otimes \mathcal{I}_B$. Then, eqn (1.58) becomes

$$p(\mathbf{r}_n) = \mathrm{tr}_{SB}\{\mathcal{P}(r_n)\mathcal{U}_{SB}(t_n, t_{n-1}) \cdots \mathcal{P}(r_1)\mathcal{U}_{SB}(t_1, 0)\mathcal{P}(r_0)\rho_{SB}(0)\}. \tag{1.59}$$

In fact, this notation is still not short enough for our purposes. Instead, we are aiming at a notation, which explicitly distinguishes between the experimentally controllable part, which is here represented by the projective measurements $\mathcal{P}(r_\ell)$ we are performing on the system, and the uncontrollable or inaccessible part of the evolution encoded in the unitary system–bath evolution $\mathcal{U}_{SB}(t_\ell, t_k)$, which is fixed in a given experimental setup. Therefore, we define

$$\begin{aligned} &\mathfrak{T}[\mathcal{P}(r_n), \ldots, \mathcal{P}(r_1), \mathcal{P}(r_0)] \equiv \\ &\qquad \mathrm{tr}_B\{\mathcal{P}(r_n)\mathcal{U}_{SB}(t_n, t_{n-1}) \cdots \mathcal{P}(r_1)\mathcal{U}_{SB}(t_1, 0)\mathcal{P}(r_0)\rho_{SB}(0)\} \end{aligned} \tag{1.60}$$

such that eqn (1.59) simply becomes $p(\mathbf{r}_n) = \mathrm{tr}_S\{\mathfrak{T}[\mathcal{P}(r_n), \ldots, \mathcal{P}(r_1), \mathcal{P}(r_0)]\}$.

The process tensor and quantum stochastic processes

In contrast to the classical case, projective measurements of a quantum system generically disturb the dynamics. Furthermore, in Sections 1.4 and 1.5 we have learned that there is a much larger class of control operations that we can implement in a lab, not only projective measurements. This motivates us to extend the definition (1.60) to include arbitrary instruments applied at times t_ℓ, which are characterized by a set of CP maps $\{\mathcal{C}(r_\ell)\}$ adding up to a CPTP map $\mathcal{C}_\ell \equiv \sum_{r_\ell} \mathcal{C}(r_\ell)$. Thus, we define

$$\boxed{\begin{aligned}&\mathfrak{T}[\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)] \equiv \\ &\qquad \mathrm{tr}_B\{\mathcal{C}(r_n)\mathcal{U}_{SB}(t_n, t_{n-1}) \cdots \mathcal{C}(r_1)\mathcal{U}_{SB}(t_1, t_0)\mathcal{C}(r_0)\rho_{SB}(0)\},\end{aligned}} \tag{1.61}$$

and call $\mathfrak{T}$ the **process tensor**, which forms the central object for our studies in the remainder of this chapter. The probability to get the results $\mathbf{r}_n = (r_n, \dots, r_1, r_0)$, i.e., the probability for applying the CP maps $\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)$, is

$$\boxed{p(\mathbf{r}_n) = \mathrm{tr}_S\{\mathfrak{T}[\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)]\},} \tag{1.62}$$

which generalizes the result for a single measurement, eqn (1.35), to multiple times. The output of the process tensor is the non–normalized system state at time t_n after $n+1$ control operations conditioned on the results $\mathbf{r}_n$. In agreement with our previous notation for a single control operation, we denote this state as

$$\boxed{\tilde{\rho}_S(t_n|\mathbf{r}_n) \equiv \mathfrak{T}[\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)].} \tag{1.63}$$

We have $p(\mathbf{r}_n) = \mathrm{tr}_S\{\tilde{\rho}_S(t_n|\mathbf{r}_n)\}$.

The process tensor is the most abstract and complex mathematical object we meet in this book. If one calls $\mathcal{C}(r_\ell)$ a superoperator, then $\mathfrak{T}$ is a *super–superoperator* and, although we seldomly attempt to compute it explicitly, it is our guiding theoretical framework in the following. Once we have appreciated its vast generality, it allows us to view the structure of many upcoming problems with greater clarity.

The process tensor encodes in an abstract way all what can happen to an open quantum system by 'interrogating' it at an arbitrary set of discrete times with instruments $\{\mathcal{C}(r_\ell)\}$, which act only on the system degrees of freedom. Thus, all the information we can locally obtain about the evolution of an open quantum system is contained in the process tensor. This neatly extends the idea of a classical stochastic process, where one also assumes the ability to perfectly measure the system at arbitrary times, to the quantum regime. Hence, we make the following postulate:

Quantum stochastic process. *Every process tensor describes a quantum stochastic process. Vice versa, every quantum stochastic process can be described by a process tensor.*

Therefore, both, a classical and a quantum stochastic processes have in common the idea to explicitly include the control operations applied in an experiment into the theoretical description, but a quantum stochastic process allows for a larger class of interventions beyond non–disturbing projective measurements. Throughout this book, we call a theoretical description, which explicitly accounts for any interventions performed in an experiment, **operational**. The rest of this section explains further properties of the process tensor (or a quantum stochastic process), which is pictorially represented in Fig. 1.5. Indeed, after having emphasized its operational character, it seems worth to first wonder how to experimentally access the process tensor.

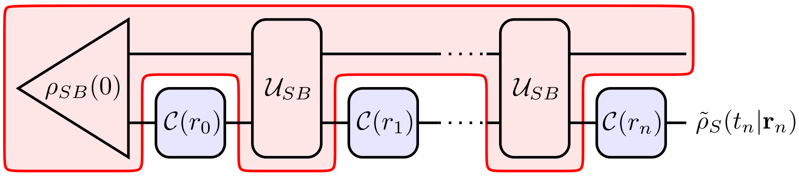

Fig. 1.5 Sketch of the process tensor with time running from left to right. Quantum systems (such as S or B) are marked with a line. The initial state is drawn as a triangle and state transformations are portrayed with boxes. Thus, the shaded red region presents all the information encoded in the process tensor, whereas the inputs or arguments of the process tensor are the interventions $\mathcal{C}(r_\ell)$ shaded in blue. For notational simplicity we dropped the time–dependence of the system–bath unitary $\mathcal{U}_{SB}$.

Experimental reconstruction of the process tensor

To experimentally reconstruct the process tensor, it is useful to note first that it really is a *tensor*, i.e., a multi–linear object with respect to its arguments. If this is not yet evident, the next exercise asks you to verify it directly. Explicit representations of the process tensor are constructed in Appendix B.3.

Exercise 1.15 Show based on definition (1.61) that for every $\ell \in \{0, 1, \dots, n\}$

$$\begin{aligned}\mathfrak{T}[\mathcal{A}_n, \dots, a_\ell\mathcal{A}_\ell + b_\ell\mathcal{B}_\ell, \dots, \mathcal{A}_0] = {} & a_\ell\mathfrak{T}[\mathcal{A}_n, \dots, \mathcal{A}_\ell, \dots, \mathcal{A}_0] \\ & + b_\ell\mathfrak{T}[\mathcal{A}_n, \dots, \mathcal{B}_\ell, \dots, \mathcal{A}_0],\end{aligned} \tag{1.64}$$

where $\mathcal{A}_0, \dots, \mathcal{A}_\ell, \dots, \mathcal{A}_n$ and $\mathcal{B}_\ell$ are arbitrary maps and $a_\ell, b_\ell \in \mathbb{C}$ two arbitrary complex numbers. Therefore, the process tensor is linear in all its entries. But on which space is the process tensor acting?

For this purpose consider a quantum system with Hilbert space $\mathcal{H}_S$ of dimension $d = \dim \mathcal{H}_S$. We denote the space of all linear maps (or operators) acting on $\mathcal{H}_S$ by $\mathcal{L}(\mathcal{H}_S)$. $\mathcal{L}(\mathcal{H}_S)$ is itself a vector (or Hilbert) space of dimension d^2. Examples for objects living in $\mathcal{L}(\mathcal{H}_S)$ are the density matrix ρ_S and the Hamiltonian H_S. Furthermore, we denote the space of all linear maps (or superoperators) acting on $\mathcal{L}(\mathcal{H}_S)$ by $\mathcal{L}(\mathcal{L}(\mathcal{H}_S))$. This again forms a Hilbert space, now of dimension d^4, and examples include all the CP and CPTP maps we have studied above such as $\mathcal{C}(r_\ell)$. The process tensor therefore maps objects from the $(n+1)$–fold tensor product space of $\mathcal{L}(\mathcal{L}(\mathcal{H}_S))$ to the state space $\mathcal{L}(\mathcal{H}_S)$, symbolically:

$$\mathfrak{T} : \underbrace{\mathcal{L}(\mathcal{L}(\mathcal{H}_S)) \otimes \cdots \otimes \mathcal{L}(\mathcal{L}(\mathcal{H}_S))}_{(n+1)\text{ times}} \to \mathcal{L}(\mathcal{H}_S). \tag{1.65}$$

Deduce that the dimension of the input space of $\mathfrak{T}$ is $d^{4(n+1)}$.

The basic idea to reconstruct the process tensor experimentally is similar to the case of a classical stochastic process, where one constructs a histogram of joint probabilities with respect to all possible measurement results. Now, however, we have to construct a 'histogram' of density matrices with respect to all kinds of possible interventions. As a preliminary step the next exercise first reviews the basics of quantum *state* tomography before we turn to the more general case of quantum *process* tomography.

Exercise 1.16 Quantum state tomography describes the experimental procedure to determine an unknown quantum state ρ. To approach it, we start with an unknown state of a classical two–level system (a 'bit'), here denoted as $\rho_{\mathrm{bit}} = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|$ with $p \in [0,1]$ unknown. Clearly, to determine p we simply need sufficiently many copies of ρ_{bit} and measure its state many times in the basis $\{|0\rangle, |1\rangle\}$. The frequency of measurement outcomes m_0/M and m_1/M (with M the total number of measurements) then approximates p and $1-p$.

Now, suppose that you have sufficiently many copies of a qubit in the state $\rho = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1| + c|0\rangle\langle 1| + c^*|1\rangle\langle 0|$ at your disposal with unknown $p \in [0,1]$ and $c \in \mathbb{C}$, which obeys $|c|^2 \leq p(1-p)$ (show that this follows from the positivity of ρ). Now, devise a measurement strategy to determine ρ. *Hint:* There are many solutions. One convenient approach is offered by the Bloch sphere representation $\rho = (I + \boldsymbol{r}\cdot\boldsymbol{\sigma})/2$ with the vector of Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and the Bloch vector $\boldsymbol{r} = \mathrm{tr}\{\boldsymbol{\sigma}\rho\}$ obeying $r_x^2 + r_y^2 + r_z^2 \leq 1$. Show also that it is sufficient to know the three probabilities $p_{x=1} = \mathrm{tr}\{|1\rangle\langle 1|_x\rho\}$, $p_{y=1} = \mathrm{tr}\{|1\rangle\langle 1|_y\rho\}$ and $p_{z=1} = \mathrm{tr}\{|1\rangle\langle 1|_z\rho\}$, where $|1\rangle_{x,y,z}$ is the eigenvector of $\sigma_{x,y,z}$ with eigenvalue $+1$, to determine ρ completely. A set of projectors such as $\{|1\rangle\langle 1|_x, |1\rangle\langle 1|_y, |1\rangle\langle 1|_z\}$ whose outcome probabilities determine the entire state of a quantum system are also known as **informationally complete**.

Despite some similarity in the quantum and classical case, there are also differences. Confirm that, given that you know that the classical bit is in a pure state, there is only a *single* measurement needed to determine its state. Convince yourself of the fact that this no longer holds true for a qubit.

Do you see how to generalize the above procedure to arbitrary d–dimensional quantum systems? In this case a convenient parametrization of ρ could be the generalized Bloch representation

$$\rho = \frac{1}{d}\left(I + \sqrt{\frac{d(d-1)}{2}}\boldsymbol{r}\cdot\boldsymbol{\Lambda}\right). \tag{1.66}$$

Here, the generalized Bloch vector $\boldsymbol{r} \in \mathbb{R}^{d^2-1}$ obeys $\sum_i r_i^2 \leq 1$ and $\boldsymbol{\Lambda}$ denotes a vector of d^2-1 traceless Hermitian matrices Λ_i obeying $\mathrm{tr}\{\Lambda_i\Lambda_j\} = 2\delta_{ij}$.

Given that we now know how to tomographically reconstruct a quantum state, how can we perform **quantum process tomography** of the full process tensor? Luckily, since the process tensor is multi–linear, it suffices to know its elements with respect to a basis of quantum operation performed at different times. For a single time, one such basis is offered by the quantum operations

$$\mathcal{B}_{\alpha\beta}\rho_S \equiv P_\alpha \mathrm{tr}\{\Pi_\beta\rho_S\}. \tag{1.67}$$

Here, the set $\{\Pi_\beta\}_\beta$ presents an informationally complete set of projectors (see last exercise). Thus, $\{\Pi_\beta\}_\beta$ has d^2-1 elements to which we add one more element such that we have a basis for the vector space of complex $d\times d$ matrices. Furthermore, $\{P_\alpha\}_\alpha$ denotes a set of d^2 independent quantum states, which span the space $\mathcal{L}(\mathcal{H}_S)$. If we fix a given basis $\{|n\rangle\}$ of $\mathcal{H}_S$, then one convenient parametrization is given by the double index $\alpha \equiv (m,n)$ such that $P_\alpha = |\psi_{m,n}\rangle\langle\psi_{m,n}|$ with $|\psi_{n,n}\rangle = |n\rangle$, $|\psi_{m,n}\rangle = (|m\rangle + |n\rangle)/\sqrt{2}$ for $m > n$ and $|\psi_{m,n}\rangle = (i|m\rangle + |n\rangle)/\sqrt{2}$ for $m < n$.

Exercise 1.17 Confirm that the above defined set of states P_α linearly spans the entire space of $d\times d$ matrices.

Physically, the control operations (1.67) correspond to measuring the quantum state and obtaining (probabilistically) the result β followed by repreparing the system in the state P_α. Every map $\mathcal{C}$ can be linearly expanded in that basis

$$\mathcal{C} = \sum_{\alpha,\beta} c_{\alpha\beta}\mathcal{B}_{\alpha\beta} \tag{1.68}$$

with in general complex coefficients $c_{\alpha\beta} \in \mathbb{C}$. If $\mathcal{C}$ is a CP or CPTP map, even more can be said about the coefficients as summarized in the next exercise.

Exercise 1.18 First, show that, if $\mathcal{C}$ preserves Hermiticity, then the coefficients $c_{\alpha\beta} \in \mathbb{R}$ are real. Next, show that, if the map $\mathcal{C}$ is trace–preserving, then $\sum_\alpha c_{\alpha\beta} = 1$.

Now, all what we have to do in order to reconstruct the full process tensor is to measure the quantum system at times t_ℓ, $\ell \in \{0, 1, \dots, n\}$, in the informationally complete basis $\{\Pi_{\beta_\ell}\}$ followed by randomly repreparing the state in one of the P_{α_ℓ}'s after the measurement. By repeating this procedure many times, we obtain the elementary process tensors $\mathfrak{T}[\mathcal{B}_{\alpha_n\beta_n}, \dots, \mathcal{B}_{\alpha_1\beta_1}, \mathcal{B}_{\alpha_0\beta_0}]$. Given them, the action of the process tensor on any set of instruments can be reconstructed by linear combination

$$\begin{aligned}&\mathfrak{T}[\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)]\\ &\qquad = \sum_{\alpha_n,\beta_n} \cdots \sum_{\alpha_1,\beta_1}\sum_{\alpha_0,\beta_0} c_{\alpha_n\beta_n}\cdots c_{\alpha_1\beta_1}c_{\alpha_0\beta_0}\mathfrak{T}[\mathcal{B}_{\alpha_n\beta_n}, \dots, \mathcal{B}_{\alpha_1\beta_1}, \mathcal{B}_{\alpha_0\beta_0}]\end{aligned} \tag{1.69}$$

for some coefficients $c_{\alpha_\ell\beta_\ell} \in \mathbb{R}$. In fact, we can now recognize that the sequence of interventions $\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)$ forms only a special subclass of all conceivable interventions, namely those that are *decorrelated*. The next exercise explains this.

Exercise 1.19 Recall eqn (1.65), which shows that the process tensor can be seen as a map acting on $\bigotimes_{i=0}^n \mathcal{L}(\mathcal{L}(\mathcal{H}_S))$. Using the basis (1.67), an arbitrary element $\boldsymbol{C}_{n:0}$ of that space can be written as

$$\boldsymbol{C}_{n:0} = \sum_{\alpha_n,\beta_n} \cdots \sum_{\alpha_1,\beta_1}\sum_{\alpha_0,\beta_0} c_{\alpha_n\beta_n,\dots,\alpha_1\beta_1,\alpha_0\beta_0}\mathcal{B}_{\alpha_n\beta_n} \otimes \cdots \otimes \mathcal{B}_{\alpha_1\beta_1} \otimes \mathcal{B}_{\alpha_0\beta_0}, \tag{1.70}$$

where the coefficients $c_{\alpha_n\beta_n,\dots,\alpha_1\beta_1,\alpha_0\beta_0}$ need not to factor as in eqn (1.69). Confirm that the element $\boldsymbol{C}_{n:0}(\mathbf{r}_n)$ corresponding to applying a sequence of control operations $\mathcal{C}(r_n), \dots, \mathcal{C}(r_0)$ can be written as a tensor product in that space: $\boldsymbol{C}_{n:0}(\mathbf{r}_n) = \mathcal{C}(r_n) \otimes \cdots \otimes \mathcal{C}(r_0)$. This can be called a decorrelated control operation or intervention.

Equation (1.70) therefore tells us that more general, correlated control operations $\boldsymbol{C}_{n:0}(\mathbf{r}_n)$ are possible. In this case we denote the process tensor as $\mathfrak{T}[\boldsymbol{C}_{n:0}(\mathbf{r}_n)] = \tilde{\rho}_S(t_n|\mathbf{r}_n)$, where $\tilde{\rho}_S(t_n|\mathbf{r}_n)$ still denotes the non–normalized system state at time t_n resulting from the action of some correlated control operation happening with probability $p(\mathbf{r}_n) = \mathrm{tr}_S\{\tilde{\rho}_S(t_n|\mathbf{r}_n)\}$. Examples for correlated control operations are, for instance, classical feedback control or conditioning of the dynamics. To be specific, let $\mathcal{P}(r_0)$ denote a projective measurement of some system observable at time t_0 giving result r_0. Let $\mathcal{C}_1(r_0)$ denote some CPTP map at time t_1, which depends on the previously recorded measurement result r_0. The corresponding control operation is $\boldsymbol{C}_{1:0}(r_0) = \mathcal{C}_1(r_0) \otimes \mathcal{P}(r_0)$, which is still decorrelated. However, the average effect of the control operation is given by $\boldsymbol{C}_{1:0} = \sum_{r_0} \mathcal{C}_1(r_0) \otimes \mathcal{P}(r_0)$, which is correlated. Correlated control operations therefore allow us to treat all conceivable scenarios of feedback control within the process tensor framework.

To conclude, the above procedure shows how to experimentally reconstruct the process tensor. This reconstruction is based on two assumptions. First, the experimentalist must be able locally measure and manipulate the open quantum system. This does not necessarily mean that one must be able to implement the specific control operations (1.67), any other basis of maps suffices as well. Second, the control operations were assumed to happen *instantaneously*, similar to the measurements in a classical stochastic process. In practice, this statement translates into the requirement that the time scales of the environmentally induced system evolution, determined by $\mathcal{U}_{SB}$, must be long compared to the time it takes to implement the control operation. This is required in order to disentangle the effect of the environment from the effect of the external controller. Even if these requirements are satisfied, experimentally reconstructing the process tensor remains a formidable challenge since the number of parameters we have to estimate grows exponentially as d^{4n} with the number n of time steps (for a classical stochastic process, it grows as d^n). Luckily, for one theoretically and experimentally important case of applications, the process tensor can be constructed in a simple manner. This case is described by quantum *Markov* processes, which we will introduce in the next section. Before turning to them, we list three further relevant properties of the process tensor.

