Martin Janßen

Generated Dynamics of Markov and Quantum Processes

Springer

Generated Dynamics of Markov and Quantum Processes

Martin Janßen

Generated Dynamics of Markov and Quantum Processes

Springer

Martin Janßen
Institut für Theoretische Physik
Universität zu Köln
Köln
Germany

ISBN 978-3-662-49694-7 ISBN 978-3-662-49696-1 (eBook)
DOI 10.1007/978-3-662-49696-1

Library of Congress Control Number: 2016937355

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer-Verlag GmbH Berlin Heidelberg

So then we just hack it all apart, take out all the complicated bits, and keep it simple

Ritchie Blackmore

To Lucia

Preface

Theoretical physics evolved from Newton's mechanics to a general theory for modeling dynamical systems. Theoretical physicists not only earn their income by investigating traditional physical systems like particles, condensed matter and star systems, but also by applying their modeling skills on economics, informatics, medicine, psychology, biology, environment, climate, language and sociology. This is to a substantial part caused by a very flexible toolbox theoretical physicists learn to use. It is this toolbox which makes physics a science with strong impact on man and nature. This book is about the organization of this toolbox. Though, it is intended as a little entertaining piece of natural philosophy and not as a nosh for the military-industrial complex.

The central aim of this book is to present Markov and quantum processes as two sides of a coin called generated stochastic processes. Quantum processes are reversible stochastic processes generated by one-step unitary operators while Markov processes are irreversible stochastic processes generated by one-step stochastic operators. The characteristic features of quantum processes are oscillations, interference, lots of stationary states in bounded systems and possible asymptotic stationary scattering states in open systems, while the characteristic features of Markov processes are relaxations to a single stationary state. Quantum processes apply to systems where all variables that control reversibility are taken as relevant variables, while Markov processes emerge when some of those variables cannot be followed and are thus irrelevant for the dynamic description. Their absence renders the dynamic irreversible. Once one realizes that Markov processes are incapable to describe reversibility, a necessity for the description of reversible stochastic processes arises and abstract quantum theory does this job in close analogy as Newton mechanics does the job for deterministic processes. Newton's invention as compared to Aristotle's view was the introduction of two properties serving as initial condition. The initial coordinate plus the initial velocity are needed to formulate deterministic reversible processes. Similarly, for stochastic processes not only the initial probability density defines the state (as in Markov processes), but also the probability current density specifies the state in order to define reversible stochastic processes. Both quantities must be independent except for the probability conservation. By generating probability density and current density from a two component pre-probability,[1] unitary quantum theory reaches this goal in a most elegant and compact way. In that sense the pre-probability as a complex wave function does have a very clear and—to me—intuitive physical interpretation: its squared modulus is the positive probability density and its phase generates the probability current density as the two components of a state for a reversible stochastic process. A similar more mathematically oriented reconstruction of quantum theory as a theory for reversible stochastic processes was formulated by Hardy in 2001.[2]

A further aim is to demonstrate that almost any subdiscipline of theoretical physics can conceptually be put in the context of generated stochastic processes. Classical mechanics and classical field theory are about deterministic processes which emerge when fluctuations in relevant variables are negligible. Quantum mechanics and quantum field theory are about genuine quantum processes. Equilibrium and non-equilibrium statistics apply to the regime where relaxing Markov processes emerge from quantum processes by omission of a large number of uncontrollable variables. Systems with many variables often self-organize such that only few slow variables can serve as relevant variables. Symmetries and topological classes are essential in identifying such relevant variables.

The third aim is to provide conceptually general methods of solutions which can serve as starting points to find relevant variables as well as to apply best practice approximation methods. Such methods are available through generating functionals.

The potential reader is a graduate student who likes to learn about quantum systems from few to many particles and about stochastic processes in a unifying way. She or he has heard already a course in quantum theory and equilibrium statistical physics including the mathematics of spectral analysis (eigenvalues, eigenvectors and Fourier and Laplace transformations) and may also have had some contact to the particle number representation of many body systems. The book does not follow the standard route of the present day's theoretical physics education[3] and does not focus on one particular subject of such education. The reader should be open for a unifying look on several topics. If she or he then likes to be educated in one particular subject like condensed matter theory or particle physics or Markov processes in many of their facets, she or he may consult the texts cited in the book at appropriate points.

[1] A notion lend from R.B. Griffiths: Consistent Quantum Theory, Cambridge University Press, 2002.

[2] L. Hardy: Quantum Theory From Five Reasonable Axioms, arXiv:quant-ph/0101012v4.

[3] See however the lecture notes of J. Chalker and A. Lukas, where quantum processes and Markov processes are discussed together: J. Chalker, A. Lukas: Lecture Notes on M. Phys Option in Theoretical Physics: C6, http://www-thphys.physics.ox.ac.uk/people/JohnChalker/theory/lecture-notes.pdf.

I was first impressed by the richness of Markov processes by a lecture in 1987 of my teacher János Hajdu and later in the 1990s by the applications in original research by my teachers John Chalker and Boris Shapiro. I came to apply them in my own work and gave a lecture course in 1998 based on these experiences. I became aware that the Chapman–Kolmogorov equation is very similar to the unitary time evolution in quantum theory and found a remark in a book of C.F. von Weizsäcker[4] which I interpret in the following way: quantum theory does not formulate a new probability theory but only a new dynamics for probabilities as compared to the Chapman–Kolmogorov dynamics. I liked to elaborate on this idea and so the original plan of writing a book on Markov processes evolved over more than 10 years into its present state.

I like to thank Claus Ascheron from Springer for his patience and encouragement to finally transform my collection of lecture notes into a book. I also wish to thank János Hajdu for his long-lasting intellectual and emotional support and for many enlightening discussions over these years. Big thanks the students of my courses who helped very much to shape the final content. Special thanks go to Stefan Brackertz and Patrick Sudowe for intensive discussions about notions and interpretations. Finally, I thank my father, Theo Dores Janssen, for having confidence in me and for initiating my desire to clean up the desk.

Krefeld Martin Janßen
April 2016

[4] C.F. von Weizsäcker: Aufbau der Physik, dtv, pp. 309–310, 1988.

Contents

About the Author

Martin Janßen is a private lecturer at the Institute of Theoretical Physics at the University of Cologne and a high school teacher at the Friedrich-Wilhelm-Gymnasium in Cologne.

He gained his doctorate in 1990 in Cologne for his work on magnetotransport and multifractality in the context of the quantum Hall effect and his Venia legendi in 1997, on completion of his postdoctoral thesis on statistics and scaling in mesoscopic electron systems. He received a DFG Postdoctoral Fellowship at Oxford University in 1993 and a MINERVA Postdoctoral Fellowship at Haifa University in 1995. He has been a member of academic staff at the University of Cologne from 1992 to 1998 and at Bochum University from 1998 to 2001. After working as an environmental physicist from 2001 to 2011, he became a high school teacher in physics and mathematics. Since 2001 he gives lectures at the University of Cologne on Theoretical Physics with an emphasis on dynamics of stochastic processes. He has co-written a book on the integer quantum Hall effect and has written a book on fluctuations and localization in mesoscopic electron systems.

Chapter 1
Introduction—Dynamics of Relevant Variables

In physical modeling one faces almost contradictory requirements. We want to catch up with reality, but by definite notions and mathematical relations. We like to describe fast dynamical and slow—or even static—situations. We try to understand the sub-microscopic down to 10^{-34} m and the universe up to 10^{26} m. We want to know the properties of single elementary particles and of complex systems coupled to environments. The complexity of modeling is drastically reduced if one can find a set of few **relevant variables** appropriate for the specific questions to be answered. It turns out that often relevant variables emerge within a more detailed theory with elementary variables. Relevant variables are typically the slow variables in a system. When dynamically time scales begin to separate, relevant variables emerge. The best known example is thermodynamics where internal microscopic variables are summed up in a partition sum and only environmental conditions of equilibrium like temperature, chemical potential, pressure and applied magnetic field are known to calculate system properties like average energy, particle density and magnetization or secondary quantities like specific heat and magnetic susceptibility.

Despite the diversification of physics into many disciplines like atomic physics, optics, nuclear physics, particle physics, astrophysics and condensed matter physics it turned out in the last decades that a common methodological frame for theoretical physics exists, which allows an overall view on basic concepts in theoretical physics. This overall view can briefly be characterized as follows.

1. Theoretical physics is about models for probabilities of varying properties in stochastic processes. These probabilities are empirically controlled by counting documentable facts. In the modeling one tries to use as few as possible relevant variables. This is the most creative job in physical modeling as the finding of relevant variables is not automatic, yet.
2. A dynamical description of a system is given in terms of a step by step evolution, which Mathematicians call a (semi-)group.
3. When **fluctuations** in the relevant variables are inessential, a time evolution can be formulated directly for the relevant variables. The process is then called a deterministic process and it is described locally in time by differential equations

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1_1

which solutions become determined paths starting at some initial value. When fluctuations are essential, the time evolution is searched for the **probability** distribution of relevant variables. Probability conservation relates the probability distribution to a probability current.

4. On each level of description one can however distinguish between two fundamental different classes of dynamics: **reversible and irreversible**.
5. Stationary states of a dynamic always play an important role, e.g. as asymptotic situations for scattering processes or as limiting situations of processes or as building blocks in analyzing the dynamics.
6. Irreversible processes with step by step evolution can be described in terms of a Chapman-Kolmogorov equation for the probability distribution and are called Markov processes. The corresponding local in time equation is called Master equation.
7. To reach reversible step by step evolution equations for processes with essential fluctuations, it turns out that it cannot be formulated directly for the probability distribution. It leads by its close relation to the current density generically to relaxation and irreversibility. Fortunately, it can instead be formulated for a two-component quantity called **pre-probability**. The components (put together as a complex number with modulus and phase) allow to calculate probability density and the current density as independent quantities, except for the probability conservation fulfilled automatically by construction. This theory of reversible step by step stochastic processes is just abstract quantum theory without explicit use of the quantum of action. The corresponding local in time equation is called Schrödinger equation. Fluctuating reversible step by step processes are called quantum processes.
8. Both, Markov and quantum processes can be solved formally by elegant and powerful methods exploiting the step by step character leading to **generating functionals** for all quantities of interest. Analyzing symmetries and topological constraints helps in moving from formal solutions by clear strategies of approximations to explicit approximate solutions.

To imagine the difference between reversible and irreversible processes consider watching a movie. A movie of reversible processes can be played in reverse and you will not take notice of this fact, while in situations of irreversible processes you will find the movie "funny". The funny things are seemingly impossible motions. In reality they could only happen after an extraordinary sophisticated rearrangement of environment and initial conditions.

In reversible dynamics the notion of **energy** plays a key role. It is the generator of motion and serves as a conserved quantity that separates possible motions from impossible motions (see Fig. 1.1).

In irreversible systems the notion of **current** through the system and the notion of **entropy** play key roles (see Fig. 1.2). The entropy measures the dispersion of states in the space of possible states. In irreversible systems this dispersion increases unless it has reached a stationary state. In regions of currents between reservoirs new

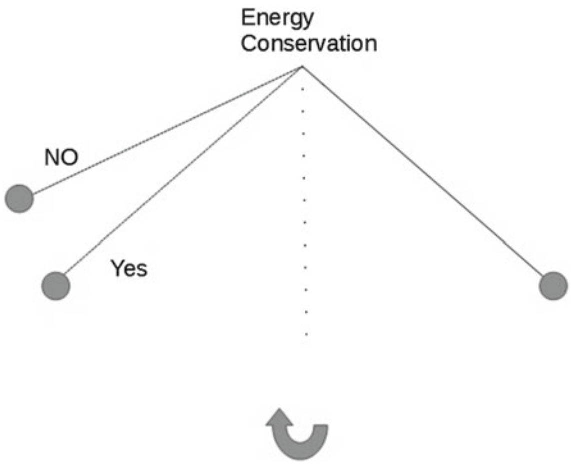


Fig. 1.1 Energy conservation

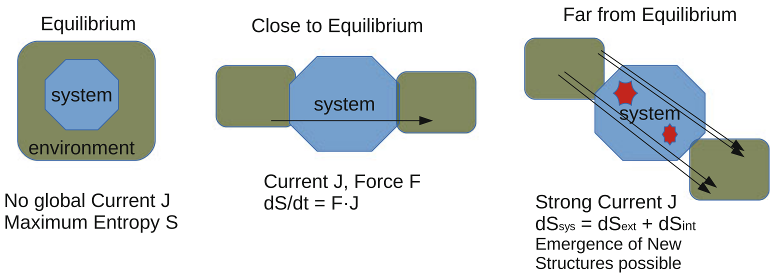


Fig. 1.2 Equilibrium and non-equilibrium

structures can emerge, while in global equilibrium global currents vanish. Therefore, entropy indicates which of several energetically allowed motions will probably take place.

In this book a physical system is defined by a set of relevant variables which form the **configuration manifold**. This manifold can be enlarged or (more often) reduced, the variables can be transformed and they have a time evolution. **Properties** of a physical system are functions on the configuration tangent bundle or cotangent bundle. The tangent bundle contains the configuration point x and local tangential vectors to describe velocities $\dot{x}$. Instead of vectors one can take a **dual** description in terms of linear forms on vectors. Actually, we usually gain information about vectors by linear forms. A basis of the vector space at a given point x is the Gaussian basis ∂_{x_k} and the dual basis is dx_j with $dx_j(\partial_{x_k}) = \delta_{jk}$. Discrete variables and their (perhaps discrete) time evolution are meant to be included in this notion; tangential objects are deviations in short time.

The methods presented here are thought to provide an organized toolbox for modeling quite general physical systems. The general strategy is: we like to calculate **expectation values** and **correlations** of properties of relevant variables evolving in time, usually under some pre-described conditions. We use models where dynamic and stationary expectation values and correlations can be calculated from generating functionals.[1] The functionals are often called **effective action**. To reach such generating functionals one exploits duality whenever possible. Duality means that variables often have dual partners with respect to functionals, e.g. coordinate x and wave number k are dual by the function e^{ikx}. Fourier-Laplace and Legendre transformations are typical examples of changing from variables to dual variables. The underlying dynamics is modeled by Markov or quantum processes and limiting behavior of such processes. Such limits can be stationary equilibrium, stationary non-equilibrium, scattering situations, decoherent situations (crossover from quantum to Markov behavior) and so called classical deterministic behavior (negligible fluctuations for relevant variables). In finding relevant variables (usually the slow ones in a system) symmetries and topology of the configuration manifold are most helpful. Topology can lead to distinguished classes on the configuration manifold which can—to a large extent—be treated separately and symmetries help optimizing the choice of coordinates for configurations. A crucial indicator for being on the right track is: a **stability analysis** based on an expansion beyond a so called Gaussian approximation (quadratic approximation around a characteristic point) in relevant variables shows the right qualitative phase structure. Such stability analysis often runs under the name of renormalization group analysis. This modeling strategy is displayed in Fig. 1.3. To illustrate the methods we try to keep the formal and calculation effort low and try to use significant but simple examples instead of trying to reach full generality. We will consider simple abstract systems, simple toy systems and some model systems for real phenomena, e.g. ink in water, Laser light, the quantum Hall effect and superconductors.

The book is organized as follows. In Chap. 2 we introduce the dynamics with semi-group or group character. States evolve step by step from an initial state. For reversible systems the group has inverse elements as part of the dynamics. For semi-groups an inverse does not necessarily exist within the semi-group. The short time steps are captured by a time homogeneous generator resulting in differential equations in continuous time. States can be configurations, probabilities or pre-probabilities for configurations. In Chap. 3 formal methods of solving the dynamics are discussed. These are of algebraic or analytic type which both have some advantages as a starting point for approximate methods. In rare cases they even allow for explicit solutions. The analytic formal solutions by generating functionals (path integrals, partition sums) are most convenient as starting points for modeling systems by appropriate relevant variables, as displayed in Fig. 1.3. To enrich the toolbox in modeling it is helpful to know exactly solvable models and a variety of methods of finding them. This is the subject of Chap. 4. Then we broader the view in Chap. 5 and work out a theory where properties and states are generalized as to have compact and flexible ways of calculation. We consider limits of stationarity and cross-over between different types of dynamics by taking system environments into account. In each type of

[1] Functionals stand for functions in perhaps infinitely many degrees of freedom.

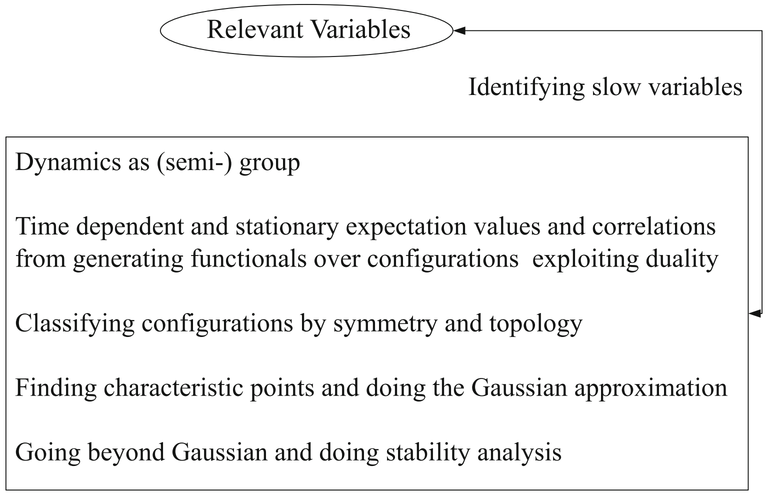


Fig. 1.3 Modeling strategy

dynamics or stationary limit, generating functionals appear as the unifying structure. When fields form the configuration space for infinitely many degrees of freedom one deals with stochastic field theories. In the case of quantum processes these are so called quantum field theories. They are met commonly in particle physics and condensed matter physics. As stressed before, one should study the topology and symmetry of the starting configuration space with respect to the generating functional to identify relevant variables. Thus, symmetry and topology are the subjects of Chaps. 6 and 7. Finally we use the toolbox in Chap. 8 for some selected applications of the author's choice to demonstrate their richness. Three appendices may help filling gaps for readers not yet familiar with probability theory (Appendix A), the method of characteristics (Appendix B) and many-body terminology (Appendix C).

Chapter 2
Generated Dynamics

Abstract We introduce dynamics with semi-group or group character. States evolve step by step from an initial state. For reversible systems the group has inverse elements as part of the dynamics. The short time steps are captured by a time homogeneous generator resulting in differential equations in continuous time. States can be configurations, probabilities or pre-probabilities for configurations. We discuss some simple prototypical systems and comment on randomness and determinism in stochastic processes.

2.1 Algebraic Structure of Causal Step by Step Dynamics

When modeling time evolution of a physical system, we look for equations of generated (semi-)group character, because they reflect **causality** and **time homogeneity** in the following sense: for each situation there is a situation earlier in time, such that it can be considered as causing the later situation. The time difference can be chosen arbitrarily. The physical laws as such should not depend on the time of application. Formally, we can incorporate this by a time-independent generator for time evolution, such that for a given initial state the time evolution follows by successive application of transformations which form a semi-group[1]

$$\boxed{T_{t_3-t_2} \cdot T_{t_2-t_1} = T_{t_3-t_1}} \tag{2.1}$$

with

$$T_0 = 1. \tag{2.2}$$

For discrete time steps of width δt, the **generator** G is from the group's tangent space and transforms a state to the next state δt ahead in time,

[1]The difference between semi-group and group is: in semi-groups not every element has an inverse.

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1_2

$$T_{\delta t} = 1 + G \cdot \delta t. \tag{2.3}$$
$$T_{k\cdot\delta t} = (1 + G \cdot \delta t)^k. \tag{2.4}$$

For continuous time t, the generator G is the derivative of the group element with respect to t at $t = 0$,

$$G = \lim_{\delta t \to 0} \frac{T_{\delta t} - 1}{\delta t}, \tag{2.5}$$

which yields a simple solution for the full time evolution operator in terms of the exponentiated generator (it solves the corresponding differential equation).

$$\boxed{T_{t-t_0} = e^{(t-t_0)\cdot G}}. \tag{2.6}$$

The natural dimension of a generator G is inverse time (frequency). Equations (2.5, 2.6) are central to the idea of (semi-)group dynamics: time evolution is step by step and solving for short times allows to calculate for long times.

The defining feature of a **state** is that it can serve as an initial condition of the (semi-)group dynamics. The time evolution operator operates on states,

$$\text{State}_t = T_{t-t_0}\, \text{State}_{t_0}. \tag{2.7}$$

In this book a state can consist of properties or of a probability for properties or of a pre-probability for properties.

We call a system reversible, if for each transformation T_{t-t_0} an inverse transformation exists, which also describes a possible time evolution of the system, otherwise irreversible. Thus, reversible systems have a time evolution with group character while irreversible systems have a time evolution with semi-group character.

2.2 Deterministic Processes

For deterministic processes the generator G acts as a local differential operator on states which are fixed by coordinates x only, or by elements of the tangential bundle (coordinates and velocities) $(x, \dot{x})$, or by elements of the co-tangential bundle (x, p), also denoted as phase space of the system. In the first case, which we like to denote as **Aristotelian processes**, the generator looks like

$$G = Ar = g(x)\partial_x \tag{2.8}$$

with some function $g(x)$, thus leading to

$$\dot{x} = g(x) \tag{2.9}$$

and more generally to an equation of motion for any property $f(x)$,

$$\dot{f}(x) = f'(x) \cdot g(x). \tag{2.10}$$

Such dynamics cannot be reversible, since at a given value of x there is only one value of $\dot{x}$ and the motion cannot be turned back. Reversible dynamics is possible with states taken from the tangent bundle. The historic invention of Newton corresponds to the following generator

$$G = N = \dot{x}\partial_x + a(x)\partial_{\dot{x}} \tag{2.11}$$

with some function $a(x)$ describing the acceleration as $\ddot{x} = a(x)$. Since the acceleration is of second order in time derivatives, at a given point, the velocity can be reversed and the motion can be turned back. The general equation of motion of **Newton processes** then reads

$$\dot{f}(x, \dot{x}) = \partial_x f(x, \dot{x}) \cdot \dot{x} + \partial_{\dot{x}} f(x, \dot{x}) \cdot a(x). \tag{2.12}$$

With the help of the phase space an additional structure besides possible reversibility can be fulfilled: the invariance of the volume element $\mathrm{d}x \wedge \mathrm{d}p$ under the time evolution. This so-called **Liouville's theorem** allows for a proper counting of states in statistical physics based on the phase space. The processes that ensure Liouville's theorem are called **Hamilton processes**, where the generator has the form of Poisson's bracket

$$G = \{H(x, p), \cdot\} := (\partial_p H(x, p))\partial_x \cdot -(\partial_x H(x, p))\partial_p \cdot, \tag{2.13}$$

with a so-called Hamilton function $H(x, p)$. The equation of motion in Hamilton dynamics together with the relation between $\dot{x}$ and p read

$$\dot{x} = \partial_p H(x, p) \;\; ; \;\; \dot{p} = -\partial_x H(x, p). \tag{2.14}$$

The general equation of motion then reads

$$\dot{f}(x, p) = \partial_x f(x, p) \cdot \partial_p H(x, p) - \partial_p f(x, p) \cdot \partial_x H(x, p). \tag{2.15}$$

Of course, the Hamilton function itself stays invariant under the dynamics. Interpreted as a property of the system it is then called energy of the system. This energy is conserved in Hamilton processes. We mention in passing that Newton and Hamiltonian dynamics are equivalent in many cases, since p and $\dot{x}$ are related, such that $\dot{p} = -\partial_x H(x, p)$ leads to a second order differential equation for x.

Thus, for deterministic processes the variable x or $(x, \dot{x})$ fulfill closed differential equations. Equations (2.11, 2.12) are just abstract in a single variable x for the much broader class of differential and partial differential equations in physics for relevant variables. Examples are the Euler equations for rigid body coordinates, Navier-Stokes equation for fluid field, Maxwell equations for electromagnetic fields, Helmholtz equation for wave fields and Einstein's equation for geometric fields. All of these equations represent deterministic (semi-)group equations for the relevant variables under consideration.

As a simple toy-example consider the Aristotelian model of motion on earth $g(x) = -kx$ with positive k. The solution reads

$$x(t) = x_0 e^{-kt} \tag{2.16}$$

and describes irreversible relaxation to rest (at 0). Another example is the logistic equation of population dynamics $g(x) = rx(1 - x/k)$ with positive growth rate r and positive k. k describes finiteness of resources, such that exponential growth can't go on forever. The solution

$$x(t) = \frac{x_0 k}{x_0 + (k - x_0)e^{-rt}} \tag{2.17}$$

approaches a stationary state $x = k$ and is irreversible.

For reversible motions the velocity $\dot{x}$ must be taken into account as state variable. A prominent example is the harmonic oscillator model of motion in Newton dynamics or Hamilton dynamics, $\ddot{x} = -\omega^2 x$. The solution reads

$$x(t) = x_0 \cos(\omega t) + (\dot{x}_0/\omega) \sin(\omega t) \tag{2.18}$$

and describes reversible harmonic oscillations with conserved energy $E = \frac{1}{2}\left(\dot{x}^2 + \omega^2 x^2\right)$ (see Fig. 1.1).

2.3 Stochastic Processes

For stochastic processes the time evolution of a probability distribution[2] $P_t(x)$ for a random variable x is searched for. $P_t(x)\mathrm{d}x$ is the positive probability to find the actual value x within the volume element $\mathrm{d}x$ at time t, given appropriate initial conditions (for an introduction to probability concepts see Appendix A). We will consider two types of stochastic processes to be defined later: Markov and quantum processes. In the following subsection we clarify notations used in both cases.

2.3.1 General Notations

The random variable can be continuous[3] or discrete. In the discrete situation the random variable will sometimes be denoted as natural number n. Formally, it gives

[2]We use the terms probability density and probability distribution synonymously.

[3]The term continuous is used in a broad sense, e.g. C^∞ if appropriate.

rise to a continuous representation as $P_t(x) = \sum_n \delta(x-n) P_t(n)$ where $P_t(n)$ is the probability to find n at time t. The random variable can have f degrees of freedom. For simplicity we often stick to $f = 1$ and switch to $f > 1$ if a generalization is not straightforward

The distribution P_t serves to calculate **expectation values** of properties $f(x)$ as a linear operation on f and can be written as a symmetric real valued bilinear form of distribution vectors $|P_t)$ and (co-) vectors of properties $(f|$

$$\boxed{\langle f \rangle_t = \int \mathrm{d}x \; f(x) P_t(x) = (f|P_t)}. \tag{2.19}$$

The expectation value of the characteristic function of some volume V, denoted as $\chi_V(x)$, is the probability to find x within the volume V.

$$\langle \chi_V \rangle_t = P_t(V). \tag{2.20}$$

The average value of x is the expectation value of the identity function $(x \mapsto x)$, denoted as id_x. This average is often written as the left hand side of

$$\langle x \rangle_t = \langle id_x \rangle_t = (id_x|P_t). \tag{2.21}$$

The identity function should not be mixed up with the peak-function at x which is $x' \mapsto \delta(x'-x)$. The vector notation of the peak function at x is $(x|$ such that we have the relations

$$(x'|x) = \delta(x'-x) \tag{2.22}$$

$$(x|P_t) = P_t(x) \tag{2.23}$$

$$(f|x) = f(x). \tag{2.24}$$

2.3.2 Constraints by Conservation of Probability

Every time evolution equation must respect the **conservation of probability**:

$$\int \mathrm{d}x \; P_t(x) = (1|P_t) = \langle 1 \rangle_t = 1, \tag{2.25}$$

$$\sum_n P_t(n) = 1. \tag{2.26}$$

For a finite volume V it follows

$$\partial_t P_t(V) = -I_t(\partial V), \tag{2.27}$$

where $I_t(\partial V)$ is the probability current leaving V through the boundary ∂V.

In continuous time and for continuous variables x a **continuity equation** with probability current density $j_t(x)$ must be fulfilled,

$$\boxed{\partial_t P_t(x) = -\partial_x j_t(x)}. \tag{2.28}$$

In discrete time steps δt and with discrete variables n the probability conservation looks similar to Kirchhoff's knot rule

$$P_{t+\delta t}(n) - P_t(n) = \left[I_{\text{gain}}(n) - I_{\text{loss}}(n)\right] \delta t, \tag{2.29}$$

where $I_{\text{gain}}(n)$ is the sum of all probability currents from other quantities n' increasing the probability at n (gain) and $I_{\text{loss}}(n)$ is the sum of all probability currents from n to other quantities n', thus decreasing the probability at n (loss). Keep in mind (2.27–2.29) cannot serve as equations of motion but are constraints on any equation of motion. An equation of motion can result as soon as the current I or j is specified as a functional of P.

2.3.3 Markov Processes

For one large class of stochastic processes, called Markov processes, the defining feature is that the semi-group property applies directly to the probability distribution. In other words, the probability distribution serves as the state of the semi-group time evolution. The corresponding equation is called **Master equation**. In continuous time it reads

$$\boxed{\partial_t P_t = M P_t}, \tag{2.30}$$

where the operator M must be linear on the space of probability distributions to preserve expectation values $\langle f(x) \rangle_t = \int \mathrm{d}x\, f(x) P_t(x)$. The M-operator is the generator G of (2.5) for Markov processes. It can be represented as a positive integral kernel $M(x', x)$ or positive Matrix. Probability conservation requires that its sum over columns must be unity for the full time evolution operator $T_t = e^{tM}$ and zero for M,

$$\int \mathrm{d}x'\, T(x', x) = 1, \tag{2.31}$$

$$\int \mathrm{d}x'\, M(x', x) = 0. \tag{2.32}$$

Such stochastic matrices T do indeed form a semi-group. However, inversion—if it works at all—does, in most cases, lead out of the stochastic matrices. Thus, for Markov processes the distribution function $P_t(x)$ fulfills a closed linear evolution equation with the semi-group character. In the continuous random variable situation the M-Operator can—under conditions to be discussed later—very often be approximated by linear differential operators with coefficient functions called **drift** and **diffusion**. The corresponding linear partial differential equation of second order in ∂_x is denoted as Fokker-Planck equation. It can be encoded in a stochastic differential equation called Langevin equation.

As an example of a phenomenological theory consider the modeling of ink in water by a current density that is approximately proportional to the gradient of the density of ink particles but points in opposite direction (Fick's law). It reflects to linear order in the gradient the observation of ink particle flow from regions of higher densities to regions of lower densities. Since the density is proportional to the local probability to find an ink particle, one has

$$j(x) = -D\partial_x P(x) \tag{2.33}$$

with the so-called diffusion constant D. The resulting Master equation is a Fokker-Planck equation with diffusion only and is known as the diffusion equation or heat equation,

$$\boxed{\partial_t P_t(x) = D\partial_x^2 P_t(x)}. \tag{2.34}$$

The solution to an initial value of delta-peaked[4] ink is an irreversible Gaussian distribution with variance increasing linear in time,

$$\boxed{P_t(x) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)}. \tag{2.35}$$

A variance increasing linear with time, $(\delta x)^2 = 2Dt$, is the signature of diffusive motion. The reader may check by differentiation that (2.35) is indeed the initial value fundamental solution.

It is instructive to discuss an easy way of finding the initial solution of (2.34). One exploits the fact that it is linear (superpositions of solutions are new solutions—a fundamental solution can serve as a basis) and that it involves the derivatives without mixing of x-dependent factors. Thus, one can use the fact that e^{ikx} is an eigenfunction of the generator ∂_x of translations, $\partial_x e^{ikx} = ike^{ikx}$. This is known as Fourier analysis, a special form of spectral analysis. The Fourier transform works between x-space and its dual k-space as

$$P_t(x) = (2\pi)^{-1/2} \int \mathrm{d}k\, \tilde{P}_t(k) e^{ikx}, \tag{2.36}$$

$$\tilde{P}_t(k) = (2\pi)^{-1/2} \int \mathrm{d}x\, P_t(x) e^{-ikx}. \tag{2.37}$$

[4]So-called fundamental solution or Green's function of the linear differential equation.

Equation (2.34) reads in k-space,

$$\partial_t P_t(k) = -Dk^2 P_t(k). \tag{2.38}$$

Equation (2.38) is an ordinary differential equation in t and solved by exponential ansatz (again Fourier analysis with respect to time t). The initial distribution in k-space, dual to a δ-peak in x-space, is uniform, $P_0(k) = (2\pi)^{-1/2}$, such that we found the initial value solution in k-space,

$$P_t(k) = (2\pi)^{-1/2} e^{-Dk^2 t}. \tag{2.39}$$

The solution (2.35) in x-space follows after performing the Fourier back-transformation as a Gaussian integral, after completing the square in the exponent, $-Dk^2t - ikx = -Dt(k + (ix/2Dt))^2 - x^2/(4Dt)$, a technique we will face several times in this book.

2.3.4 *Quantum Processes*

The most general class of stochastic processes known to date is characterized by a linear unitary time evolution U_t for a pre-probability (also called wave function) $\psi_t(x)$, generated by a hermitian operator. This generator is called Hamilton operator or Hamiltonian H. Such processes are called quantum processes for historical reasons on which we like to comment here.

Quantum processes were were first studied in physics after the discovery of the discrete nature of the energy of light (1900–1905 by Planck and Einstein) and the discrete nature of stationary bound states of discrete microscopic constituents of matter (1913 by Bohr). These discrete objects are called photons and atoms. The charged constituents of an atom are also discrete and are called electron and proton. A crucial feature of these discrete objects is that they are completely characterized by a few quantities in discrete units of elementary quantities. These characterizing numbers are thus called quantum numbers. Two of such quantum objects are completely indistinguishable from each other as soon as they share the same quantum numbers. It was found in 1925–1927 by Heisenberg, Schrödinger, Born, Dirac and others that the dynamics of these quantum objects can successfully be described as generated reversible stochastic processes.[5] This very formulation was able to explain those quantum numbers that are associated with the dynamics. For example, the universal relation between energy and frequency and the discrete nature of energy in a bounded system. In a generated dynamics the natural dimension of the generator is frequency (inverse time) and Planck's constant $h \approx 6,63 \cdot 10^{-34}$ Js in the relation $E = h\nu$ between energy E and frequency ν tells how to recalculate energy = frequency from natural units into standard international units. Other quantum numbers, such as the charge

[5] Although it was never called that way.

and mass of electrons, still to this day remain to be explained by a special theory of matter. The discovery of quantum processes started from observations of light and the theory of light is now established as a quantum field theory called quantum electrodynamics. The configurations in this theory are numbers of photons with certain polarization and frequency within a volume element in space. The dynamics is described as stochastic process because the numbers fluctuate. The reversible nature of the dynamics excludes a Markov process description. Fortunately, the description as a quantum process works out nicely. Because of the development of the theory of reversible stochastic processes as a physical theory of the quantum nature of matter and interaction, the name quantum theory got stuck with it and—as far as the author knows—mathematicians do not consider it as a mathematical discipline within stochastic processes. This may change when reversible stochastic processes are discovered outside of genuine quantum field physics. However, the observation of reversible stochastic processes is hampered, because the reversibility is unstable against environmental contact.

The pre-probabilities are complex functions and their space (Hilbert space) is equipped with a scalar product, $\langle\phi|\psi\rangle := \int \mathrm{d}x\, \phi^*(x)\psi(x)$. The pre-probability must be normalizable, such that $|\psi(x)|^2$ can serve as a probability distribution. This is the Born-rule in quantum theory. With the short-hand notation $|\, x\rangle$ for a delta-function peaked at position x this means:

$$P_t(x) = |\langle x \mid \psi_t\rangle|^2\,, \tag{2.40}$$

$$\psi_t = U_t\psi_0 = e^{-iHt}\psi_0, \tag{2.41}$$

$$\boxed{\partial_t\psi_t = -iH\psi_t}\,. \tag{2.42}$$

The differential time version (2.42) is called **general Schrödinger equation**. Here, by construction, the probability is conserved and time reversibility is guaranteed by

$$U_t^{-1} = U_{-t} = U_t^\dagger\,. \tag{2.43}$$

Quantum processes are reversible stochastic processes. They do not fulfill the Markov property of (2.30), they do not provide a closed equation for $P_t(x)$, but rather a closed equation for the pre-probability with full group character. Thus, in quantum processes the pre-probabilities are the states which fulfill a closed linear evolution equation of group character. We have written the generator in such a form that the hermitian character of $H = H^\dagger$ goes with the unitarian character of U_t. Note, that so far we do not rely on any presumed relation between the generator H here and the Hamilton function of deterministic processes. Their relation will be derived later. Note also that the pre-probability does not introduce a new concept of probability. Two different values x_1 and x_2 of variable x are still exclusive properties of a system and a state $\psi_t(x)$ which is finite for both of them does not mean that a new property of x_1 and x_2 is described, but simply that the probabilities of finding one of them are finite. Note also, that the probability current density is not necessarily a functional of $P_t(x)$, but both, $P_t(x)$ and $j_t(x)$, are independent quantities following from the pre-probability $\psi_t(x)$. This opens another way to realize that quantum processes can be time reversible stochastic processes.

As the most basic comparison between Markov and quantum processes we consider the toy models of two value systems in the following subsections. A comparison for continuous variables in one dimension (1D) is discussed subsequently.

2.3.5 Markov: Two Values

The random variable n can take two values, called $+$ and $-$. The process is defined by two transition rates w_{+-} from $-$ to $+$ and w_{-+} from $+$ to $-$. The Master equation in continuous time then reads (see later)

$$\dot{P}_t(+) = w_{+-}P_t(-) - w_{-+}P_t(+), \tag{2.44}$$

$$\dot{P}_t(-) = w_{-+}P_t(+) - w_{+-}P_t(-). \tag{2.45}$$

Since $P_t(+) = 1 - P_t(-)$ a closed equation for each of them is possible. We choose $P_t(+)$. It reads

$$\dot{P}_t(+) = w_{+-} - (w_{+-} + w_{-+})P_t(+), \tag{2.46}$$

and can be solved by exponential ansatz and variation of constant. The solution is

$$P_t(+) = \frac{w_{+-}}{w_{+-} + w_{-+}}\left[1 - e^{-(w_{+-}+w_{-+})t}\right] + P_0(+)e^{-(w_{+-}+w_{-+})t}. \tag{2.47}$$

For $P_t(-)$ the solution follows after interchanging $+$ and $-$.

The solution relaxes to the stationary state

$$P_\infty(+) = \frac{w_{+-}}{w_{+-} + w_{-+}}, \tag{2.48}$$

with **relaxation time** $(w_{+-}+w_{-+})^{-1}$. There is no way to get time reversal symmetric solutions within the Markov scheme for a two value system.

On the other hand, measurement of relaxation time and stationary state yield the parameters of the Master operator. Thus, observing and measuring relaxation to stationary states opens the possibility to model the process by a Master equation, without measuring the short time dynamics yielding the transition rates.

If the transition rates are symmetric, $w_{+-} = w_{-+} = w$, then $P_\infty = 0.5$ and the relaxation time is $1/(2w)$. If, in addition, $P_0(+) = P_0(-) = 0.5$, then the distribution stays constant. Thus, in the Markov case to much symmetry leads to boring dynamics.

2.3.6 *Quantum: Two Values*

The time evolution is unitary and the generator H is hermitian with real eigenvalues (called energies or eigenfrequencies) ω_m and a complete set of eigenstates $\mid m\rangle$. With the help of the eigenstates $C_{xm} := \langle x \mid m\rangle$ the time evolution reads

$$\psi_t(x) = \sum_m C_{xm} e^{-i\omega_m t} \langle m \mid \psi_0\rangle \,, \tag{2.49}$$

$$\langle m \mid \psi_0\rangle = \sum_{x'} C^\star_{x'm} \psi_0(x'). \tag{2.50}$$

For two values $x = +, -$ and $m = 1, 2$ the diagonal elements of H are real numbers H_{++} and H_{--}. The off-diagonal elements are complex conjugated $H_{-+} = H^\star_{+-}$. The frequencies are

$$\omega_{1,2} = \frac{H_{++} + H_{--}}{2} \pm \sqrt{\frac{(H_{++} - H_{--})^2}{4} + \mid H_{+-} \mid^2}, \tag{2.51}$$

and the eigenstates are

$$C_{+1} = \frac{-H_{+-}}{\sqrt{(\omega_1 - H_{++})^2 + \mid H_{+-} \mid^2}}, \tag{2.52}$$

$$C_{+2} = C_{+1} \cdot \frac{\omega_1 - H_{++}}{H_{+-}}, \tag{2.53}$$

$$C_{-2} = \frac{-H_{-+}}{\sqrt{(\omega_2 - H_{--})^2 + \mid H_{+-} \mid^2}}, \tag{2.54}$$

$$C_{-1} = C_{-2} \cdot \frac{\omega_2 - H_{--}}{H_{-+}}. \tag{2.55}$$

Choosing the initial state as $\psi_0 = +$ one finds so-called Rabbi oscillations in the probability of a two value quantum system (frequently called two level system),

$$P_t(+) = 1 - 4 \mid C_{+1} \mid^2 \cdot (1 - \mid C_{+1} \mid^2) \cdot \sin^2\left(\frac{(\omega_1 - \omega_2)t}{2}\right). \tag{2.56}$$

For degenerate states $\omega_1 = \omega_2$, of course, there are no oscillations. Starting with an eigenstate, of course, the probability stays 1.

Oscillations rather than relaxation is the indicator of reversible stochastic processes. As an example think of neutrino oscillations or spin precession in a magnetic field.

To model a reversible stochastic two value system, one can gain the Hamiltonian from observing and measuring strength and frequency of oscillations. This yields the difference $H_{++} - H_{--}$ and the absolute value of H_{+-}. However, the sum $H_{++} + H_{--}$

and the phase of H_{+-} remain undetermined. This indicates a general important feature of quantum systems: the zero of energy remains free and a gauge freedom of a global phase remains.

For systems with translation invariance one can choose $H_{++} = H_{--} = 0$ and finds $\omega_{1,2} = \pm \mid H_{+-} \mid$ with $\mid C{+}1 \mid^2 = 1/2$ and

$$P_t(+) = 1 - \sin^2(\mid H_{+-} \mid t)\,. \tag{2.57}$$

Thus, on time averaging, the same average probability of 1/2 appears as in the Markov situation.

2.3.7 *Comparison Between Diffusion and Free Quantum Propagation*

As an important and far reaching example we consider a **free particle** with spatial coordinate x. To model a free quantum system we cannot directly write an ansatz for the current density as in the diffusion model, since we need an equation for the pre-probability. Instead, we argue with symmetries, which is *the* appropriate way to model quantum processes from scratch. The very notion of free particle means that translation invariance and rotational (in 1D reflection) invariance should be fulfilled. This means that the Hamiltonian can be chosen as a function of the squared translation generator, $H(\partial_x^2)$, and does not explicitly depend on x. Thus, it has eigenvalues $\omega(k^2)$, where k belongs to the translation eigenfunction e^{ikx}. The mean velocity

$$\langle \dot{x} \rangle_t := \mathrm{d}_t \langle x \rangle_t \tag{2.58}$$

in such eigenstates can be found as the slope of $\omega(k)$,

$$\mathrm{d}_t \langle x \rangle_t = \partial_{ik}(i\omega(k^2)), \tag{2.59}$$

where we have assumed that the eigenstates e^{ikx} can be normalized to some finite support and that $xe^{ikx} = \partial_{ik}e^{ikx}$. If, in addition, we rely on a theory of inertial symmetry, we may be able to further specify this function. Here, we take a Galilei type symmetry which means that velocities add: when $\dot{x}$ changes to $\dot{x} + v$, then k should change to $k + \delta k(v)$ in a compatible way, such that the shift δk is a function of v alone. This works out only if $w(k^2)$ is of first order in k^2, otherwise the shift δk will also depend on $\dot{x}$. This scenario of a free particle with Galilei inertia leads uniquely (up to an irrelevant constant) to the standard non-relativistic free Hamilton operator,

$$\boxed{H = \frac{-1}{2m}\partial_x^2,\ \omega(k^2) = \frac{k^2}{2m},\ \langle \dot{x} \rangle = \frac{k}{m}}\,. \tag{2.60}$$

Here m is a parameter controlling the inertia and usually called mass. In our units its dimension is time per squared length. There is no need to rely on a so-called classical to quantum correspondence principle to find the Hamiltonian, only symmetry restrictions are needed. The corresponding Schrödinger equation reads

$$\boxed{\partial_t \psi_t(x) = \frac{i}{2m} \partial_x^2 \psi_t(x)}. \tag{2.61}$$

It looks like a diffusion equation when we identify D with $i/2m$. Indeed, we can find a fundamental solution (Green's function) for the free Schrödinger equation by similar Fourier analysis as for the diffusion equation. It reads

$$\boxed{G(x, x_0, t) = \sqrt{\frac{m}{2\pi i t}} \exp\left(-\frac{mx^2}{2it}\right)}. \tag{2.62}$$

Note, this is not quite the solution of the initial value problem for a particle initially peaked at x_0, but for a pre-probability function which is δ-peaked initially at x_0. Its absolute square is not normalizable to unity. Before we discuss the true initial value problem, we have a look at the probability current. It cannot be red of the continuity equation immediately. One firstly has to write down the continuity equation following from the Schrödinger equation. For Hamiltonians, where the gradient appears as in the free model (2.60) (called kinetic energy) and the Hamiltonian may include a translation symmetry breaking term $V(x)$ (called potential energy)

$$H = \frac{-1}{2m} \partial_x^2 + V(x), \tag{2.63}$$

the probability current density $j_t(x)$ is simply related to the phase gradient of the pre-probability $\psi = \sqrt{P} e^{i\varphi}$,

$$\boxed{j_t(x) = \frac{1}{2im} \left(\psi_t^*(x)(\partial_x \psi_t(x)) - \psi_t(x)(\partial_x \psi_t^*(x))\right) = P_t(x) \frac{\partial_x \varphi}{m}}. \tag{2.64}$$

You should check this by verifying the continuity equation using this current and the Schrödinger equation. Note, the current density must be defined in another way, according to the continuity equation, for more general Hamiltonians. A general current density definition will be given in (5.12).

Now, we can compare the dynamics of diffusive propagation and free quantum propagation. In both cases we take an initial normalized Gaussian distribution of width σ,

$$P_0^{[d]}(x) = (2\pi\sigma^2)^{-1/2} \exp -\frac{(x - x_0)^2}{2\sigma^2}. \tag{2.65}$$

As to the diffusion problem, this fixes the initial condition. In the free quantum case we have the freedom to add a phase factor to the modulus and we take it such that the initial probability current is k_0/m,

$$\psi_0^{[f]}(x) = (2\pi\sigma^2)^{-1/4} \exp\left[-\frac{(x-x_0)^2}{4\sigma^2} + ik_0 x\right]. \tag{2.66}$$

The fact that the phase allows to give an initial condition to the current independently of the density is related to the fact that quantum processes can describe reversible processes. When reversing the process one can reverse the initial current appropriately. With the fundamental solutions $G^{[d]}$ of (2.35) and $G^{[f]}$ of (2.62) one can find the probability densities and pre-probability densities by integration,

$$P_t^{[d]}(x) = \int \mathrm{d}x'\, G^{[d]}(x, x', t) P_0^{[d]}(x'), \tag{2.67}$$

$$\psi_t^{[f]}(x) = \int \mathrm{d}x'\, G^{[f]}(x, x', t) \psi_0^{[f]}(x'). \tag{2.68}$$

Again, one has to calculate Gaussian integrals by completing the square in the exponents. We leave the details as an exercise and state the answer:

$$P_t^{[d]}(x) = (2\pi\hat{\sigma}^2)^{-1/2} \exp -\frac{(x-x_0)^2}{2\hat{\sigma}^2} \tag{2.69}$$

$$\begin{aligned}\psi_t^{[f]}(x) &= (2\pi\hat{\sigma}^2)^{-1/4} \exp\left[-\frac{(x-(x_0+vt))^2}{4\tilde{\sigma}^2}\left(1-\frac{it}{m\sigma^2}\right)\right] \times \\ &\times \exp\left(+ik_0 x - i\omega(k_0)t\right).\end{aligned} \tag{2.70}$$

Here $\hat{\sigma}^2 = \sigma^2 + 2Dt$ and $\tilde{\sigma}^2 = \sigma^2 + \left(\frac{t}{m\sigma}\right)^2$. It shows already that the width of the quantum wave packet grows linearly in time with velocity $1/(m\sigma)$ while the peak moves with velocity $v = k_0/m$. The diffusive wave packet has no drift at all and its width grows only as a square root in time. The current density in the diffusive case is given by the density gradient,

$$j_t^{[d]}(x) = \frac{x-x_0}{\hat{\sigma}^2} P_t(x), \tag{2.71}$$

and the current density in the free quantum case is given by the phase gradient,

$$j_t^{[f]}(x) = \left[\frac{k_0}{m} + \frac{t(x-(x_0-vt))}{\tilde{\sigma}^2 m^2 \sigma^2}\right] P_t(x). \tag{2.72}$$

So far, the behavior of quantum propagation shows faster spreading of the wave packet plus a motion of its center as compared to the diffusive process.

To catch the more important **interference** aspect of quantum propagation we now take an initial distribution of two Gaussian peaks (width σ) separated at a distance $2d$, say at $x = \pm d$, and with initial momentum $\mp k_0$, equal in strength (wave length), but pointing in opposite directions. For better comparison we also shift the centers of the diffusive motion by the same velocity $\mp k_0/m$ and calculate what happens at times where the two packages meet. In the diffusive case one can simply add both solutions corresponding to the initial Gaussians at $x = \pm d$, because the diffusion equation is linear for the density. In the quantum case one has a corresponding linear superposition for the pre-probabilities and must calculate the resulting densities of probability and current afterwards. This results in interference patterns which become most pregnant at meeting time $t = d/v$, provided the spreading is slower than the movement of the packages and the wavelength is shorter than the spreading. We leave the explicit calculations as a valuable exercise and only display the resulting probability densities and current densities in a qualitative way in Fig. 2.1. They capture an essential difference between Markov (irreversible fluctuations) and quantum processes (reversible fluctuations and oscillations). Figure 2.1 also shows two interesting facts: the current density in the Markov case just follows from the gradient of the probability density while the current density in the quantum case has no resemblance to the probability density. It is generated by the phase of the wave function not visible in the probability density. However, after smearing out the interference oscillations in the quantum case, the Markov case is recovered with a current following the gradient of the probability density. We will come back to this in Sect. 3.4.2.

2.3.8 External and Internal Randomness and Deterministic Representations

In this section we look at the interpretation of randomness in Markov and quantum processes.

An electron position in an atom, a quasi-electron momentum in a conducting wire, a car position in traffic, a number of radioactive atoms in a substance, a stock index, a weather parameter form examples of dynamic random variables. An irregular time evolution is indeed more general than a seemingly regular motion. Whenever fluctuations in a system are an essential part of the description, we describe it as a stochastic process. This does not mean that a deterministic description is absent or that a deterministic description is impossible. Even in cases where we we have a deterministic description we may use it only to extract the equations for the stochastic process in terms of fluctuating relevant variables.

Throughout this book we will distinguish between external and internal randomness in the following ways. By **external randomness** we mean that the system variables x interact with external variables y which are not treated dynamically. Their effect on x was integrated out, such that the system variables x become distributed at

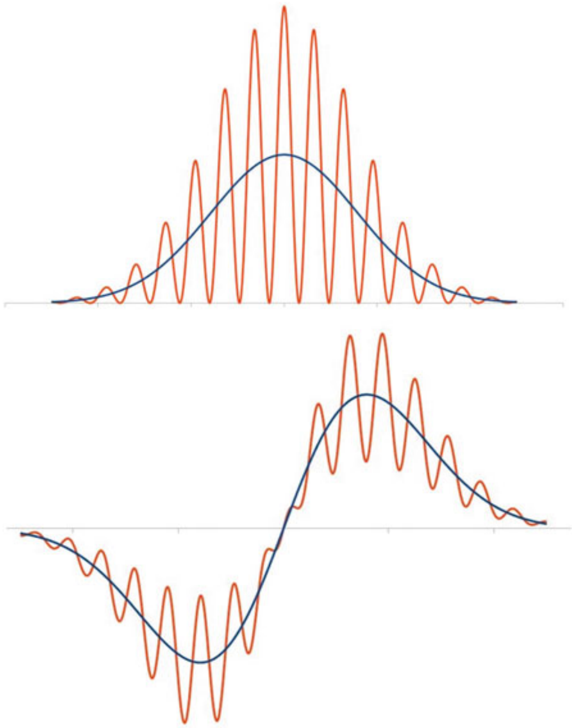


Fig. 2.1 Comparison of diffusive Markov and free quantum motion for two oppositely moving Gaussian packets. The probability densities and the current probability densities are shown as functions of coordinate in 1D at meeting time

every instant of time and are described by a distribution $P_t(x)$. As an example think of a car in traffic where its particular motion depends on many other participants. The relevant variable x as the possible position of a car is now distributed. Another example we have already addressed: the position x of a tiny volume of possible ink particles pushed around by water molecules in thermalized water. Often, like in our phenomenological treatment of ink in water, the integration over external variables is not made explicit, but the result is incorporated statistically in a distribution of parameters for the system under consideration or in fixed parameters like the diffusion constant D. As a further example think of an quasi-electron in a conducting wire with elastic scattering events. These events can be described by a distribution of random potentials. Also here, the randomness is related to external variables which are changed without explicit notice. The modeling will eventually lead to a certain generator G for the stochastic process.

If the fluctuation of x is negligible, then the external variables y can or cannot influence the reversibility of the x dynamics. However, as soon as fluctuations in x are essentially due to the y variables, reversibility of the x dynamics is hardly possible, because for a replay of a time sequence in reality the information about the positions and velocities of the interacting y variables is necessary. In the dynamics of x the information is lost and recurrence times for x become astronomic. However, as long as we are interested in not to small time intervals (where abrupt changes are out of control) we can follow the time evolution of the distribution $P_t(x)$ step by step by means of transition rates. Consequently, a Markov process description is convenient for prognostication in systems with external randomness. We will see that for continuous variables it often suffices to consider a deterministic drift of the whole distribution and time dependent fluctuations around it, called diffusion. The corresponding equation is the **Fokker-Planck equation** or its representation as a **Langevin equation**. Often, external randomness is easy to identify as in the case of ink in water. The thermalized water molecules are the eliminated partners of the ink molecules.

By **internal randomness** we mean: interacting external partners are not identified or there are no such partners. Nevertheless, the system shows relevant fluctuations. In the absence of interacting partners randomness can e.g. show up after coarse graining in deterministic chaos, because of a strong sensitivity on initial conditions. Here, the Markov process description may apply and typically irreversibility emerges on a coarse grained level of description due to the lack of information about the fine grain dynamics. Such situation of internal randomness is very similar to external randomness and the lost fine grain dynamics is similar to the external variables y.

In the case of reversible time evolution with fluctuations we have a true situation of internal randomness and it is hardly possible to imagine that hidden variables y cause fluctuations in x and do not destroy the time reversibility for the distribution of x.[6] This is the situation of quantum processes. Quantum processes have a complete description by the unitary time evolution and there is no need to think about hidden variables. But where do the fluctuations come from? This question can lead to long philosophical debates. It simply cannot be answered within the theory of quantum processes, but needs further interpretation. Here we like to stress that many deterministic representations are possible, where randomness is entirely due to unknown initial positions x_0.

To clarify the notion, we define a **deterministic representation of a stochastic process** as follows. The stochastic process is characterized by an initial distribution $P_{t_0}(x)$ and corresponding time dependent distribution $P_t(x)$ for each time $t > t_0$. If one manages to find for each initial value $x(t_0)$ a unique path $x(t)$, such that for each distribution $P_{t_0}(x)$ of initial values $x(t_0)$ the resulting paths $x_k(t)$ (k labeling such corresponding paths) lead to the time dependent distribution on averaging over quasi-continuously many paths

$$P_t(x) = \lim_{N\to\infty} \frac{1}{N} \sum_k^N \delta(x - x_k(t)), \tag{2.73}$$

we call this ensemble of paths a deterministic representation of the stochastic process. It is obvious that a deterministic representation is by no means unique for a given

[6] This has to be distinguished from a situation where an reversible interacting system is approximated by an effective non-interacting reversible system where each constituent moves in a mean field.

stochastic process. Think of changes in paths that have no effect on the averaging in (2.73).

Nevertheless, it is interesting that for every stochastic process with continuous variable in continuous time a deterministic representation can be explicitly constructed. The corresponding paths $x(t)$ are simply the integral curves of the velocity field $v_t(x) := j_t(x)/P_t(x)$,

$$\dot{x}(t) = v_t(x(t)). \tag{2.74}$$

In the case of external randomness, however, the interpretation does not give a realistic motion. There, in principle, we can observe the paths and their irregularity due to external interactions. Usually it does not coincide with the smooth behavior of the integral curves in (2.74). In the case of internal randomness and quantum systems the deterministic representation by integral curves of the velocity field is known as **de Broglie-Bohm theory** or Bohmian mechanics (see [1, 2]). It is a completely legitimate interpretation of quantum processes and its appealing feature is that the stochastic velocity flow is also the deterministic flow and no other variables than the original configuration variables have to be taken into account. Randomness just stems from the unknown initial conditions of configuration variables. This interpretation keeps the philosophical principle of sufficient reason intact: every event has a precursor event which determines it sufficiently. Two predictions within this interpretation are: (1) In every stationary state the deterministic realization stays at rest, although distributed according to the initial distribution. In this interpretation it seems plausible that stationary states of charged particles do not radiate. (2) Paths do not intersect each other, because the velocity field is unique. This allows to identify paths in a double slit experiment from each slit to the position of detection. However, it does not mean that we can actually pin down this motion in a probabilistic prognostic sense. For example, the conditional probabilities for finding an interference pattern at detectors with particles entering through known initial slit positions vanishes. Of course, it is speculative that this deterministic representation describes the true particle motion, because it is not unique and it seems difficult to experimentally test the priority of this interpretation as long as the paths cannot be resolved to accuracies better than allowed by the uncertainty relation of quantum theory (see Sect. 5.1). Furthermore, in the discrete case, the construction of a deterministic realization is more difficult. The velocity field can take any real value but the discrete numbers must change by discrete differences in a given time step. Thus, the velocity field does not lead in a unique deterministic way to the discrete quantities in the next time step. Lacking a more fundamental theory than quantum theory, we have to leave its interpretation beyond the stochastic process level as open.

So, when we say that our variable is found to be at x at some time t, we may imagine some deterministic representation compatible with $P_t(x)$ and $j_t(x)$, but we don't need an explicit representation when calculating the time evolution of a stochastic process. We are also allowed to think that there is no realistic deterministic representation at all but only pre-probabilities or probabilities and probability currents evolve in time steps with (semi-)group properties. In this view, events come into existence or leave existence within the range of possibilities[7] described by these probabilistic tools. This latter view is taken when we speak of creation and annihilation of discrete quanta (e.g. photons) in a quantum field theory describing infinitely many degrees of freedom.

2.4 Exercises

Exercise 1: Examples for stochastic processes
Find examples for each of the mentioned equations in books or other media. Try to answer: Why is the process stochastic? What is the fluctuating variable and why are fluctuations essential to the problem. Is there oscillation or relaxation?

Exercise 2: Meaning of the velocity field and deterministic representation
Consider a vector coordinate $\boldsymbol{x}$ with components x^{μ}. Show

$$\langle \boldsymbol{v_t}(\boldsymbol{x}) \rangle_t = \partial_t \langle \boldsymbol{x} \rangle_t$$

where averaging is with respect to $P_t(\boldsymbol{x})$. Argue, that the knowledge of $\boldsymbol{j}_t(\boldsymbol{x})$ for all t and $\boldsymbol{x}$ and the initial distribution $P_{t_0}(\boldsymbol{x})$ suffices to obtain $P_t(\boldsymbol{x})$ by the continuity equation and thus also $\boldsymbol{v}_t(\boldsymbol{x})$. Show that for the densities and current densities related to a number N of paths $\boldsymbol{x}_k(t)$ by

$$\varrho_t(\boldsymbol{x}) := \frac{1}{N} \sum_k \prod_\mu \delta(x_k^\mu(t) - x^\mu), \tag{2.75}$$

$$j_t^\mu(\boldsymbol{x}) := \frac{1}{N} \sum_k \prod_{\nu \neq \mu} \dot{\Theta}(x_k^\mu(t) - x^\mu)\delta(x_k^\nu(t) - x^\nu), \tag{2.76}$$

a continuity equation holds in the sense of distributions. Argue that, therefore, the integral curves of $\boldsymbol{v}_t(\boldsymbol{x})$ lead—on averaging over the initial distribution—to the full distribution $P_t(\boldsymbol{x})$.

Exercise 3: Stochastic matrices
Show that stochastic matrices form a semi-group. Give an example where no inverse exists or the inverse is no longer a stochastic matrix.

Exercise 4: Discrete time in Markov and quantum two value systems
Consider two value systems with discrete time step dynamics for Markov and quantum processes for one step δt. Specialize to $w_{+-} = 0.5 = w_{-+}$ and $w_{+-} = 0$ with $w_{-+} = 1$ and for the quantum case to $H_{+-} = 1$ and $H_{++} = H_{--} = 0$.

Exercise 5: Continuous free fluctuations: reversible and irreversible
Find the fundamental solution for the free particle Schrödinger equation and the diffusion equation by yourself in 1D by Fourier analysis. Find the time evolution

[7] Some people like to call it many worlds.

for the probability distribution $P_t(x)$ and the probability-current density $j_t(x)$ for Gaussian initial distribution of width σ_0 centered at $x = 0$. In the quantum process, the initial momentum can be captured in an initial phase factor e^{ik_0x}. Keep the right normalizations in mind. Compare the behavior of fluctuations.

Exercise 6: Interference in reversible stochastic processes
Generalize your solutions of Exercise 5 to an initial distribution consisting of separated Gaussian peaks at $x = \pm d$. In the quantum process the initial momentum $\mp k_0$ should be chosen equal in strength (wave lengths), but pointing in opposite directions. Pay attention to commensurability of d and the wavelength. For the diffusion process add a velocity $v = \mp k_0/m$ to the mean value of the peaks for better comparison with the quantum process. Take the movement by this velocity faster than the spreading of the wave packets, such that the packets can meet at some meeting time $t = d/v$. Compare the possibility of constructive and destructive interference between Markov and quantum processes (Fig. 2.1 gives a qualitative picture).

References

1. D. Dürr, S. Teufel, *Bohmian Mechanics—The Physics and Mathematics of Quantum Theory* (Springer, Berlin, Heidelberg, 2009)
2. A.S.Sanz, S.Miret-Artes, *A Trajectory Description of Quantum Processes. Vol. I Fundamentals and Vol. II Applications* (Springer 2012 and 2014)

Chapter 3
Formal Solutions

Abstract Formal methods of solving the dynamics are discussed. These are of algebraic (Lie series) or analytic (generating functional) type which both have some advantages as a starting point for approximate methods. In rare cases they even allow for explicit solutions. The analytic formal solutions by generating functionals (path integrals, partition sums) are most convenient as starting points for modeling systems. They provide a basis for interpreting Markov processes by the chain rule for probabilities and for interpreting quantum processes by Huygens' principle in combination with Born's rule. They also allows to discuss the emergence of Markov behavior in quantum processes (decoherence) and of classical deterministic behavior.

3.1 Generator as Differential Operator

In deterministic processes the generator G acts as a local differential operator on states which are fixed by coordinates x, coordinates and velocities $(x, \dot{x})$, or by elements of the co-tangential bundle (x, p), also denoted as phase space of the system.

For Markov processes the generator $G = M$ can be represented as a kernel $M(x, x')$,

$$\partial_t P_t(x) = \int \mathrm{d}x'\, M(x, x') P_t(x'). \tag{3.1}$$

For quantum processes the Hamiltonian H as generator $G = -iH$ can also be represented as a kernel $H(x, x')$,

$$\partial_t \psi_t(x) = -i \int \mathrm{d}x'\, H(x, x') \psi_t(x'). \tag{3.2}$$

Such kernels can alternatively be represented by a series of local differential operators of arbitrary high order, because ∂_x is nothing but the generator of translations h in variable x, leading to the following useful relations

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1_3

$$f(x+h) = e^{h\partial_x} f(x) = \sum_{n=0}^{\infty} \frac{h^n (\partial_x)^n}{n!} f(x), \tag{3.3}$$

$$\int \mathrm{d}x' \, f(x,x') = \int dh \, f(x, x+h) = \sum_{n=0}^{\infty} (\partial_x)^n \int dh \, \frac{h^n}{n!} f(x-h, x). \tag{3.4}$$

In the Markov case, the diagonal part of the kernel $M(x,x')$ must be singular like a delta-function and it is related to the sum over all off-diagonal elements by the conservation of probability, (2.33). Furthermore, it is positive and consequently the off-diagonal terms are just transition rates from x' to x per unit time, $w(x' \to x)$, and the Master equation becomes an equation of gain and loss,

$$\boxed{\partial_t P_t(x) = \int \mathrm{d}x' \, \{w(x' \to x) P_t(x') - w(x \to x') P_t(x)\}}. \tag{3.5}$$

Exploiting the translational group content of (3.4) one arrives for Markov processes at the so called Kramers-Moyal representation

$$\boxed{\partial_t P_t(x) = \sum_{n=1}^{\infty} (\partial_x)^n \left[D^{[n]}(x) P_t(x) \right]}, \tag{3.6}$$

which is a differential equation of infinite order. The **Kramers-Moyal coefficients** are defined as the moments of the transition rate in deviations $\Delta x = x' - x$ and can suggestively be written as

$$D^{[n]}(x) := \lim_{\Delta t \to 0} \frac{(-1)^n}{n!} \left\langle (\Delta x)^n \right\rangle_w / \Delta t. \tag{3.7}$$

For obvious reasons $D^{[1]}$ is called drift coefficient (deviation in linear time) and $D^{[2]}$ diffusion coefficient (quadratic fluctuation in linear time). It can happen that only $D^{[1]}$ and $D^{[2]}$ are non-zero. In such case (3.6) is called a Fokker-Planck equation and the short time dynamics of (3.7) captured as drift and diffusion is the corresponding Langevin equation. The positivity of the probability ensures that all other coefficients have to be non-zero, as soon as one of them for $n > 2$ is non-vanishing.