Further properties of the process tensor

In Section 1.6 we have seen that the joint probabilities of a classical stochastic process form a hierarchy. The same is also true for the process tensor, which satisfies a *containment property* as explored in the next exercise. We remark that this containment property is the basis to show that there exists a generalized Daniell–Kolmogorov extension theorem also for quantum stochastic processes.

Exercise 1.20 The process tensor $\mathfrak{T}$ was defined on the set of times $\{t_0, t_1, \dots, t_n\}$. Consider any subset of times $T \subset \{t_0, t_1, \dots, t_n\}$. Show that the process tensor $\mathfrak{T}_T$ defined on this subset of times is *contained* in the original $\mathfrak{T}$. By this we mean that all probabilities predictable from $\mathfrak{T}_T$ can be also recovered from $\mathfrak{T}$. Thus, process tensors $\mathfrak{T}_{T_1}, \dots, \mathfrak{T}_{T_N}$ for discrete sets of times $T_1 \subset \cdots \subset T_N$ form a hierarchy with $\mathfrak{T}_{T_\ell}$ containing $\mathfrak{T}_{T_k}$ for $\ell \geq k$.

Furthermore, one can extend the operator–sum representation and the unitary dilation theorem to the process tensor, but we are not going to write down the corresponding operator–sum representation theorem here and the unitary dilation theorem of the process tensor is only pictorially presented in Fig. 1.6. Mathematically, this is possible because the process tensor satisfies requirements similar to those imposed on a single–time control operation in Section 1.5 [requirements (i'), (ii) and (iii)].

First, the process tensor preserves complete positivity [requirement (i')] in the following sense. Let ρ_{SA} be an arbitrary initial system–ancilla state and let $\boldsymbol{C}^{SA}_{n:0}(\mathbf{r}_n)$ be any $(n+1)$–time control operation acting on the system–ancilla state. We can then

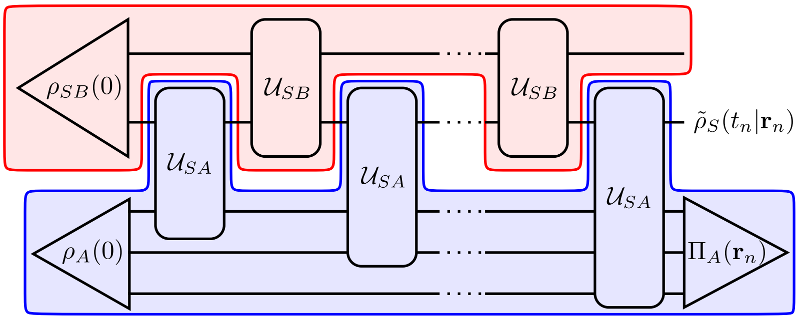

Fig. 1.6 Similar to the unitary dilation theorem, also an arbitrary correlated control operation $\boldsymbol{C}_{n:0}(\mathbf{r}_n)$ can be simulated by introducing a sufficiently large ancilla state $\rho_A(0)$, which is initially decorrelated from the system and usally contains multiple ancillas (represented by the different lines in the figure) and which interacts unitarily with the system through $\mathcal{U}_{SA}$. Note that we are a bit sloppy here and use the same symbol $\mathcal{U}_{SA}$ for in general different system–ancilla unitaries. Finally, the joint ancilla state is measured using some projector $\Pi_A(\mathbf{r}_n)$. The blue and red object together represent the unitary dilation of the process.

define an extended process tensor $\mathfrak{T}_S \otimes \mathfrak{I}_A$ as in eqn (1.61) by replacing $\rho_{SB}(0)$ by $\rho_{SBA}(0)$ and $\mathcal{U}_{SB}(t_\ell, t_k)$ by $\mathcal{U}_{SB}(t_\ell, t_k) \otimes \mathcal{I}_A$. Thus, $\mathfrak{T}_S$ equals $\mathfrak{T}$ as defined in eqn (1.69) and $\mathfrak{I}_A$ is the 'identity process.' It then follows that the output state $\tilde{\rho}_{SA}(t_n|\mathbf{r}_n) = \mathfrak{T}_S \otimes \mathfrak{I}_A(\boldsymbol{C}_{n:0}^{SA}) \geq 0$ is always positive.

Second, the trace non–increasing property (ii) is clearly satisfied for the process tensor and it also satisfies a modified requirement (iii) of linearity by recalling that the process tensor is linear with respect to the applied interventions. In fact, those interventions are the objects, which we can freely control in an experiment, in contrast to the initial system state $\rho_S(0)$. This resolves the conundrum of Exercise 1.11.

Exercise 1.21 The process tensor does not depend linearly on the initial system state $\rho_S(0)$ in general. However, show that it does for an initial state of the form $\rho_{SB}(0) = \rho_S(0) \otimes \rho_B(0)$. Then, convince yourself that in this case the first control operation $\mathcal{C}(r_0)$ becomes redundant and one can define the process tensor as $\mathfrak{T}[\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \rho_S(0)]$, where $\rho_S(0)$ is now taken arbitrary. Beyond that case, the present approach provides an operational resolution to the conundrum of Exercise 1.11 by realizing that *quantum dynamics is linear with respect to the state preparation* $\mathcal{C}(r_0)$ of an experiment, but not with respect to the initial system state.

The final point we want to make is that the process tensor can be used to compute correlation functions of the form

$$\langle A(t)B(0)\rangle = \mathrm{tr}_{SB}\{AU_{SB}(t,0)B\rho_{SB}(0)U_{SB}^\dagger(t,0)\}. \tag{1.71}$$

Here, A and B are two arbitrary system observables. The reader is asked to explicitly verify this in the next exercise, which concludes this section.

Exercise 1.22 We write the spectral decomposition of A as $A = \sum_a a|a\rangle\langle a|$. Since

$$\langle A(t)B(0)\rangle = \sum_a a\mathrm{tr}_{SB}\{|a\rangle\langle a|U_{SB}(t,0)B\rho_{SB}(0)U_{SB}^\dagger(t,0)\}, \tag{1.72}$$

it is clear that the final control operation at time t_1 has to be a projective measurement of the observable A. We therefore write $\langle A(t)B(0)\rangle = \sum_a a\mathrm{tr}_S\{\mathfrak{T}[\mathcal{P}(a),\mathcal{B}_0]\}$, where $\mathfrak{T}[\cdot,\cdot]$ is the two–time process tensor defined at times 0 and t and the control operation $\mathcal{B}_0$ is defined by $\mathcal{B}_0\rho_{SB}(0) = B\rho_{SB}(0)$. Unfortunately, $\mathcal{B}_0$ is not CP and does not even preserve Hermiticity. Therefore, it cannot directly be implemented in a lab using a suitably tailored system–ancilla interaction. Nevertheless, by linearity we can find a set of experimentally implementable CP maps $\mathcal{B}_{\alpha\beta}$ with coefficients $c_{\alpha\beta}$ such that $\mathcal{B}_0 = \sum_{\alpha,\beta} c_{\alpha\beta}\mathcal{B}_{\alpha\beta}$, cf. eqn (1.68). To see this explicitly, we use $B = \sum_b b|b\rangle\langle b|$ and $I = \sum_b |b\rangle\langle b|$ to write

$$\mathcal{B}_0\rho_{SB}(t_0) = B\rho_{SB}(t_0) = \sum_b b|b\rangle\langle b|\rho_{SB}\sum_{b'}|b'\rangle\langle b'| = \sum_{b,b'} b|b\rangle\langle b'|\mathrm{tr}_S\{|b'\rangle\langle b|\rho_{SB}(0)\}. \tag{1.73}$$

Now, this looks already close to a linear combination of the elementary control operations (1.67) with the difference that the elements $|b\rangle\langle b'|$ in general do not belong to the sets of $\{P_\alpha\}_\alpha$ and $\{\Pi_\beta\}_\beta$. However, as Exercise 1.17 has shown, we can always write

$$|b\rangle\langle b'| = \sum_\alpha c_\alpha^{bb'}P_\alpha, \quad |b'\rangle\langle b| = \sum_\beta \tilde{c}_\beta^{b'b}\Pi_\beta \tag{1.74}$$

for some (in general complex) coefficients $c_\alpha^{bb'}$ and $\tilde{c}_\beta^{b'b}$. Thus, in terms of the elementary control operations (1.67) we have

$$\langle A(t)B(0)\rangle = \sum_{a,b,b',\alpha,\beta} abc_\alpha^{bb'}\tilde{c}_\beta^{b'b}\mathrm{tr}_S\{\mathfrak{T}[\mathcal{P}(a),\mathcal{B}_{\alpha\beta}]\}. \tag{1.75}$$

Now, the process $\mathfrak{T}[\mathcal{P}(a),\mathcal{B}_{\alpha\beta}]$ is implementable in a lab using only local measurements and state preparations. Furthermore, the coefficient $abc_\alpha^{bb'}\tilde{c}_\beta^{b'b}$ is known. Hence, the correlation function $\langle A(t)B(0)\rangle$ is measurable and its value is encoded in the process tensor.

Readers, who had problems to follow the steps above, are asked to explicitly verify them for a qubit and the linear map $\mathcal{B}_0\rho = \sigma_z\rho$ using a basis of your choice for the elementary control operations $\mathcal{B}_{\alpha\beta}\rho = P_\alpha\mathrm{tr}\{\Pi_\beta\rho\}$. Furthermore, convince yourself of the fact that the above statement can be extended to arbitary multi–time correlation functions $\langle A_n(t_n)\dots A_1(t_1)A_0(t_0)\rangle$ as long as all A_ℓ are system observables.

1.8 Quantum Markov Processes and Dynamical Maps

Markov processes, may they be quantum or classical in nature, play an important role in physics. In part, this seems to be caused by the fact that they considerably simplify the life of a theoretician and typically allow for at least some analytical progress in the description. Also in this book we will encounter Markov processes, albeit a considerable part of this book is devoted to showing that all our main results continue to hold for non–Markovian processes. Colloquially, Markov processes are associated with *memoryless* processes. This means that the environment quickly *forgets* the state of the system in the past such that the system's future evolution is only influenced by its current state. We now make this reasoning rigorous.

To approach the problem, we first of all introduce the notion of a **causal break**. A causal break is an intervention, which reprepares the system in a state, which is independent of all past interventions. They are in general written as

$$\mathcal{B}_{\alpha\beta}\rho_S \equiv \sigma_S^{(\alpha)}\mathrm{tr}_S\{P_\beta\rho_S\}. \tag{1.76}$$

Here, P_β is an arbitrary element of a POVM and $\sigma_S^{(\alpha)}$ an arbitrary system density matrix. Thus, a causal break describes an intervention, where we read out the state of the system in an arbitary way (remember that $P_\beta = I_S$ is a legitimate choice too), then discard the system state, and finally prepare a fresh state $\sigma_S^{(\alpha)}$, which is *independent* of the previous system state or the result of the measurement P_β. This ensures that $\sigma_S^{(\alpha)}$ can have no memory about the past. Note that the operations introduced in eqn (1.67) are causal breaks and hence, causal breaks can be used as a basis to span the space of linear maps.

Furthermore, we introduce the following notation to denote the *normalized* system state after an arbitrary sequence $\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)$ of interventions:

$$\rho_n[\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)] \equiv \frac{\tilde{\rho}_S(t_n|\mathbf{r}_n)}{p(\mathbf{r}_n)} = \frac{\mathfrak{T}[\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)]}{\mathrm{tr}_S\{\mathfrak{T}[\mathcal{C}(r_n), \dots, \mathcal{C}(r_1), \mathcal{C}(r_0)]\}}. \tag{1.77}$$

We now define:

Quantum Markov process. *A quantum stochastic process is Markovian if the normalized system state at time t_ℓ after a causal break (1.76) at time $t_k < t_\ell$ depends only on the input state $\sigma_S^{(\alpha_k)}$ for any set of previous interventions $\mathcal{C}(r_{k-1})$, …, $\mathcal{C}(r_0)$. In equations,*

$$\rho_\ell[\mathcal{B}_{\alpha_k\beta_k}, \mathcal{C}(r_{k-1}), \dots, \mathcal{C}(r_0)] = \rho_\ell[\sigma_S^{(\alpha_k)}]. \tag{1.78}$$

This definition captures the idea that everything which has happened to the system in the past does not influence its future after any causal connection at the system level is cut. Thus, if eqn (1.78) is violated, this must be due to the fact that the *environment* kept some memory about what has happend to the system in the past. To get familiar with this definition, it is best to confirm an intuitve result such as the following.

Exercise 1.23 Verify that an isolated (i.e., unitarily evolving) system is Markovian.

The following important result, which the reader is asked to prove in an exercise below, shows that quantum Markov processes have a particularly simple mathematical structure.

Factorization of the process tensor. *For a Markovian process the process tensor 'factorizes':*

$$\boxed{\mathfrak{T}[\mathcal{C}(r_n), \dots, \mathcal{C}(r_0)] = \mathcal{C}(r_n)\mathcal{E}(t_n, t_{n-1}) \dots \mathcal{E}(t_1, 0)\mathcal{C}(r_0)\rho_S(0).} \tag{1.79}$$

Here, $\rho_S(0) = \mathrm{tr}_B\{\rho_{SB}(0)\}$ is the initial system state and $\mathcal{E}(t_\ell, t_k)$ are CPTP maps independent of $\mathcal{C}(r_n), \dots, \mathcal{C}(r_0)$.

The physical meaning of the CPTP maps $\mathcal{E}(t_\ell, t_k)$ is to propagate the system state forward in time. This becomes transparent by considering the process tensor obtained by applying the identity maps restricted to the subset of times $\{t_k, 0\}$ with $k > 0$:

$$\rho_S(t_k) = \mathfrak{T}_{k,0}[\mathcal{I}_k, \mathcal{I}_0] = \mathcal{E}(t_k, 0)\rho_S(0). \tag{1.80}$$

Furthermore, we can use the interventions $\mathcal{C}(r_k)$ to prepare arbitrary system states at any time t_k. Since eqn (1.79) holds for all interventions and all subsets of times $t_\ell > t_k > t_j > t_0$, we infer that the CPTP maps obey the composition rule

$$\mathcal{E}(t_\ell, t_j) = \mathcal{E}(t_\ell, t_k)\mathcal{E}(t_k, t_j). \tag{1.81}$$

In fact, whenever it is possible to define a set of cptp maps $\{\mathcal{E}(t_k, t_j)\}$ for all times $t_k > t_j$ that propagate the system state $\rho(t_k) = \mathcal{E}(t_k, t_j)\rho(t_j)$ and obey eqn (1.81) one calls the dynamics **CP divisible**. Note that a dynamics can be non-Markovian but CP divisible because the notion of CP divisibility does not rely on interventions.

Note that a CPTP map $\mathcal{E}(t_k, 0)$ propagating the system state forward in time can be *always* defined if the system–bath state at time t_0 factorizes. Then, we can write

$$\rho_S(t_k) = \mathrm{tr}_B\{U_{SB}(t_k, 0)\rho_S(0) \otimes \rho_B(0)U^\dagger_{SB}(t_k, 0)\} \equiv \mathcal{E}(t_k, 0)\rho_S(0) \tag{1.82}$$

and by virtue of the unitary dilation theorem the map $\mathcal{E}(t_k, 0)$ is CPTP. Markovianity precisely says that we can always write $\rho_S(t_\ell) = \mathcal{E}(t_\ell, t_k)\rho_S(t_k)$ for all pairs of times $t_\ell > t_k$ with $\mathcal{E}(t_\ell, t_k)$ CPTP and independent of what has happened in the past. Since the maps $\mathcal{E}(t_\ell, t_k)$ play such an important role for the evolution of open quantum systems, they are called **dynamical maps**. In quantum information theory they are also often called **channels** to signify that they can be used to *communicate* a quantum state from one laboratory to another. That is to say, the CPTP maps $\mathcal{E}$ cannot only be used to propagate the system state forward in time, but also forward in *space*–time. In non–relativistic quantum mechanics $\mathcal{E}$ describes therefore the most general time evolution obeying the properties (i'), (ii) and (iii) of Section 1.5. The proof that Markov processes factorize is relegated to an exercise.

Exercise 1.24 First, show that, if the process tensor factorizes as in eqn (1.79), then the process is Markovian. Conversely, let us assume that the process is Markovian. Consider first an elementary process tensor obtained by applying only causal breaks. Note that the action of a causal breaks implies that the system–bath state becomes decorrelated: $\mathcal{B}_{\alpha\beta}\rho_{SB} = \sigma_S^{(\alpha)} \otimes \mathrm{tr}_S\{P_\beta \rho_{SB}\}$. We can therefore always write

$$\begin{aligned}\mathfrak{T}[\mathcal{B}_{\alpha_n\beta_n}, \dots, \mathcal{B}_{\alpha_1\beta_1}, \mathcal{B}_{\alpha_0\beta_0}] = {}& \\ \sigma_S^{(\alpha_n)}\mathrm{tr}_S\{P_{\beta_n}\tilde{\mathcal{E}}(t_n, t_{n-1})\sigma_S^{(\alpha_{n-1})}\} \dots \mathrm{tr}_S\{P_{\beta_1}\tilde{\mathcal{E}}(t_1, t_0)\sigma_S^{(\alpha_0)}\}&\mathrm{tr}_S\{P_{\beta_0}\rho_S(t_0)\}.\end{aligned} \tag{1.83}$$

Here, the $\tilde{\mathcal{E}}(t_\ell, t_k)$ are CPTP maps which can be reconstructed by quantum process tomography by preparing a set of basis states $\{\rho_S^{(\alpha_k)}\}$ and by measuring an informationally complete set of POVMs $\{P_{\beta_\ell}\}$. In general, however, the maps $\tilde{\mathcal{E}}(t_\ell, t_k)$ depend on all previous interventions $\beta_k, \alpha_{k-1}, \beta_{k-1}, \dots, \alpha_0, \beta_0$ because the reduced state of the bath at time t_k carries information about the history of the system. Therefore, the maps $\tilde{\mathcal{E}}(t_\ell, t_k)$

are usually not very helpful. However, for Markovian processes the claim is precisely that these maps are *independent* of the history of the system. Prove this! *Hint:* It might be useful to try a proof by contradiction, i.e., assume that there are two different histories $\mathbf{h} \equiv (\beta_k, \alpha_{k-1}, \beta_{k-1}, \ldots, \alpha_0, \beta_0)$ and $\mathbf{h}' \equiv (\beta'_k, \alpha'_{k-1}, \beta'_{k-1}, \ldots, \alpha'_0, \beta'_0)$ of causal breaks with $\mathbf{h} \neq \mathbf{h}'$ such that $\tilde{\mathcal{E}}(t_\ell, t_k) \equiv \tilde{\mathcal{E}}(t_\ell, t_k|\mathbf{h}) \neq \tilde{\mathcal{E}}(t_\ell, t_k|\mathbf{h}') \equiv \tilde{\mathcal{E}}'(t_\ell, t_k)$. Show that this leads to a contradiction for a Markov process.

It is important to remark that the Markov property is purely defined in terms of the process tensor. Hence, it is a property *inherent* to the process itself. In particular, the question whether the process is Markovian or not is *independent* of the control operations applied to the system. This holds even true for correlated control operations, for instance, if we apply feedback control at time t_n depending on previous measurement results $\mathbf{r}_k$ $(k < n)$. The fact that the environment for a Markov process does not keep any memory about previous interventions is not changed by the decision of an external agent to keep a memory about them. The connection between classical and quantum Markov processes is explored in the next section.

1.9 Classical Quantum Stochastic Processes

In the final section of this chapter we connect the notion of quantum stochastic processes to classical stochastic processes. We unravel that quantum stochastic processes look classical in some measurement basis whenever coherences do not influence the dynamics in that basis. Later on in this book, we will indeed see that there is a preferred basis in which at least weakly coupled open quantum systems behave ‘classical.’ This basis is the energy eigenbasis, which is related to the fact that the thermal equilibrium state $\pi_S = e^{-\beta H_S}/\mathcal{Z}_S$ is diagonal in that basis. In the second part of this section we connect the notion of quantum Markovianity to classical Markovianity.

Non–classicality and coherence

To investigate the question when does a quantum stochastic process mimic a classical stochastic process, we return to the case of a projectively measured system observable R_S with a joint probability $p(\mathbf{r}_n)$ as defined in eqns (1.59) and (1.60). It turns out that our answer depends on the question whether the observable R_S is degenerate or not. For the moment we assume that it is non–degenerate, i.e., all projectors are of rank one, which means that $R_S = \sum_r r|r\rangle\langle r|_S$. To approach the problem, let us first consider a case in which the quantum stochastic process evidently looks classical. This case is described by assuming that at each time t_ℓ, $\ell \in \{0, 1, \ldots, n\}$, the joint system–bath state can be written as

$$\rho_{SB}(t_\ell) = \sum_{r_\ell} p(r_\ell, t_\ell)|r_\ell\rangle\langle r_\ell|_S \otimes \rho_B(t_\ell|r_\ell). \tag{1.84}$$

This describes a state with classical but no quantum correlations. The system is in state $|r_\ell\rangle$ with probability $p(r_\ell, t_\ell)$ and conditioned on that the state of the bath is $\rho_B(t_\ell|r_\ell)$ on which we put no further restriction. A unique characteristic of the state (1.84) is that a projective measurement of R_S does not change it *on average*, i.e.,

$$\rho_{SB}(t_\ell) = \sum_{r_\ell} |r_\ell\rangle\langle r_\ell|_S \rho_{SB}(t_\ell)|r_\ell\rangle\langle r_\ell|_S. \tag{1.85}$$

Put differently, $\rho_{SB}(t_\ell)$ is characterized by the fact that we can find a local measurement basis (in this case $\{|r_\ell\rangle_S\}$), which has no quantum backaction, i.e., does not disturb the state. Bipartite states, which have this property, are also said to possess *zero quantum discord*. It is interesting to remark that such states allow to extend the definition (1.82) of a dynamical map, originally given only for decorrelated system–bath states of the form $\rho_{SB}(0) = \rho_S(0) \otimes \rho_B(0)$, to classically correlated cases, but in general not beyond. This is shown in the next exercise.

Exercise 1.25 Consider a system–bath state with zero quantum discord with respect to a complete set of system projectors $|j\rangle\langle j|_S$ such that

$$\rho_{SB}(0) = \sum_j |j\rangle\langle j|_S \rho_{SB}(0)|j\rangle\langle j|_S = \sum_j p_j |j\rangle\langle j|_S \otimes \rho_B(j). \tag{1.86}$$

Here, p_j is a probablity distribution and $\rho_B(j)$ the state of the bath given the state $|j\rangle\langle j|_S$ of the system. Show that the reduced system dynamics $\rho_S(t) = \mathrm{tr}_B\{U_{SB}\rho_{SB}(0)U_{SB}^\dagger\}$ is CPTP for any unitary U_{SB}. *Hint:* Show that you can write

$$\begin{aligned}&\rho_S(t) = \\ &\sum_{b,b'} \left[\sum_j \left\langle b \left| U_{SB}\sqrt{\rho_B(j)}\right| b' \right\rangle |j\rangle\langle j|_S\right] \rho_S(0) \left[\sum_k |k\rangle\langle k|_S \left\langle b' \left| \sqrt{\rho_B(k)}U_{SB}^\dagger \right| b \right\rangle\right],\end{aligned} \tag{1.87}$$

where $\{|b\rangle\}$ and $\{|b'\rangle\}$ are arbitrary bases in the bath Hilbert space and the square root of $\rho_B(j)$ is well–defined since $\rho_B(j)$ is a positive operator. Then, put eqn (1.87) into operator–sum representation.

Another consequence of the assumption (1.84) is that the projective measurement statistics of $R_S = \sum_r r|r\rangle\langle r|_S$ are classical because they satisfy the Kolmogorov consistency condition. The reader is asked to verify this in the next exercise.

Exercise 1.26 Show, assuming eqn (1.84) for all t_ℓ, that the joint probabilities (1.59) satisfy the Kolmogorov consistency condition (1.53).

While states of the form (1.84) provide a sufficient criterion to decide that $p(\mathbf{r}_n)$ cannot be distinguished from a classical stochastic process, the answer is not yet fully satisfactory for two reasons. First, deciding whether eqn (1.84) applies requires explicit knowledge about the system–bath correlations, which is usually not available in an experiment. Second, even if the system–bath state is not of the form (1.84), the resulting measurement statistics $p(\mathbf{r}_n)$ might nevertheless be indistinguishable from a classical stochastic process. We now show that this happens whenever *coherences* in the system state with respect to the basis $\{|r_\ell\rangle_S\}_{r_\ell}$ do not influence the dynamics of the *populations*.

Recall that for a given basis $\{|r\rangle\}_r$ the density matrix can always be written as

$$\rho = \sum_r \rho_{rr}|r\rangle\langle r| + \sum_{r'>r}(\rho_{rr'}|r\rangle\langle r'| + \text{h.c.}) = \begin{pmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1n} \\ \rho_{12}^{*} & \rho_{22} & & \vdots \\ \vdots & & \ddots & \rho_{n-1n} \\ \rho_{1n}^{*} & \cdots & \rho_{n-1n}^{*} & \rho_{dd} \end{pmatrix}, \tag{1.88}$$

where the diagonal elements of the matrix are called populations and the off-diagonal elements coherences. The average effect of a porjective measurement of an observable R is called a **dephasing operation**, denoted by $\mathcal{D}_R$ in the following. Its action on the previous state ρ is to delete all coherences:

$$\mathcal{D}_R\rho \equiv \sum_r |r\rangle\langle r|\rho|r\rangle\langle r| = \sum_r \rho_{rr}|r\rangle\langle r| = \begin{pmatrix} \rho_{11} & 0 & \dots & 0 \\ 0 & \rho_{22} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \dots & 0 & \rho_{dd} \end{pmatrix}. \tag{1.89}$$

We now introduce the notion of an **incoherent process**, which is supposed to capture the absence of observable effects of the coherences on the population dynamics. Namely, we call a quantum stochastic process n–incoherent (with respect to the system observable R_S), if all process tensors

$$\mathfrak{T}\left[\mathcal{D}_{R_n}, \begin{Bmatrix} \mathcal{D}_{R_{n-1}} \\ \mathcal{I}_{n-1} \end{Bmatrix}, \dots, \begin{Bmatrix} \mathcal{D}_{R_1} \\ \mathcal{I}_1 \end{Bmatrix}, \mathcal{C}_0\right] \tag{1.90}$$

are equal, where the curly bracked notation $\{\cdot\}$ signifies that we are free to choose to apply either a dephasing operation $\mathcal{D}_{R_\ell}$ or nothing (i.e., the identity operation $\mathcal{I}_\ell$) at time t_ℓ. Remember our convention to leave away the subscript S on operations that act only on the system space. Furthermore, $\mathcal{C}_0$ describes an arbitrary but fixed initial state preparation (recall Exercise 1.21). Therefore, an n–incoherent process is characterized by the fact that the populations of its output state $\rho_S(t_n|\mathcal{C}_0)$ given any initial state preparation at time t_0 are insensitive to the question whether we erased all coherences at any intermediate time step t_ℓ, $\ell \in \{1, \dots, n-1\}$, or not. Put differently, the coherences do not affect the dynamics of the populations. In the following we are only interested in processes, which are ℓ–incoherent for all $\ell \in \{1, 2, \dots, n\}$, and call them *incoherent.*

Finally, we recall that the probability to get the measurement results $r_n, \dots, r_1$ for a given state preparation $\mathcal{C}_0$ is $p(r_n, \dots, r_1|\mathcal{C}_0) = \text{tr}_S\{\mathfrak{T}[\mathcal{P}(r_n), \dots, \mathcal{P}(r_1), \mathcal{C}_0]\}$. After these preliminary considerations, we can formulate the first main result of this section, whose proof is left as an exercise.

Classicality implies incoherence. *If the hierarchy of probabilities $p(r_n, \dots, r_1|\mathcal{C}_0)$ obeys the Kolmogorov consistency condition (1.53), then the process is incoherent.*

Exercise 1.27 Prove this statement. *Hint:* Since $R_S = \sum_r r|r\rangle\langle r|_S$ is assumed to be non–degenerate, it follows that $\mathfrak{T}[\mathcal{P}(r_n), \dots, \mathcal{P}(r_1), \mathcal{C}_0] = p(r_n, \dots, r_1|\mathcal{C}_0)|r_n\rangle\langle r_n|$.

Thus, we see that the requirement of classicality as characterized by the Kolmogorov consistency condition is quite strong as it immediately implies that coherences can have no detectable effect on the populations dynamics. However, experimentally confirming the Kolmogorov consistency condition can become quite involved, whereas confirming the notion of incoherent dynamics only requires to probe the response of a system to one or multiple dephasing operations. The second main result of this section specifies under which condition incoherent dynamics are sufficient to conclude that the measurement statistics are classical.

Classicality from incoherence. *If the dynamics are Markovian, invertible, and incoherent for all preparations $\mathcal{C}_0$, then the statistics are classical for any preparation.*

To understand the notion of invertibility, recall eqn (1.79), which shows that Markovian dynamics are characterized by a set of dynamical maps $\{\mathcal{E}(t_\ell, t_k) | n \geq \ell \geq k \geq 0\}$. *Invertible* Markovian dynamics are then defined by the requirement that the dynamical maps $\mathcal{E}_{\ell,k}$ are invertible (in the usual sense of an invertible matrix), where here and in the rest of this chapter we use the abbreviation $\mathcal{E}_{\ell,k} \equiv \mathcal{E}(t_\ell, t_k)$. This puts us in a position to prove the above statement.

Using that the process is incoherent and Markovian, we confirm that

$$\mathcal{D}_{R_{\ell+1}} \mathcal{E}_{\ell+1,\ell} \mathcal{D}_{R_\ell} \mathcal{E}_{\ell,0} \mathcal{C}_0 \rho_S(t_0) = \mathcal{D}_{R_{\ell+1}} \mathcal{E}_{\ell+1,\ell} \mathcal{I}_\ell \mathcal{E}_{\ell,0} \mathcal{C}_0 \rho_S(t_0) \tag{1.91}$$

must hold for all preparations $\mathcal{C}_0$. Since the dynamics are invertible, this becomes a superoperator identity: $\mathcal{D}_{R_{\ell+1}} \mathcal{E}_{\ell+1,\ell} \mathcal{D}_{R_\ell} = \mathcal{D}_{R_{\ell+1}} \mathcal{E}_{\ell+1,\ell}$. By multiplying this equation with $\mathcal{P}(r_{\ell+1})$, we obtain the relation

$$\sum_{r_\ell} \mathcal{P}(r_{\ell+1}) \mathcal{E}_{\ell+1,\ell} \mathcal{P}(r_\ell) = \mathcal{P}(r_{\ell+1}) \mathcal{E}_{\ell+1,\ell}, \tag{1.92}$$

where we used that $\mathcal{D}_{R_\ell} = \sum_{r_\ell} \mathcal{P}(r_\ell)$. Based on this, it is easy to show that the Kolmogorov consistency condition is satisfied:

$$\begin{aligned}\sum_{r_\ell} p(r_n, \ldots, r_1 | \mathcal{C}_0) &= \sum_{r_\ell} \mathrm{tr}_S \left\{ \mathcal{P}(r_n) \mathcal{E}_{n,n-1} \ldots \mathcal{P}(r_{\ell+1}) \mathcal{E}_{\ell+1,\ell} \mathcal{P}(r_\ell) \ldots \mathcal{E}_{1,0} \mathcal{C}_0 \rho_S(t_0) \right\} \\ &= \mathrm{tr}_S \left\{ \mathcal{P}(r_n) \mathcal{E}_{n,n-1} \ldots \mathcal{P}(r_{\ell+1}) \mathcal{E}_{\ell+1,\ell} \mathcal{I}_\ell \ldots \mathcal{E}_{1,0} \mathcal{C}_0 \rho_S(t_0) \right\} \\ &= p(r_n, \ldots \cancel{r_\ell}, \ldots, r_1 | \mathcal{C}_0). \end{aligned} \tag{1.93}$$

This concludes the proof.

The question remains whether it is possible to relax some conditions above, for instance, by looking at Markovian dynamics, which are incoherent only for some preparations $\mathcal{C}_0$ or not invertible. The following exercise excludes this possibility.

Exercise 1.28 Find examples of non-classical processes, which are Markovian and incoherent with respect to a restricted set of preparations $\mathcal{C}_0$ or not invertible. *Hint:* It suffices to consider the unitary evolution of a two-level system prepared in the maximally mixed state $\rho_S(t_0) = (|0\rangle\langle 0| + |1\rangle\langle 1|)/2$.

Finally, we briefly discuss the case of degenerate observables $R_S = \sum_r r\Pi_S(r)$, where some projectors $\Pi_S(r)$ have a rank larger than one. One easily confirms that the proof above made no use of the fact that the observable is non–degenerate. Thus, classicality continues to follow from incoherence under the assumptions spelled out above, even for degenerate observables. On the other hand, our first main result that classicality implies incoherence can break down. The reason is that coherence could affect the system state in the degenerate subspaces with respect to R_S, whereas the probabilities $p(r_n, \dots, r_1|\mathcal{C}_0)$ do not reveal any information about these subspaces.

Classical Markov Processes

Our exposition of quantum stochastic and Markov processes would be quite incomplete without mentioning the definition of a classical Markov processes.

Classical Markov process. *We call a classical stochastic process described by probabilities* $p(\mathbf{r}_n)$ *on a set of times* $\{t_0, t_1, \dots, t_n\}$ *Markovian if*

$$\boxed{p(r_n|\mathbf{r}_{n-1}) \equiv \frac{p(\mathbf{r}_n)}{p(\mathbf{r}_{n-1})} = p(r_n|r_{n-1}),} \tag{1.94}$$

holds for all joint probabilities in the hierarchy, i.e., for all subsets of times $T \subset \{t_0, t_1, \dots, t_n\}$.

Equation (1.94) encodes the fact that the conditional probability $p(r_n|\mathbf{r}_{n-1})$ of a Markov process depends only on the *last* measurement result r_{n-1}, but not on previous ones $r_{n-2}, \dots, r_0$. It is important to note that we assumed in our definition the probabilities $p(\mathbf{r}_n)$ to actually describe a *classical* stochastic process, i.e., we assumed the Kolmogorov consistency condition (1.53) to hold. The description of processes satisfying only eqn (1.94) but *not* the consistency condition is more involved and differs significantly from the standard theory of classical Markov processes. An example for such a kind of process is an isolated, unitarily evolving system interrupted by rank–1 projective measurements. This process satisfies eqn (1.94), and it is also a *quantum Markov* process (recall Exercise 1.23), but the probabilities $p(\mathbf{r}_n)$ in general violate the consistency condition because the projective measurements disturb the dynamics.

The connection between a quantum Markov process and a classical Markov process is indeed subtle. At least, however, a statement analogous to eqn (1.79) holds also for classical Markov processes. Namely, using the definition of conditional probabilities, we can always write the joint probability $p(\mathbf{r}_n)$ as

$$\begin{aligned} p(\mathbf{r}_n) &= \frac{p(\mathbf{r}_n)}{p(\mathbf{r}_{n-1})} \frac{p(\mathbf{r}_{n-1})}{p(\mathbf{r}_{n-2})} \cdots \frac{p(\mathbf{r}_1)}{p(r_0)} p(r_0) \\ &= p(r_n|\mathbf{r}_{n-1}) p(r_{n-1}|\mathbf{r}_{n-2}) \dots p(r_1|r_0) p(r_0). \end{aligned} \tag{1.95}$$

Now, for a classical Markov process we can simplify that to

$$p(\mathbf{r}_n) = p(r_n|r_{n-1}) p(r_{n-1}|r_{n-2}) \dots p(r_1|r_0) p(r_0), \tag{1.96}$$

where the conditional probabilities $p(r_\ell|r_k)$ play an analogous role to the dynamical maps $\mathcal{E}_{\ell,k}$: they also propagate the system state, now described by a vector of probabilities $p(r_k)$, forward in time. In the next chapter we will often use these conditional probabilities $p(r_\ell|r_k)$ and call them *transition matrices.*

Now, the third and last main result of this section establishes the connection between quantum stochastic processes, classical stochastic processes and the Markov property (1.94).

Classical from quantum Markovianity. *Consider a quantum stochastic process, which yields for a fixed set of interventions the probabilities $p(\mathbf{r}_n)$. It is true that:*

1. *If the quantum stochastic process is Markovian and if all interventions are causal breaks, then the probabilities $p(\mathbf{r}_n)$ satisfy the Markov property (1.94).*
2. *If we add to the assumptions of point (1.) that the probabilities $p(\mathbf{r}_n)$ also satisfy the Kolmogorov consistency condition, then these probabilities describe a classical Markov process.*

If these statements are clear and understandable to the reader, you have successfully mastered the entire first chapter of this book. If there is some scepticism left, it helps to try to prove them.

Exercise 1.29 Prove the statement above. *Hint:* For the first part it is helpful to note the following equivalent statement: *If for some set of interventions, which are causal breaks, the probabilities $p(\mathbf{r}_n)$ do not satisfy the Markov property (1.94), then the quantum stochastic process is non–Markovian.*

Further reading

1. The first section should be part of the standard quantum mechanics curriculum.

2. Introducing open quantum systems by partitioning an isolated 'universe' into a system and an environment is also fairly standard. Indeed, this idea is already inherent to thermodynamics itself and therefore, it was used long before the advent of microscopic system–bath theories. Which particular assumption and gauge is implied by splitting the Hilbert space of the universe into a *tensor product* of a system and a bath Hilbert space is discussed by Stokes and Nazir (2020). The picture on the right in Fig. 1.1 was taken from Josefsson *et al.* (2018).

3. In our discussion about equilibrium states of open quantum systems we left open how to justify the use of ensembles at first place given that any isolated quantum system in some pure state. Readers interested in this non–trivial question can find a large body of recent reviews on this topic (Gemmer *et al.*, 2004; D'Alessio *et al.*, 2016; Borgonovi *et al.*, 2016; Gogolin and Eisert, 2016; Goold *et al.*, 2016; Deutsch, 2018; Mori *et al.*, 2018). Furthermore, readers interested in a proof of Poincaré's recurrence theorem can look, e.g., at the work of Wallace (2015). Calculating the exact Poincaré recurrence time for a given model is very hard, but estimates can be found at various places (Reimann, 2008; Venuti, 2015). The Hamiltonian of mean force was first discussed almost hundred years ago by Onsager, Kirkwood, and others, and the concept is widely used in chemical physics (Roux and Simonson, 1999), but the terminology has not yet become standard in the wider physics community. The Caldeira–Leggett Hamiltonian, which we introduced in Exercise 1.2 and which we will meet from time to time again, became a standard model to describe the dynamics of open quantum systems, for in–depth treatments see, e.g., the books of Nitzan (2006) and Weiss (2008).

4. Section 1.4 reviewed well–known results covered in greater detail elsewhere (Nielsen and Chuang, 2000; Holevo, 2001; Wiseman and Milburn, 2010; Jacobs, 2014).