Without general proof we report that the Fokker-Planck situation occurs in continuous systems provided a separation of time scales occurs, such that the short time dynamics is already randomized in a Gaussian way. It means that a central limit theorem[1] holds and higher moments vanish. When many additive random elements are already at work on some time scale τ, the process on times larger than τ may very well be described by a Fokker-Planck equation of second order in ∂_x. A simplified demonstration is given in Sect. 4.2.6.

[1]See Appendix A.9.

Due to probability conservation there is no $D^{[0]}$ and the current density $j_t(x)$ of the continuity equation (2.29) can be red off the right hand side of (3.6) by reducing the power of $-\partial_x$ by one. It is an essential insight that the current density in a Markov process can be expanded in derivatives of the probability. It is not an independent quantity and it shows the irreversible character of Markov processes as soon as they show fluctuations. Fluctuations automatically make the diffusion coefficient non-zero. The corresponding current contribution will point in the direction of decreasing probability, a signature of irreversibility.

By using the calculus for δ-functions, already used in one of the previous exercises, one can show the intuitive result: as long as only drift is non-zero, the dynamics stems from a deterministic process of Aristotelian type and is given by $\dot{x} = -D^{[1]}(x)$. Thus, in the absence of fluctuations a first order generator for a deterministic process is indeed sufficient.

In the quantum process case we don't have to care about positivity and conservation of probability since this is guaranteed by unitarity of the time evolution and hermiticity of the Hamiltonian. Nevertheless, we can exploit the translational group content of (3.7) and arrive at

$$\boxed{\partial_t \psi_t(x) = -i \sum_{n=0}^{\infty} (\partial_x)^n \left[\mathcal{H}^{[n]}(x)\psi_t(x)\right]}, \tag{3.8}$$

which, again, is a differential equation of infinite order. The coefficients are determined as

$$\mathcal{H}^{[n]}(x) = \frac{(-1)^n}{n!} \int \mathrm{d}x' \, (x' - x)^n \left\langle x' | H | x \right\rangle . \tag{3.9}$$

Now, there is no restriction on these coefficients apart from hermiticity of H which means

$$\int \mathrm{d}x \, \mathcal{H}^{[n]}(x) = (-1)^n \int \mathrm{d}x \, \left[\mathcal{H}^{[n]}(x)\right]^* . \tag{3.10}$$

On average over x even coefficients are real and odd coefficients are imaginary. In constructing Hamiltonians we will not rely on a classical to quantum correspondence principle. We start from scratch and we have to develop tools to further specify the coefficients which we like to denote as **Hamilton coefficients**. Kramers-Moyal coefficients are moments of positive transition rates and separation of time scales and the central limit theorem can help in specifying them. The Hamiltonian coefficients don't have an interpretation as moments of rates, but rather as moments of complex rate amplitudes. Thus, only restrictions like symmetries can help in specifying the coefficients. As an important and far reaching example we have already discussed in Sect. 2.3.7 the particle propagation in 1D with Galilei inertia and a translation symmetry breaking potential $V(x)$,

$$H = \frac{-1}{2m}\partial_x^2 + V(x), \tag{3.11}$$

where m is the mass. Here, the probability current is given by the phase gradient of the pre-probability (2.65).

Since each of the generators for Markov and quantum processes can be written as series of differential operators (3.6, 3.8) we arrive at the conclusion that the generator of a (semi-)group dynamics can be written as a differential operator of possibly infinite order,

$$G\cdot = \sum_{n=0}^{\infty} (\partial_x)^n \left[\mathcal{G}^{[n]}(x)\cdot\right], \tag{3.12}$$

with coefficients uniquely determined by the kernel representation $\langle x'|G|x\rangle = \int d\tilde{x}\, \delta(\tilde{x}-x')(G\delta(\tilde{x}-x))$,

$$\mathcal{G}^{[n]}(x) = \frac{(-1)^n}{n!} \int \mathrm{d}x'\, (x'-x)^n \langle x'|G|x\rangle. \tag{3.13}$$

Alternatively, the coefficients can be determined by requirements when modeling a certain system. By partial integration and using $\partial_{\tilde{x}} f(\tilde{x}-x') = -\partial_{x'} f(\tilde{x}-x')$ we can rewrite the kernel in a nice way appropriate for integration

$$\langle x'|G|x\rangle = \sum_{n=0}^{\infty} \left[(\partial_{x'})^n \delta(x'-x)\right] \cdot \mathcal{G}^{[n]}(x). \tag{3.14}$$

As quite general results we can state.

- Deterministic (semi-)group type equations of motion correspond to the case where only the first order term is non-vanishing. In such case the probability or pre-probability $\delta(x-x(t))$ with drift equation $\dot{x} = -\mathcal{G}^{[1]}(x)$ solves the equation of motion. Such distribution shows no fluctuations along the deterministic drift path $x(t)$.
- In the quantum case a pure zeroth-order term yields a pure phase factor in pre-probabilities, such that probabilities don't change in time at all.
- In the Markov case there is no zeroth order term due to probability conservation.
- The case of a zeroth order plus a first order term in the quantum case combines a phase factor in the pre-probability and a non-fluctuating probability peaked along the drift path.
- In the Markov case the current density can be red of the right hand side of (3.6) by reducing the power of $-\partial_x$ by one. Thus, it is not an independent quantity and it shows the irreversible character of Markov processes as soon as they show fluctuations.
- In the quantum case the current density is not related to derivatives of the probability, but generated by the phase of the pre-probability (for a general definition see Sect. 5.1).

3.2 Lie-Series

In all of the mentioned dynamics the generated (semi-)group character allows for the formal solution of $\dot{f} = Gf$ by exponentiation

$$f(t) = e^{tG} f(0), \tag{3.15}$$

where $f(t)$ stands short for $f(x(t))$ or $f(x(t), \dot{x}(t))$, $f(x(t), p(t))$, $P_t(x)$, or $\psi_t(x)$ and $f(0)$ for $f(x)$ or $f(x, \dot{x})$, $f(x, p)$, $P_0(x)$ or $\psi_0(x)$ as the initial values. The exponential function can be taken serious by its series representation and thus provides a formal solution of the dynamics. It also has practical relevance [1, 2]. In the literature of differential equations it is called **Lie series**. The solution reads

$$f(t) = \sum_{m=0}^{\infty} \frac{t^m G^m}{m!} f(0), \tag{3.16}$$

$$\boxed{f(t) = \sum_{m=0}^{\infty} \frac{t^m}{m!} \left(\sum_{n=0}^{\infty} (\partial_x)^n \left[\mathcal{G}^{[n]}(x) \right] \right)^m f(0)}. \tag{3.17}$$

Notice, the series solution is defined by pure differentiation and thus can be carried out to arbitrary high order by (computer-) algebra. In some special cases the summation can be done completely and in all other cases it can be used as a quite effective tool for approximations.

As an example with a complete analytical solution we consider the Aristotelian model for motion on earth: $G = -kx\partial_x$. The Lie series applied to an initial x yields $x(1 + (-kx)t + (1/2)(-k)^2 t^2 + \cdots)$ and coincides with the series of the exponential decay xe^{-kt} to rest. Notice, the Lie series doesn't need a special ansatz, but only algorithmic differentiation. As an exercise try the harmonic oscillator, which also works out nicely.

An advantage of the Lie series for approximations is: for short times one can restrict to few terms in the series and take the result as a new starting point for the next time step. To capture fluctuations, the second order derivatives in G have to be taken into account. This gives a tool with flexible step width. It works best for deterministic processes where G is of first order in derivatives and the state is just the variable which is differentiated. Then, higher terms can often be calculated by recursive means.

In addition, it can serve as the starting point for perturbation theory when $G = G_0 + \delta G$ with some G_0 for which solutions are known and allows for expansions in powers of δG. This goes along the same lines as time dependent perturbation theory in ordinary quantum mechanics (see e.g. Chap. XVII in [3]) and will not be repeated here.

3.3 Path Integrals

There is another general method of formal solutions which opens a wide range of further treatment: path integral solutions (see e.g. [4–7]). It exploits two central ideas: (1) the (semi-)group property by iterating on short time solutions (short time propagator for a single time step) and (2) by solving the short time propagator with spectral analysis of translations and linear approximations in time steps. We treat Markov processes and quantum processes together by denoting T_{tt_0} as the (semi-)group element, $G(x', x)$ as the generator kernel and $\mid x\rangle$ as the state peaked at position x. We like to calculate the transition(-amplitude) (called **propagator**)

$$\left\langle x', t|x, t_0\right\rangle := \left\langle x'|T_{tt_0}|x\right\rangle . \tag{3.18}$$

The (semi-)group property now yields in kernel representation an equation which is well known from quantum theory ($1 = U_t^\dagger 1 U_t = \int d\tilde{x} \mid \tilde{x}, \tilde{t}\rangle\langle\tilde{x}, \tilde{t} \mid$) and also well known in Markov theory as the **Chapman-Kolmogorov equation**.

$$\left\langle x', t|x, t_0\right\rangle = \int d\tilde{x} \left\langle x', t|\tilde{x}, \tilde{t}\right\rangle\left\langle \tilde{x}, \tilde{t}|x, t_0\right\rangle . \tag{3.19}$$

This can be iterated as often as one likes thanks to the (semi-)group property. After a large number N of steps each propagator becomes a short-time propagator which can be treated to linear order in the time step $\Delta t = (t - t_0)/(N + 1)$

$$\left\langle x', t + \Delta t|x, t\right\rangle := \left\langle x'|1 + G\Delta t|x\right\rangle . \tag{3.20}$$

Now we use the kernel representation (3.14) and use the spectral representation (a concept of **duality**) of the delta-function.

$$\left\langle x', t + \Delta t|x, t\right\rangle = \int (dk/2\pi)\, e^{ik(x'-x)} \left[1 + \Delta t \sum_{n=0}^{\infty} (ik)^n \mathcal{G}^{[n]}(x)\right] . \tag{3.21}$$

The expression

$$\sum_{n=0}^{\infty} (ik)^n \mathcal{G}^{[n]}(x) =: G(x, k) \tag{3.22}$$

will be called generator function. In the quantum case it will be called (quantum) Hamilton function. This function depends on the definition of the coefficients $\mathcal{G}^{[n]}(x)$ and therefore on the ordering of derivatives and coefficients in G. The variable k is just an integration variable and has, so far, no meaning as a canonical conjugate of x as in classical Hamilton mechanics. Such meaning only emerges under certain conditions to be discussed in Sect. 3.4.2.

The term $1 + \Delta t G(x, k)$ can be re-exponentiated in the order Δt, such that we finally arrive at a complete integral solution

$$\langle x', t|x, t_0\rangle = \lim_{N\to\infty} \frac{1}{(2\pi)^{N+1}} \int \mathrm{d}x_N \ldots \int \mathrm{d}x_1 \int \mathrm{d}k_{N+1} \ldots \int \mathrm{d}k_1 \cdot \left[\cdot \exp\left\{\sum_{j=1}^{N+1} G(x_{j-1}, k_j)\Delta t + \frac{ik_j(x_j - x_{j-1})}{\Delta t}\Delta t\right\}\right]. \tag{3.23}$$

As a short-hand notation such **path integral** can be written as

$$\boxed{\langle x', t|x, t_0\rangle = \int\limits_{x\to x'} Dx(\tau)Dk(\tau)\, e^{\int_{t_0}^{t} \mathrm{d}\tau \{G(x(\tau),k(\tau)) + ik(\tau)\dot{x}(\tau)\}}}. \tag{3.24}$$

Let us stress the importance of this formal solution by some remarks.

- The integration over elements of paths $Dx(\tau)$ is restricted to intermediate steps; the initial value x and final value x' are kept fix (a visualization is in Fig. 3.1).
- The propagation over an arbitrary time step is expressed as an integral (although high-dimensional) where only functions on the sliced configuration manifold complemented by dual coordinates k are involved. It forms a dual solution to the solution by Lie series where no integration but only differentiation was involved. In terms of programming it only involves ordinary numerics (e.g. Monte Carlo integration) while Lie series involve computer algebra.

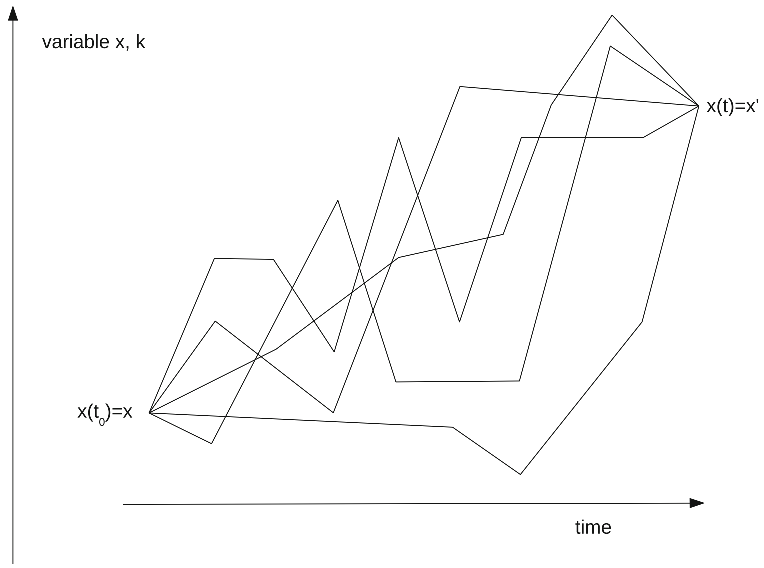


Fig. 3.1 The propagator is a sum over many paths. Each path contributes a factor. The factor is positive in Markov processes and complex in quantum processes

- As a warning and as a guideline for further treatment: the path integral is uniquely defined by the partitioning in (3.23). The short-hand notation (3.24) can only be used as a short-hand notation. It does not prescribe the discretization in a unique way as (3.23) does. There are no tables for path integrals. Only integrals up to second order in k or x variables can be integrated in closed form by Gaussian integrals.
- The path integral has a similar look and status in stochastic dynamics as the **partition sum** in equilibrium statistical physics. With the help of additional source terms it can serve as a generating functional for almost any expectation value one likes to calculate (see Sect. 5.5).
- All known approximation schemes can be applied: perturbation in small parameters and expansion about a solved generator G_0 as with Lie series.
- Further approximation schemes show up: expansion around characteristic points of functionals, exploiting symmetries and topology of functionals, reducing to relevant variables by integrating out irrelevant variables, enlarging variable space with auxiliary variables (see Sect. 8.5) to re-express difficult terms or constraints via Lagrange multipliers.

3.4 Chain Rule and Huygens-Born Principle

In (3.23, 3.24) the integrations are over paths in the configuration variable x and in the dual variable k. We can get rid of the dual variable by formally carrying out this integration at each intermediate step as a kind of Fourier-Laplace transform changing the variable $k(\tau)$ to $\dot{x}(\tau)$,

$$\boxed{\int Dk(\tau)\, e^{\int_{t_0}^{t} \mathrm{d}\tau \{ G(x(\tau),k(\tau)) + ik(\tau)\dot{x}(\tau)\}} =: e^{\int_{t_0}^{t} \mathrm{d}\tau L^{[G]}(x(\tau),\dot{x}(\tau))}}. \tag{3.25}$$

The function resulting from this transformation is called the L-function and its integral over time is a functional of a path $x(\tau)$ and is called the S-functional,

$$S^{[G]}[\mathrm{x}(\tau)] := \int_{t_0}^{t} \mathrm{d}\tau\, L^{[G]}(x(\tau), \dot{x}(\tau)). \tag{3.26}$$

Note, L is not necessarily the Legendre-transform of G, but more generally defined by the Fourier-Laplace transform of (3.25). For Markov processes ($G = M$) the negative of the L-function is called **Onsager-Machlup function** and the exponents are written with a minus sign, $L^{[G]} = -L^{[OM]}$ and $S^{[G]} = -S^{[OM]}$. For quantum processes the L-function is (with a factor of (i) called (quantum) **Lagrange function** and written as

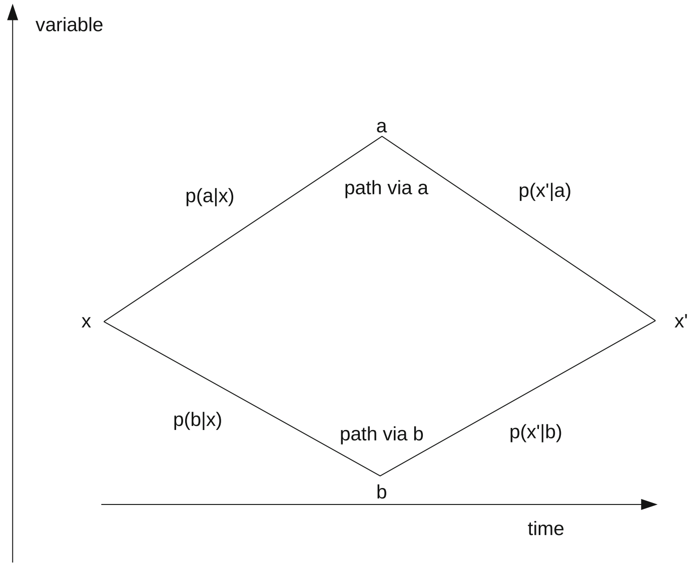


Fig. 3.2 A Markov process with only two paths. The path integral represents the usual chain rule

$L^{[G]} = iL$ and the corresponding S-functional as **action functional** $iS[x(\tau)] = i\int_{t_0}^{t} \mathrm{d}\tau L(x(\tau), \dot{x}(\tau))$. Thus, the propagator of a Markov process can be written as

$$\boxed{\left(x', t|x, t_0\right) = \int\limits_{x\to x'} Dx(\tau) e^{-\int_{t_0}^{t} \mathrm{d}\tau\, L^{[OM]}(x(\tau),\dot{x}(\tau))}}. \tag{3.27}$$

Similarly, the propagator of a quantum process can be written as

$$\boxed{\left\langle x', t|x, t_0\right\rangle = \int\limits_{x\to x'} Dx(\tau) e^{i\int_{t_0}^{t} \mathrm{d}\tau\, L(x(\tau),\dot{x}(\tau))}}. \tag{3.28}$$

To illustrate the meaning of a path integral with only the configuration variable we have a look at a process with only one intermediate time step and with only two possible values a, b for the configuration variable at that time, resulting in a restriction to just two paths (see Fig. 3.2).

In the Markov case, where $e^{-S^{[OM]}}$ is a positive weight with probabilistic meaning for each path, the path integral simply represents the usual chain rule to calculate the probability to find x' when started at x, denoted as $p(x'|x)$: multiply the conditional probabilities along each path and sum them up, resulting in

$$p(x'|x) = p(x'|a)p(a|x) + p(x'|b)p(b|x) = p_a + p_b. \tag{3.29}$$

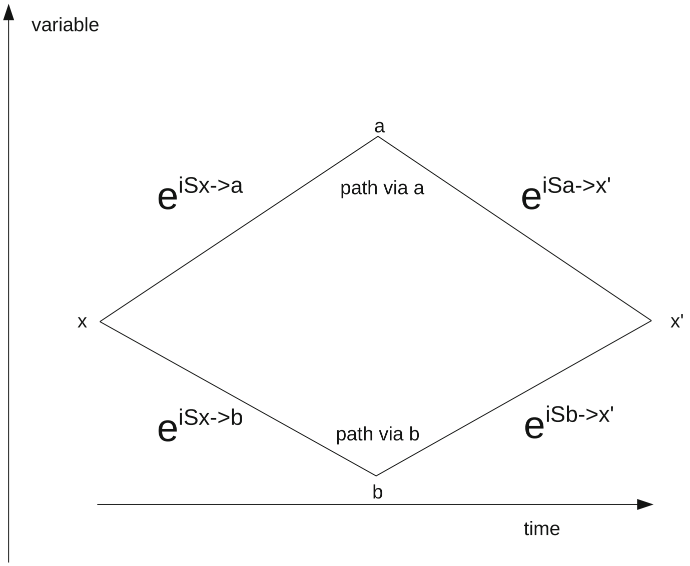


Fig. 3.3 A quantum process with only two paths. The path integral represents the Huygens-Born principle

In the quantum case, e^{iS} is not a positive weight and it cannot be interpreted as a probability attached to a path. But the path integral represents the complex amplitude for the process from x to x' as Huygen's principle: the amplitude is a superposition of amplitudes with phases accumulated along paths starting at x and ending at x' (see Fig. 3.3). Since the resulting amplitude of the full process has probabilistic meaning in the sense of Born's rule, we can view the path integral as the realization of Huygen's principle and Born's rule to interpret wave intensities as probabilities.

$$\begin{aligned}\sqrt{p(x'|x)}e^{i\phi} &= \sqrt{I_a}e^{iS_{x\to a}+iS_{a\to x'}} + \sqrt{I_b}e^{iS_{x\to b}+iS_{b\to x'}} \\ &= \sqrt{I_a}e^{iS_a} + \sqrt{I_b}e^{iS_b}.\end{aligned} \tag{3.30}$$

For two paths with equal absolute intensities $I_a = I_b = I$ we get for the transition probability a simple interference pattern

$$\boxed{p(x'|x) = 2I(1 + \cos(S_a - S_b))}. \tag{3.31}$$

The total intensity (probability) oscillates between 0 (destructive interference) and $4I$ (constructive interference), while an averaging over phases yields $2I$, as for a Markov process with equal probabilities for each of two paths.

Note, in quantum processes there is no immediate probabilistic measure attached to paths between two values x and x' with intermediate steps. The natural way, how paths enter the formalism is via the group property for pre-probabilities. Then paths appear as elements of path integration and its interpretation is along Huygen's principle with Born's rule and it incorporates interference. This leads frequently to the misunderstanding that quantum theory introduces a novel probability theory with violation of Kolmogorov axioms. This is not true, since two different values a and b of property x are mutually exclusive at any time and weighted by a probability measure in the Kolmogorov sense. The novel aspect of quantum theory is that the dynamical evolution is non-Markovian in a way that allows for a full group property and reversibility. Independently from path integrals as realization of the Huygens-Born principle it is also possible to explicitly attach probabilities to paths along discrete time steps in a meaningful way within quantum theory. This requires additional consistency conditions on top of the Huygens-Born principle. For an elaboration on this so called consistent histories approach see for example [8, 9]. We will not elaborate on this, as it has no practical value for the topics addressed in this book.

3.4.1 The L-Function for Second Order Derivatives

When generators are up to quadratic in derivatives the generator function reads

$$G(x,k) + ik\dot{x} = G^{[0]}(x) + k\left(iG^{[1]}(x) + i\dot{x}\right) - k^2 G^{[2]}(x). \tag{3.32}$$

Now the important Gaussian integral relation (valid for arbitrary complex numbers a, b, c as long as the real part of a is positive)

$$\int \mathrm{d}x\, e^{-ax^2+bx+c} = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a}+c} \tag{3.33}$$

allows to perform the Fourier-Laplace transform explicitly and leads to

$$L^{[G]}(x,\dot{x}) = G^{[0]}(x) + \frac{-\left(\dot{x} + G^{[1]}(x)\right)^2}{4G^{[2]}(x)}. \tag{3.34}$$

Also here we can see that in processes with vanishing fluctuations ($G^{[2]}(x) \to 0$) we arrive at a deterministic process with drift $\dot{x} = -G^{[1]}(x)$, since the L-function acts as Gaussian with shrinking width in the path integral, thus leading to a δ-function distribution along the drift path.

In the Markov situation $G^{[0]}$ vanishes due to probability conservation and the Onsager-Machlup function reads

$$L^{[OM]}(x,\dot{x}) = \frac{\left(\dot{x} + D^{[1]}(x)\right)^2}{4D^{[2]}(x)} \tag{3.35}$$

In the quantum situation of a Galilei particle ($G^{[2]}(x) = -i\frac{-1}{2m}$) with translation symmetry breaking terms $G^{[0]} = -iV(x)$ (V is called potential energy) and $G^{[1]} = -i\mathcal{H}^{[1]}(x)$ ($\mathcal{H}^{[1]}$ is called gauge field) we get the Lagrange function

$$L(x, \dot{x}) = \frac{m}{2}\left(\dot{x} - i\mathcal{H}^{[1]}(x)\right)^2 - V(x). \tag{3.36}$$

Note, that we did not use any correspondence principle or any "quantization" of a classical theory. Equation (3.36) states the exact quantum Lagrange function of a Galilei particle in a translation symmetry breaking potential and gauge field. From this Lagrange function the full quantum propagator can be calculated as a path integral.

Note also, that the L-function for up to second order generators is indeed the Legendre transform of the generator function with respect to $\partial_{-ik}G(x, k) = \dot{x}$. This is a general mathematical property of Fourier-Laplace transformsfor Gaussian integrands. Still, this does not define a deterministic equation of motion for $x(t)$. Such equation only results as a limiting situation when fluctuations are negligible.

3.4.2 Emergence of a Quantum to Classical Correspondence

Fluctuations in the path integral can become negligible as a consequence of the characteristic physical parameters for the relevant variable x under consideration. It means that the integral is dominated by a certain path from $x(t_0)$ to $x(t)$. Since the functional $e^{iS[x(t)]}$ is a strongly oscillating quantity the path integral will sum up many oscillating contributions. A path $x_c(t)$ that leaves the action stationary can serve as the starting point for an expansion in deviations from this stationary solution, $\eta(t) := x(t) - x_c(t)$,

$$S[x(t)] = S[x_c(t)] + S_2[\eta(t)] + \delta S[\eta(t)]. \tag{3.37}$$

where $S_2[\eta]$ contains quadratic fluctuations in η and $\delta S[\eta]$ all higher orders. By definition there are no linear order terms left at a stationary path and the stationary path fulfills the Lagrange equation of classical mechanics,

$$\frac{\delta S[x(t)]}{\delta x(t)} = \frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} = 0. \tag{3.38}$$

The quadratic fluctuations are determined by the Hessian of the action at the stationary action solution,

$$S_2[\eta] = \frac{1}{2}\int_{t_0}^{t} \mathrm{d}t' \int_{t_0}^{t} \mathrm{d}t'' \, \frac{\delta^2 S[x(t)]}{\delta x(t')\delta x(t'')}|_{x_c(t)}\eta(t')\eta(t''). \tag{3.39}$$

When $\delta S[\eta(t)]$ turns out to be sub-leading, the path integral can be approximated by the so-called stationary action approximation with Gaussian fluctuations as

$$\langle x_b, t_b \mid x_a, t_a \rangle \approx \exp\{iS_c(x_b, t_b; x_a, t_a)\}\, F(x_b, t_b; x_a, t_a), \tag{3.40}$$

where $S_c(x_b, t_b; x_a, t_a)$ is the action for the stationary path under the boundary conditions

$$x_c(t_a) = x_a,\;\; x(t_b) = x_b \tag{3.41}$$

and $F(x_b, t_b; x_a, t_a)$ is a factor resulting from a Gaussian integral with fluctuations $S_2[\eta]$. Since Gaussian integrals in many variables are evaluated in eigenvalue coordinates of the corresponding quadratic form and involve the determinant of this form (see Sect. 5.5.3), the factor will be called determinant factor. In the present case, a simple expression for this determinant factor can be derived by a sophisticated and clever analysis which, however, is of no further use for our purposes. The proof can be collected from Chaps. 6, 12 and 13 of Schulman's classic text [6]. We simply state the result where the Hessian of the stationary action with respect to initial and final coordinates is involved,

$$\boxed{\langle x_b, t_b \mid x_a, t_a \rangle \approx \sum_k e^{iS_c^{[k]}(x_b, t_b; x_a, t_a)} \sqrt{\det\left(\frac{i}{2\pi}\frac{\partial^2 S_c^{[k]}}{\partial x_a \partial x_b}\right)}}. \tag{3.42}$$

Since it often happens (for an example see Sect. 8.1) that a stationary action solution for the boundary conditions (3.41) is not unique, a summation over distinct stationary action solutions (labeled by k) can be performed—provided the corresponding extrema can be separated. We mention that an integer multiple of $\pi/2$ (so-called Maslov correction) must be subtracted from the action in (3.42) when an integer number of so-called focal points exist along the path of stationary action. At focal points the second derivative $\frac{\partial^2 S_c^{[k]}}{\partial x_a \partial x_b}$ becomes infinite (see [10]).

Equation (3.42) shows that there are always fluctuations in the propagator due to the determinant factor. If they are negligible or undetectable for practical reasons the system can best be described by the classical deterministic Lagrange equation. This is a consequence of system parameters and is an emergent phenomenon like the emergence of Gaussian distributions with tiny variance in real statistical ensembles (central limit theorem, see Appendix A.9). The corresponding classical Hamilton function $H(x, p)$ is the Legendre transform of $L(x, \dot{x})$ and coincides, of course, with the quantum Hamilton function in those cases where it is of up to second order in k (denoted as p in classical mechanics).

Thus, the quantum-classical correspondence might emerge for some relevant variable. To take it as a construction principle for quantum time evolution is dangerous because of its limitations. For the historical development of quantum theory it was a very helpful guide. However, to model quantum time evolution one should directly model the quantum Hamilton operator from characteristic parameters of oscillations and symmetry requirements or model some of its derivatives like the quantum Hamilton function or the quantum action.

3.4.3 Emergence of a Quantum to Markov Behavior

Consider the time evolution of a wave function in discrete representation

$$\psi_n(t) = \sum_m \langle n, t|m, t_0\rangle \, \psi_m(t_0). \tag{3.43}$$

For the corresponding probability distribution this means a non-Markovian non-closed time evolution

$$\boxed{P_n(t) = \sum_{mm'} \langle n, t|m, t_0\rangle \left\langle m', t_0|n, t\right\rangle \psi_m(t_0)\psi^*_{m'}(t_0)}\,. \tag{3.44}$$

The diagonal terms ($m = n$) do not contain phase factors, but the off-diagonal terms do. They are essential for the possibility to describe a time reversible stochastic process. This can be seen easily, once we assume that the off-diagonal parts in this sum can be neglected. We arrive at a Chapman-Kolmogorov equation characteristic for Markov processes,

$$\boxed{P_n(t) = \sum_m w(n, t; m, t_0) P_m(t_0)}\,, \tag{3.45}$$

with positive transition rate,

$$w(n, t; m, t_0) = |\langle n, t|m, t_0\rangle|^2. \tag{3.46}$$

In systems coupled only very tiny to some environment the phases are typically much more sensitive to the coupling than the amplitudes. After a characteristic time scale, called **decoherence time** τ_{dec}, the phases become effectively random and a coarse grained description for P_n cannot resolve the filigree information buried in the rapidly fluctuating off-diagonal contributions. Because of large sums over randomly fluctuating phases with smoothly varying amplitudes, the systems dynamics can effectively be described by a Markov process instead of the original quantum process. Thus, on a time scale larger than the decoherence time τ_{dec}, the tiny coupling to the environment, not captured explicitly in the dynamics, will finally lead to the typical behavior of Markov processes, which means some relaxation and irreversibility. A related and more elaborated discussion will be presented in Sect. 5.4.2.

Here we have a closer look at the different roles of the probability current density $j(n, t)$ in Markov and quantum processes. We simplify the discussion by restricting to the case where the quantum current density is only first order in gradients of the phases of wave-functions $\psi = e^{0{,}5 \ln P + i\phi}$,

$$j^{\mathrm{Q}}(n,t) = \frac{i}{2m}\left\{\psi(n,t)\partial_n\psi^*(n,t) - \psi^*(n,t)\partial_n\psi(n,t)\right\}$$
$$= P(n,t)\frac{\partial_n\phi(n,t)}{m}, \tag{3.47}$$

and the Markov current density is only first order in gradients of the probability,

$$j^{\mathrm{M}}(n,t) = -D\partial_n P(n,t). \tag{3.48}$$

Exploiting the quantum dynamics of (3.43) and writing the transition amplitudes as $\langle n,t|m,t_0\rangle = e^{0,5\ln w(n,m)+i\varphi(n,m)}$ yields for the quantum current

$$j^{\mathrm{Q}}(n,t) = \frac{1}{m}\sum_{n',m'}\left(w(n,n')w(n,m')P(n')P(m')\right)^{0,5}$$
$$\times\left[\sin\left(\varphi(n,n')-\varphi(n,m')+\phi(n')-\phi(m')\right)(\partial_n(0,5\ln w(n,n'))\right.$$
$$\left.+\cos\left(\varphi(n,n')-\varphi(n,m')+\phi(n')-\phi(m')\right)(\partial_n\varphi(n,n'))\right]. \tag{3.49}$$

The Markov dynamics of (3.45) yields for the Markov current

$$j^{\mathrm{M}}(n,t) = -D\sum_{n'} w(n,t;n',t_0)(\partial_n \ln w(n,t;n',t_0))P(n',t_0). \tag{3.50}$$

In the decoherent situation, the dominating diagonal part of the quantum dynamics leads to a coarse grained current density dynamics

$$j^{\mathrm{QDC}}(n,t) = \frac{1}{m}\sum_{n'} w(n,t;n',t_0)P(n',t_0)(\partial_n\varphi^{QDC}(n,t;n',t_0)). \tag{3.51}$$

Thus, after coarse graining and decoherence, a reversible dynamics with quantum currents from phase gradients turns to an irreversible situation with Markov currents from rate gradients,

$$\boxed{\frac{1}{m}\partial_n\varphi^{QDC}(n,t;n',t_0)) \to -D\partial_n \ln w(n,t;n',t_0))}. \tag{3.52}$$

3.5 Exercises

Exercise 1: Lie Series for Harmonic Oscillator

Solve for $x(t)$ with Lie series for the harmonic oscillator $Gx = \{H,x\}$ with $H(x,p) = \frac{1}{2}\left(p^2+\omega^2x^2\right)$.

Exercise 2: Pure Drift
Show that $\delta(x - x(t))$ with drift equation $\dot{x} = -\mathcal{G}^{[1]}(x)$ solves the equation of motion, if only $\mathcal{G}^{[1]}$ is non-zero in the generator expansion.

Exercise 3: Basic Gaussian Integral
Show (3.33) in two steps: First $b = c = 0$ and considering the square of the integral as performed in 2d with polar coordinates and then by quadratic extension for b, c finite.

Exercise 4: Path Integral for Free Particle
Follow the calculation of the propagator for a free quantum particle $H = -\frac{-1}{2m}\partial_x^2$ by the path integral method along the lines presented in books (e.g. [11]) with pen and paper. You also get to know Gaussian integrals there.

Exercise 5: Fourier-Laplace and Legendre
Show that the L-function of (3.34) is the Legendre transform of the generator function with respect to $\partial_{-ik} G(x, k) = \dot{x}$.

References

1. W. Gröbner, *Die Lie-Reihen und ihre Anwendungen* (VEB, Berlin, 1960)
2. H. Mitter, *Mechanik, Vorlesungen über Theoretische Physik I* (BI Wissenschaftsverlag, Mannheim, 1989)
3. A. Messiah, *Quantum Mechanics II* (North-Holland, Amsterdam, 1965)
4. J. Chalker, A. Lukas, *Lecture Notes on M. Phys Option in Theoretical Physics: C6* (Oxford University, Oxford, 2011)
5. T.P. Cheng, L.-F. Li, *Gauge Theory of Elementary Particles* (Clarendon Press, Oxford, 1984)
6. L.S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981)
7. S. Weinberg, *The Quantum Theory of Fields I* (Cambridge University Press, Cambridge, 1996)
8. R.B. Griffiths, *Consistent Quantum Theory* (Cambridge University Press, Cambridge, 2002)
9. P.C. Hohenberg, Rev. Mod. Phys. **82**, 2835 (2010)
10. P.A. Horvathy, Central. Eur. J. Phys. **9**, 1 (2011)
11. U. Mosel, *Path Integrals in Field Theory, An Introduction* (Springer, Berlin, 2003)

Chapter 4
Special Solutions

Abstract The Lie series solution and the path integral solution of the (semi-)group dynamics are formal solutions which show the way for approximation schemes. Rarely, these series or integrals can be performed exactly leading to explicit solutions. Even then, quicker solutions by an appropriate ansatz can be found. To enrich the toolbox in modeling it is helpful to know exactly solvable models and a variety of methods of finding them. We will discuss such special solutions which can be derived without the use of path integrals. However, sometimes it helps to know the path integral to find a short-cut. We firstly consider discrete variables in deterministic and Markov processes. Here the translation operator is also discrete and the generator of translations is the hopping between nearest neighbor variables. Secondly, we consider the important continuous models of Markov and quantum processes which are the Ornstein-Uhlenbeck process and the quantum well and harmonic oscillator models.

4.1 Discrete Few States Deterministic Processes

In deterministic situations with discrete time steps and a discrete variable the dynamic equation is of the form

$$n(t + \delta t) = n(t) + G(n(t))\delta t, \tag{4.1}$$

with a function $G(n)$. Consider only two states $n = 0, 1$. There are only four possible time steps: $0 \to 0$, $0 \to 1$, $1 \to 0$, and $1 \to 1$. For a time homogeneous group dynamics we have three possible motions: (A) **constant**, (B) **periodic** and (C) **relaxing** to (A). For (A) we have 0 stays 0 and 1 stays 1 and for (B) we have 0 followed by 1 followed by 0 etc. or starting with 1 followed by 0. The corresponding functions are

$$G(n) = 0 \quad \text{(A)}, \tag{4.2}$$

$$G(n) = (1 - 2n)/\delta t \quad \text{(B)}. \tag{4.3}$$

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1_4

The solutions of (A) and (B) are reversible. The constant solution has the full time translational symmetry. The time homogeneity is broken spontaneously by the periodic solutions (B) with finite period of 2 steps.[1] However, they don't survive the limit $\delta t \to 0$. On averaging over periodic solutions or coarse graining over periods, the time translational symmetry is restored. In this sense, the time translational symmetry is hidden in the periodic solutions with finite period. The motion (C) happens when one starts with 0 followed by 1 followed by 1 and thus staying at 1 or one starts with 1 followed by 0 staying at 0. Here relaxation in finite time (1 step) to a stationary state occurs.

For three states we have also (A) stationary solutions and (B) periodic solutions with periods of 2 or 3 steps and also (C) solutions with relaxation to stationary solutions in finite time (1 step or 2 steps). For each periodic solution a time reversed solution exists. The relaxing solutions break time reversal symmetry. Again, the finite period solutions don't survive the limit $\delta t \to 0$ and they spontaneously break the time translational symmetry and restore it on averaging. Similar statements hold for any finite number of states.

4.2 Discrete Nearest Neighbor Markov Processes

This section contains mainly standard applications. You can find similar and more applications in [1, 2]. Here we elaborate a little more on stationary solutions with external currents.

The Master equation for discrete random variables reads in the form of a gain–loss rate equation

$$\partial_t P_t(n) = \sum_{n'} w_{nn'} P_t(n') - w_{n'n} P_t(n), \tag{4.4}$$

where $w_{nn'}$ is the transition rate per unite time from state n' to n. It doesn't need to be symmetric. A simpler local situation corresponds to so-called **one-step processes**, where transitions only occur between successive states or nearest neighbors:

$$w_{nn'} = l_{n'} \delta_{n,n'-1} + g_{n'} \delta_{n,n'+1}, \tag{4.5}$$

where l_n measures the strength of loss at n (**death rate** in the case of n species) and g_n the strength of gain at n (**birth rate** in case of n species). You may interpret it as hopping on a 1D lattice with **hopping rates** l_n to the left and g_n to the right (see Fig. 4.1). Then the change at position n is due to 4 steps: one to the left from n to $n-1$ (loss at n), one from the right $n+1$ to n (gain), one to the right from n to $n+1$ (loss) and one to the right from $n-1$ to n (gain). Thus, the Master equation reads for such discrete nearest neighbor (one-step) processes

[1] If a symmetry of the dynamics is not present in the solutions it is called a spontaneously broken symmetry (see Chap. 6).

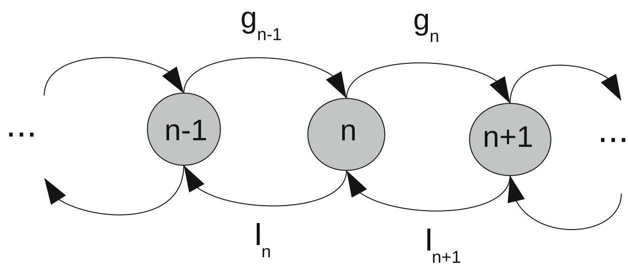


Fig. 4.1 The nearest neighbor (one-step) process and its transition rates

$$\boxed{\partial_t P_t(n) = l_{n+1} P_t(n+1) + g_{n-1} P_t(n-1) - (g_n + l_n) P_t(n)}. \tag{4.6}$$

The discrete natural number n can range from $-\infty$ to ∞ (unbounded variables), or from $n = 0$ to ∞ (bounded from one side variables). If it terminates after a finite number N it corresponds to a variable that is bounded from both sides. For the bounded situation (4.6) is completed by the boundary conditions

$$\partial_t P_t(0) = l_1 P_t(1) - g_0 P_t(0) = J(t), \tag{4.7}$$

$$\partial_t P_t(N) = g_{N-1} P_t(N-1) - l_N P_t(N) = -J(t). \tag{4.8}$$

Here $J(t)$ corresponds to a possible **external probability current** flowing from higher n to lower n (from right to left). In unbounded situations one requires that $P_t(n)$ goes to zero fast enough for $n \to \pm\infty$.

It is now quite interesting that the **stationary solution** can be found in closed form and that external currents can be very important. Stationarity, $\partial_t P_t(n) = 0$ within the system, means

$$l_{n+1} P(n+1) - g_n P(n) = l_n P(n) - g_{n-1} P(n-1) = J, \tag{4.9}$$

where J is a constant independent of n (and t). The equation with $J = 0$ is identical to a situation in certain closed isolated systems at equilibrium where $P(n)$ is the equilibrium distribution and transition probabilities have to fulfill $l_n P(n) = g_{n-1} P(n-1)$ as a constraint, called **detailed balance** (see [1] Chap. V.6 and XVII.7). However, here we like to study the more general case with $J \geq 0$. We consider the bounded situation. When we come to the boundary at $n = 0$, we have $l_1 P(1) - g_0 P(0) = J$ and $J > 0$ describes a probability current from 0 and to the left environment. At the boundary $n = N$ we find $l_N P_N - g_{N-1} P_{N-1} = J$. Thus, an external current $J \geq 0$ flows from right to left through the system.

To study the local change of the stationary solution $P(n)$ we rewrite (4.9)[2] as

$$\boxed{P(n+1) - P(n) = \frac{1}{l_{n+1}} \left[J + (g_n - l_{n+1}) P(n) \right]}. \tag{4.10}$$

A stationary solution can become uniform, $P(n) \equiv P$, for a perfect balance between death and birth rate,

$$l_{n+1} - g_n = \frac{J}{P}, \tag{4.11}$$

In the absence of external current J a uniform stationary solution can only exist in the exceptional situation of the equality of death and birth rates. In non-uniform situations (4.10) tells:

- If $g_n - l_{n+1}$ stays positive, then $P(n)$ will increase as a function of n.
- If $g_n - l_{n+1}$ stays negative, then J plays an important role. Without an external current, $P(n)$ would decrease as a function of n, but a finite external current can change the situation.
- For certain values of n it may happen, that $J - (l_{n+1} - g_n) P(n)$ changes its sign and the stationary solution shows some internal structure due to an external current. Take for example a situation where the birth rate can be neglected in comparison with the death rate, $g_n \ll l_{n+1}$. Then

$$P(n) = \frac{J}{l_n}. \tag{4.12}$$

In case of non-linear l_n this solution can show structure. An illustrative example with l_n of fourth order with two minima is shown in Fig. 4.2.

Since (4.10) has a semi-group structure the stationary solution can be given in closed form for arbitrary $l_n \neq 0$ and $g_n \neq 0$ by iteration, starting from $P(0)$,

$$\boxed{P(n) = \frac{1}{g_n} \left\{ J \sum_{r=1}^{n} \prod_{k=r}^{n} \frac{g_k}{l_k} + (l_0 P(0)) \prod_{k=0}^{n} \frac{g_k}{l_k} \right\}}. \tag{4.13}$$

Equation (4.10) has a continuum limit ($n \to x$ and $l(x)$, $g(x)$ slowly varying on the scale of 1) as a linear (inhomogeneous) ordinary differential equation,

$$\frac{\mathrm{d}}{\mathrm{d}x} P(x) = a(x) - b(x) P(x), \tag{4.14}$$

[2] assuming that $l_n \neq 0$.

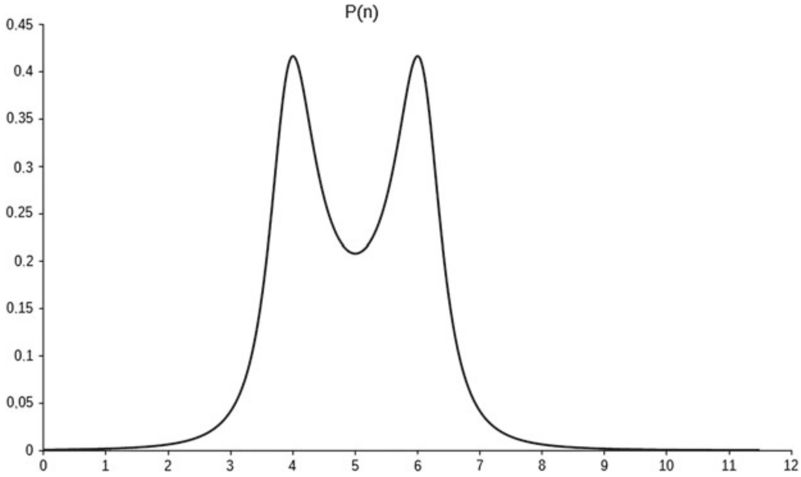


Fig. 4.2 An external current can lead to structure in stationary distributions

with $a(x) = J/l(x)$ and $b(x) = 1 - g(x)/l(x)$. It is solved by standard methods as

$$P(x) = e^{-B(x)} \left\{ P(0) + \int_0^x \mathrm{d}t\, a(t) e^{B(t)} \right\}, \tag{4.15}$$

where $B(x) = \int_0^x \mathrm{d}t\, b(t)$.

The full time dependent solutions can only be given in closed form for **linear n-dependence** of birth and death rates

$$l_n = l_0 + l \cdot n, \tag{4.16}$$

$$g_n = g_0 + g \cdot n. \tag{4.17}$$

There are two tracks for finding time dependent solutions: (A) equations of motions for moments (or linear combinations) and (B) solving for a generating function. On the first track (A) one writes down time evolution equations for moments $\langle n^k \rangle_t$ by virtue of (4.6). For mean and variance they read in an unbounded situation (n from $-\infty$ to $+\infty$)

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle n \rangle_t = \langle g_n \rangle_t - \langle l_n \rangle_t , \tag{4.18}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle (\delta n)^2 \right\rangle_t = 2 \left\langle (\delta n)(g_n - l_n) \right\rangle_t + \langle l_n \rangle_t + \langle g_n \rangle_t , \tag{4.19}$$

where $\delta n := n - \langle n \rangle$. In the linear case such equations become closed differential equations in time. In the non-linear case the equations for low moments involve higher moments and one can find approximate solutions by truncation. In bounded situations additional terms may appear when re-indexing sums. The second track (B) rests on a generating function, a basic concept in theoretical physics that we will meat several times. We consider the unbounded situation for simplicity. The generating function is defined as a Laurent series[3] for complex variable z with $P_t(n)$ as coefficients,

$$F(z,t) := \sum_{n=-\infty}^{\infty} z^n \cdot P_t(n). \tag{4.20}$$

It exploits the group character of the hopping operators $f(n) \mapsto f(n \pm 1)$ by introducing z^n as eigenfunctions of $z\partial_z$ and as states on which z and ∂_z act as **raising and lowering operators** with respect to variable n.

$$(z\partial_z)z^n = nz^n, \; zz^n = z^{n+1}, \; \partial_z z^n = nz^{n-1}. \tag{4.21}$$

The order of z and ∂_z counts, because they do not commute. Their **commutator** acting on some function $f(z)$ is

$$[\partial_z, z] f(z) := (\partial_z z - z\partial_z) f(z) = f(z). \tag{4.22}$$

This is usually written without explicit notice of an arbitrary function as

$$[\partial_z, z] = 1. \tag{4.23}$$

The master equation transforms to a partial differential equation for the generating function,

$$\partial_t F(z,t) = \left[\left(\frac{1}{z} - 1 \right) l_{(z\partial_z)} + (z-1)\, g_{(z\partial_z)} \right] F(z,t). \tag{4.24}$$

Here the variable n has been replaced in l_n and g_n by the differential operator $z\partial z$. Once $F(z,t)$ is known, one can generate moments simply by differentiation

$$\left\langle n^k \right\rangle_t = (z \cdot \partial_z)^k \, F(z,t) \mid_{z=1} . \tag{4.25}$$

Even the full distribution can point-wise be calculated by inversion of the Laurent series,

$$P_t(n) = \frac{1}{2\pi i} \oint_C \frac{F(\xi,t)}{\xi^{n+1}} \mathrm{d}\xi, \tag{4.26}$$

[3]for complex analysis see e.g. the excellent and efficient book by Cartan [3].

where C is a closed loop around $z = 0$ within the radii of convergence. In the linear case the partial differential equation for $F(z, t)$ is of first order and can thus be solved by the **method of characteristics** (see Appendix B). It reads

$$\boxed{\partial_t F(z,t) = (1-z)(l-gz)\partial_z F(z,t) + (1-z)(l_0/z - g_0)F(z,t)}. \tag{4.27}$$

The fundamental solution for an initial sharp position at $n = m$ ($P_0(n) = \delta_{nm}$, $F(z, 0) = z^m$) reads in terms of the generating function (for a derivation see [1] Chap. VI.6 and Appendix B)

$$F(z,t) = z^m \left[\frac{le^{(g-l)t} - g + l(1-e^{(g-l)t})z^{-1}}{l-g}\right]^{m+\frac{l_0}{l}} \times \left[\frac{l - ge^{(g-l)t} - g(1-e^{(g-l)t})z}{l-g}\right]^{-m-\frac{g_0}{g}}. \tag{4.28}$$

It is now time to apply our findings to a number of interesting examples.

4.2.1 Random Walk

The random walk is characterized by constant hopping rates to the left and right,

$$l_n = l_0, \;\; g_n = g_0. \tag{4.29}$$

For $g_0 = l_0 = w$ the random walk is symmetric.

In a bounded situation with vanishing external current J, due to (4.13), the stationary solution reads

$$P(n) = P(0)\left(\frac{g_0}{l_0}\right)^n \tag{4.30}$$

which increases (decreases) to the right for stronger (weaker) hopping to the right. For $g_0 = l_0$ the stationary distribution stays uniform.

In the unbounded situation, the time evolution for average and variance (4.18, 4.19) allow to conclude

$$\langle n \rangle_t = n_0 + (g_0 - l_0)t, \tag{4.31}$$

and

$$\left\langle (\delta n)^2 \right\rangle_t = (l_0 + g_0)t + (\delta n)_0^2. \tag{4.32}$$

For the initial condition of a sharp start at $n = 0$, one has $n_0 = (\delta n)_0^2 = 0$. Both, mean and variance increase linear in time. The mean stays at rest for symmetric hopping, while the variance is insensitive to the hopping direction and shows the characteristics of diffusion (linear time dependence of the variance). The unbounded random walk has no stationary limit, since the distribution keeps spreading out diffusively.

For a discussion of the full dynamic solution we restrict to the symmetric random walk $w = l_0 = g_0$. The generating function $F(z,t)$ can easily be found from (4.27) as

$$F(z,t) = F(z,0)e^{wt(z+1/z-2)}. \tag{4.33}$$

We take the initial condition of a sharp position at $n = 0$, which means $P_0(n) = \delta_{n0}$ and $F(z,0) = 1$. To identify the distribution as Laurent coefficients we use the series of the exponential function and write

$$\mathbf{F}(z,t) = e^{-2wt}\left(\sum_{k=0}^{\infty}\frac{(wt)^k z^k}{k!}\right)\left(\sum_{l=0}^{\infty}\frac{(wt)^l z^{-l}}{l!}\right) = \tag{4.34}$$

$$= e^{-2wt}\sum_{n=-\infty}^{\infty} z^n \left(\sum_{k=0}^{\infty}\frac{(wt)^{n+2k}}{k!(k+n)!}\right), \tag{4.35}$$

where we made use of the fact that the variable $n = k - l$ runs from $-\infty$ to $+\infty$ and n could be replaced by $-n$ in the last sum over k. We can now read off $P_t(n)$ as a power series,

$$P_t(n) = e^{-2wt}\sum_{k=0}^{\infty}\frac{(wt)^{n+2k}}{k!(k+n)!} = e^{-2wt}I_{|n|}(2wt), \tag{4.36}$$

where one can identify this series with a special function, known as special Bessel function $I_{|n|}(x) = \sum_{k=0}^{\infty}\frac{(x/2)^{n+2k}}{k!(k+n)!}$. By analyzing this Bessel function in the limit $t \to \infty$ with fixed ratio n^2/t one can show that the random walk is described by the fundamental solution of the diffusion equation,

$$P_t(n) = \frac{1}{\sqrt{4\pi wt}}\exp\left(-\frac{n^2}{4wt}\right), \tag{4.37}$$

with diffusion constant $D = w$. We will give a short-cut argument for this finding in Sect. 4.2.6.

4.2.2 Population Dynamics

A simple model of population dynamics is characterized by birth and death rates being proportional to the number n of species,

$$l_n = ln, \;\; g_n = gn. \tag{4.38}$$

The number n is usually bounded, at least from below by $n = 0$. Ignoring any environmental resources captured in boundary conditions we consider the dynamics of mean and variance first (see (4.18, 4.19)). The mean shows exponential increase ($g > l$) or decrease ($l > g$),

$$\langle n \rangle_t = n_0 e^{(g-l)t}, \tag{4.39}$$

and the variance obeys a similar linear differential equation with an inhomogeneity,

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle (\delta n)^2 \right\rangle_t = (g-l) \left\langle (\delta n)^2 \right\rangle_t + (g+l) \langle n \rangle_t \,. \tag{4.40}$$

It can be solved by variation of parameters for the particular solution. We assume that initially $n(t_0) = n_0$ is sharp,

$$\left\langle (\delta n)^2 \right\rangle_t = n_0 e^{(g-l)t} \frac{l+g}{g-l} \left(e^{(g-l)t} - 1 \right). \tag{4.41}$$

The variance shows exponential increase for $g > l$ and exponential decrease for $g < l$, too. Thus, the linear population model becomes unrealistic when $r = g - l > 0$ would cause exponential growth while resources are limited. Then, at least a nonlinear modification in death- and birth rates and/or specific boundary conditions have to be taken into account. In Sect. 2.3.8 we have already presented the logistic equation as a nonlinear replacement for the evolution of the average number n.

In the linear case, (4.13) also tells that stationary states at $n \neq 0$ do not exist for vanishing currents $J = 0$, since $l_0 = 0$. Thus, in the decreasing case, $P(n) = \delta_{n0}$ is the stationary limit. With finite external current J, the linear case yields,

$$P(n) = \frac{J}{gn} \sum_{r=1}^{n} \left(\frac{g}{l} \right)^{n-r+1} . \tag{4.42}$$

As we have discussed in Sect. 4.2 already, the stationary solution can show some internal structure (changes from increase to decrease) when the rates become non-linear.

As to the full dynamics of the distribution $P_t(n)$ the solution for the generating function (4.28) can be used, but it does not give more insight as the discussion of mean and variance.

4.2.3 Radioactive Decay

A model of radioactive decay is characterized by death rates being proportional to the number n of kernels which did not decay yet,

$$l_n = ln, \;\; g_n = 0. \tag{4.43}$$

The number n is bounded from below by $n = 0$.

The solution for the generating function (4.28) can be used for this case and yields

$$F(z, t) = \left[1 - (1 - z)e^{-lt}\right]^{n_0} \tag{4.44}$$

where n_0 is the sharp value of kernels at $t = 0$. Since $n \geq 0$ the generating function is a series in nonnegative powers of n, and the full distribution can be found by differentiation,

$$P_t(n) = \frac{1}{n!}\frac{\mathrm{d}^n}{\mathrm{d}z^n} F(z, t) \mid_{z=0} = \frac{n_0!}{(n_0 - n)!n!} e^{-nlt} \left(1 - e^{-lt}\right)^{n_0 - n}. \tag{4.45}$$

Note, that this distribution equals the conditional probability from n_0 at $t = 0$ to n at t. Thus, it provides a complete solution of the Markov process for radioactive decay.

For mean and variance one finds from the generating function by virtue of (4.25, 4.26),

$$\langle n \rangle_t = n_0 e^{-lt}, \tag{4.46}$$

$$\left\langle (\delta n)^2 \right\rangle_t = n_0 e^{-lt} \left(1 - e^{-lt}\right). \tag{4.47}$$

The decay goes on until the last kernel has decayed. Thus, the stationary limit is $P(n) = \delta_{n0}$.

4.2.4 Fluctuations in an Ideal Gas

A model of fluctuations of ideal gas molecules in a volume element ΔV is characterized by leaving rates l_n proportional to the number n of molecules and entering rates g_n, being independent of n,

$$l_n = ln, \;\; g_n = g_0. \tag{4.48}$$

The number n is bounded from below by $n = 0$.

Here, the stationary state corresponding to an equilibrium situation (no external current J) is most interesting. The stationary distribution follows from (4.13) as

$$P(n) = \frac{(g_0)^n}{n! l^n} P(0), \tag{4.49}$$

which is known as a Poisson distribution. In terms of its mean value (which also results as stationary limit of (4.18))

$$\langle n \rangle = \frac{g_0}{l} \tag{4.50}$$

and after normalization it can be written as

$$P(n) = \frac{\langle n \rangle^n \, e^{-\langle n \rangle}}{n!}. \tag{4.51}$$

For the variance one finds by clever summation that it equals the mean

$$\left\langle (\delta n)^2 \right\rangle = \langle n \rangle \, . \tag{4.52}$$

We mention without proof that for a Poisson distribution special combinations of moments called cumulants (see Appendix A) are all equal to the mean. This can serve as a defining feature of the Poisson distribution.

4.2.5 Shot Noise

As our last example of discrete linear one-step processes we consider the problem of classical shot noise. It corresponds to the incoherent excitation of a number n of discrete charges q from a source that move to a drain, thus giving rise to an average electric current $\langle I \rangle = q \frac{\mathrm{d}\langle n \rangle}{\mathrm{d}t}$. The creation rate is constant and no charges get destroyed,

$$l_n = 0, \;\; g_n = g_0. \tag{4.53}$$

As initial value we take $n_0 = 0$ particles. The average is by (4.18)

$$\langle n \rangle_t = g_0 t, \tag{4.54}$$

such that

$$\langle I \rangle = q g_0. \tag{4.55}$$

From (4.19) we find that variance and mean are equal,

$$\left\langle (\delta n)^2 \right\rangle_t = g_0 t = \langle n \rangle_t \, . \tag{4.56}$$

This reminds us of a Poisson distribution. As a check we calculate the generating function $F(z, t)$ from (4.27)

$$F(z,t) = e^{g_0(z-1)t} = e^{-g_0 t} \sum_0^\infty \frac{z^n (g_0 t)^n}{n!}, \tag{4.57}$$

from which we can read off (recall the definition of $F(z,t)$) the full time dependent distribution to the sharp initial value at $n = 0$,

$$P_t(n) = \frac{(\langle n \rangle_t)^n \, e^{-\langle n \rangle_t}}{n!}. \tag{4.58}$$

It is indeed a Poisson distribution. Such processes are therefore also called Poisson processes.

When analyzing stochastic process experimentally one very often considers the spectral content of random functions like the current $I(t)$ and studies the auto-correlation spectral function $S_I(\omega)$ defined by

$$S_I(\omega) := \int \mathrm{d}t \; \langle \delta I(0) \delta I(t) \rangle \, e^{-i\omega t} \tag{4.59}$$

For Markov processes the auto correlation function is a function of the time difference only and it can be shown[4] that $S_I(\omega)$ is equal to the power spectrum defined by

$$S_I(\omega) := \lim_{T\to\infty} \frac{1}{T} \left\langle |I_T(\omega)|^2 \right\rangle, \;\; I_T(\omega) := \int_{-T}^{T} \mathrm{d}t \; I(t) e^{-i\omega t}. \tag{4.60}$$

For the shot noise problem we have

$$q \, \langle I \rangle_t = \left\langle (\delta n)^2 \right\rangle_t = \int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \, \langle \delta I(t_1) \delta I(t_2) \rangle \, . \tag{4.61}$$

The characteristic time for the auto-correlation of $n(t)$ is given by the time scale $(g_0)^{-1}$ due to exponential time behavior in $P_t(n)$. Therefore, the current as derivative can be correlated only on even shorter time scales and we may assume that it is approximately δ-correlated in time, or white noise when talking about its spectrum. With this white noise assumption we find by replacing t_2 with the new variable $\Delta t = t_2 - t_1$ that average current times charge equals the white noise spectral function in a shot noise situation,

$$q \, \langle I \rangle = S_I(\omega). \tag{4.62}$$

[4]known as Wiener-Khintchine theorem.

4.2.6 Fokker-Planck Equation in the Continuum Limit

Non-linear cases of l_n and g_n are difficult to solve. However, one can get further in the continuum limit. We use again the translation property,

$$f(n+a) = e^{a\partial_n} f(n) \tag{4.63}$$

with arbitrary a. For the original one-step process we have to take $a = 1$ in the end. We perform a Kramers-Moyal expansion of the Master equation. This yields kth order coefficients

$$D^{[k]}(n) = \frac{(-1)^k}{k!} a^k \left[g_n + (-1)^k l_n \right]. \tag{4.64}$$

Thus, for $a = 1$ there is no truncation criterion for high orders. All orders k contribute.

However, in a continuum limit, where $a = \frac{\Delta x}{\delta L} \ll 1$ with a scale of resolution δL and rates l_n and g_n for hopping on the scale Δx, one can conclude that the first two coefficients dominate and a Fokker-Planck equation with $D^{[1]} = a(l_n - g_n)$ and $D^{[2]} = a^2(l_n + g_n)$ yields a reasonable description of the Markov process on scales larger than δL. Scales larger than δL means in the discretized picture that we look for changes on large scales δn within time t when studying the dynamics of $P_t(n)$. For the symmetric random walk the resulting Fokker-Planck equation is the diffusion equation and (4.36) in this limit is no surprise. The advantage of the continuum approach is that non-linear one-step processes can be addressed by the approximation methods for Fokker-Planck equations to be presented in Sect. 5.5.4.

4.3 The Ornstein-Uhlenbeck Process

The Ornstein-Uhlenbeck process in a one component variable x is characterized by the following Fokker-Planck equation,

$$\partial_t P_t(x) = \gamma \partial_x \left[x P_t(x) \right] + D\partial_x^2 P_t(x), \tag{4.65}$$

with $\gamma = \tau^{-1}$ an inverse relaxation time and D a diffusion constant with dimension $[x^2]/[t]$. It can alternatively be described by a stochastic differential equation, called Langevin equation,

$$\dot{x} = -\frac{x}{\tau} + \sqrt{C}\eta,$$

where $C = 2D$ is the fluctuation strength of a Gaussian white noise random rate (also called white noise random force) η,

$$\langle \eta(t) \rangle = 0, \; \left\langle \eta(t)\eta(t') \right\rangle = \delta(t - t'). \tag{4.66}$$

On the equivalence of both descriptions we comment a little later. The Fokker-Planck equation (4.65) is of second order in ∂_x and has a linear in x drift. Thus, one can study its Fourier transformed which yields a first order partial differential equation in Fourier variable k, which can be solved by the method of characteristics. Alternatively, one can calculate the path integral by Gaussian integration, since k and x are not higher than second order in the generator function. The path integral representation also shows that the Ornstein-Uhlenbeck process is the Markov pendant to the harmonic oscillator of quantum mechanics. Without doing this integral explicitly we can infer from this that the solution of the initial value problem $P_0 = \delta(x_0)$ for the Fokker-Planck equation must be Gaussian and reads

$$\boxed{P_t(x) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} \exp\left[\frac{-(x - \langle x\rangle_t)^2}{2\sigma^2(t)}\right]}, \tag{4.67}$$

where the time evolution of average and variance still have to be calculated. This can either be done with the help of the Langevin equation, solving it and performing the average over η in calculating average and variance of x at time t, or it can be derived from integrating the Fokker-Planck equation over x and x^2 and doing integral per parts to reach closed differential equations for average and variance of x at time t. Either of these methods yields the desired answer:

$$\langle x\rangle_t = x_0 \cdot e^{-\gamma t};\ \sigma^2(t) = \left\langle(\Delta x)^2\right\rangle_t = \frac{D}{\gamma}\left[1 - e^{-2\gamma t}\right]. \tag{4.68}$$

For short time intervals $\Delta t \ll \tau$ one reproduces the defining features of drift and diffusion in the Fokker Planck equation,

$$\langle \Delta x\rangle = -\gamma x \cdot \Delta t;\ \left\langle(\Delta x)^2\right\rangle = 2D \cdot \Delta t. \tag{4.69}$$

To see the equivalence of the Langevin equation with the Fokker Planck equation it is sufficient to see that the Langevin equation as a differential equation leads to the short time behavior for drift and diffusion as displayed by (4.69). Therefore, the drift and diffusion expressions are just another way to define a Langevin equation for a Fokker-Planck equation. In the long time limit the variable relaxes to zero with constant variance $D\tau$—which is a stationary equilibrium state.