5. The content of Section 1.5 is reviewed at many places in greater detail (Nielsen and Chuang, 2000; Holevo, 2001; Wiseman and Milburn, 2010; Jacobs, 2014). An early influential book was written by Kraus (1983). For this reason, the operators K_α appearing in eqn (1.45) are sometimes called *Kraus operators* and the entire operation is sometimes called a *Kraus map*. We did not follow this terminology here as those maps and operators were studied already earlier. In general, the historical development of the field is quite intertwined involving many mathematicians and physicists (re)discovering the same results from different perspectives. The proof of the operator–sum representation can be found, e.g., in the book of Nielsen and Chuang (2000) (Theorem 8.1 therein). This proof makes use of the Choi–Jamiołkowski isomorphism, an elegant mathematical construction reviewed also in Appendix B. For a proof of the unitary dilation theorem see Nielsen and Chuang (2000) or Holevo (2001).

6. The field of classical stochastic processes is covered in many textbooks, but only a very few prove the extension theorem mentioned in Section 1.6, see, e.g., the original work of Kolmogorov (2018). A standard book covering many aspects of classical causal modeling was written by Pearl (2009).

7. In contrast to the previous sections, the treatment of quantum stochastic processes as done in Section 1.7 has not yet become standard material, although the basic idea is quite old (Lindblad, 1979). However, only recently this approach regained independent attention from many different directions, see Milz and Modi (2021) for a detailed introduction citing many references. The generalized extension theorem for quantum stochastic processes is discussed by Milz *et al.* (2020*b*). The generalized Bloch representation (1.66) is due to Byrd and Khaneja (2003).

8. The definition of a quantum Markov process has caused some debate, see Li *et al.* (2018) for the latest review of many different perspectives. Our definition coincides with the one of Pollock *et al.* (2018*b*). It has the advantage that it reduces to the conventional Markov definition for a classical stochastic process in its respective limit. In fact, for classical systems it coincides with the *causal Markov condition* of classical causal models (Pearl, 2009).

9. In the first part of the last section we followed Strasberg and Díaz (2019) and Milz *et al.* (2020*a*). Putting multi–time statistics aside, the influence of initial system–bath correlations as quantified by quantum discord on the definition of a dynamical map (Exercise 1.25) was investigated by Rodríguez-Rosario *et al.* (2008).

Appendix A

Concepts from Information Theory

We briefly review some basic concepts of classical and quantum information theory and afterwards present some useful, advanced theorems without proof. Below, we denote by $d = \dim \mathcal{H}$ the dimension of the Hilbert space of the system or, in the classical case, d denotes the dimension of the space in which the vector of probabilities $\boldsymbol{p} \in \mathbb{R}^d$ lives. Furthermore, $d_{X,Y,\dots}$ refers to the dimension of a subsystem $X, Y, \dots$.

A.1 Basic Concepts

Classical information theory

We define the **Shannon entropy** of a probability distribution $\{p_x\}$ with probabillity vector $\boldsymbol{p}$ as

$$S_{\text{Sh}}(\{p_x\}) = S_{\text{Sh}}(\boldsymbol{p}) \equiv -\sum_x p_x \ln p_x. \tag{A.1}$$

Note that we use the natural logarithm in the definition (measuring entropy in 'nats'), whereas in information theory it is customary to use the logarithm $\log_2$ with respect to base 2 (measuring entropy in 'bits' $= \ln 2$ nats ≈ 0.69 nats).

If the state of a physical system X is described by probabilities $\{p_x\}$, then the Shannon entropy can be interpreted as the *information content* that the system has to offer to an external observer upon a measurement of the system. Switching perspective, from the observer's point of view the Shannon entropy can be interpreted as the *uncertainty* one has about a system X *before* measuring it. There is no uncertainty about a system (or the system contains no information for the observer, respectively) if the system is for sure in the state x^*: $p_x = \delta_{x,x^*}$. Then, it follows from the convention $0 \ln 0 \equiv 0$, which can be justified by the limit $\lim_{x\searrow 0} x \ln x = 0$, that $S_{\text{Sh}}(\{\delta_{x,x^*}\}) = 0$. Furthermore, one can verify the following four properties:

(1) The Shannon entropy is bounded from above and below: $0 \le S_{\text{Sh}}(\boldsymbol{p}) \le \ln d$.

(2) The Shannon entropy $S_{\text{Sh}}(\{p_x\})$ is continuous in each p_x.

(3) If $S_{\text{Sh}}(d)$ denotes the Shannon entropy of the uniform distribution $p_x = 1/d$ for all x, then $S_{\text{Sh}}(d) < S_{\text{Sh}}(d+1)$. Thus, the uncertainty of a system always increases if it can be in more different states about which we have no prior information.

(4) Let us divide the system X into 'subsystems' $X = \bigoplus_\alpha X_\alpha$ and decompose the probabilities as $p_x = p_{x|\alpha} P_\alpha$, where P_α is the probability to be in subsystem X_α and $p_{x|\alpha}$ is the conditional probability to be in x given α. Then, the Shannon entropy 'additively' decomposes as

$$S_{\mathrm{Sh}}(\{p_x\}) = S_{\mathrm{Sh}}(\{P_\alpha\}) + \sum_\alpha P_\alpha S_{\mathrm{Sh}}(\{p_{x|\alpha}\}). \tag{A.2}$$

The above properties can be regarded as natural properties that a measure of uncertainty or information should satisfy, but in fact, Shannon *deduced* eqn (A.1) (up to an overall positive factor) from the properties (2), (3) and (4).

Furthermore, there are a number of important information theory concepts related to Shannon entropy. First, we define the **classical relative entropy** between two probability vectors $\boldsymbol{p}$ and $\boldsymbol{q}$ of the same system X as

$$D(\boldsymbol{p}|\boldsymbol{q}) \equiv \sum_x p_x \ln \frac{p_x}{q_x} \geq 0. \tag{A.3}$$

The positivity of relative entropy can be derived from properties that we discuss at the beginning of Section 4.6; namely, that the convex function $f(x) \equiv x \ln x$ satisfies Jensen's inequality (4.117). Furthermore, eqn (A.3) can diverge whenever $q_x = 0$ but $p_x \neq 0$. Since $D(\boldsymbol{p}|\boldsymbol{q}) = 0$ if and only if $\boldsymbol{p} = \boldsymbol{q}$, relative entropy can be interpreted as measuring the 'distance' or 'difference' between the two probability vectors $\boldsymbol{p}$ and $\boldsymbol{q}$, i.e., the larger $D(\boldsymbol{p}|\boldsymbol{q})$ the easier it is to tell them apart. Nevertheless, relative entropy is not a metric in the mathematical sense because it is not symmetric: $D(\boldsymbol{p}|\boldsymbol{q}) \neq D(\boldsymbol{q}|\boldsymbol{p})$.

Another important concept is the **classical mutual information**, which is defined for a bipartite system XY with joint probability vector $\boldsymbol{p}_{XY}$ as

$$I(\boldsymbol{p}_{XY}) \equiv S_{\mathrm{Sh}}(\boldsymbol{p}_X) + S_{\mathrm{Sh}}(\boldsymbol{p}_Y) - S_{\mathrm{Sh}}(\boldsymbol{p}_{XY}) = \sum_{x,y} p_{x,y} \ln \frac{p_{x,y}}{p_x p_y}, \tag{A.4}$$

where $\boldsymbol{p}_X$ and $\boldsymbol{p}_Y$ describe the marginal distributions of $\boldsymbol{p}_{XY}$. We remark that we often write $I_{X:Y} \equiv I(\boldsymbol{p}_{XY})$ if the probability vector $\boldsymbol{p}_{XY}$ is clear from context. Classical mutual information is bounded from above and below by

$$0 \leq I(\mathbf{p}_{XY}) \leq \ln \min\{d_X, d_Y\}. \tag{A.5}$$

The first inequality follows after noting that $I(\boldsymbol{p}_{XY}) = D(\boldsymbol{p}_{XY}|\boldsymbol{p}_X \otimes \boldsymbol{p}_Y)$, which also establishs the fact that mutual information quantifies the *correlations* contained in $\boldsymbol{p}_{XY}$. To derive the second inequality, we suppose that $d_X \leq d_Y$ without loss of generality. Next, we write

$$I(\boldsymbol{p}_{XY}) = S_{\mathrm{Sh}}(\{p_x\}) - \sum_y p_y S_{\mathrm{Sh}}(\{p_{x|y}\}). \tag{A.6}$$

The claim is now that there exists a legitimate probability distribution $p_{x,y}$, which (simultaneously) maximizes the first term and minimizes the second term in eqn (A.6). To see this, consider any injective function $f : X \to Y$ (note that this step requires $d_X \leq d_Y$) and define $\tilde{p}_{x,y} \equiv \delta_{y,f(x)}/d_X$. This gives $\tilde{p}_{x|y} = \delta_{x,f^{-1}(y)}$ for all x, y such that $f(x) = y$. For all y for which no x exists such that $f(x) = y$, we have $\tilde{p}_y = 0$. In either case, the second term in eqn (A.6) vanishs. Thus, this distribution satisfies $I(\tilde{\boldsymbol{p}}_{XY}) = \ln d_X$.

Quantum information theory

The subsequent quantum concepts in information theory follow from the classical case by analogy. We start with the **von Neumann entropy**, which is defined as

$$S_{\mathrm{vN}}(\rho) \equiv -\mathrm{tr}\{\rho \ln \rho\} = -\sum_k \lambda_k \ln \lambda_k = S_{\mathrm{Sh}}(\{\lambda_k\}), \tag{A.7}$$

where we used the spectral decomposition of $\rho = \sum_k \lambda_k |k\rangle\langle k|$ at the end. The von Neumann entropy of a quantum system is therefore measures the *classical* uncertainty an external observer has about the state of the system. Equivalently, the classical information content of a system in state ρ equals its von Neumann entropy. The von Neumann entropy has a couple of elementary properties, which we will occasionally use in this book and which we state here without proof.

1. The von Neumann entropy is bounded from above and below: $0 \leq S_{\mathrm{vN}}(\rho) \leq \ln d$.
2. The von Neumann entropy is invariant under any unitary transformation U: $S_{\mathrm{vN}}(U\rho U^\dagger) = S_{\mathrm{vN}}(\rho)$.
3. For a bipartite quantum system in a state ρ_{XY} with marginal states $\rho_{X/Y} = \mathrm{tr}_{Y/X}\{\rho_{XY}\}$ we have

   $$S_{\mathrm{vN}}(\rho_{XY}) \leq S_{\mathrm{vN}}(\rho_X) + S_{\mathrm{vN}}(\rho_Y) \tag{A.8}$$

   with equality if and only if $\rho_{XY} = \rho_X \otimes \rho_Y$. Equation (A.8) is known as **subadditivity** of von Neumann entropy.
4. The von Neumann entropy is concave, i.e., for any convex combination $\sum_j \lambda_j \rho_j$ of density matrices ρ_j with weights $\lambda_j \geq 0$ such that $\sum_j \lambda_j = 1$,

   $$\sum_j \lambda_j S_{\mathrm{vN}}(\rho_j) \leq S_{\mathrm{vN}}\left(\sum_j \lambda_j \rho_j\right). \tag{A.9}$$

Further concepts are directly related to the von Neumann entropy. First, the **quantum relative entropy** between two states ρ and σ is defined as

$$D(\rho|\sigma) \equiv \mathrm{tr}\{\rho(\ln \rho - \ln \sigma)\} \geq 0. \tag{A.10}$$

Its positivity follows from *Klein's inequality*, which we do not discuss or derive here. Furthermore, $D(\rho|\sigma) = 0$ if and only if $\rho = \sigma$. As in the classical case, relative entropy measures the statistical difference between two quantum states. For instance, let $\sigma = I/d$ be the maximally mixed state. Then,

$$D\left(\rho \middle| \frac{I}{d}\right) = \ln d - S_{\mathrm{vN}}(\rho), \tag{A.11}$$

which is intuitively appealing: the larger the uncertainty about ρ, the less it can be distinguished from a maximally mixed or uninformative state. However, since the relative entropy is not symmetric, $D(\rho|\sigma) \neq D(\sigma|\rho)$, it does not define a metric.

Furthermore, it diverges whenever the support of ρ is not contained in the support of σ as in the classical case. Like the von Neumman entropy, relative entropy is invariant under any unitary transformation U: $D(U\rho U^\dagger|U\sigma U^\dagger) = D(\rho|\sigma)$. In contrast to von Neumann entropy, it is not concave but convex: $D(\rho|\sigma) \leq \sum_j \lambda_j D(\rho_j|\sigma_j)$ for convex combinations $\rho = \sum_j \lambda_j \rho_j$ and $\sigma = \sum_j \lambda_j \sigma_j$.

A second important concept is the **quantum mutual information** of a bipartite state ρ_{XY}:

$$I(\rho_{XY}) \equiv S_{\text{vN}}(\rho_X) + S_{\text{vN}}(\rho_Y) - S_{\text{vN}}(\rho_{XY}) \geq 0. \tag{A.12}$$

We also write $I_{X:Y} \equiv I(\rho_{XY})$ if the state ρ_{XY} is clear from context. Furthermore, positivity follows from subadditivity, eqn (A.8), or after noting that $I(\rho_{XY}) = D(\rho_{XY}|\rho_X \otimes \rho_Y)$, which shows that quantum mutual information measures the correlations between X and Y as in the classical case. However, in contrast to the classical case, cf. eqn (A.5), quantum mutual information is upper bounded by (note the factor 2)

$$I(\rho_{XY}) \leq 2 \ln \min\{d_X, d_Y\}. \tag{A.13}$$

This implies that quantum correlations can be twice as strong as classical correlations. To prove the bound, we need to find again a state that simultaneously maximizes the first two terms and minimizes the last term in eqn (A.12). At least in the case that $d_X = d_Y$, it is easy to see that these conditions are satisfied by a *maximally entangled state* $\rho_{XY} = |\psi\rangle\langle\psi|_{XY}$ with $|\psi\rangle_{XY} = \sum_{k=1}^{d_X} |k\rangle_X|k\rangle_Y/\sqrt{d_X}$. Here, $|k\rangle_X$ ($|k\rangle_Y$) denotes an arbitrary set of orthonormal states in $\mathcal{H}_X$ ($\mathcal{H}_Y$).

It is interesting to note that we used a *pure* state to maximize the mutual information in the quantum case, whereas in the classical case we used a *mixed* state. In fact, the classical mutual information of any classical pure state, which is always of the form $p_{x,y} = \delta_{x,x^*}\delta_{y,y^*}$ for some $x^* \in X$ and $y^* \in Y$, is *zero*—in strong contrast to the quantum case. The origin of this striking difference between the quantum and classical world comes from the fact that the reduced state $\rho_X = \text{tr}_Y\{|\psi\rangle\langle\psi|_{XY}\}$ of a joint pure state is in general not pure anymore.

Finally, we will sometimes also need to quantify correlations of an N–partite state $\rho_{12\dots N}$ with $N > 2$. This can be done in many different ways and in this book we will sometimes encounter the **total information**

$$I_{\text{tot}}(\rho_{12\dots N}) \equiv \sum_{i=1}^{N} S_{\text{vN}}(\rho_i) - S_{\text{vN}}(\rho_{12\dots N}). \tag{A.14}$$

This quantity also has a variety of properties. A few of them are explored in the next exercise.

Exercise A.1 Show that the total information can be written in the two alternative forms

$$\begin{aligned} I_{\text{tot}}(\rho_{12\dots N}) &= D(\rho_{12\dots N}|\rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_N) \\ &= I_{1:2} + I_{12:3} + \cdots + I_{12\dots N-1:N}. \end{aligned} \tag{A.15}$$

Notice that eqn (A.15) implies that the total information is positive.

A.2 Advanced Inequalities

We here state a couple of useful inequalities without proof, which will be used at certain points in this book and which are good to know in general. Since not all of these inequalities have a (simple memorable) name, we label them as ‘Theorem A.1,’ ‘Theorem A.2’, etc. for later reference in the main text.

The first inequality bounds the entropy of a mixture of quantum states and should be compared with eqn (A.9):

Theorem A.1 *Let* $\rho = \sum_n \lambda_n \rho_n$ *be a convex combination of density matrices. Then,*

$$S_{\mathrm{vN}}(\rho) \leq \sum_n \lambda_n S_{\mathrm{vN}}(\rho_n) + S_{\mathrm{Sh}}(\boldsymbol{\lambda}). \tag{A.16}$$

Equality holds if and only if the ρ_n *have support on mutually orthogonal subspaces.*

Closely related to the previous theorem is also the next one. To state it, we need the notion of a positive operator–valued measure (POVM) from Section 1.4.

Theorem A.2 *Let* $\{P_n\}$ *be a set of positive operators such that* $\{P_n^2\}$ *is a POVM (i.e.,* $\sum_n P_n^2 = I$*). Then, for any state* ρ*,*

$$S_{\mathrm{vN}}(\rho) \leq S_{\mathrm{vN}}\left(\sum_n P_n \rho P_n\right). \tag{A.17}$$

The content of the last two theorems can be neatly summarized in one equation. Defining $\rho_n \equiv P_n \rho P_n / \lambda_n$ with $\lambda_n \equiv \mathrm{tr}\{P_n^2 \rho\}$, we obtain

$$S_{\mathrm{vN}}(\rho) \leq S_{\mathrm{vN}}\left(\sum_n \lambda_n \rho_n\right) \leq \sum_n \lambda_n S_{\mathrm{vN}}(\rho_n) + S_{\mathrm{Sh}}(\boldsymbol{\lambda}). \tag{A.18}$$

Exercise A.2 Show that projective measurements increase the von Neumann entropy of the *average* post–measurement state.

The next result is known as **monotonicity of relative entropy**. If you are not yet familiar with the notion of CPTP maps, postpone the rest of this section until you are familiar with the content of Section 1.5.

Theorem A.3 *For any CPTP map* $\mathcal{C}$ *and all states* ρ, σ *we have*

$$\boxed{D(\mathcal{C}\rho|\mathcal{C}\sigma) \leq D(\rho|\sigma).} \tag{A.19}$$

This theorem is so important that we put a box around it: It appears in many microscopic derivations of the second law in the main text. Some insights into the derivation and the use of it can be gained from the following exercise.

Exercise A.3 Consider two arbitrary bipartite states ρ_{AB} and σ_{AB} and show that eqn (A.19) implies

$$D(\rho_A|\sigma_A) \leq D(\rho_{AB}|\sigma_{AB}). \tag{A.20}$$

Then, use eqn (A.20) to derive eqn (A.19) in general. *Hint:* Remember the unitary dilation theorem, eqn (1.49).

We also use the classical counterpart of Theorem A.3 in this book, for which we need the notion of a stochastic matrix T defined by the requirement that $T_{x,x'} \geq 0$ for all x, x' and $\sum_x T_{x,x'} = 1$ for all x'.

Theorem A.4 *For any stochastic matrix T and any two probability distributions $\boldsymbol{p}$ and $\boldsymbol{q}$ we have*

$$D(T\boldsymbol{p}|T\boldsymbol{q}) \leq D(\boldsymbol{p}|\boldsymbol{q}). \tag{A.21}$$

Finally, a useful theorem to bound the quantum relative entropy is the following.

Theorem A.5 *For arbitrary states ρ and σ acting on a Hilbert space with dimension d we have*

$$D(\rho|\sigma) \geq \frac{[S_{\text{vN}}(\rho) - S_{\text{vN}}(\sigma)]^2}{3(\ln d)^2}. \tag{A.22}$$

Further reading

The fields of classical and quantum information theory are enormous and better covered elsewhere (Cover and Thomas, 1991; Nielsen and Chuang, 2000). That they are intimately linked to the field of statistical mechanics was, in some sense, even noticed before the advent of information theory. The origin of the word entropy goes back to Clausius and some of the definitions given above were already used by Boltzmann, Gibbs and others.

The proof of Theorem A.1 can be looked up in the book of Nielsen and Chuang (2000) (Theorem 11.10 therein) and the proof of Theorem A.2 can be found in the book of Jacobs (2014) (Theorem 11 therein). Whereas the proofs of the previous theorems are not too complicated, the proof of Theorem A.3 is involved (Lindblad, 1975; Ruskai, 2002). The last Theorem A.5 was discovered recently by Reeb and Wolf (2015).

Appendix B

Superoperators

Maps that map matrices onto matrices (or operators onto operators) are often called **superoperators** and we denote them by calligraphic letters such as $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}\dots$ throughout this book. The goal of this appendix is to show that superoperators are simply 'big matrices' and to provide some background information useful for practical calculations and numerical implementations.

Recall that, whenever you have a vector space V and a map $\Phi : V \to V$ acting linearly on it, then this map can be represented by a matrix. To see this, consider an arbitrary vector $\mathbf{v} = \sum_i v_i \mathbf{e}_i \in V$ decomposed in an arbitrary basis $\{\mathbf{e}_i\}$ of that vector space. Since Φ acts linearly, we have

$$\Phi(\mathbf{v}) = \sum_i v_i \Phi(\mathbf{e}_i). \tag{B.1}$$

The components of $\Phi(\mathbf{v}) \in V$ can be read off by taking the scalar product

$$\Phi(\mathbf{v})_j \equiv \langle \mathbf{e}_j | \Phi(\mathbf{v}) \rangle = \sum_i v_i \langle \mathbf{e}_j | \Phi(\mathbf{e}_i) \rangle \equiv \sum_i \hat{\Phi}_{ji} v_i. \tag{B.2}$$

In the last step we introduced the matrix $\hat{\Phi}$ with components $\hat{\Phi}_{ji} = \langle \mathbf{e}_j | \Phi(\mathbf{e}_i) \rangle$. In order to distinguish it from the abstract map Φ and in order to emphasize that the representation of $\hat{\Phi}$ depends on the chosen basis, we put a 'hat' on it. In that basis the action of Φ is given by ordinary matrix multiplication and we identify $\Phi(\mathbf{v}) \leftrightarrow \hat{\Phi}\mathbf{v}$.

Now, the same recipe can be also applied to superoperators since the set of complex $d \times d$ matrices (where d equals the dimension of the underlying Hilbert space in quantum mechanical applications) forms a vector space. All what we have to do is to fix a basis and a scalar product for the vector space of complex $d \times d$ matrices. Below, we will review two popular choices: one is typically used for numerical manipulations, whereas the other has additional mathematical and structural advantages.

B.1 Numerically Convenient Superoperator Mapping

For the first choice consider an arbitrary matrix ρ written in some basis $\{|k\rangle\}$ as

$$\rho = \sum_{k,l} \rho_{kl} |k\rangle\langle l|. \tag{B.3}$$

Now, we wish to map the set of matrix coefficients $\{\rho_{kl}\}$ to a vector, a procedure also known as **vectorization**. One way to do so is offered by identifying the basis element

$|k\rangle\langle l|$ in the space of matrices with the tensor product of the two vectors $|k\rangle$ and $|l\rangle^*$. Here, the star denotes complex conjugation in case that $|l\rangle$ has complex coefficients. This choice turns out to be convenient, but other choices are possible too. Henceforth, we identify $|k\rangle\langle l| \leftrightarrow |k\rangle \otimes |l\rangle^* \equiv |kl\rangle\rangle$, where we used a 'double–ket' notation to denote vectorized operators. Thus, we identify

$$\rho \leftrightarrow |\rho\rangle\rangle = \sum_{k,l} \rho_{kl} |kl\rangle\rangle = \sum_{k,l} \rho_{kl} |k\rangle \otimes |l\rangle^*. \tag{B.4}$$

The dual vectors $\langle\langle kl| = \langle k| \otimes \langle l|^* = (|k\rangle \otimes |l\rangle^*)^\dagger$, denoted by a 'double–bra,' are constructed as usual by taking the conjugate transpose: $\langle\langle \rho| = \sum_{k,l} \rho^*_{kl} \langle k| \otimes \langle l|^*$.

Next, we introduce a scalar product $(\rho|\sigma)$ between two matrices ρ and σ (assumed to be of equal size) by defining

$$(\rho|\sigma) \equiv \mathrm{tr}\{\rho^\dagger \sigma\}. \tag{B.5}$$

This scalar product is known as the Frobenius or Hilbert–Schmidt scalar product.

Exercise B.1 Show that $(\rho|\sigma) = \langle\langle \rho|\sigma\rangle\rangle$, where $|\rho\rangle\rangle$ and $|\sigma\rangle\rangle$ are the vectorized matrices introduced above and $\langle\langle \rho|\sigma\rangle\rangle$ denotes the usual scalar product of two complex vectors. Next, introduce the vector $|I\rangle\rangle \equiv \sum_k |k\rangle \otimes |k\rangle^*$. Show that $|I\rangle\rangle$ is the vectorization of the identity matrix I. Show also that the trace can be written in superoperator space as $\langle\langle I|A\rangle\rangle = \mathrm{tr}\{A\}$, where A is an arbitrary matrix.

In order to use ordinary matrix calculus for superoperators, we need to know the matrix representation $\hat{\mathcal{A}}$ of an arbitrary superoperator $\mathcal{A}$ with respect to the above chosen basis. For this purpose we use the fact that the action of every superoperator $\mathcal{A}$ can be written as

$$\mathcal{A}\rho = \sum_k X_k \rho Y_k \tag{B.6}$$

for some set of (not further specified) matrices $\{X_k\}$ and $\{Y_k\}$. The proof of this statement follows from our considerations below as we discuss later. Consequently, in order to write $\mathcal{A}$ as a matrix $\hat{\mathcal{A}}$, we need to know how to represent the operation $X\rho Y$ for arbitrary X and Y as a matrix. To this end, we look at its matrix elements:

$$\begin{aligned}(X\rho Y)_{mn} &= \sum_{k,l} \rho_{kl} \langle m|(X|k\rangle)\langle l|(Y|n\rangle) = \sum_{k,l} \rho_{kl} \langle m|(X|k\rangle)[\langle n|(Y^\dagger|l\rangle)]^* \\ &= \langle m| \otimes \langle n|^* X \otimes Y^T \sum_{k,l} \rho_{kl} |k\rangle \otimes |l\rangle^* = \langle\langle mn|\big(X \otimes Y^T|\rho\rangle\rangle\big).\end{aligned} \tag{B.7}$$

Here, a superscript T denotes the transpose of a matrix. Note that X and Y need not be Hermitian, which is the reason why we were extra careful and wrote, for instance, $\langle m|(X|k\rangle)$ to make clear on which side of the scalar product X is acting. From eqn (B.7) we then infer the following matrix representation of the superoperator $\mathcal{A}$:

$$\mathcal{A}\rho = X\rho Y \leftrightarrow \hat{\mathcal{A}} = X \otimes Y^T. \tag{B.8}$$

Obviously, the matrix representation of the superoperator in eqn (B.6) follows as $\hat{\mathcal{A}} = \sum_k X_k \otimes Y_k^T$.

Finally, we show that the concatenation of two superoperators $\mathcal{A}_2 \circ \mathcal{A}_1$ corresponds to ordinary matrix multiplication $\hat{\mathcal{A}}_2 \cdot \hat{\mathcal{A}}_1$, here explicitly denoted with a dot. We do so by considering the superoperators $\mathcal{A}_1\rho = X_1\rho Y_1$ and $\mathcal{A}_2\rho = X_2\rho Y_2$. The more general case of eqn (B.6) follows from linearity. Then, to see this, we define $\mathcal{B}\rho \equiv \mathcal{A}_2 \circ \mathcal{A}_1\rho = X_2X_1\rho Y_1Y_2$ and from eqn (B.8) it follows that

$$\hat{\mathcal{B}} = X_2X_1 \otimes (Y_1Y_2)^T = X_2X_1 \otimes Y_2^T Y_1^T = (X_2 \otimes Y_2^T)(X_1 \otimes Y_1^T) = \hat{\mathcal{A}}_2 \cdot \hat{\mathcal{A}}_1. \quad \text{(B.9)}$$

Another direct but tidious way is to confirm that for any ρ it holds that $\langle i|(\mathcal{A}_2 \circ \mathcal{A}_1\rho)|j\rangle = \sum_{k,l} \langle\langle ij|\hat{\mathcal{A}}_2|kl\rangle\rangle\langle\langle kl|\hat{\mathcal{A}}_1|\rho\rangle\rangle$.

Let us now return to eqn (B.6) by going the reverse way. We saw that any superoperator $\mathcal{A}$ can be represented by a matrix $\hat{\mathcal{A}}$. If we denote by $\{B_k\}$ a basis for the vector space of $d \times d$ matrices on which $\mathcal{A}$ acts, then the space of $d^2 \times d^2$ matrices $\hat{\mathcal{A}}$ is spanned by the basis $\{B_k \otimes B_l^T\}$. In particular, any matrix representation of the superoperator $\mathcal{A}$ can be expanded as

$$\hat{\mathcal{A}} = \sum_{k,l} a_{kl} B_k \otimes B_l^T \quad \text{(B.10)}$$

for some complex coefficients a_{kl}. It follows from our representation (B.8) that the corresponding superoperator $\mathcal{A}$ reads

$$\mathcal{A}\rho = \sum_{k,l} a_{kl} B_k \rho B_l, \quad \text{(B.11)}$$

which is of the general form (B.6) if we define $X_k \equiv B_k$ and $Y_k \equiv \sum_l a_{kl} B_l$.

While the above exposition provides all the necessary tools to deal with superoperators numerically, the devil is (as usual) in the detail and simply requires further practice. As a first lesson the reader is therefore asked to confirm the following results.

Exercise B.2 An important superoperator in quantum mechanics results from considering the time evolution of an isolated system, which is given by $\mathcal{U}\rho \equiv U\rho U^\dagger$ for some unitary matrix U. According to the above construction, the matrix representation of $\mathcal{U}$ is given by $\hat{\mathcal{U}} = U \otimes U^*$. Show that $\hat{\mathcal{U}}$ is unitary in the usual sense of $\hat{\mathcal{U}} \cdot \hat{\mathcal{U}}^\dagger = \hat{\mathcal{U}}^\dagger \cdot \hat{\mathcal{U}} = \hat{\mathcal{I}}$, where $\hat{\mathcal{I}} = I \otimes I$ is the identity matrix in superoperator space. On the other hand, according to the definitions (i) and (i') of Section 1.5 the map $\mathcal{U}\rho \equiv U\rho U^\dagger$ is CP. Show that this does *not* imply that the matrix $\hat{\mathcal{U}}$ is positive.

B.2 The Choi–Jamiołkowski Isomorphism

We now consider another way to represent superoperators by matrices, which somehow reverses the properties found out in the foregoing exercise. This representation plays an outstanding role in mathematical physics and is typically refered to as the Choi–Jamiołkowski isomorphism.

To introduce it, let $\mathcal{A}$ be a superoperator acting on quantum states ρ_1 defined over a Hilbert space $\mathcal{H}_1$. Next, we consider the tensor product space $\mathcal{H}_1 \otimes \mathcal{H}_0$ where $\mathcal{H}_0 = \mathcal{H}_1$ is just a copy of the original Hilbert space. It turns out, however, to be convenient to use a different index ‘0’ instead of ‘1’ in the notation. A central role in the following is played by the non–normalized maximally entangled state

$$|\psi^+\rangle \equiv \sum_i |i\rangle \otimes |i\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_0, \tag{B.12}$$

where $\{|i\rangle\}$ is an arbitrary orthonormal basis in $\mathcal{H}_1$ or $\mathcal{H}_0$, respectively. The vectorization procedure for an arbitrary operator X_1 acting on $\mathcal{H}_1$ in the Choi–Jamiołkowski isomorphism is accomplished via the mapping

$$|X\rangle\rangle \equiv (X_1 \otimes I_0)|\psi^+\rangle = \sum_i (X|i\rangle) \otimes |i\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_0. \tag{B.13}$$

Similarly, a superoperator $\mathcal{A}$ is mapped to a matrix A via the prescription

$$\mathsf{A} \equiv (\mathcal{A}_1 \otimes \mathcal{I}_0)|\psi^+\rangle\langle\psi^+| = \sum_{i,j} \mathcal{A}(|i\rangle\langle j|) \otimes |i\rangle\langle j|, \tag{B.14}$$

which is a matrix acting on the vector space $\mathcal{H}_1 \otimes \mathcal{H}_0$. In this context, A is known as the *Choi matrix.* To recover the action of $\mathcal{A}$ on a state ρ, one uses the relation

$$\mathcal{A}\rho = \mathrm{tr}_0\{(I_1 \otimes \rho_0^T)\mathsf{A}\}, \tag{B.15}$$

which is easy to confirm by direct calculation.

Working with the Choi matrix (B.14) has an important advantage: The superoperator $\mathcal{A}$ is CP if and only if its Choi matrix is positive: $\hat{\mathcal{A}} \geq 0$. In fact, the direction “$\Rightarrow$” is easy to see, but the converse direction requires more work. To get further acquainted with Choi matrices, the reader is asked to do the following exercise.

Exercise B.3 Show that, if $\mathcal{A}$ is trace–preserving, then the trace of the Choi matrix is $\mathrm{tr}\{\hat{\mathcal{A}}\} = d$, where $d = \dim \mathcal{H}_1$. Thus, recalling that $\hat{\mathcal{A}} \geq 0$, we can view $\hat{\mathcal{A}}/d$ as a quantum state of a bipartite system, which is in one–to–one correspondence with the map $\mathcal{A}$. However, in contrast to our earlier construction, the Choi matrix of a unitary time evolution map $\mathcal{U}\rho = U\rho U^\dagger$ is no longer unitary. Convince yourself of this.

We proceed by looking at the concatenation of superoperators, which can be described using the **link product** $*$. To this end, it turns out to be convenient to explicitly include the spaces on which the Choi matrices are defined in the notation. Thus, let A_{10} act on two spaces labeled 1 and 0 and B_{21} acts on two spaces labeled 2 and 1. Their link product is defined as

$$\mathsf{B}_{21} * \mathsf{A}_{10} = \mathrm{tr}_1\{(I_2 \otimes \mathsf{A}_{10}^{T_1})(\mathsf{B}_{21} \otimes I_0)\}, \tag{B.16}$$

where T_1 means transpose on space 1 only, i.e., $\mathsf{A}_{10}^{T_1} = \sum_{i,j} \mathcal{A}(|i\rangle\langle j|)_1^T \otimes |i\rangle\langle j|_0$. In words, the link product takes two Choi matrices, puts them in reverse order, appends them with identity matrices to make them act on the same joint space (here, the space 210), performs a partial transpose of one matrix with respect to the common space (here, the space 1), and finally traces them over the common space.

The link product satisfies a number of elementary properties, which can be checked by direct calculation. For instance, it is associative if the three matrices share *no* common space, which we write as

$$\mathsf{C}_{32} * \mathsf{B}_{21} * \mathsf{A}_{10} = (\mathsf{C}_{32} * \mathsf{B}_{21}) * \mathsf{A}_{10} = \mathsf{C}_{32} * (\mathsf{B}_{21} * \mathsf{A}_{10}). \tag{B.17}$$

Moreover, if two matrices have no space in common, the link product reduces to the tensor product:

$$\mathsf{B}_{2} * \mathsf{A}_{0} = \mathsf{B}_{2} \otimes \mathsf{A}_{0}. \tag{B.18}$$

If they act on the same space instead, one obtains the Hilbert–Schmidt scalar product

$$\mathsf{B}_{0} * \mathsf{A}_{0} = \mathrm{tr}_0\{\mathsf{B}_0^T \mathsf{A}_0\}. \tag{B.19}$$

Finally, the link product is commutative up to relabeling of Hilbert spaces,

$$\mathsf{B}_{21} * \mathsf{A}_{10} = S_{2,0}\mathsf{A}_{10} * \mathsf{B}_{21} S_{2,0}, \tag{B.20}$$

where $S_{2,0} = S_{2,0}^{\dagger}$ is the unitary swap operator between spaces 2 and 0, defined as $S_{2,0}|j\rangle_2 \otimes |k\rangle_0 = |k\rangle_0 \otimes |j\rangle_2$. In particular, the link product is commutative if the participating spaces are traced over in the final expression. For instance, for arbitary different spaces 0, 1, 2, 3, 4 and 5 it is true that

$$\mathrm{tr}_3\{\mathsf{D}_{54} * \mathsf{C}_{432} * \mathsf{B}_{21} * \mathsf{A}_{10}\} = \mathrm{tr}_3\{\mathsf{D}_{54} * \mathsf{B}_{21} * \mathsf{C}_{432} * \mathsf{A}_{10}\}. \tag{B.21}$$

To connect the link product to the concatenation of superoperators acting on a state ρ it is useful to introduce some conventions. First of all, we identify the Choi matrix of ρ with ρ itself. Equation (B.15) then implies $\mathcal{A}\rho = \mathrm{tr}_0\{(I_1 \otimes \rho_0^T)\mathsf{A}_{10}\} = \mathsf{A}_{10} * \rho_0$. Moreover, although the state space of ρ is always the same, it is useful to denote state spaces at different times with different labels, i.e., we formally associate to each time a different space. Thus, instead of writing $\mathcal{C} \circ \mathcal{B} \circ \mathcal{A}\rho$, we write $\mathcal{C}_{32} \circ \mathcal{B}_{21} \circ \mathcal{A}_{10}\rho_0$, and we call, e.g., space 1 the *output space* of $\mathcal{A}$ and the *input space* of $\mathcal{B}$. With this identification we have

$$\mathcal{C}_{32} \circ \mathcal{B}_{21} \circ \mathcal{A}_{10}\rho_0 = \mathsf{C}_{32} * \mathsf{B}_{21} * \mathsf{A}_{10} * \rho. \tag{B.22}$$

B.3 Matrix Representations of the Process Tensor

We return to the process tensor introduced in Section 1.7, which we can now express in a neat form. To this end, we label the input space of the nth control operation $\mathcal{C}(r_n)$ with S_n and its output space with S'_n (remember that the control operations only act on the system). The bath space during the nth control operation is labeled B_n. This convention is illustrated in Fig. B.1. The process tensor defined in eqn (1.61) is then written as

$$\begin{aligned}&\mathfrak{T}[\mathcal{C}(r_n), \ldots, \mathcal{C}(r_1), \mathcal{C}(r_0)] = \\ &\mathrm{tr}_{B_n}\left\{\mathcal{C}_{S'_n,S_n}\mathcal{U}_{S_nB_n,S'_{n-1}B_{n-1}} \cdots \mathcal{C}_{S'_1,S_1}\mathcal{U}_{S_1B_1,S'_0B_0}\mathcal{C}_{S'_0,S_0}\rho_{S_0B_0}\right\}.\end{aligned} \tag{B.23}$$

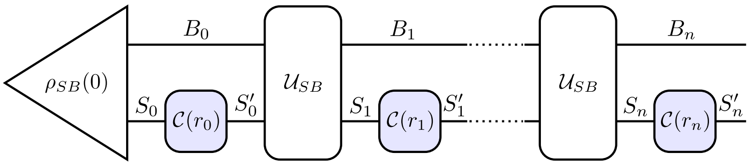

Fig. B.1 Process tensor with input and output spaces labeled according to our convention.

where we dropped any dependence on time or the measurement results r_n for notational simplicity. Now, observe that each space in eqn (B.23) appears exactly twice (except of S_n', which appears only once). This allows us to write

$$\mathfrak{T}[\mathcal{C}(r_n),\dots,\mathcal{C}(r_1),\mathcal{C}(r_0)] = \tag{B.24}$$
$$\mathrm{tr}_{B_n}\left\{\mathsf{C}_{S_n',S_n} * \mathsf{U}_{S_nB_n,S_{n-1}'B_{n-1}} * \cdots * \mathsf{C}_{S_1',S_1} * \mathsf{U}_{S_1B_1,S_0'B_0} * \mathsf{C}_{S_0',S_0} * \rho_{S_0B_0}\right\}.$$

Next, observe that we can apply eqn (B.21) to rearrange terms into

$$\mathfrak{T}[\mathcal{C}(r_n),\dots,\mathcal{C}(r_1),\mathcal{C}(r_0)] = \tag{B.25}$$
$$\mathsf{C}_{S_n',S_n} * \cdots * \mathsf{C}_{S_1',S_1} * \mathsf{C}_{S_0',S_0} * \mathrm{tr}_{B_n}\left\{\mathsf{U}_{S_nB_n,S_{n-1}'B_{n-1}} * \cdots * \mathsf{U}_{S_1B_1,S_0'B_0} * \rho_{S_0B_0}\right\}.$$

We can write this concisely as

$$\mathfrak{T}[\mathcal{C}(r_n),\dots,\mathcal{C}(r_1),\mathcal{C}(r_0)] = \mathsf{C}(\mathbf{r}_n) * \mathsf{T} \tag{B.26}$$

with $\mathsf{C}(\mathbf{r}_n) = \mathsf{C}(r_n) \otimes \cdots \otimes \mathsf{C}(r_0)$, where we used eqn (B.18) and introduced the dependence on the measurement results again, and $\mathsf{T} = \mathrm{tr}_B\{\mathsf{U}_{n-1} * \cdots * \mathsf{U}_0 * \rho_0\}$, where the subscripts now denote the time steps, tacitly assuming the association of input and output spaces as illustrated in Fig. B.1.