In the limit $\gamma \to 0$ the Ornstein-Uhlenbeck process tends to a **Wiener process** which has no relaxation but only diffusive fluctuation,

$$\langle \Delta x\rangle_t = 0\ ;\ \left\langle(\Delta x)^2\right\rangle_t = 2D \cdot t. \tag{4.70}$$

The corresponding Langevin equation as a stochastic differential equation reads

$$\dot{x} = \sqrt{C}\eta. \tag{4.71}$$

The resulting Fokker-Planck equation is, of course, the diffusion equation (2.35).

The Ornstein-Uhlenbeck process has two prominent realizations:

1. The variable is a velocity v in a Brownian motion.[5] For short times ($t \ll \tau$) the velocity behaves diffusive with $D_v = C/2$ and for long times it relaxes to equilibrium, such that $\langle (\Delta v)^2 \rangle = \langle v^2 \rangle = C\tau/2$ can be identified with the equipartition law[6] T/m. The corresponding spatial coordinate x with $v = \dot{x}$ will also behave diffusive in the long time limit with diffusion constant $D_x = C\tau^2/2$. Thus, a relation (called Einstein relation) between diffusion constant, relaxation time, mass and temperature follows:
$$D_x = \frac{T}{m}\tau. \tag{4.72}$$
We will come back to this realization in a slightly more general context with two variables x and v in the next chapter.
2. The variable is the spatial coordinate of a stochastically relaxing particle in the presence of a harmonic oscillator potential with strong friction (negligible acceleration),
$$0 \approx \dot{v} = -\frac{v}{\tau} + F(x)/m + \sqrt{C}\eta, \tag{4.73}$$
which leads via $\dot{x} = v$ and $F(x) = -kx$ to the Langevin equation for x,
$$\dot{x} = -\frac{\tau k}{m}x + \tau\sqrt{C}\eta. \tag{4.74}$$

4.4 Elementary Quantum Systems

For quantum systems the normalized eigenstates $\mid E_\alpha\rangle$ of the Hamilton operator H (energy eigenstates with energy eigenvalue E_α) are the stationary states in the sense that their time dependence is simply a phase factor,

$$\mid E_\alpha\rangle_t = e^{-iE_\alpha t} \mid E_\alpha\rangle_0 \,, \tag{4.75}$$

and the corresponding probability distribution $P_\alpha(x) = |E_\alpha(x)|^2$ is stationary. These states can be used for a spectral representation of H and thus for the spectral representation of the dynamics for any initial state $\psi_0(x)$ as

$$\psi_t(x) = \sum_\alpha e^{-iE_\alpha t} C_\alpha^0 E_\alpha(x), \tag{4.76}$$

[5] A suspended particle is kicked around by lighter fast moving thermalized particles.

[6] T is temperature in units of frequency ($k_B = \hbar = 1$) and m is mass in units of time/length^2 or equivalently in units of frequency/velocity^2.

where $C^0_\alpha = \langle E_\alpha|\psi_0\rangle$ and $E_\alpha(x) = \langle x|E_\alpha\rangle$. The resulting probability density has stationary contributions from diagonal contributions and shows quasi-periodic[7] oscillations from non-diagonal contributions,

$$\begin{aligned} P_t(x) = &\sum_\alpha |C^0_\alpha|^2 |E_\alpha(x)|^2 \\ &+ \sum_{\alpha\neq\beta} \mathrm{Re}\ \left\{C^0_\alpha E_\alpha(x)(C^0_\beta)^* E_\beta(x)^*\right\} \cos\big((E_\alpha - E_\beta)t\big) \\ &- \mathrm{Im}\left\{C^0_\alpha E_\alpha(x)(C^0_\beta)^* E_\beta(x)^*\right\} \sin\big((E_\alpha - E_\beta)t\big)\,. \end{aligned} \tag{4.77}$$

Here α can be a discrete index of summation or a continuous index for integration. Only energy differences regulate the quasi-periodic time dependence. To represent the dynamics this way is helpful for theoretical considerations (like quasi-periodicity) and helpful for practical calculations if the eigenstates are known and their overlaps C^0_α with the initial state can be calculated exactly or approximately.

4.4.1 Quantum Well

The model of a Galilei particle with mass m and piecewise constant potential $V(x) = V_{ab}$ for $x \in [a, b]$ in one dimension serves as a solvable toy model to capture essential qualitative features of quantum systems,

$$H = -\frac{\partial_x^2}{2m} + V(x). \tag{4.78}$$

On each interval $[a, b]$ the eigenvalue problem for energy eigenvalue E has (because of piecewise translational invariance) solutions of the form e^{ikx} with piecewise eigenvalue $E(k) = k^2/(2m) + V_{ab}$. The possible values k are related to the energy as

$$k(E) = \pm\sqrt{2m(E - V_{ab})}. \tag{4.79}$$

For $E \geq V_{ab}$ they describe waves of wavelength $\lambda = 2\pi/k$ directed left or right. For $E \leq V_{ab}$ they describe exponential modes with characteristic lengths of exponential decay $l = i/k$ to the left or right. On each interval a solution for a given energy eigenvalue E is possible as a linear combination of two eigenfunctions corresponding to (4.79). To reach a solution on the conjunction of intervals, one has to fulfill continuity conditions for the eigenfunction and its first derivative to guarantee the continuity of the probability density and the current probability density. Thus, matching conditions have to be fulfilled at the boundaries of the intervals. These matching conditions cannot always be solved analytically but by accurate approximate methods.

[7] Quasi-periodicity means a superposition of periodic oscillations of non-commensurate periods.

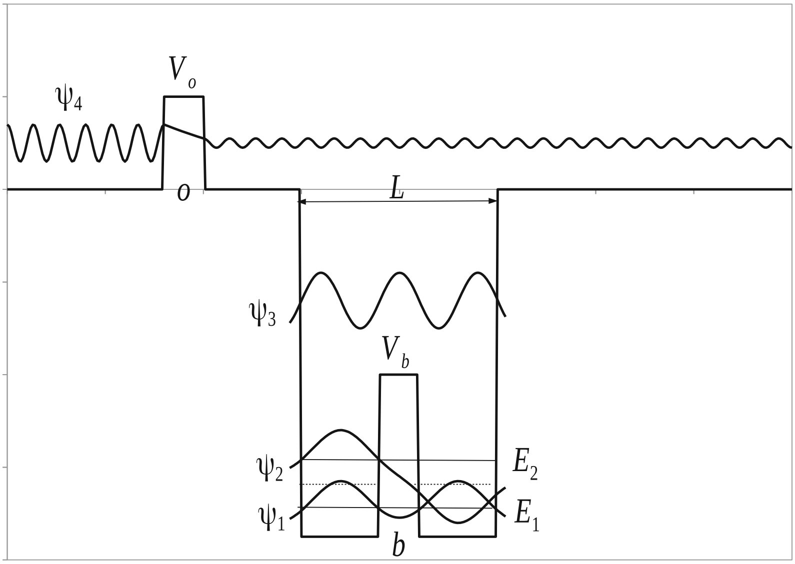


Fig. 4.3 Illustration of eigenstates in a piecewise constant potential in 1D. Eigenstates ψ_1 (symmetric with respect to smaller wells) and ψ_2 (anti-symmetric with respect to smaller wells) are nearly degenerate in their energies E_1 and E_2 for large barrier height V_b. Bound states ψ_3 with energies above the barrier V_b are standing waves fitting within the well of size L. Extended states ψ_4 have exponential modes within an obstacle as long as their energy is lower than the obstacle potential V_o (for simplicity the effect of the well is not shown in ψ_4)

Furthermore, these matching conditions are responsible for discrete bound states as they cannot be fulfilled for a continuum of energy eigenvalues in the case of bound states. Examples can be found in most textbooks on quantum mechanics, e.g. in Chap. 2 in [4]. In Fig. 4.3 a potential landscape with piecewise constant potentials is shown. The far left and far right with $V = 0$ can serve as ingoing and outgoing regions of scattering processes. The region of width o with potential V_o serves as an obstacle to propagation and the region of width L and depth V_w serves as a so-called quantum well model for bound states. Within the quantum well a barrier of width b and height V_b is placed at the bottom of the well. For a given value of energy E eigenstates may be constructed from the piecewise solutions under the matching conditions. For $0 > E > -V_w$ only discrete values are allowed by the matching conditions, while for $E > 0$ extended eigenstates exist at any energy. The discrete energies correspond to stationary bound states and the discreteness of the energy eigenvalues explains the energy quantization phenomenon for bound states. The extended eigenstates cannot be normalized on the infinite line and are thus called improper eigenstates. It is also possible to close the system at some very large embedding length $\mathcal{L}$ and normalize the eigenstates to that system size. The resulting quasi-continuous energies are discrete with a level spacing vanishing for infinite $\mathcal{L}$. The following conclusions about possible qualitative behavior can be drawn.

- For $E < -V_w$ no eigenstates exist. It is impossible to construct a non-vanishing eigenfunction from only exponential modes.
- For $-V_w < E < -V_w + V_b$ discrete eigenstates exist. In the two wells of width $(L-b)/2$ they are wavelike and within the barrier region of width b they consist of exponential modes. The probability within the barrier region gets rapidly smaller as the barrier height V_b gets larger. The probability decays exponentially into the region outside the wells and vanishes when the well depth V_w becomes infinite. Thus, the particle is localized to the well of width L up to exponentially small corrections. It is concentrated in the two wells of width $(L-b)/2$ but has some smaller but finite chance to be found between the two wells. The discrete allowed wave lengths within the two wells get smaller for larger energy and the largest is approximately twice the width of the wells for sufficiently large barrier height V_b. It becomes exact for infinite V_b and V_w. For sufficiently large barrier height V_b the lowest lying energies occur in almost degenerate pairs of energies. Their eigenstates can be approximated by linear superpositions of eigenstates located in individual wells. The two possible unbiased superpositions (the sum and the difference) have nearly the same energy (see ψ_1 and ψ_2 in Fig. 4.3). The sum state has higher probability within the barrier and is thus often called binding state while the difference state is called unbinding state because of lower probability within the barrier. It turns out that also the energy of the sum state is a bit lower as that of the difference state.[8] A further characteristic feature of quantum systems with few degrees of freedom can be seen: although the energy is below the potential barrier, the sum and difference states, as stationary states, have equal probability in both wells and the particle cannot have a stationary state in only one of the wells. These statements can easily be substantiated within a two level approximation as discussed in Sect. 2.3.6. The dynamics of a particle starting in one well will show Rabbi oscillations between two wells. Such process is called tunneling with the misleading imagination that particles tunnel through a barrier violating energy conservation. One should keep in mind that we are talking stationary states when addressing fixed energies. When talking the dynamics from one well to the other the superposition of at least two eigenstates with some maybe small energy difference $\Delta\epsilon$ is involved leading unavoidably to oscillations with frequency $\Delta\epsilon$. For larger barriers the frequency decreases drastically. One should also keep in mind that couplings of a particle to some environment may effectively localize it into one of the wells (see the discussion on quantum Master equations in Sect. 5.4.2).
- For $-V_w + V_b < E < 0$ discrete eigenstates with wavelike behavior within the well exist. The wavelength is a bit larger in the region of the barrier. The barrier becomes insignificant when $V_b \ll E + V_w$ and the width L is approximately an integer multiple of half of the wavelength (see ψ_3 in Fig. 4.3). This becomes exact for $V_b = 0$ and $V_w \to \infty$.

[8] The model can be used to illustrate atomic binding.

- For $0 < E < V_0$ a continuous spectrum of energies E is allowed with wavelike behavior of improper extended eigenstates outside the region of the obstacle. Within the region of the obstacle exponential modes exist (see ψ_4 in Fig. 4.3). In a scattering situation with ingoing wave from the left the stationary situation is such that on the left side of the obstacle a superposition of ingoing and reflected waves exists, where the amplitude of the reflected wave is r times the amplitude of the ingoing wave. On the right of the obstacle and the quantum well a transmitted wave with an amplitude of t times the amplitude of the ingoing wave results. The squared absolute values of r and t can be interpreted as reflection and transmission probability and they sum up to 1. The effect of the obstacle in this energy regime is to drastically decrease the transmission amplitude. The transmission is non-vanishing despite the fact that E is smaller than the obstacles potential energy V_o. This fact is also denoted as tunneling. When considering a propagating wave from the left it consists of a spectrum of energy modes and the obstacle leads to energy dispersion. The effect of the following quantum well is that the transmission gets some resonance peaks when the wave length becomes commensurate with the width L of the well.
- For $V_0 < E$ the situation is similar to the regime before, except that no exponential modes have to be taken into account and the transmission is not so drastically diminished.

4.4.2 Harmonic Oscillator and Occupation Numbers

The harmonic oscillator is that model in theoretical physics on which almost any method of solution gets tested and to which one would like to map almost any given problem. Its main feature is the symmetry between configuration coordinate and translation operator or velocity. Both appear in second order in the Hamiltonian resulting in an oscillation between kinetic energy and potential energy with one characteristic parameter, the period T. In terms of the corresponding frequency $\omega = 2\pi/T$ the Hamiltonian reads

$$H = \frac{-\partial_x^2}{2m} + \frac{m\omega^2 x^2}{2}. \tag{4.80}$$

Since it is quadratic in the hermitian generator of translation $p := -i\partial_x$ with real eigenvalue k and in x, one can find the propagator from the path integral by Gaussian integration in k and x paths. In that sense, the harmonic oscillator problem is the reversible stochastic process pendant to the irreversible Ornstein-Uhlenbeck process. In doing the path integral calculation one can start from the discretized version and perform the continuum limit in the end. Alternatively, one can use the quantum to classical correspondence in the sense of Sect. 3.4.2. This is demonstrated e.g. in part 6 of the classic text on path integrals by Schulman [5]. One has to solve the stationary action differential equation (classical equation of motion) and calculate the action of such solutions from one location to another in time t. In addition one has to calculate a multicomponent Gaussian fluctuation integral yielding a determinant (see (3.42)). We leave these lengthy calculations as an exercise and only state the result here,

$$\langle x, t \mid \mathrm{x}_0, t_0\rangle = \sqrt{\frac{m\omega}{2\pi i \sin(\omega(t-t_0))}} \times \tag{4.81}$$

$$\times \exp\left\{\frac{im\omega}{2\sin(\omega(t-t_0))}\left[(x^2+x_0^2)\cos(\omega(t-t_0)) - 2xx_0\right]\right\}. \tag{4.82}$$

It is possible to extract eigenvalues and eigenvectors of H from the propagator by Fourier-Laplace transformation and integrations in the complex energy plane. However, these are tedious and sophisticated calculations. For the purpose of extracting eigenvalues and eigenvectors a much more elegant way is provided by an algebraic method based on creation, annihilation and number operators. We present this also because it can be generalized to quantum field theories for an arbitrary number of oscillating particles whose interactions can be expressed with the help of these operators. This algebraic method is presented in many textbooks on quantum mechanics and we follow the compact treatment in [6].

From the shape of the parabolic potential $V(x)$ and our experience with the quantum well we expect that the Hamiltonian has discrete positive energy eigenvalues, as the parabola could be interpreted as a particle confining potential. Firstly, we introduce the length scale $l := 1/\sqrt{m\omega}$ and a factorization of the positive quadratic Hamiltonian with dimensionless linear factor operators

$$a := \frac{x}{l\sqrt{2}} + i\frac{pl}{\sqrt{2}}, \tag{4.83}$$

$$a^\dagger = \frac{x}{l\sqrt{2}} - i\frac{pl}{\sqrt{2}}, \tag{4.84}$$

such that we can write

$$H = \omega\left(a^\dagger a + \frac{1}{2}\left[a, a^\dagger\right]\right). \tag{4.85}$$

The commutator $\left[a, a^\dagger\right]$ appears, because the order of infinitesimal translation with ∂_x and multiplication with x counts. When applied to a function, the commutator of these elementary operations reads

$$[\partial_x, x] = 1. \tag{4.86}$$

and as a consequence we have

$$\left[a, a^\dagger\right] = 1, \tag{4.87}$$

such that the Hamiltonian shows explicitly its positive spectral character,

$$H = \omega\left(a^{\dagger}a + \frac{1}{2}\right). \tag{4.88}$$

It is now crucial to realize that the operators a and $a^{\dagger}$ transform an eigenstate of the operator

$$\hat{N} := a^{\dagger}a \tag{4.89}$$

into another eigenstate with a shift in the eigenvalue by just ± 1. This follows from the commutation relations

$$\left[\hat{N}, a\right] = -a, \tag{4.90}$$

$$\left[\hat{N}, a^{\dagger}\right] = a^{\dagger}, \tag{4.91}$$

as a result of the fundamental commutation relation of (4.87). When operating on an eigenstate $\mid N\rangle$ of hermitian positive $\hat{N}$ with $\hat{N}a$ we can apply the commutation relation and find that

$$\hat{N}(a \mid N\rangle) = (N-1)(a \mid N\rangle). \tag{4.92}$$

Thus, the operator a has transformed an eigenstate of $\hat{N}$ with eigenvalue N to another eigenstate with eigenvalue $N-1$. Similarly, we find that

$$\hat{N}(a^{\dagger} \mid N\rangle) = (N+1)(a^{\dagger} \mid N\rangle), \tag{4.93}$$

and the operator $a^{\dagger}$ has transformed an eigenstate of $\hat{N}$ with eigenvalue N to another eigenstate with eigenvalue $N+1$. Since N is positive, there must be a minimum eigenvalue for it and we call this state $\mid N_0\rangle$. Since a cannot lower this eigenvalue the application of a on this state must vanish,

$$a \mid N_0\rangle = 0. \tag{4.94}$$

On operating from the left with $a^{\dagger}$ we see that the eigenvalue N_0 of $\hat{N}$ must be zero. Therefore this state can be written as $\mid 0\rangle$. By successive applications of $a^{\dagger}$ we get all other eigenstates and we know the spectrum of $\hat{N}$: it just consists of all natural numbers including 0 as the ground state level. These marvelous findings justify to call $\hat{N}$ the number operator and $a^{\dagger}$ a creation operator and a an annihilation operator. They create and destroy quanta. For the harmonic oscillator these quanta are related by (4.88) to the energies. The eigenenergies (or eigenfrequencies) are equidistant with distance ω and ground-state value $\omega/2$,

$$E_N = \omega(N + \frac{1}{2}). \tag{4.95}$$

To get properly normalized states from the normalized ground state one finds by recursion

$$\boxed{\mid N\rangle = \frac{1}{\sqrt{n!}} \left(a^\dagger\right)^N \mid 0\rangle}. \tag{4.96}$$

Also, the coordinate representation $\langle x \mid 0\rangle =: \varphi_0(x)$ can be found from the resulting differential equation

$$\langle x \mid a \mid 0\rangle = 0 = \left[\frac{x}{l\sqrt{2}} + \frac{l\partial_x}{\sqrt{2}}\right]\varphi_0(x) \tag{4.97}$$

as a Gaussian which reads

$$\varphi_0(x) = \frac{1}{\sqrt{l\sqrt{\pi}}} \exp\left(-\frac{x^2}{2l^2}\right). \tag{4.98}$$

All higher eigenvalue eigenfunctions (Hermite polynomials) can be generated by (4.96).

The algebra of creation, annihilation and number operators can be used to describe systems where discrete states, labeled as index j, are occupied with certain natural numbers. Such systems are called many particle systems or many body systems because the discrete states can be viewed as the states of a single of many indistinguishable quantum objects and the occupation number N_j tells how many of these quantum objects occupy the single object state j.[9] Defining the vacuum state $\mid 0\rangle$ as ground-state for the particle number operator $\hat{N}_j = a_j^\dagger a_j$ to eigenvalue 0 one can create a convenient many particle basis of the many body system by applications of the creation operators $a_j^\dagger$ on the vacuum state. The algebra

$$\boxed{\left[a_j, a_l^\dagger\right] = \delta_{lk}} \tag{4.99}$$

together with

$$\boxed{\hat{N}_j = a_j^\dagger a_j} \tag{4.100}$$

is sufficient to express the dynamics of a many body system with natural numbers as occupation numbers. Such particle types are called Bosons. Their wave function must

[9]To call a quantum object a real particle does however need some further ingredients of spatial symmetries and the possibility to find the object in a finite region of space.

be symmetric against interchanging the coordinate of two of its indistinguishable particles.

To represent Fermions (the wave function must be antisymmetric against interchanging the coordinate of two of its indistinguishable particles) one can use a similar algebra of creation ($b_j^\dagger$), annihilation (b_j) and number operators,

$$\boxed{\hat{N}_j := b_j^\dagger b_j} \tag{4.101}$$

where for Fermions the algebra is defined with anti-commutator[10] relations,

$$\boxed{\left\{b_j, b_l^\dagger\right\} = \delta_{jl}} \tag{4.102}$$

and a rule of antisymmetry in state indices

$$\boxed{\left\{b_j^\dagger, b_l^\dagger\right\} = 0 = \left\{b_j, b_l\right\}}. \tag{4.103}$$

Equations (4.102, 4.103) define an algebra of creation and annihilation for Fermion many particle systems. The basis states for an index j are just $\mid 0_j\rangle$ with no particle (vacuum state) and $\mid 1_j\rangle$ with one particle in state j. The algebra suffices to show that $\hat{N}_j$ is the particle number operator for state j and that $b_j^\dagger$ creates a particle from the vacuum and that b_j annihilates a particle in j state. Both operators applied twice to any state yields zero, consistent with the possible particle occupation numbers 0, 1 for each state j.

An algebraic setup of a quantum field theory can then be formulated with the help of local creation, $a^\dagger(x)$, annihilation, $a(x)$, and particle density operator, $\hat{N}(x) = a^\dagger(x)a(x)$, where creation/annihilation means creation/annihilation of a particle at configuration coordinate x within the volume element dx such that $\hat{N}(x)\mathrm{d}x$ is the number operator in volume element dx. We remark that the local creation and annihilation operators $a^\dagger(x)$ and $a(x)$ are often simply called field operators and written with letters known from wave functions like $\Psi^\dagger(x)$ and the completely inadequate notion of second quantization is still widespread for the **occupation number representation** of many body physics.

4.5 Exercises

Exercise 1: Few States Deterministic

Consider deterministic motions in the case of 3 states for discrete time homogeneous dynamics ($n = 0, 1, 2$) and discuss their solutions along the line of Sect. 4.1.

---

[10]The anti-commutator of two algebra elements A and B is defined as $\{A, B\} := AB + BA$.

Exercise 2: Generating Function for One Step Processes
Discuss why the non-linear case of l_n and g_n is difficult to solve.

Exercise 3: Poisson Distribution
Calculate mean and variance for the Poisson distribution $P(n) = \frac{\mu^n e^{-\mu}}{n!}$ by clever summation.

Exercise 4: Wiener-Khintchine Theorem
Show the equality of expressions (4.59) and (4.60) for sufficiently fast decay of the auto-correlation function at infinity.

Exercise 5: Ornstein-Uhlenbeck Process
Derive closed differential equations for mean and variance from the Fokker-Planck equation for the Ornstein-Uhlenbeck process and solve them for a sharp initial value at x_0.

Exercise 6: Propagator for the Harmonic Oscillator
Follow the calculation of the propagator for the harmonic oscillator model in the sense of Sect. 3.4.2 as outlined e.g. in part 6 of [5] and also in Sect. 3.5 of [7]. You may alternatively do the calculation directly from the discretized path integral of (3.23) with Gaussian integrations in x and k.

References

1. N.G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 3rd edn. (North-Holland, Amsterdam, 2007)
2. G. Roepke, *Statistische Mechanik für das Nichtgleichgewicht* (VEB, Berlin,1987); *Nonequilibrium Statistical Physics* (Wiley, 2013)
3. H. Cartan, *Elementary Theory of Analytic Functions of One or Several Complex Variables* (Dover Publications, New York, 1995)
4. M. Alonso, E.J. Finn, *Fundamental University Physics: III Quantum and Statistical Physics* (Addison-Wesley, 1968)
5. L.S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981)
6. H. Mitter, *Quantentheorie, Vorlesungen über Theoretische Physik III* (Spektrum Akademischer Verlag, Heidelberg, 1994)
7. A. Altland, B. Simons, *Condensed Matter Field Theory*, 2nd edn. (Cambridge University Press, Cambridge, 2010)

Chapter 5
Observables, States, Entropy and Generating Functionals

Abstract We broader the view and work out a theory where properties and states are generalized as to have time derivatives of properties and reduced states (density operators) included with compact and flexible ways of calculation. We introduce the notion of entropy as a dispersion measure and consider its time evolution in Markov and quantum processes. We consider limits of stationarity and cross-over between different types of dynamics by taking system environments into account. In each type of dynamics or stationary limit generating functionals appear as the unifying structure. When fields form the configuration space for infinitely many degrees of freedom one deals with stochastic field theories. In the case of quantum processes these are so called quantum field theories met commonly in particle physics and condensed matter physics. Modeling strategies are discussed that start with a Gaussian approximation around stationary action solutions, supplemented with a stability analysis.

5.1 Time Derivatives, Compatibility and Uncertainty

To treat time derivatives of properties on the same level as properties we like to define observables $\dot{f}$ that correspond to the time derivatives of properties in the following sense: their expectation value at a given time should be equal to the time derivative of the property expectation value at that time,

$$\left\langle \dot{f} \right\rangle_t = \partial_t \left\langle f \right\rangle_t. \tag{5.1}$$

In the Markov case we can write

$$\partial_t \left\langle f \right\rangle_t = (f|\partial_t P_t) = (f|MP_t) = (M^{\mathrm{T}} f|P_t) =: \left\langle \dot{f} \right\rangle_t, \tag{5.2}$$

where M^{T} is the transposed operator (partial integration in kernel notation) to the generator M. Again, the time derivative observable

$$\dot{f}(x) := M^{\mathrm{T}} f(x) \tag{5.3}$$

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1_5

is a function of x and can be viewed as a property compatible with any other property, since their values can be addressed simultaneously. Nevertheless, the system shows fluctuations which are controlled by the Kramers-Moyal coefficients of order two or higher; characteristic is the diffusive fluctuation for short times,

$$\left\langle (\delta x)^2 \right\rangle = 2D^{[2]}\delta t. \tag{5.4}$$

Note, that the operator ∂_x is relevant in the theory as it generates translations and the commutation relation $[\partial_x, x] = 1$ expresses the incompatibility of addressing simultaneously values to a position and a translation, resulting in the well known uncertainty relations between Fourier transformed

$$|\delta x| \cdot |\delta k| \geq 1/2. \tag{5.5}$$

Either the spectrum of positions is sharp or the spectrum of translations is sharp; both cannot be sharp as position and translation are strictly incompatible notions. This can be clearly seen for Gaussian functions by (3.33), where the equality is met. Another intuitive reading of (5.5) is: with one wave of wave-length λ you cannot resolve objects smaller than $\approx\lambda/2$. However, in Markov dynamics this uncertainty has no direct manifestation with observables, as they can all be represented by functions of the configuration variable.

In the quantum case we write the property $f(x)$ as an operator in spectral decomposition

$$f = \int \mathrm{d}x f(x) \mid x\rangle \langle x \mid \tag{5.6}$$

and use the Leibniz rule for differentiation,

$$\begin{aligned} \partial_t \langle f \rangle &= \partial_t \langle \psi \mid f \mid \psi \rangle \\ &= \langle -iH\psi \mid f \mid \psi \rangle + \langle \psi \mid f \mid -iH\psi \rangle \\ &= i \langle \psi \mid Hf \mid \psi \rangle - i \langle \psi \mid fH \mid \psi \rangle \\ &= i \langle [H, f] \rangle. \end{aligned} \tag{5.7}$$

Thus, in quantum processes an observable can be defined which represents the time derivative of some property f by

$$\dot{f} := i[H, f]. \tag{5.8}$$

Now, something very interesting has happened: the time derivative of a property is no longer a property in the usual sense as a function of the configuration variable—as soon as fluctuations are present: the Hamilton operator is of second or higher order in the translation generator ∂_x, resulting in a dependence of $\dot{f}$ on ∂_x of order one or higher. Therefore, within fluctuating quantum processes time derivatives are no longer compatible observables with those properties where they stem from.

Their values cannot simultaneously be addressed, since they do not commute and do not have a common spectral decomposition. Depending on the Hamiltonian coefficients the uncertainty relation between Fourier transformed translates to uncertainty relations between properties and their time derivatives. For example, in the case of a Galilei particle with mass m, the uncertainty between local coordinate x and velocity $\dot{x}$ reads

$$|\delta x| \cdot |\delta \dot{x}| \geq \frac{1}{2m}. \tag{5.9}$$

This sets a limit to the resolution of observations of smooth paths in quantum processes. If m becomes large, the uncertainty shrinks, but also the fluctuations as such. In quantum processes the fluctuations and the resolution of paths are controlled by the same Hamiltonian coefficients.

From now on we will denote as generalized property or **observable** O such hermitian operators which are either properties (diagonal in x), or are time derivatives of such properties, or are functions of properties and their derivatives. Their time derivatives fulfill also

$$\dot{O} = i[H, O]. \tag{5.10}$$

From now on we will denote the hermitian translation operator $k := -i\partial_x$ as **momentum operator** and the Hamiltonian as **energy operator**, since they can be seen as observables in fluctuating quantum processes. The spectral content of momentum is provided by Fourier analysis. The eigenvalues of momentum k have dimension $[x]^{-1}$. The momentum eigenstates $\mid k\rangle$ read in x-representation $\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$. The spectral content of energy is the frequency spectrum ω_n (dimension $[t]^{-1}$) of stationary states $U_t \mid \omega_n\rangle = e^{-i\omega_n t} \mid \omega_n\rangle$.

With the notion of generalized properties (observables) we can also define in a completely general way the property density operator for some s-component property $\boldsymbol{O}$ (components are listed as O^μ) and an associated property current density operator. To distinguish the property operator from its spectrum we use $\hat{O}$ for the operator and O for its eigenvalue. Then the property density operator is given as

$$\boxed{\hat{\varrho}(\boldsymbol{O}) := \prod_\mu \delta\left(\hat{O}^\mu - O^\mu\right)}. \tag{5.11}$$

Its expectation value in some state yields the spectral density of property $\boldsymbol{O}$ in that state in a probabilistic sense: the probability to find $\boldsymbol{O}$ in the volume element $\mathrm{d}^s O$ in that state is given by $\langle \varrho(\boldsymbol{O})\rangle\, \mathrm{d}^s O$. The configuration probability is given as $P_t(\boldsymbol{x}) = \left\langle \hat{\varrho}(\boldsymbol{x})\right\rangle_t$. As the most general definition of an associated conserved property current density operator we can define

$$\boxed{\hat{j}^\mu(\boldsymbol{O}) := \dot{\Theta}\left(\hat{O}^\mu - O^\mu\right) \prod_{\nu\neq\mu} \delta\left(\hat{O}^\nu - O^\nu\right)}. \tag{5.12}$$

By comparing $\sum_\mu \partial_{O^\mu}\hat{j}^\mu(\boldsymbol{O})$ with $\partial_t\hat{\varrho}(\boldsymbol{O})$ and exploiting $\partial_O\dot{\Theta}(\hat{O}-O) = -\dot{\delta}(\hat{O}-O)$ and the Leibniz rule of differentiating commuting operators one finds that a continuity equation holds already on the level of operators,

$$\boxed{\sum_\mu \partial_{O^\mu}\hat{j}^\mu(\boldsymbol{O}) + \partial_t\hat{\varrho}(\boldsymbol{O}) = 0}. \tag{5.13}$$

Thus, the continuity equation must also hold for expectation values (a linear operation) of such densities. As a special case, the configuration probability current density can be expressed as $j_t^\mu(\boldsymbol{x}) = \left\langle \hat{j}^\mu(\boldsymbol{x})\right\rangle_t$.

With (5.12, 5.10) we are able to find explicit expressions for the probability current density $j_t(x)$ in terms of the wave function for a given Hamiltonian in terms of its Hamiltonian coefficients. As an exercise show that we get back (2.65) for Hamiltonians of the form of (3.11).

5.2 Reduction of Variables and the Density Operator

In our notation of expectation values for quantum processes $\langle O\rangle = \langle\psi \mid O \mid \psi\rangle$ the dual character of observables and states is not obvious. For the discussion to follow it is very instructive to rewrite the expectation value in the following way

$$\langle O\rangle_\psi = \mathrm{Tr}\,\left\{OP_\psi\right\} \tag{5.14}$$

where Tr is a unitarian invariant matrix operation called trace and reads

$$\mathrm{Tr}\cdot = \int \mathrm{d}x\,\langle x \mid \cdot \mid x\rangle = \sum_n \langle n \mid \cdot \mid n\rangle. \tag{5.15}$$

The trace has the important cyclic invariance

$$\mathrm{Tr}\,\{ABC\} = \mathrm{Tr}\,\{CAB\} = \mathrm{Tr}\,\{BCA\}\,. \tag{5.16}$$

The hermitian operator P_ψ is the projector on state ψ,

$$P_\psi := \mid\psi\rangle\,\langle\psi\mid \tag{5.17}$$

It has eigenvalues 0 and 1 and fulfills the important projector condition

$$P^2 = P. \tag{5.18}$$

When we are not interested in all variables of a system but in a reduced set (relevant variables) we like to set up the theory in terms of the reduced variables. In terms of a probability distribution for the reduced variable $A(x)$ (typically the number of degrees of freedom of A is much lower than that of x) the construction of the distribution for A in terms of the distribution for x is straightforward

$$P_t(A) := \langle \delta(A - A(x)) \rangle_{P_t(x)} \,. \tag{5.19}$$

If $P_t(x)$ follows a Master equation, so does $P_t(A)$ and the Kramers-Moyal coefficients can easily be derived by studying the moments of deviations δA in short time. Nothing spectacular happens to the formalism as such.

In terms of pre-probabilities or corresponding projectors something very interesting happens: the state for the reduced variable is no longer described by a projector but by a so called **density operator** ϱ which fulfills three conditions: (1) it is hermitian, (2) positive and (3) normalized to unity ($\mathrm{Tr}\,\varrho = 1$). This can be understood by the following discussion of a vector-state in a product Hilbert space $\mathcal{H}_A \times \mathcal{H}_B$

$$\mid \psi \rangle = \sum_{A_i, B_j} \psi(A_i, B_j) \mid A_i \rangle \mid B_j \rangle \,. \tag{5.20}$$

The corresponding projector reads

$$P_\psi = \sum_{A_i, B_j, A_k, B_l} \psi^*(A_k, B_l) \psi(A_i, B_j) \mid A_i \rangle \mid B_j \rangle \langle B_l \mid \langle A_k \mid . \tag{5.21}$$

Once we consider observables belonging to A and not to B we can calculate their expectation values with the help of a state ϱ_A defined by the following constraint:

$$\langle f(A) \rangle = \mathop{\mathrm{Tr}}_{AB} \left\{ P_\psi f(A) \right\} = \mathop{\mathrm{Tr}}_{A} \{ \varrho_A f(A) \}, \tag{5.22}$$

and ϱ_A results from a partial trace along B over P_ψ,

$$\varrho_A \cdot := \mathop{\mathrm{Tr}}_{B} \left\{ P_\psi \cdot \right\}. \tag{5.23}$$

The matrix representation of ϱ_A is then

$$(\varrho_A)_{ki} = \sum_{B_l} \psi^*(A_k, B_l) \psi(A_i, B_l). \tag{5.24}$$

We leave it as an exercise to show that this a density matrix. Density matrices which reduce to projectors $\varrho = \varrho^2$ are called pure states.

In the following we consider quantum processes in relevant variables x as characterized by density operators ϱ as states and observables O which are functions of properties or of their corresponding time derivatives $\dot{O}$. Expectation values can be calculated as

$$\boxed{\langle O \rangle = \mathrm{Tr}\ \{\varrho O\}}. \tag{5.25}$$

If the dynamics can be considered as closed for the relevant variables the group property is given by either the Schrödinger equation for states or the Heisenberg equation for observables. The Schrödinger equation for the density operator is often called von Neumann equation.

$$\boxed{\dot{\varrho} = -i\,[H, \varrho]\,, \;\; \dot{O} = i\,[H, O]}. \tag{5.26}$$

5.3 Entropy

Entropy is a measure for the degree of dispersion of a state over possible states. The degree of dispersion is proportional to the degree of information one gains in taking notice of the actual state. Depending on the character of state we distinguish between configuration entropy and quantum entropy. With configuration entropy $S(x = \xi)$ we mean the degree of information we gain when ξ is the actual configuration state, while the configuration states are distributed according to some distribution $P(x)$. With quantum entropy $S(P_j)$ we mean the degree of information we gain when the actual state is given by projector P_j, while the states are distributed according to some density operator ϱ having P_j as a projector in its spectral decomposition.

The definition of entropy is motivated by the following special situation: a variable can take N different values with equal probability $P = 1/N$. Somebody knows the actual value. He or she already has the information that we can get by asking him or her binary questions. How many binary questions do we need to ask? The answer is that $\log_2(N) = -\log_2(P)$ is always enough, because that is the number of digits of N.

A requirement for the definition of entropy is that it should be additive for independent variables. This leads to the logarithm's functional equation. The choice of basis is arbitrary as it just defines the unit of a dimensionless entropy. In thermodynamics, for historical reasons, the entropy has the dimension of energy/temperature and the logarithm is multiplied by the Boltzmann constant. We use the natural logarithm and dimensionless entropy.

5.3.1 Configuration Entropy

We define the **configuration entropy** as

$$S(x) := -\ln(P(x)), \tag{5.27}$$

where $P(x)$ is a dimensionless probability density.[1] Accordingly the **average configuration entropy** is

$$\boxed{\mathrm{S} := \langle S(x)\rangle = -\int \mathrm{d}x\, P(x) \ln P(x)}. \tag{5.28}$$

Note that $S(x)$ is, like the probability $P(x)$, not an original property, but a **meta property** of the system (depending on what we know about the system). The average configuration entropy is a functional of the probability $P(x)$. In calculations to follow we will use the following relations

$$P(x) = e^{-S(x)};\ \mathrm{d}P = -P\mathrm{d}S;\ \mathrm{d}\ln P = -\mathrm{d}S. \tag{5.29}$$

To study the time evolution of the average configuration entropy we make use of the continuity equation and then specify to certain processes.

$$\dot{\mathrm{S}} = -\int \mathrm{d}x\, \dot{P}(x)(1 + \ln P(x)) = \int \mathrm{d}x\, \partial_x j(x)(1 + \ln P(x)). \tag{5.30}$$

By partial integration we get an edge term which can only survive in open systems plus a volume term over a scalar product of two vectors: the current density and the entropy gradient,

$$\boxed{\dot{\mathrm{S}} = \dot{\mathrm{S}}_{\mathrm{Edge}} + \int \mathrm{d}x\, j(x) \cdot \partial_x S(x)}. \tag{5.31}$$

Equation (5.31) is the most general statement about the dynamics of the average configuration entropy for continuous variables in continuous time. It is also true for quantum processes, where j is not a functional of the distribution P. However, for quantum processes the configuration entropy is not of great importance for characterizing the process. Therefore, we now consider Markov processes and further simplify to Fokker-Planck processes which captures the main ingredients drift and diffusion for continuous configurations. It is always possible [1] to transform to variables such that the diffusion $D^{[2]}$ is independent of x. Thus, we can write for the current density

$$j(x) = -D^{[1]}(x)P(x) - D^{[2]}\partial_x P(x), \tag{5.32}$$

and for the entropy rate

$$\begin{aligned}
\dot{\mathrm{S}} &= \dot{\mathrm{S}}_{\mathrm{Edge}} + \int \mathrm{d}x\, \left[-D^{[1]}(x) \cdot (\partial_x S(x))\, P(x) - D^{[2]}\partial_x P(x) \cdot \partial_x S(x)\right], \\
\dot{\mathrm{S}} &= \dot{\mathrm{S}}_{\mathrm{Edge}} - \left\langle \partial_x D^{[1]}(x)\right\rangle + \left\langle \partial_x S(x) \cdot D^{[2]} \cdot \partial_x S(x)\right\rangle.
\end{aligned} \tag{5.33}$$

[1] The integral measure dx can be made dimensionless by a convenient unit for variable x.

In the last step we made use of (5.28) and partial integration.

In a closed system the edge term vanishes and the diffusion term is a quadratic form with positive coefficient (matrix) $D^{[2]}$ thus leading to an increase in entropy. The drift term vanishes for a reversible Hamiltonian dynamics, since this expresses Liouville's theorem: the divergence of the vector $D^{[1]}(x, p) = (\partial_p H, \partial_x H)$ vanishes due to $\partial^2_{xp} H = \partial^2_{px} H$.

Thus, for closed deterministic reversible Hamiltonian dynamics without fluctuations the average entropy stays constant. For irreversible dynamics with reversible deterministic drift and diffusive fluctuations the entropy increases with time.

We mention that for purely deterministic but irreversible processes the entropy may increase or decrease depending on the divergence of the drift. For example in 1D with $\dot{x} = -kx$ all motions come to rest at $x = 0$ and thus the distribution gets finally pinned at $x = 0$ and the entropy decreases with time.

For the exactly solvable Ornstein-Uhlenbeck process with linear drift (friction), $D^{[1]} = x/\tau$ and diffusion constant D the solution is a Gaussian[2] with time dependent variance $\sigma_t^2 = D\tau(1 - e^{-2t/\tau})$. The drift term contributes $-1/\tau$ to the entropy derivative. However, the diffusive term with squared entropy gradients yields[3] $D\frac{\sigma_t^2}{(\sigma_t^2)^2} = [\tau(1 - e^{-2t/\tau})]^{-1}$. Thus, the time derivative of entropy starts strongly positive with $1/2t - 1/\tau$ for short times ($t \ll \tau$), reaches $1/\tau$ at $t = (\tau/2)\ln(2)$ and finally approaches $1/\tau - 1/\tau = 0$ for infinitely large times. During the whole irreversible process the entropy increases. This generalizes to a multidimensional variable x.

Systems far from equilibrium are not closed and characterized by strong currents of energy, material and entropy from its environment, as depicted in Fig. 1.2. For such systems the edge term in (5.33) is of great importance and one can write down a non-equilibrium entropy equation as

$$\boxed{\mathrm{d}S = \mathrm{d}S_{\mathrm{ext}} + \mathrm{d}S_{\mathrm{int}}}, \tag{5.34}$$

where $\mathrm{d}S$ means the systems entropy change in total, $\mathrm{d}S_{\mathrm{int}}$ the internal entropy change and $\mathrm{d}S_{\mathrm{ext}}$ the entropy change due to input and output through the edge between system and environment. The internal entropy change is always non-negative, as discussed before,

$$\boxed{\mathrm{d}S_{\mathrm{int}} \geq 0}. \tag{5.35}$$

The external change can be arbitrary. We can qualitatively distinguish three situations.

1. The system exports more entropy then it imports and lowers its entropy in total,

$$\mathrm{d}S_{\mathrm{ext}} < 0, \ |\mathrm{d}S_{\mathrm{ext}}| > \mathrm{d}S_{\mathrm{int}}, \ \mathrm{d}S < 0. \tag{5.36}$$

[2] See [1–3], note the opposite sign convention in the definition of $D^{[1]}$.

[3] The entropy as ln of the Gaussian is quadratic in deviations from the average.

In such a situation within the system new order and structures can emerge (self-organized).

2. Similar to the first case, but with constant total entropy,

$$\mathrm{d}S_{\mathrm{ext}} < 0,\ |\mathrm{d}S_{\mathrm{ext}}| = \mathrm{d}S_{\mathrm{int}},\ \mathrm{d}S = 0. \tag{5.37}$$

The new structures reach a stationary non-equilibrium state.

3. Finally the situation, where the system entropy increases in total,

$$\mathrm{d}S_{\mathrm{ext}} > 0,\ \mathrm{d}S > 0. \tag{5.38}$$

The order will disappear.

To describe a non-equilibrium stationary state with a Master equation one has to consider finite current boundary conditions.

5.3.2 *Quantum Entropy*

To get an entropy for the pre-probability as a meta-observable we define it with respect to the spectral content of the density operator as

$$S := -\ln \varrho. \tag{5.39}$$

For an eigenvalue ϱ_n the corresponding entropy S_n fulfills

$$\varrho_n = e^{-S_n}. \tag{5.40}$$

The average quantum entropy is defined accordingly,

$$\boxed{\mathrm{S} = -\langle \ln \varrho \rangle = -\mathrm{Tr}\ \{\varrho \ln \varrho\}}. \tag{5.41}$$

By the cyclic invariance of the trace one can show (exercise) that in reversible quantum processes the quantum entropy stays constant

$$\dot{\mathrm{S}} = 0. \tag{5.42}$$

The density operator evolves in time, but the degree of dispersion over states stays constant like in deterministic reversible Hamiltonian processes.

5.4 Stationary States and Equilibrium

In this section we study how stationary states can represent an equilibrium situation. We begin with the exactly solvable case of an Ornstein-Uhlenbeck process and then see how quantum systems can be described by a Master equation as soon as the dynamics is not a closed one in relevant variables by contact to some environment. The relaxation to stationarity in Markov processes is generic. This route gives support for the use of the maximum entropy principle in systems at global or local equilibrium. Another situation of irreversible stationarity is with scattering states to be discussed at the end of this section.

5.4.1 Stationary State in Ornstein-Uhlenbeck Processes

For the exactly solvable Ornstein-Uhlenbeck process we can see how the distribution reaches a stationary state. For an initial value peaked at x_0 the Gaussian distribution is centered around the average value $\langle x \rangle_t = e^{-t/\tau} x_0$ with the variance $\sigma_t^2 = D\tau(1 - e^{-2t/\tau})$ discussed already for the entropy production. For long times the distribution becomes stationary with stationary average $\langle x \rangle_\infty = 0$ and stationary variance $\sigma_\infty^2 = D\tau$. Thus, the entropy increases unless the distribution has reached a stationary state where the entropy stays constant. Such situation is called equilibrium.

It is even more instructive to consider an Ornstein-Uhlenbeck process in two degrees of freedom: $x_1 = x$ and $x_2 = v = \dot{x}$. The diffusion can be restricted to $D_{vv} = D$. The velocity drift can incorporate friction and a linear Newton force $F(x) = -V'(x) = -kx = m\dot{v}$ for a particle with mass m, which means

$$D_v^{[1]} = v/\tau + V'(x)/m. \tag{5.43}$$

The drift in the coordinate x is simply $D_x^{[1]} = -v$ for consistency. The stationary equilibrium limit can be written as

$$P_{eq}(x, v) = \frac{1}{Z} \exp - \frac{(1/2)v^2 + V(x)/m}{D\tau}, \tag{5.44}$$

which remarkably coincides with the **canonical equilibrium distribution** of a particle subject to a potential force $F(x) = -V'(x)$, once we identify the diffusion constant times the friction time with temperature T over mass m (T in units where the Boltzmann constant is 1),

$$D\tau = T/m. \tag{5.45}$$

The friction time τ serves as **relaxation time** to reach equilibrium. The relation (5.45) is quite famous and also known as Einstein relation between the product of diffusion and relaxation time, and the temperature. We have argued with the help of the exactly solvable case with linear force, but the validity of the canonical equilibrium distribution can also be shown for more general potential forces (see [1, 2]).

5.4.2 Quantum Master Equation

Quantum systems reduced to relevant variables may not be describable by a unitary time evolution, because of the missing irrelevant variables. The irrelevant variables are irrelevant in the sense that we cannot follow them and we have to concentrate on the slow macroscopically relevant degrees of freedom. They are however not irrelevant for the reversibility of the whole system. The idea is to get rid of them by formally integrating out their dynamics. The price to pay is the loss of closed unitary dynamics. But this price fits well as we get a Markov type dynamics with relaxation to macroscopically stationary solutions. We follow the quite general projector formalism developed by Zwanzig for quantum processes. The formalism as such is of great importance in many applications of linear algebra. Its generality is advantageous for getting the right general structure of quantum Master equations. On the other hand, it is not explicit about the couplings between relevant and irrelevant variables. Therefore, we will later rely on certain assumptions about separation of time scales in the system without exemplifying these assumptions on specific models.

Our relevant variables belong to a certain linear subspace of the full Hilbert space and we project onto this subspace by a projection operator $\mathcal{P}$. All expectation values of relevant observables can be calculated with the help of the **relevant density operator**

$$\varrho_{\mathrm{rel}} := \varrho_{\mathcal{P}} := \mathcal{P}\varrho\mathcal{P}. \tag{5.46}$$

The projector on the complement to the relevant variables is denoted as $\mathcal{Q} := 1 - \mathcal{P}$. The full density operator that fulfills a von Neumann equation with full Hamiltonian H can be decomposed as

$$\varrho = \varrho_{\mathrm{rel}} + \varrho_{\mathcal{Q}} + \varrho_{\mathcal{PQ}} + \varrho_{\mathcal{QP}} \tag{5.47}$$

with obvious notation. We like to construct the dynamic equation for ϱ_{rel}.

To concentrate on the structure we simplify the notation. The von Neumann equation can be written as

$$\partial_t \varrho_t = -i\mathcal{L}\varrho_t \tag{5.48}$$

with the so called Liouville operator $\mathcal{L}\cdot = [H, \cdot]$ as the generator. The formal solution is the time evolution operator for states,

$$\varrho_t = e^{-i\mathcal{L}t}\varrho_0. \tag{5.49}$$

The spectral content of such time evolution operator is captured in the frequency dependent **resolvent** $\mathcal{R}(z)$ ($-$i times the Laplace transformed of the time evolution)

$$\mathcal{R}(z) := [z - \mathcal{L}]^{-1} = -i \int_0^\infty \mathrm{d}t\, e^{izt} e^{-i\mathcal{L}t} = [i \int_{-\infty}^0 \mathrm{d}t\, e^{iz^*t} e^{-i\mathcal{L}t}]^*. \tag{5.50}$$

On the real valued spectrum $\mathcal{R}(z)$ is singular and analytic in the upper plane $z = \omega + i\epsilon$ or lower plane $z^* = \omega - i\epsilon$. At isolated eigenvalues $\mathcal{R}(z)$ has poles (states are normalizable), along the continuous spectrum (states are non normalizable in infinite systems) it has branch cuts. The resolvent's matrix elements are usually called **Green's function** of the linear dynamic or frequency dependent **propagator**. These notions are even more common on the level of the Schrödinger equation with H as generator.

Now, the evolution of the full density operator reads in frequency space

$$\varrho(z) = i\,[z - \mathcal{L}]^{-1}\,\varrho_0. \tag{5.51}$$

For the relevant density operator a similar equation holds for purely algebraic reasons

$$\varrho_{\mathrm{rel}}(z) = i\left[z - \mathcal{L}_{\mathit{eff}}(z)\right]^{-1} \varrho_{\mathrm{rel}0}. \tag{5.52}$$

Here the effective Liouville operator $\mathcal{L}_{\mathit{eff}}(z)$ lives on $\mathcal{P}$ space only, but depends on the spectrum. It is, in general, no longer hermitian but develops complex eigenvalues for each value of z. Therefore, eigenstates can decay with characteristic life time. As long as eigenvalues are discrete and close to the real axis, the imaginary part can be identified with the inverse lifetime. This is, of course, due to the coupling to the $\mathcal{Q}$ degrees of freedom, which have only formally been integrated out. Therefore, within the effective dynamics the reversibility can get lost and irreversibility shows up.

The most simple non-trivial situation is, that $\mathcal{L}_{\mathit{eff}}(z)$ does not significantly depend on z (time scale separation), but develops imaginary parts in its eigenvalues leading to relaxation to a stationary state. This is an emergent behavior—it is not by our choice, but by organization within a complex system, that some degrees of freedom emerge as the slow variables such that we can identify them as relevant to characterize it. The effective Liouville reads

$$\boxed{\mathcal{L}_{\mathit{eff}}(z) = \mathcal{L}_{\mathcal{P}} + \mathcal{L}_{\mathcal{P}\mathcal{Q}}\left[z - \mathcal{L}_{\mathcal{Q}}\right]^{-1} \mathcal{L}_{\mathcal{Q}\mathcal{P}}}. \tag{5.53}$$

The terms have a very intuitive interpretation. The first term is the bare Liouville in $\mathcal{P}$ space. It would be the full Liouville in the absence of any couplings to $\mathcal{Q}$-degrees. The second term is due to **virtual processes** in $\mathcal{P}$-space. They are produced by hops from $\mathcal{P}$-space to $\mathcal{Q}$-space, there taking a lift with the propagator $[z - \mathcal{L}_{\mathcal{Q}}]^{-1}$ in $\mathcal{Q}$ space, followed by hoping back onto $\mathcal{P}$-space (see Fig. 5.1). Equation (5.52) could be called quantum Master equation in frequency space. One can use the so-called

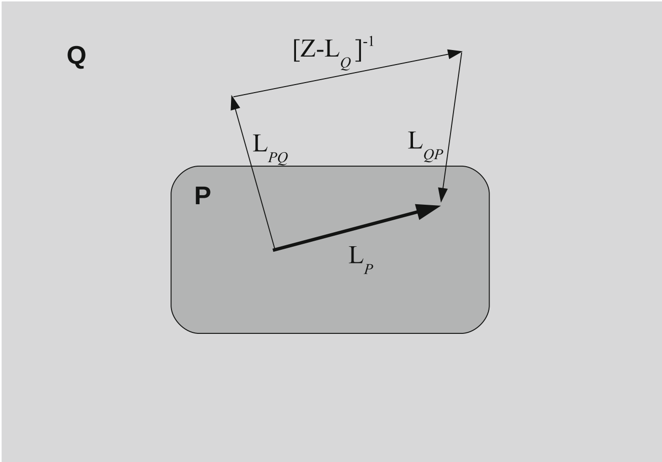


Fig. 5.1 Visualizing the effective Liouville in $\mathcal{P}$ space by direct processes and virtual processes via propagation in $\mathcal{Q}$ space

Sokhotski-Plemelj decomposition for $\epsilon \to 0$ of the resolvent in $\mathcal{Q}$ space to separate real and imaginary parts,

$$\lim_{\epsilon \to 0} \left[z - \mathcal{L}_{\mathcal{Q}} \right]^{-1} = \mathrm{P} \left[\omega - \mathcal{L}_{\mathcal{Q}} \right]^{-1} - i\pi\delta(\omega - \mathcal{L}_{\mathcal{Q}}), \tag{5.54}$$

where P stands for the Cauchy value on integration. Thus, the real eigenvalues of $\mathcal{L}_{\mathcal{P}}$ gain some negative imaginary parts, as soon as the spectrum of $\mathcal{L}_{\mathcal{Q}}$ is much denser as that of $\mathcal{L}_{\mathcal{P}}$ and summation can be replaced by integration. Negative imaginary parts $1/\tau$ in eigenvalues of the effective Liouville means that the former eigenstates of the pure $\mathcal{L}_{\mathcal{P}}$ begin to decay with characteristic time scale τ (Fig. 5.2).

Before switching to the time dependent picture we will give a sketch of a proof for the effective Liouville operator. It relies on the algebraic relation

$$[A - B]^{-1} = A^{-1} + A^{-1}B[A - B]^{-1}. \tag{5.55}$$

which can be shown by multiplying with $A - B$ from the right. It is also the basis of the famous Dyson equation in perturbation theory and diagrammatics. The proof relies in addition on the projector properties $\mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0$ and $\mathcal{Q}^2 = \mathcal{Q}$ and $\mathcal{P}^2 = \mathcal{P}$. The proof needs three steps:

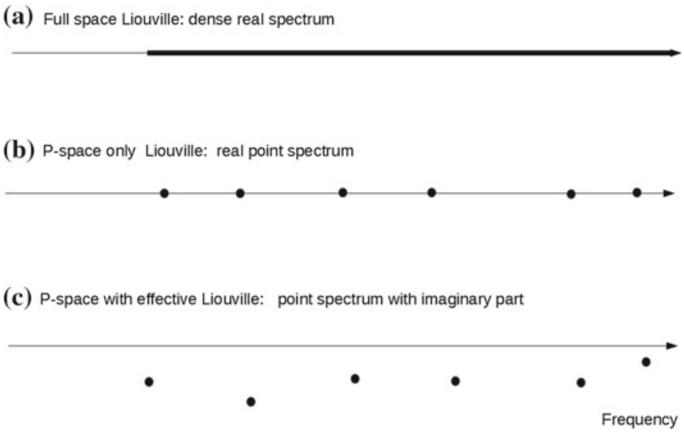


Fig. 5.2 The spectrum of **a** the full Liouville operator, **b** the closed part Liouville operator on $\mathcal{P}$ space, and **c** the complex valued spectrum of the effective Liouville operator

$$
\begin{aligned}
[z-\mathcal{L}]^{-1}{}_{\mathcal{P}\mathcal{P}} &= [z-\mathcal{L}_{\mathcal{P}}]^{-1} \\
&\quad + [z-\mathcal{L}_{\mathcal{P}}]^{-1}\left(\mathcal{L}_{\mathcal{Q}}+\mathcal{L}_{\mathcal{P}\mathcal{Q}}+\mathcal{L}_{\mathcal{Q}\mathcal{P}}\right)[z-\mathcal{L}]^{-1}\mathcal{P}, \\
[z-\mathcal{L}]^{-1}{}_{\mathcal{Q}\mathcal{P}} &= \left[z-\mathcal{L}_{\mathcal{Q}}\right]^{-1} \\
&\quad + \left[z-\mathcal{L}_{\mathcal{Q}}\right]^{-1}\left(\mathcal{L}_{\mathcal{P}}+\mathcal{L}_{\mathcal{P}\mathcal{Q}}+\mathcal{L}_{\mathcal{Q}\mathcal{P}}\right)[z-\mathcal{L}]^{-1}\mathcal{P}, \\
[z-\mathcal{L}]^{-1}{}_{\mathcal{P}\mathcal{P}} &= [z-\mathcal{L}_{\mathcal{P}}]^{-1} \\
&\quad + [z-\mathcal{L}_{\mathcal{P}}]^{-1}\left(\mathcal{L}_{\mathcal{P}\mathcal{Q}}\left[z-\mathcal{L}_{\mathcal{Q}}\right]^{-1}\mathcal{L}_{\mathcal{Q}\mathcal{P}}\right)[z-\mathcal{L}]^{-1}\mathcal{P}.
\end{aligned}
\tag{5.56}
$$

In the time dependent picture the evolution reads (see also Sect. 2.4.1 in [4])

$$
\partial_t \varrho_{\mathrm{rel}}(t) = -i\mathcal{L}_{\mathcal{P}}\varrho_{\mathrm{rel}}(t) + \int_0^t \mathrm{d}\tau\, \mathcal{L}_{\mathcal{P}\mathcal{Q}} e^{-i\mathcal{L}_{\mathcal{Q}}(t-\tau)}\mathcal{L}_{\mathcal{Q}\mathcal{P}}\,\varrho_{\mathrm{rel}}(\tau), \tag{5.57}
$$

which shows a retardation effect: all times between initial time 0 and time t contribute from the $\mathcal{Q}$ journey.

To get back a simple local in time dynamics the system has to manage a separation of time scales, such that the retardation has a short time scale. A source for this is offered by the oscillatory nature of quantum processes whenever phases are involved. Therefore, we now consider the following special situation: the projector projects onto diagonal elements of the density operator in some relevant basis:

$$
(\varrho_{\mathrm{rel}})_{nm} = \varrho_n \delta_{nm}. \tag{5.58}
$$

These diagonal elements ϱ_n are not affected by phase fluctuations and are non-negative like probabilities. Due to the conservation of $\sum_n \varrho_n = 1$ the time evolution can be written in the form of gain and loss as a **retarded Master equation**

$$\boxed{\partial_t \varrho_n(t) = \sum_{n' \neq n} \int_0^t d\tau \, \{W_{nn'}(t-\tau)\varrho_{n'}(\tau) - W_{n'n}(t-\tau)\varrho_n(\tau)\}}, \tag{5.59}$$

where

$$W_{nn'}(t-\tau) := \left(\mathcal{L}_{\mathcal{PQ}} e^{-i\mathcal{L}_{\mathcal{Q}}(t-\tau)} \mathcal{L}_{\mathcal{QP}}\right)_{nn'} . \tag{5.60}$$

For the choice to be really relevant, the following assumption about separation of time scales has to be fulfilled. There is a time scale τ_{dec} over which $W_{nn'}(t)$ is concentrated. Outside of it $W_{nn'}(t)$ is nearly zero due to random phase summations and on the other hand $\varrho_n(t)$ does not change significantly over this time scale. This time scale τ_{dec} can be called **decoherence time**, because this time separation allows to approximate the dynamics for the diagonal elements ϱ_n without big quantitative errors by a dynamics of the Master type:

$$\partial_t \varrho_n(t) = \sum_{n' \neq n} \left\{\overline{W}_{nn'} \varrho_{n'}(t) - \overline{W}_{n'n} \varrho_n(t)\right\} , \tag{5.61}$$

where $\overline{W}_{nn'} = \int_{-\tau_{dec}}^{0} \mathrm{d}\tau \, W(\tau)$. The dynamics for the rapidly varying off-diagonal elements cannot be approximated this way. Their filigree rapid quantum oscillations have been neglected and treated as zero because of random phase summations. Thus, decoherence does not mean that quantum oscillations really die out but rather they become very hard to be observed in the dynamics of macro observables. The corresponding oscillations only lead to very very small deviations from the slowly varying values calculated by the effective Master equation. The irreversibility is *real* in the sense, that it is impossible to reverse the dynamics of the slowly varying relevant variables without knowledge about the fast irrelevant variables. A simpler discussion of the possible emergence of a Markov dynamics from a quantum dynamics by random phase summation was given in Sect. 3.4.3.

5.4.3 Stationarity in Markov Processes

Our demonstrations that solutions of the Master equation finally become stationary states are not artificial. On the contrary, one can proof[4] (see [2] for enlightening proofs): all solutions of a Master equation tend to a stationary solution in the infinite time limit. The stationary solution is unique on an irreducible subspace of probability

[4] An elementary treatment is given in Appendix A.7.

densities.[5] This is strictly true only for a finite number of states. For an infinite number or for a continuous state space there are special exceptions like the pure diffusive system, which does not reach a stationary state but keeps on spreading out. In a generic situation with a bit of friction the statement of asymptotic stationarity still holds. Therefore, the maximum entropy principle for equilibrium or local equilibrium statistics is not only a principle of unbiased guessing of distributions or density operators, but motivated by the semi-group dynamics of Master equations.

5.4.4 Maximum Entropy Principle

For a stationary density operator in energy representation ϱ_n the maximum entropy principle states that the average entropy should be at a maximum with respect to all possible values of ϱ_n. On fixing appropriate average values $\langle A \rangle$ by Lagrange multipliers λ (called fields) one can find the maximum entropy from minimizing

$$F[\varrho_n] = \sum_n -\varrho_n \ln(\varrho_n) + \lambda \sum_n \varrho_n A_n, \tag{5.62}$$

which leads to a (grand)-canonical equilibrium distribution (Gibbs distribution),

$$\boxed{\varrho_n = \frac{1}{Z} \exp\left(\lambda A_n\right)}. \tag{5.63}$$

The well known normalized canonical equilibrium density operator,

$$\varrho_{\text{can}} = \frac{1}{Z} \exp\left(-H/T\right);\ \ Z = \text{Tr}\ \left\{e^{-H/T}\right\} \tag{5.64}$$

can be identified as the unbiased guess for the system's state when, by its energetic contact to the environment, the average value of energy can be held fixed by an external (thermodynamical dual) field, called temperature T (measured in units of energy). The environment is kept at constant temperature as a thermostat for the system in equilibrium. The partition sum Z as a function of T and other relevant macroscopic parameters like particle number, volume, field strengths of magnetic and electric fields acts as the generating function(al) for average values and correlations (see Sect. 5.5.2 and Appendix C).

---

[5] In a reducible space one has several independent systems treated as one system.