Taking the trace over the final output space and using eqn (B.19), we can compactly write

$$p(\mathbf{r}_n) = \mathrm{tr}_S\{\mathfrak{T}[\mathcal{C}(r_n),\dots,\mathcal{C}(r_1),\mathcal{C}(r_0)]\} = \mathrm{tr}\{\mathsf{C}(\mathbf{r}_n)^T\mathsf{T}\}, \tag{B.27}$$

where the final trace is over the spaces $S_n', S_n, \dots, S_0', S_0$. Equation (B.27) can be interpreted as a generalization of the Born rule to multiple time steps. Indeed, at a single time the Born rule says that $p(r) = \mathrm{tr}\{P(r)\rho\}$ for some POVM element $P(r)$ and state ρ. By analogy, $\mathsf{C}(\mathbf{r}_n)^T$ corresponds to a multitime POVM element and T corresponds to a multitime 'state.' In particular, we note that both objects are positive.

Thus, we can conclude that the link product defined on Choi states acting on multiple input/output spaces allows for a convenient separation of the process T itself, which captures all the effects of the environment, and the external control operations $\mathsf{C}(\mathbf{r}_n)$. The probability to get a sequence of outcomes $\mathbf{r}_n$ can be obtained by matrix multiplication of the two objects followed by a trace. This separation is, of course, not a particular consequence of the Choi–Jamiołkowski isomorphism—it follows from any representation as we illustrate now, which further elucidates the meaning of the link product and of eqn (B.25).

For this purpose we consider an explicit matrix representation of the state and superoperators. Let $\rho(0) = \sum \rho_{a_0,b_0}^{\alpha_0,\beta_0} |\alpha_0 a_0\rangle\langle\beta_0 b_0|$ be the initial state, where Greek (Latin) indices label the bath (system) degrees of freedom (thus, the index b_0 does *not* label bath degrees of freedom), and summation symbols $\sum$ without subscripts correspond to sums over all indices in the following. Note that we do not specify a particular basis for the representation. The unitary time evolution operator in the first time step from 0 to t_1 is written as $U_0 = \sum U^{\alpha_1,\alpha_0}_{a_1,a_0} |\alpha_1 a_1\rangle\langle\alpha_0 a_0|$ and the action of the time evolution superoperator on the initial state is written as $\mathcal{U}_0\rho(0) = \sum \mathcal{U}^{\alpha_1\alpha_0,\beta_1\beta_0}_{a_1a_0,b_1,b_0} \rho^{\alpha_0,\beta_0}_{a_0,b_0} |\alpha_1 a_1\rangle\langle\beta_1 b_1|$.

For simplicity, we consider only a three–step process in the following; the generalization to an n–step process is mathematically straightforward but cumbersome to write down. We find (again dropping the dependence on $\mathbf{r}_n$ in the notation)

$$\begin{aligned}&\mathcal{C}_2\mathcal{U}_1\mathcal{C}_1\mathcal{U}_0\mathcal{C}_0\rho(0) = \\ &\quad \sum \mathcal{C}_{a_2'a_2,b_2'b_2}\mathcal{U}^{\alpha_2\alpha_1,\beta_2\beta_1}_{a_2a_1',b_2b_1'}\mathcal{C}_{a_1'a_1,b_1'b_1}\mathcal{U}^{\alpha_1\alpha_0,\beta_1\beta_0}_{a_1a_0',b_1b_0'}\mathcal{C}_{a_0'a_0,b_0'b_0}\rho^{\alpha_0,\beta_0}_{a_0,b_0}|\alpha_2 a_2'\rangle\langle\beta_2 b_2'|.\end{aligned} \tag{B.28}$$

Tracing over the system and bath degrees of freedom and regrouping terms, we find

$$\begin{aligned}p(r_2,r_1,r_0) &= \sum_{\text{Latin}}\left(\sum_{\text{Greek}}\mathcal{U}^{\epsilon\alpha_1,\epsilon\beta_1}_{a_2a_1',b_2b_1'}\mathcal{U}^{\alpha_1\alpha_0,\beta_1\beta_0}_{a_1a_0',b_1b_0'}\rho^{\alpha_0,\beta_0}_{a_0,b_0}\right)\mathcal{C}_{ea_2,eb_2}\mathcal{C}_{a_1'a_1,b_1'b_1}\mathcal{C}_{a_0'a_0,b_0'b_0} \\ &\equiv \sum_{\text{Latin}}\mathfrak{T}_{a_2a_1'a_1a_0'a_0,b_2b_1'b_1b_0'b_0}\mathfrak{C}_{a_2a_1'a_1a_0'a_0,b_2b_1'b_1b_0'b_0} = \mathrm{tr}\{\mathfrak{T}\mathfrak{C}^T\}.\end{aligned} \tag{B.29}$$

Here, we have again separated the influence of the environment from the control operations. In fact, the trace over the Latin indices corresponds precisely to the trace on the right hand side of eqn (B.27). Furthermore, the term in the brackets presents an explicit matrix representation of the process tensor $\mathfrak{T}$, which can be associated to $\mathrm{tr}_B\{\mathcal{U}_1 * \mathcal{U}_0 * \rho(0)\}$ if one interprets the link product as a matrix product in the environment space and a tensor product in the system space. Likewise, the term $\mathfrak{C}$ containing the control operations can be associated to $\mathcal{C}_2 * \mathcal{C}_1 * \mathcal{C}_0 = \mathcal{C}_2 \otimes \mathcal{C}_1 \otimes \mathcal{C}_0$. This analogy can be even further strengthened by tracing out only the bath degrees of freedom in eqn (B.28) and by noting that

$$\begin{aligned}&\mathrm{tr}_B\{\mathcal{C}_2\mathcal{U}_1\mathcal{C}_1\mathcal{U}_0\mathcal{C}_0\rho(0)\} = \\ &\quad\mathrm{tr}_{S_2S_1'S_1S_0'S_0}\Bigg\{I_{S_2'}\otimes\sum_{\text{Latin}}\sum_{\text{Greek}}\mathcal{U}^{\epsilon\alpha_1,\epsilon\beta_1}_{a_2a_1,b_2,b_1}\mathcal{U}^{\alpha_1\alpha_0,\beta_1\beta_0}_{a_1a_0,b_1,b_0}\rho^{\alpha_0,\beta_0}_{a_0,b_0}|a_2a_1'a_1a_0'a_0\rangle\langle b_2b_1'b_1b_0'b_0| \\ &\qquad\times\sum_{\overline{\text{Latin}}}\mathcal{C}_{\bar a_2'\bar a_2,\bar b_2'\bar b_2}\mathcal{C}_{\bar a_1'\bar a_1,\bar b_1'\bar b_1}\mathcal{C}_{\bar a_0'\bar a_0,\bar b_0'\bar b_0}|\bar a_2'\bar a_2\bar a_1'\bar a_1\bar a_0'\bar a_0\rangle\langle\bar b_2'\bar b_2\bar b_1'\bar b_1\bar b_0'\bar b_0|\Bigg\}\end{aligned} \tag{B.30}$$

Exercise B.4 Show that eqn (B.30) is identical to eqn (B.25) if we use the Choi representation for superoperators, i.e., if we identify $\mathcal{U} \leftrightarrow \mathsf{U}$ and $\mathcal{C} \leftrightarrow \mathsf{C}$.

To complete our exposition, we turn to another equivalent representation of the process tensor, which shows that the process tensor can be seen as a state of a suitable quantum many–body system. Specifically, we convert an n–step process to a state living on $\mathcal{H}_S^{\otimes(2n+1)}$, which is isomorphic to our previous representations. To motivate the

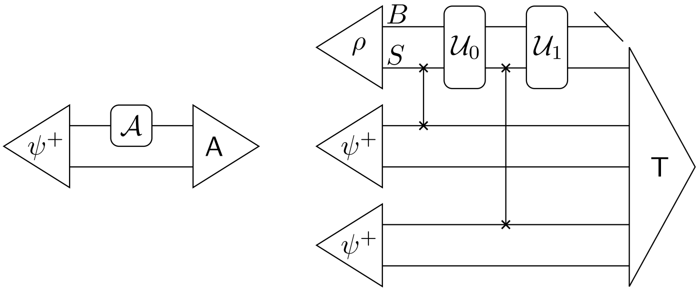

Fig. B.2 **Left:** Circuit diagram of the Choi matrix representation of a superoperator $\mathcal{A}$. **Right:** Circuit diagram to construct the Choi matrix of the process tensor according to a generalized Choi–Jamiołkowski isomorphism. The vertical lines denote a swap between state spaces marked with a cross.

following, we return to the Choi matrix A corresponding to a superoperator $\mathcal{A}$, which was constructed by letting $\mathcal{A}$ act on one half of an (unnormalized) maximally entangled state, see eqn (B.14). Furthermore, recall that the Choi matrix can be naturally interpreted as the (unnormalized) state of a bipartite quantum system (Exercise B.3). This is graphically depicted in Fig. B.2.

Similarly, to turn the process tensor into its corresponding Choi matrix, we let it interact at each intervention time t_j with one half of a maximally entangled state. This is achieved by *swapping* at each time the current system state with a fresh state, which forms one half of a maximally entangled ancilla state A_j. Precisely, let $\psi_j^+ = \sum |a'_j a'_j\rangle\langle b'_j b'_j|$ denote the (unnormalized) maximally entangled state of A_j and let the unitary swap superoperator be

$$\mathcal{S}_{S,A_j}(\rho_S \otimes \psi_j^+) = \mathcal{S}_{S,A_j} \sum \rho_{a,b} |a a'_j a'_j\rangle\langle b b'_j b'_j| \equiv \sum \rho_{a,b} |a'_j a a'_j\rangle\langle b'_j b b'_j|, \tag{B.31}$$

which exchanges the system with the first half of the ancilla. Then, the final claim of this section is

$$\begin{aligned} \mathsf{T} &= \mathrm{tr}_{B_2}\{\mathsf{U}_{S_2B_2,S'_1B_1} * \mathsf{U}_{S_1B_1,S'_0B_0} * \rho_{S_0B_0}\} \\ &\cong \mathrm{tr}_B\{\mathcal{U}_1\mathcal{S}_{SA_1}\mathcal{U}_0\mathcal{S}_{SA_0}\rho_{SB}(0) \otimes \psi_0^+ \otimes \psi_1^+\}, \end{aligned} \tag{B.32}$$

where $\cong$ means that the result is identical up to reordering of the Hilbert spaces and if the superoperators are given in Choi representation. Furthermore, we have restricted ourselves again to the first three control operations, but the generalization to n interventions is straightforward.

Exercise B.5 Derive eqn (B.32). Furthermore, show that the Choi matrix corresponding to a quantum Markov process defined in Section 1.8 is isomorphic to $\mathcal{E}(t_n, t_{n-1}) \otimes \cdots \mathcal{E}(t_1, 0) \otimes \rho_S(0)$, i.e., a many–body state where correlations only exist between a preparation and its subsequent measurement or, in view of the terminology of this appendix, between an output state S'_{j-1} and an input state S_j.

Further reading

Pedagogical accounts on how to represent quantum operations by matrices can be found at many places. As the name suggests, the Choi–Jamiołkowski isomorphism is due to the work of Jamiołkowski (1972) and Choi (1975). The link product was introduced by Chiribella *et al.* (2009) and the process tensor representation in terms of a many–body state was given by Pollock *et al.* (2018*a*); see also Milz and Modi (2021) and references therein for a detailed exposition.

Appendix C

Time–Reversal Symmetry

We show that the equations of motion of classical and quantum mechanics have a remarkable property, which we call *time–reversal symmetry* or *microreversibility.* Its consequences for the arrow of time and the second law of thermodynamics are also discussed at the end.

In both cases, classically and quantum mechanically, the notion of time–reversal symmetry will be introduced with respect to the following abstract thought experiment, which is also depicted as a diagram in Fig. C.1. It is important to note here that this thought experiment can be carried out in the real world without the need to actually 'reverse' the time. The reader therefore should *not* take the terminology 'time–reversal' literally (cf. the discussion in Section C.3). As usual in physics, there are two main players involved. Initial states, here abstractly denoted by S_0, and some dynamical law, here abstractly denoted by $\mathcal{E}(\tau)$, which maps the initial states to some final states $S_\tau = \mathcal{E}(\tau)S_0$ after a time τ has elapsed. Now, suppose that we find an invertible map Θ, which we call the time–reversal operator, and some conjugate dynamics $\mathcal{E}_\Theta(\tau)$ such that

$$S_0 = \Theta^{-1}\mathcal{E}_\Theta(\tau)\Theta\mathcal{E}(\tau)S_0. \tag{C.1}$$

In words: we get back to the initial state S_0 if we let the system evolve in time for a duration τ, then time–reverse the state followed by an evolution for a duration τ with respect to the conjugate dynamics and, finally, apply the inverse of the time–reversal operator. We now define:

Time–reversal symmetry. *A physical system defined by some dynamical law $\mathcal{E}(\tau)$ is said to possess time–reversal symmetry if there exists an invertible time–reversal operator Θ and a conjugate dynamical law $\mathcal{E}_\Theta(\tau)$ such that eqn (C.1) holds under the following three conditions:*

$$\begin{tikzcd}
S_0 \arrow[r, "\mathcal{E}(\tau)"'] & S_\tau \arrow[d, "\Theta"'] \\
\Theta S_0 \arrow[u, "\Theta^{-1}"'] & \Theta S_\tau \arrow[l, "\mathcal{E}_\Theta(\tau)"]
\end{tikzcd}$$

Fig. C.1 Abstract diagram of the thought experiment related to the notion of time–reversal symmetry.

1. *Equation (C.1) holds for all legitimate initial conditions* S_0.
2. *The states* S_τ, ΘS_τ *and* ΘS_0 *are legitimate physical states.*
3. *The conjugate dynamical law* $\mathcal{E}_\Theta(\tau)$ *is a legitimate physical evolution law, which can be (in principle) implemented in a lab.*

Here, the word 'legitimate' has to be defined by the physical context at the end, e.g., legitimate states or evolution laws should not give rise to negative probabilities. Furthermore, the conjugate dynamics $\mathcal{E}_\Theta(\tau)$ must be realizable in a lab in principle (e.g., generated by a legitimate Hamiltonian). As we see below, this excludes the choice $\Theta = I$ and $\mathcal{E}_\Theta(\tau) = \mathcal{E}(\tau)^{-1}$, which would trivially satisfy eqn (C.1).

C.1 Time–Reversal Symmetry in Classical Mechanics

The state of a classical system with N particles and $2f$ degrees of freedom per particle is described by its phase space coordinates $(\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2Nf}$, where $\mathbf{q} = (q_1, \ldots, q_{Nf})$ are the generalized coordinates and $\mathbf{p} = (p_1, \ldots, p_{Nf})$ the conjugate momenta. Note that we here restrict the discussion to 'pure' states, which are represented by a single point in phase space. Since mixtures evolve via Liouville's equation linearly in classical mechanics, this assumption does not entail any loss of generality. In addition, to focus on the essential ingredients of time–reversal symmetry, we set $N = 1$ and $f = 1$ in the following (i.e., a single particle moving in one dimension). The generalization to many particles and multiple degrees of freedom is indeed just a matter of notation. Thus, we denote the Hamiltonian of the system by $H(q, p)$ and Hamilton's equations of motion become

$$\dot{q} = \frac{\partial H(q,p)}{\partial p}, \quad \dot{p} = -\frac{\partial H(q,p)}{\partial q}. \tag{C.2}$$

To be particularly cautious and in view of what follows, we write Hamilton's equations in difference form as

$$q_{t+dt} = q_t + dt\, \frac{\partial H}{\partial p}\bigg|_{(q_t,p_t)}, \quad p_{t+dt} = p_t - dt\, \frac{\partial H}{\partial q}\bigg|_{(q_t,p_t)}, \tag{C.3}$$

assuming dt to be small enough such that terms of order $\mathcal{O}(dt^2)$ are negligible throughout. Note that we explicitly keep the information at which phase space point the partial derivative is evaluated, which turns out to be crucial.

We now define define the time–reversal operator Θ via its action on a phase space point (q, p) as

$$\Theta(q,p) \equiv (q, -p), \tag{C.4}$$

i.e., we leave the coordinate unchanged, but flip the momentum. We see that this definition implies that Θ is an *involution*: $\Theta^2 = I$. Put differently, the time–reversal operator is its own inverse: $\Theta = \Theta^{-1}$. This will be true for the rest of this section, but it is no longer the case for quantum systems in general. Fig. C.2 explains the concept of time–reversal for the case of a simple harmonic oscillator.

Furthermore, we start with the simplest situation and assume a Hamiltonian, which obeys the symmetry $H(q, -p) = H(q, p)$. This is often satisfied, e.g., when the Hamiltonian $H(q, p) = p^2/2m + V(q)$ describes the motion of a particle in some external

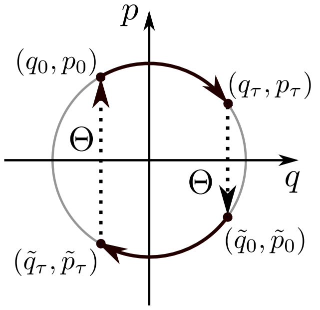

Fig. C.2 Time–reversal symmetry illustrated in the phase space of a harmonic oscillator. The grey circle defines a ‘surface’ of constant energy. Time–reversal symmetry of the dynamics means that one can go back from (q_τ, p_τ) to (q_0, p_0) by, first, mapping (q_τ, p_τ) to its time–reversed image $(\tilde{q}_0, \tilde{p}_0) = (q_\tau, -p_\tau)$, then, letting the system evolve for a time τ, and finally, mapping $(\tilde{q}_\tau, \tilde{p}_\tau)$ back to $(q_0, p_0) = (\tilde{q}_\tau, -\tilde{p}_\tau)$.

potential $V(q)$, but we treat exceptions soon. We then postulate the conjugate dynamics to be also described by Hamilton's equations with respect to the *same* Hamiltonian

$$H_\Theta(q, p) \equiv H(q, p). \tag{C.5}$$

We now check the validity of the diagram C.1 for a small time step dt from $t = 0$ to dt. We introduce the notation

$$(\tilde{q}_0, \tilde{p}_0) \equiv \Theta(q_{dt}, p_{dt}) = (q_{dt}, -p_{dt}). \tag{C.6}$$

This choice might seem unconventional, but it has the advantage that the time parameter also increases in the time–reversed experiment as it would in any actual experiment. Our goal is now to show that the time–reversed state, evolved for a small time step dt with respect to the Hamiltonian (C.5), obeys $(\tilde{q}_{dt}, \tilde{p}_{dt}) = \Theta(q_0, p_0) = (q_0, -p_0)$. To see this, we start by writing down Hamilton's equation for the time–reversed evolution with $H_\Theta = H$

$$\tilde{q}_{dt} = \tilde{q}_0 + dt\, \frac{\partial H}{\partial p}\bigg|_{(\tilde{q}_0, \tilde{p}_0)}, \quad \tilde{p}_{dt} = \tilde{p}_0 - dt\, \frac{\partial H}{\partial q}\bigg|_{(\tilde{q}_0, \tilde{p}_0)}. \tag{C.7}$$

Next, we use definition (C.6) and the fact that any differentiable function obeying $f(x) = f(-x)$ satisfies $f'(-x) = -f'(x)$. Applied to $H(q, p) = H(q, -p)$, this implies

$$\tilde{q}_{dt} = q_{dt} - dt\, \frac{\partial H}{\partial p}\bigg|_{(q_{dt}, p_{dt})}, \quad \tilde{p}_{dt} = -p_{dt} - dt\, \frac{\partial H}{\partial q}\bigg|_{(q_{dt}, p_{dt})}. \tag{C.8}$$

Using furthermore our assumption that terms of order $\mathcal{O}(dt^2)$ are negligible allows us to evaluate the partial derivatives at (q_0, p_0) instead of (q_{dt}, p_{dt}). Multiplying the second equation with -1, we end up with

$$\tilde{q}_{dt} = q_{dt} - dt\, \frac{\partial H}{\partial p}\bigg|_{(q_0, p_0)}, \quad -\tilde{p}_{dt} = p_{dt} + \frac{\partial H}{\partial q}\bigg|_{(q_0, p_0)}. \tag{C.9}$$

$$\begin{tikzcd}
q_0, p_0 \arrow[r, "H"] \arrow[d, leftrightarrow, "\Theta"] & q_{dt}, p_{dt} \arrow[r, "H"] \arrow[d, leftrightarrow, "\Theta"] & q_{2dt}, p_{2dt} \arrow[r, "H"] \arrow[d, leftrightarrow, "\Theta"] & \cdots \arrow[r, "H"] & q_{\tau-dt}, p_{\tau-dt} \arrow[r, "H"] \arrow[d, leftrightarrow, "\Theta"] & q_\tau, p_\tau \arrow[d, leftrightarrow, "\Theta"] \\
\tilde{q}_\tau, \tilde{p}_\tau & \tilde{q}_{\tau-dt}, \tilde{p}_{\tau-dt} \arrow[l, "H_\Theta"] & \tilde{q}_{\tau-2dt}, \tilde{p}_{\tau-2dt} \arrow[l, "H_\Theta"] & \cdots \arrow[l, "H_\Theta"] & \tilde{q}_{dt}, \tilde{p}_{dt} \arrow[l, "H_\Theta"] & \tilde{q}_0, \tilde{p}_0 \arrow[l, "H_\Theta"]
\end{tikzcd}$$

Fig. C.3 Commutative diagram describing time–reversal symmetry for a finite interval $[0, \tau]$.

But this is equation is identical—after some rearrangement—to eqn (C.3) at $t = 0$ if we identify $(\tilde{q}_{dt}, \tilde{p}_{dt}) = (q_0, -p_0)$. To conclude, we have shown that we end up at the initial phase space coordinate (q_0, p_0) if we start a time step dt later with (q_{dt}, p_{dt}), apply the time–reversal operator Θ, let the time–reversed state evolve forward in time for a step dt with respect to the Hamiltonian (C.5), and finally apply Θ again.

Is the above argument sufficient to conclude that time–reversal symmetry applies also to a *finite* interval from 0 to τ? It is if we recall that we can always discretize any trajectory (q_t, p_t), $t \in [0, \tau]$, with a sufficiently small time step dt and if we use the fact that the time reversal operator obeys $\Theta^2 = I$. This means that each step shown in the diagram of Fig. C.3, where we used the notation

$$(\tilde{q}_t, \tilde{p}_t) \equiv \Theta(q_{\tau-t}, p_{\tau-t}) = (q_{\tau-t}, -p_{\tau-t}), \tag{C.10}$$

obeys the mapping described above. Thus, the process obeys time–reversal symmetry.

It is interesting to wonder whether the time–reversal symmetry relation worked out above is unique or whether other choices for Θ and H_Θ are possible as well. As the next exercise shows, other choices are indeed possible.

Exercise C.1 Assume that the Hamiltonian obeys the symmetry $H(q, p) = H(-q, p)$, which is, for instance, the case for a harmonic oscillator. Now, consider the time–reversal operator $\Theta'(q, p) \equiv (-q, p)$, which flips the coordinate, but not the momentum, and define the reversed dynamics via $H_{\Theta'}(q, p) \equiv H(q, p)$. By following the same steps as above, show that these transformations also lead to the notion of time–reversal symmetry. Flipping the coordinates and not the momenta might seem awkward at first sight. However, recall the flexibility that is offered by Hamilton's framework of classical mechanics. In particular, remember that any canonical transformation preserves the form of Hamilton's equations and describes the same physics in a different coordinate system. Convince yourself of the fact that the mapping $(Q, P) \equiv (p, -q)$ is a canonical transformation.

We have so far considered time–independent Hamiltonians obeying the symmetry $H(q, p) = H(q, -p)$. Two generalizations are important. First, it might be that $H(q, p) \neq H(q, -p)$. A prominent example is a particle with charge q in an external electromagnetic field described by an electric potential ϕ and a vector potential $\boldsymbol{A}$, which creates a magnetic field via $\boldsymbol{B} = \nabla \times \boldsymbol{A}$. Such a system is described by the Hamiltonian

$$H(\boldsymbol{q}, \boldsymbol{p}; \boldsymbol{B}) = \frac{1}{2m}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}\right)^2 + q\phi(\boldsymbol{q}), \tag{C.11}$$

where $\boldsymbol{p} \in \mathbb{R}^3$ ($\boldsymbol{q} \in \mathbb{R}^3$) describes the three–dimensional momentum (position) and c is the speed of light. Clearly, $H(\boldsymbol{q}, -\boldsymbol{p}; \boldsymbol{B}) \neq H(\boldsymbol{q}, \boldsymbol{p}; \boldsymbol{B})$. However, if we recall that any magnetic field is created by moving charges and if we would include those in our description as well, then the time–reversal operator Θ would flip the velocity of those charges and hence, the direction of the magnetic field. Therefore, eqn (C.11) obeys the symmetry $H(\boldsymbol{q}, -\boldsymbol{p}; -\boldsymbol{B}) = H(\boldsymbol{q}, \boldsymbol{p}; \boldsymbol{B})$. To describe time–reversal symmetry for the situation where we treat the magnetic field as an *external* parameter, we can keep the definition of Θ from eqn (C.4) and define the conjugate dynamics by applying Θ to the Hamiltonian (C.11):

$$H_\Theta(q,p;B) \equiv H(q,-p;B) = H(q,p;-B). \tag{C.12}$$

Here, we returned to a scalar notation (i.e., $\boldsymbol{q} \to q$, etc.) for simplicity. Due to the symmetry $H(q,p;B) = H(q,-p;-B)$, the conjugate dynamics are therefore generated by a Hamiltonian, which describes the same system but with an inverted magnetic field. Also due to that symmetry, we can confirm that

$$\left.\frac{\partial H_\Theta(q,p;B)}{\partial p}\right|_{(q_t,-p_t)} = -\left.\frac{\partial H(q,p;B)}{\partial p}\right|_{(q_t,p_t)}. \tag{C.13}$$

This relation is sufficient to repeat the same steps as above and to show the time–reversal symmetry of the dynamics.

The second generalization concerns explicitly time–dependent Hamiltonians of the form $H(q,p;B,\lambda_t)$, where λ_t is some externally specified driving protocol. To include this scenario in our description, remember that our calculation above holds for any Hamiltonian at a fixed time t. In particular, we could replace $H(q,p)$ by $H(q,p;\lambda_t)$ in eqns (C.5) to (C.9) without invalidating any argument. For a finite time interval $[0,\tau]$ and with respect to the diagram in Fig. C.3 this means that the time argument of the Hamiltonian $H(q,p;B,\lambda_t)$ in the forward process must match with the time argument of the Hamiltonian $H_\Theta(q,p;B,\lambda_t)$ in the backward process. Together with the convention (C.10) that the time–reversed trajectory starts at $t=0$ and ends at $t=\tau$ this implies that the time–reversed Hamiltonian is given by

$$H_\Theta(q,p;B,\lambda_t) \equiv H(q,p;-B,\lambda_{\tau-t}), \tag{C.14}$$

i.e., the protocol is executed in the reverse order, starting with λ_τ and ending with λ_0.

We end this section with a remark and a small exercise. The remark concerns the observations that the notion of time–reversal symmetry is closely linked to Liouville's theorem, which states that the flow of points in phase space generated by Hamilton's equations is divergence–free and preserves the volume. Since this fact is used in the main text, we state it here without proof (which can be looked up in any standard textbook on classical mechanics):

Liouville's theorem. *Consider a classical Hamiltonian system of N particles with $2f$ degrees of freedom per particle. Let $\Gamma = (\boldsymbol{q}, \boldsymbol{p}) \in \mathbb{R}^{2Nf}$ denote a point in the phase space. Furthermore, let $\Gamma^t = \phi^t(\Gamma^0)$ denote the time evolved point in phase space given* *initial condition* Γ^0*. Then, the Jacobian of this transformation equals one, i.e., using a compact notation*

$$J = \det\left(\frac{\partial\Gamma^t}{\partial\Gamma^0}\right) = 1. \tag{C.15}$$

In particular, this implies for any function $f(\Gamma)$

$$\boxed{\int d\Gamma_0 f[\Gamma_t(\Gamma_0)] = \int d\Gamma_t f(\Gamma_t).} \tag{C.16}$$

Roughly speaking, Liouville's theorem states that *no information is lost* during the evolution of a Hamiltonian system. This idea is closely related to time–reversal symmetry since the latter principle states that we can find for each 'forward' trajectory a conjugated 'reversed' trajectory, which also obeys Hamiltonian dynamics. The fact that conservation of information plays a crucial role here is exemplified by the following exercise.

Exercise C.2 Consider a master equation $d_t\boldsymbol{p}(t) = R\boldsymbol{p}(t)$ described by a time–independent rate matrix R. The solution of the dynamics is given by the transition matrix e^{Rt}. Thus, the dynamics are clearly *invertible* as we can associate to each final state $\boldsymbol{p}(t)$ a unique initial state $\boldsymbol{p}(0)$ via $\boldsymbol{p}(0) = e^{-Rt}\boldsymbol{p}(t)$. Now, it is tempting to conclude that the dynamics of a master equation obeys time–reversal symmetry by setting $\Theta = I$ and by postulating the time–reversed dynamics to obey the 'master equation' $d_t\boldsymbol{p}(t) = -R\boldsymbol{p}(t)$. While the above steps are mathematically correct, show that the above construction does not satisfy the requirements of time–reversal symmetry. What is wrong with the time–reversed master equation? What is the difference between Hamiltonian dynamics and master equation dynamics (compare, e.g., the physical insight obtained from Liouville's theorem with respect to Theorem A.4)?

C.2 Time–Reversal Symmetry in Quantum Mechanics

We introduce time–reversal symmetry in quantum mechanics by postulating that there exists a time–reversal operator Θ such that $|\psi(0)\rangle = \Theta^{-1}U_\Theta(\tau,0)\Theta U(\tau,0)|\psi(0)\rangle$ holds for any initial state $|\psi(0)\rangle$. Here, $U(\tau,0)$ is the unitary time evolution for the forward dynamics and $U_\Theta(\tau,0)$ is the unitary time evolution of a suitably defined conjugate or backwards dynamics. In words, the relation $|\psi(0)\rangle = \Theta^{-1}U_\Theta(\tau,0)\Theta U(\tau,0)|\psi(0)\rangle$ says that, if we let an arbitrary state evolve for a time τ, time–reverse it, let it evolve for a time τ using the conjugate dynamics, and apply the inverse time–reversal, then we end up with the same state. Since this relation is supposed to hold for any initial state, we can also write it as an operator identity:

$$\boxed{\Theta^{-1}U_\Theta(\tau,0)\Theta U(\tau,0) = I.} \tag{C.17}$$

How to define Θ and U_Θ remains, of course, the open question.

To approach it, we consider the simplest situation first and rely on some classical intuition. Consider a single particle with mass m moving in a potential V with Hamiltonian $H = P^2/2m + V(X)$, where X and P are the position and momentum operators. For this case we found classically that the time–reversal operator is an involution, $\Theta^{-1} = \Theta$, and we have good reasons to believe that the conjugate dynamics is identical to the forward dynamics, i.e., $U_\Theta(\tau) = U(\tau) = e^{-iH\tau/\hbar}$. We use this as our hypothesis now and investigate its consequences. Expanding eqn (C.17) for small τ, we arrive at

$$I + \Theta(-iH\tau\Theta - \Theta iH\tau) + \mathcal{O}(\tau^2) = I, \tag{C.18}$$

where we used $\Theta^2 = I$. From this equation we obtain the condition $-iH\tau\Theta = \Theta iH\tau$. Now, if Θ was a linear operator, the last condition reduces to $-H\Theta = \Theta H$, i.e., the time–reversal operator anti–commutes with the Hamiltonian. This conclusion, however, causes troubles because one immediately confirms that for any eigenstate $|E\rangle$ of the Hamiltonian with eigenenergy $E > 0$ there exist another eigenstate $\Theta|E\rangle$ with negative eigenenergy $-E$. This is problematic because we expect the spectrum of every reasonable physical Hamiltonian to be *bounded from below* (otherwise it would be thermodynamically unstable and we could draw an infinite amount of energy from it). Thus, our assumption that Θ is a linear operator must have been wrong. Therefore, we consider the alternative possibility that Θ is *anti–linear*, by which we mean that $\Theta i = -i\Theta$. With this assumption the condition $-iH\tau\Theta = \Theta iH\tau$ reduces to $H\Theta = \Theta H$, i.e., the time–reversal operator commutes with the Hamiltonian. This, indeed, does not give rise to any paradoxical situations for the spectrum of the Hamiltonian.

Anti–linear operators are somewhat bizarre objects, they cannot be represented by a matrix and typically one does not encounter them in quantum mechanics. To get familiar with them, we consider a simple example, namely the complex conjugation operator denoted by K. It is clear that $K^2 = I$, but K is not yet well–defined if we do not specify in which basis it causes complex conjugation. Within the context of time–reversal symmetry and for the example considered above of a particle in a potential V, the most reasonable choice turns out to be complex conjugation with respect to the coordinate representation of the wavefunction. Thus, we set $\Theta = K$ and, by expanding any state in the coordinate representation, $|\psi\rangle = \int dx \langle x|\psi\rangle |x\rangle = \int dx \psi(x)|x\rangle$, we define K as $K|\psi\rangle = \int dx \psi(x)^*|x\rangle$. The motivation for this choice comes from the fact that the position and momentum operators X and P then transform as expected from the classical case (C.4):

$$\Theta X\Theta = X, \quad \Theta P\Theta = -P. \tag{C.19}$$

In this context, X is said to be an *even* observable and P an *odd* observable. Proving $\Theta X\Theta = X$ is simple. To prove $\Theta P\Theta = -P$, consider a momentum eigenstate $\psi_k(x) = e^{ikx/\hbar}$ with eigenvalue k in the coordinate representation (this is a plane wave). We then obtain the chain of equalities

$$\Theta P\Theta\psi_k(x) = \Theta P e^{-ikx/\hbar} = \Theta(-k)e^{-ikx/\hbar} = -k\psi_k(x) = -p\psi_k(x), \tag{C.20}$$

where we used that the momentum operator has the coordinate representation $P = -i\hbar\frac{\partial}{\partial x}$. Since the $\psi_k(x)$ form an (over)complete set of basis vectors, we can conclude from eqn (C.20) that $\Theta P\Theta = -P$. Furthermore, we see that a Hamiltonian of the form $H = P^2/2m + V(X)$ obeys $\Theta H\Theta = H$ and hence, it is invariant under time–reversal. This also allows us to easily prove eqn (C.17) for $U_\Theta(\tau) = U(\tau)$ and $\Theta^{-1} = \Theta$:

$$\Theta e^{-iH\tau/\hbar}\Theta e^{-iH\tau/\hbar} = \Theta^2 e^{iH\tau/\hbar}e^{-iH\tau/\hbar} = I. \tag{C.21}$$

Unfortunately, the time–reversal operator Θ is not always given by complex conjugation in the position representation. It has, however, a couple of general features. The first is related to anti–linearity and is called *anti–unitarity.* It is defined by the requirement that for any two states $|\psi\rangle$ and $|\phi\rangle$

$$\langle\Theta\psi|\Theta\phi\rangle = \langle\psi|\phi\rangle^* = \langle\phi|\psi\rangle. \tag{C.22}$$

This property ensures that $|\langle\Theta\psi|\Theta\phi\rangle| = |\langle\psi|\phi\rangle|$, i.e., all probabilities are left unchanged. To get further acquainted with the 'bizarreness' of anti–unitarity, the reader is asked to do the following three small exercises.

Exercise C.3 Show that anti–unitarity implies anti–linearity.

Exercise C.4 Show for any operator O that $\mathrm{tr}\{\Theta O\Theta^{-1}\} = \mathrm{tr}\{O\}^* = \mathrm{tr}\{O^\dagger\}$. *Hint:* You can use that, if Θ is anti–unitary, then also Θ^{-1} is.

Exercise C.5 Show for any observable O that the time–reversed observable $\Theta O\Theta^{-1}$ is also an observable, i.e., it is Hermitian. *Hint:* Show this directly by confirming $\langle\psi|\Theta O\Theta^{-1}\phi\rangle = \langle\Theta O\Theta^{-1}\psi|\phi\rangle$ for any $|\psi\rangle$ and $|\phi\rangle$. We remark that it is unclear how and never necessary to define the Hermitian conjugate of the anti–unitary operator Θ.

Furthermore, show for any observable O that $\Theta O\Theta^{-1}$ has the same spectrum as O, i.e., the same eigenvalues, but not necessarily the same eigenvectors.

It is clear from definition (C.22) that the product of two anti–unitary operators is unitary. This insight makes the following result intuitively appealing. Namely, every anti–unitary operator can be written in the standard form

$$\Theta = UK, \tag{C.23}$$

where K denotes as above complex conjugation in some fixed basis and U is a unitary operator. We will, however, not prove eqn (C.23) here. Furthermore, we demand that applying Θ twice to a wave function should give back the same wave function apart from a phase factor: $\Theta^2|\psi\rangle = e^{i\varphi}|\psi\rangle$. This requirement leads to an interesting conclusion. First, from $\Theta^2 = UKUK = e^{i\varphi}$ one derives $U^* = KUK = e^{i\varphi}U^\dagger = e^{i\varphi}(U^*)^T$. Iterating the last relation once, we obtain $U^* = e^{i\varphi}[e^{i\varphi}(U^*)^T]^T = e^{2i\varphi}U^*$. Hence, $e^{2i\varphi} = 1$, which implies $e^{i\varphi} = \pm 1$. Thus, we arrive at the conclusion

$$\Theta^2 = \pm I. \tag{C.24}$$

The case $\Theta^2 = I$ appeared already above, but as we will see now the case $\Theta^2 = -I$ becomes important to describe time–reversal of a spin 1/2 particle.