5.4.5 Quantum Scattering

Asymptotic states in scattering theory are always meant in the sense of a **long time average limit**—a simple limit of $t \to \pm\infty$ is usually not well defined. One should note that a long time average cannot be reversed and a reversed movie of a scattering process with asymptotic ingoing states (e.g. a plane wave of fixed wavelength) scattered by a target leading to an outspread of outgoing asymptotic waves in several directions looks as impossible as the reversed movie of a drop of ink put into water. The long time average of a function $f(t)$,

$$\lim_{t\to\pm\infty} f(t) := \lim_{T\to\infty} (1/T) \int_{0;-T}^{T;0} \mathrm{d}t f(t) \tag{5.65}$$

can be calculated in a gentle way by the ϵ-prescription,

$$\lim_{t\to\pm\infty} f(t) := \lim_{\epsilon\to 0^+} \epsilon \cdot \int_{0;-\infty}^{\infty;0} \mathrm{d}t f(t) e^{\mp\epsilon t}. \tag{5.66}$$

In spectral decomposition, $f(t) = \sum_{\omega_n} \tilde{f}_{\omega_n} e^{i\omega_n t}$, one sees that only the zero modes survives (see Fig. 5.3).

$$\lim_{t\to\pm\infty} f(t) = \lim_{\epsilon\to 0^+} \sum_{\omega_n} \frac{\epsilon \cdot (\mp\tilde{f}_{\omega_n})}{\mp\epsilon + i\omega_n} = \sum_{\omega_n=0} \tilde{f}_{\omega_n=0} \tag{5.67}$$

We will, if not stated otherwise, assume that the zero mode is non-degenerate,

$$\lim_{t\to\pm\infty} f(t) = \tilde{f}(\omega_n = 0). \tag{5.68}$$

The zero energy ground state is called **vacuum state** and its wave function is denoted as

$$\phi_0(x) = \langle x|0\rangle\,. \tag{5.69}$$

One finds by a similar calculation for the asymptotic stationary limit of the propagator

$$\lim_{t\to\infty} \lim_{t_0\to-\infty} \langle x, t|x_0, t_0\rangle = \phi_0(x)\phi^*(x_0). \tag{5.70}$$

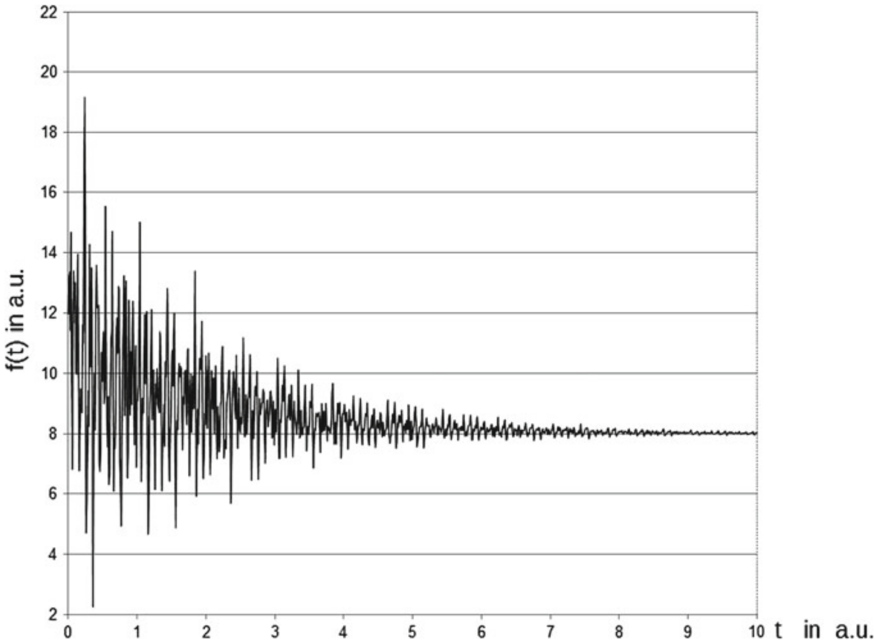


Fig. 5.3 In the long time average of a function its zero mode emerges, free of oscillations

On an operator level it reads[6]

$$\boxed{\lim_{t\to\infty}\lim_{t_0\to-\infty} e^{-iH(t-t_0)} = \lim_{\epsilon\to 0^+}\frac{-\epsilon^2}{H^2-\epsilon^2} = \delta_{H0}}. \tag{5.71}$$

In scattering theory all quantities of interest like scattering rates can be calculated from the time ordered correlation functions (moments) in the vacuum state (see e.g. [5] Sect. 6.3), called **n-point Green's functions**

$$\langle 0|O(t_1,\ldots,t_n)|0\rangle := \left\langle 0|\hat{T}\left\{x(t_n)\ldots x(t_1)\right\}|0\right\rangle, \tag{5.72}$$

where $\hat{T}$ is the time ordering symbol meaning that all the observables are taken at successive times starting from the right with t_1 and ending with t_n at the left. We want to express the Green's functions by the n-point propagator $\langle x,t|O(t_1,\ldots,t_n)|x_0,t_0\rangle$ for which we can write path integral representations. This is done in two steps. Firstly, we use completeness and write

[6]Convergence can be expected only after sandwiching with states.

$$\langle 0|O(t_1,\ldots,t_n)|0\rangle = \int \mathrm{d}x_0\mathrm{d}x\,\langle 0|x,t\rangle\,\langle x,t|O(t_1,\ldots,t_n)|x_0,t_0\rangle\,\langle 0|x_0,t_0\rangle \tag{5.73}$$

and use again completeness in the n-point propagator for $t \to \infty$ and $t_0 \to -\infty$ as in (5.70),

$$\begin{aligned} &\langle x,t|O(t_1,\ldots,t_n)|x_0,t_0\rangle \\ &= \int dQ_0 dQ\,\langle x,t|Q,T\rangle\,\langle Q,T|O(t_1,\ldots,t_n)|Q_0,T_0\rangle\,\langle Q_0,T_0|x_0,t_0\rangle \\ &= \phi_0(x)\phi^*(x_0)\,\langle 0|O(t_1,\ldots,t_n)|0\rangle\,. \end{aligned} \tag{5.74}$$

The final expression is

$$\langle 0|O(t_1,\ldots,t_n)|0\rangle = \lim_{t\to\infty}\lim_{t_0\to-\infty}\frac{\langle x,t|O(t_1,\ldots,t_n)|x_0,t_0\rangle}{\langle x,t|x',t_0\rangle}. \tag{5.75}$$

Note, the ratio is independent of x and x_0 and we may integrate over them in the nominator and the denominator. As we will argue in the next section, the right hand side can be expressed by a generating functional represented by a path integral.

5.5 Generating Functionals All Over

The main idea behind generating functionals is well established in equilibrium statistics. Instead of calculating many correlation functions by integration (summation) one can calculate only one integral (partition sum) for a system in the presence of a so called source field J dual to the relevant variable x and then generate all of the correlation functions of that variable by (functional) differentiation. The duality of the source field J is by Fourier-Laplace or Legendre transformation and one can change the roles of x and J, if appropriate. Thus, the generating functionals can depend on external fields J or on the average relevant variable $\varphi = \langle x\rangle$. The cumulant generating functional as a functional of external field J is denoted as $W[J]$ and its Legendre transformed as a functional of the average value $\varphi = \langle x\rangle$ is called effective action and denoted as $\Gamma[\varphi]$. More explicit definitions will follow. We start with scattering theory for a configuration variable x.

5.5.1 Scattering Theory

Recall from Sects. 3.3 and 3.4 the restricted path integral expression for the propagator

$$\left\langle x', t | x, t_0 \right\rangle = \int\limits_{x \to x'} Dx(\tau) \;\; e^{iS[x(\tau)]}, \tag{5.76}$$

where the action S is defined via the Lagrange function L as

$$S[\mathrm{x}(\tau)] = \int\limits_{t_0}^{t} \mathrm{d}\tau \, L(x(\tau), \dot{x}(\tau)). \tag{5.77}$$

In general, the Lagrangian is related by a Fourier-Laplace transformation to the Hamilton function $H(x, k)$ which is, by the discretization procedure, uniquely related to the Hamilton operator. However, for up to quadratic in k Hamilton functions the Lagrange function is simply the Legendre transformed of the Hamilton function,

$$L = (\partial_k H)k - H; \;\; \dot{x} = \partial_k H. \tag{5.78}$$

By repeating all the steps in deriving the path integral representation of the propagator one can see that the n-point propagator can be represented by the path integral correlation function[7]

$$\left\langle x', t | O(t_1, \ldots, t_n) | x, t_0 \right\rangle = \int\limits_{x \to x'} Dx(\tau) \;\; x(t_n) \ldots x(t_1) e^{iS[x(\tau)]}. \tag{5.79}$$

Instead of operators on the left hand side one has functions on the right hand side. This opens up for the following generating idea:

$$\frac{\delta \left[\int \mathrm{d}\tau \, J(\tau) \cdot x(\tau) \right]}{\delta J(t_a)} = x(t_a). \tag{5.80}$$

By adding a so-called source term to the action consisting of additive multiplicative couplings between the variable $x(\tau)$ and a dual auxiliary variable $J(\tau)$ (called **source field**) one arrives at the generator formula for the n-point correlator

$$\left\langle x', t | O(t_1, \ldots, t_n) | x, t_0 \right\rangle = \lim_{J \to 0} \frac{\delta^n \left\langle x, t | x_0, t_0 \right\rangle_J}{\delta i J(t_1) \ldots \delta i J(t_n)}, \tag{5.81}$$

where the source-dependent propagator is defined via the action with source term

$$S[x(\tau); J(\tau)] := S[x(\tau)] + \int\limits_{t_0}^{t} \mathrm{d}\tau \, J(\tau) \cdot x(\tau). \tag{5.82}$$

[7]The time ordering is essential in the discretization procedure.

With the help of (5.75) we can now generate every n-point Green's function of scattering theory from the source dependent partition sum, defined as an unrestricted path integral with long time averages for t_0 and t

$$Z[J] := \int Dx(\tau)\; e^{iS[x(\tau);J(\tau)]} = \langle 0|0\rangle_J\,. \tag{5.83}$$

$$\langle 0|O(t_1,\ldots,t_n)|0\rangle \;=\; \lim_{J\to 0}\frac{1}{Z[J]}\frac{\delta^n Z[J]}{\delta iJ(t_1)\ldots\delta iJ(t_n)}. \tag{5.84}$$

In statistics one is usually not so much interested in moments but in cumulants. Cumulants are generated by the logarithm of the partition sum. As the cumulant generating functional $W[J]$ in scattering theory we take

$$W[J] := \ln Z[J] \tag{5.85}$$

and the cumulants are generated accordingly,

$$\boxed{\langle 0|O(t_1,\ldots,t_n)|0\rangle_c = \lim_{J\to 0}\frac{\delta^n W[J]}{\delta iJ(t_1)\ldots\delta iJ(t_n)}}. \tag{5.86}$$

For reasons of graphical representations they are also called connected Green's functions. The relation between cumulants and moments follows by differentiation and the cumulant of nth order combines moments of up to nth order. For example, the first moment equals the first cumulant and the second cumulant is the correlator,

$$\langle 0|x(t_1)|0\rangle_c = \langle 0|x(t_1)|0\rangle \tag{5.87}$$

$$\langle 0|x(t_2)x(t_1)|0\rangle_c = \langle 0|x(t_2)x(t_1)|0\rangle - \langle 0|x(t_2)|0\rangle\,\langle 0|x(t_1)|0\rangle\,. \tag{5.88}$$

As we will see, partition sums can be calculated exactly for quadratic form actions (and some relatives) and for all other situations one relies on approximative or exact but macroscopic methods. For such methods it turns out to be more advantageous to consider a generating functional $\varGamma$ as a functional of the average value $\varphi(t) := \langle 0|x(t)|0\rangle$. Motivated by its implicit definition it is called **effective action** $\varGamma[\varphi]$,

$$e^{i\varGamma[\varphi]} := \int D\eta\; e^{iS[\varphi+\eta]+i\int \mathrm{d}t\,\frac{\delta\varGamma}{\delta\varphi}(t)\cdot\eta(t)}, \tag{5.89}$$

where $\eta = x - \varphi$ is the deviation of variable x from its average value φ. Equation (5.89) is solved when the effective action $\varGamma[\varphi]$ is a Legendre transformed of $W[J]$,

$$\varGamma[\varphi] = -iW[J[\varphi]] + \int \mathrm{d}t\, J[\varphi(t))]\cdot\varphi(t), \tag{5.90}$$

with

$$\frac{\delta\Gamma[\varphi]}{\delta\varphi} = J[\varphi]\,;\;\; \varphi[J] = \frac{\delta W[J]}{i\delta J}. \tag{5.91}$$

Once we know the effective action as a functional of macroscopic average fields, we can calculate every n-point Green's function we like. In other words, $\Gamma[\varphi]$ solves the scattering problem. The effective action is in the focus of most qualitative and quantitative approximate treatments. If the integrand in (5.89) allows for a Gaussian approximation around the average value, the effective action can be calculated (see Sect. 5.5.3). Omitting the Gaussian fluctuations, the crudest approximation Γ^0 is simply the original action at the mean value φ.

$$\Gamma^0[\varphi] = S[\varphi]. \tag{5.92}$$

5.5.2 Canonical Equilibrium

In canonical equilibrium we have to calculate expectation values

$$\langle A\rangle = \mathrm{Tr}\;\{A\varrho\} = \int \mathrm{d}x\;\langle x|A\varrho|x\rangle = \int \mathrm{d}x\mathrm{d}x'\;A(x,x')\varrho(x',x) \tag{5.93}$$

The Equilibrium theory is solved once we have calculated the density matrix $\varrho(x,x')$. In canonical equilibrium the density matrix has the same structure

$$\varrho(x,x') = \left\langle x \mid e^{-\beta H} \mid x'\right\rangle \tag{5.94}$$

as the propagator $\left\langle x \mid e^{-iHt} \mid x'\right\rangle$ on identifying the inverse temperature as an imaginary time,

$$\beta = it, t = -i\beta. \tag{5.95}$$

It can be represented as a restricted path integral. Using again a source field J, which typically has real meaning as a thermodynamical conjugate field to a physical observable F, we can generate moments of such observable from the source dependent partition sum,

$$\langle F(\lambda_1)\ldots F(\lambda_n)\rangle = \frac{1}{Z[J]}\frac{\delta^n Z[J]}{\delta J(\lambda_1)\ldots\delta J(\lambda_n)} \tag{5.96}$$

$$Z[J] = \int\limits_{x\to x} Dx(\lambda)\; e^{-\int_0^\beta \mathrm{d}\lambda\left\{\tilde{L}(x(\lambda),\dot{x}(\lambda)-J(\lambda)\cdot F(\lambda)\right\}}. \tag{5.97}$$

Note, that a term $\dot{x}^2$ in the original Lagrange function L appears with a minus sign in $\tilde{L}$ since the integration variable is $\lambda = it$. For a particle with Galilei inertia m and a translation symmetry braking potential $V(x)$ it reads

$$\tilde{L}(x, \dot{x}) = \frac{m\dot{x}^2}{2} + V(x). \tag{5.98}$$

Note also, one has to fulfill periodicity conditions in imaginary time, $x(0) = x(\beta)$. This has lead to the Matsubara technique by exploiting this periodicity. We will not elaborate on it here, but present a discussion in Appendix C. In addition, a many body partition sum should respect the particle permutation laws (different for Fermions and Bosons). These conditions can be fulfilled better within a coherent states path integral approach to equilibrium statistics, which is also reviewed in the same appendix. Canonical equilibrium is treated there for many body systems in Matsubara technique and functionals are carried out in coherent states representation.

Finally, we comment on the formal analogies between equilibrium partition sum,

$$\boxed{Z = \int\limits_{x \to x} Dx(\lambda)\; e^{-\int\limits_0^\beta \mathrm{d}\lambda\, \tilde{L}(x(\lambda), \dot{x}(\lambda))}}, \tag{5.99}$$

and Markov and quantum propagators (3.27) and (3.28). The analogies can be technically exploited when analytical continuations in the complex plane of the variables temperature λ (originally along the imaginary axis) and time τ (originally along the real axis) and of the integrand (real valued in the partition sum and the Markov case and complex in the quantum case) can be performed. In the quantum case the particle is moving in time while in the partition sum of equilibrium the time is absent. However, the parameter λ can also be interpreted as a one-dimensional coordinate of a classical field $x(\lambda)$ in $1D$ (a string). The partition sum is the classical equilibrium partition sum of that string. This analogy between quantum propagators and partition sum has lead to the following slogan: a quantum field theory in d dimensions is equivalent to an equilibrium classical field system in $d + 1$ dimensions. The analogy between quantum and Markov propagators has led to the technical method of so called stochastic quantization, which means that one can set up a Markov process and calculate from it quantum propagators by analytical continuation (if possible).

5.5.3 Field Theory and Gaussian Fluctuations

So far, the configuration variable x could have been discrete, multicomponent discrete or even multicomponent continuous and products as $x \cdot J$ are always meant as sums or integrals of products $\sum_k \int \mathrm{d}s\, x_k(s) J_k(s)$. For later use it is convenient to distinguish between **external** indices and **internal** indices. Following the usual nomenclature the external indices are in principle multicomponent continuous (external space) and now denoted as $\boldsymbol{x}$, while the internal indices are discrete. The configuration variable is than called a **field** and written as $\phi(x)$, where x is short for time t and space coordinate $\boldsymbol{x}$. The action $S[\phi]$ is then an integral over time and the external space over a **Lagrange density** $\mathcal{L}(\phi, \partial_x\phi)$. Usually, x is multicomponent real and ϕ is (perhaps multicomponent) real or complex. In situations of Fermion permutation constraints the field components can be of anti-commuting, nilpotent, Grassmann type[8] instead of commuting complex number type. The fields ϕ and their arguments x may be subject to symmetry constraints, e.g. $\boldsymbol{x}$ is a vector in Euclidean space or x is a four vector in Minkowski space (written as x^μ, μ running from 0 to 3) and ϕ is a vector or a spinor or in general a tensor representation with respect to external symmetry.[9] With this nomenclature, the scattering field theoretic connected n-point Green's functions are generated as

$$\left\langle 0|\hat{T}\left\{\phi(x_1)\ldots\phi(x_n)\right\}|0\right\rangle_c = \lim_{J\to 0}\frac{\delta^n W[J]}{\delta iJ(x_1)\ldots iJ(x_n)} \tag{5.100}$$

with

$$e^{W[J]} = \int D\phi\; e^{iS[\phi]+i\int \mathrm{d}x\, J(x)\cdot\phi(x)}. \tag{5.101}$$

Here the $\cdot$ between J and ϕ means an appropriate contraction over internal indices. Often you will find in the literature the generating functionals written with an imaginary time $\tau = it$ coordinate to change from fluctuating phases to relaxing amplitudes and the prescription of analytical continuation at the end, usually by a simple rotation back to real time (so-called Wick rotation). The action is then called Euclidean action, since a quadratic form of type $-t^2 + x^2$ becomes an Euclidean quadratic form $\tau^2 + x^2$. To the author's knowledge this is not really a technical advantage as only Gaussian integrals have to be performed explicitly for which analytic results are available anyway. Nevertheless, we make use of the Euclidean action as it unifies notation. In many body physics at finite temperature in equilibrium one can use the Matsubara technique with coherent state path integrals, as reviewed in Appendix C. The generating functionals have the same structure, except that integrations over time are not from $-\infty \to \infty$ but can be deformed in the complex plane to take the finite temperature equilibrium ground state into account. For such systems, the question of analytic deformation of contours is really important. It is possible to consider non-equilibrium states (Keldysh formalism) as well. Also, as we have seen, solutions of Markov processes have path integral representations. Their stationary limits are not restricted to equilibrium.

Thus, in almost any area of theoretical physics (dynamics, scattering limits, equilibrium, non-equilibrium) quantities of interest, expectation values and correlations, can be expressed by cumulants generated from a source field dependent functional integral. In a unified notation for equilibrium statistics and the Euclidean version of scattering field theory the cumulants (n-point Green's functions) can be generated as

---

[8] For a compact introduction to Grassmann variables in field theory see [6, 7].

[9] Representations of symmetry are elucidated in Sect. 6.2.

$$\boxed{\left\langle \hat{T}\left\{\phi(x_1)\ldots\phi(x_n)\right\}\right\rangle_c = \lim_{J\to 0}\frac{\delta^n W[J]}{\delta J(x_1)\ldots J(x_n)}} \tag{5.102}$$

with

$$\boxed{e^{W[J]} = \int D\phi\; e^{-S[\phi]+\int \mathrm{d}x\, J(x)\cdot\phi(x)}}. \tag{5.103}$$

The action $S[\phi]$ is specified for a system at hand by a Lagrange density $\mathcal{L}(\phi(x), \partial_x\phi(x))$ which has to be summed (integrated) over all external indices. In the Lagrange density the internal indices and discrete external indices were already summed over to make $\mathcal{L}$ a scalar with respect to discrete indices,

$$\boxed{S[\phi] = \int \mathrm{d}x\, \mathcal{L}(\phi(x), \partial_x\phi(x))}. \tag{5.104}$$

The effective action $\Gamma[\varphi]$ is defined as the Legendre transformed of the cumulant generating functional $W[J]$,

$$\boxed{\Gamma[\varphi] = -W[J[\varphi]] + \int \mathrm{d}x\, J(x)\cdot\varphi(x);\;\; \frac{\delta\Gamma[\varphi]}{\delta\varphi(x)} = J(x)}. \tag{5.105}$$

For non-interacting systems the action $S[\phi]$ is at most quadratic in the fields and the path integral is a multidimensional Gaussian integral which can be calculated in closed form. The essential formulas are given in the following.

The elementary Gaussian integral

$$\int \mathrm{d}x\, e^{-\frac{1}{2}a(x-x_0)^2} = \sqrt{\frac{2\pi}{a}} \tag{5.106}$$

generalizes to higher dimensions. Let the commuting field configurations be ϕ_i constituting a (large but finite dimensional) vector space. Defining a real valued Gaussian distribution with real symmetric matrix A,

$$\boxed{e^{-S[\phi]} = \exp -\frac{1}{2}\left[\sum_{kl} A_{kl}\phi_k\phi_l\right]}, \tag{5.107}$$

the real valued generating function(al)

$$Z[J] = \int \prod_n \mathrm{d}\phi_n\, e^{-S[\phi]} \exp\sum_k J_k\phi_k \tag{5.108}$$

is evaluated to be

$$Z[J] = \sqrt{\det(A/(2\pi))}^{-1} \exp -\frac{1}{2}\left(\sum_{kl} J_k A^{-1}_{kl} J_l\right), \tag{5.109}$$

where A^{-1} is the inverse of matrix A. Notice that the normalization is given by the determinant of A. The integration could be carried out as a product of one-dimensional Gaussian integrals by changing to eigenvalues and eigenvectors of matrix A. This isometric variable change does not change the integration measure. The determinant is just the product of eigenvalues. This separability qualifies a quadratic action as an action of a non-interacting system. The cumulant generating functionall $W = \ln Z$ is

$$\boxed{W[J] = -\frac{1}{2}\ln(\det(A/(2\pi))) + \frac{1}{2}\left(\sum_{kl} J_k A^{-1}_{kl} J_l\right)}. \tag{5.110}$$

The field average is

$$\varphi_l[J] = \frac{\partial W[J]}{\partial J_l} = \sum_k A^{-1}_{lk} J_k \tag{5.111}$$

which vanishes for vanishing source field,

$$\langle \phi \rangle = \lim_{J \to 0} \frac{\delta W[J]}{\delta J} = 0, \tag{5.112}$$

and fluctuations of ϕ are determined by the inverse of the defining symmetric operator A of the Gaussian distribution,

$$\langle \phi_1 \phi_2 \rangle = \frac{\delta^2 W[J]}{(\delta J_1)\,(\delta J_2)} = A^{-1}_{12}. \tag{5.113}$$

Note, the vanishing of all higher but second order cumulants is the characteristic feature of a Gaussian distribution. The effective action $\Gamma[\varphi] = -W[\varphi]\sum_k J_k \varphi_k$ turns out to be the original Gaussian action up to a field independent logarithm, since the fluctuation matrix does not depend on φ,

$$\Gamma[\varphi] = S[\varphi] + \text{const}. \tag{5.114}$$

In the case of a hermitian operator $A = A^\dagger$ we require two fields, ϕ and its complex conjugate ϕ^*, to define

$$\begin{aligned} Z[J, \bar{J}] &= \int \prod_n \mathrm{d}\phi_n^* \mathrm{d}\phi_n \, \exp\left\{-\sum_{kl} \phi_k^* A_{kl} \phi_l \sum_k J_k \phi_k \sum_k J_k^* \phi_k^*\right\} \\ &= (\det(A/(2\pi)))^{-1} \exp\left\{\sum_{kl} J_k^* A^{-1}_{kl} J_l\right\} \end{aligned} \tag{5.115}$$

In the case of Grassmann fields (see e.g. [6] Chap. 4) the integral expression

$$
\begin{aligned}
Z[\bar{\xi}, \xi] &= \int \prod_n \mathrm{d}\bar{\eta}_n \mathrm{d}\eta_n \exp\left\{-\sum_{kl} \bar{\eta}_k A_{kl} \eta_l \sum_k \bar{\eta}_k \bar{\xi}_k \sum_k \eta_k \xi_k\right\} \\
&= (\det A)^{+1} \exp\left\{\sum_{kl} \bar{\xi}_k A^{-1}_{kl} \xi_l\right\}
\end{aligned}
\tag{5.116}
$$

is the Grassmann analog of the Gaussian integrals for commuting numbers. Notice, the determinant appears now in the nominator instead of the denominator.

5.5.4 Stationary Action and Expansions

When the action is not quadratic one can try perturbation theory around a stationary action solution. The stationarity of the action is solved by a field configuration ϕ_0 which fulfills the **Euler-Lagrange equations**,

$$
\boxed{\frac{\delta S[\phi]}{\delta \phi} = 0 = \frac{\partial \mathcal{L}}{\partial \phi(x,t)} - \partial_t \frac{\partial \mathcal{L}}{\partial\left(\partial_t \phi(x,t)\right)} - \sum_k \partial_{x_k} \frac{\partial \mathcal{L}}{\partial\left(\partial_{x_k} \phi(x,t)\right)}}\,. \tag{5.117}
$$

A stationary action solution is a deterministic drift solution of the dynamics neglecting any fluctuations. The corresponding Euler-Lagrange equations are often called classical field equations or classical equations of motion, because they were studied historically before fluctuations of Markov and quantum types came into focus. Using these stationary action solution as a starting point, one can incorporate fluctuations on a Gaussian level first, and then one can perform a perturbational calculation beyond the Gaussian level. Thus, one can expand the source dependent action in the following way,

$$
S[\phi, J] = S_0^{\phi_0^J} + \frac{1}{2} \int \mathrm{d}x \mathrm{d}x'\, \eta(x') \cdot \mathcal{S}_2^{\phi_0^J}(x, x') \cdot \eta(x) + \delta S[\eta], \tag{5.118}
$$

where $S_0^{\phi_0^J}$ is the action at the stationary source dependent action solution and $\mathcal{S}_2^{\phi_0^J}(x, x')$ is the Hessian of the source independent Lagrange density at the source dependent stationary action solution. It describes Gaussian fluctuations in the deviation field $\eta = \phi - \phi_0^J$ around the stationary solution and $\delta S[\eta]$ contains all higher order terms in η. Note, the stationary action solution in the presence of the source field fulfills the duality relation

$$
\frac{\delta S[\phi]}{\delta \phi}[\phi_0^J] = J. \tag{5.119}
$$

In a first step one solves the Gaussian part, resulting in a Gaussian partition sum.[10] For commuting field variables it can be written as

$$\boxed{W_0[J] = -S_0^{\phi_0^J} + \int \mathrm{d}x\, J(x) \cdot \phi_0^J(x) - \frac{1}{2}\mathrm{Tr}\,\log(\mathcal{S}_2^{\phi_0^J})}. \tag{5.120}$$

Note, the Gaussian approximation does already include source independent fluctuations via $\mathcal{S}_2^{\phi_0}$ and the second quadratic term of the r.h.s. of (5.120) can also be written as

$$\int \mathrm{d}x\, J(x) \cdot \phi_0^J(x) = -\frac{1}{2} \int \mathrm{d}x\mathrm{d}x'\, J(x') \cdot \left[\mathcal{S}_2^{\phi_0^J}\right]^{-1}(x, x') \cdot J(x). \tag{5.121}$$

due to (5.119). To go beyond the Gaussian level one can use the fact that any polynomial in η under the path integral in front of the source factor can be written as a polynomial in functional derivatives with respect to J, because of the duality between J and η. Thus, one may write the full partition sum in the following way

$$\boxed{\exp W[J] = \exp\left(-\delta S\left[\frac{\delta}{\delta J}\right]\right) \exp W_0[J]}. \tag{5.122}$$

This short equation actually defines in a unique way a perturbation expansion of the full partition sum in terms of the solved Gaussian part around a stationary action solution. The Gaussian part can be expressed solely in terms of Gaussian level two-point Green's functions, which can graphically be represented by a line connecting two points (or loops, when points meet). The perturbation expansion thus corresponds to summation over graphs of combined lines and loops. Equation (5.122) tells the so called Feynman rules for the graphical perturbation expansion. As an example see the ϕ^4-treatment in [7], Chap. 1.2 and the Appendix B there. For a compact treatment within the effective action formalism see [8].

Rigorous statements about the accuracy of perturbation expansions are difficult or impossible. Its validity rests on a good choice of the relevant variable and corresponding stationary solution, such that the higher orders can hopefully be controlled by a small parameter. Studying symmetries can help a lot in finding a good choice for the relevant variable. The review [8] gives an overview about the state of the art within the effective action formalism.

The expansion of the fields around the stationary action can often be justified by the presence of a large parameter (called N) such that the action can be written as

$$S[\phi] = N\tilde{S}[\phi]. \tag{5.123}$$

[10] The logarithm of a matrix determinant, $\ln\det A$, of some matrix A can be written as $\mathrm{Tr}\,\log A$—as can be seen by diagonalizing it. The latter version is better for further expansions of the log, if necessary.

If $\tilde{S}[\phi]$ is independent of N and has some stationary action solution, the large prefactor will make this stationary solution much more important. This can be seen by expanding $\tilde{S}$ around the stationary solution,

$$\tilde{S}[\phi_0 + \eta] = \tilde{S}[\phi_0] + \tilde{S}_2[\phi_0]\eta^2 + \mathcal{O}\left(\eta^3\right), \tag{5.124}$$

and introducing the rescaled field $\tilde{\eta} := \eta\sqrt{N}$, resulting in an expansion for the large action S,

$$S[\phi] = N\tilde{S}[\phi_0] + \tilde{S}_2[\phi_0]\tilde{\eta}^2 + \mathcal{O}\left(\tilde{\eta}^3 N^{-1/2}\right). \tag{5.125}$$

Now it can be seen that the action is dominated by the stationary action and the sub-leading quadratic term and that higher contributions die out asymptotically with large N. Thus, asymptotically with large N the Gaussian approximation becomes exact. As to the question of negligible fluctuations one can see that their ratio to the drifting stationary action solution is typically of order $1/\sqrt{N}$. This is either due to massive phase cancellations in quantum path integrals (large fluctuating imaginary exponents lead to randomly oscillating contributions in the sum over paths), or due to exponential suppression in weights of path integrals for Markov processes or statistical partition sums. In that case, the deterministic solution ϕ_0 captures the essential physics behind the path integral with suppressed fluctuations. In quantum processes this corresponds to the classical limit and was historically described in the WKB approximation for wave functions, where only the action for the stationary path was taken into account. In Markov processes this corresponds to the limit of negligible diffusion, and in thermodynamic equilibrium this corresponds to the zero temperature limit where the energetic ground state characterizes the thermodynamic ground-state.

The condition for non-fluctuating behavior in real systems is that typical process scales like wavelength, relaxation time and temperature are very small as compared to the systems global scales like effective system size, measurement time and excitation energy. To illustrate the condition of non-fluctuating behavior for quantum processes we compare two systems: (1) A billard ball of mass 0.15 kg in standard units and typical velocity of 5 m/s on a table of typical dimensions of 1.5 m. The wavelength is $h/(mv) = 8.8 \cdot 10^{-34}$ m and the ratio of the wavelength to the table size is approximately $6 \cdot 10^{-34}$. (2) An electron in a quantum dot of size 10 nm. Its (Fermi-) wavelength is of the same order of magnitude and hence the relation of wavelength to effective system size is of order 1. Obviously in case (1) quantum fluctuations are irrelevant, while they are essential in case (2).

An enlightening example of the large N limit is also the emergence of the central limit theorem, where N is the number of weakly correlated random numbers summed up to an average random number which fluctuations become more and more Gaussian as N increases. The mathematical way to show this is along the generating function for cumulants, which is additive. N appears in the partition sum in exactly the way discussed here (see also Appendix A on large numbers I and II).

5.6 Modeling Strategies

Recall that for a physical system at hand, showing fluctuations in relevant variables, one wants to calculate conditional expectation values, stationary and dynamic correlation functions, propagators, susceptibilities and/or scattering rates. These quantities can be expressed as Green's functions which can be generated from a cumulant generating functional, or equivalently from its Legendre transformed with respect to the dual source field. This Legendre transformed is the effective action. The whole machinery for a physical system at hand is defined by the Lagrange density in terms of the configuration field variable and its derivatives. The Lagrange density can be uniquely[11] constructed from the systems dynamic or equilibrium generator, encoded in coefficients with respect to polynomials in ordered products of powers of the variable and its deviations (Hamiltonian coefficients or Kramers-Moyal coefficients) or in ordered products of powers of excitation and annihilation operators (occupation number representation of many body systems). The modeling can thus set in at different levels: the generator coefficients or the Lagrange density or the effective action can be starting points for the modeling.

On all modeling levels the first choice is the set of relevant variables. On all modeling levels symmetries play a fundamental role in identifying relevant variables and their couplings. Symmetry means that performing a related transformation (symmetry transformation) of the variables may leave some quantities invariant (symmetry invariants), almost invariant, or they vary in an easily controlled manner, e.g. by continuity equations. Almost invariant means a slower or smoother variation of some quantities as compared to the change in the original variables. Thus, finding symmetries and corresponding invariants or almost invariant quantities helps to identify the slow and smooth variables as candidates for macroscopic relevant variables. On the other hand, those quantities which change rapidly under the symmetry transformation can be considered as irrelevant and one tries to "integrate them out". Relevant variables may be classifiable with respect to topology into distinct classes, either as a consequence of boundary conditions or as a consequence of the topology of symmetry invariant subspaces of the original configuration space. We will have a closer look at symmetry in Chap. 6 and at topology in Chap. 7.

On the level of the generator, the modeling has to respect symmetries and the algebraic structure of operators, which makes it a sophisticated task to find transformations to relevant variables. Nevertheless, a number of successful techniques like the projector formalism used in Sect. 5.4.2 or the Bogoluibov transformation in the superfluid/superconductor problem (see e.g. [9]) have been developed. However, in this book we like to focus on the advantages of the modeling by generating functionals.

On the slow and long ranged scales (macroscopic scales) a phenomenological modeling may start right away with a choice of the mean field φ as the most macroscopic relevant variable and one constructs the effective action. Here, symmetry is the guide to find an appropriate effective action. As a simple model for the phase

[11] In the discretized version with time ordering prescription.

transition to spontaneous magnetization Landau introduced a quartic action function (called Landau free energy) of a homogeneous order parameter field M for the one dimensional caricature of the magnetization in a ferromagnet,

$$\Gamma(M) = -\tau\alpha^2 M^2 + \frac{\lambda}{4}M^4, \tag{5.126}$$

with positive parameters α^2 and λ and a real parameter τ as a dimensionless measure of deviation from the transition temperature. The effective action function is symmetric under reflection $M \to -M$, because the magnetization mechanism does not single out a magnetization direction. It is thus expanded in a series of even powers of M. It is stopped after the second term, because this suffices to model the occurrence of spontaneous magnetic ordering into one of two symmetric possible directions, as long as the system is in the ordered phase ($\tau > 0$). It also describes the smooth transition at $\tau = 0$ to an disordered phase of vanishing magnetization. It is depicted in Fig. 5.4. We will also discuss a modified version including fluctuations in Sect. 6.3.

The modeling of the Lagrangian density can start from a level of microscopic degrees with known interactions and one proceeds by reducing to relevant macroscopic variables. The reduction to relevant macroscopic variables is most easily done within this formulation because of "summations first" instead of "algebra first". The prescriptions, to be exemplified in subsequent chapters, are given here.

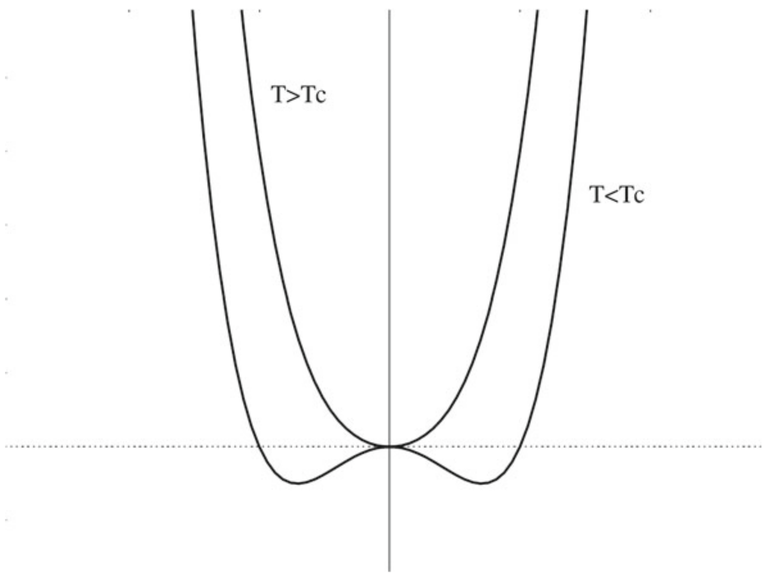


Fig. 5.4 Effective potential for systems with continuous phase transitions for temperatures below and above criticality

- Having found by symmetry considerations a candidate for the macroscopic relevant field Ψ as a function(al) of the microscopic fields ϕ, $\Psi = F[\phi]$, one constructs a partition sum for the macroscopic field Ψ by introducing the Fourier duality trick,[12]

$$1 = \int D\Psi\, \delta(\Psi - F[\phi]) = \int D\Omega D\Psi\, \exp\left[i\left(\Psi - F[\phi]\right) \cdot \Omega\right], \qquad (5.127)$$

and interchanging the order of integration over configurations

$$\exp W[J = 0] = \int D\Omega \int D\psi \int D\phi\, e^{-S[\phi[\Psi]]+[i(\Psi - F[\phi])\cdot\Omega]}. \qquad (5.128)$$

If one manages to integrate out exactly or approximately the original microscopic variable ϕ and one of the dual partners Ψ or Ω, one ends up with a generating functional in the macroscopic relevant field, which can be either Ψ or its dual partner Ω. In case of Ω being the remaining variable, the generating functional of cumulants in Ω has again the usual form with a reduced action $\tilde{S}[\Omega]$,

$$\exp W[J_\Omega] = \int D\Omega\, e^{-\tilde{S}[\Omega]+\int \mathrm{d}x\, \Omega(x)\cdot J_\Omega(x)}. \qquad (5.129)$$

The action follows from performing the integrations over the original variable ϕ and one of the dual macroscopic partners, say Ψ. In doing the integrations one has to be aware of determinant factors from a symmetry induced change of the integration variables. These determinant factors can be re-exponentiated as Tr log-terms in the action. The ϕ integral can be performed exactly for quadratic couplings $F[\phi]$ and one writes the remaining functionals by the duality of Ψ and Ω in such a way that one can integrate out one of them in a Gaussian way. The remaining reduced action[13] $\tilde{S}[\Omega]$ will usually be non-Gaussian and hast to be further analyzed.
- Analyzing the reduced action $\tilde{S}[\Omega]$ with respect to its symmetries and the topology of these configurations one may separate further into few component slow modes $\tilde{\phi}$ and fast field modes and integrates out the fast modes, at least formally by redefining the coefficients in front of polynomials in products of powers of the field $\tilde{\phi}$ and its derivatives $\partial_x\tilde{\phi}$. Sometimes, an infinite power series can be recast into the form of a special function.
- If one has finally arrived at a reduced action $\tilde{S}[\tilde{\phi}]$ in a relevant slow mode field $\tilde{\phi}$, one proceeds with the expansion starting from the stationary action solution, as outlined before. Here, the stationary action, $\Gamma_0[\tilde{\phi}_0]$, as a function of the homogeneous

[12]The Fourier duality trick is a bit more general than the Hubbard-Stratonovitch transformation (see e.g. [6]) for quadratic F.

[13]The reduced action of the macroscopic field, $\tilde{S}[\Omega]$, is also often called effective action, but should not be mixed up with the Legendre transform $\Gamma[\langle\Omega\rangle]$ which we denoted as effective action.

stationary action solution $\tilde{\phi}_0$, is already a candidate for a mean field modeling with a Landau free energy.

- The perturbative analysis beyond the Gaussian level has to be accompanied by topological considerations and by a stability analysis, usually called renormalization group analysis. Topological considerations mean that one must respect distinct topological classes of configurations when calculating the partition sum. An example will be discussed in Sect. 7.3.3. Action contributions from discrete topological field configurations can be overlooked in an ordinary perturbational expansion, because a continuous perturbation cannot change a discrete contribution.

5.7 The Renormalization Semi-Group

To study the stability of the model in a simple way one would look at the change of the cumulants with increasing order of the perturbation series. However, in many models of interest even the Gaussian level leads to diverging quantities when the continuity of the external space is taken literally. For example,[14] in the ϕ^4-model,

$$S[\phi] = \int \mathrm{d}^3x \left[\sum_{l=1}^{3} (\partial_l \phi(\mathrm{x}))^2 + \frac{m^2}{2}\phi^2(\mathrm{x}) + \frac{\lambda}{8}\phi^4(\mathrm{x}) \right], \tag{5.130}$$

the effective action in a Gaussian level approximation around the stationary homogeneous action solution φ reads

$$\Gamma[\varphi] = \int \mathrm{d}^3x \left\{ \frac{m^2}{2}\varphi^2 + \frac{\lambda}{8}\varphi^4 + \frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3} \ln\left[k^2 + m^2 + \frac{3}{2}\varphi^2\right] \right\}. \tag{5.131}$$

The integral shows a simple divergence due to infinite system size, called infrared divergence, and a more serious divergence due to infinite k, called ultraviolet divergence. The notions refer to wavelengths of light (infrared for long wavelengths and ultraviolet for short wavelengths). One can regularize the integral by introducing a finite macroscopic cubic system size L to cure the infrared divergence and a finite shortest length l_0 with corresponding wave number $K = 2\pi/l_0$ and finds for the integral

$$\begin{aligned} &\frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3} \ln\left[k^2 + m^2 + \frac{3}{2}\varphi^2\right] \\ &= \frac{1}{4\pi^3}K^3 \left(3\ln(K^2 + a) - 2\right) + \frac{3}{2\pi^2}aK - \frac{1}{12\pi}a^{3/2}, \end{aligned} \tag{5.132}$$

[14]We follow here the discussion in [8].

where $a = m^2 + 3/2\varphi^2$. If one tries to incorporate the Gaussian approximation in the stationary action by renormalizing the coefficients m^2 and λ as the first and second derivative of the action with respect to $\frac{1}{2}\varphi^2$ at $\varphi = 0$, one finds for these renormalized coefficients (as long as $m_R^2 > 0$),

$$m_R^2 = m^2 + \frac{3\lambda K}{4\pi^2} - \frac{3\lambda m}{8\pi}, \tag{5.133}$$

$$\lambda_R = \lambda - \frac{9\lambda^2}{16\pi m}. \tag{5.134}$$

These equations show two interesting things. First, the mass parameter m sets an inverse length scale to the problem, as contributions of K for $K \approx m$ cause relevant changes. This length scale can become infinite as the mass approaches zero, where the phase transition occurs. Thus, the length scale can be identified with a correlation length ξ over which local quantities are correlated in the system. Second, for large couplings the corrections to the coupling become large and naive perturbation theory must break down. In addition, the coupling grows with mass going to zero, consistent with the interpretation of mass as an increasing correlation length. This example shows that a stability analysis must be based on an analysis of the scaling behavior of the theory. The idea that characteristic length scales emerge in interacting systems helps a lot in setting up analyzing tools for the stability analysis. It turns out that the key, the so called renormalization group, is again a generated semi-group. As an introductory text to scaling and the renormalization group we recommend Cardy's book [10]. Let us sketch the main ideas behind this tool.

One of the two central ideas is to introduce a probing length scale L into the formalism such that one can consider the effective action or related quantities as a scale dependent quantity. On the most general level an effective action can be defined, $\Gamma_L[\varphi]$, that takes into account the full fluctuations of fields on scales up to L while fluctuations on larger scales are suppressed. As a lower limit for the scale one takes the microscopic scale of the problem l_0. When reaching this microscopic limit the scale dependent effective action equals the pure action because fluctuations are inessential at this scale,

$$\lim_{L\to l_0} \Gamma_L[\varphi] = S[\varphi]. \tag{5.135}$$

For large probing length$L$ the full effective action is recovered,

$$\lim_{L\to\infty} \Gamma_L[\varphi] = \Gamma[\varphi]. \tag{5.136}$$

It is indeed possible, by a clever use of the Gaussian level approximation, to introduce a Gaussian scale probing term with kernel R_L into the partition sum to reach the desired limits and to write down an exact scaling equation for the flow of the effective action as a functional differential equation. This is achieved by the following construction that takes the Legendre transform property, accompanied by a smooth cut-off at length scale L,

$$\exp -\Gamma_L[\varphi] = \int D\eta \; \exp\left\{ -S[\varphi+\eta] + \int \mathrm{d}x \, \frac{\delta \Gamma_L}{\delta \varphi}(x) \cdot \eta(x) \right. \\ \left. - \int \mathrm{d}x\mathrm{d}x' \, \eta(x') R_L(x',x) \eta(x) \right\} . \tag{5.137}$$

Here the kernel $R_L(x,x')$ has to fulfill two limiting requirements: for $|x-x'| << L$ the kernel is negligible and fields at these separations are correlated in the same way as in the original model. In the opposite limit, $|x-x'| >> L$ the kernel becomes very large to suppress any fluctuations at such large separations. The precise form of the kernel can be chosen appropriately for a model at hand. In any case the functional equation (5.137) leads to an exact flow equation (see [8] Sect. 2) for the effective action, usually formulated in wave numbers $K = 2\pi/L$,

$$\partial_K \Gamma_K = \mathrm{Tr} \left\{ \left[\Gamma_K^{[2]} + R_K \right]^{-1} \partial_K R_K \right\} . \tag{5.138}$$

The trace stands for sums over all indices. Such equations are exact but hard to solve in closed form as they are equivalent to a set of infinitely many coupled non-linear partial differential equations. They can however serve as a solid and flexible starting point for meaningful approximations. Approximations become meaningful when one has found the appropriate relevant variables for the system at hand. Then it will be possible to characterize the effective action by a few coefficients in terms of an expansion into a series build of powers of the field and perhaps its derivative. In general, these coefficients will be functions of external coordinates. As an example consider the so called vertex expansion which is the effective actions Taylor expansion around the stationary solution φ_0 of the effective action,

$$\Gamma_L[\varphi] = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\prod_{j=0}^{n} \int \mathrm{d}x_j \, (\varphi(x_j) - \varphi_0) \right) \Gamma_L^{[n]}(x_1, \ldots x_n). \tag{5.139}$$

The so called vertex functions $\Gamma_L^{[n]}(x_1, \ldots x_n)$ are such coefficients characterizing the effective action in an expansion. The first non-trivial one is $\Gamma_L^{[2]}(x_1, x_2)$. Other expansions are possible, for example with respect to symmetry invariants of the model.

In the vicinity of homogeneous stationary action solutions it often suffices to consider parameters characterizing those coefficients. These parameters do not depend on the external coordinates, but only on the probing scale L. In such cases the scaling behavior is captured in a set of few coupled ordinary differential equations for such parameters, then called **scaling variables**. Examples are the mass m and the coupling constant λ in our introductory example (5.130).

Let us give a heuristic motivation for this second central idea behind the renormalization group: the scaling flow of the scaling variables $\boldsymbol{g}(L)$ is given by a set of ordinary autonomous differential equations. This behavior can be recast in an assumption about the functional dependence of scaling variables on characteristic macroscopic lengths $\boldsymbol{\xi}$. For simplicity, we take a single relevant length ξ and its relevance is manifest when the single relevant scaling variable $g(L)$ can be expressed as a universal function of the ratio ξ/L,

$$g(L) = f(\xi_c/L). \tag{5.140}$$

All parametric details enter through the macroscopic length ξ. Such behavior may describe the dominating behavior relevant in a macroscopic description; deviations may be present but negligible asymptotically with $\xi/l_0 \gg 1$. Such behavior is emergent and known as the universality phenomenon. It is found that macroscopic behavior for different systems with different microscopic details can lead asymptotically to the same macroscopic behavior. It might even turn out that systems with seemingly unrelated microscopic variables lead to the same effective action in relevant variables. An example is the liquid gas transition and the transition to spontaneous magnetization which—on a level of homogeneous mean fields—is described by the same Landau model (see (5.126) and Fig. 5.4) with quartic self-interaction potential. In the case of universality, described by (5.140), the ratio ξ/L can be expressed as the inverse function

$$\hat{f}(g) = \xi/L. \tag{5.141}$$

To be precise, one has to allow for branches of the scaling function f; each branch belongs to a separate phase of the model. The branches meet at a critical point, where ξ diverges. With (5.140) a so called β-function can be defined as a function of g alone,

$$\beta(g) := -\frac{f'(\hat{f}(g))}{f(\hat{f}(g))}\hat{f}(g). \tag{5.142}$$

Calculating $\mathrm{d}g(L)/\mathrm{d}L$ and using the scaling behavior (5.140) with (5.141) one finds a flow equation for $g(L)$ as an ordinary autonomous differential equation in terms of the β-function. The generalization to a number of scaling variables $\boldsymbol{g}$ reads

$$\frac{\mathrm{d}\boldsymbol{g}}{\mathrm{d}t} = \boldsymbol{\beta}(\boldsymbol{g}). \tag{5.143}$$

Note that the logarithmic length scale $t = \ln(L/l_0)$ is the appropriate variable to make the differential equations autonomous, i.e. the function on the r.h.s. does not explicitly depend on $t = \ln(L/l_0)$.

Equation (5.143) show that the scaling is captured by a semi-group of Aristotelian deterministic dynamic type in the time like variable t. In an abstract notation the renormalization group operator $\hat{\mathcal{R}}_{\delta t}$ for a rescaling from t to $t + \delta t$ does not depend on t explicitly, but only on δt. The infinitesimal generator $\hat{R} := \lim_{\delta t \to 0}(\hat{\mathcal{R}}_{\delta t} - 1)/\delta t$ is then independent of t, such that a renormalization group transformation on the scaling variables $\boldsymbol{g}$ reads

$$\boldsymbol{g}(t+\delta t) = \hat{\mathcal{R}}_{\delta t}\boldsymbol{g}(t) = e^{\delta t \hat{R}}\boldsymbol{g}(t), \tag{5.144}$$

leading to the differential equations

$$\frac{\mathrm{d}\boldsymbol{g}}{\mathrm{d}t} = \hat{R}\boldsymbol{g}(t) =: \boldsymbol{\beta}(\boldsymbol{g}(t)). \tag{5.145}$$

The β-functions correspond to the infinitesimal semi-group action of the renormalization group on the level of scaling variables $\boldsymbol{g}(\ln(L/l_0))$. The dynamics in the time like variable $t = \ln L/l_0$ is irreversible as the differential equation is of first order and autonomous. It is thus capable to describe the phenomenon of universality as the asymptotic stationary limit of the renormalization group can turn out to be unique for different initial model systems. The zeroings of the $\boldsymbol{\beta}$-functions are **fixed points** of scaling. The fixed points can have stable, repulsive or marginal directions. In the vicinity of fixed points one can study the stability and the scaling by linear approximation of the $\boldsymbol{\beta}$-functions. The linear regime around a fixed point $\boldsymbol{g}^*$ of the flow ($\beta\,(\ln g^*) = 0$) defines the critical regime (see Fig. 5.5). The positive linear coefficient β' for a repulsive flow direction g leads to an exponential growth in the variable $|g(l_0) - g^*)|$ away from the fixed point, corresponding to a power law behavior in the ratio L/l_0 with power β',

$$|g(L) - g^*| = |g(l_0) - g^*)|(L/l_0)^{\beta'}. \tag{5.146}$$

Power law behavior is the indicator of the absence of an intrinsic length scale in the system and the power law must bend over to a scale dependent behavior when the probing length L approaches the correlation length ξ_c of the system. Reversing this argument tells that the correlation length ξ_c diverges with power $\nu = 1/\beta'$ when

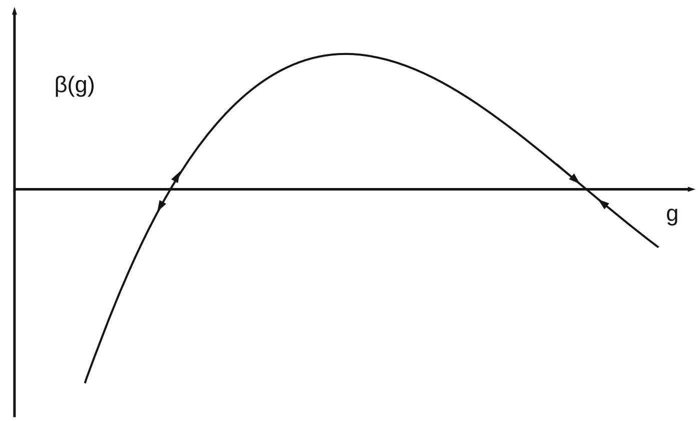


Fig. 5.5 Sketch of a β-function with two fixed points. At the *left* fixed point value the flow is repulsive, at the *right* fixed point value the flow is attractive

approaching the critical point,

$$\xi_c \propto |g - g^*|^{-\nu}. \tag{5.147}$$

Thus, also the critical exponents of a systems critical behavior can be extracted from the renormalization group analysis. However, an exact calculation of $\boldsymbol{\beta}$ functions is usually not possible. Within the effective action approach one should start from the exact flow equation (5.138) with clever truncation of some appropriate expansion. The calculations are based on the Gaussian approximation around stationary action solutions and expansions in auxiliary parameters such as deviations from integer dimensions or in real small parameters of the problem such as the dimensionless electromagnetic fine structure constant $\alpha = 1/137$.

Once the generating functional approach has put the finger on appropriate scaling variables $\boldsymbol{g}(L)$ one is free to use simplified approaches to focus on these variables and tries to set up the $\boldsymbol{\beta}$ functions as the result of a deterministic semi-group process. This opens a great flexibility for several tools developed for dynamical deterministic systems including, of course, numerical calculations for lattice models with explicit introduction of a microscopic scale l_0 as the lattice constant and finite system size L. In numerics, the ratio L/l_0 is usually restricted by computer power, but the variation may already give valuable information about the scaling behavior when parameters are varied such that the system exhibits different phases (see e.g. Chap. 4 in [10]).

Models with a duality in coupling constants are very convenient for such stability analysis. One can treat a strong coupling limit of one model as the weak coupling limit of the other model. By this one may also be able to interpolate the β functions for one model between two limits and make meaningful statements about the intermediate regime where critical behavior might or might not occur. An example is the modeling of the Anderson localization problem (see Sect. 8.7).

5.8 Exercises

Exercise 1: Hermiticity
Show that $\dot{f}$ and k are hermitian operators.

Exercise 2: Uncertainty
Show the uncertainty relation (5.9) from (5.5) for Galilei particles.

Exercise 3: Continuity Equation
Show by the general definitions of density (5.11) and current density (5.12) that we get back (2.65) for Hamiltonians of the form of (3.11).

Exercise 4: Trace
Show the cyclic invariance and the unitary invariance of the trace and verify (5.14).

Exercise 5: Projector
Show the property $P^2 = P$ for the projector P_ψ.

Exercise 6: Distribution for a Reduced Variable
Show that (5.19) is the appropriate distribution for all functions of reduced variable $A(x)$.

Exercise 7: Density Matrix
Show that (5.24) is a density matrix. Construct it for two two-value systems with originally pure states for

(a) product state

$$|\,\psi\rangle = |\,A+\rangle\;|\,B-\rangle\,,$$

(b) entangled states

$$|\,\psi\rangle = \sqrt{\frac{1}{2}}\,(|\,A+\rangle\;|\,B-\rangle \pm |\,A-\rangle\;|\,B+\rangle)\,.$$

Exercise 8: Quantum Entropy and von Neumann's Equation
Show that the quantum entropy stays constant when the density matrix dynamics is given by von Neumann's equation $\dot{\varrho} = -i\,[H, \varrho]$

Exercise 9: Entropy of Gaussian
Calculate the entropy for a Gaussian distribution

$$P(x) = (1/\sqrt{2\pi\sigma^2})\exp -\frac{(x-x_0)^2}{2\sigma^2},$$

where σ is dimensionless, measured in the units of variable x.

Exercise 10: Effective Action for Gaussian Fluctuations Around Stationary Solutions
Recapitulate the derivation of the Euler-Lagrange equations as following from stationarity, interchange of linear approximations and partial integrations with vanishing boundary terms. Then calculate the effective action $\Gamma[\phi]$ for the Gaussian partition sum of (5.120).

Exercise 11: Effective Action for Gaussian Fluctuations in the ϕ^4-Model
Derive (5.131) from the Gaussian approximation around the homogeneous stationary action solution of the ϕ^4-model by using Fourier transformation to diagonalize the derivative $\partial_l\phi(\mathrm{x})$.

Exercise 12: Phases from β Functions
A generating functional for a one component mean field φ with homogeneous action of the form

$$\Gamma_L[\varphi] = \frac{\lambda_L}{2}\left(\varphi^2 - \varphi_{0L}^2\right)^2$$

has two positive scaling parameters λ and φ_0^2 with approximate β-functions

$$\beta_\lambda(\varphi_0^2, \lambda) = 0,9\lambda - \frac{\lambda^2}{3(1+2\lambda\varphi_0^2)}; \;\; \beta_{\varphi_0^2}(\varphi_0^2, \lambda) = 1.05\varphi_0^2 - \frac{1}{6(1+2\lambda\varphi_0^2)}.$$

Discuss the fixed points and their stability character and possible phases of the model. Calculate the critical exponent ν of the correlation length as the positive eigenvalue of the Jacobian matrix for the β-functions at the critical point with a direction of instability.

References

1. H. Risken, *The Fokker-Planck Equation* (Springer, 1996)
2. N.G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 3rd edn. (North-Holland, Amsterdam, 2007)
3. G. Roepke, *Statistische Mechanik für das Nichtgleichgewicht* (VEB, Berlin,1987); *Nonequilibrium Statistical Physics* (Wiley, 2013)
4. D. Zubarev, V. Mozorov, G. Roepke, *Statistical Mechanics of Nonequilibrium Processes*. Basic Concepts, Kinetic Theory, vol. 1 (Akademie Verlag, Berlin, 1996)
5. J. Chalker, A. Lukas, *Lecture Notes on M. Phys Option in Theoretical Physics: C6* (Oxford University, Oxford, 2011)
6. A. Altland, B. Simons, *Condensed Matter Field Theory*, 2nd edn. (Cambridge University Press, Cambridge, 2010)
7. T.P. Cheng, L.-F. Li, *Gauge Theory of Elementary Particles* (Clarendon Press, Oxford, 1984)
8. J. Berges, N. Tetradis, C. Wetterich, Phys. Rept. **363**, 223 (2002)
9. C.P. Enz, *A Course in Many Body Theory Applied to Solid State Physics* (World Scientific, Singapore, 1992)
10. J. Cardy, *Scaling and Renormalization in Statistical Physics* (Cambridge University Press, Cambridge, 1996)

Chapter 6
Symmetries and Breaking of Symmetries

Abstract Symmetries help to reduce complexity of calculations. A familiar example is the use of spherical polar coordinates in calculating integrals of quantities which are spherical symmetric. If one manages to find coordinates fitting to symmetries, some of them disappear from the invariant functions and this reduces the calculation task drastically. The same idea is behind the use of symmetries in representation theory to classify (and thus simplify the calculation of) eigenspaces and eigenvalues of invariant observables. The next task is to identity relevant variables and regimes or phases of its states with the help of the system?s symmetrics. Finally, symmetrics can appear as local symmetrices together with a field controlling the correct gauge to identify the symmetry at all. When spontaneous symmetry breaking occurs with gauge symmetrices the gauge modes can become massive (Anderson - Higgs mechanism).

The next task is to identify relevant variables and regimes or phases of its states with the help of the system's symmetries. In a macroscopic treatment of a system one keeps watching for symmetries and related constants of motion by Noether's theorem. In highly excited states (high temperature) these symmetries are manifest. Low energy long wavelength excitations in these highly excited states can be described hydro-dynamically, where continuity equations of conserved quantities dominate the slow macroscopic modes. For low lying excitations (low temperature) the process of spontaneous symmetry breaking is indicated by appropriate order parameters. It is further accompanied by defects, dislocations and dynamic modes which try to restore the symmetry (Goldstone modes). These dominate the slow mode macroscopic behavior, e.g. elastic behavior.

Finally, symmetries can appear as local symmetries together with a field controlling the correct gauge to identify the symmetry at all. This introduces a very strong geometric principle of identifying interactions in nature. These symmetries might only appear as subgroups after a process of broken symmetry. Actually, the celebrated standard model of elementary particle physics is exactly of this type (see [1]) and also gravitation theory (going beyond general relativity) can be viewed as a gauge theory (see [2]). When spontaneous symmetry breaking occurs with gauge symmetries the gauge modes can become massive (Anderson-Higgs mechanism). This is observed in superconductivity and electroweak interaction.

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1_6

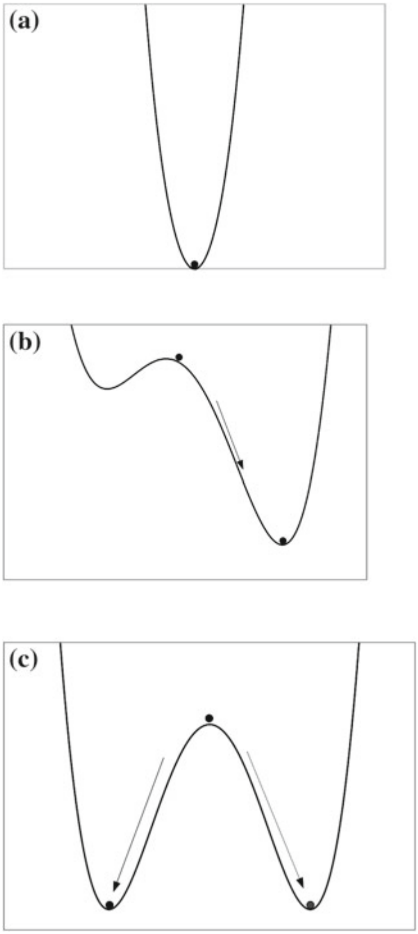


Fig. 6.1 Sketch of symmetry (reflection or rotation) from full (dynamics and ground-state) (**a**) over explicitly broken (**b**) to spontaneously broken (dynamics yes, ground-states no, but hidden) (**c**)

6.1 General Definitions

We start with a general definition in words complemented with figures with reflection symmetry (Fig. 6.1).

1. A symmetry of a system is a **group** G **of transformations** g acting on the configuration variables $\phi(x)$ (external or internal), properties $F[\phi]$, states $\mid \Phi\rangle$ of the corresponding Hilbert space[1] and/or observables $O(a^\dagger(x), a(x))$, where $a^\dagger(x)$ creates a state[2] from the vacuum with property x and its hermitian conjugate $a(x)$ annihilates such particle, leaving the time evolution operator T—and/or some other important system observable—**invariant**.

[1]For fields the Hilbert space of infinite particle numbers is called Fock space.

[2]usually called particle.

2. A symmetry is **explicitly broken** (perhaps to a subgroup H of G) if the former invariant quantity I is changed by an amount δI, such that $I' = I + \delta I$ is no longer invariant under G (but perhaps under the action of the subgroup H).
3. A symmetry is **spontaneously broken** (perhaps to a subgroup H of G) if the dynamics T is still invariant under the full group G, but the **ground-state** is not invariant under G (but perhaps under H). Rather, the symmetry is **hidden** in the sense, that the ground-state is a member of degenerate ground-states which can be transformed into each other by the action of the factor space $G/H = \{gH|g \in G\}$ (H acts as a 1).

If a system shows many symmetry relations it has less special relations between its configuration variables. In this sense it shows more disorder. For example, in a gas all continuous translations and rotations are symmetry operations of the state; this is also true for a liquid. But in a liquid a symmetry between occupied positions and unoccupied positions is already broken that was present in the gas state. Thus, there is a subtle difference in symmetry between both fluid phases. In a piece of condensed matter the state is only symmetric under discrete translations and rotations. It has more structure and less disorder. As a rule of thump with only few exceptions one finds that states with higher thermodynamic entropy (configuration entropy in phase space or quantum entropy) and higher temperature have more symmetry.

In the context of phase transitions there are transitions of first order with a jump in one of the thermodynamic potentials (e.g. latent heat) and so-called second order transitions with smooth behavior of thermodynamic potentials (although singularities appear in derivatives). For first order transitions the breaking of symmetry can be to a different symmetry group which is not a subgroup of the larger symmetry group. For second order transitions this is not possible. The smaller symmetry must be a subgroup H of the larger symmetry group G. In any case symmetries apply or don't apply. With second order transitions the **order parameter** shrinks continuously to zero, while it jumps for first order transitions.

6.2 Transformation Groups and Representations

The paradigm of a symmetry is mirror symmetry. As a simple mathematical realization consider the discrete group $\mathbf{Z}_2$ consisting of two elements $\{-1, +1\}$. As a transformation group acting on variables it looks like

$$1: \quad x \mapsto x := g_1(x), \tag{6.1}$$

$$-1: x \mapsto -x := g_{-1}(x). \tag{6.2}$$

As an invariant I we can take every function $I = f(x)$ with mirror symmetry with respect to the y-axis, e.g.

$$f(x) = x^2 - \frac{1}{4}x^4 = f(-x). \tag{6.3}$$

The symmetry is explicitly broken for

$$I + \delta I(j, \epsilon) = x^2 - \frac{1}{4}x^4 + jx + \epsilon x^3, \tag{6.4}$$

where j and ϵ are **coupling constants** that measure the strength of the explicit symmetry breaking.

As an important example for a **continuous group** consider translations in $\mathbf{R}^d$,

$$g_{\boldsymbol{a}} : \boldsymbol{x} \mapsto \boldsymbol{x} + \boldsymbol{a}. \tag{6.5}$$

For a deterministic free Galilei particle of inertia m in d dimensions the Hamilton function is translation invariant,

$$H(\boldsymbol{x}, \boldsymbol{p}) = \frac{1}{2m}\boldsymbol{p}^2 = H(\boldsymbol{x} + \boldsymbol{a}, \boldsymbol{p}). \tag{6.6}$$

The momentum as the generator of translations in canonical mechanics fulfills

$$\{\boldsymbol{p}, H\} = 0 \tag{6.7}$$

and therefore the momentum $\boldsymbol{p}$ is a conserved quantity in systems of translational invariant dynamics (an example of Noether's theorem). To implement symmetries from configuration variables on the space of states (probabilities or pre-probabilities) they have to be represented on the space of states. Since probabilities are just functions of the configuration, there is nothing new and we switch to Hilbert spaces of states. A symmetry representation $\pi(g)$ on a Hilbert space is an operator acting on states that respects the original group structure (homomorphism)

$$\begin{aligned} \pi(g_1 g_2) &= \pi(g_1)\pi(g_2) \\ \pi(g^{-1}) &= (\pi(g))^{-1}, \\ \pi(1) &= 1. \end{aligned} \tag{6.8}$$

The Wigner theorem (for a detailed discussion see Chap. 2 in [3]) states that in order to respect the scalar product of the Hilbert space, the representing matrices have to be unitary linear or anti-unitary anti-linear. An anti-unitary anti-linear matrix changes the scalar product to its complex conjugated value. Anti-unitary transformations are only relevant if a change of direction of time's flow is involved. Besides the so-called ray-representations of (6.8) there are also projective representations, where the representation of a product may involve an additional phase. We will briefly comment on this possibility a little later in the context of Lie algebras.

A trivial representation is always possible: $\pi(g) = 1$. Thus, representations need some qualifying attributes. Representations of practical relevance are the **irreducible representations**. These leave no subspace invariant under their action, while reducible representations do leave some true subspace $\mathcal{H}_1$ invariant, $\pi(G)\mathcal{H}_1 = \mathcal{H}_1$. The group itself can be classified into **symmetry classes** $[g]$ by an equivalence relation $g \sim g' = bgb^{-1}$ with some group element b.

$$[g] := \left\{a \in G | b \in G \,\text{exist} : bab^{-1} = g\right\}. \tag{6.9}$$

Two representations of the same group are called unitarily or anti-unitarily equivalent if $\pi_2(G) = U\pi_1(G)U^{-1}$ for all g with the same unitary or anti-unitary operator U. There are some helpful theorems (see [4]):

- For discrete (and also for compact[3] continuous) groups any representation can be decomposed as a direct sum of irreducible representations.
- For discrete finite groups there are as many nonequivalent irreducible representations as number of classes. With the definition of the character

  $$\chi_g := \mathrm{Tr}\ \pi(g), \tag{6.10}$$

  which is a class invariant, χ_1 provides the dimension of the representation. The criterion for irreducibility is: the average scalar product of characters over the group of N elements is just unity,

  $$(\chi, \chi) := N^{-1} \sum_{g \in G} \chi_g (\chi_g)^* = 1. \tag{6.11}$$

- Once one knows the irreducible representations of group G that leaves the dynamics invariant,

  $$\pi(G) H \pi^{-1}(G) = H \tag{6.12}$$

  one can conclude:

  $$[H, \pi(G)] = 0. \tag{6.13}$$

  Thus, the representations and H can be diagonalized simultaneously in a common basis. The dimension of the irreducible representation is the minimum degeneracy factor of energy eigenvalues. H can be brought to block-diagonal form where each block acts on an invariant subspace, where its eigenvalue is totally degenerate,

[3] closed and bounded.

$$H = \begin{pmatrix} [H_1] & [0] & [0] & [0] \\ [0] & [H_2] & [0] & [0] \\ [0] & [0] & [H_3] & [0] \\ [0] & [0] & [0] & [H_4] \end{pmatrix}. \tag{6.14}$$

By accident eigenvalues on different invariant subspaces can coincide, too. Such coincidences however disappear, as soon as parameters are changed that leave the symmetry untouched.

These theorems have broad applications e.g. in classifying atomic levels with respect to the angular momentum and spin quantum numbers and also in classifying energy bands of crystals with their specific point group symmetries and in classifying elementary particles with their specific symmetry groups of e.g. flavour and isospin.

Continuous groups that form a topological manifold of dimension d_G and that can be described locally by generators X_a,

$$g_{\boldsymbol{\alpha}} = \exp\left[i \sum_a \alpha^a X_a \right], \tag{6.15}$$

such that group members are analytic in the parameters α^a, are called **Lie groups** with a corresponding Lie algebra of the generators,

$$[X_a, X_b] = \sum_c i C^c_{ab} X_c. \tag{6.16}$$

Here C^c_{ab} are the so-called **structure constants** of the Lie algebra. The generators live in the group's tangent bundle and describe the group locally. The structure constants will be respected by any reasonable representation. For so-called projective representations (up to a phase products) there can appear a so-called central charge in addition to the right side of (6.16); however not for single connected groups[4] (see Chap. 2.7 in [3]).

The Lie algebra does, by the exponential map (6.15), lead back to the full group if the group's topology is connected.[5] Many physically relevant groups have however several disconnected components. But, they are distinguished by certain discrete transformations like reflection and can thus be reconstructed from the connected group component containing the 1. For each connected group there is a universal covering group which has the same Lie algebra and is single connected. The covering property means that some discretely separated members of the covering group correspond by the covering map to a single element of the covered group. As an

[4] Single connected: every closed path can be continuously deformed to a single point without leaving the topological space.

[5] Connected means here: every two points can be connected by a path within the group.

example take the circle $\mathbf{S}^1$ covered by the full line $\mathbf{R}^1$ by the covering map $\alpha \mapsto e^{i\alpha}$, where all real numbers with step-width 2π are mapped to the same circle point. Some topology notion is captured in Fig. 7.2.

Needless to say that there is a big machinery of mathematical theory about Lie groups, algebras and their representations for physical systems. If you are familiar with the classification of the rotation group $SO(3)$ by spherical harmonics, the corresponding angular momentum algebra and quantum numbers, developed from raising and lowering operators, you have already seen it at work. How strong symmetry classifications are, can be demonstrated by the fact that the form of a free particle Lagrangian density is almost completely determined by the constraint of relativistic Lorentz invariance. Usually this is presented under the label of classical field theory but it holds true as well for the Lagrangian density of quantum field theoretic generating functionals. No correspondence principle or quantization procedure has to be defined in order to see the importance of symmetry constraints in relativistic quantum field theory. We give some hints how to proceed and summarize some of the findings. A compact and insightful discussion is presented in [5] and a deep and self contained discussion is presented in [3].

For concreteness we use four vector notation. An event is characterized by four coordinates x^μ for $\mu = 0, 1, 2, 3$, where (x^1, x^2, x^3) are the spatial coordinates and $x^0 = t$ is the time coordinate. For small deviations $\mathrm{d}x^\mu$ the spatial deviations give rise to a distance $\mathrm{d}x$ in a (locally) Euclidean manner: $\mathrm{d}\boldsymbol{x} = (\mathrm{d}x^1, \mathrm{d}x^2, \mathrm{d}x^3)$ with $(\mathrm{d}x)^2 = \mathrm{d}\boldsymbol{x} \cdot \mathrm{d}\boldsymbol{x}$. While events as such are absolute, their coordinates depend on a spatial and temporal reference frame. Using the same metric units in all reference frames a fundamental observational law states: for two events with infinitesimal deviation, which happen at the same location $\mathrm{d}\boldsymbol{x'} = \mathbf{0}$ in a certain reference frame, there is a **proper time** $\mathrm{d}\tau$ that does not depend on the reference frame and equals the time $\mathrm{d}t'$ in the reference frame with $\mathrm{d}\boldsymbol{x'} = \mathbf{0}$ (like a clock in a co-moving reference frame). In any other reference frame the invariant proper time can be calculated as

$$(\mathrm{d}\tau)^2 = \sum_{\mu\nu} g_{\nu\mu} \mathrm{d}x^\mu \mathrm{d}x^\nu =: \sum_\nu \mathrm{d}x_\nu \mathrm{d}x^\nu \tag{6.17}$$

where $g_{\mu\nu}$ is a pseudo-Euclidean (local) metric which by itself has to be determined by equations of motion (e.g. Einstein's equation of gravitation). When the local gravitational interaction can be neglected the metric reduces to the Minkowski metric $g = \eta$ for all non-accelerated reference frames and one finds

$$(\mathrm{d}\tau)^2 = (\mathrm{d}t)^2 - c^2 (\mathrm{d}\boldsymbol{x})^2, \tag{6.18}$$

where c is a universal constant with the dimension of a velocity. It is convenient to use units in which $c = 1$. In these units the Minkowski metric can be written as,

$$\eta = \mathrm{diag}(1, -1, -1, -1). \tag{6.19}$$

The symmetry transformations on $\mathrm{d}x^\mu$ that leave the pseudo scalar product $\sum_\nu \mathrm{d}x_\nu \mathrm{d}x^\nu$ invariant form the group of Poincare transformations, also called inhomogeneous Lorentz transformations. They contain translations and homogeneous Lorentz transformations which consist of rotations in space and Lorentz boosts. Lorentz boosts describe the transformation between reference frames with relative constant velocities $\boldsymbol{v}$. In addition, there are some discrete transformations like reflection and time reversal. A Lorentz boost in x^1 direction which doesn't alter x^2 and x^3 can be written as

$$(x')^1 = \gamma(v)(x^1 - vx^0),\ (x')^0 = \gamma(v)(x^0 - vx^1),\ \gamma(v)^{-2} = 1 - v^2. \tag{6.20}$$

Other four component quantities a^μ which give rise to similar **Lorentz invariants** $\sum_\nu a_\nu a^\nu$ like $\sum_\nu \mathrm{d}x_\nu \mathrm{d}x^\nu$ for $\mathrm{d}x^\mu$ are called four vectors of Minkowski space. The generators of translation in time and space (energy and momentum) can be combined to a four vector

$$\partial_\mu = (\partial_t, \partial_{\boldsymbol{x}}), \tag{6.21}$$

since the duality $\sum_\mu \partial_\mu x^\mu = 4$ holds. For free particles there must be common eigenvalues of energy and momentum $(\omega, \boldsymbol{k})$ and the four vector character yields

$$\omega^2 - \boldsymbol{k}^2 = m^2, \tag{6.22}$$

where m is an invariant called the **rest mass** of the particle. Thus, the free particle motion in a Lorentz invariant dynamics defines the property of inertia. For small k^2 compared to m^2 the energy approximates to

$$\omega = m + \frac{k^2}{2m} \tag{6.23}$$

which is the Galilei form of energy for free particles (up to a constant energy due to the rest mass). For particles of zero rest mass (like photons) the invariance of (6.22) gives rise to the Doppler formula for the frequency shift between reference frames moving with relative velocity v.

Another example of a four vector is the combination of charge and current density $j^\mu = (\varrho, \boldsymbol{j})$. An invariant is the continuity equation

$$\sum_\mu \partial_\mu j^\mu = 0 = \dot{\varrho} + \partial_{\boldsymbol{x}} \cdot \boldsymbol{j}. \tag{6.24}$$

Note, the charge density ϱ alone is not an invariant under Lorentz boosts.

Representing the Poincare group on field configurations we know the translation part is generated by ∂_μ and rotations are represented on finite dimensional irreducible spaces characterized by angular momentum quantum numbers $0, 1/2, 1, \ldots$. They are now called spin, because they do not relate to the orbiting of an object around some fixed center in space. The spin of a free particle and its rest mass are invariants and the energy momentum relation (6.22) as a relation between translations in time and space dictates the possible invariant actions (up to prefactor conventions and gauge freedoms in the Lagrangian), which we summarize for the two cases we need later. A spin 0 particle of rest mass m is described by a (complex) scalar field $\phi(x)$ and the Lagrangian is the **Klein-Gordon** Lagrangian

$$\mathcal{L} = \sum_{\mu} \left(\partial_\mu \phi^*(x)\right) (\partial^\mu \phi(x)) - m^2 \phi^*(x)\phi(x). \tag{6.25}$$

A spin 1 and massless particle like the photon is described by a vector field A^μ with a so-called gauge freedom,[6] such that the Lagrangian is expressed in terms of a tensor[7] $F^{\mu\nu} := \partial^\mu A^\nu - \partial^\nu A^\mu$,

$$\mathcal{L} = \frac{-1}{4} \sum_{\mu\nu} F_{\mu\nu} F^{\mu\nu}. \tag{6.26}$$

Identifying A^μ with the electromagnetic vector potential, $\mathcal{L} = \frac{1}{2}\left(E^2 - B^2\right)$ with $\boldsymbol{E}, \boldsymbol{B}$ the electric and magnetic fields, respectively. A spin 1/2 particle with mass m is represented by a spinor field (it is convenient to use 4 components) and its Lagrangian is the Dirac Lagrangian which we will not write down explicitly, because we will not use it.

6.3 Noether-, Ward- and Goldstone-Theorems

The essence of Emmy Noether's glorious theorem (derived originally in the context of deterministic Lagrangian mechanics) can be seen most clearly on an operator level valid in any dynamical theory. Consider the action of the symmetry group on the dynamical generator H

$$\pi^{-1}(g_\alpha) H \pi(g_\alpha) = H(\alpha), \tag{6.27}$$

which yields for the generators X

$$\boxed{\partial_\alpha H(\alpha) = i\,[X, H] = -i\,[H, X] = -\partial_t X(t)}. \tag{6.28}$$

Thus, as soon as the dynamics is invariant under the group, the generators are **constants of motion**. In the context of inner symmetries the generators X multiplied by

[6]One can put a constraint on the components of A^μ because the spin has only two transversal polarization degrees of freedom. This is caused by the vanishing mass, such that the particles travel at maximum possible speed c and components of spin in the moving direction are void.

[7]Tensor means that it transforms under the group like the product $\mathrm{d}x^\mu \mathrm{d}x^\nu$ does.

a convenient unit q are often called **charge operators**. In field theories one would like to round out global conserved charges with local current densities and charge densities fulfilling a continuity equation. Here we follow the modern text of [6], Chap. 5, together with [7], Chap. 2.4.

On the level of deterministic stationary action solutions the construction of local currents can be defined in the following way. For a given local linear transformation (x stands short for $x^\mu = (t, \boldsymbol{x})$ as event coordinates in Minkowski space—or for $\boldsymbol{x}$ as point coordinate in Euclidean space)

$$\delta_{\alpha(x)}\phi(x) = -i\alpha(x)F(\phi, \partial_\mu\phi) \tag{6.29}$$

the Lagrangian density changes as

$$\begin{aligned}\delta_{\alpha(x)}\mathcal{L} = &\frac{\partial\mathcal{L}}{\partial\phi}\left(-i\alpha(x)F(\phi, \partial_\mu\phi)\right)\\ &+\sum_\mu \frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\phi\right)}\left(\partial_\mu\left(-i\alpha(x)F(\phi, \partial_\mu\phi)\right)\right).\end{aligned} \tag{6.30}$$

For stationary action solutions the Euler Lagrange equations (5.117) allow to rewrite the change as

$$\begin{aligned}\delta_{\alpha(x)}\mathcal{L} = &\sum_\mu\left[\partial_\mu\frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\phi\right)}\right]\left(-i\alpha(x)F(\phi, \partial_\mu\phi)\right) +\\ &+\frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\phi\right)}\left(\partial_\mu\left(-i\alpha(x)F(\phi, \partial_\mu\phi)\right)\right).\end{aligned} \tag{6.31}$$

One can see by partial integration and vanishing boundary conditions that indeed the action is stationary, but here we like to identify the local current density. By defining it as

$$j^\mu(x) := -iF(\phi, \partial_\mu\phi)\frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\phi\right)} \tag{6.32}$$

one can rewrite the change in (6.31) as

$$\delta_{\alpha(x)}\mathcal{L} = \sum_\mu j^\mu(x)\partial_\mu\alpha(x) + \alpha(x)\partial_\mu j^\mu(x). \tag{6.33}$$

From here we can read off a generalized current definition, which can be useful even when it is not conserved:

$$j^\mu(x) = \frac{\partial\left(\delta_{\alpha(x)}\mathcal{L}\right)}{\partial\left(\partial_\mu\alpha(x)\right)}. \tag{6.34}$$

Therefore, we can conclude Noether's theorem for stationary action field configurations. If the action is invariant under a global continuous group, $\delta_\alpha S = 0$ and $\partial_\mu \alpha(x) = 0$, then for stationary action field configurations the current density of (6.34) obeys a continuity equation, $\sum_\mu \partial_\mu j^\mu = 0$.

To see the current identification (6.34) at work, we consider the $U(1)$ invariant Lagrangian for a complex Boson field $\phi(x)$ in the presence of some potential V:

$$\mathcal{L} = \sum_\mu \left(\partial_\mu \phi\right)^* (\partial^\mu \phi) - V(|\phi|). \tag{6.35}$$

The field changes are

$$\delta\phi = -i\alpha(x)\phi;\ \ \delta\phi^* = i\alpha(x)\phi^*, \tag{6.36}$$

$$\delta\partial_\mu \Phi = -i\partial_\mu(\alpha(x)\phi);\ \delta\partial_\mu \Phi^* = i\partial_\mu(\alpha(x)\phi^*). \tag{6.37}$$

The resulting change of the Lagrangian allows to identify the current as

$$j^\mu(x) = \frac{\partial\left(\delta_{\alpha(x)}\mathcal{L}\right)}{\partial\left(\partial_\mu \alpha(x)\right)} = i\left[\phi(x)^*(\partial^\mu \phi(x)) - \phi^*(x)(\partial^\mu \phi(x))\right]. \tag{6.38}$$

The current identification can be generalized to the complete theory in terms of the path integral by noticing that a symmetry—in general—means that the **combination of action and measure** is an invariant under a global symmetry transformation,

$$D\phi' e^{iS[\phi']} = D\phi e^{iS[\phi]}. \tag{6.39}$$

Making this transformation local allows to identify the current as field within the path integral via

$$\boxed{D\phi' e^{iS[\phi']} = D\phi e^{iS[\phi]}\left(1 + \int dx \sum_\mu (\partial_\mu \alpha(x))\, j^\mu(x)\right)}. \tag{6.40}$$

Note, that the current may contain contributions from a change of the measure as well. Equation (6.40) is the most general way to define a symmetry related current density in quantum theory via functional integration. The current density $j^\mu(x)$ corresponding to a continuous symmetry group is identified as the dual field to the gradient of the parameter field $\partial_\mu \alpha(x)$. On performing a partial integration one can conclude the continuity equation for global symmetries,

$$\sum_\mu \partial_\mu \langle j^\mu(x)\rangle = 0. \tag{6.41}$$

If the path integral is invariant under a global group action ($\partial_\mu \alpha(x) = 0$), then the current density of (6.40) obeys a continuity equation on average. This can be generalized to constraints for correlation functions, known as Ward identities or anomalous Ward identities (when measure changes are involved). For details see Chap. 5 in [6].

Now, we have a look at the ground state (vacuum) of a system with a dynamic symmetry generated by a charge operator Q with corresponding local current density operator $j^\mu(x)$, such that $Q = \int \mathrm{d}^3x\, \varrho(x)$, as usual. We assume that it commutes with the four momentum P^μ $(H, -i\partial_{\boldsymbol{x}})$. The vacuum state is assumed to be a state of zero energy and momentum.

Then a theorem known as Fabri-Picasso theorem (see [7]) tells: either the charge operator annihilates the vacuum or its action on the vacuum is not normalizable. In the first case the symmetry of the vacuum is manifest (since it is not changed), but in the second case it is unconventional. The symmetry is said to be realized in the Nambu-Goldstone way. To prove the theorem one considers

$$\langle 0 \mid QQ \mid 0\rangle = \int \mathrm{d}^3x\ \langle 0|\varrho(x)Q|0\rangle\,. \tag{6.42}$$

Since the vacuum is translation invariant the integrand is a constant. Either it is zero or it is finite. In the first case Q annihilates the vacuum, in the second case it can not be normalizable, since the integral diverges.

As a next step in investigating the Nambu Goldstone vacuum we make a further reasonable assumption in view of our definition of spontaneous symmetry breaking. We assume that there is some field operator $\Phi(x)$ which is not invariant under the action of Q,

$$\Phi'(x) = -i[Q, \Phi(x)], \tag{6.43}$$

and which has -even under the action of Q-a finite expectation value in the vacuum

$$\left\langle 0|\Phi'(x)|0\right\rangle \neq 0. \tag{6.44}$$

If the continuous symmetry is realized in the Nambu Goldstone way, there exist **soft modes** in the system above the ground state. We will proof this famous Goldstone theorem for a situation with spontaneous symmetry breaking after explaining its meaning. Soft modes are states which momentum goes to zero (long wavelengths) when the energy goes to zero: $k \to 0$ for $\omega \to 0$. In other words: the frequency momentum dispersion relation $\omega(k)$ is some positive power for low momenta (long wavelengths). Such states are also called **massless** particles, since a mass term in field theories corresponds to short ranged excitations even for low energies. This can be seen as follows. A relativistic field equation for a free particle of mass m reads in frequency momentum notation

$$\omega^2(k)\phi(\omega, k) = [k^2 + m^2]\phi(\omega, k), \tag{6.45}$$

which yields the dispersion relation

$$\omega(k) = \sqrt{k^2 + m^2}. \tag{6.46}$$

On the other hand, a static excitation ϕ_k from a δ-point source has to fulfill in Fourier terms the condition

$$[k^2 + m^2]\phi_k = 1, \tag{6.47}$$

such that it coincides (up to a constant factor) with the Fourier transform of a r_0-ranged Yukawa potential $V(r) = (e^{-r/r_0})/r$,

$$\phi_k = V_k = 1/[k^2 + (1/r_0)^2], \tag{6.48}$$

when we identify mass and inverse range

$$m = 1/r_0. \tag{6.49}$$

For mass going to zero or range going to infinity, we get the infinite range Coulomb potential and a dispersion $\omega \sim |k|$.

The proof of the Goldstone theorem considers

$$\left\langle 0|\Phi'(x)|0\right\rangle = \left\langle \int \mathrm{d}^3x' \, [\varrho(x'), \Phi(x)] \right\rangle_0 . \tag{6.50}$$

With the help of the continuity equation one can show that the expression does not depend on time t'. Introducing eigenstates of the four-momentum $P\,|n\rangle = p_n\,|n\rangle$, translating x' to 0 and performing the integration one can write (6.50) as

$$\begin{aligned} \left\langle 0|\Phi'(x)|0\right\rangle = \sum_n \delta^3(\boldsymbol{p}_n) \big[&\langle 0|\varrho(0)|n\rangle \, \langle n|\Phi(x)|0\rangle \, e^{i\omega_n t'} \\ &- \langle 0|\Phi(x)|n\rangle \, \langle n|\varrho(0)|0\rangle \, e^{-i\omega_n t'} \big]. \end{aligned} \tag{6.51}$$

That this expression is non-vanishing and independent of t' can only happen for finite matrix elements $\langle 0|\Phi(x)|n\rangle \, \langle n|\varrho(0)|0\rangle$, when the frequency ω_n tends to zero as the momentum $\boldsymbol{p}_n$ does (by the delta function).

As two qualitative examples for the Goldstone theorem let us have a look at the fluid condensation to a crystal and at ferromagnetism. Both, in the fluid and in the crystalline phases the dynamics of particles is translational invariant under the full translation group, as the forces are two-body potential forces with potential type $V(\boldsymbol{x}_i - \boldsymbol{x}_k)$. When the fluid becomes a crystal, the ground state's symmetry is broken to a discrete crystal group. However, there are soft mode excitations, the acoustic phonon excitations with long wavelengths for small frequencies. Both, in the ferromagnetic phase as well as in the paramagnetic phase, the dynamics of spins becomes rotational invariant, $H = \sum_{<kl>} J_{kl} \boldsymbol{S}_k \cdot \boldsymbol{S}_l + \sum_k \boldsymbol{h} \cdot \boldsymbol{S}_k$, when the magnetic field h is switched off. However, in the ferromagnetic phase the ground state is not invariant but singles out a spontaneous direction. There are soft modes in the system, the magnons (also called spin waves) with long wavelengths for small frequencies.

The most general way to discuss spontaneous symmetry breaking with generating functionals is by considering the effective action, since it can also incorporate symmetry breaking that occurs after quantum fluctuations have been taken into account. On the level of an effective action $\Gamma[\varphi]$ a spontaneously broken symmetry corresponds to an **effective potential** as described by c) in Fig. 6.1.

Let us consider a relative of the Landau model (5.126), the following φ^4 model for complex φ,

$$\boxed{\Gamma[\varphi] = \int dx \left[\sum_{\mu} \left(\partial_\mu \varphi\right) \left(\partial^\mu \varphi^*\right) + V(\varphi) \right]}. \tag{6.52}$$

Here the Landau potential is

$$V(\varphi) = -\tau\alpha^2 |\varphi|^2 + \frac{\lambda}{4} |\varphi|^4 \tag{6.53}$$

with positive parameters α^2 and λ and a tuning parameter τ that can be varied from positive values to negative values. As long as τ stays positive the homogeneous stationary state of the effective action is given by

$$M := |\varphi_0| = \sqrt{\frac{2\tau\alpha^2}{\lambda}}. \tag{6.54}$$

This is an appropriate order parameter for the symmetry breaking. It vanishes smoothly as τ is going to zero and stays zero in the disordered phase, $\tau < 0$. To study fluctuations around the stationary solution we take advantage of the factor space G/H which is still $U(1)$ in this case and write the field with small real valued deviations η and θ from the stationary solution

$$\varphi = e^{i\theta}(M + \eta). \tag{6.55}$$

Expanding the effective action up to second order in the deviations leads to

$$\begin{aligned} \Gamma[\eta, \theta] = \int \mathrm{d}x \; V(M) + \Bigg[\sum_{\mu} \big\{ M^2 (\partial_\mu \theta)(\partial^\mu \theta) \; + \\ + \; (\partial_\mu \eta)(\partial^\mu \eta) \big\} + 2\tau\alpha^2 \eta^2 \Bigg]. \end{aligned} \tag{6.56}$$

This effective action of fluctuations around the broken ground state clearly demonstrates:

1. The excitation η is massive (short ranged) due to the curvature $4\tau\alpha^2$ at the symmetry broken mimima.
2. The excitation θ establishes the hidden symmetry by going along different possible minima. It is massless, as no term proportional to θ^2 appears in the effective action.

This model is actually a reasonable phenomenological model for the thermodynamics of a superconductor/superfluid with order parameter field φ representing the macroscopic complex wave function of Cooper pairs/superfluid bosons. The effective potential of this φ^4 model is of the same Landau type potential that we discussed already for continuous phase transitions in terms of order parameters and effective potentials in Sect. 5.6. The parameter $\tau = T_c - T$ corresponds to the deviation of temperature below the critical temperature T_c, as depicted in Fig. 5.4. The order parameter is the density of Cooper pairs/superfluid bosons below the transition temperature. The Goldstone modes are soft sound modes in the superfluid.

6.4 The Gauge Principle

A special form of symmetries are the so-called gauge symmetries because they allow to introduce an interaction between the original configuration variables (fields) and a Boson field which ensures the symmetry of the dynamics. As a reference we recommend [1, 7]. The interaction is usually long ranged, but—as we will see—can be effectively short ranged in the situation of spontaneously broken symmetries. The idea behind gauge symmetries is geometric: a symmetry group G that normally acts on the internal degrees of freedom of the field ϕ,

$$\phi'(x) = g\phi(x), \tag{6.57}$$

is made local by gauging the unit element at every value of the external space x in a slightly different way,

$$\phi'(x) = g(x)\phi(x). \tag{6.58}$$

The different choices of gauge are incorporated in a so-called **connection** or **gauge potential field** $A(x)$ which re-gauges the translation operator ∂_μ to a gauge-covariant translation operator. A change of gauge is compensated by a change of the gauge potential. For unitary representations the equations read

$$\phi'(x) = e^{-i\sum_a \alpha^a(x) X_a}\phi(x), \tag{6.59}$$

where X_a are the hermitian generators of the gauge group and $\alpha^a(x)$ the corresponding local parameters of re-gauging. Since it is not assumed that the generators commute one has in linear order of α^a,

$$g(x)X_a g^{-1}(x) = X_a - i\sum_b \alpha^b[X_b, X_a] = \sum_{bc}\alpha^b C^c_{ba}X_c, \tag{6.60}$$

where C^c_{ab} are the Lie algebra structure constants, as before. The gauge-covariant translation operator for fields $\phi(x)$ is defined as (for concreteness in four-vector notation)

$$\boxed{D_\mu := \partial_\mu + iqA_\mu(x)}, \tag{6.61}$$

where q is a free coupling constant, called **charge** and $A_\mu(x)$ is the gauge potential. It takes values in the Lie algebra of the generators and can be represented as

$$A_\mu = \sum_a \mathrm{A}^a_\mu X_a. \tag{6.62}$$

In the combination $qX_a = Q_a$ the generators are also called charge operators, as mentioned earlier. The gauge potential transforms under the local action of G in a definite way to make the procedure consistent,

$$D'_\mu = \partial_\mu + iqA'_\mu(x) = g(x)D_\mu g^{-1}(x), \tag{6.63}$$

which leads to the transformation law

$$\sum_a (A')^a_\mu X_a = \sum_a \left[A^a_\mu X_a + \frac{1}{q}(\partial_\mu\alpha^a(x))X_a + \sum_{bc}\alpha^b C^c_{ba}X_c\right] \tag{6.64}$$

and for A' alone to

$$\boxed{(A')^a_\mu = A^a_\mu + \frac{1}{q}(\partial_\mu\alpha^a(x)) + \sum_{bc}\alpha^b C^a_{bc}A^c_\mu}. \tag{6.65}$$

For the Abelian group $U(1)$ there is only one component, $X = 1$, $C = 0$, and the third term in (6.65) vanishes.

As a consequence of the local gauge transformation, terms of the form

$$[\partial_\mu\phi(x)]' = \partial_\mu(g(x)\phi(x)) \tag{6.66}$$

cannot be combined to invariants $[\partial_x\phi(x)]'[\partial_x\phi(x)]'^*$. However, on replacing the translation with the gauge-covariant translation of (6.63) one finds

$$\boxed{D'_\mu\phi'(x) = [D_\mu\phi(x)]' = g(x)D_\mu\phi(x)}. \tag{6.67}$$

This can be easily combined to invariants

$$[D'_\mu \phi'(x)][D'^\mu \phi'(x)]^* = [D_\mu \phi(x)][D^\mu \phi(x)]^*. \tag{6.68}$$

It is also important to know that the identification by (6.34) of current (in unit of charges q) generalizes in the presence of gauge fields simply to

$$\boxed{j^{a\mu}(x) = -\frac{\partial \mathcal{L}}{\partial A^a_\mu}}. \tag{6.69}$$

Note, that here no change of integration measure is included. This can be cured by considering the full change of the measure and the action: the current density $j^\mu(x)$ corresponding to a continuous symmetry group is identified as (minus) the dual field to the corresponding gauge potential $A_\mu(x)$.

In geometrically invariant notation the gauge potential corresponds to a 1-form $A = \sum_\mu A_\mu dx^\mu$. Its exterior covariant derivative $F = DA = dA + iqA \wedge A$ is the curvature 2-form (it measures differences in parallel transport along closed paths) and is in physics denoted as **field strength tensor**. It reads explicitly

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + q \sum_{cb} C^a_{cb} A^c_\mu A^b_\nu. \tag{6.70}$$

Its action on a field $\phi(x)$ can be written in covariant form as

$$\sum_a F^a_{\mu\nu} X_a \phi = (D_\mu D_\nu - D_\nu D_\nu)\phi. \tag{6.71}$$

The free dynamics of the gauge field is captured in a Lagrangian density

$$\mathcal{L}_A = -\frac{1}{4} \sum_{\mu\nu a} F^a_{\mu\nu} F^{a\mu\nu}. \tag{6.72}$$

Again this choice is (up to the prefactor) dictated by symmetry. The free deterministic field equations are $\delta \mathcal{L}_A = 0$ yielding

$$\sum_\mu \mathrm{d}_\mu F^{a\mu\nu} = 0, \tag{6.73}$$

where the covariant derivative on the level of the field strengths is

$$\mathrm{d}_\lambda F^{a\mu\nu} := \partial_\lambda F^{a\mu\nu} + q \sum_{bc} C^a_{bc} A^c_\lambda F^{b\mu\nu} \tag{6.74}$$

The field equations (6.73) show (1) that free gauge bosons are always massless, because all terms involve derivatives of A and no term proportional A^2 appears. This is necessary to guarantee gauge invariance. They show (2) that the free field is self-interacting since the covariant derivative acting on derivatives of A contains a factor of A in the non Abelian situation (finite structure constants). In other words: non Abelian gauge fields are charged and self interacting. However, in the Abelian U(1) gauge theory the structure constants vanish and the U(1) gauge field is not charged and thus not self interacting. Equation (6.73) simplifies in the U(1) situation to

$$\sum_{\mu} \partial_{\mu} F^{\mu\nu} = 0 \tag{6.75}$$

Taking $A^{\mu} = (V, \boldsymbol{A})$ and $\boldsymbol{E} = \dot{\boldsymbol{A}} - \partial_{\boldsymbol{x}} V$ and $\boldsymbol{B} = \partial_{\boldsymbol{x}} \times \boldsymbol{A}$ one finds from (6.75) exactly the free of charge and current Maxwell equations for the fields $\boldsymbol{E}$ and $\boldsymbol{B}$

$$\partial_{\boldsymbol{x}} \cdot \boldsymbol{E} = \partial_{\boldsymbol{x}} \cdot \boldsymbol{B} = 0, \tag{6.76}$$

$$\partial_{\boldsymbol{x}} \times \boldsymbol{E} = -\dot{\boldsymbol{B}}, \tag{6.77}$$

$$\partial_{\boldsymbol{x}} \times \boldsymbol{B} = \dot{\boldsymbol{E}}. \tag{6.78}$$

Because of (6.69) A^{μ} also couples to the matter field in the same way as electromagnetic fields. Thus, the **U(1) gauge theory** can be identified with electromagnetic quantum field theory.

The standard model of elementary particle physics treats the strong quark interactions as a SU(3) gauge theory and the unification of electromagnetism and weak interactions as a SU(2) $\times$ U(1) gauge theory. The gravitational force can also be written as a gauge theory involving gauges for the Poincare group. It is not impossible that physicists might find a grand unified gauge theory in the near future capturing the four fundamental forces. It is likely that supersymmetry (a theory symmetric in bosons and fermions) will be an ingredient, too. There are calculation reasons for that and observational puzzles like dark matter which might be solvable along supersymmetry.

6.5 Anderson-Higgs Mechanism

Now, we combine the gauge symmetry of electromagnetism with the φ^4 model of spontaneous symmetry breaking. As an application think of a superconductor in a magnetic field. Since we have gauge covariant expressions it is easy to set up a gauge invariant effective action corresponding to the model (6.52) including U(1) electromagnetism,

$$\boxed{\Gamma[\varphi; A_\mu] = \int dx \left[\sum_\mu \left(D_\mu\varphi\right)\left(D^\mu\varphi^*\right) + V(\varphi) - \frac{1}{4}\sum_{\mu\nu} F_{\mu\nu}F^{\mu\nu} \right]}. \tag{6.79}$$

Note, in the superconductor case the elementary charge must be $q = -2e$. Again, we consider the stationary state with respect to φ and A_μ, where the latter is vanishing. Now we look for fluctuations around the stationary solution

$$\varphi(x) = e^{i\theta(x)}(M + \eta(x)), \;\; A_\mu(x) \tag{6.80}$$

and exploit the fact that we can re-gauge $A_\mu(x)$ in such a way as to eliminate the Goldstone mode $\theta(x)$

$$A'_\mu(x) = A_\mu(x) + \frac{1}{2e}\partial_\mu(\theta(x)). \tag{6.81}$$

Expanding the action again to second order in the remaining fields one arrives at

$$\Gamma[\eta, A_\mu] = \int dx \left[\sum_\mu \left(\boxed{4e^2M^2A_\mu A^\mu} + (\partial_\mu\eta)(\partial^\mu\eta) \right) + 2\tau\alpha^2\eta^2 + V(M) \right.$$
$$\left. -\tfrac{1}{4}\sum_{\mu\nu} F_{\mu\nu}F^{\mu\nu} \right]. \tag{6.82}$$

Something very interesting has happened. The former massless gauge field has **acquired a mass** m proportional to the ground-state value M of the order parameter in the spontaneously broken phase while the Goldstone mode disappeared. This mechanism is known as Anderson-Higgs mechanism and has at least two prominent applications with experimental evidence. In the model here it describes the Meissner-Ochsenfeld effect of a finite penetration width of a magnetic field into the superconductor (an uncharged superfluid cannot undergo the Anderson-Higgs mechanism) and the stationary point equation of motion for $\boldsymbol{A}$ is the London equation for superconductors, $(\partial_{\boldsymbol{x}})^2\boldsymbol{A} = \text{const.} \cdot e^2M^2\boldsymbol{A}$. In a model with non Abelian gauge group U(1) $\times$ SU(2) for fermion fields (Salam-Weinberg model) it describes the presence of massive gauge particles of the weak interaction (W and Z Bosons) and the presence of a massive particle, the famous Higgs Boson, described by the scalar field η with a mass term proportional to $\sqrt{\tau}\alpha$ in our simplified model.

It is believed, that a Anderson-Higgs mechanism is at work to make elementary particles massive and that spontaneous symmetry breaking is responsible for the low energy symmetry groups that we observe nowadays in particle physics. According to standard models of modern cosmology spontaneous symmetry breaking may have occurred in the earliest very hot phases of our universe. One can fairly say that theories about symmetry, its breaking and gauging are one of the most important contributions to physics by the late 20th and beginning 21st century.

6.6 Exercises

Exercise 1: Spontaneous Symmetry Breaking
Find examples for spontaneous symmetry breaking in nature: for single particle systems, equilibrium and self organizing systems far from equilibrium.

Exercise 2: Current Identification in Global U(1) Invariant Cases
Calculate the expression in terms of fields and perhaps their derivatives for the current density $j^{\mu}(x)$ for the U(1) global invariant Lagrange densities of a complex spin 0 boson (Klein Gordon Lagrange density) and for an electron (Dirac Lagrange density) by (6.34).

Exercise 3: Current identification in Local U(1) Invariant Cases
Calculate the current density $j^{\mu}(x)$ in terms of fields and perhaps their derivatives for the U(1) local invariant Lagrange densities of a complex spin 0 boson (Klein Gordon Lagrange density with covariant derivatives) by (6.69).

Exercise 4: Stationary Field Equations in Local U(1) Invariant Cases
Derive the full set of field equations for a U(1) local invariant Lagrange density of a complex spin 0 boson in the presence of electromagnetic fields (Klein Gordon Lagrange density with covariant derivative and free field strength action).

References

1. T.P. Cheng, L.-F. Li, *Gauge Theory of Elementary Particles* (Clarendon Press, Oxford, 1984)
2. F.W. Hehl, *Gauge Theory of Gravity and Spacetime*, arXiv: 1204.3672v2, 2014
3. S. Weinberg, *The Quantum Theory of Fields I* (Cambridge University Press, Cambridge, 1996)
4. W. Fulton, J. Harris, *Representation Theory: A first course*, Corr. edn. (Springer, 1999)
5. J. Chalker, A. Lukas, *Lecture Notes on M. Phys Option in Theoretical Physics: C6* (Oxford University, Oxford, 2011)
6. D. Skinner, *Quantum Field Theory II, Lecture Notes* (Cambridge University, Cambridge, 2015)
7. I.J.R. Aitchison, *An Informal Introduction to Gauge Field Theories* (Cambridge University Press, Cambridge, 1982)

Chapter 7
Topology

Abstract Topology addresses local and global neighborhood aspects of sets. Consider the mapping from $\mathbf{R}$ to a circle $\mathbf{S^1}$ where each real number t is mapped to e^{it}. By this mapping many formerly distinct real numbers $t + 2\pi\mathbf{Z}$ become identical points on the circle. Continuous deformations may change metric aspects of sets but leave topological aspects invariant. Continuous mappings are therefore the homomorphisms of topology. Global aspects of topology are of special interest in physics when quantities become discrete (quantized) for topological reasons and thus distinguished classes of these quantities exist or/and when (discrete) topological invariants like winding numbers (indexes) are represented as integrals that occur in the context of generating functionals. An obvious invariant in topological spaces is there topological dimension (=number of parameters to describe it locally). We start with three introductory examples and summarize some basics about topology before we discuss few of a bunch of known topological aspects with the integer quantum Hall effect (IQHE).

7.1 Kinks, Quantization and Magnetic Monopoles

Consider a rope on a corrugated iron sheet as sketched in Fig. 7.1. Shown are three different situations with 0, 1 and 2 kinks. By continuously deforming the paths one cannot get rid of the 1 kink situation. However, the 2 kink situation is actually a situation of kink and anti-kink, because it can be continuously deformed into a 0 kink situation. Thus the number of kinks with a grading of orientation is a topological invariant for a rope on a corrugated iron sheet. It resembles a situation in an instanton path integral description of tunneling (see e.g. Chap. 3 in [1] and our discussion in Sect. 8.1) between symmetric potential minima.

As a second example consider the wave equation in 1D for a field $\phi(x,t)$

$$\left[\partial_t^2 - c^2\partial_x^2\right]\phi(x,t) = 0. \tag{7.1}$$

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1_7

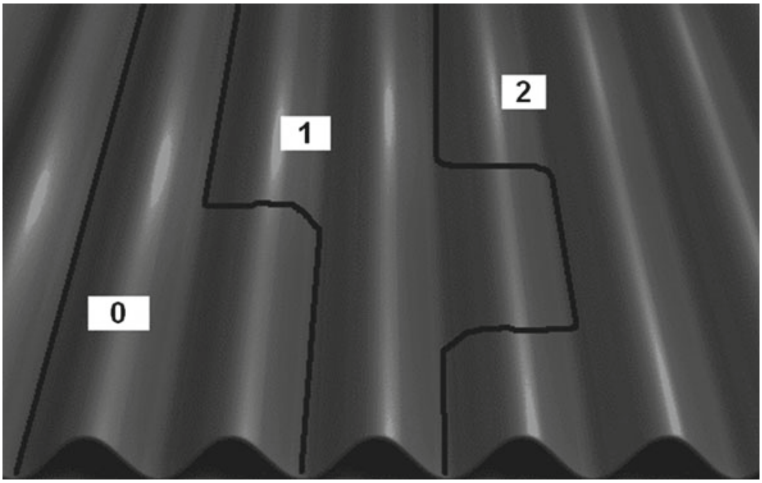


Fig. 7.1 A rope on a corrugated iron sheet for three different situations: 0, 1 and 2 kinks. The situation with 2 kinks (kink and anti-kink) can be continuously deformed to the 0 kink situation

As long as $\phi(x,t)$ is defined on the full 1D line $x \in \mathbf{R}$ one knows that there are infinitely many solutions. Actually, any differentiable functions $f(x-ct)$ and $g(x+ct)$ solve the equation and linear superpositions do it as well. Also, exploiting the translational invariance in time and space, a Fourier spectral representation

$$\phi(x,t) = \int \mathrm{d}k\, \mathrm{d}\omega\, e^{ikx-i\omega t} \tilde{\phi}(k,\omega) \tag{7.2}$$

solves the wave equation provided the dispersion relation

$$\omega^2(k) = c^2 k^2 \tag{7.3}$$

is fulfilled. However, as soon as we put the equation on a circle S^1, which means some periodic boundary conditions like

$$\phi(x=-L/2,t) = \phi(x=L/2,t), \tag{7.4}$$

the possible solutions are discretized and momentum k and energy ω become quantized with a quantum number $n \in \mathbf{Z}$,

$$\omega_n^2(k) = c^2 k_n^2;\; k_n = \frac{2\pi n}{L}. \tag{7.5}$$

Thus, the **topology** of $\mathbf{S^1}$ being characterized by winding numbers $n \in \mathbf{Z}$ has the consequence that some physical quantities living on $\mathbf{S^1}$ become quantized.

As a third example we have a look at Dirac's monopole (we follow the presentation in [2]). A magnetic monopole of strength g sitting at the origin $\boldsymbol{r} = (x, y, z) = \mathbf{0}$ should fulfill

$$\partial_{\boldsymbol{r}} \cdot \boldsymbol{B}(\boldsymbol{r}) = 4\pi g \delta(\boldsymbol{r}). \tag{7.6}$$

The solution is—as we know from electrostatics

$$\boldsymbol{B}(\boldsymbol{r}) = g\frac{\hat{r}}{r^2}, \tag{7.7}$$

where $\hat{r} = \boldsymbol{r}/r$. This field is defined everywhere except at the origin. Its corresponding 2-form is

$$B = \boldsymbol{B} \cdot \mathrm{d}\boldsymbol{S} = g\mathrm{d}\Omega, \tag{7.8}$$

where $\mathrm{d}\Omega = \sin\theta \mathrm{d}\theta \mathrm{d}\phi$ is the solid angle 2-form, θ is the polar angle against the z axis and ϕ the azimuth angle in the x, y plane. Equation (7.8) with the Stokes-Gauss theorem shows that the monopole fulfills the desired Poisson equation. However, for magnetic fields we should have a vector potential $\boldsymbol{A}(\boldsymbol{r})$ and a corresponding 1 form

$$A = \boldsymbol{A}(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{r} \tag{7.9}$$

such that

$$B = \mathrm{d}A \; ; \; \boldsymbol{B}(\boldsymbol{r}) = \partial_{\boldsymbol{r}} \times \boldsymbol{A}(\boldsymbol{r}). \tag{7.10}$$

One can define such vector potential, but one cannot define it on the full space $\mathbf{R^3} - 0$. One must leave out a full ray. For example, one can define two vector potentials

$$A^{N,S} := \frac{g}{r(r \pm z)} - y\mathrm{d}x + x\mathrm{d}y \; ; \; \boldsymbol{A}^{N,S}(\boldsymbol{r}) = \frac{g(1 \mp \cos\theta)}{r \sin\theta}\hat{\phi}, \tag{7.11}$$

where $\hat{\phi} = (-\sin\phi, \cos(\phi), 0)$ is the unit vector along the ϕ coordinate. A^N is defined everywhere except at the negative z axis and A^S everywhere except at the positive z axis. Indeed, everywhere where $A^{N,S}$ are defined, they yield the monopole field by the curl,

$$\partial_{\boldsymbol{r}} \times \boldsymbol{A}^{N,S}(\boldsymbol{r}) = \boldsymbol{B}(\boldsymbol{r}) + \delta(x)\delta(y)\Theta(\mp z). \tag{7.12}$$

Interestingly, both vector potentials are related by a gauge transformation,

$$A^N - A^S = 2g\mathrm{d}\phi, \tag{7.13}$$

which is defined everywhere except at the poles $\theta = 0, \pi$. Along the equator it is well behaved and we can write the total flux Φ as a sum of flux through the north hemisphere and the south hemisphere and can express this via Stokes theorem by the pure gauge field $d\phi$,

$$\Phi = \int_N \mathrm{d}A^N + \int_S \mathrm{d}A^S = \int_{\partial N} 2g\mathrm{d}\phi = 2g \cdot 2\pi, \tag{7.14}$$

as it should be. It shows that, by restricting to appropriate maps, one can find vector potentials for magnetic monopoles. They cannot be defined everywhere, but they have a common region where a gauge transformation relates them. One has to be careful with applying Stokes theorem and check where the differential forms are defined. Once a magnetic monopole exists, one can consider an electron in its vicinity. Its wave function acquires a phase change for each winding around the monopole,

$$\delta\phi = 4eg\pi. \tag{7.15}$$

To keep its wave-function single valued, the phase must be an integer multiple of 2π and the **electric and magnetic charges are quantized**,

$$\boxed{eg = \mathbf{Z}/2}. \tag{7.16}$$

This theory suggests that the quantization of charge might be caused by topological quantization.

7.2 Sketch of Topological Vocabulary

Here we sketch some vocabulary which occurs frequently in the context of topology in physics and try to give some hints how it is used and how it may help. A good reference for physicists is [2]. The first notions of compact, connected and single-connected are exemplified in Fig. 7.2.

- A **compact** space M is closed and bounded. If it has an edge ∂M, the edge belongs to M. The important property is that every continuous function f into real numbers takes its maximum and minimum on M and its image $f(M)$ is compact, too. One can compactify spaces like the real numbers; e.g. in an affine way with two infinite points $\pm\infty$, or in a projective way with one infinite point ∞ where both negative and positive numbers meet. The projective compactification of $\mathbf{R}$ is topologically equivalent to a circle $\mathbf{S^1}$.
- A **connected** space M cannot be disassembled in several separated components. The important property is that every continuous function into discrete number spaces is constant. Sometimes the weaker notion of arc-connected is used, which means that every two points can be connected by a continuous path. Arc-connected spaces are connected and the inverse holds except for some interesting pathological exceptions which—as far as the author knows—have not yet popped up in physics.
- In a **single-connected** space M every closed loop can be continuously deformed to a point. If a space is not single-connected one usually finds some hole of appropriate dimensionality in M, such that certain closed loops wind around it and cannot be deformed to overcome it.

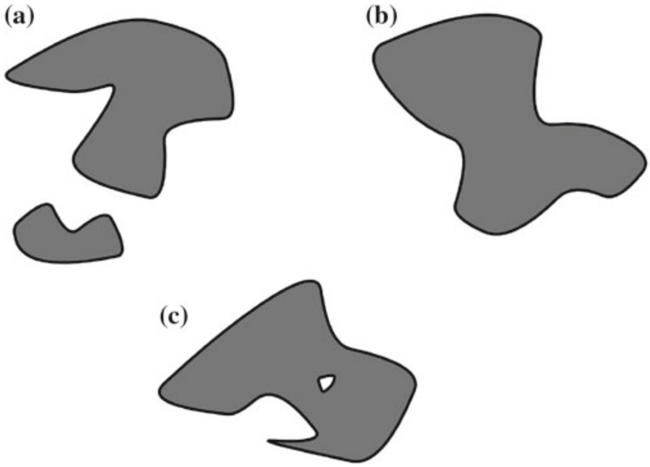
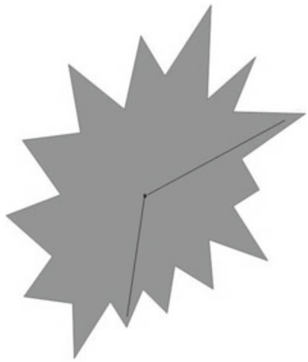


Fig. 7.2 Sketch of topological notions: **a** compact (bounded and closed with boundary) but disconnected, **b** compact and single connected (and of course connected), **c** compact and connected but not single connected (a path around the hole cannot be contracted within the space)

Fig. 7.3 Sketch of a star shaped space. From a certain point every other point can be reached by a straight line



There is a type of spaces, called **star shaped**, which are single-connected and have in addition a stronger property: there is one point from which every other point can be reached by a straight line within it (see Fig. 7.3 for an example). For such star shaped spaces a fundamental theorem holds, which is known as **Poincare's lemma**: On a star shaped space M every closed differential form ω (closed means $\mathrm{d}\omega = 0$) is exact (in physical terms: has a potential),

$$\boxed{\omega = \mathrm{d}\eta}. \tag{7.17}$$

If you are unfamiliar with forms you may consult [2], Chap. 5.4. You may also just consider forms as multilinear alternating differentials which represent little volumes like a determinant of coordinate differentials $\mathrm{d}x_k$ which like to be integrated over. The main rules are: $\mathrm{d}f(x) \wedge \mathrm{d}g(x) = \left(\sum_k \partial_k f \, \mathrm{d}x_k\right) \wedge \left(\sum_l \partial_l g \, \mathrm{d}x_l\right)$, $\mathrm{d}x_k \wedge \mathrm{d}x_l = -\mathrm{d}x_l \wedge \mathrm{d}x_k$ and for m-dimensional M: $\int_M f(x) \, \mathrm{d}x_1 \wedge \ldots \wedge \mathrm{d}x_m = \int_M f(x) \, \mathrm{d}x^m$. Applying the exterior differentiation d twice to a form nullifies it[1]:

$$\boxed{\mathrm{d}\mathrm{d}\omega = 0}. \tag{7.18}$$

The most beautiful theorem of calculus on manifolds, the general **Stoke's theorem**, reads in forms

$$\boxed{\int_M \mathrm{d}\omega = \int_{\partial M} \omega}. \tag{7.19}$$

It shows the dual relation between forms and manifolds and it shows a nice immediate topological property: Boundaries don't have boundaries, $\partial\partial M = 0$.

In mathematics one likes to find functors from one structure to another, hoping to deal with heavy problems easier after transformation. In algebraic topology one considers several such functors from topology to algebra. Two very important functors in physical contexts are given by group functors: homotopy groups Π_n and de-Rham cohomology groups H_n. The elements of the homotopy group Π_n over a manifold M are given by mappings from an n-sphere $\mathbf{S^n}$ to M, $f : \mathbf{S^n} \to M$. Two such mappings g, f are equivalent, $g \sim f$, if they can be continuously deformed into each other; they wrap the manifold similarly with an n-sphere. Π_1 is called the fundamental group. The most important example is

$$\Pi_1(\mathbf{S^1}) = \mathbf{Z}. \tag{7.20}$$

It means that the functions are equivalent as long as they have the same winding number $n \in \mathbf{Z}$. For a function with winding number n,

$$f_n(\phi) = e^{in\phi} \tag{7.21}$$

the winding number can be represented as an integral,

$$n = \frac{1}{2\pi i} \int_{\mathbf{S^1}} \mathrm{d}\phi \, f^{-1}(\partial_\phi f). \tag{7.22}$$

Note, the winding angle form $\mathrm{d}\phi$ may appear in disguised form, for example in 2D as

$$\mathrm{d}\phi = \frac{-y\mathrm{d}x + x\mathrm{d}y}{x^2 + y^2}. \tag{7.23}$$

[1]For example: $\mathrm{d}\mathrm{d}f(x, y) = \mathrm{d}\left[(\partial_x f)\mathrm{d}x + (\partial_y f)\mathrm{d}y\right] = (\partial^2_{xy} f)\mathrm{d}x \wedge \mathrm{d}y + (\partial^2_{yx} f)\mathrm{d}y \wedge \mathrm{d}x = 0.$

Some general results are:

$$\Pi_n(\mathbf{S^n}) = \mathbf{Z}, \tag{7.24}$$

$$\Pi_n(\mathbf{S^m}) = 0 \text{ for } n < m. \tag{7.25}$$

Since the group $U(1)$ is topologically equivalent to $SO(2)$ (its universal covering group in the terminology of Lie groups) and to a circle $\mathbf{S^1}$, the fundamental group (in the sense of algebraic topology) of $U(1)$, $SO(2)$ and $\mathbf{S^1}$ is the group of integer winding numbers $\mathbf{Z}$. The Lie group $SO(3)$ has $SU(2)$ as its universal covering group and $SU(2)$ is topologically equivalent to a 3-sphere $\mathbf{S^3}$, such that $SU(2)$ and $\mathbf{S^3}$ are single-connected ($\Pi_1 = 0$), but have integer wrapping numbers with respect to 3-spheres, $\Pi_3 = \mathbf{Z}$.

With de-Rham cohomology groups we come to differential forms which can, by Stokes theorem, tell something about the underlying topology. $H_k(M)$ is the group of all closed k-forms over the manifold M which form equivalence classes with respect to being identical up to a potential term

$$d\omega_1 = \mathrm{d}\omega_2 = 0 \tag{7.26}$$

$$\omega_1 \sim \omega_2 \ \text{ iff } \ \omega_1 = \omega_2 + \mathrm{d}\eta. \tag{7.27}$$

If all closed forms have potentials (are exact), then they are all equivalent, $\mathrm{d}\eta_1 = \mathrm{d}\eta_2 + \mathrm{d}(\eta_1 - \eta_2)$ and the group consists of one element, denoted as 0. Thus, on star-shaped manifolds M Poincare's lemma tells us: $H_k(M) = 0$ for all k up to the dimension of M. For single-connected manifolds 1-forms have potentials, thus $H_1(M) = 0$.

Important examples of cohomology groups containing more than one element are the first cohomology group on 2D areas with holes or in 3D spaces with missing complete lines, because the angle 1-form $d\phi$ has no potential, e.g.

$$H_1(\mathbf{R^2} - 0) \neq 0. \tag{7.28}$$

The solid angle 2-form $\mathrm{d}\Omega$ tells that $H_2(\mathbf{R^3} - 0) \neq 0$. It turns out that curvature 2-forms $F = \mathrm{d}A$ in gauge theories can lead to non-trivial topological invariants when they appear as terms $F \wedge F$ in the action and can be reduced to edge terms. The connection 1-form A approaches a pure gauge at the edge (where the curvature has to vanish to guarantee finite action) $A \to U^{-1}\partial_\mu U$, similar to the situation with Dirac's monopole. This can lead to integrals over a phase 1-form and thus to winding numbers. For an easy to read introduction see [3], Chap. 16.

7.3 Topology and the Quantum Hall Effect

In this section we use standard units. We will consider three aspects of topology: (1) The phase transition underlying the quantum Hall effect can be described as a transition from closed loops with zero windings around a circular system direction

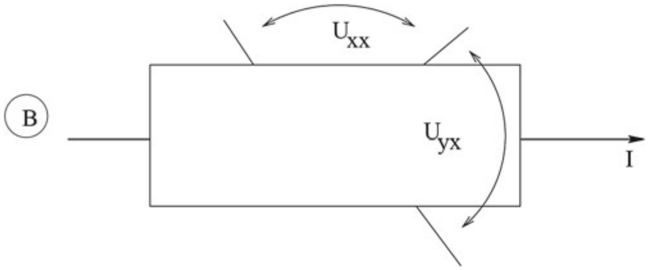


Fig. 7.4 Setup to measure current voltage characteristics of 2 D electrons in perpendicular magnetic fields B. From these characteristics the conductances are determined

to extended loops with one winding around a circular system direction. (2) The Hall conductivity can be described as a topologically quantized loop invariant. While (1) and (2) are demonstrated within a deterministic dynamics approximation with separation of time and length scales provided by very strong magnetic fields, we consider (3) the more general fully quantum mechanical field theory approach to the underlying quantum phase transition; however in a drastically simplified caricature of this field theory. The caricature contains a similar topological term as the full field theory. Our discussion follows closely the presentations in [4, 5].

7.3.1 Quantum Hall Effect

The integer quantum Hall effect (IQHE) was discovered by von Klitzing [6] in a 2D electron system in the presence of strong perpendicular magnetic fields at temperatures below 1K when investigating conductances from current voltage characteristics (see Fig. 7.4). The effect is characterized by a step-function like behavior of the **Hall conductance** g_H (see Fig. 7.5) as a function of the so called filling factor. The filling factor ν is a dimensionless quantity proportional to carrier concentration n and inversely proportional to the magnetic field B. It also describes the ratio of the number of electrons in the system N_e to the number of magnetic flux quanta through the system N_ϕ,

$$\nu = \frac{hn}{eB} = \frac{N}{N_\phi}. \tag{7.29}$$

The plateau values of the Hall conductance turned out to be exactly quantized in units of the quantum unit of conductance (conductivity)[2]

$$g_H = j\frac{e^2}{h}, \quad j = 1, 2, 3, \ldots . \tag{7.30}$$

[2]In 2D we do not need to distinguish between Hall conductivity σ_H and conductance g_H.

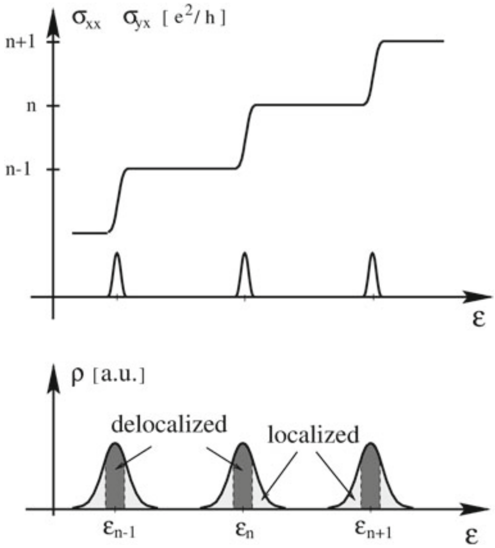


Fig. 7.5 Qualitative picture visualizing the explanation of the QHE being due to a sequence of localization-delocalization transitions occurring at the Landau levels. In finite systems the range of extended states on the energy scale has finite width. This width shrinks to zero in the thermodynamic limit

Remarkably, each integer j corresponds to a small region around integer filling factors $\nu = j$. In addition, the IQHE is characterized by a vanishing dissipative conductivity σ in the Hall plateau regimes (see Fig. 7.5).[3] The peaks in the dissipative conductivity as a function of the filling factor have a clear interpretation in terms of a **zero temperature quantum phase transition** where electrons change from immobile and **localized** to mobile and **delocalized**. This transition is called after his discoverer [7] Anderson transition or more technically LD transition.

The IQHE can be described within an effective model of independent electrons subject to a random potential $V(x, y)$. Treating electrons as independent Fermi particles the thermodynamics is described by the Fermi distribution function for single particle states. For simplicity we ignore the spin degree of freedom.

Since dissipative electric currents are due to transitions of charge carriers from occupied to empty states, at zero temperature, only states at the Fermi energy contribute to the conductivity. In other words, the conductivity is a Fermi level quantity. If the Fermi energy, in a macroscopic system, is situated in an energy range of localized states no electric current can be carried through the system. Consequently, the zero temperature conductivity vanishes.

Now, recall from a quantum mechanics course that strong magnetic fields quantize the energies of free electrons into highly degenerate **Landau levels**[4]

[3] Note, that for non-vanishing Hall conductivity a vanishing dissipative conductivity causes also the vanishing of the longitudinal resistivity, since the current flow is perpendicular to an applied electric field.

[4] a harmonic oscillator problem with independence on a continuous quantum number.

$$\epsilon_j = \hbar\omega_c\left(j + \frac{1}{2}\right) \tag{7.31}$$

where $\omega_c = eB/m$ is the cyclotron energy. Any amount of disorder in the system will break the degeneracy and broaden these levels into **Landau bands** for the density of states (see Fig. 7.5). The IQHE occurs when the Landau level broadening Γ does not wash out the structure of separated Landau bands ($\Gamma < \hbar\omega_c$). In addition, the temperature must be low enough to keep thermal transitions from localized to delocalized states low ($k_B T \ll \Gamma, \hbar\omega_c$). The filling factor ν is an integer for each fully occupied Landau band. According to the observed behavior of the longitudinal conductivity in the IQHE it seems that states situated between the Landau levels, corresponding to the plateau regions of the Hall conductance, are localized, while states in the vicinity of Landau levels are delocalized. The latter correspond to the transition regimes between subsequent plateaus (see Fig. 7.5). The IQHE is thus interpreted in terms of localization-delocalization (LD) transitions which occur close to the Landau band centers. Localization in 2D disordered quantum systems at very low temperature is by no means an unusual phenomenon. On the contrary, in a 2D system with sufficiently strong disorder states are localized. Delocalization can only happen for certain topological reasons—as is the case in the IQHE (see [8] for an up to date review). The delocalization at the band centers occurring in the IQHE is attributed to the strong magnetic field which puts an orientation to the area and to certain states. In a finite system, the Hall conductance can be represented as a Fermi level quantity, too. In this case, so called (oriented) **edge states** occur. They alone cannot cause any dissipation, but contribute to the Hall conductance. Now we will have a more quantitative look at the problem.

7.3.2 Winding Paths

The most simple and illuminating approach to the quantum Hall effect is provided by the **high field model** which will be discussed now.

In the high field limit the cyclotron radius which is proportional to the magnetic length ℓ_B[5] shrinks and electrons move along equipotential lines of potentials which vary smoothly on the scale of l_B. To see this one introduces center coordinates (X, Y) and rapidly varying relative coordinates ($\zeta = v_y/\omega_c, \eta = -v_x/\omega_c$) of the (distorted) cyclotron orbit

$$x = X + \zeta, \quad y = Y + \eta. \tag{7.32}$$

The following commutation relations result

$$[X,\ Y] = i\ell_B^2, \quad [\zeta,\ \eta] = -i\ell_B^2. \tag{7.33}$$

[5]The magnetic length is defined by a square containing one flux quantum.