From eqn (C.19) we infer that angular momentum $\mathbf{J} = \mathbf{X} \times \mathbf{P}$ of a particle moving in three dimensions is odd under time–reversal: $\Theta\mathbf{J}\Theta = -\mathbf{J}$. By analogy, we postulate the same for the spin: $\Theta\boldsymbol{\sigma}\Theta = -\boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices. If $\Theta = K$, this is not possible independent of the basis, which we choose for K. We therefore set $\Theta = UK$ and assume that K denotes complex conjugation in the coordinate representation *and* in the σ_z representation, where the Pauli matrices take on the standard form:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{C.25}$$

In this representation the condition $\Theta\boldsymbol{\sigma}\Theta = -\boldsymbol{\sigma}$ yields three equations:

$$\Theta\sigma_x\Theta^{-1} = U\sigma_x U^{-1} = -\sigma_x \quad \Leftrightarrow \quad \{U, \sigma_x\} = 0, \tag{C.26}$$

$$\Theta\sigma_y\Theta^{-1} = -U\sigma_y U^{-1} = -\sigma_y \quad \Leftrightarrow \quad [U, \sigma_y] = 0, \tag{C.27}$$

$$\Theta\sigma_z\Theta^{-1} = U\sigma_z U^{-1} = -\sigma_z \quad \Leftrightarrow \quad \{U, \sigma_z\} = 0. \tag{C.28}$$

Now, every complex 2×2 matrix can be written as $U = \alpha\sigma_x + \beta\sigma_y + \gamma\sigma_z + \delta I$ with $\alpha, \beta, \gamma, \delta \in \mathbb{C}$. Inserting this ansatz in the above three equations and evaluating the (anti–)commutators reveals that $\alpha = \delta = 0$ (from the first equation) and $\gamma = 0$ (from the second equation). The third equation is then automatically satisfied and we are left with $U = \beta\sigma_y$. The parameter β can be chosen freely as long as U is unitary, which implies $|\beta| = 1$. The conventional choice is $\beta = i$ such that

$$\Theta = i\sigma_y K = e^{i\pi\sigma_y/2} K. \tag{C.29}$$

One easily confirms that $\Theta^2 = -I$. Moreover, for a system with N spin 1/2 particles the time–reversal operator becomes $\Theta = \exp[i\pi(\sigma_y^{(1)} + \cdots + \sigma_y^{(N)})/2]K$ and we have $\Theta^2 = I$ if N is even and $\Theta^2 = -I$ if N is odd.

It is instructive to consider the distinction between systems with $\Theta^2 = I$ and $\Theta^2 = -I$ a little more in detail. We start with $\Theta^2 = I$ and assume that $[\Theta, H] = 0$. As the next exercise shows, it is then possible to always write the Hamiltonian as a real–valued matrix *without* explicit knowledge of the energy eigenbasis.

Exercise C.6 Show that any Hamiltonian, which obeys $[\Theta, H] = 0$ for an anti–unitary operator Θ with $\Theta^2 = I$, can be given a real matrix representation without knowing the eigenbasis (remember that, in general, a Hamiltonian matrix has *complex* entries although its eigenvalues are always real since $H = H^\dagger$). For this purpose start with an arbitrary vector $|\phi_1\rangle$ and complex number a_1 and set $|\psi_1\rangle = a_1|\phi_1\rangle + \Theta a_1|\phi_1\rangle$, which is clearly Θ–invariant: $\Theta|\psi_1\rangle = |\psi_1\rangle$. Next, take a second vector $|\phi_2\rangle$ *orthogonal to* $|\psi_1\rangle$ and set $|\psi_2\rangle = a_2|\phi_2\rangle + \Theta a_2|\phi_2\rangle$. Show that $\langle\psi_2|\psi_1\rangle = 0$. Continued application of this recipe results in a set of basis vectors $\{|\psi_n\rangle\}$, which obey $\langle\psi_m|\psi_n\rangle = \delta_{m,n}$ for an appropriate choice of the a_n. Finally, show that the Hamiltonian is real in that basis by proving that $H_{mn} = \langle\psi_m|H|\psi_n\rangle = H_{mn}^*$. Hamiltonians which can be given such a real–valued matrix representation are said to possess *time–reversal invariance* or *time–reversal symmetry*. This notion should not be confused with our notion of time–reversal symmetry: Also a Hamiltonian, which does not obey $[\Theta, H] = 0$ for an anti–unitary operator Θ with $\Theta^2 = I$, gives rise to a time–reversal symmetry of the *dynamics* as defined at the beginning of this appendix.

As a consequence of the previous exercise, we can choose without loss of generality $|E\rangle = \Theta|E\rangle$ for any energy eigenstate $|E\rangle$ if $[\Theta, H] = 0$ and $\Theta^2 = I$. In contrast, let us now consider the second option: $[\Theta, H] = 0$ with $\Theta^2 = -I$. We then confirm

$$\langle E|\Theta E\rangle = \left\langle \Theta E|\Theta^2 E\right\rangle^* = -\langle\Theta E|E\rangle^* = -\langle E|\Theta E\rangle. \tag{C.30}$$

Hence, $\langle E|\Theta E\rangle = 0$, which implies that $|E\rangle$ and $\Theta|E\rangle$ are two *orthogonal* states with the same energy eigenvalue. Thus, all eigenvalues of a Hamiltonian obeying $[\Theta, H] = 0$ with $\Theta^2 = -I$ are doubly degenerate. This result is known as *Kramer's degeneracy.*

After this excursion how to define the time–reversal operator Θ for quantum systems, let us return to the dynamical picture. Consider a Hamiltonian $H(\lambda_t)$ with some driving protocol λ_t, $t \in [0, \tau]$. The time evolution operator for the forward time evolution can be approximated as

$$U(\tau, 0) \approx e^{-iH(\lambda_{N-1})\delta t/\hbar} \dots e^{-iH(\lambda_0)\delta t/\hbar}, \tag{C.31}$$

where we divided the time interval into steps of size $\delta t = \tau/N$ and implicitly keep in mind the limit $N \to \infty$ in which eqn (C.31) becomes exact. From our basic equation (C.17) we can then infer that the conjugate dynamics are described by the time evolution operator

$$\begin{aligned} U_\Theta(\tau, 0) &= \Theta U^\dagger(\tau, 0)\Theta^{-1} \\ &= \Theta e^{iH(\lambda_0)\delta t/\hbar} \dots e^{iH(\lambda_{N-1})\delta t/\hbar}\Theta^{-1} \\ &= e^{-iH_\Theta(\lambda_0)\delta t/\hbar} \dots e^{-iH_\Theta(\lambda_{N-1})\delta t/\hbar}. \end{aligned} \tag{C.32}$$

In the last equation, we defined $H_\Theta(\lambda_t) \equiv \Theta H(\lambda_t)\Theta^{-1}$. Thus, as expected from the classical case, the conjugate dynamics are defined by changing the protocol backwards in time from λ_τ to λ_0 with respect to the time–reversed Hamiltonian. Again in unison with the classical case, the time–reversed Hamiltonian describing a particle in an external magnetic field B can be obtained by simply flipping the magnetic field: $\Theta H(B, \lambda_t)\Theta^{-1} = H(-B, \lambda_t)$. Note, however, that it is *not* true that $\Theta B \Theta^{-1} = -B$. Treated as an *external* field, B is simply a real–valued parameter, which remains unaffected by the time–reversal operator Θ.

Finally, in the last exercise we prove and generalize a statement, which we used in Section 2.3 to derive the important relation of *local detailed balance.*

Exercise C.7 Consider first two observables $X = \sum_x x\Pi(x)$ and $Y = \sum_y y\Pi(y)$ and their time–reversal $\Theta X \Theta^{-1} = \sum_x x\Pi_\Theta(x)$ and $\Theta Y \Theta^{-1} = \sum_y y\Pi_\Theta(y)$. Show the validity of the following identity:

$$\text{tr}\{\Pi(y)U(t, 0)\Pi(x)U^\dagger(t, 0)\} = \text{tr}\{\Pi_\Theta(x)U_\Theta(t, 0)\Pi_\Theta(y)U_\Theta^\dagger(t, 0)\}. \tag{C.33}$$

Now, recall that the rate to jump from a coarse–grained state x' to x under the assumption of time scale separation was computed in eqn (2.41) and, writing $\Pi(E, x) = \Pi_{E,x}$, reads:

$$R_{x,x'} = \frac{1}{\delta t}\frac{1}{V_{E,x'}}\text{tr}\{\Pi(E, x)U(\delta t)\Pi(E, x')U^\dagger(\delta t)\}. \tag{C.34}$$

We now consider the time–reversed process. The rate to jump from a time–reversed coarse–grained state x_Θ to x'_Θ under the assumption of time scale separation becomes

$$R^\Theta_{x'_\Theta, x_\Theta} = \frac{1}{\delta t}\frac{1}{V_{E,x}}\text{tr}\{\Pi_\Theta(E, x')U_\Theta(\delta t)\Pi_\Theta(E, x)U_\Theta^\dagger(\delta t)\}. \tag{C.35}$$

Note that the number of microstates remains unchanged by the time–reversal operator: $V_{E,x_\Theta} = \mathrm{tr}\{\Theta\Pi_{E,x}\Theta^{-1}\} = \mathrm{tr}\{\Pi_{E,x}\}^* = V_{E,x}$. From eqn (C.33) it follows directly that

$$\frac{R_{x,x'}}{R^{\Theta}_{x'_\Theta,x_\Theta}} = \frac{V_{E,x}}{V_{E,x'}} = \exp\left[\frac{S_B(E,x) - S_B(E,x')}{k_B}\right], \tag{C.36}$$

which is the local detailed balance relation in full generality. The conventionally considered case from Section 2.3 assumes that the observable is even, $X = \Theta X \Theta^{-1}$, and the Hamiltonian has time–reversal invariance, $H = \Theta H \Theta^{-1}$. Under these circumstances $R^{\Theta}_{x'_\Theta,x_\Theta} = R_{x',x}$ and eqn (C.36) reduces to the conventional local detailed balance condition (2.43).

C.3 The Arrow of Time

After the mathematical treatment of time–reversal symmetry, we discuss some physical and philosophical implications. In fact, the world around us does not seem to obey time–reversal symmetry: ageing, the ability to remember the past but not the future, and the fact that the rich get richer and the poor poorer are three simple examples, which demonstrate our inability to reverse the **arrow of time** in our everyday life. Evolution, the second law of thermodynamics and the expansion of the universe are three further examples, which seem to show a clear arrow of time. But how can such an arrow of time emerge, when the underlying equations of motion obey time–reversal symmetry?

This apparent paradox was articulated by Loschmidt and Zermelo, who critically questioned Boltzmann's attempt in 1872 to derive the second law of thermodynamics on a purely mechanical and microscopic basis. Loschmidt in 1876 pointed out that a purely mechanical derivation to reach (and maintain) a stationary (i.e., equilibrium) state from some arbitrary initial state contradicts time–reversal symmetry. This argument is known as Loschmidt's *Umkehreinwand*, i.e., Loschmidt's *objection* based on (time–)*reversal*. In addition, Zermelo in 1896 pointed out that Poincaré's recurrence theorem forbids the derivation of a stationary state from an initial non–stationary state as the state of an isolated mechanical system must eventually return (very close) to its initial state. This argument is known as Zermelo's *Wiederkehreinwand*, i.e., Zermelo's *objection* based on *recurrences*.

However, both, Loschmidt and Zermelo, seemed to be unaware of the fact how *unlikely* these arguments are for macroscopic systems. The vast majority of states of a macroscopic isolated mechanical system with a fixed energy closely resemble a maximum entropy state and the Poincaré recurrence time becomes immeasurably large (compare also with Section 1.3). Boltzmann instead seemed to be fully aware of these arguments and emphasized the statistical character of the second law (as also Maxwell did) in his replies.

Nevertheless, even more than hundred years after these objections, controversies about the origin of the arrow of time are still not fully settled. As the major purpose of this book is to clarify the foundations of quantum and classical stochastic thermodynamics, which necessarily includes also various arguments used to 'derive' the second law of thermodynamics, it seems worthwhile to point out a few interesting observations—without any intention to provide a complete resolution.

A first question one could wonder about is whether the mathematical construct of time–reversal symmetry actually describes well the philosophical or human idea we associate with it. In fact, often time–reversal symmetry is epitomized by the transformation '$t \mapsto -t$,' but as we saw above this very simple mapping does not correctly describe time–reversal symmetry, which is a much more complicated construction in general. Perhaps due to this reason some people prefer to speak about 'microreversibility' instead of 'time–reversal symmetry' and Wigner himself noted that it would be more appropriate to speak about "reversal of the direction of motion." Putting this question aside, let us proceed by assuming that the mathematical construct above correctly describes time–reversal symmetry.

Next, one could wonder whether the second law of (phenomenological) thermodynamics can be actually used to prove the arrow of time. In fact, the second law of thermodynamics is probably *the* outstanding physical law, which does not possess time–reversal symmetry. However, remember that the laws of phenomenological thermodynamics are *postulates* or *axioms* in accordance with human experience (in the same way as Newton's or Schrödinger's equation are axioms in classical or quantum mechanics). Thus, saying that the second law proves the arrow of time is a tautology in so far as it simply shifts the problem from proving the arrow of time to proving the increase in entropy. At least, however, it gives us evidence that the arrow of time is linked to another physical concept, namely *entropy.* Thus, let us accept the idea that the second law of thermodynamics relates to the arrow of time.

But now, when we try to derive the second law from an underlying microscopic theory, we are back to Boltzmann's problem. Undeniably, our knowledge how to 'derive' the second law of thermodynamics has improved since Boltzmann and many ways to do so are presented in this book. However, all the ways the author is aware of share one common feature: The increase in entropy is only proven with respect to some special initial state. Thus, whereas we might be nowadays able to prove the second law under increasingly mild assumptions, we were *not* yet able to prove the arrow of time since all our derivations rely on a particularly chosen boundary condition. To put it differently: We could replace in this book the original Hamiltonian with its time–reversed counterpart, yet we were still able to prove the second law in the same way as before. The second laws in this book do *not* explain the arrow of time.

This insight strongly suggest that the second law is *not a consequence of the microsopic equations of motion*, as already clearly stated by Boltzmann: "The Second Law can never be proved mathematically by means of the equations of dynamics alone." But of what is the second law then a consequence? One of Boltzmann's ideas, which he attributes to his assistant Schuetz, was the following. First, they assumed that the entire universe is in global equilibrium. Then, since they knew about the *statistical* character of thermodynamics, they concluded that there must be local fluctuations in the entropy of the universe. If the universe is sufficiently large, the chances for the existence of a very low entropy region somewhere in the universe could be sufficiently high. The fact that we experience a second law, and the fact that we even exist, is then a consequence of living in such a rare entropy fluctuation. This scenario is illustrated in part (a) of Fig. C.4.

This idea has been met with scepticism. One point of criticism is that a small

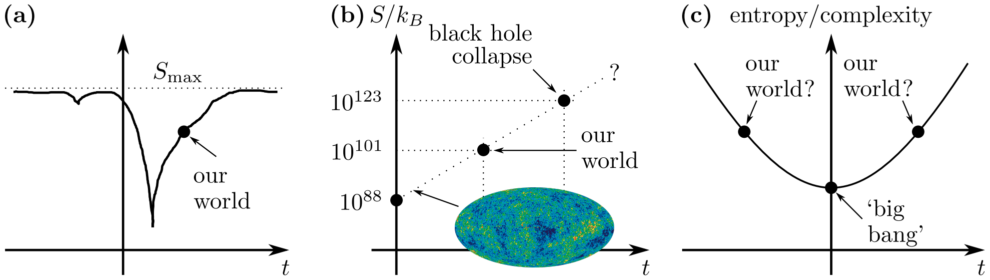

Fig. C.4 Three scenarios explaining the arrow of time in the cosmological universe. (a) An eternal and infinite universe showing a large spatiotemporal downward fluctuation in entropy away from its maximum value $S_{\max}$. (b) The big bang initialized the universe in a low entropy state of approximately $S_0 = 10^{88} k_B$ ('past hypothesis'). Shortly afterwards, the universe becomes transparent and the image of the cosmic microwave background (NASA/WMAP Science Team) shows radiation in almost perfect equilibrium (puzzle: why is this state not already close to maximum entropy in this scenario?). The entropy value $10^{123} k_B$ is computed by collapsing all matter and energy of the universe into a black hole. However, since black holes evaporate, this is not the end of the story. (c) Cosmological model that is time–reversal symmetric on large scales with a low entropy (or complexity) value at the centre (the 'big bang') and arrows of time emerging from there in both directions.

local entropy fluctuation, which only creates a *single* observer, whose brain gives the *impression* that we live in the current universe, is much *more likely* than a large local entropy fluctuations, which creates a low entropy observer together with a low entropy earth together with a low entropy solar system together with a low entropy galaxy, etc. The creation of such a single conscious observer by spontaneous thermal fluctuations is known as the **Boltzmann brain** problem.

Therfore, most researchers believe today that it is much more likely that the second law is *a consequence of the initial state of the universe right after the Big Bang* (the concept of the Big Bang was not known to Boltzmann and his contemporaries). In fact, if the thermodynamic entropy of the initial state of the universe was sufficiently low, an increase of thermodynamic entropy could be observed for a *very long* time, thus effectively explaining the second law of thermodynamics. This is also known as the **past hypothesis**. This scenario is illustrated in part (b) of Fig. C.4.

Notice that, even if the past hypothesis was true, it does not seem to explain why the *concept of time* (independent of any *arrow*) exists at all. Perhaps it turns out that the Hamiltonian of the universe is not time–reversal invariant. In fact, violations of time–reversal invariance *were observed* in systems described by electroweak interactions. Electroweak interactions could therefore explain the fundamental asymmetry between time and space. Furthermore, although the past hypothesis explains the *thermodynamic* arrow of time, it is not clear whether it also explains, e.g., the biological arrow of time: Is evolution, ageing, or the ability to remember the past but not the future a consequence of the second law?

We conclude by mentioning a third alternative to explain the emergence of an arrow of time on a cosmological scale, where a time–reversal symmetric universe has two branches, each locally defining its own arrow of time. This is illustrated in part (c) of Fig. C.4. In fact, it has been argued that this situation could be generic. Also doubts has been expressed about the applicability of the entropy concept to the universe as a whole because the general definition of gravitational entropy (except for the case of a black hole) remains unclear. Perhaps another concept (loosely called ‘complexity’ in Fig. C.4) is required to explain the arrow of time in the universe?

Further reading

Much of our knowledge about time–reversal symmetry, and symmetries in general in quantum mechanics, goes back to Wigner (1959). Finding pedagogically useful accounts of time–reversal symmetry in standard textbooks on quantum mechanics is, however, not so easy, but see, for instance, the book of Sakurai (1994) for an exception. The question whether a Hamiltonian is invariant under time–reversal is also very important in the field of quantum chaos and part of my exposition was inspired by the book of Haake (2010).

The phrase ‘arrow of time’ was popularized in a book by Eddington (1928). Another historically important review about statistical mechanics, including many citations to the original references from Boltzmann, Loschmidt, Zermelo, and others, can be found in the treatise of Ehrenfest and Ehrenfest (1911), which was translated into English by Moravcsik (Ehrenfest and Ehrenfest, 1959). I also directly quoted from Boltzmann (1895). Another modern and less technical account of many of the ideas I discussed above is given by Lebowitz (1993). I should also mention here the numerous research efforts showing why and how isolated quantum systems can effectively equilibrate, even if they are initialized out of equilibrium in a pure quantum state (Gemmer *et al.*, 2004; D’Alessio *et al.*, 2016; Borgonovi *et al.*, 2016; Gogolin and Eisert, 2016; Goold *et al.*, 2016; Deutsch, 2018; Mori *et al.*, 2018). To the best of my knowledge, however, also this complementary line of research cannot establish an asymmetry in time: Isolated quantum systems initialized out of equilibrium seem to equilibrate in both directions of time. Cosmological considerations about entropy and the arrow of time can be found at various places. The name ‘past hypothesis’ was coined by Albert (2000). The entropy estimates in part (b) of Fig. C.4 are due to Penrose (1989). A time–symmetric universe explaining an entropic arrow of time was suggested by Carroll and Chen (2004). Criticsim about the use of the entropy concept in cosmology can be found, e.g., in the article by Earman (2006). A generic explanation of a time–symmetric scenario with an arrow of time in terms of a complexity measure was found by Barbour *et al.* (2014). For further research on the question how the concept of time can emerge at all see Vaccaro (2016) and references therein.

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