The Hamiltonian reads

$$H = \frac{m{\omega_c}^2}{2}\left(\zeta^2 + \eta^2\right) + V\left(X + \zeta,\ Y + \eta\right). \tag{7.34}$$

Since the expectation values of ζ and η are of the order $\ell_B \sim 1/\sqrt{B}$, in the limit $B \to \infty$, for smooth potentials, the Hamiltonian (7.34) separates. Under the boundary conditions of the Landau model the eigenvalues of the first term are the Landau energies ε_n. Thus, in the limit $B \to \infty$, (7.34) is equivalent to

$$H = \varepsilon_n + V(X, Y). \tag{7.35}$$

Furthermore, in the limit $B \to \infty$ the commutator of X and Y vanishes like $1/B$ and thus the quantities X and Y can be treated approximately as commuting variables with vanishing fluctuations. For this so called classical approximation the corresponding canonical equations of motion are

$$\dot{X} = \frac{\ell_B^2}{\hbar}\frac{\partial V}{\partial Y}, \quad \dot{Y} = -\frac{\ell_B^2}{\hbar}\frac{\partial V}{\partial X}. \tag{7.36}$$

Obviously $\mathrm{d}V/dt = 0$, i.e. the electron moves along equipotential orbits $V(X, Y) =$ const. (see Fig. 7.6). We shall assume that the random potential is symmetrically distributed around $V = 0$ and its variation $\Delta V := V_{\max} - V_{\min}$ is small compared with the Landau level splitting, $\Delta V \ll \hbar\omega_c$.

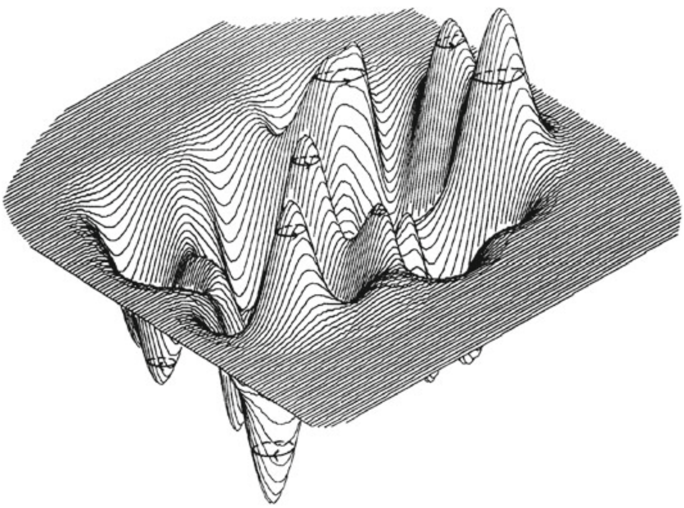


Fig. 7.6 Equipotential orbits near the *bottom* and near the *top* of a smooth random potential. *Arrows* indicate the direction of the motion

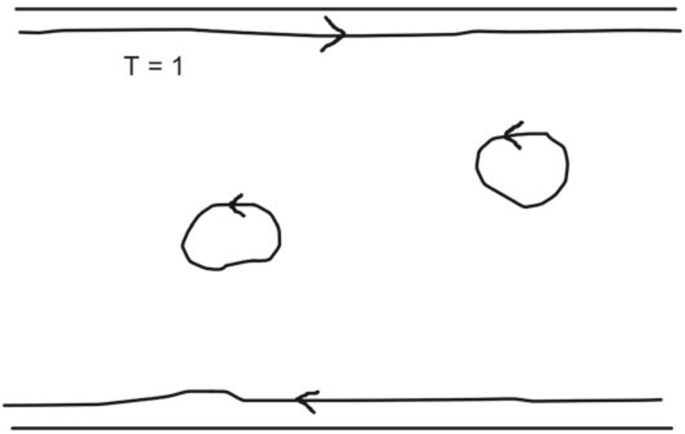


Fig. 7.7 In a system with edges directed equipotential lines exist which cannot backscatter in a regime of bulk localization and therefore have transmission probability $T = 1$

Then, in the limit of infinite system size we have a topological classification: all equipotential orbits with $V \neq 0$ are closed (see Fig. 7.6) while percolating open equipotential orbits can only exist for $V = 0$, i.e. at energy $E = \varepsilon_n$. Thus, in an infinite system there is a localization-delocalization transition which is in the high field model a topological transition between closed and open percolating paths. If the system is finite with one periodic direction, then the open percolating paths wind around the periodic direction. Note however, that the percolating path meets several saddle points where paths come close of the order of a magnetic length and therefore the classical approximation, ignoring tunneling, becomes invalid. Let us concentrate on a situation where the Fermi energy is in a regime of bulk localized states, where the high field model is fine. In finite systems with contacts at two opposite sites and boundaries macroscopically separated, there appear, due to the steep rising edge potentials, directed equipotential lines along the edge (see Fig. 7.7). These edge states are oriented according to the magnetic field and the gradient of the edge potential. At opposite edges the direction is opposite. In a regime off the Landau energies, where only closed equipotential lines exist in the bulk of the system, there is no way for backscattering of an electron on its way along an edge state. Thus, in finite systems also in the regime of bulk localization there are—due to their orientation-**topologically protected open edge states** which are topologically distinguished from bulk localized states. Both types cannot be transformed continuously into each other without changing the winding number around a periodic system direction. It has become popular to call such system a topological insulator. The impossibility for an edge state to backscatter (the transmission probability is one) can be used to demonstrate the quantization and stability of the Hall conductance in a scattering theoretical approach to multi probe conductors pioneered by Landauer and Büttiker

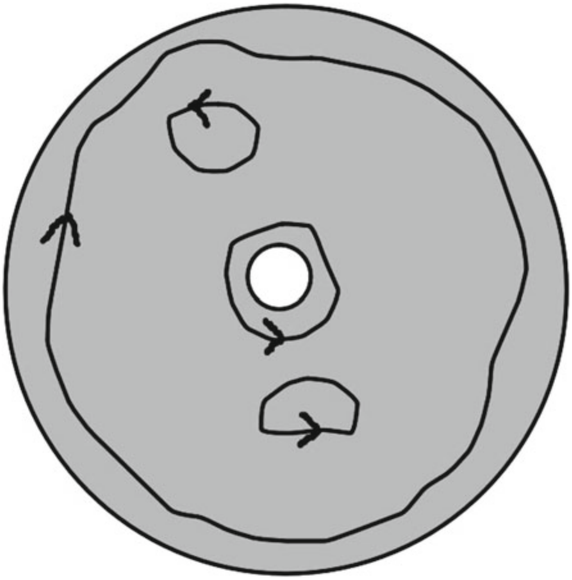


Fig. 7.8 In a Corbino Disc geometry at the edges directed edge states exist in a regime of bulk localized states

(for a review see e.g. [9]). Here we like to demonstrate that the quantization can be captured by integration with topological content. For that purpose we put the 2D system on the surface of a finite cylinder or-topologically equivalent—on a so called Corbino disc as displayed in Fig. 7.8. We take the periodic direction along the current direction (y direction). The current occurs in response to an applied electric field in x direction. We start from the Kubo formula for the Hall conductivity σ_H without detailed derivation (which is possible along the lines presented in Appendix C.1, (C.20))

$$\sigma_H = \frac{e^2}{\mathrm{Ar}} \int \frac{dXdY}{2\pi \ell_B^2} \frac{\partial f(E)}{\partial E} \dot{Y} \overline{X}, \tag{7.37}$$

where $f(E)$ is the Fermi distribution, which at zero temperature is the step function

$$f(E) = \Theta\left(\varepsilon_F - E\right), \; E = \varepsilon_n + V(X, Y), \tag{7.38}$$

and $\overline{X}$ is the long time limit of center coordinate X. The formula can be made plausible by pointing out that in the Kubo susceptibilities two operators enter: the current $-e\dot{Y}$ and the long time limit of the coupling operator to the driving field, which is here the dipole moment $-eX$. The phase space in the high-field limit is the (X, Y) space with unit size $2\pi \ell_B^2$. The derivative of the step function shows the Fermi edge character of conductivity. We can use the equation of motion for $\dot{Y}$ and write

$$\sigma_{yx} = -\frac{e^2}{h\mathrm{Ar}} \int \mathrm{d}X\mathrm{d}Y \, \frac{\partial f}{\partial X} \overline{X} \tag{7.39}$$

and, on integrating by parts,[6]

$$\sigma_{yx} = \frac{e^2}{h\mathrm{Ar}} \int \mathrm{d}X\mathrm{d}Y \, f(H) \frac{\partial \overline{X}}{\partial X}. \tag{7.40}$$

At $T = 0$ the Fermi function limits the 2D integration to an area called $\mathcal{B}(\varepsilon_F)$

$$\begin{aligned} \int dXdY \, f \frac{\partial \overline{X}}{\partial X} &= \int\limits_{\mathcal{B}(\varepsilon_F)} \mathrm{d}X\mathrm{d}Y \frac{\partial \overline{X}}{\partial X} \\ &= \int\limits_{\mathcal{B}(\varepsilon_F)} \mathrm{d}\overline{X} \wedge dY. \end{aligned} \tag{7.41}$$

Let the Fermi energy lie above the Landau level. The area $\mathcal{B}(\varepsilon_F)$ is the filling between equipotentials at the Fermi edge. We can now apply Stoke's theorem and find

$$\int \mathrm{d}X\mathrm{d}Y \, f \frac{\partial \overline{X}}{\partial X} = \int\limits_{\partial\mathcal{B}(\varepsilon_F)} \overline{X}(s)\dot{Y}(s)\mathrm{d}s. \tag{7.42}$$

The boundaries $\partial\mathcal{B}$ include all boundaries of $\mathcal{B}$ with proper orientation (see Fig. 7.8), i.e. in particular also those at $\pm L_x/2$. The geometry of the system is equivalent to that of a cylinder of length L_x, there are no boundaries with respect to y. The set $\partial\mathcal{B}(\varepsilon_F)$ consists of contours which either wind around the cylinder and thus cannot be contracted to a single point or do not wind and so can be contracted to one point. Obviously, the latter do not contribute to the Hall conductivity (and thus represent localized states), whereas each of the former (delocalized edge states) contributes an amount proportional to

$$\int \mathrm{d}s\overline{X}(s)\dot{Y}(s) = (\pm L_x/2)(\pm L_y) = \mathrm{Ar} \tag{7.43}$$

where the sign reflects the handedness. Thus, each occupied Landau level contributes via its edge contours one quantum e^2/h to the Hall conductivity in a regime of localized bulk states.

[6]The boundary value term vanishes since the potential energy right at the geometric boundary is larger than the Fermi energy. Furthermore, a "would be" compensating term had already been omitted in deriving (7.37).

7.3.3 *Field Theory with Topological Term*

The aim of the field theoretical approach to the QHE invented by Pruisken [10] is to explain the LD transitions by an appropriate generalization of the field theoretical method applied to the metal-insulator transition in disordered systems at zero temperature (Anderson transition) for strong magnetic fields. As shown by Wegner [11] averaging of Green's functions with respect to a short-range correlated random potential $V(\mathbf{r})$,

$$\left\langle V(\mathbf{r})V(\mathbf{r}')\right\rangle = c\,\delta(\mathbf{r}-\mathbf{r}'), \tag{7.44}$$

can be formally carried out on the generating functional for disorder averaged Green's functions.

We sketch the main steps which follow the prescriptions of Sect. 5.6.

1. As we have learned already, the one particle Green's function-as an inverse operator-can be represented as a Gaussian integral over commuting fields, where a determinant appears in the denominator. One likes to average out the potentials which is hard to do for the determinant. Therefore one likes to get rid of it.
2. One can either introduce several copies of the model (replicas) and let formally the number n of replicas goes to zero which is mathematically dangerous. Or one introduces anticommuting fields to get rid of the determinant and stays with a supersymmetric field theory in fields of Bosonic and Fermionic type, $\overline{\Psi}$, Ψ.
3. Now one averages over disorder which results in a quartic coupling of fields. These fields are not the appropriate long range fields of the problem. To get those, one reduces by integration to matrix variables quadratic in field combinations, $X = \overline{\Psi}\Psi$. By taking also their dual Fourier partners $\tilde{Q}$ into account and integrating Gaussian variables out, one ends up with an effective theory in the dual supermatrix field $\tilde{Q}$.
4. The next step is the search for stationary points and quadratic fluctuations. One finds a situation of broken symmetry where the Goldstone matrix modes Q are the candidates for describing transport modes in the system.
5. The final action is quadratic in gradients plus an oriented boundary term which can be neglected in the absence of handedness in the system. However, the fields are subject to constraints ($Q^2 = 1$) which makes the theory non-linear. In systems with magnetic fields there is an orientation and the boundary term becomes important. The resulting action is mainly dictated by symmetry constraints and the requirement of keeping only second order gradients. What remains to be calculated explicitly are the **coupling constants**. It turns out that they are related to the dissipative conductance g and the Hall conductance g_H measured in quantum units e^2/h and evaluated at the mean field level.

The structure of the action of Pruisken's **non-linear sigma model** is shown here[7]

$$S[Q] = \int \mathrm{d}x \left[g \left(\mathrm{sTr} \left\{ \left(\partial_\mu Q \right) \left(\partial_\mu Q \right) \right\} \right) + \frac{g_H}{2} \left(\mathrm{sTr} \left\{ Q \left[\partial_y Q, \partial_x Q \right] \right\} \right) \right]. \quad (7.45)$$

As discussed in Sect. 5.7 with such model one tries to find the **renormalization flow** of the coupling constants g and g_H as a function of system size L to study the phase transition. We briefly recapitulate the main ideas. The scale dependence is introduced into the generating functional by a regulator that takes the full fluctuations of fields on scales up to L into account while fluctuations on larger scales are suppressed. The form of the Lagrangian will change by this procedure, but one hopes that one can recast it in the same form as before with renormalized couplings. These renormalized couplings will become scale dependent **running couplings**. This renormalization step may be iterated and forms the renormalization semi-group action on the running couplings, giving rise—when done in small steps—to differential equations with respect to a continuous change of scale,

$$\frac{\mathrm{d} \ln g}{\mathrm{d} \ln L} = \beta_g(g, g_H); \quad \frac{\mathrm{d} \ln g_H}{d \ln L} = \beta_{g_H}(g, g_H). \quad (7.46)$$

The β-functions contain the scaling behavior of the coupling constants and the zeroings are the fixed points of scaling. They can be either stable or repulsive (in certain directions), or marginal. In the vicinity of fixed points one can study the scaling by linear approximation of the β-functions, giving rise to scaling exponents. However, an exact calculation of β-functions is usually not possible. The integration over irrelevant fields can, of course, only be done by relying on Gaussian integration and meets restrictions of applicability. This renormalization program for Pruisken's model (7.45) could be done so far only approximately in the vicinity of the delocalized phase, where the mean field conductances are large numbers and the Goldstone modes describe long ranged electron diffusion. However, a reliable qualitative consistent picture for the scaling behavior in the IQHE emerged from that (see e.g. the discussion in [12] or in [1], Chap. 9). For this qualitative picture the second term in the Lagrangian turned out to be of great importance. It shows the handedness due to the magnetic field since it breaks the symmetry against interchanging x and y. This goes together with its character being a total derivative, thus representing an edge term. This edge term turns out to be **topologically quantized**. The resulting two-parameter flow diagram compatible with the theory must then be periodic in g_H and must show a transition between different quantized Hall conductances. These two hard facts of the model allow to sketch a qualitative form of the renormalization flow, as predicted shortly after the model was found. It is shown in Fig. 7.9. The precise position g^* of the separating unstable fixed point and precise scaling exponents could not be derived so far from the model. However, alternative ways relying on a numerical finite size scaling analysis were developed (for overviews see [8, 13]).

[7] sTr stands for a trace respecting supersymmetry requirements.

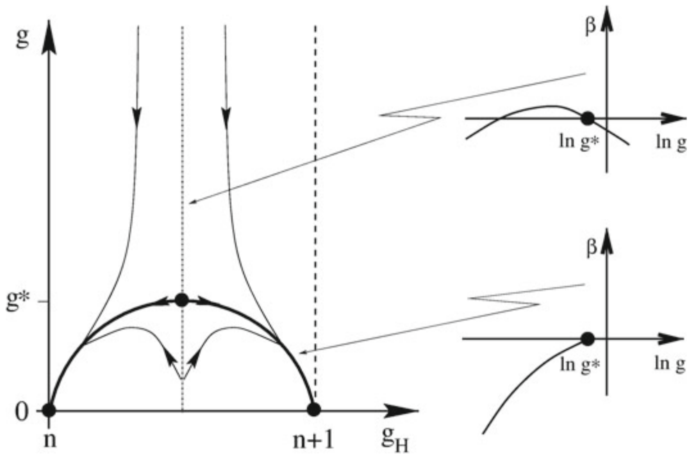


Fig. 7.9 Flow diagram of conductance g and Hall conductance g_H compatible with the quantum Hall effect. On the *right* β-functions ($\beta(g) = d \ln g / d \ln L$) are shown corresponding to a fixed half-integer value of g_H (*top*) and to the asymptotic one-parameter regime, drawn as bold semi-circle (*bottom*)

To illustrate the interrelation of symmetry breaking, boundary condition and topological quantization let us consider a simple one-dimensional caricature model for a complex scalar field $\varphi(x)$ with the U(1) global invariant Lagrangian

$$\boxed{\mathcal{L} = \left(\partial_x \varphi^*\right)\left(\partial_x \varphi\right) + V(\varphi^* \varphi) + \frac{1}{2i}\left[\varphi^*\left(\partial_x \varphi\right) - \varphi\left(\partial_x \varphi^*\right)\right]} \tag{7.47}$$

depending on φ and its first derivative $\partial_x \varphi$ (and their complex conjugates). In (7.47) $V(\varphi^* \varphi)$ is an arbitrary potential taking minimal values along a circle $\varphi_0^* \varphi_0 = M^2$ in the complex φ-plane (see e.g. the φ^4-model of (6.52)) and the third term on the r.h.s. introduces a handedness by breaking the symmetry against space reflection $x \to -x$. To study fluctuations around the stationary constant solution M we write again—as with the discussion of Goldstone modes

$$\varphi(x) = (M + \eta(x)) e^{i\alpha(x)} \tag{7.48}$$

and expand to second order in the fields η and α,

$$\begin{aligned} \mathcal{L} = V(M^2) + \left[(\partial_x \eta)^2 + (\frac{1}{2} V''|_{M^2})\, \eta^2\right] \\ + M^2 (\partial_x \alpha)^2 + (\partial_x \alpha)\,(M^2 + 2M\eta), \end{aligned} \tag{7.49}$$

which indicates again that $\alpha(x)$ is a massless Goldstone mode. Integrating out the short-ranged field $\eta(x)$[8] we end up with the reduced Lagrangian

$$\mathcal{L}_{\text{eff}} = \tilde{M}^2(\partial_x\alpha)^2 + \boxed{M^2(\partial_x\alpha)}. \tag{7.50}$$

Thus, the contribution of the reflection symmetry breaking part of the effective Lagrangian ($M^2(\partial_x\alpha)$) to the effective action,

$$\Gamma_{\text{eff}} = \int \mathrm{d}x\, \mathcal{L}_{\text{eff}}, \tag{7.51}$$

is a pure **boundary term** which has no effect on the level of Euler-Lagrange equations. However, for the generating functional—defined by the effective action— the boundary conditions become essential. Once we consider finite action solutions we compactify the line $\mathbf{R}$ to a circle $\mathbf{S^1}$ and the corresponding periodic boundary conditions,

$$\lim_{x\to\infty} e^{i\alpha(x)} = \lim_{x\to-\infty} e^{i\alpha(x)} \tag{7.52}$$

lead to

$$\lim_{x\to\infty} (\alpha(x) - \alpha(-x)) = 2\pi \cdot \mathbf{Z} \tag{7.53}$$

and quantized values for the boundary term result. A proof for the quantization of the topological term in the field theory of (7.45) follows very similar lines [14].

7.4 Exercises

Exercise 1: Topological Classes
Find examples for topological classes by considering closed paths on manifolds.

Exercise 2: Dirac Monopole I
What could be concluded if the vector potential for the monopole could be defined everywhere without any singularity? Think of Poincare's Lemma.

Exercise 3: Dirac Monopole II
Verify that the magnetic field fulfills the equations with A^N and A^S and that both vector potentials are related by the given gauge transformation. Clarify the range of definition of this gauge transformation. Repeat the argument about the quantized charges.

Exercise 4: Quantization of Hall Conductivity
Go through the calculations which lead to (7.42) and argue carefully, why closed bulk contours do not contribute and why edge states contribute one quantum.

[8] The linear coupling $2M\eta\partial_x\alpha$ changes the prefactor M^2 of $(\partial_x\alpha)^2$ to some $\tilde{M}^2$.

Exercise 5: Quantization of Topological Term in Caricature Field Theory
Repeat the argument about the quantization of the topological term in the caricature field theory (7.47). Why must such term break a discrete symmetry? Which discrete symmetry is it in Pruisken's model (7.45) and why can that happen?

References

1. A. Altland, B. Simons, *Condensed Matter Field Theory*, 2nd edn. (Cambridge University Press, Cambridge, 2010)
2. M. Nakahara, *Geometry, Toplology and Physics* (IOP Publishing, 2003)
3. T.P. Cheng, L.-F. Li, *Gauge Theory of Elementary Particles* (Clarendon Press, Oxford, 1984)
4. M. Janßen, O. Viehweger, U. Fastenrath, J. Hajdu (eds.), *Introduction to the Theory of the Integer Quantum Hall Effect* (VCH, Weinheim, 1994)
5. M. Janssen, *Fluctuations and Localization in Mesoscopic Electron Systems* (World Scientific, Singapore, 2001)
6. K. von Klitzing et al., Phys. Rev. Lett **45**, 494 (1980)
7. P.W. Anderson, Phys. Rev. **109**, 1492 (1958)
8. F. Evers, A. Mirlin, Rev. Mod. Phys. **80**, 1355 (2008)
9. M.V. Moskalets, *Landauer-Büttiker Formalism*. Scattering Matrix Approach to Non-Stationary Quantum Transport (Imperial College Press, 2011), pp. 1–33
10. A.M.M. Pruisken, Nucl. Phys. B **235**, 277 (1984)
11. F. Wegner, Z. Phys. B **35**, 207 (1979)
12. A.M.M. Pruisken, Topological Principles in the Theory of Anderson Localization. In: E. Abrahams (ed.), *50 years of Anderson Localization* (World Scientific, Singapore, 2010), pp. 503–558
13. B. Kramer, T. Ohtsuki, S. Kettemann, Phys. Rept. **417**, 211 (2005)
14. M. Janßen, Z. Phys. B **69**, 227 (1987)

Chapter 8
Selected Applications

Abstract We will have a look at selected applications of the methods developed so far. Tunneling in a double well potential shows the importance of topological instanton solutions as stationary action solutions. We have a look at the generating role of entropy as a generalized thermodynamic potential close to equilibrium. A paradigmatic model for non-equilibrium phase transitions is the Laser model where we meet again the Landau potential and the interplay of drift and diffusion. That the concept of semi-group dynamics cannot only be used for real time Markov processes will be demonstrated within random matrix theory where a pseudo time Markov process helps in simplifying the formulation of limiting distributions in different variables, avoiding tedious measure transformations. Markov processes can be set up for evolution processes in other real parameters such as disorder strength s in a random Hamiltonian problem or as system length L in a quasi-one dimensional (quasi-1D) system for a so called transfer matrix. In the context of the dynamics for matrix variables we demonstrate the construction of an effective field theory that captures—in a certain regime—the essential physical phenomenon: universal fluctuations in additive macroscopic variables. Finally, we look at a simplified renormalization group analysis for the localization-delocalization quantum phase transition, bringing ideas of quantum processes (interference) and Markov processes (renormalization group) together in a single application.

8.1 Tunneling in a Double Well

The problem of tunneling of a particle with coordinate x in a one-dimensional (1D) double well can be analyzed with the help of a Landau potential as displayed in Fig. (6.1c),

$$V(x) = -\frac{\alpha}{2}x^2 + \frac{\lambda}{4}x^4 + \frac{\alpha^2}{4\lambda}, \tag{8.1}$$

for $\alpha, \lambda > 0$ and further simplifying approximations. We will only keep the following characteristics of this potential: the positions $x = \pm a := \sqrt{\alpha/\lambda}$ of the two minima (where $V = 0$), the curvature $m\omega^2 := V''(\pm a) = 2\alpha$ at the minima and the barrier height $V_0 := \alpha^2/(4\lambda)$.

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1_8

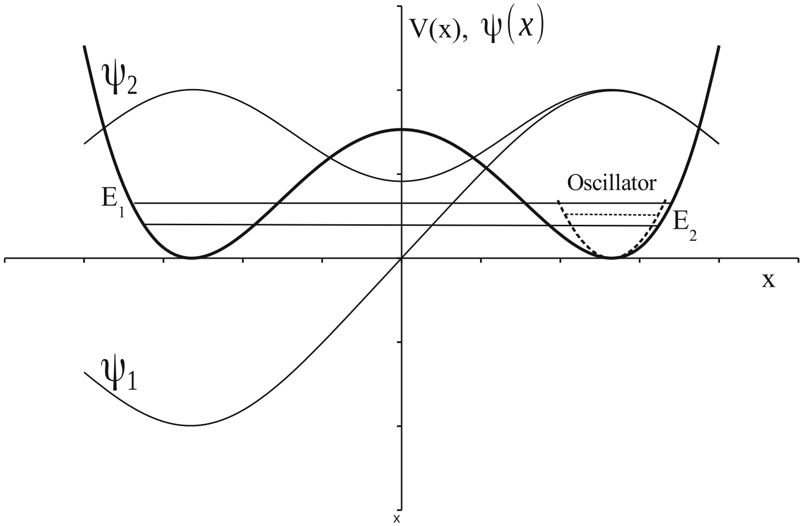


Fig. 8.1 Visualization of the two level approximation for the eigenvalue problem in a double well potential

One knows from 1D quantum eigenvalue problems (see the listing in Sect. 4.4.1) that the two lowest energy eigenstates are an almost degenerate pair of symmetric and antisymmetric linear combination of ground states (energy E_0) of a single well centered at opposite positions $\pm a$. These ground states of single wells will be called $|\pm\rangle$ for obvious reasons. We will approximate the general tunneling problem by restricting the dynamics to the two level problem of Sect. 2.3.6. Thus, in the $|\pm\rangle$ representation the Hamiltonian is the 2×2 matrix with identical diagonal elements $H_{++} = H_{--} = E_0$ and identical off-diagonal elements $H_{+-} = H_{-+} =: \Delta\epsilon/2$. This $\Delta\epsilon$ is, according to (2.52), the so-called tunneling splitting energy,

$$E_{1,2} = E_0 \pm \frac{\Delta\epsilon}{2}. \tag{8.2}$$

In this approximation (see Fig. 8.1) the tunneling splitting energy can be calculated as twice the Hamiltonian matrix element

$$\Delta\epsilon = 2H_{+-} = \int \mathrm{d}x\, \psi_+(x) \left[-\frac{\mathrm{d}_x^2}{2m} + V(x) \right] \psi_-(x). \tag{8.3}$$

Since $\psi_\pm(x)$ are concentrated on opposite sites, one can approximate this integral very well by omitting the overlap with $V(x)$ and doing partial integrations with the kinetic energy term. As a result one has

$$\Delta\epsilon \approx m^{-1} \left[\psi_-(0)\psi'_+(0) - \psi_+(0)\psi'_-(0) \right]. \tag{8.4}$$

In this approximation the splitting energy is uniquely determined by the single well wave functions centered at $\pm a$. The probability amplitude for a particle to start at a and reach $-a$ after time t is the propagator (Green's function) $G(-a, a, t) = \langle -a \mid e^{-iHt} \mid a \rangle$. From the calculations in Sect. 2.3.6 we know the answer in the two-level approximation:

$$G(-a, a, t) = \frac{1}{2}\left(e^{-i(E_0 - \Delta\epsilon/2)t} - e^{-i(E_0 + \Delta\epsilon/2)t}\right) = e^{-iE_0 t} \sin\left(\frac{\Delta\epsilon}{2} t\right). \tag{8.5}$$

The Green's function can alternatively be calculated as a path integral via the stationary action method as given by (3.42). We have a look at this calculation, because we will see the importance of topological classes of such stationary action solutions by direct comparison with (8.5). In a first step we have to find the stationary action solution from a to $-a$ in time t which solves the classical equation of motion $m\ddot{x} = -V'(x)$. By multiplying this with $\dot{x}$ and integrating over time from 0 to t and noting that $V(a) - V(-a) = 0$, we have

$$\frac{m}{2}\dot{x}_c^2 + V(x_c) = 0 \tag{8.6}$$

and the action of such path with a one-to-one correspondence between time and coordinate is purely imaginary,

$$S_{\text{inst}} = i \int_{-a}^{a} \mathrm{d}x \, \sqrt{2mV(x)}. \tag{8.7}$$

It is independent of the details of how the path is parametrized except that it must be in a one-to-one correspondence. Such stationary action solution with a one-to-one correspondence between time and coordinate is called **single instanton action** or single ant-instanton action (if the path is reversed keeping the action the same). The name was chosen by t'Hooft to point out that, for such single instanton action path, the essential change from a to $-a$ is localized in time at some intermediate time t_1 over a time scale of order $2\pi/\omega$ set by the time period of motions in one of the minima. Usually we look at probing times $t \gg 1/\omega$. In such case one must take into account that not only this single instanton is a stationary solution, but many instanton solutions with several bounces back and forth from a to $-a$ exist. They can be taken into account by summing them up in the stationary action method, as written in (3.42). It is assumed that typically they are separated in time and thus contribute independently (dilute instanton gas). The consistency of this assumption can be justified by comparison to our previous result for the propagator for arbitrary times t. A typical multi-instanton solution is displayed in Fig. 8.2 and shows the topological character of kinks very much the same as in our example of a corrugated iron sheet in Sect. 7.1. The total kink number must be -1 as we have a motion from

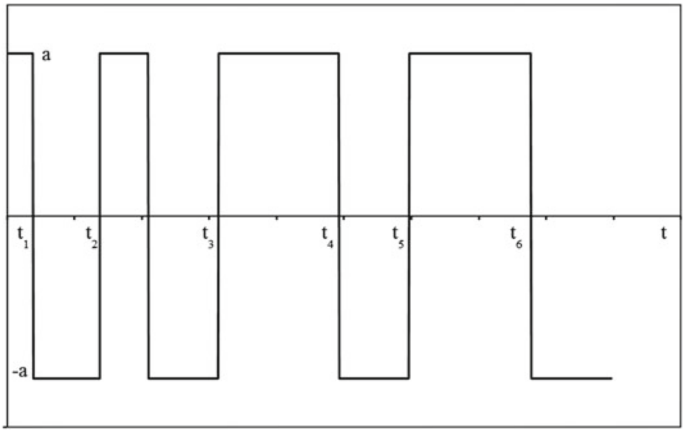


Fig. 8.2 Visualization of a multi-instanton solution with total kink number -1

a to $-a$. Consequently, the instanton action can contain an odd number n of instantons and anti-instantons. Thus, the contribution from k (anti-) instantons (k odd) is simply

$$S^{[k]} = kS_{\text{inst}}. \tag{8.8}$$

The calculation of the determinant factor is a bit tricky because we have to solve for the eigenvalues of the Hessian of the action at stationarity (see (3.42)) and here we simply lend it from the oscillator problem in one minimum which is found for large times t to be proportional to e^{-iE_0t} where E_0 is the ground state energy of such oscillator. It can be written in the presence of k instantons as (for details see [1])

$$(Ct)^k e^{-iE_0t} \tag{8.9}$$

where C is a constant which remains to be calculated. Finally we must take care of the fact that the positions of instantons in time are arbitrary and we cannot distinguish them. For that reason we have to devide the contribution of k instantons by $k!$ to avoid double counting.[1] Now we apply (3.42) and find, after identifying the series over odd k as the series for the sin function, for the propagator

$$\boxed{G(-a, a, t) \approx e^{-iE_0t} \sin\left(Cte^{iS_{\text{inst}}}\right)}. \tag{8.10}$$

By comparison with (8.5) we see how important the incorporation of many instanton stationary action solutions is to get the correct functional dependence of the

[1] An alternative view is performing an average over intermediate times $t^{-k} \int_o^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \ldots \int_0^{t_{k-1}} \mathrm{d}t_k = 1/k!$.

propagator for arbitrary large times. In addition, we have learned that the tunneling splitting energy

$$\Delta\epsilon = 2Ce^{iS_{\text{inst}}} \tag{8.11}$$

can be expressed by the instanton stationary action and the constant C to be determined from the determinant factor.

8.2 Entropy Close to Equilibrium

We consider the entropy S (quantum or configuration) with respect to a relevant density operator or relevant distribution over configurations. To simplify notations we write equations for the quantum case with traces over operators. This can easily be translated to integration over functions. We consider further a situation of hydrodynamics, which means that the times t considered are separated from microscopic times τ_0 where individual collisions could be resolved as well as from large time scales τ_{eq} of global equilibrium. However, the time t may be in a regime, where the system has locally relaxed to some kind of local equilibrium. It is also important that macroscopic currents I_m are driven through the system. These currents are the expectation values of time derivatives of some relevant observables O_m,

$$X_m(t) = \langle O_m \rangle (t) = \text{Tr}\ \{O_m \varrho_{rel}(t)\}, \tag{8.12}$$

$$I_m(t) = \partial_t X_m(t), \tag{8.13}$$

$$\varrho_{rel}(t) = e^{-S(t)}. \tag{8.14}$$

Now, we anticipate that $X_m = \langle O_m \rangle$ are convenient coordinates within a maximum entropy ansatz for the non-equilibrium operator ϱ_{rel}. Thus, we can write

$$\varrho_{rel}(t) = e^{-\Phi(t) - \sum_m F_m(t) O_m}, \tag{8.15}$$

where $F_m(t)$ are Lagrange multipliers to guarantee the average values X_m. They are called **forces** in this context. $\Phi(t)$ is a non-equilibrium thermodynamic potential.

It is now easy to show that the average entropy serves as a non-equilibrium thermodynamic potential,

$$\mathrm{S}(t) = \Phi(t) + \sum_m F_m(t) X_m(t), \tag{8.16}$$

and that (8.12) requires the variational relation

$$\frac{\delta\Phi}{\delta F_m} = -X_m. \tag{8.17}$$

Thus, (8.16) generalizes the equilibrium Legendre transformation to this non-equilibrium case (see [2]). The analogy goes further, as any variation of the average entropy results in

$$\delta S(t) = \sum_m F_m(t)\delta X_m(t) \tag{8.18}$$

showing that forces and coordinates are thermodynamically conjugate to each other,

$$F_m(t) = \frac{\delta S(t)}{\delta X_m(t)}. \tag{8.19}$$

Consequently, the positive average entropy rate within the system is bilinear in currents and forces

$$\boxed{\dot{S}(t) = \sum_m F_m(t) I_m(t) \geq 0}. \tag{8.20}$$

An example is the entropy rate in the heat exchange between two reservoirs with temperature difference ΔT. The current is the heat current $\dot{q}$ and the force is $1/T - 1/(T + \Delta T) \approx \Delta T/T^2$. A second example is the entropy rate of an electric current I for a voltage U. Here, the force is voltage per temperature, U/T.

Very often the currents can be expanded in powers of the forces and the **linear response** regime has a macroscopic range of applicability. In terms of the Fourier coefficients $f(\omega)$ of time dependent functions $f(t) = \int \mathrm{d}t\, f(\omega)e^{i\omega t}$, the linear relations can be written as

$$I_m(\omega) = \sum L_{mn}(\omega) F_n(\omega), \tag{8.21}$$

where $L_{mn}(\omega)$ are called **kinetic coefficients**. They often fulfill symmetry conditions, known as Onsager relations, due to the reversibility of the microscopic dynamics. In the Appendix C explicit linear response formulas for such kinetic coefficients are presented as Kubo susceptibilities. To see the relevance of such coefficients in calculating physical effects consider a situation with heat exchange and electric voltage. The electric current I and the heat current $\dot{q}$ can be expanded as

$$I = L_{ee}\frac{U}{T} + L_{eq}\frac{\Delta T}{T^2}, \tag{8.22}$$

$$\dot{q} = L_{qe}\frac{U}{T} + L_{qq}\frac{\Delta T}{T^2}. \tag{8.23}$$

Now, the Seebeck effect corresponds to a potential drop related to the temperature difference at vanishing electric current,

$$U = \frac{L_{eq}}{L_{ee}}\frac{\Delta T}{T}. \tag{8.24}$$

In addition, the Peltier effect corresponds to a heat current at vanishing temperature difference due to the presence of a voltage,

$$\dot{q} = L_{qe}\frac{U}{T} = \frac{L_{qe}}{L_{ee}}I. \tag{8.25}$$

An interesting conclusion, called **minimal entropy production principle**, can be drawn for systems in the linear regime close to equilibrium. From (8.20) we have for constant forces

$$\dot{\mathrm{S}} = \sum_{mn} L_{mn}F_m F_n \geq 0. \tag{8.26}$$

In full equilibrium all currents vanish, as well as the entropy production. Keeping one current, say I_1, non-vanishing, while the others, say I_2 tend to vanish, allows to write for this state

$$\frac{\partial \dot{\mathrm{S}}}{\partial F_2} = 2I_2 = 0;\ \frac{\partial^2 \dot{\mathrm{S}}}{\partial F_2^2} = 2L_{22}. \tag{8.27}$$

Since diagonal elements L_{22} are positive (due to positive entropy production), one concludes that the entropy production is minimal with respect to driving forces. This can help in modeling non equilibrium processes close to equilibrium.

In systems close to full equilibrium the equilibrium state is reached with minimal entropy production. However, no new structure can emerge, as long as alternative stationary states, separated by instability regions, are missing. As a prototype of the emergence of new structures in non-equilibrium situations we consider the Laser phenomenon in the following section.

8.3 Self-organized Laser Far from Equilibrium

The Laser problem can serve as a paradigm for self-organizing systems far from equilibrium (see e.g. [3]). Before discussing this problem in some detail we like to summarize the main ingredients of such systems in words and by a mathematical model, the Haken-Zwanzig model. A much more detailed discussion, capturing quantitatively the fluctuating aspects, can be found in Chap. 12 of Risken's book [4].

Self-organized systems can be described by a slowly varying relevant variable X, called order parameter. The order parameter X is coupled to (many) fast relaxing variables y, which follow the order parameter instantaneously. This leads to a non-linear feedback for the order parameter which may then have more than one stable region. The stable (attractive) regions are separated by unstable (repulsive) regions. The dynamics of the order parameter may be described by a deterministic drift part and a stochastic diffusive part. The drift part dynamics is characterized by a non-equilibrium phase transition scenario of Landau potential type (see Sect. 6.3). The fluctuation part is dominating in the regime of vanishing (mean) order parameter and it is responsible for triggering the spontaneous transition into a new stable ordered phase, when the system is situated in the instability region.

The **Haken-Zwanzig model** captures the deterministic part of this scenario. It is defined by two coupled (positive coupling constants a, b) deterministic differential equations,

$$\dot{X} = \epsilon X - aXy, \tag{8.28}$$

$$\dot{y} = -y/\tau + bX^2. \tag{8.29}$$

The relaxation time τ of the fast relaxing variable y is assumed to be much smaller than the long repulsion time $1/\epsilon$ of the slow order parameter X. Then, for $|\dot{y}| \ll |y/\tau|$, the fast relaxing variable follows the order parameter instantaneously,

$$y = \tau b X^2, \tag{8.30}$$

and the order parameter fulfills an effective closed deterministic equation with **Landau potential**,

$$\dot{X} = \epsilon X - ab\tau X^3 = -V'(X) \tag{8.31}$$

$$V(X) = \frac{-\epsilon}{2} X^2 + \frac{ab\tau}{4} X^4 \tag{8.32}$$

The Landau potential has three local extrema, one local maximum at $X = 0$ and two absolute minima at

$$X = \pm\sqrt{\frac{\epsilon}{\tau ab}}, \tag{8.33}$$

provided the small parameter ϵ is positive. Then, the system shows order with non-vanishing order parameter. It will, triggered by stochastic fluctuations, finally reach one of two finite valued minimal positions. If the system is tuned to negative values ϵ, only one minimum at vanishing order parameter, $X = 0$ survives. When crossing the threshold, $\epsilon = 0$, stochastic fluctuations become very important (see Chap. 12.5 in [4]).

In a lamp oscillating dipoles of N atoms are sending photons which electric field amplitude E is a superposition of waves. It reads in a one component 1D plane wave approximation

$$E^{\text{lamp}}(x, t) = \sum_{l=1}^{N} e_l(t) \sin\left(\omega_l(x/c - t) + \phi_l(t)\right). \tag{8.34}$$

The amplitudes $e_l(t)$ and phases $\phi_l(t)$ are drifting and fluctuating quantities. Their drift dynamics is typically much slower than the very fast wave oscillations,

$$\frac{|\dot{e}_l|}{|e_l|}, \frac{|\dot{\phi}_l|}{|\phi_l|} \ll \omega_l. \tag{8.35}$$

Thus, we completely separate off the fast oscillating wave dynamics and look at the slow drift dynamics. The stochastic fluctuations will be treated only qualitatively. For an incoherent lamp light the field amplitudes and phases are only weakly correlated random numbers resulting in a small common field amplitude $E^{\text{lamp}}(t)$, as qualitatively shown in Fig. 8.3. However, a laser light source manages to self-organize in such a way that all amplitudes, frequencies and phases become synchronized up to some stochastic fluctuations,

$$E^{\text{laser}}(x,t) = Ne(t)\sin\left(\omega(x/c - t) + \phi(t)\right), \tag{8.36}$$

The resulting field amplitude is qualitatively shown in Fig. 8.4. To see how this comes about we sketch a semi-phenomenological treatment of the drift aspect of laser dynamics (see e.g. [5]). In a two level laser system with atomic energy level difference $\epsilon_2 - \epsilon_1 = \omega$ and level occupation numbers N_1 and N_2, three types of processes can

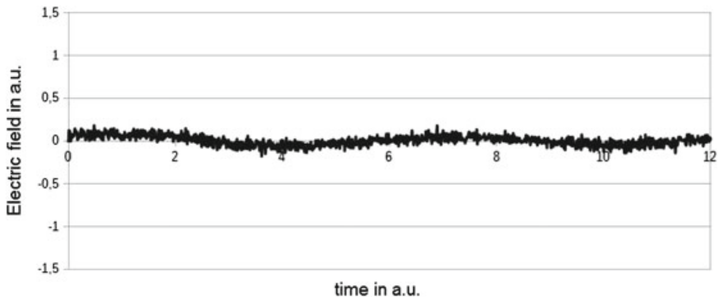


Fig. 8.3 Qualitative sketch of the fluctuating field amplitude of an incoherent light source

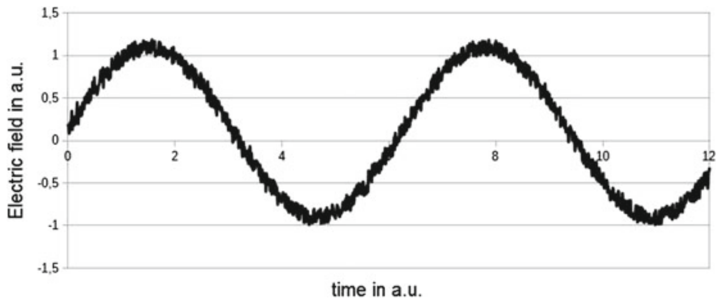


Fig. 8.4 Qualitative sketch of the fluctuating field amplitude of a coherent laser light source

occur: (1) spontaneous emission of a photon such that an electron changes from ϵ_2 to ϵ_1, (2) absorption of a photon with frequency ω to raise an electron from ϵ_1 to ϵ_2, (3) and stimulated emission of a photon with an electron moving from level ϵ_2 to level ϵ_1. While the spontaneous emission is independent of the field strength E and occupation number, the absorption and induced emission depend on the field strength and the occupation number of the initial level. The change of the electric field is due to the coupling to the dipole fields and has some relaxation,

$$\dot{E} = -\kappa E + g \sum_l e_l, \tag{8.37}$$

where κ is a relaxation parameter and g a coupling constant. On the other hand, the electric field E changes the dipole fields due to absorption and spontaneous emission

$$\dot{e}_l = -\gamma e_l + gdE, \tag{8.38}$$

where γ is a relaxation parameter for the dipoles and d measures the difference in occupation numbers $D := N_2 - N_1$ over the number of dipoles N,

$$d = \frac{N_2 - N_1}{N} = \frac{D}{N}, \tag{8.39}$$

Usually, d is negative, because the lower level has higher occupation numbers in an equilibrium situation. However, if one manages to get an occupation number inversion by external pumping, one can reach a non-equilibrium situation with $d > 0$. Furthermore, the occupation number difference will decrease as the energy of the electric field becomes larger. The energy is quadratic in the field strength. Thus, the difference can be modeled as

$$D = D_0 - cE^2, \tag{8.40}$$

where c is some positive constant. We see, that (8.37–8.40) look similar to the Haken-Zwanzig model. Provided the dipoles relax fast, $|\dot{e}_l| \ll \gamma |e_l|$, we conclude that the dipoles follow the external field instantaneously,

$$e_l = \frac{gd}{\gamma} E, \tag{8.41}$$

having the same frequency and phase as the field E. We finally arrive at a drift equation for the electric field of Landau model type,

$$\boxed{\dot{E} = -V'(E)\ , \ \ V(E) = \left(\frac{g^2 D_0}{2\gamma} - \frac{\kappa}{2}\right) E^2 - \frac{g^2 c}{4\gamma} E^4.} \tag{8.42}$$

Now, as soon as the lasing condition,

$$\frac{g^2 D_0}{\gamma} - \kappa > 0, \tag{8.43}$$

is fulfilled, one finds two stable finite lasing field strength minima, separated by an unstable maximum at $E = 0$. In the non-lasing regime, the stable field strength is $E = 0$ and fluctuations make the incoherent light.

8.4 Brownian Motion in Random Matrix Theory

Systems with disorder or complex dynamics can be captured by a stochastic modeling and are described by an ensemble of Hamiltonian matrices in a certain matrix representation. The relevant physical quantities can be obtained from the statistical properties of the Green's function $G^+(\boldsymbol{x}, \boldsymbol{x}'; E) = \langle \boldsymbol{x} \mid [E + i0 - H]^{-1} \mid \boldsymbol{x}' \rangle$ as the matrix representation of the resolvent $[z - H]^{-1}$ at energies that approach the real spectrum from the upper complex half plane $z = E + i0$. The field theoretic approach to the quantum Hall effect briefly described in Sect. 7.3.3 stems from a mapping of such random matrix problem. Here we will look at a simpler modeling focusing on some universal properties of complex or disordered systems in a certain limit of their dynamics, called ergodic limit. Owing to the energy eigenstate representation of the resolvent,

$$[E + i0 - H]^{-1} = \sum_{\alpha_n} \frac{\mid \psi_{\alpha_n} \rangle \langle \psi_{\alpha_n} \mid}{E - \alpha_n + i0}, \tag{8.44}$$

the statistics of $G^+(\boldsymbol{x}, \boldsymbol{x}'; E)$ is contained in the joint probability distribution of eigenvalues, ε_α, and eigenvectors, ψ_α,

$$\mathcal{P}\left(\varepsilon_{\alpha_1}, \psi_{\alpha_1}, \varepsilon_{\alpha_2}, \psi_{\alpha_2}, \varepsilon_{\alpha_3}, \psi_{\alpha_3}, \ldots\right). \tag{8.45}$$

To get some feeling about the nature of the statistical problem we consider the Hamiltonian in a finite basis $\{|i\rangle\}_{i=1,\ldots,N}$ as hermitian $N \times N$ matrix $H_{ik} = \langle i \mid H \mid k \rangle$. The diagonalizing unitary matrix $U \in \mathcal{U}(N)$ with matrix elements $U_{k\boldsymbol{a}}$ fulfills

$$\sum_{ik} U^\dagger_{\beta i} H_{ik} U_{k\alpha} = \varepsilon_\alpha \delta_{\alpha\beta}. \tag{8.46}$$

It is related to the amplitude of an eigenstate ψ_α in the $\{|k\rangle\}$ basis by

$$\psi_\alpha(k) := \langle k | \psi_\alpha \rangle = U_{k\alpha}. \tag{8.47}$$

We can think of the randomness of H as being controlled by a large number of independent parameters, e.g. strength and position of point scatterers in space for a spatially disordered system. We can also think of the matrix elements H_{ik} as random transition amplitudes in a complex system of states labeled by quantum numbers i. Each realization of the Hamiltonian represents one point in a high dimensional parameter space.

As to the problem of the statistics of eigenvectors one can easily imagine two extreme situations. In the first situation the probability distribution of U is peaked at a single fixed matrix. This matrix singles out a certain basis of eigenstates. We choose this matrix as the unit matrix, such that the Hamiltonian is diagonal in this basis

$$H_{ik} = \varepsilon_i \delta_{ik}. \tag{8.48}$$

The corresponding **eigenstates are localized** to certain quantum number states, i.e.

$$\psi_\alpha(k) = \delta_\alpha k. \tag{8.49}$$

The second extreme situation corresponds to an isotropic distribution for the unitary matrix. By this we mean that the probability density, $\mathcal{P}(U)$, to find a certain unitary matrix U within the volume element, $d[\mathcal{U}(N)]$, is equal for all elements $U \in \mathcal{U}(N)$. The volume element itself stays invariant under the action of group transformations (invariant measure) $d[\mathcal{U}(N)]$, i.e. it does not single out any particular element. The corresponding **eigenstates are isotropically distributed** among all possible eigenstates, no basis is preferred. Such systems are called ergodic. Of course, both extreme situations are not generic ones, but can serve as limiting situations (phases) in a stability analysis of complex or disordered systems. Therefore, to model an ergodic phase we assume the distribution of the Hamiltonian matrix to be unitarian invariant. One of the simplest possible choices is the so-called Gaussian unitary ensemble (GUE) introduced by Wigner [6] when studying the level statistics of complex nuclei,

$$\mathcal{P}\left(\{\mathrm{Re}\ H_{ik}, \mathrm{Im} H_{ik}\}\right) \mathrm{d}\,[H] = \tilde{C}_N \exp\left(-\frac{N}{2\mathcal{E}_0^2} \mathrm{Tr}\ H^2\right) \mathrm{d}\,[H]\,. \tag{8.50}$$

Here $\tilde{C}_N$ is a normalization constant, $\mathcal{E}_0$ some arbitrary energy scale and the volume element is defined in terms of the independent matrix elements of H as

$$\mathrm{d}\,[H] = \prod_1^N \mathrm{d}H_{ii} \prod_{i<k}^N \mathrm{d}\,(\mathrm{Re}\ H_{ik})\, \mathrm{d}\,(\mathrm{Im} H_{ik}). \tag{8.51}$$

Since $\mathrm{Tr}\ H^2 = 2\sum_{i<k} \left[(\mathrm{Re}\ H_{ik})^2 + (\mathrm{Im} H_{ik})^2\right] + \sum_i H_{ii}^2$ the GUE describes a random matrix with all its elements uncorrelated. Each of the elements vanishes on average and its absolute value fluctuates, $\left\langle |H_{ik}|^2 \right\rangle = \mathcal{E}_0^2/N$. If we think of the model in a site-representation we see that by (8.50) transition amplitudes from from one site to another are equally probable independent of the distance between sites. This

means that we can associate a vanishing traveling time scale t_D to travel through the whole system. Ergodic systems are systems where the traveling time through the system is much smaller than any other relevant probing time scale. In the absence of intrinsic time scales one expects universal behavior.

Introducing eigenvalues ε_α and eigenvectors $\psi_\alpha(k) = U_{k\alpha}$ one can transform the probability $\mathcal{P}(\{\text{Re } H_{ik}, \text{Im} H_{ik}\})\text{d}\,[H]$ to these variables at the expense of introducing a Jacobian between the set of variables. To calculate this Jacobian one needs precise knowledge about the parametrization of the continuous group $U(N)$. Fortunately, these parametrizations are known and the Jacobian can be calculated (see [7]), the integration over $\text{d}[\mathcal{U}(N)]$ being a trivial normalization (since $\text{Tr } H^2$ is unitarian invariant), and one obtains for the joint probability of eigenvalues

$$\mathcal{P}(\varepsilon_1, \ldots, \varepsilon_N) = C_N \prod_{\alpha<\beta} \left(\varepsilon_\alpha - \varepsilon_\beta\right)^2 \exp\left(-\sum_\alpha^N \frac{N}{2\mathcal{E}_0^2}\varepsilon_\alpha^2\right). \tag{8.52}$$

The factors in front of the exponential are due to the Jacobian and describe that the probability to find two levels close to each other vanishes; a phenomenon which is denoted as **level repulsion**. The factors can be rewritten as $\exp\left(2\sum_{\alpha<\beta}\ln|\varepsilon_\alpha - \varepsilon_\beta|\right)$ such that the joint probability describes a classical **Gibbs ensemble**,

$$\mathcal{P}(\{\varepsilon_{\boldsymbol{a}}\}) = C_N \exp\left[-\beta\mathcal{H}(\{\varepsilon_\alpha\})\right], \tag{8.53}$$

of a gas of particles with coordinates ε_α and a Hamiltonian

$$\boxed{\mathcal{H}(\{\varepsilon_\alpha\}) = \frac{1}{2}\sum_{\alpha\neq\beta} U(\varepsilon_\alpha, \varepsilon_\beta) + \sum_\alpha V(\varepsilon_\alpha)} \tag{8.54}$$

that contains a logarithmic two-body interaction $U(x, y) = -\ln|x - y|$ and a one-body (confining) potential $V(x) = Nx^2/(2\beta\mathcal{E}_0^2)$. The inverse temperature is $1/T = 2$ for the GUE. A related ensemble of real symmetric matrices, reflecting time inversion symmetry, denoted as Gaussian orthogonal ensemble (GOE), gives rise to the same Gibbs ensemble, the only change being $1/T = 1$ ($1/T = 4$ corresponds to spin systems with time reversal symmetry, for more details and review see [7]). From a symmetry classification point of view, adopted in [8], further matrix ensembles have been introduced and extensively investigated since. The interpretation of the joint probability distribution of levels as a Gibbs-ensemble has led to an important mean-field approach to level statistics which we will embed into a field theoretic description in the following Sect. 8.5.

In the standard random matrix ensembles a number of results are well known which we will not repeat here (for a short overview see e.g. Sect. IIIA in [9]). The main result is that ideal ergodic systems (with vanishing time scale t_D) are characterized by an incompressible spectrum of correlated energies. Here, we like to present a stochastic process that leads to the GUE as its equilibrium state and which avoids the tedious calculation of Jacobians and allows a direct way, by perturbation theory of second order, to find the Fokker-Planck equations for reduced variables. The construction goes back to Dyson who constructed an Ornstein-Uhlenbeck process for matrices in fictitious time s that relaxed to the Wigner Dyson equilibrium ensemble [10]. The general ansatz for a stepwise change of the Hamiltonian is

$$\delta H = \sqrt{\delta s} H_1 + \delta s H_2 \tag{8.55}$$

with statistical properties of drift and diffusion,

$$\langle H_1 \rangle = 0, \; \langle H_2 \rangle = D^{[1]}, \; \langle H_{1kl} H_{1k'l'} \rangle = 2D^{[2]}_{kl,k'l'}. \tag{8.56}$$

Note, that $D^{[1,2]}$ will in general depend on $H(s)$. This general ansatz can be used for drift and diffusion of any property derived from H, e.g. for the resolvent $G = [z - H]^{-1}$ by perturbation theory up to second order in δH by terminating the Dyson equation after two terms

$$\delta G = G\delta H G + G\delta H G\delta H G. \tag{8.57}$$

This leads to drift and diffusion of a Fokker-Planck equation for the distribution of the resolvent with respect to the evolution parameter s,

$$\frac{\langle \delta G_{kl} \rangle}{\delta s} = \sum_{k'l'} G_{kk'} G_{ll'} D^{[1]}_{k'l'} + 2 \sum_{mnm'n'} G_{km} G_{m'n} G_{n'l} D^{[2]}_{mm',nn'} \tag{8.58}$$

$$\frac{\langle \delta G_{kl} \delta G_{k'l'} \rangle}{\delta s} = 2 \sum_{mnm'n'} G_{km} G_{nl} G_{k'm'} G_{n'l'} D^{[2]}_{mn,m'n'}. \tag{8.59}$$

The corresponding Fokker-Planck equation may be useful as a starting point to investigate the distribution of matrix elements of the resolvent, e.g. the imaginary part of diagonal elements which captures the local density of states. In this general non-linear form it cannot be solved and further approximations are necessary; e.g. linearization and decoupling. One may also have a direct look at the eigenvalues by second order perturbation theory and one finds that, in the general case, the eigenvalue statistics is coupled to the eigenvector statistics. To the authors knowledge, this general concept of Brownian motion in random matrix theory has not been fully exploited yet. However, in the extreme situation of a fully isotropic ensemble with respect to unitary rotations, the situation simplifies and has been studied by Dyson.

The following choice by Dyson guarantees that diffusion with strength D is uncorrelated and equal for all absolute values of the complex matrix H with uncorrelated real parts H^1 and imaginary parts H^2.

$$\left\langle \delta H^{1,2}_{ik} \delta H^{1,2}_{lm} \right\rangle = \delta_{il} \delta_{km} (1 + \delta_{ik}) D \delta s. \tag{8.60}$$

The drift

$$\delta H_{ik} = -H_{ik}\frac{\delta s}{\tau} \tag{8.61}$$

serves to relax to an equilibrium situation for large s with relaxation time τ. The corresponding Ornstein-Uhlenbeck process for H and initial H_0 has the solution

$$P_s(H) = \text{const.}(1-q^2)^{-f/2}\exp\left\{\frac{-\text{Tr }(H-qH_0)^2}{2D\tau(1-q^2)}\right\}, \tag{8.62}$$

where $q = e^{-s/\tau}$ and f is the number of independent matrix elements. The stationary solution just equals the standard isotropic Gaussian ensemble of (8.50) with parameters D and τ appropriately identified.

For the eigenvalues Dyson's choice of diffusion and drift of H leads to the following drift and diffusion for the eigenvalues by second order perturbation

$$\langle\varepsilon_k\rangle = -\varepsilon_k\frac{\delta s}{\tau} + \sum_{l\neq k}\frac{D}{\varepsilon_l - \varepsilon_k} \tag{8.63}$$

$$\langle\varepsilon_k\varepsilon_l\rangle = \delta_{kl}2D\delta s \tag{8.64}$$

Consequently, the equilibrium level distribution is just the standard isotropic Gaussian ensemble level distribution (8.52) with parameters appropriately identified.

Note, the level repulsion term is now a result of simple second order perturbation theory and not a result of sophisticated investigations about invariant measures.

8.5 A Field Theory for Universal Fluctuations

We have a look at the Gibbs ensemble in (8.54) and want to set up a field theory for fluctuations of a general dimensionless macroscopic additive variable X which can be written as a so-called **linear statistics** of the N microscopic level variables x_i, $X = \sum_i f(x_i)$ in a Gibbs ensemble of a classical gas determined by a parameter free (universal) two-body potential (which can be chosen to be symmetric) and a parameter-dependent one-body (confining) potential which contains the prefactor N,

$$\begin{aligned}
\mathcal{P}(X) &= \int \mathrm{d}^N x\, \mathcal{P}(\{x_i\})\,\delta\left(X - \sum_i f(x_i)\right),\\
\mathcal{P}(\{x_i\}) &= Z^{-1}\exp -\beta\mathcal{H}(\{x_i\}),\\
\mathcal{H}(\{x_i\}) &= \frac{1}{2}\sum_{m,n}U(x_n,x_m) + \sum_i V(x_i).
\end{aligned} \tag{8.65}$$

As an example, think of the number of energy levels in some energy interval, $N(\delta E; E_0)$. In this context x_i are energy levels and $f(x)$ could be chosen as a characteristic function of an interval of width δE centered around E_0; as a smooth function it could be a Gaussian,

$$N((\delta E; E_0) = \sum_i f(x_i);\ f(x) = \exp[-(x - E_0)^2/2(\delta E)^2]. \tag{8.66}$$

Another example is the total transmittance T of a wave guide with a large number of traveling wave modes in a prescribed direction. The total transmittance is the sum of the eigenvalues $\mathcal{T}_i$ of the transmission probability matrix. Explicit expressions will be discussed in subsequent sections. Such wave modes can be charged or uncharged modes like electron modes, electromagnetic modes and sound modes. For charged modes the transmittance is the conductance in dimensionless units, as found by Landauer [11] and generalized by Büttiker [12].

In a work on electron conductance Beenakker pointed out [13] that the one-body potential in the Gibbs ensemble can be viewed as a source term in the partition sum

$$Z[V] = \int \mathrm{d}^N x \exp\left[-\beta \mathcal{H}\left(\{x_i\}\right)\right]. \tag{8.67}$$

All cumulants[2] of the level density, $\varrho(x) := \sum_i \delta(x - x_i)$, can be obtained by functional derivatives

$$\langle\langle \varrho(x_1) \dots \varrho(x_k) \rangle\rangle = \frac{\delta^k \ln Z}{\delta\left(-\beta V(x_1)\right) \dots \delta\left(-\beta V(x_k)\right)}. \tag{8.68}$$

Cumulants of a linear statistics $X = \sum_i f(x_i)$ are given by integration

$$\langle\langle X^k \rangle\rangle = \int dx_1 \dots dx_k \,\langle\langle \varrho(x_1) \dots \varrho(x_k) \rangle\rangle\, f(x_1) \dots f(x_k). \tag{8.69}$$

The whole distribution $\mathcal{P}(X)$ can be obtained from a modified partition sum $Z(\kappa)$,

$$\mathcal{P}(X) = \int d\kappa\, e^{i\kappa X} Z(\kappa), \tag{8.70}$$

where $Z(\kappa)$ follows from Z through a simple shift in the one-body potential

$$V_\kappa(x) := V(x) + i\frac{\kappa}{\beta} f(x). \tag{8.71}$$

[2]Recall that cumulants $\langle\langle X^n \rangle\rangle$ are linear combinations of moments of order $k \leq n$. While moments can be generated from a partition sum Z, the corresponding cumulants are generated by $\ln Z$. The Gaussian distribution is characterized by vanishing cumulants for $n \geq 3$.

In order to work with functional derivatives one has to know Z (or $Z(\kappa)$) as an explicit functional of the one-body potential. Alternatively, the knowledge of the average level density as a functional of the one-body potential would be enough,

$$\nu(x) := \langle \varrho(x) \rangle = \nu[V_\kappa(x)]. \tag{8.72}$$

A field theoretic approach by the author [14] will be discussed now. Starting from the partition sum Z, or $Z(\kappa)$, one proceeds along the prescriptions of Sect. 5.6 which is also analog to the derivation of the field theory for the quantum Hall Effect, briefly discussed in Sect. 7.3.3, albeit with much less technicalities.

1. The Hamiltonian is expressed by the level density $\varrho(x)$, replacing sums by integration. Here the absence of self-interaction is ignored in a first step and cured later on an effective potential level,

$$\sum_{n \neq m} U(x_n, x_m) \approx \int \mathrm{d}x\, \mathrm{d}y\, \varrho(x)\varrho(y)U(x, y). \tag{8.73}$$

2. With the help of a δ-functional,

$$\delta[\nu - \phi]D\phi \tag{8.74}$$

a field $\phi(x)$ is introduced that takes the role of the level density.
3. The δ-functional is replaced by its Fourier representation,

$$\exp\left\{ i \int \mathrm{d}x\, \psi(x)\, [\nu(x) - \phi(x)] \right\}, \tag{8.75}$$

on introducing a dual field $\psi(x)$.
4. Now, the original integration over the set $\{x_i\}$ can be carried out leaving a field theoretical partition function in terms of two field degrees of freedom, $\phi(x)$ and $\psi(x)$.
5. Due to the two-body character of the original $\mathcal{H}$ the field $\phi(x)$ can be integrated out by a Gaussian integration. The final result is a path integral representation of the partition sum Z or of the complete distribution function $\mathcal{P}(X)$, where the integration runs over field configurations of $\psi(x)$. We concentrate on $\mathcal{P}(X)$ which reads

$$\begin{aligned}
\mathcal{P}(X) &= \int D\,[\psi] \exp -S\,[\psi; X], \\
S\,[\psi; X] &= \frac{-1}{2\beta}\,(\psi|\, K\, |\psi) + \frac{1}{2}\,(f|\, K\, |f)\; Q^2(\psi; X) \\
&\quad + F_N\,[\psi + \beta V]\,.
\end{aligned} \tag{8.76}$$

Here we made use of a short-hand scalar product notation,

$$(f|A|g) := \int \mathrm{d}x\,\mathrm{d}y\, f(x)A(x,y)g(y), \quad (f|g) := \int \mathrm{d}x\, f(x)g(x). \tag{8.77}$$

K denotes the inverse operator of U ($U(x,y) = (x|\,U\,|y)$), the functional $Q(\psi; X)$ is defined as

$$Q(\psi; X) := \frac{X - \beta^{-1}\,(f|\,K\,|\psi)}{\beta^{-1}\,(f|\,K\,|f)}, \tag{8.78}$$

and the functional F_N is a free energy of N independent particles with one-body-potential $\psi + \beta V$,

$$F_N\,[\psi + \beta V] := -N \ln\left[\int \mathrm{d}x\, \exp\left[-\left(\psi(x) + \beta V(x)\right)\right]\right]. \tag{8.79}$$

The omission of the self-interaction can be cured on an effective potential level. By shifting the one-body-potential $V(x)$ to $\tilde{V}(x) = V(x) - \frac{1}{2}U(x, x + \Delta(x))$ where $\Delta(x)$ is the average level spacing at x, the theory is able to account for those quantities that are smooth on the scale of $\Delta(x)$. For example, with the logarithmic interaction, $U(x,y) = -\ln\mid x - y\mid$ the effective potential reads $\tilde{V}(x) = V(x) - \frac{1}{2}\ln\nu(x)$.

The path integral in (8.76) cannot be calculated exactly. However, for large N one can use the method of stationary action. Recall that $V(\lambda)$ contains the prefactor N which we assume to be large: $N \gg 1$. Introducing the **mean-field** level density ν_X^0 as

$$\nu_X^0 := \frac{N}{Z_X^0}\exp\left[-\left(\psi_X^0 + \beta V\right)\right], \tag{8.80}$$

$$Z_X^0 := \int d\lambda\, \exp\left[-\left(\psi_X^0(\lambda) + \beta V(\lambda)\right)\right], \tag{8.81}$$

corresponding to the stationary solution,

$$\left.\frac{\delta S}{\delta\psi}\right|_{\psi_X^0} = 0, \tag{8.82}$$

the mean-field equation reads[3]

$$\mid\nu_X^0) = -\tilde{K}\left|V + \beta^{-1}\ln\nu_X^0\right) + \beta^{-1}Q(X)\tilde{K}\,|f) + \frac{NK\,|1)}{(1|\,K\,|1)}. \tag{8.83}$$

[3]Equation (8.83) is identical to the one obtained by Dyson in the standard random matrix ensemble [10].

Here the kernel $\tilde{K}$ is defined as

$$\tilde{K} = K - \frac{K\,|1)\,(1|\,K}{(1|\,K\,|1)}, \quad \tilde{K}\,|1) = (1|\,\tilde{K} = 0, \tag{8.84}$$

and $Q(X)$ as

$$Q(X) := \frac{X - \overline{X}_X}{\beta^{-1}\,(f|\,\tilde{K}\,|f)} \tag{8.85}$$

with

$$\overline{X}_X := -\,(f|\,\tilde{K}\,\big|V + \beta^{-1}\ln\nu_X^0\big) + \frac{N\,(f|\,K\,|1)}{(1|\,K\,|1)}. \tag{8.86}$$

In deriving these equations it has been used that the mean-field level density is normalized $\left(1 \mid \nu_X^0\right) = N$ and yields the current X as an expectation value $\left(f \mid \nu_X^0\right) = X$.

Now one can draw the following conclusions:

1. For $|V(\lambda)| \gg \beta^{-1}\ln\nu_X^0$ the expression $\overline{X}_X$ equals the average value of X, independently of current X. Since V contains the large factor N the inequality is satisfied as long as
$$|\delta X| \ll \langle X\rangle, \quad \langle X\rangle \gg 1. \tag{8.87}$$
2. The stationary point of S is then given by
$$S\left[\psi_X^0; g\right] = \frac{1}{2}\frac{(X - \langle X\rangle)^2}{\beta^{-1}\,(f|\,\tilde{K}\,|f)} + S_{\langle X\rangle}, \tag{8.88}$$
where $S_{\langle X\rangle}$ is independent of current X.
3. One can also analyze fluctuations around the stationary solution and show that they give sub-leading contributions to the path integral. Finally, one arrives at the conclusion that the distribution of the linear statistics in a Gibbs ensemble with universal two-body interaction and a parameter dependent one-body potential is, for $|\delta X| \ll \langle X\rangle \gg 1$,
$$\mathcal{P}(X) = \text{const.}\exp\left[-\frac{(X - \langle X\rangle)^2}{2\beta^{-1}\,(f|\,\tilde{K}\,|f)}\right] \tag{8.89}$$
up to $\mathcal{O}(\ln X)$ corrections in the exponent.

Therefore, the distribution of the dimensionless linear statistics in the regime of a large average value is described by a Gaussian with a variance,

$$\left\langle(\delta X)^2\right\rangle = \beta^{-1}\,(f|\,\tilde{K}\,|f), \tag{8.90}$$

being independent of the average value and only depending on the inverse kernel of the two body potential in a quadratic form with the defining function f of the linear statistics. In the context of standard random matrices the variance of the number of levels in an interval with large average number $\langle N \rangle \gg 1$ thus turns out to be of order 1,[4]

$$\left\langle (\delta N)^2 \right\rangle \approx 1. \tag{8.91}$$

This result is plausible as the strong level repulsion in ergodic systems, captured by the parameter free two body interaction potential $U(x, y)$, makes the spectrum of levels incompressible such that the number in a given window cannot fluctuate strongly and the level number variance is of order 1, independent of the large number of levels in that window. In the context of large average transmittance $\langle T \rangle \gg 1$ the variance is, for similar reasons, of order unity, too,

$$\left\langle (\delta T)^2 \right\rangle \approx 1. \tag{8.92}$$

Thus, these type of fluctuations run under the name of universal fluctuations.

8.6 Transfer Matrix as Semi-Group Dynamics

When systems have a preferred long direction and transverse short directions (like a wire or a wave guide) it can be helpful to consider the system as quasi-one-dimensional (quasi-1D) with a finite number N_c of quantum numbers labeling the quantum states due to the finite extension in transverse direction. We will assume that this number does not change along the preferred long direction. To exploit the quasi-1D character one can try to do calculations of partition sums, or eigenvalue problems, or scattering problems by a step by step procedure in the preferred direction. This step by step procedure has a one-parameter continuous semi-group character if the units can be defined as individual units coupled at their boundaries. The parameter is the increasing system length L in the preferred direction. If the semi-group elements can be represented by matrices and the group operation by multiplication such matrices are called transfer matrices. We will exemplify this for wave guides in a scattering set up with random locally weak scatterers to calculate transmission probabilities. Thereby we make contact with the previously mentioned transmission matrix formulation of transmittance and in Sect. 8.7 we look at an explicit renormalization group treatment of the Anderson localization problem in 1D and of a quantum Hall effect in a setup of two intertwined chiral 1D wave guides.

In a scattering problem for N_c wave modes (channels) a scattering matrix can be defined,

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \tag{8.93}$$

[4] When f is smooth; for a sharp step function a weak logarithmic dependence on the average level number remains.

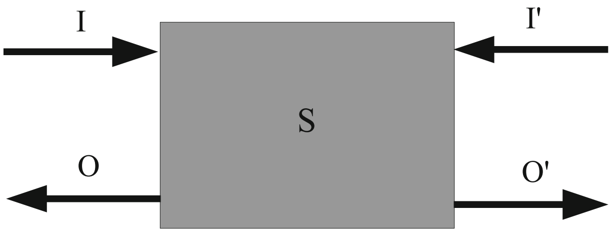


Fig. 8.5 Visualizing the S-matrix relating incoming and outgoing scattering fluxes from *left* and *right*

connecting incoming and outgoing fluxes left and right of a scattering region, t, r, t' and r' being $N_c \times N_c$ matrices of transmission and reflection coefficients for scattering from left to right and vice versa, respectively (see Fig. 8.5),

$$\begin{pmatrix} O \\ O' \end{pmatrix} = S \begin{pmatrix} I \\ I' \end{pmatrix}. \tag{8.94}$$

The probability flux conservation $|I|^2 + |I'|^2 = |O|^2 + |O'|^2$ requires the S-matrix to be unitary,

$$SS^\dagger = 1_{2N_c}. \tag{8.95}$$

Let us briefly mention how this S-matrix is related to a Hamiltonian dynamics (see textbooks on formal scattering theory in quantum mechanics, e.g. [15]). The Hamiltonian can be decomposed into a part that describes wave guides free of any scattering, H_0, and a part H_1 that describes the finite scattering region. The scattering states of the wave guides have a continuous energy spectrum which can be chosen to obey energy normalization

$$\langle \alpha(E) | \alpha(E') \rangle = \delta(E - E'). \tag{8.96}$$

The S-matrix as defined by (8.94) at conserved energy E is given as

$$S_{\alpha\beta} = \delta_{\alpha\beta} - 2\pi i \mathrm{T}_{\alpha\beta} \tag{8.97}$$

where the transition operator T is related to the Hamiltonian's resolvent (Green's function) $G^+ = (E + i0^+ - H)^{-1}$ by

$$\mathrm{T} = H_1 + H_1 G^+ H_1. \tag{8.98}$$

Note that $|\,\alpha\rangle$ describe the incoming and outgoing modes corresponding to H_0 and the matrix elements of T are taken with these modes. Thus, the S-matrix is a well defined object capturing the long time averaged scattering amplitudes following from the Hamiltonian dynamics of a finite scattering region attached to wave guides. Here, however, we consider the matrix elements as starting point of the modeling and don't bother how they might have been calculated from a Hamiltonian.

The idea of a transfer matrix can be exploited by writing the relation between in and out modes as a relation between left and right modes. We define the transfer matrix M

$$\begin{pmatrix} I' \\ O' \end{pmatrix} = M \begin{pmatrix} O \\ I \end{pmatrix}. \tag{8.99}$$

By algebra one finds from the S-matrix that the transfer matrix M can be expressed as

$$M = \begin{pmatrix} \left(t^{\dagger}\right)^{-1} & r' t'^{-1} \\ -t'^{-1} r & t'^{-1} \end{pmatrix}. \tag{8.100}$$

The probability flux conservation requires the symmetry property

$$M \sigma_z M^{\dagger} = \sigma_z, \tag{8.101}$$

with σ_z being the Pauli matrix, which is diagonal, $(1_{N_c}, -1_{N_c})$. The semi-group character of the transfer matrix becomes obvious when two scattering regions are put together,

$$M_{1+2} = M_2 M_1, \tag{8.102}$$

as shown in Fig. 8.6.

As a macroscopic observable of great practical relevance we will address the (total) transmittance,

$$\boxed{T := \mathrm{Tr}\left\{ t t^{\dagger} \right\}}. \tag{8.103}$$

For charged modes this total transmittance equals the dimensionless conductance g of a two-probe linear response setup. The conductance in standard units is then given by g times the natural unit of conductance, e.g. e^2/h for electron modes. This relation of transmittance to conductance has been found by Landauer [11] and was

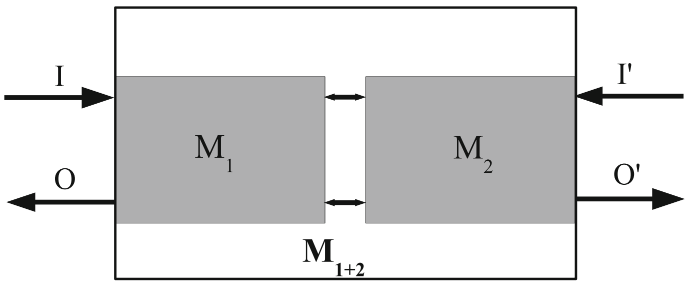


Fig. 8.6 Visualizing the composite transfer matrix M_{1+2} of two scattering regions connected by wave guides

generalized to a scattering matrix theory of admittance for multi-probe setups by Büttiker and coworkers (for review see [16]). The relation between the S-matrix and the transfer matrix M allows to express the transmittance as

$$T = \mathrm{Tr}\, \frac{2}{MM^\dagger + (MM^\dagger)^{-1} + 2}. \tag{8.104}$$

The matrices $tt^\dagger$ and $MM^\dagger$ occurring in the transmittance formulas (8.103, 8.104) are hermitian and, thus, can be diagonalized. The positive eigenvalues are denoted as $0 \leq \mathcal{T}_i \leq 1$ (for $tt^\dagger$) and as $0 \leq e^{\nu_i} < \infty$ (for $MM^\dagger$). The eigenvalues of $MM^\dagger$ appear in inverse pairs and we can restrict to those with $\nu_i \geq 0$. The transmittance reads in the corresponding eigenvalue representation

$$g = \sum_i \mathcal{T}_i = \sum_i \frac{2}{1 + \cosh \nu_i}. \tag{8.105}$$

Here we see, as announced in the foregoing section on universal statistics, that in these S-matrix models the transmittance appears as a linear statistics. Therefore, the results on universal fluctuations apply to transmittance in ergodic regimes (where the traveling time through the disordered system is much shorter than any probing time scale).

8.7 Quantum and Markov: Anderson Localization

In the following we will look at the opposite limit where the modes become unable to travel through a disordered system because of destructive interference after multiple scattering events. This Anderson localization is a generic phase in quasi-1D coherent disordered wave guides. From the point of view of this book it is interesting that this generic quantum phenomenon can be best captured by a Markov process in the pseudo-time variable system size L. We thus have a closer look at the modeling in quasi-1D based directly on the scattering matrix or, equivalently, on the transfer matrix. The modeling of the coherent disordered wave guide goes by

1. fixing the statistical properties of the S-matrix corresponding to a small strip of length δL, denoted as strip S-matrix $S(\delta L)$ and
2. the composition of the whole wave guide by putting statistically independent strip S-matrices in series by the multiplication of corresponding strip transfer matrices $M(\delta L)$.

The assumption of statistical independence is justified if the strip length δL is larger than the microscopic disorder potential correlation length l_V. Furthermore, the modeling allows for a simple description of the mean free path corresponding to the strip S-matrix. As long as the corresponding reflection probabilities $\mid r_{\boldsymbol{a}\beta} \mid^2 =: R_{\boldsymbol{a}\beta}$ are small compared to 1 the mean free path l_m is large compared to δL and can be defined as follows

$$\boxed{\frac{\delta L}{l_m} := N_c^{-2} \sum_{\boldsymbol{a}\beta} \left\langle R_{\boldsymbol{a}\beta}(\delta L) \right\rangle}. \tag{8.106}$$

This situation is called local weak scattering as the mean free path is larger than the strip length.

The S-matrix fulfills the requirement of unitarity. To model systems with specific symmetry properties one can impose further symmetry constraints on S. Internal degrees of freedom, such as spin, can also be incorporated by taken the corresponding quantum numbers of wave modes into account.

Thus, the modeling rests on a microscopic length scale, the mean free path l_m, and symmetry properties. The statistical problem is thus defined by (A) fixing the distribution of the strip S-matrix $S(\delta L)$ and (B) by applying the semi-group composition law for the corresponding transfer matrices,

$$\boxed{M(L + \delta L) = M(\delta L) M(L)}. \tag{8.107}$$

This defines a stochastic multiplicative process where the pseudo-time parameter is the system length L. The statistical properties of the increment

$$\delta M(L, \delta L) = M(L + \delta L) - M(L) \tag{8.108}$$

are known by construction and hence it is always possible to construct a Fokker-Planck equation for the distribution function $\mathcal{P}(M; L)$ (see e.g. [17]). This is, in the local weak scattering situation, an exact equation as higher orders of a Kramers-Moyal expansion vanish in the continuous limit $\delta L \to 0$. Still, a general solution of this equation is presently not available and we will not discuss it in detail. Before looking at the simpler situation of $N_c = 1$ a little later we collect some general results for the case of an arbitrary number N_c of channels. Under the additional assumption of isotropic scattering with respect to the N_c channels a Fokker-Planck equation can be constructed in terms of only so-called radial parameters λ_i of the transfer matrix. It is known as the DMPK equation (for a review see Chap. C in [9]) and it is known that a solution has the form of a Gibbs ensemble with universal two-body potential and a parameter dependent one-body potential, as discussed in the forgoing section. This corresponds to an ergodic behavior in the transversal directions of the wave guide. For large average transmission the universal transmission fluctuations can be explicitly calculated. However, the average transmission does depend on the system length L and is large only for system lengths shorter as the localization length ξ_l to be discussed now.

The semi-group property of the transfer matrix $M(L)$ for $L = N\delta L$ contains the key to localization because eigenvalues of $MM^\dagger$ larger than 1 describe growth of amplitudes, those smaller than 1 decay. Now, mathematical theorems (see [18]) as extensions of the central limit theorem (see Appendix A.9) for large products (large sums of logarithms) to the case of products of independent random transfer matrices guarantee the existence of eigenvalues of the diagonalizable limiting matrix

$$\lim_{N\to\infty} (M(N)M^{\dagger}(N))^{\frac{1}{2N}} \tag{8.109}$$

of the form

$$(e^{\gamma_{N_c}}, \ldots, e^{\gamma_1}, e^{-\gamma_1}, \ldots, e^{-\gamma_{N_c}}). \tag{8.110}$$

The quantities $\gamma_1 < \cdots < \gamma_{N_c}$ are called Lyapunov exponents. The inverse of the smallest Lyapunov exponent serves us to define the relevant localization length of the problem

$$\xi_l := \gamma_1^{-1}\delta L. \tag{8.111}$$

In the limit of large system sizes, $N\delta L,\ N \to \infty$, following (8.104), the transmittance shows the behavior

$$\lim_{N\to\infty} \frac{1}{N} \log \mathrm{Tr}\ tt^{\dagger} = -2\gamma_1. \tag{8.112}$$

This means that the transmittance becomes exponentially small for $L \gg \xi_l$,

$$T \propto e^{-2L/\xi_l}. \tag{8.113}$$

This is interpreted as a localization of the probability to find the corresponding transport quanta in energy eigenstates to some finite region within the wave guide. Indeed, numerical calculations of the stationary eigenstates of the corresponding closed disordered wave systems show this spatial localization in typical eigenstates at the corresponding energies (for a review see [19]).

As an instructive and paradigmatic example we consider the case of $N_c = 1$. The composition law (8.107) yields, after some algebra, the composition law for the transmission (see Fig. 8.6)

$$t_{12} = \frac{t_1 t_2}{1 - r_1' r_2}. \tag{8.114}$$

Exploiting unitarity of S yields for the transmission probability

$$T = |t|^2;\ R = |r|^2;\ T = 1 - R \tag{8.115}$$

and

$$T_{12} = \frac{T_1 T_2}{1 - 2\cos(\phi)\sqrt{(1-T_1)R_2} + (1-T_1)R_2}, \tag{8.116}$$

where ϕ is the sum of phases of r_1' and r_2. Based on (8.116) one can derive an evolution equation for the probability distribution of T with increasing length L. We take $T_1 = T(L)$ and $T_2 = T(\delta L)$ and expand the denominator with respect to the small quantity $2\cos\phi\sqrt{(1-T(L))R(\delta L)}+(1-T(L))R(\delta L)$ up to second order, such that orders of $(R(\delta L))^{1/2}$ and $R(\delta L)$ are kept consistently. The result is

$$\begin{aligned}\delta T(L) := T(L+\delta L) - T(L) = T(L)\Big[&2\cos(\phi)\sqrt{1-T(L)}\sqrt{R(\delta L)}\\ &+ R(\delta L)\left(4\cos^2(\phi)(1-T(L)) - (1-T(L)) - T(L)\right)\Big]\end{aligned} \tag{8.117}$$

Averaging over realizations of increments of width δL means averaging over random phases ϕ and random $R(\delta L)$. The latter is characterized by the mean free path l_m,

$$\langle R(\delta L)\rangle = \frac{\delta L}{l_m}. \tag{8.118}$$

The resulting Kramers-Moyal coefficients stop after the second term in the continuum limit $\delta L \to 0$ and read for drift and diffusion:

$$-\frac{\langle \delta T(L)\rangle}{\delta L} = D_T^{[1]} = \frac{T^2(L)}{l_m}, \tag{8.119}$$

$$\frac{\left\langle(\delta T(L))^2\right\rangle}{2\delta L} = D_T^{[2]} = \frac{(1-T(L))T^2(L)}{l_m}. \tag{8.120}$$

The Fokker-Planck equation for the distribution of $P_L(T)$ depending on system length L can be easily brought to the form of a continuity equation

$$\boxed{\partial_L P_L(T) = (l_m)^{-1}\partial_T\left[(1-T)\,\partial_T\left(T^2 P_L(T)\right)\right]}, \tag{8.121}$$

where the current density is $J_L(T) = -(l_m)^{-1}\left[(1-T)\,\partial_T\left(T^2 P_L(T)\right)\right]$. This distribution depends on only one parameter, the mean free path l_m. The Fokker-Planck equation has two fixed points at vanishing current: T is δ-peaked at $T=1$ or alternatively at $T=0$. The fixed point at $T=1$ is unstable and any small deviation leads to a flow to the stable solution peaked at $T=0$. This can be seen in the two limiting cases: (A) $T \ll 1$ and (B) $R = 1-T \ll 1$.

For case (A) the solution is a **log-normal distribution**,

$$P_L(T)\mathrm{d}T = \frac{1}{\sqrt{4\pi L/l_m}}\exp\left[-\frac{(\ln T - (-L/l_m))^2}{2(2L/l_m)}\right]\mathrm{d}\ln T, \tag{8.122}$$

with a typical value $T_\mathrm{t} := \exp\langle \ln T\rangle = \exp(-L/l_m)$. This solution corresponds to a typical localization length of $\xi = 2l_m$. Interesting is the fact that the second parameter of the log-normal distribution, the log-variance $2L/l_m$, is simply related to the log-average value

$$\left\langle(\ln T - \langle\ln T\rangle)^2\right\rangle = 2\langle \ln T\rangle = 2L/l_m. \tag{8.123}$$

For case (B) the solution is an exponential distribution for the variable R,

$$P_L(R) = \frac{l_m}{L} \exp\left(-Rl_m/L\right) \tag{8.124}$$

with average value $\langle R(L)\rangle = L/l_m$. This solution is valid only for very small system sizes $L \ll l_m$ and becomes invalid very quickly for increasing system size L. When the system size reaches the mean free path, a cross over to the log-normal distribution with exponential localization behavior evolves. The stability of exponential localization can also be concluded by looking at the time evolution of average values of functions of T, $\langle F(T)\rangle_L$, which follows uniquely from the Fokker-Planck equation,

$$\partial_L \langle F(T)\rangle_L = (l_m)^{-1} \left\{\left\langle T^2(1-T)F''(T)\right\rangle_L - \left\langle T^2 F'(T)\right\rangle_L\right\}, \tag{8.125}$$

where F' and F'', stand for first and second derivatives with respect to T, respectively. Taking the variable $F(T) = \ln T$ yields a very simple exact equation:

$$\boxed{\partial_L \langle \ln T\rangle_L = -(l_m)^{-1}}. \tag{8.126}$$

This proofs unambiguously that the typical transmission decays exponentially for large system sizes and that the localization length is

$$\xi_l = 2l_m \tag{8.127}$$

in the 1D disordered wave guide. Notice that the distributions in both limits (A) and (B) are very broad as can be concluded from the strong growth of moments. The occurrence of broad distributions is central in disordered coherent systems (see e.g. [20]).

For arbitrary channel numbers N_c the above 1D result of a localization length of only twice the mean free path does not apply. For ergodic systems with respect to the transverse directions it turns out, as one might expect from a parallel composition law, that the localization length is

$$\xi_l(N_c) \approx N_c l_m. \tag{8.128}$$

We now switch to a related model of two intertwined chiral 1D wave guides which captures the qualitative essence of the localization-delocalization mechanism of the quantum Hall effect as discussed in Sect. 7.3. The idea goes back to the Chalker-Coddington model for the quantum Hall effect in 2D [21] which picks up the high field limit of Sect. 7.3.2, but allows for tunneling at each saddle point where equipotential lines with opposite orientation come close of about a magnetic length l_B (see [22]). The Chalker-Coddington model consists of a regular network of scatterers as displayed in Fig. 8.7.

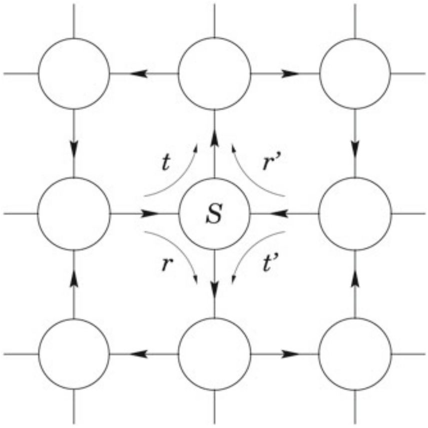


Fig. 8.7 The graphical representation of the Chalker-Coddington network model. Wave amplitudes propagating on links can be scattered either to the *left* with transmission coefficient t or to the *right* with reflection coefficient r by unitary scattering matrices situated at the nodes of the network

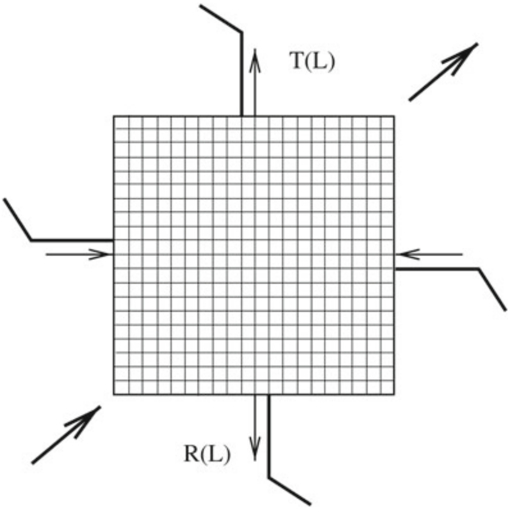


Fig. 8.8 Schematic representation of a renormalized Chalker-Coddington network of size $L \times L$ in a two-terminal set up having the same terminal structure as a cell in the original network

These scatterers, interpreted as 2D scatterers in a rectangular network, have only two ingoing modes and two outgoing modes like a scatterer in 1D. However, with the topology of the 2D network such scatterers allow for $T = 1 - R \approx 0$ only clockwise motion and for $T \approx 1$ only counter-clockwise motion, resembling equipotential orbits in the high field limit (see Fig. 7.6) for states with energy eigenvalues below or above the percolating energy level, respectively. The possibility of finite transmission or reflection at a scatterer makes the Chalker-Coddington model a quantum model for the assumed universal quantum phase transition responsible for the quantum Hall effect. Now, a real space renormalization of the Chalker-Coddington model could be build on the study of the system size L dependence of the two-terminal transmission $T(L)$ as displayed in Fig. 8.8. The calculation of macroscopic transmission to the left or to the right is, so far, possible only numerically (see [23]). However, a caricature

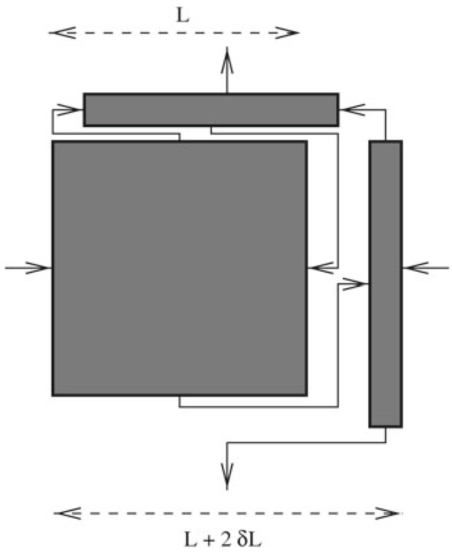


Fig. 8.9 Construction of a network of an intertwined chiral set up of two 1D wave guides by adding infinitesimal networks to a square network of linear size L. The infinitesimal networks are characterized by a small extension δL in one direction. The network is composed according to series and parallel composition laws (see text)

can be set up (see [24]) by attaching infinitesimal blocks at two sides of the 2D system as displayed in Fig. 8.9. This set up ignores lots of scatterers but keeps the chirality of clockwise or counterclockwise edge states intact. It can no longer be considered as a fully 2 dimensional Chalker-Coddington network but as a an intertwined chiral set up of two 1D wave guides. We now proceed in analogy to the one-dimensional case and take the average of the infinitesimal strips as

$$\begin{aligned} \langle R(L, \delta L)\rangle &= \langle -\ln T\rangle_L \cdot (\delta L/L), \\ \langle T(\delta L, L+\delta L)\rangle &= \langle -\ln(1-T)\rangle_L \cdot (\delta L/L). \end{aligned} \tag{8.129}$$

With this setting and taking the composition laws of 1D wave guides (8.116) in an alternating way for T in the 2D setup (now called series composition) and than for $R = 1 - T$ (now called parallel composition) the resulting Fokker-Planck equation reads

$$\partial_L P_L = -\partial_T J_L(T), \tag{8.130}$$

where the current density $J_L(T)$ is given by

$$\begin{aligned} J_L(T) = &\langle \ln T\rangle_L \frac{1-T}{2L}\,\partial_T \left\{T^2 P_L(T)\right\} \\ &+ \langle \ln(1-T)\rangle_L \frac{T}{2L}\,\partial_L \left\{(1-T)^2 P_L(T)\right\}. \end{aligned} \tag{8.131}$$

The results that one can obtain from the Fokker-Planck equation (8.131) are:

- There are three fixed point distributions: $\delta(T)$, $\delta(1-T)$, and a uniform very broad critical distribution $P^*(T) \equiv 1$.
- The δ-like solutions correspond to stable separated percolating edge states.
- The broad uniform critical distribution is unstable and describes large fluctuations at criticality. As soon as the system is slightly off criticality the distribution flows to one of the stable distributions under increasing system size L.
- To extract the critical exponent ν of the localization length one may take

$$\boxed{X_L = \langle \ln(1-T) \rangle_L - \langle \ln T \rangle_L} \tag{8.132}$$

  as a scaling variable. It has a fixed point value $X^* = 0$. Linearizing the flow equation around the fixed point distribution gives rise to a β-function for X_L which reads

$$\boxed{\frac{\mathrm{d}X_L}{\mathrm{d}\ln L} = \beta(X_L) = X_L} \,. \tag{8.133}$$

  Consequently, the critical exponent of the correlation length is $\nu = 1$.

Although this intertwined setup of two chiral 1D wave guides does not lead to the full Chalker-Coddington network, it is able to describe the correct qualitative physics of the localization-delocalization transition reminiscent of the quantum Hall effect: separated chiral edge states where the localization for one orientation means delocalization for the other and a transition with delocalization in both is unavoidable for topology reasons.

8.8 Exercises

Exercise 1: Tunneling in a Double Well
Show for a two level system with identical diagonal elements and identical off-diagonal elements that the eigenfunctions are symmetric and antisymmetric superpositions of the basis states in which the matrix was set up (see Sect. 2.3.6).

Exercise 2: Self-organized Candle Flame
The self-organized candle flame is a paradigmatic example of a so called dissipative structure where a system is subject to currents of energy and material. In the stationary state the wick supplies the flame with a liquid wax stream, evaporates in the burning zone and reacts with the oxygen of the air. This releases energy which can be transformed to light in the area of the candle flame. Argue that the internal entropy production ΔS_i scales with the volume of the flames size and argue that the exported entropy ΔS_e scales with the surface of the flames size. Find an argument of stationarity such that a certain stable flame size results.

Exercise 3: Drift and Diffusion for Green's Function
Derive a Fokker-Planck equation for the distribution of Green's function starting from (8.56) and (8.57). Specialize to a Fokker-Planck equation for the distribution of the local density of states $\varrho(E; x)$,

$$\begin{aligned}\varrho(E; x) &:= \langle x \mid \delta(E - H) \mid x\rangle \\ &= \frac{i}{2\pi}\left\langle x \mid [E - H + i0]^{-1} - [E - H - i0]^{-1} \mid x\right\rangle.\end{aligned}$$

Exercise 4: Range of Universal Fluctuations
Analyze fluctuations around the stationary solution of the model defined by (8.76) and show that they give sub-leading contributions to the approximation

$$\mathcal{P}(X) = \text{const.} \exp\left[-\frac{(X - \langle X\rangle)^2}{2\beta^{-1}\,(f|\,\tilde{K}\,|f)}\right]$$

as long as $|\delta X| \ll \langle X\rangle \gg 1$ (up to $\mathcal{O}(\ln X)$ corrections in the exponent).

Exercise 5: Typical Quantum Transmittance
In 1D the phase average yields for the logarithm of the series composition the simple additive result:

$$\langle \ln T_{12}\rangle_\phi = \ln T_1 + \ln T_2.$$

Iterating this procedure tells that the logarithm of the transmission will be distributed in a Gaussian way according to the central limit theorem for independent additive random numbers. This motivates to call $T_\mathrm{t} := \exp\langle \ln T\rangle$ the typical transmission, and to write down a quantum series composition law for transmittance in 1D wave guides

$$T_\mathrm{t}(L_1 + L_2) = T_\mathrm{t}(L_1)T_\mathrm{t}(L_2).$$

Now combine this with a subsequent parallel composition, where $R = 1 - T$ takes the role of T. Look at an infinitesimal increase of systems length: $L_1 = L$, $L_2 = \delta L$. Conclude that a β-function for the typical transmittance of such combination of series and parallel composition reads

$$\beta(T_\mathrm{t}) := \frac{\mathrm{d}\ln T_\mathrm{t}}{\mathrm{d}\ln L} = T_\mathrm{t}\ln T_\mathrm{t} - (1 - T_\mathrm{t})\ln(1 - T_\mathrm{t}).$$

Analyze its fixed point behavior and calculate the critical exponent ν for this β-function.

References

1. S. Coleman, in *The Uses of Instantons*. Proceedings of International School of Subnuclear Physics (Erice, 1977)
2. D. Zubarev, V. Mozorov, G. Roepke, *Statistical Mechanics of Nonequilibrium Processes*. Basic Concepts, Kinetic Theory, vol. 1 (Akademie Verlag, Berlin, 1996)
3. H. Haken, *Synergetics* (Springer, Berlin, 1977)
4. H. Risken, *The Fokker-Planck Equation* (Springer, 1996)
5. H. Haken, A. Wunderlich, *Die Selbststrukturierung der Materie: Synergetik in der unbelebten Materie* (Vieweg, Braunschweig, 1991)
6. E.P. Wigner, Ann. Math. **53**, 36 (1951)
7. M.L. Mehta, *Random Matrices* (Academic, New York, 1991)
8. A. Altland, M.R. Zirnbauer, Phys. Rev. Lett. **76**, 3420 (1996)
9. T. Guhr, A. Mueller-Groeling, H.A. Weidenmüller, Phys. Rept. **299**, 189 (1998)
10. F.J. Dyson, J. Math. Phys. **13**, 90 (1972)
11. R. Landauer, IBM J. Res. Dev. **1**, 223 (1957); Philos. Mag. **21**, 863 (1970)
12. M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986)
13. C.W.W. Beenakker, Phys. Rev. Lett. **70**, 1155 (1993)
14. M. Janßen, Phys. Rept. **295**, 1 (1998)
15. A. Messiah, *Quantum Mechanics II* (North-Holland, Amsterdam, 1965)
16. M.V. Moskalets, *Landauer-Büttiker Formalism*. Scattering Matrix Approach to Non-Stationary Quantum Transport (Imperial College Press, 2011), pp. 1–33
17. P.A. Mello, S. Tomsovic, Phys. Rev. Lett. **67**, 342 (1991)
18. R. Johnston, H. Kunz, J. Phys. C **16**, 4565 (1983)
19. E. Abrahams (ed.), *50 Years of Anderson Localization* (World Scientific, Singapore, 2010)
20. M. Janssen, *Fluctuations and Localization in Mesoscopic Electron Systems* (World Scientific, Singapore, 2001)
21. J.T. Chalker, P.D. Coddington, J. Phys. C **21**, 2665 (1988)
22. H.A. Fertig, Phys. Rev. B **38**, 996 (1988)
23. B. Kramer, T. Ohtsuki, S. Kettemann, Phys. Rept. **417**, 211 (2005)
24. D.P. Arovas, M. Janssen, B. Shapiro, Phys. Rev. B **56**, 4751 (1997)

Appendix A
Random Variables

Quantities that change in time in stochastic processes are called random variables. Random variables in general with no explicit reference to time are the subject of statistics and probability theory, the basic concepts of which we introduce in this appendix. Some overlap with the main part is tolerated for better readability.

A.1 Facts, Frequencies, Mean and Fluctuation

In a scientific approach to reality there are at least two good reasons for using statistical methods. (1) We like to classify events which have taken place and are known through documents. In classifying such **facts** we describe them in terms of properties and then make a choice which properties are relevant for us. Counting facts with some relevant properties is elementary in any scientific discipline and is the basis of **descriptive statistics**. (2) We like to prognosticate or even predict properties of potential events that could become facts in the future.

Usually, for practical or general reasons, we cannot exactly predict an event to take place at a definite time. Thus, we call it a **random event**. A prognostication based on a descriptive statistics of facts and theoretical insight is the area of **probability theory**.

A random event ε is an element of a space of events with f degrees of freedom forming a configuration space. For a quantitative description we assume that random events can be represented by real coordinates $x^l(\varepsilon)$, $l = 1, \ldots, f$, forming a vector of coordinates $\boldsymbol{x}(\varepsilon) \in \mathbf{R}^f$. The coordinates $\boldsymbol{x}$ of the random event ε are called random numbers or **random variables**. They can be either discrete or continuous.

To describe facts associated with random events we consider M non-overlapping classes Q_j, $j = 1, \ldots, M$ which are either identical to the random numbers in the discrete case or form an f-dimensional hypercube,

$$Q_j := I_j^1 \times \cdots \times I_j^f, \tag{A.1}$$

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1

where I_j^l is some interval for coordinate x^l. The total space S of random numbers is called coordinate space of events (sometimes "coordinate" is dropped for simplicity), or in short sample space. It is made up by all classes

$$S = \dot{\bigcup}_{j=1}^{M} Q_j. \tag{A.2}$$

We assume to know how to decide if an event has taken place and has become a fact. The registration of a fact is what we call a measurement, or in short a **trial**. Surely, a reliable measurement that meets scientific standards can only be done on the basis of some theory, or at least a pre-theory, that is open to improvements. The theory tells which documents are to be accepted in order to decide if an event with certain properties has become a fact. Performing measurements under controlled conditions that could be met again later within some accepted range of validity is what we call an **experiment**.

The number of facts with random variables to be found in class Q_j is denoted as H_j and called the absolute frequency of class Q_j. Often, each class Q_j will be represented by a discrete random number $\boldsymbol{x}_j$ within that class.

The total number of facts $N := \sum_{j=1}^{M} H_j$ should equal the total number of trials in the experiment, assuming that each of N trials leads to a definite result within the M classes. Thus, the **relative frequencies** $h_j := H_j/N$ are normalized to unity,

$$\sum_{j=1}^{M} h_j = 1. \tag{A.3}$$

The well known example for a discrete random event is the outcome of throwing a dice, which can be described by a one-dimensional variable represented by a coordinate x that can take discrete values, for example two values 0 and 1. The outcome of an experiment where the dice is thrown 100 times may be $H(0) = 34$ and $H(1) = 66$. The relative frequencies are $h(0) = 0.34$ and $h(1) = 0.66$, summing up to one.

As an example for a continuous random event, we take the weight of a certain sort of bread that we buy on many days in the same bakery, say 682 times. The bread is announced to have a weight of 500 g. Thus, we have a one-dimensional variable x which can take positive real numbers in units of g. The precision of our scale may suggest to take classes of intervals of width 5 g. A possible outcome of the experiment is depicted in Fig. A.1. What to do with the outcome of an experiment, the relative frequencies? The relative frequencies allow to calculate the **mean** of any property $A(\boldsymbol{x})$ being a function of $\boldsymbol{x}$, i.e.

$$\langle A \rangle_{\mathrm{d}} := \frac{1}{N} \sum_{i=1}^{N} A(\boldsymbol{x}_{\{i\}}), \tag{A.4}$$

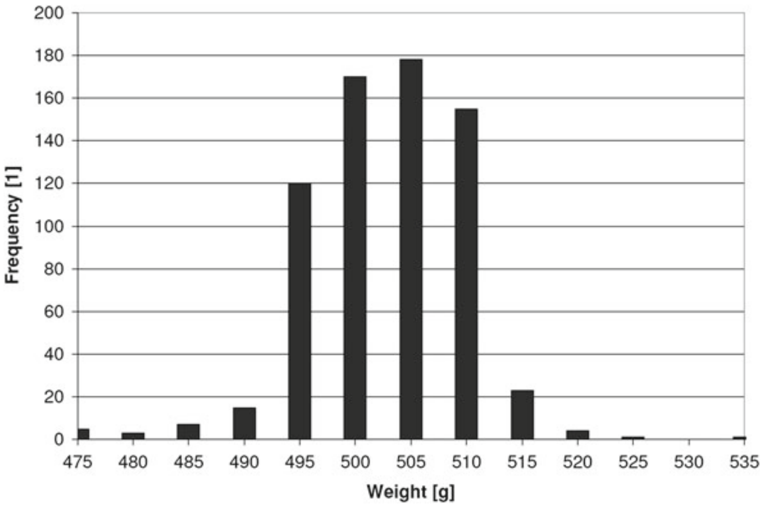


Fig. A.1 Frequencies for weight of a sort of bread

where the sum runs over N trials with outcome $\boldsymbol{x}_{\{i\}}$, $i = 1, \ldots, N$. With the relative frequencies it can be calculated as a sum over the M classes as

$$\langle A \rangle_{\mathrm{d}} = \sum_{j=1}^{M} A(\boldsymbol{x}_j) h_j. \tag{A.5}$$

The following special functions are sometimes useful for formal derivations: the characteristic function χ_j of a class Q_j which equals unity, if $\boldsymbol{x} \in Q_j$ and vanishes otherwise, and the 1-function which equals unity on all classes, i.e. $1 = \sum_j \chi_j$. The mean of the characteristic function is nothing but the relative frequency,

$$\left\langle \chi_j \right\rangle_{\mathrm{d}} = h_j, \tag{A.6}$$

and the mean of the 1-function yields the normalization of relative frequencies,

$$\langle 1 \rangle_{\mathrm{d}} = 1. \tag{A.7}$$

The mean is a linear operation,

$$\langle \lambda_1 A_1 + \lambda_2 A_2 \rangle_{\mathrm{d}} = \lambda_1 \langle A_1 \rangle_{\mathrm{d}} + \lambda_2 \langle A_2 \rangle_{\mathrm{d}}. \tag{A.8}$$

In the above examples of throwing a dice 100 times and of buying many days a certain type of bread, the means are $\langle x \rangle_{\mathrm{d}} = 0.66$ and $\langle x \rangle_{\mathrm{d}} = 502.8$, respectively.

Whenever a random number fluctuates in our experiment, i.e. the relative frequency is not simply 1 for just one class ($h_j \not\equiv \delta_{jj_0}$ for some j_0), the descriptive **variance** $\sigma_{A\mathrm{d}}^2$ of any $\boldsymbol{x}$-sensitive quantity $A(\boldsymbol{x})$ is non-vanishing,

$$\sigma_{A\mathrm{d}}^2 := \left\langle (\delta A)^2 \right\rangle_\mathrm{d} := \left\langle (A - \langle A \rangle_\mathrm{d})^2 \right\rangle_\mathrm{d} = \left\langle A^2 \right\rangle_\mathrm{d} - \langle A \rangle_\mathrm{d}^2 \geq 0. \tag{A.9}$$

The square root $\sigma_{A\mathrm{d}} := \sqrt{\sigma_{A\mathrm{d}}^2}$ is called descriptive **standard deviation**. In the above examples of throwing a dice 100 times and of buying many days a certain type of bread, the standard deviations are $\sigma_{x\mathrm{d}} = 0.47$ and $\sigma_{x\mathrm{d}} = 7.0$, respectively.

Fluctuations in two quantities $A(\boldsymbol{x})$ and $B(\boldsymbol{x})$ show up in the descriptive **correlation**,

$$C_{AB\mathrm{d}} := \langle \delta A\, \delta B \rangle_\mathrm{d} = \langle AB \rangle_\mathrm{d} - \langle A \rangle_\mathrm{d} \langle B \rangle_\mathrm{d}\,. \tag{A.10}$$

The resulting descriptive correlator

$$R_{AB\mathrm{d}} := \frac{C_{AB\mathrm{d}}}{\sigma_{A\mathrm{d}}\sigma_{B\mathrm{d}}} \tag{A.11}$$

is a number between -1 and 1. We denote A and B as uncorrelated, if $R_{AB\mathrm{d}}$ vanishes, as totally correlated, if $R_{AB\mathrm{d}} = 1$, or as totally anti-correlated, if $R_{AB\mathrm{d}} = -1$.

The relative frequencies h_j contain the complete knowledge about a system in descriptive statistics. Naturally, one tries to characterize the system by few characteristic parameters, such as mean $\left\langle x^l \right\rangle_\mathrm{d}$, standard deviation $\sigma_{x^l\mathrm{d}}$, correlations $C_{x^l x^k \mathrm{d}}$ and possibly higher moments $\left\langle x^l \ldots x^m \right\rangle_\mathrm{d}$ of the random variable $\boldsymbol{x}$. However, high moments usually don't add very much to the understanding.

Instead, in the case of a one-dimensional random variable x the so-called **quantiles** can be very helpful in characterizing. The α-quantile x_α is defined as that (in an infimum sense) value of the variable x, for which the summed histogram has reached the value $\alpha \in [0, 1]$,

$$\sum_{j=1}^{M'(x_\alpha)} h_j \ngtr \alpha. \tag{A.12}$$

In particular, $x_{0.5}$ is called median and can often serve as a **typical value** of the histogram, even when the mean is strongly influenced by rare events far from typical values. Furthermore, positions were the histogram has local maxima and minima may be of importance.

Before we turn to prognostication and probability theory, let us stress that randomness is not necessarily in conflict with determinism. To clarify the notion, we call a set of random numbers $\boldsymbol{x}_{\{i\}}$, $i = 1, \ldots, N$ **deterministic**, if we know a law which determines each value in a definite way. For example, a time series $\boldsymbol{x}_{\{i\}} = \boldsymbol{x}(t_i)$ of a motion $\boldsymbol{x}(t)$ obeying a differential equation $\dot{\boldsymbol{x}} = F(\boldsymbol{x})$ with continuous F yields a deterministic set of numbers. Even in this case, we can study mean values and fluctuations. When we talk about random numbers we simply do not know an underlying deterministic law, or we know such law, but its to complicated to study, or its of no use for the questions we like to ask. In some cases, as in quantum theory, there might be good reasons to assume that there is no underlying deterministic theory at all, but this is to some extent a matter of taste.

A.2 Potential Events, Probability, Mean and Fluctuation

Probability theory is a mathematical discipline. However, when applied to practice, probability has the following meaning directed to the future: the probability $P_j \geq 0$ of potential events in class Q_j is a prognostication for the relative frequencies h_j to be found when potential events have become facts.

For continuous random variables a **probability distribution**, with $P(\boldsymbol{x}) \geq 0$, yields the probability P_j of class Q_j

$$P_j := \int \mathrm{d}^f x \; P(\boldsymbol{x}) \chi_j(\boldsymbol{x}). \tag{A.13}$$

Prognostic mean values for quantities $A(\boldsymbol{x})$ are commonly called **expectation values**. For probability distribution $P(\boldsymbol{x})$ they are defined as

$$\langle A \rangle := \int \mathrm{d}^f x \; P(\boldsymbol{x}) A(\boldsymbol{x}). \tag{A.14}$$

It is linear in A and must fulfill the normalization

$$\langle 1 \rangle = \int \mathrm{d}^f x \; P(\boldsymbol{x}) = 1. \tag{A.15}$$

Equation (A.13) can be written as

$$P_j = \langle \chi_j \rangle . \tag{A.16}$$

Expected fluctuations in quantities $A(\boldsymbol{x})$ and $B(\boldsymbol{x})$ are given by the correlation,

$$C_{AB} := \langle \delta A \, \delta B \rangle = \langle AB \rangle - \langle A \rangle \langle B \rangle , \tag{A.17}$$

or, in case of a single quantity, by the variance,

$$\sigma_A^2 := \left\langle (\delta A)^2 \right\rangle = \left\langle A^2 \right\rangle - \langle A \rangle^2 . \tag{A.18}$$

For a one-dimensional random variable the α-quantile x_α is defined as that (in an infimum sense) value of the variable x, for which the integrated probability distribution has reached the value $\alpha \in [0, 1]$,

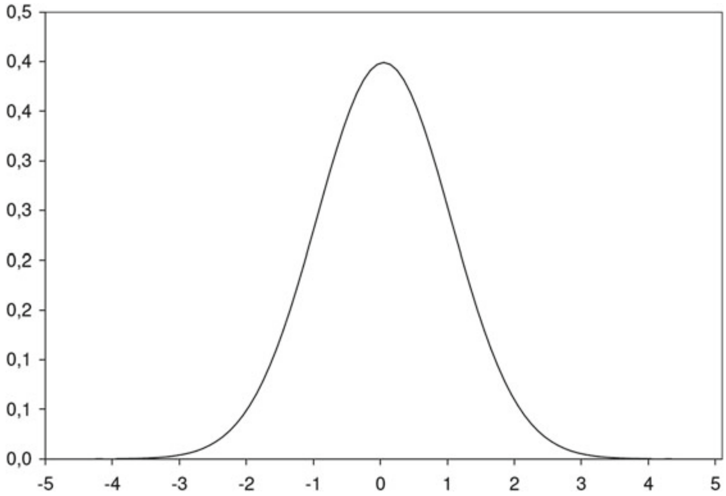


Fig. A.2 Gauss-distribution in a.u.

$$\int_{-\infty}^{x_\alpha} \mathrm{d}x\, P(x) = \alpha. \tag{A.19}$$

In particular the median $x_{0.5}$ can often serve as a typical value of the distribution, even when the mean $\langle x \rangle$ is strongly influenced by rare events in **fat tails** far from typical values. However, quantiles are difficult to calculate, because one has to invert the integrated probability with respect to the upper limit.

The well known **Gaussian distribution** (also called normal-distribution) is a prototypic probability density. It is defined for $f = 1$ by

$$P_{\text{Gauss}}(x) = (2\pi\sigma^2)^{-1/2} \exp -(x - x_0)^2/(2\sigma^2). \tag{A.20}$$

It is displayed in Fig. A.2. The Gauss-distribution is centered around its maximum at the average position $\langle x \rangle = x_0 = x_{0.5}$ with exponentially small tails. Its variance is indeed the parameter σ^2 with $x_0 + \sigma \approx x_{0.84}$, $x_0 + 2\sigma \approx x_{0.98}$ and $x_0 + 3\sigma \approx x_{0.999}$.

A probability fulfills its purpose, if it yields reliable expectation values for descriptive means,

$$\langle A \rangle_{\mathrm{d}} \longrightarrow \langle A \rangle\,. \tag{A.21}$$

The "limit" is an empirical limit, not a mathematical one. To test a probability we have to perform N trials under "similar conditions", take the relative frequencies $h_j(N)$ and check empirically for large N if we find

$$h_j(N) - P_j = \delta_j(N) \longrightarrow_{N\to\infty} 0. \tag{A.22}$$

Notice that this empirical limit involves not only a large number N of trials, but they have to be performed under similar conditions. That similar conditions lead to similar facts is the central observation on which any science is based. In its sharpest form, where equal conditions lead to equal facts it is the reason to formulate philosophical categories as **causality**, **continuity** and **homogeneity of time**. In reverse, we expect from equal facts that equal conditions had been fulfilled leading to the principle of **sufficient reason**.

In practice, we can never be sure, that we have met similar conditions. But if seemingly similar conditions do not lead to similar facts, we expect that either we missed something essential in preparing similar conditions, or we face a phenomenon with very sensitive dependence on the variation of conditions. In the latter case we try to fix in a quantitatively controlled manner the conditions and look for the quantitative fluctuations in facts, which should at least shrink in a systematic way.

What does "large N" mean? If we are able to perform an experiment of N trials under similar conditions, then we expect that for each trial the expectation value can be estimated by the **same** distribution $P(\boldsymbol{x})$. If that is true, a mathematical result, known as **law of large numbers** helps in fulfilling the empirical limit of (3.8). An elementary version of this law will be discussed in the following section.

In most cases of constructing time-independent probabilities, if not all, one starts from some a-priori probability distribution for elementary situations with high symmetry or **no preferential outcome**. For such elementary situations the probability is equally distributed or biased in a specific way if constraints have to be fulfilled. They can be constructed on the basis of**maximum information** as discussed in Sect. A.10.

As an example consider throwing a dice with say 6 sides and corresponding numbers. For a good dice all 6 sides should be made the same way and no side is distinguished. Even, if we take little variations into account, by throwing the dice in an unpredictable way, we expect that all numbers have the same a-priori probability. If we have very much detailed knowledge about the design of the dice and all of the conditions when throwing it, we might be able to predict which number becomes a fact, i.e. the underlying dynamics might be fully deterministic. However, the sensitivity to slight variations in the conditions of throwing is such, that after many trials the resulting facts do not seem to prefer any specific number.

In such cases, where the outcome of each of N possible events has no preferential outcome the **golden rule of probability** applies. It states that the probability of a class Q is the ratio of advantageous elements (M) to all possible elements (N),

$$P(Q) = M/N. \tag{A.23}$$

Before we proceed, a few remarks on notation. In mathematical statistics ε is called elementary event; more generally any subset ω of the set S of elementary events is called an event. Probability is introduced as a real valued function $\mathrm{P}(\omega)$ satisfying Kolmogorov's axioms 1–3.

1. $\mathrm{P}(\omega) \geq 0$
2. $\mathrm{P}(S) = 1$
3. $\mathrm{P}(\dot{\bigcup}_l \omega_l) = \sum_l \mathrm{P}(\omega_l)$

Within our notation the first axiom means positivity of the probability distribution, the second means normalization and the third allows for the introduction of a distribution to be summed up by integration. For a 1D-continuous set of random numbers $\mathcal{P}(x) = \int^x \mathrm{d}x' \, P(x')$ is called probability of the set with random numbers smaller than x. While mathematicians prefer this probability, physicists prefer the density $P(\boldsymbol{x})$ with the understanding that $P(\boldsymbol{x})\mathrm{d}^f x$ is the probability to find $\boldsymbol{x}$ in the infinitesimal[1] volume element $\mathrm{d}^f x$. For discrete random numbers $\boldsymbol{x}_n$, the density has delta-peaks $P(\boldsymbol{x}) = \sum P_n \delta(\boldsymbol{x} - \boldsymbol{x}_n)$, such that P_n is the probability to find the discrete value $\boldsymbol{x}_n$. Mathematicians dislike the notion of δ-function, since it is an ill defined function. Its sound definition is via the notion of distributions (linear functionals), but physicists like to think of a family of strongly peaked normalized functions which shrink to a point-like support and keep in mind that the corresponding limit has to be performed after some integral has been carried out.

A.3 Large Numbers I

As a consistency check for the interpretation of probability as relative frequency for large N we consider the following situation.

We have N random numbers $\{x_l\}$ each of which could have been predicted by the same distribution $P(x)$. Then we find for the predicted mean and variance of the relative frequencies $h_j = 1/N \sum_{l=1}^N \chi_j(x_l)$

$$\langle h_j \rangle = P_j, \tag{A.24}$$

$$\left\langle (\delta h_j)^2 \right\rangle = \frac{1}{N}\left(P_j - P_j^2\right). \tag{A.25}$$

The first of these equations is nothing but repeating the interpretation, but the second equation is deep. It tells two interesting things.

Whenever $P_j = P_j^2$, which means $P_j = 0$ or $P_j = 1$, there are no fluctuations in frequencies, independent of N. More importantly, if relative frequencies fluctuate at all, the fluctuations die out with large N as $1/\sqrt{N}$ and h_j reaches asymptotically its mean value P_j, i.e. relative frequencies become self-averaging.

This mathematical result is a law of large numbers. It ensures that the interpretation of probability as relative frequency for large N is no nonsense. However, it does not prove the empirical finding of convergence of relative frequencies to probabilities, since we can never be sure, that each random number is well predicted by the same distribution, i.e. measured under similar conditions.

[1] Infinitesimal is short hand for: where linearity rules.

A.4 Or, And, and Conditional

So far we considered non-overlapping classes Q_j which exhaust the full space S of random events. Since $Q_j \cap Q_k = \emptyset$ we have $P(Q_j \cup Q_k) = P(Q_j) + P(Q_k)$ and $\sum_k P(Q_k) = 1$. Non-overlapping classes mean that the corresponding events of $Q_j \cup Q_k$ are either in Q_j or in Q_k. Thus the simple summation of probabilities corresponds to "either-or" of events.

Now, consider an arbitrary class Q of events which may have some overlap with class Q_k. Since we can always decompose Q into non-overlapping classes as $Q = Q \setminus (Q \cap Q_k) \cup (Q \cap Q_k)$, we have $P(Q \setminus (Q \cap Q_k)) = P(Q) - P(Q \cap Q_k)$. Then we decompose $Q \cup Q_k$ into three non-overlapping classes $Q \cup Q_k = (Q \setminus (Q \cap Q_k)) \cup (Q \cap Q_k) \cup (Q_k \setminus (Q \cap Q_k))$ and get the generalized **sum rule for probabilities** corresponding to "or" of events,

$$P(Q \cup Q_k) = P(Q) + P(Q_k) - P(Q \cap Q_k). \tag{A.26}$$

For the latter probability corresponding to "and" of the events in Q and Q_k a **multiplication rule** can be formulated

$$P(Q \cap Q_k) = P(Q) \cdot P_Q(Q_k), \tag{A.27}$$

where $P_Q(Q_k)$ is denoted as the **conditional probability** of class Q_k under the condition that class Q is already known as a fact. Equation (A.27) is indeed the definition for the conditional probability. Why does it make sense?

To motivate the meaning of conditional probability let us consider an example, before we investigate its formal properties. In an urn we have three balls of three different colors, say yellow (y), blue (b) and red (r). We take out one ball by chance, keep it, and then another ball by chance. What is the probability to have first a yellow ball and then a red ball. By the golden rule (A.23) we have in the first step $P(y) = 1/3$. Given the fact, that we have already the yellow ball, the probability to find the red ball is (by the golden rule) the conditional probability $P_y(r) = 1/2$, since there are two possible balls left to be taken. By the golden rule we can also calculate the probability to find the ordered pair of yellow and red, just by counting the possible events of the two-step experiment. It equals $P(y \,\text{and}\, \text{r}) = 1/6$ and coincides with the product of $P(y)$ and $P_y(r)$.

As to the formal properties of $P_Q(Q_k)$ we look at the situations where (1) Q and Q_k have no common events, (2) Q is within Q_k. In case (1) the product in (A.27) has to vanish, either because $P(Q)$ is zero already, or the conditional probability $P_Q(Q_K)$ has to vanish, which meets the interpretation of conditional probability for there is no chance to have an event of class Q_k, when it is sure to have found the event in non-overlapping class Q. In case (2) $Q \cap Q_k = Q$ and the conditional probability $P_Q(Q_k) = 1$, which also meets the interpretation, for there is evidence in having an event in Q_k after knowing it took place in Q which is within Q_k.

Furthermore, Q can always be decomposed into non-overlapping classes denoted as Q^{in} and Q^{out} as $Q = Q^{\text{in}} \dot{\cup} Q^{\text{out}}$, such that $Q \cap Q_k = Q^{\text{in}}$. As a consequence, we can write $P(Q \cap Q_k) = P(Q^{\text{in}}) = \left[P(Q^{\text{in}}) + P(Q^{\text{out}})\right] \cdot P_Q(Q_k)$ such that

$$0 \leq P_Q(Q_k) = \frac{P(Q^{\text{in}})}{P(Q^{\text{in}}) + P(Q^{\text{out}})} \leq 1, \tag{A.28}$$

which meets the interpretation of a probability.

Finally, summing over all classes Q_k yields $\sum_k P(Q \cap Q_k) = P(Q \cap S) = P(Q)$, such that the conditional probability is normalized in an adequate way,

$$\sum_k P_Q(Q_k) = 1. \tag{A.29}$$

Consider the urn example, but this time we put the ball back after we have documented its color. This time the probability to have first a yellow ball and then a red ball can be found by similar steps as before. By the golden rule (A.23) we have in the first step $P(y) = 1/3$. This time, the fact that we have already the yellow ball does not influence the probability to find the red ball. By the golden rule the conditional probability $P_y(r) = 1/3 = P(r)$, since there are again three possible balls left to be taken. By the golden rule we can also calculate the probability to find the ordered pair of yellow and red, just by counting the possible events of the two-step experiment. It equals $P(y \text{ and r}) = 1/9$ and coincides with the product of $P(y)$ and $P_y(r) = P(r)$.

Thus, it makes sense to call a situation where the conditional probability $P_Q(Q_k) = P(Q_k)$ is insensitive to the condition a situation where class Q_k is **statistically independent** of Q. Then a simple multiplication rule can be formulated corresponding to "and" of statistically independent events in Q and Q_k,

$$P(Q \cap Q_k) = P(Q) \cdot P(Q_k). \tag{A.30}$$

Consequently, the relation of statistical independence is also symmetric, while the conditional probability in general must not be symmetric.

Quite often the conditional probability $P_Q(Q')$ (to find class Q' given that class Q is a fact) is written as $P(Q' \mid Q)$ or as $P(Q \mid Q')$. We avoid this notation which may suggest a symmetric role of Q and Q'. Instead of general symmetry we have

$$P_{Q'}(Q) = P_Q(Q')\frac{P(Q)}{P(Q')}. \tag{A.31}$$

A.5 Joint, Reduction, Change and Conditional

The considerations of the foregoing section were general for events in classes, now we stick to the notion of probability distributions $P(\boldsymbol{x})$. Here $\boldsymbol{x}$ is again shorthand for f degrees of freedom $x^1, \ldots x^f$ and $P(\boldsymbol{x}) = P(x^1, \ldots x^f)$ is called the

joint-probability density of the f random variables. The interpretation is that it yields the probability to find x^1 and x^2, ..., and x^f in the conjoint infinitesimal volume element $dx^1 \wedge \cdots \wedge dx^f$. The wedge product of differentials in a volume element is antisymmetric and reminds us that a volume element is a determinant of differentials along different coordinates. This volume element is abbreviated as $\mathrm{d}^f x$ or as $d\boldsymbol{x}$. The probability of a class Q is given by the appropriate integration over its characteristic function, as displayed in (A.13).

As an example consider the probability density to find a point with coordinates (x^1, x^2) on a plane within a given area A. The probability density is by the golden rule $P(x^1, x^2) = (1/A)\chi_A(x^1, x^2)$ with χ_A the characteristic function of the area. The density is normalized to unity. By partial summations we can construct **reduced probability densities**, e.g.

$$P(x^{k_f+1}, \ldots, x^f) = \int dx^1 \wedge \ldots \wedge dx^{k_f} \; P(x^1, \ldots, x^f). \tag{A.32}$$

In the example of points on a 2D area we can ask for the probability density of only coordinate x^1, and to be concrete we assume a rectangular $A = L_1 L_2$. Then, by (A.32), $P(x^1) = (1/L_1)\chi_{L_1}(x^1)$, as expected by the golden rule.

In general, we can construct a **reduced probability** distribution $P(\mathrm{A})$ for a given function $\mathrm{A}(\boldsymbol{x})$ with $F < f$ degrees of freedom by the expression

$$P(\mathrm{A}) = \langle \delta\,(\mathrm{A} - \mathrm{A}(\boldsymbol{x}))\rangle = \int \mathrm{d}\boldsymbol{x}\; P(\boldsymbol{x})\delta\,(\mathrm{A} - \mathrm{A}(\boldsymbol{x}))\,. \tag{A.33}$$

which yields the same mean values for any function of $A(\boldsymbol{x})$ as the original $P(\boldsymbol{x})$. When A has much less degrees of freedom than $\boldsymbol{x}$ ($F \ll f$), the reduced probability $P(\mathrm{A})$ is much easier to handle than the original $P(\boldsymbol{x})$.

As an example, consider the case of points on a 2D disc area of size πR^2. We can ask for the probability density of finding a certain radius r, while the total probability density of finding any point there is $1/\pi R^2$. By the one to one mapping of cartesian coordinates to polar coordinates ($0 \le r \le R, 0 \le \phi < 2\pi$)

$$x^1 = r\cos\phi,\;\; x^2 = r\sin\phi,\;\; dx^1 \wedge dx^2 = r dr \wedge d\phi, \tag{A.34}$$

we find a non-constant probability density

$$P(r)dr = \frac{2r}{R^2}dr. \tag{A.35}$$

Interestingly, the density vanishes for $r \to 0$.[2] Furthermore, it shows that non-trivial probability densities often (if not always) arise from originally trivial probability densities (e.g. by the golden rule of no preferential outcome) by reduction.

Equation (A.33) is very important, whenever we are able to foresee the relevant variables A of a problem at hand, which was set up from a model with detailed variables $\boldsymbol{x}$. It is extensively used e.g. in quantum and statistical **field theories** based on the so called **path integral** approach. It allows to get rid of complexity in calculations and to concentrate on relevant variables by simple integration (see Sect. 5.6).

As a special case, (A.33) also tells how to perform a change of coordinates from f-dimensional $\boldsymbol{x}$ to f-dimensional $\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{x})$ in a one to one way,

$$P(\boldsymbol{y}) = \langle \delta\left(\boldsymbol{y} - \boldsymbol{y}(\boldsymbol{x})\right)\rangle = P\left(\boldsymbol{x}(\boldsymbol{y})\right) \mid \det\left(\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{y}}\right) \mid . \tag{A.36}$$

The last equation can be captured by the short hand notation

$$P(\boldsymbol{y})d\boldsymbol{y} = P(\boldsymbol{x})\mathrm{d}\boldsymbol{x}, \tag{A.37}$$

with $\mathrm{d}\boldsymbol{x} =\mid \det\left(\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{y}}\right) \mid d\boldsymbol{y}$. It states that probability of an infinitesimal class expressed as density times volume element is invariant with respect to change of coordinates.

As an example, consider again the case of points on a 2D disc area of size πR^2. The mapping of Cartesian coordinates to polar coordinates tells

$$P(r, \phi)dr \wedge d\phi = \frac{1}{\pi R^2} r dr \wedge d\phi. \tag{A.38}$$

Besides joint and reduced probability densities we can also construct **conditional probability densities** $P_{x^1,\ldots,x^e}(x^{e+1}, \ldots, x^f)$. They are defined similarly to (A.27) by

$$P(x^1, \ldots, x^f) =: P(x^1, \ldots, x^e) P_{x^1,\ldots,x^e}(x^{e+1}, \ldots, x^f). \tag{A.39}$$

It is interpreted as the probability for finding $x^{e+1}, \ldots, x^f$ in the conjoint volume $\mathrm{d}x^{e+1} \wedge \ldots \wedge \mathrm{d}x^f$ knowing that $x^1, \ldots, x^e$ are conjoint facts. Sometimes it is denoted as $P(x^1, \ldots, x^e \mid x^{e+1}, \ldots, x^f)$ or as $P(x^{e+1}, \ldots, x^f \mid x^1, \ldots, x^e)$, depending on pure convention. Note, that it is not symmetric. This is best expressed by an asymmetric notation. For example, normalization means

$$\int \mathrm{d}x^{e+1} \wedge \cdots \wedge \mathrm{d}x^f \; P_{x^1,\ldots,x^e}(x^{e+1}, \ldots, x^f) = 1, \tag{A.40}$$

[2]This phenomenon is known in the context of random matrix theory as level repulsion: When a matrix has random entries, the mapping to eigenvalue coordinates as radial coordinates shows that the probabilities to find close eigenvalues goes to zero.

while

$$\int dx^1 \wedge \cdots \wedge dx^e \; P(x^1, \ldots, x^e) \; P_{x^1,\ldots,x^e}(x^{e+1}, \ldots, x^f) \tag{A.41}$$

$$= P(x^{e+1}, \ldots, x^f). \tag{A.42}$$

In the case of points on a 2D area we find for the conditional probability of finding an angle ϕ, given a fixed radius r

$$P_r(\phi) = P(r, \phi)/P(r) = \frac{1}{\pi R^2} r \frac{R^2}{2r} = 1/2\pi. \tag{A.43}$$

It turns out, as expected from symmetry, that it is independent of r and equals the unconditional probability $P(\phi)$. For a non-trivial example of conditional probability see the exercises.

A.6 Correlation

The probabilistic correlation of two quantities A and B is defined in the same way as the descriptive correlation (A.10).

$$C_{AB} := \langle \delta A \delta B \rangle = \langle AB \rangle - \langle A \rangle \langle B \rangle . \tag{A.44}$$

For $C_{AB} = 0$, A and B are called to be **statistically uncorrelated**. If for a set of random numbers $\boldsymbol{x}$ and $\boldsymbol{y}$ every pair of functions $A(\boldsymbol{x})$ and $B(\boldsymbol{y})$ turn out to be statistically uncorrelated, then the random numbers are called to be **statistically independent**.

An equivalent characterization of statistical independence is, that the conditional probability equals the unconditional one and thus the joint probability factorizes,

$$P_{\boldsymbol{x}}(\boldsymbol{y}) = P(\boldsymbol{y}), \;\; P_{\boldsymbol{y}}(\boldsymbol{x}) = P(\boldsymbol{x}), \;\; P(\boldsymbol{x}, \boldsymbol{y}) = P(\boldsymbol{x})P(\boldsymbol{y}). \tag{A.45}$$

To show the equivalence it is helpful to use variational arguments in C_{AB} with respect to the functions $A(\boldsymbol{x})$ and $B(\boldsymbol{y})$.

Note however, that the pure vanishing of a single correlation between two quantities does not necessarily mean that they are statistically independent: "uncorrelated" is only a necessary, but not a sufficient condition for "independent".

In the case of points on a 2D area we have uncorrelated cartesian coordinates for a rectangular area $A = L_1 L_2$

$$P(x^1, x^2) = \frac{1}{L_1 L_2} = \frac{1}{L_1}\frac{1}{L_2} = P(x^1)P(x^2). \tag{A.46}$$

For the circular area $A = \pi R^2$ the polar coordinates are uncorrelated,

$$P(r, \phi) = \frac{1}{\pi R^2} r = \frac{2r}{R^2} \frac{1}{2\pi} = P(r)P(\phi). \tag{A.47}$$

In both cases the uncorrelated nature stems from the orthogonality of the directions related to a change of only one coordinate and the adapted symmetry of the area, such that the golden rule can be applied to each coordinate separately.

A.7 Compact Notation and Structure

Equation (A.37) allows to express the coordinate independent meaning of expectation values with the help of the scalar product notation for real valued functions f, g,

$$(g \mid f) := \int \mathrm{d}\boldsymbol{x}\, g(\boldsymbol{x}) f(\boldsymbol{x}), \tag{A.48}$$

$$\langle A \rangle = (A \mid P) = \int \mathrm{d}\boldsymbol{x}\, A(\boldsymbol{x}) P(\boldsymbol{x}) = \int \mathrm{d}\boldsymbol{y}\, A(\boldsymbol{x}(\boldsymbol{y})) P(\boldsymbol{y}). \tag{A.49}$$

A (continuous) function f is a (infinite dimensional) vector, and with respect to the scalar product one can introduce dual vectors by the linear form $g^*(f) := (g \mid f)$. Physicists like the notation $\mid f)$ for f and $(g \mid$ for g^* melting to the scalar product $(g \mid f)$ when they are multiplied in the corresponding manner. When they are multiplied the other way $\mid f)\,(g \mid$ they can act as a bilinear mapping $\left(g' \mid \cdot \mid f\right) (g \mid \cdot \mid f') = \left(g' \mid f\right) \left(g \mid f'\right)$.

The following functions need special attention: the 1-function which is constantly 1 for any event ε and the coordinate-function $\mathrm{id}_{\boldsymbol{x}}$ which just gives $\boldsymbol{x}(\varepsilon)$, the specific coordinate representation of the events ε. With the 1-function normalization of probability is expressed as

$$\langle 1 \rangle = (1 \mid P) = 1, \tag{A.50}$$

and the average of coordinates $\boldsymbol{x}$ as

$$\langle \boldsymbol{x} \rangle = (\mathrm{id}_{\boldsymbol{x}} \mid P)\,, \tag{A.51}$$

A basis in the vector space of functions is given by the set of all delta-functions $\{\delta_{\boldsymbol{x}}\}_{\boldsymbol{x} \in S}$ where $\delta_{\boldsymbol{x}}(\boldsymbol{x}') = \delta(\boldsymbol{x} - \boldsymbol{x}')$ is peaked at $\boldsymbol{x}$. Its expectation value just picks out $P(\boldsymbol{x})$,

$$\langle \delta_{\boldsymbol{x}} \rangle = (\delta_{\boldsymbol{x}} \mid P) = P(\boldsymbol{x}), \tag{A.52}$$

Motivated by a similar convention in quantum mechanics we will use the short-hand $\mid \boldsymbol{x})$ for $\delta_{\boldsymbol{x}}$, such that

$$(\boldsymbol{x} \mid P) = P(\boldsymbol{x}) \tag{A.53}$$

is the projected vector component of vector P. Note, that in order to avoid inconsistencies one should not use the abbreviation $\mid \boldsymbol{x})$ for $\mathrm{id}_{\boldsymbol{x}}$, since $\langle \boldsymbol{x} \rangle \neq P(\boldsymbol{x})$. Orthogonality of the basis $\{\delta_{\boldsymbol{x}}\}_{\boldsymbol{x}\in S}$ is expressed by

$$\left(\boldsymbol{x} \mid \boldsymbol{x}'\right) = \delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{A.54}$$

In case that the probability $\mid P)$ is a conditional one of type $\mid P_{\boldsymbol{x}'})$ we can define in a unique way a linear "operator" D, denoted as **distributor**. It maps the sharp conditional probability $\mid x'\big)$ to the distribution $\mid P_{\boldsymbol{x}'})$,

$$\mathrm{D} \mid x'\big) = \mid P_{\boldsymbol{x}'}) \;\text{ and }\; \left(\boldsymbol{x} \mid \mathrm{D} \mid \boldsymbol{x}'\right) = P_{\boldsymbol{x}'}(\boldsymbol{x}). \tag{A.55}$$

In discrete matrix notation the mth column of D forms a probability vector P_m with components $P_m(n) = \mathrm{D}_{mn}$. Thus, conditional probability densities $P_{\boldsymbol{x}'}(\boldsymbol{x})$ can be viewed as matrix elements of a in general non-symmetric distributor. A distributor has the following properties

$$\left(\boldsymbol{x} \mid \mathrm{D} \mid \boldsymbol{x}'\right) \geq 0, \tag{A.56}$$
$$(1 \mid \mathrm{D} = (1 \mid, \tag{A.57}$$

where the latter equation (normalization) reads in discrete matrix notation

$$\sum_n \mathrm{D}_{nm} = 1. \tag{A.58}$$

Such square-matrices with non-negative elements and each row summing to one are commonly called **stochastic matrices**, sometimes probability matrices or transition matrices. We prefer the name distributor for the discrete as well as for the continuous case.

As to eigenvalues and eigenvectors of distributors we find from the ansatz $\mathrm{D} \mid v) = \lambda \mid v)$ and (A.57)

$$(1 \mid v) = \lambda\,(1 \mid v)\,. \tag{A.59}$$

Thus, if v is an eigenvector with non-vanishing $(1 \mid v)$ its eigenvalue is $\lambda = 1$, or $\mid v)$ is an eigenvector with $(1 \mid v) = 0$. Since $(1 \mid \mathrm{D} \mid \boldsymbol{x})$ is non-negative, $\sup_{\boldsymbol{x}}\,(1 \mid \mathrm{D} \mid \boldsymbol{x})$ defines a matrix-norm $\|\mathrm{D}\|$, which is induced by the maximum norm $\|v\| = sup_{\boldsymbol{x}} \mid (\boldsymbol{x} \mid v) \mid$. Then, one has the inequality $\|\mathrm{D} \mid v)\,\| \leq \|\mathrm{D}\|\,\|v\|$. Here $\|\mathrm{D}\| = 1$ and eigenvalues must fulfill $\mid \lambda \mid \leq 1$. For the transposed operator

$| \, 1)$ is by (A.57) an eigenvector with eigenvalue 1. By transposing the secular equation, $\det\left(\mathrm{D}^{\top} - \lambda 1\right) = 0$, for the determination of eigenvalues we also have 1 as an eigenvalue for D. Without proof we state a more refined result from matrix theory (Perron-Frobenius theorem): $\lambda = 1$ is non-degenerate provided all elements of D are strictly positive.

Thus we can summarize:

- Distributors have an eigenvector $| \, v)$ with eigenvalue $\lambda = 1$ and non-vanishing element summation,

$$\exists \, | \, v \,) \; : \; \mathrm{D} \, | \, v) = | \, v) \, , \text{with} \; (1 \, | \, v) \neq 0. \tag{A.60}$$

- For strictly positive elements of D, $\lambda = 1$ is non-degenerate.
- All eigenvalues fulfill

$$| \, \lambda \, | \leq 1. \tag{A.61}$$

-

$$\lambda \neq 1 \Longrightarrow (1 \, | \, v) = 0. \tag{A.62}$$

It is of great importance for the theory of stochastic Markov processes (see Sect. 2.3.3) that distributors can be multiplied forming a semi-group, provided the vector spaces of $\boldsymbol{x}$ and $\boldsymbol{x}'$ can be identified. Semi-group means that we have an associative multiplication the result of which stays within the group (see (A.57, A.58)), but in general the elements have no inverse with respect to the 1-operator which belongs to the semi-group. In the discrete notation where n and m may run over N elements it is easy to see that by normalization we have $N(N-1)$ degrees of freedom in the group of distributors. Viewing this group geometrically as a manifold one is interested in the group elements $\mathrm{D} = 1 - \alpha \mathrm{G}$ that lie in the infinitesimal (linear order of the parameter α) vicinity of 1. By the exponential map, $\exp\left(-\sum_k \alpha_k \mathrm{G}_k\right)$ and a complete algebra of generators G_k, one can generate the group. The generators have to nullify the $(1 \, |$ states,

$$(1 \, | \, \mathrm{G}_k = 0. \tag{A.63}$$

A.8 Generating Function

Integrating is typically much more difficult than differentiating, since the first is an inverse of the second, and only for differentiating we have algorithmic rules based on differentiating elementary functions, that lead to definite results. Only in few cases this algorithmic rules can be reversed to simple rules for integration.

To calculate expectation values with respect to a probability distribution we have to integrate or to sum up. But, this is exactly what distributions are designed fo. To characterize a probability distribution by averages we may have to calculate many averages. For example, if we want to characterize the distribution by its moments we need infinitely many of them. It is therefore highly advantageous when calculating averages to do that in one run for a whole family characterized by parameters,

$$G(\alpha) := \langle G(\boldsymbol{x};\alpha)\rangle = \int \mathrm{d}\boldsymbol{x}\; G(\boldsymbol{x};\alpha)P(\boldsymbol{x}). \tag{A.64}$$

The result can also be used to **generate** further expectation values by differentiating the family with respect to the parameters, provided convergence allows to commute averaging and differentiating. Also, in many circumstances it may be much easier to formally manipulate the family of averages than the probability distribution to reach theoretical insight about the distribution. In that case one doesn't care to much about convergence, but rather sticks to the formal properties.

All moments can be generated from the **moment generating function**

$$Z(\mathrm{k}) := \langle \exp(i\mathrm{k}\cdot\boldsymbol{x})\rangle = \int d\boldsymbol{x}\;\exp(i\mathrm{k}\cdot\boldsymbol{x})P(\boldsymbol{x}). \tag{A.65}$$

The factor i in the exponent is conventional to work with Fourier transformed of $P(\boldsymbol{x})$. It may help for convergence but may also be assisted by a convergence generating $\mathrm{k}+i\varepsilon$ prescription with $\varepsilon \to 0+$. The generating feature of $Z(\mathrm{k})$ goes with differentiating with respect to $i\mathrm{k}$ and finally putting $\mathrm{k}=0$,

$$Z(0) = 1, \tag{A.66}$$

$$Z(\mathrm{k}) = \left\langle \sum_n \frac{(i\mathrm{k}\cdot\boldsymbol{x})^n}{n!}\right\rangle, \tag{A.67}$$

$$\left\langle (x^l)^m (x^j)^n \ldots\right\rangle = \frac{\partial^{[m+n+\cdots]}Z(\mathrm{k})}{(\partial^m ik_l)(\partial^n ik_j)\ldots}\Big|_{\mathrm{k}=0}. \tag{A.68}$$

The fact, that $Z(\mathrm{k})$ is the Fourier transformed of $P(\boldsymbol{x})$ allows to reconstruct $P(\boldsymbol{x})$ from $Z(\mathrm{k})$ by backward transformation,

$$P(\boldsymbol{x}) = (2\pi)^{-f}\int \mathrm{dk}\;\exp(-i\mathrm{k}\cdot\boldsymbol{x})Z(\mathrm{k})\;. \tag{A.69}$$

Thus, if the moments exist they form the Taylor series of $Z(\mathrm{k})$ and therefore determine the distribution. In addition, we can generate any expectation of an observable $A(\boldsymbol{x})$ given its Taylor expansion as a series in moments. Apart from these more formal properties high moments are not very interesting on their own.

A better characterization of distributions is by **cumulants** which are defined via the **cumulant generating function** $W(\mathrm{k})$,

$$W(\mathrm{k}) := \ln Z(\mathrm{k}), \tag{A.70}$$

in a similar way to moments,

$$W(0) = 0, \tag{A.71}$$

$$W(\mathrm{k}) = \sum_n \left\langle \frac{(i\mathrm{k} \cdot \boldsymbol{x})^n}{n!} \right\rangle_{\mathrm{c}}, \tag{A.72}$$

$$\left\langle (x^l)^m (x^j)^n \dots \right\rangle_{\mathrm{c}} := \frac{\partial^{[m+n+\dots]} W(\mathrm{k})}{(\partial^m i k_l)(\partial^n i k_j) \dots} \Big|_{\mathrm{k}=0}. \tag{A.73}$$

Cumulants of order s (order defined by the number of derivatives) are linear combinations of moments up to order s, but not higher. In particular, the first moment equals the corresponding first cumulant, i.e. the mean

$$\langle \boldsymbol{x} \rangle_{\mathrm{c}} = \langle \boldsymbol{x} \rangle, \tag{A.74}$$

and the second order cumulants yield the correlation matrix C_{ij},

$$\left\langle x_i x_j \right\rangle_{\mathrm{c}} = \left\langle \left(\delta x_i \delta x_j \right) \right\rangle =: C_{ij}. \tag{A.75}$$

Since $P(\boldsymbol{x})$ can be expressed by $W(\mathrm{k})$ as

$$P(\boldsymbol{x}) = (2\pi)^{-f} \int \mathrm{dk}\ \exp(-i\mathrm{k} \cdot \boldsymbol{x} + W(\mathrm{k})). \tag{A.76}$$

we conclude:

- A distribution $P(\boldsymbol{x})$ which has no fluctuations at all but is δ-peaked at its average value $\langle \boldsymbol{x} \rangle$, $P(\boldsymbol{x}) = \delta(\boldsymbol{x} - \langle \boldsymbol{x} \rangle)$, corresponds in a unique way to a purely linear cumulant generating function $W(\mathrm{k}) = i\mathrm{k} \cdot \langle \boldsymbol{x} \rangle$.
- A distribution $P(\boldsymbol{x})$ which has vanishing cumulants for order three and higher corresponds in a unique way to a second order cumulant generating function $W(\mathrm{k}) = i\mathrm{k} \cdot \langle \boldsymbol{x} \rangle + \frac{1}{2}\mathrm{k} \cdot C\mathrm{k}$.
- It can be written in closed form and is a Gaussian distribution

$$P(\boldsymbol{x}) = (2\pi)^{-f} \sqrt{\det C} \exp\left[-\frac{1}{2} (\boldsymbol{x} - \langle \boldsymbol{x} \rangle) \cdot C^{-1} (\boldsymbol{x} - \langle \boldsymbol{x} \rangle) \right]. \tag{A.77}$$

where C^{-1} is the inverse of the symmetric matrix C, where the latter is the correlation matrix corresponding to the Gaussian distribution.

In other words, Gaussian distributions are those distributions which have only first and second order cumulants. All higher cumulants vanish. This is not true for the moments which are generally non-vanishing to all orders. This fact is one advantage of cumulants over moments.

A.9 Large Numbers II

Another important property of cumulants is the following: for a sum of additive uncorrelated random numbers

$$X = \sum_{l=1}^{N} x_l, \tag{A.78}$$

the cumulant generating function is additive too and so are the cumulants:

$$W(K) = \sum_{l=1}^{N} W_l(K), \tag{A.79}$$

$$\langle X^n \rangle_C = \sum_{l=1}^{N} \langle x_l^n \rangle_C. \tag{A.80}$$

Again, this is not true for the moments and $Z(K)$. The remarkable property for a large sum of uncorrelated random numbers is that every cumulants scale as N times a single cumulant independent of its order. By normalizing the variance to unity, every higher order cumulant scales with a negative power of $\sqrt{N}$ with respect to the variance and can thus be neglected in a large N limit provided the cumulants do not grow two fast with increasing order n such that they cannot compensate for the negative powers of $\sqrt{N}$. We thus conclude a version of the **central limit theorem** as our second law of large numbers: as long as the individual cumulants $\langle x^n \rangle_c$ do not grow faster than sub-linear exponential with n, the distribution $P(X)$ of a large sum of uncorrelated random numbers will approach a gaussian for large N.

A final remark on generating functions in mathematics: a generating function is a formal power series whose coefficients encode information about a sequence that is indexed by natural numbers. In mathematical statistics our generating function (A.65), the Fourier transform, is denoted as characteristic function while the same expression with real value kappa instead of ik is denoted as moment generating function. Canonical and grand-canonical partition functions in equilibrium statistics are special generating functions where parameters are external control parameters like temperature, pressure or chemical potential. Path integrals can be viewed as generating functions where variables are paths or other field configurations (see Sect. 5.5). The appropriate tool for numerical calculations of generating functions and functionals as high-dimensional integrals is the **Monte Carlo integration** method (see [1]).

A.10 Information

We gain information when an event takes place which, for us, was not sure to happen. To quantify the gain of information we like to define a quantifier function depending on $\boldsymbol{x}$ as well as a quantifier for the whole distribution $P(\boldsymbol{x})$. It should fulfill the following constraint: given N equally probable events, an information quantifier with no further preference to one of the outcomes must be a monotonic increasing function of N. The most basic representation of a natural number in digital representation tells us that with $\log_2(N)$ we are done.

In the continuous case we must specify a class Q_j around $\boldsymbol{x}_j$ such that the digitalization is finite. We can do that in two different ways. Either we integrate the density $P(\boldsymbol{x})$ times the characteristic function yielding P_j of that class and are back to the discrete case, or we keep the continuity description and simply multiply the density $P(\boldsymbol{x})$ with an appropriately chosen small volume element Γ_0 yielding an approximate probability (≤ 1) to find the value $\boldsymbol{x}$ in the volume Γ_0 around it. For this to be reasonable the probability density has to be nearly constant within Γ_0. We thus, come to the following definition of a non-negative **information** function as

$$I_j := -\log_2\left(P_j\right), \tag{A.81}$$

$$I(\boldsymbol{x}) := -\log_2\left(P(\boldsymbol{x})\Gamma_0\right). \tag{A.82}$$

The first line corresponds to the discrete case and the second line to the continuous case. This notion goes back to Boltzmann, Gibbs and Einstein in treating entropy in thermodynamics in the context of statistical mechanics and to Shannon in the context of information in general probability theory. As a quantifier for the information corresponding to the whole distribution we take the unbiased average value of the information function

$$I := (I) = \sum_{j=1}^{M} -\log_2\left(P_j\right) P_j, \tag{A.83}$$

and in the continuous case

$$I := -\int d\boldsymbol{x} \log_2\left(P(\boldsymbol{x})\Gamma_0\right) P(\boldsymbol{x}). \tag{A.84}$$

One **bit** is the information gain when we get to know the result of a binary alternative with equal probability of 1/2. Three bits is the information gain when we get to know the result of throwing a perfect eight-sided dice with probability 1/8 for each of its eight sides.

We must note that the definition of information does depend on the choice of Γ_0 in the continuous case, but it does also depend on the choice of classes in the discrete case. In the continuous case it is obvious from the definition that a change of Γ_0 by a factor a yields a change of I by $-\log_2(a)$. Similar changes happen in the discrete case when we divide classes into subclasses or join them to form superclasses. In both cases, the probability P_j changes accordingly and so does the information. For example, dividing a class into two classes of equal weight leads to half of the former probability of the whole class and hence increases the information in each class by an amount of 1 bit. Thus, classes and volume element Γ_0 have to be chosen appropriately for the problem at hand or for a class of similar problems for which we like to compare the information I. But one should be careful with comparison of information values without specifying classes or volume elements. This warning is in the same spirit as the warning not to compare probabilities without clarifying their conditional character. Once the classes or the volume element Γ_0 are chosen, we can quantitatively compare the information for different probability distributions.

Information has by its logarithmic character the very helpful property of being additive for independent random variables

$$P(\boldsymbol{x}, \boldsymbol{y}) = P(\boldsymbol{x})P(\boldsymbol{y}) \quad \longrightarrow \quad I(x, y) = I(\boldsymbol{x}) + I(\boldsymbol{y}). \tag{A.85}$$

The great advantage of the concept of information of the whole distribution is its additive and macroscopic character: it measures the overall distributiveness of the distribution. A uniform distribution has maximum information and a singular distribution (with probability 1 for one class and zero for all others) has zero information. Distributiveness and information have the same meaning in probability theory. Indeed, we can use distributiveness as a construction principle for distributions as it helps to quantify the **ignorance principle** of no preferential outcome. This principle goes back to Gibbs and has been stressed as a general principle in probability theory by Jayne.

A.11 Exercises

Exercise 1: Reduced Variable

Consider the probability of finding a point in the 2D disc of area $A = \pi R^2$, but within a mixture of Cartesian and polar coordinates, say x and angle ϕ. The relation between coordinates is $x = r\cos\phi$, $y = r\sin\phi$ and the disc A is defined by $x^2 + y^2 \le R^2$.
(a) Show that

$$P(x, \phi) = \frac{1}{\pi R^2}\frac{x}{\cos^2\phi}\chi_{R^2}\left(x^2\right)\chi_{(R/x)^2}\left(\tan^2\phi + 1\right)$$

with the characteristic function $\chi_Y(X) = 1$ if $0 \le X \le Y$ and zero otherwise.
(b) Show by reduction that $P(\phi) = 1/2\pi$ and

$$P(x) = \frac{2\sqrt{R^2 - x^2}}{\pi R^2}\chi_{R^2}\left(x^2\right)$$

Exercise 2: Conditional Probability

Verify the conditional probability for finding the angle ϕ for given x coordinate in the 2D plane to be

$$P_x(\phi) = \frac{\chi_{(R/x)^2}\left(\tan^2\phi + 1\right)}{2\cos^2\phi\sqrt{R^2/x^2 - 1}}$$

and show it is different from the unconditional $P(\phi)$. Show that x and ϕ are correlated random numbers.

Appendix B
Method of Characteristics

The method of characteristics is a method of solving homogeneous partial differential equations of first order.

B.1 Hamilton-Jacobi

A well known example is the Hamilton-Jacobi equation in mechanics. The momentum p is the partial derivative of the generating action function $S(x, t)$ with respect to the configuration coordinate x,

$$p(x, t) = \partial_x S(x, t). \tag{B.1}$$

The dynamics can be captured in the Hamilton-Jacobi equation,

$$H(x, \partial_x S(x, t)) + \partial_t S(x, t) = 0, \tag{B.2}$$

where $H(x, p)$ is the known Hamilton function of the system. This equation is a partial differential equation of first order for the unknown function $S(x, t)$. From a solution with constant value $S(x, t) = S_0$ one can find a possible solution $x(t)$ and also $p(t)$. The Hamilton-Jacobi equation is intimately connected with the Hamilton equations, which are ordinary differential equations,

$$\dot{x} = \partial_p H; \;\; \dot{p} = -\partial_x H. \tag{B.3}$$

This connection is just an expression of the method of characteristics: the Hamilton equations are the characteristic equations of the Hamilton-Jacobi equation.

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1

B.2 Characteristics

The method of characteristics can be summarized as follows. Given a homogeneous partial differential equation of first order for an unknown function $u(x, y)$ (we treat two variables for simplicity),

$$a(x, y)\partial_x u(x, y) + b(x, y)\partial_y u(x, y) = 0, \tag{B.4}$$

one studies its lines of constant value $u(x(t), y(t)) = u_0$ and finds from $\mathrm{d}u = 0$ and (B.4), that $(x(t), y(t))$ have to solve the **characteristic equations**,

$$\dot{x} = a(x, y);\ \ \dot{y} = b(x, y). \tag{B.5}$$

These equations are ordinary differential equations and can typically be solved easier than the original partial differential equation. The corresponding solutions $(x(t), y(t))$ are called **characteristic curves** and the constant solution $u(x(t), y(t)) = u_0$ is called **characteristic**. Once a solution of the characteristic equations is found for arbitrary initial values x_0, y_0 one can construct characteristics $u(x(t), y(t))$ which are constants along the characteristic curves by rewriting the solutions in terms of the constant initial values. This is the searched for characteristic.

As an example we consider the radioactive decayof Sect. 4.2.3,

$$l_n = ln,\ \ g_n = 0, \tag{B.6}$$

for the Master equation (4.6), such that the partial differential equation for the generating function $F(z, t)$ of (4.20) reads,

$$\partial_t F(z, t) = l(1 - z)\partial_z F(z, t). \tag{B.7}$$

The number n is bounded from below by $n = 0$. We introduce the parameter s as a fictitious time and apply the method of characteristics,

$$\dot{t} = 1;\ \ \dot{z} = l(z - 1). \tag{B.8}$$

The first equation is solved as $t(s) = s + t_0$ and the second is equivalent to $\mathrm{d}_t(z - 1) = l(z - 1)$ and therefore solved as $z(s) - 1 = (z_0 - 1)e^{ls}$. Both solutions can be put together in

$$z(s) - 1 = (z_0 - 1)e^{l(t-t_0)} \tag{B.9}$$

allowing to re-express the constants as

$$(z_0 - 1)e^{-lt_0} \equiv (z - 1)e^{-lt}. \tag{B.10}$$

Thus, a general solution for $F(z,t)$ is a function $f((z-1)e^{-lt})$. The generating function has to fulfill $F(z=1,t)=1$ due to probability normalization and $F(z,t=0)=z^{N_0}$, because $P_0(N)=\delta_{N_0,N}$. This fixes the choice of the function f and we arrive at the solution

$$F(z,t)=\left((z-1)e^{-lt}+1\right)^{N_0}. \tag{B.11}$$

This generating function allows to calculate the full conditional distribution function

$$P_{N_0,t_0}(N,t)=\frac{1}{N!}\frac{\mathrm{d}^N}{\mathrm{d}z^N}F(z,t)\mid_{z=1}=\frac{N_0!e^{-Nlt}(1+e^{-lt})^{N_0-N}}{(N_0-N)!N!}. \tag{B.12}$$

B.3 Exercise

Exercise: Hamilton-Jacobi Theory
Show that the Hamilton equations are the characteristic equations of the Hamilton-Jacobi equation.

Appendix C
Many-Body Green's Functions

In this Appendix usual unit conventions are used unless otherwise stated. The many-body Green's functions are treated in Matsubara technique within a functional perturbation theory following mainly [2]. The machinery of perturbation theory for $H = \tilde{H}^{[0]} + \tilde{U}$ is the subject of Sect. C.2, where the non-combinatorial method of generating functionals is used. The path integral functional representation in coherent states of Sect. C.3 follows mainly [3].

C.1 Susceptibilities and Matsubara Technique

Green's functions in real time t, $G(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n; \boldsymbol{x}_1, \ldots, \boldsymbol{x}_n; t)$, describe the quantum mechanical **probability amplitude** for n particles (excitations/quasi-particles) that are created at $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$, propagate a time t, and are annihilated at points $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n$. A definite expression requires the notion of quantum state and time evolution. The quantum state can be an equilibrium state described by a grand canonical ensemble, the time evolution is described by the Schrödinger equation, usually as time evolution of operators, called operators in Heisenberg picture. For time dependent perturbations on a system, the time evolution is split between the operators evolving according to the unperturbed Hamiltonian and the density operator evolving with the perturbation such that expectation values contain the full dynamics. Such decomposition runs under the name interaction picture or interaction representation. Operators will be decomposed into linear combinations of products of creation and annihilation operators. Since both, the Heisenberg time evolution as well as the grand canonical density operator involve the form

$$e^{-i\lambda H} \tag{C.1}$$

where $\lambda = (1/\hbar)t$ is purely real for time evolution, or $\lambda = -i\beta$ is purely imaginary for density operators, it turns out to be advantageous to treat Green's functions in so-called complex time. Transforming from time to energies introduces

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1

Fourier/Laplace transformed Green's functions of complex energy/frequency. The basic formalism of these objects will be introduced for the linear response two-operator Green's functions. In non-interacting systems they can be related to the one-particle Green's function $\langle \boldsymbol{x}'| \left(E - H(1) \pm i0\right)^{-1} |\boldsymbol{x}\rangle$ which is the real space representation of the **resolvent**, $(E - H(1) \pm i0)^{-1}$, of the one-particle Hamiltonian $H(1)$.

The most general object to be called Green's function in theoretical physics is the **n-operator time-ordered Green's function**,

$$\left\langle \hat{T} \prod_{j=1}^{n} X_j(t_j) \right\rangle, \tag{C.2}$$

where $X_j(t_j)$ are operators in Heisenberg picture and $\langle \ldots \rangle$ is a convenient statistical average (e.g. grand-canonical) and $\hat{T}$ is the time ordering operator which means that all operators to its right are to be ordered in increasing order of times, e.g.

$$\hat{T}\left(X_1(t_1)X_2(t_2)\right) = \Theta(t_1 - t_2)X_1(t_1)X_2(t_2) \pm \Theta(t_2 - t_1)X_2(t_2)X_1(t_1) \tag{C.3}$$

where $(+)$ is for bosons and $(-)$ for fermions. Time ordered n-operator Green's functions appear in the iterative solution of the integral equation of the form

$$S(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt'\, H_1(t')S(t', t_0) \tag{C.4}$$

which solution can formally be written as the **Dyson series**,

$$S = \hat{T} \exp\left[\frac{-i}{\hbar} \int \mathrm{d}t' H_1(t')\right]. \tag{C.5}$$

Here S is the time evolution operator in interaction representation, i.e. there is some decomposition $H = H_0 + H_1$ where the time evolution with H_0 is assumed to be known,

$$\Psi(t) = \left[e^{-(i/\hbar)H_0 t} S(t, t_0) e^{(i/\hbar)H_0 t_0}\right] \Psi(t_0) \tag{C.6}$$

and

$$H_1(t) = e^{(i/\hbar)H_0 t} H_1 e^{-(i/\hbar)H_0 t} \tag{C.7}$$

(H_1 may have also an explicit time dependence which is suppressed in the notation). Such integral equations follow from the Schrödinger equation directly and we mention that a similar to (C.4) integral equation holds for the time dependent density operator in linear response theory and its first order iterative solution yields the Kubo formula to be discussed soon. The special case of n-particle propagation corresponds to the choice of field creation and annihilation operators $\Psi^\dagger(\boldsymbol{x})$, $\Psi(\boldsymbol{x})$,[3]

$$\begin{aligned} &G(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n; \boldsymbol{x}_1, \ldots, \boldsymbol{x}_n; t) \\ &:= \left\langle \hat{T}\left[\Psi(\boldsymbol{y}_1; t) \ldots \Psi(\boldsymbol{y}_n; t)\Psi^\dagger(\boldsymbol{x}_n) \ldots \Psi^\dagger(\boldsymbol{x}_1)\right]\right\rangle. \end{aligned} \tag{C.8}$$

In linear response theory one faces a so-called retarded two-operator Green's function

$$G^{\mathrm{ret}}_{XY}(t) := \frac{-i}{\hbar}\Theta(t)\,\langle[X(t), Y]\rangle\,. \tag{C.9}$$

Linear response theory is a theory to calculate **susceptibilities** like magnetic susceptibilities, polarizabilities and conductivities. In general, susceptibilities are introduced as the linear coefficients between the expectation value of some observable $\langle Y\rangle$ and a driving field F. To calculate the expectation of Y we may start from a many-body Hamiltonian $H = H(F) =: H_0$, and we expand it with respect to an increment δF,

$$H(F + \delta F) = H_0 - X(F)\delta F;\;\; X(F) := -\partial_F H(F). \tag{C.10}$$

Here $X(F)$ is the dual operator to the field F which, in general, may depend on F and may not commute with H_0. There are two different ways to proceed which yield **isothermal** or **Kubo susceptibilities**. In the first case one considers a system that, under variation of F, will equilibrate fast enough, such that, at any value of F, it can be described by an equilibrated grand-canonical density operator

$$\varrho_0 = \exp - [\beta(H_0 - \mu N)]e^{\beta\Omega} \tag{C.11}$$

where $\beta = 1/(k_B T)$ is the inverse temperature, k_B the Boltzmann constant, μ the chemical potential, N the particle number operator, and

$$\Omega(F, T, \mu, V) = -k_B T \ln \mathrm{Tr}\, \exp - [\beta(H(F) - \mu N)] \tag{C.12}$$

is the grand-canonical potential. One may generate the equilibrium value $\langle Y\rangle$ by solving for the grand-canonical potential depending on a dual field J that is coupled to Y in $H(F)$. Very often, one is interested in the observable $Y = X$ and in that case $F = J$ and the **isothermal** susceptibility in $\partial_F\,\langle X(F)\rangle_F = \chi_{XX}$ is simply the (negative) second derivative of Ω with respect to F. A different way to calculate a general thermodynamic susceptibility

$$\chi_{YX} := \partial_F\,\langle Y(F)\rangle = \partial_F \mathrm{Tr}\,\{\varrho(F)Y(F)\} \tag{C.13}$$

[3]The are defined such that the combination $\Psi^\dagger(\boldsymbol{x})\Psi(\boldsymbol{x})$ is the particle number density operator and the charge density operator of particles with charge q is given as $\varrho(\boldsymbol{x}) = q\Psi^\dagger(\boldsymbol{x})\Psi(\boldsymbol{x})$.

is founded on a perturbation theory for the density operator (similar to the time dependent perturbation theory of the time evolution operator $e^{-(i/\hbar)Ht}$ in quantum mechanics) and expresses susceptibilities as correlators in the absence of the perturbing field. To safe writing, from now on, we will not explicitly write down the argument F in operators or expectation values. We state the result for the susceptibility without derivation (the derivation is a valuable exercise),

$$\boxed{\chi_{YX} = \langle \partial_F Y \rangle + \beta \langle \Delta X; \Delta Y \rangle}. \tag{C.14}$$

Here we have allowed for an explicit field dependence of observable Y, and $\Delta O := O - \langle O \rangle$ stands for fluctuations around the average. The Kubo scalar product of two operators is defined as[4]

$$\langle X; Y \rangle := \frac{1}{\beta} \int_0^\beta d\lambda \; \langle XY(i\hbar\lambda) \rangle = \langle Y; X \rangle^*. \tag{C.15}$$

The imaginary time evolution is meant in the Heisenberg picture with respect to H_0, $Y(t) = e^{(i/\hbar)H_0 t} X e^{-(i/\hbar)H_0 t}$. The Kubo scalar product resembles the expectation value of the simple product of X and Y and one can interpret: isothermal susceptibilities are time independent correlations in equilibrium. The correlation is between the quantity Y to be measured and the quantity X dual to the varied field. Usually, the thermodynamic susceptibilities are real and therefore symmetric.

The second way to consider susceptibilities is by considering a dynamical opening of the system. In the Kubo linear response theory a time dependent field increment $\delta F(t)$ is slowly switched on at t_0. To introduce the loss of information about an arbitrary initial condition by a long time average procedure leading to entropy production and stationarity, the initial time is sent to $t_0 = -\infty$ by an ϵ-prescription,

$$H_F(t) = H_0 - X \delta F(t) e^{\epsilon t}, \tag{C.16}$$

where ϵ is infinitesimally small and will be sent to zero after the thermodynamic limit has been performed in the sense that the energy spectrum has become quasi-continuous. At $t_0 = -\infty$ the system has been in equilibrium, described by the grand-canonical density operator, $\varrho_0 = \varrho(\delta F = 0)$. Now the density operator evolves in time according to the von-Neumann equation

$$\dot{\varrho}(t) = \frac{-i}{\hbar} \left[H_F(t), \varrho(t) \right]. \tag{C.17}$$

The solution linear in δF, keeping only a single Fourier component,

$$\delta F(t) = \delta F e^{-i\omega t}, \tag{C.18}$$

[4] Note, that X and Y are hermitian operators here, otherwise the definition has to be slightly modified.

yields for the linear increment of the expectation value

$$\langle Y\rangle_{\delta F}(t) = \left\{\langle \partial_F Y\rangle + \chi_{YX}(z)\right\}\delta F(t) \tag{C.19}$$

with the **Kubo susceptibility** $\chi_{YX}(z)$ given by the Kubo formula

$$\boxed{\chi_{YX}(z) = \frac{i}{\hbar}\int_0^\infty dt\, e^{izt}\,\langle [Y(t), X]\rangle}. \tag{C.20}$$

The so called Kubo-identity

$$\langle \dot{X}; Y\rangle = \frac{-i}{\beta\hbar}\langle [X, Y]\rangle . \tag{C.21}$$

turns out to be helpful in calculations. The susceptibility, in time representation, is thus identical to minus the two-operator retarded Green's function

$$\boxed{\chi_{YX}(t) = -G^{\mathrm{ret}}_{YX}(t) = \Theta(t)\frac{i}{\hbar}\langle [Y(t), X]\rangle .} \tag{C.22}$$

Isothermal and Kubo susceptibilities are generally not identical and it depends on the physical problem which one should be used. As a rule of thumb one may say that susceptibilities in closed equilibrated systems (e.g. magnetic susceptibility) are described by isothermal susceptibilities while in situations with driving currents through the system, susceptibilities (e.g. conductance) are better described by Kubo susceptibilities.

The definition (C.9) is useful for bosons operators X, Y. In fact, in linear response only densities of observables are possible candidates for X, Y, and these must be bosonic, i.e. they fulfill $X^\dagger X = XX^\dagger$ since $X^\dagger = X$ (and the same for Y). However, in view of (C.2, C.8) it makes sense to extend the definition to Fermion operators, for which $X^\dagger X = -XX^\dagger$. In case that X, Y are Fermion operators, we replace the commutator by the anti-commutator. To cover both cases by one symbol one often introduces $[X, Y]_\mp$ where—is for Bosons (commutator) and + for Fermions (anti-commutator). A mixed case will not be defined. The relation to the time-ordered two-operator Green's function (also often called causal Green's function)

$$G_{XY}(t) := \frac{-i}{\hbar}\left\langle \hat{T}\left(X(t)Y\right)\right\rangle \tag{C.23}$$

will soon become clear. As an example consider the Green's function corresponding to the charge density response $G_{\varrho(\boldsymbol{x}')\varrho(\boldsymbol{x})}$ and express it by field operators. The result is

$$G_{\varrho(\boldsymbol{x}')\varrho(\boldsymbol{x})}(t) = \frac{-ie^2}{\hbar}\left\langle \hat{T}\left(\Psi^\dagger(\boldsymbol{x}'; t)\Psi(\boldsymbol{x}'; t)\Psi^\dagger(\boldsymbol{x})\Psi(\boldsymbol{x})\right)\right\rangle \tag{C.24}$$

which is close to the **two-particle propagator** of (C.8). For $G_{XY}(t)$ one can introduce its Fourier transformed, called $G_{XY}(\omega)$,

$$G_{XY}(\omega) := \int \mathrm{d}t\, e^{i\omega t} G_{XY}(t) \tag{C.25}$$

It becomes well defined when using an infinitesimal damping in the auxiliary Green's function (being analytic in the half-plane $\Im z > 0$)

$$\Gamma_{XY}(z) := \frac{-i}{\hbar} \int_0^\infty \mathrm{d}t\, e^{izt} \langle X(t)Y \rangle\,, \quad z = \omega + i\epsilon \tag{C.26}$$

such that

$$G_{XY}(\omega) = \lim_{\epsilon\to 0^+} \Gamma_{XY}(z) \pm \Gamma_{YX}(-z^*) \tag{C.27}$$

(where $+$ for Bosons, $-$ for fermions). On the other hand, the Fourier transformed retarded Green's function, being also analytic in $\Im z$, can as well be expressed by Γ_{XY},

$$G^{\mathrm{ret}}_{XY}(z) := \int \mathrm{d}t\, e^{izt} G^{\mathrm{ret}}_{XY}(t) = \Gamma_{XY}(z) \pm \left(\Gamma_{X^\dagger Y^\dagger}(-z^*)\right)^*. \tag{C.28}$$

The last two equations rest on the time translation invariance

$$\left\langle X(t+t_0)Y(t'+t_0)\right\rangle = \left\langle X(t)Y(t')\right\rangle \tag{C.29}$$

for any t_0. Let us summarize the resulting strategy to obtain susceptibilities: knowing the time-ordered two-operator Green's function $G_{XY}(t)$ is enough to calculate $\Gamma_{XY}(z)$, and hence the retarded two-operator Green's function $G^{\mathrm{ret}}_{XY}(z)$. The latter yields the linear response susceptibilities,

$$\boxed{G_{XY}(t) \longrightarrow \Gamma_{XY}(z) \longrightarrow -G^{\mathrm{ret}}_{XY}(z) = \chi_{XY}(z)}\,, \tag{C.30}$$

as the most interesting observables in many-body systems. For brevity we will, in the following, call G_{XY} the propagator (although this relates more appropriate to the special case $X = \Psi(\boldsymbol{x}')$, $Y = \Psi^\dagger(\boldsymbol{x})$) and G^{ret}_{XY} the retarded Green's function.

Although there are methods to directly calculate the propagator in real time (mostly approximately) it is often more advantageous to calculate the frequency dependent retarded Green's function in a direct attack. To do that a trick was invented by Matsubara in the 1950s and others which makes the calculations most easy, in particular with respect to analytical properties. The imaginary-time propagator (also called **temperature Green's function** or Matsubara Green's function). The Matsubara technique relies on the similarity of time evolution and density operator. To make this similarity in the grand canonical case most closely, one modifies the Heisenberg picture ruled by the Hamiltonian H to a time evolution given by

$$H^{\mu} := H - \mu N. \tag{C.31}$$

That means, in the following we take the time evolution of any operator $X(t)$ with respect to H^{μ} instead of H. This must be kept in mind. Fortunately, for susceptibilities this will not change anything as long as either X or Y do commute with N, and this is the case for realistic physical densities. For Bose systems with vanishing μ there is, of course, no effect. If X, Y, do not commute with N, then one has to take the change into account. In the relevant cases, e.g. when X, Y are simply creation and annihilation operators, one finds simple relations between Green's functions with Heisenberg and Matsubara time evolution, such that the evaluation of the latter is always sufficient to obtain the former.

With the Matsubara time evolution we define the imaginary-time propagator by

$$\begin{aligned} -\hbar\mathcal{G}_{XY}(\tau) &:= \left\langle \hat{T}\left(X(-i\hbar\tau)Y\right)\right\rangle \\ &= \Theta(\tau)\left\langle X(-i\hbar\tau)Y\right\rangle \pm \Theta(-\tau)\left\langle YX(-i\hbar\tau)\right\rangle, \end{aligned} \tag{C.32}$$

where τ is a real number with the physical dimension of inverse energy. To make the writing more transparent we will take $\hbar = 1$ in the following. It can be re-introduced by simple dimensional analysis. The crucial property of the Matsubara time evolution is the property

$$\left\langle X(-i\tau)Y(-i\tau')\right\rangle = \left\langle Y(-i\tau')X(-i\tau + i\beta)\right\rangle, \tag{C.33}$$

in addition to (C.29) (this can be shown by using the cyclicity of the trace). As a consequence, a periodicity-property of the imaginary-time propagator follows

$$\boxed{\mathcal{G}_{XY}(\tau + \beta) = \pm\mathcal{G}_{XY}(\tau)}. \tag{C.34}$$

Therefore a discrete Fourier expansion with respect to imaginary-time (temperature) can be introduced

$$\boxed{\mathcal{G}_{XY}(\tau) = \frac{1}{\beta}\sum_{n=0,\pm1,\pm2,\dots}\mathcal{G}_{XY}(i\nu_n)\, e^{-i\nu_n\tau}}, \tag{C.35}$$

where the **Matsubara frequencies** are

$$\nu_n = \frac{2\pi n}{\beta} \qquad \text{(Bosons)}, \tag{C.36}$$

$$\nu_n = \frac{(2n+1)\pi}{\beta} \quad \text{(Fermions)}. \tag{C.37}$$

The frequency dependent temperature Green's function is obviously

$$\mathcal{G}_{XY}(i\nu_n) = \int_0^\beta d\tau\, \mathcal{G}_{XY}(\tau)\, e^{i\nu_n\tau}. \tag{C.38}$$

The nice feature of the temperature Green's function is that it equals, after analytic continuation in the half-plane $\Im z > 0$, the retarded Green's function,

$$\boxed{\mathcal{G}_{XY}(i\nu_n \to z) = G^{\text{ret}}_{XY}(z)}. \tag{C.39}$$

The proof of the last equality is easiest in energy representation, $|\,\mathcal{E}_\lambda\rangle$ of total H, and left as an exercise.

The equality (C.39) is very important, since in practice one tries to find the temperature Green's function at the Matsubara frequencies first, then analytically continues to arbitrary complex frequencies $\Im z > 0$, a process which becomes unique by the requirement $\mathcal{G}_{XY}(z) \to 0$ for $|z| \to \infty$.

We mention, that the temperature Green's function appears directly in isothermal susceptibilities[5]

$$\boxed{\chi_{XY} = \chi_{YX} = \beta\langle Y; X\rangle = -\mathcal{G}_{XY}(i\nu_n = 0) = -\int_0^\beta d\tau\ \langle X(-i\tau)Y\rangle}. \tag{C.40}$$

Thus, the thermodynamic Green's function at zero frequencies determine the thermodynamics. In particular, one can calculate the thermodynamic potential from special Green's functions, e.g. from that of $X = Y = N$.

As an important application we calculate the so-called **unperturbed Green's functions** or unperturbed one-particle propagator corresponding to creation and annihilation operators for X, Y and a non-interacting Hamiltonian $H^{[0]}$ with one-particle spectrum ε_j and eigenstates $|\,\alpha_j\rangle$, e.g.

$$\mathcal{G}^0_{jj'}(\tau) := -\left\langle \hat{T}\left(a^0_j(-i\tau)a^\dagger_{j'}\right)\right\rangle^0 \tag{C.41}$$

(the superscript ^{0} indicates the non-interacting dynamics and state). They form the elementary objects of any perturbation theory. The time evolution of a_j can be calculated with the help of (3.21), since $H^{[0]} = \sum_j \varepsilon_j a^\dagger_j a_j$,

$$a^0_j(t) = e^{i(H^{[0]}-\mu N)t} a_j e^{-i(H^{[0]}-\mu N)t} = e^{-i(\varepsilon_j-\mu)t} a_j. \tag{C.42}$$

[5] We have neglected an explicit field dependence of Y and assumed that the zero-field equilibrium expectation of X, Y vanishes.

Thus, we find for $\tau > 0$

$$\mathcal{G}^0_{jj'}(\tau) = -e^{(\varepsilon_j-\mu)\tau}\left\langle a_j a^\dagger_{j'}\right\rangle^0 . \tag{C.43}$$

Since $\left\langle a_j a^\dagger_{j'}\right\rangle^0 = \big(b(\varepsilon_j)+1\big)\,\delta_{jj'}$ for Bosons, and $\left\langle a_j a^\dagger_{j'}\right\rangle^0 = \big(1-f(\varepsilon_j)\big)\,\delta_{jj'}$ for Fermions, and at the Matsubara frequencies $e^{i\beta\nu_n} = \pm 1$, one finds for the unperturbed one-particle temperature Green's function, and for the unperturbed retarded one-particle Green's function,

$$\boxed{\mathcal{G}^0_{jj'}(i\nu_n) = [i\nu_n - \varepsilon_k + \mu]^{-1}\,\delta_{jj'}}, \tag{C.44}$$

$$\boxed{G^{\mathrm{ret}\,0}_{jj'}(z) = [z - \varepsilon_k + \mu]^{-1}\,\delta_{jj'}}. \tag{C.45}$$

Note, that the Bose/Fermi-distribution functions exactly cancel, due to the Matsubara time evolution; for the Heisenberg time evolution they don't. Interesting enough, the unperturbed retarded single-particle Green's function equals the usual retarded Green's function of the single-particle Hamiltonian $H(1)$ at an energy ε shifted from the chemical potential, i.e. the energy representation of the resolvent operator $G(z = \mu + \varepsilon + i0) := [(\mu+\varepsilon) - H(1) + i0]^{-1}$,

$$\boxed{G^{\mathrm{ret}\,0}_{jj'}(z = \mu + \varepsilon + i0) = \left\langle \alpha_j \mid [z - H(1)]^{-1} \mid \alpha_{j'}\right\rangle}. \tag{C.46}$$

This justifies the name Green's function for the many-body case as a generalizing one. The above unperturbed retarded Green's function does not depend on the statistics and we will refer to it as the **free electron propagator**.

For phonons, as introduced in condensed matter lectures, one needs also the **free phonon propagator**. However it is not defined with respect to the pure creation and annihilation operators of phonon modes, but with respect to the quantized normal mode coordinates

$$Q_{\mathrm{k}} = \frac{1}{\sqrt{2}}\left(b_{\mathrm{k}} + b^\dagger_{-\mathrm{k}}\right) = Q^\dagger_{-\mathrm{k}}, \tag{C.47}$$

where b_{k} annihilates bosons of wave-vector k. The free phonon propagator is defined as

$$\mathcal{D}^0(\tau, \mathrm{k}) := -\left\langle \hat{T}\left(Q_{\mathrm{k}}(-i\tau)Q^\dagger_{\mathrm{k}}\right)\right\rangle^0 . \tag{C.48}$$

Recall that a phonon Hamiltonian reads

$$H^{[0]}_{\mathrm{ph}} = \sum_{\mathrm{k}} \hbar\omega_{\mathrm{k}}\left(N_{\mathrm{k}} + \frac{1}{2}\right), \tag{C.49}$$

where ω_{k} is the frequency of phonon mode k. For small k and acoustic phonons, the dispersion is linear. With this Hamiltonian the free phonon propagator reads (the chemical potential is zero since the number of phonons is not conserved)

$$\boxed{\mathcal{D}^0(\tau,\mathrm{k}) = -\frac{1}{2}\left[e^{-\omega_{\mathrm{k}}\tau}\left\langle b_{\mathrm{k}}b^{\dagger}_{\mathrm{k}}\right\rangle^0 + e^{\omega_{\mathrm{k}}\tau}\left\langle b_{-\mathrm{k}}b^{\dagger}_{-\mathrm{k}}\right\rangle^0\right]}, \tag{C.50}$$

leading to the retarded free phonon Green's function

$$\boxed{\mathcal{D}^{\mathrm{ret}\,0}(z,\mathrm{k}) = \frac{1}{2}\left[\frac{1}{z-\omega_{\mathrm{k}}} - \frac{1}{z+\omega_{\mathrm{k}}}\right] = \frac{\omega_{\mathrm{k}}}{z^2-(\omega_{\mathrm{k}})^2}}. \tag{C.51}$$

C.2 Generating Functional and Perturbation Theory

Recall the main expressions for the many-body temperature Green's functions,

$$\mathcal{G}_{XY}(\tau) = -\left\langle \hat{T}\,(X(-i\tau)Y)\right\rangle = \pm\mathcal{G}_{XY}(\tau+\beta), \tag{C.52}$$

$$\mathcal{G}_{XY}(\tau) = \frac{1}{\beta}\sum_n \mathcal{G}_{XY}(i\nu_n)e^{-i\nu_n\tau}, \tag{C.53}$$

$$\mathcal{G}_{XY}(i\nu_n) = \int_0^{\beta} \mathrm{d}\tau\, \mathcal{G}_{XY}(\tau)e^{i\nu_n\tau}, \tag{C.54}$$

where $\nu_n = 2\pi n/\beta$ ($\nu_n = 2(n+1)/\beta$) are Matsubara frequencies for Bosons (Fermions). The time evolution is with some many-body Hamiltonian H_μ and the expectation value is given by

$$\langle\ldots\rangle = \frac{\mathrm{Tr}\, e^{-\beta H_\mu}\ldots}{Z},\quad Z = \mathrm{Tr}\, e^{-\beta H_\mu}. \tag{C.55}$$

So far, we only know to calculate these Green's functions for additive (non-interacting) systems described by $H^{[0]}$, e.g.

$$\mathcal{G}^0_{a_k a^{\dagger}_k}(i\nu_n) = (i\nu_n - \varepsilon_k + \mu)^{-1}\,. \tag{C.56}$$

To develop approximate schemes for calculating Green's functions we proceed in three steps. (1) We represent them as functional derivatives of a source dependent partition sum $Z\,[j]$. The source is introduced by an additional term in H_μ. In the non-interacting case $Z^0\,[j]$ can be given in closed form as a Gaussian functional.

(2) We can represent $Z\,[j]$ as a perturbation series from $Z^0\,[j]$, which is well defined for a given interaction term U in $H = H^{[0]} + U$. As a result, one has a well defined operational (in contrast to combinatorial) perturbation series for Green's functions. Each term can be represented by graphs which contain lines of unperturbed propagators and vertices describing the interaction. To each graph a weight factor is attached, that follows uniquely from the operational scheme The graphs can help to comprehend the perturbation series and to visualize elementary processes that build the series. In step (3) we represent the partition sum $Z\,[j]$ by field theoretic integrals (path integrals). This opens new approximation schemes that can go beyond perturbation theory as outlined in Sect. 5.6.

The n-operator Green's function can be represented as a functional derivative

$$\left\langle \hat{T}\left(\prod_{l=1}^{n} X_l(-i\tau)\right)\right\rangle = (-)^n \frac{\delta^n}{\delta j_1(\tau)\ldots j_n(\tau)} \left\langle \hat{T} e^{-\int\limits_0^\beta \mathrm{d}\tau \sum\limits_l j_l(\tau) X_l(-i\tau)} \right\rangle\Bigg|_{j=0}, \tag{C.57}$$

which follows by differentiating the exponential functional. Here $j_l(\tau)$ are commuting (e.g. complex) numbers for Bosons and anticommuting (Grassmann) numbers for Fermions, i.e. $j_l j_k = -j_k j_l$ to preserve the commuting/anti-commuting nature of operators X_l, X_k in the Green's function (for details on Grassmann numbers see e.g. [4]). Note, for Grassmann numbers the order of performing derivatives does count. Defining a source dependent partition function by

$$Z[j] := \mathrm{Tr}\left\{ e^{-\beta H_\mu} \hat{T} e^{-\int\limits_0^\beta \mathrm{d}\tau \sum\limits_l j_l(\tau) X_l(-i\tau)} \right\}, \tag{C.58}$$

one can write

$$\boxed{\left\langle \hat{T}\left(\prod_{l=1}^{n} X_l(-i\tau)\right)\right\rangle = \frac{1}{Z[0]} (-)^n \frac{\delta^n}{\delta j_1(\tau)\ldots j_n(\tau)} Z[j]\Bigg|_{j=0}}, \tag{C.59}$$

where $Z[0] = Z$ is the ordinary partition sum, free of source terms. Since we know how to deal with non-interacting systems, it is not surprising that one can find the unperturbed source dependent partition sum in closed form. Without proof we state here the result, a Gaussian functional,

$$\boxed{Z^0[j] = Z^0[0] \exp\left\{ \frac{1}{2} \int\limits_0^\beta \mathrm{d}\tau \int\limits_0^\beta \mathrm{d}\tau' \sum_{ll'} j_l(\tau) \mathcal{G}^0_{X_l X_{l'}}(\tau, \tau') j_{l'}(\tau') \right\}}. \tag{C.60}$$

It is easy to verify that this indeed generates the unperturbed propagator, but it needs more effort to show, by using equations of motion with $H^{[0]}$, that it does not contain higher polynomials of j in the exponent. The proof, however, is much easier in the field theoretic formulation of the following subsection. From the last two equations it immediately follows that any n-operator unperturbed Green's function factorizes into (sums and integrals of) products of unperturbed propagators. The explicit formulas are known as Wick's theorem, which has been proved in a combinatorial way first.

Due to the fact that (a) any realistic interaction term U in $H = H^{[0]} + U$ is a polynomial in some basic operators X_l, e.g.

$$U = \sum_{klmn} V_{klmn} a_k^\dagger a_l^\dagger a_m a_n, \tag{C.61}$$

and (b) that any polynomial in the operators X_l can be generated by plugging the derivative with respect to the dual source field $\delta/\delta j_l$ as an differential operator into that polynomial, the interaction can act on the exponential source and finally the source is put to zero. Expanding the exponential function into its defining series and comparing term by term one can then show the identity

$$\boxed{Z[j] = e^{-\int\limits_0^\beta \mathrm{d}\tau U[\frac{\delta}{\delta j(\tau)}]} Z^0[j]}. \tag{C.62}$$

This formula is the pendant for finite temperature equilibrium to the scattering state formula (5.122). It yields, by expanding the exponential function, an operative perturbative expansionof $Z[j]$ in terms of powers of $\mathcal{G}^0$ connected by those terms (V_{klnm} in the example above) defining the interaction. Each term can be represented graphically by a diagram, in which lines represent propagators and vertices represent the interaction. Each diagram can be classified with respect to the order of powers of U entering, and with respect to the loop-order of diagrams. A loop represents a perturbation term, where propagators have the same initial and final point. The perturbative formula above has the great advantage over combinatorial diagrammatics, that the weight of each diagram can be read of the formula by using the exponential series and Laplace's chain rule for derivatives. The only ingredients needed for this operational perturbation scheme are the unperturbed propagators and the polynomial structure of the interaction U; each term is generated from that by (C.59, C.60, C.62). Although, for pure perturbative purposes in a $H^{[0]} + U$ decomposition, there is no need to introduce a field theoretic formulation of the partition sum, we will do so in order to open new approximation routes.

C.3 Field Theoretic Partition Sum

The trace in the partition sum Z can be expressed with the help of the energy representation, but for this to be useful one needs to diagonalize the problem first. Also, one could use the occupation number representation $\{\mid n\rangle\}$

$$\mathrm{Tr}\, e^{-\beta H_\mu} = \sum_n \langle n \mid e^{-\beta H_\mu} \mid n\rangle \,. \tag{C.63}$$

Due to the exponential form, the matrix elements are not easy to calculate. One could use a partition of the identity $1 = \sum_n \mid n\rangle \langle n \mid$ and divide the finite value of β into a large number of small pieces $\delta = \beta/\mathcal{N}$. On each short piece evolution $e^{-\delta H_\mu}$ one may introduce the partition of the identity and approximate the exponential by $1 - \delta H_\mu$. Finally, one has to send $\mathcal{N}$ to infinity. The matrix elements can then be calculated. Nevertheless, this leads to a mess of combinatorics with all possible occupation number combinations. Although this route may be helpful for particular interactions U, we will search for a more general approach in terms of integrals over continuous quantum numbers.

Such representation is opened by the so-called **coherent states** representation of many-body systems. Coherent states are defined as eigenvectors for a complete set of annihilation operators $\hat{a}_l$. Such eigenstates, if they exist, must be a linear combination of occupation number states. By this one notices that creation operators $\hat{a}^\dagger$ cannot have eigenstates, since the lowest occupation number will in any case be raised by one. A similar problem does not exist for annihilation, as there is no maximum occupation number, and the minimum occupation number can be taken as zero. It turns out that coherent states can be constructed by

$$\mid \psi\rangle = e^{\pm \sum_l \psi_l \hat{a}_l^\dagger} \mid 0\rangle \tag{C.64}$$

($\pm$ distinguishes between Bosons and Fermions). They are right-eigenstates for the annihilators

$$\hat{a}_l \mid \psi\rangle = \psi_l \mid \psi\rangle \tag{C.65}$$

and left-eigenstates for the creators

$$\langle \psi \mid \hat{a}_l^\dagger = \langle \psi \mid \overline{\psi}_l . \tag{C.66}$$

Here the right(left)-eigenvalues ψ ($\overline{\psi}$) are commuting/anti-commuting numbers for Bosons/Fermions. For commuting numbers $\overline{\psi}$ can be identified with the complex conjugate of ψ. A coherent state is determined by the set of numbers (fields) $\left\{\psi_l, \overline{\psi}_l\right\}$ where the label l runs over the complete set of one-particle quantum numbers. In case of field-operators $\hat{\Psi}(\boldsymbol{x})$ they become fields over real space $\psi(\boldsymbol{x}), \overline{\psi}(\boldsymbol{x})$.

Two different coherent states are not orthogonal to each other, but have a finite overlap

$$\langle \psi' \mid \psi \rangle = e^{\sum_l \overline{\psi}'_l \psi_l}. \tag{C.67}$$

Furthermore, they form an over-complete set of states, when the fields run over all possible numbers. Nevertheless, the coherent states allow for a partition of unity

$$1 = \int \left(\prod_l \pi^{-(1\pm 1)/2} \mathrm{d}\overline{\psi}_l \mathrm{d}\psi_l \right) e^{-\sum_l \overline{\psi}_l \psi_l} \mid \psi \rangle \langle \psi \mid . \tag{C.68}$$

For the definition of integrals over Grassmann numbers we only mention that it obeys simple rules because Grassmann variables vanish to second order, for details see e.g. [4]. For details on coherent states see [3]. With the help of coherent states the partition sum reads

$$Z = \int D[\overline{\psi}, \psi], e^{-\sum_l \overline{\psi}_l \psi_l} \langle \pm\psi \mid e^{-\beta H_\mu} \mid \psi \rangle, \tag{C.69}$$

where we have abbreviated the measure $\prod_l \pi^{-(1\pm 1)/2} \mathrm{d}\overline{\psi}_l \mathrm{d}\psi_l$ by $D[\overline{\psi}, \psi]$. Since the matrix elements of a Hamiltonian in occupation number representation $H = \sum_{lk} h^{mu}_{lk} a^\dagger_k a_l + \sum_{klmn} V_{klmn} a^\dagger_k a^\dagger_l a_m a_n$ become simple in coherent states (operators are replaced by the fields)

$$\frac{\langle \psi \mid H_\mu \mid \psi' \rangle}{\langle \psi \mid \psi' \rangle} = \sum_{lk} h^{mu}_{lk} \overline{\psi}_l \psi'_l + \sum_{klmn} V_{klmn} \overline{\psi}_k \overline{\psi}_l \psi'_m \psi'_n =: H_\mu(\overline{\psi}, \psi'). \tag{C.70}$$

Therefore, one uses the above mentioned idea of cutting the finite β into a large number $\mathcal{N}$ of small pieces δ and introduces for each point τ_i on that **path** a partition of unity. By this procedure one arrives finally at the **coherent states path integral representation** of Z

$$\boxed{Z = \int D(\overline{\psi}, \psi) e^{-S(\overline{\psi}, \psi)}}. \tag{C.71}$$

Here the measure $D(\overline{\psi}, \psi)$ is an abbreviation for the product $\prod_i^{\mathcal{N}} d[\overline{\psi}(\tau_i), \psi(\tau_i)]$. The **action** of the path integral is given by

$$\boxed{S(\overline{\psi}, \psi) = \int_0^\beta \mathrm{d}\tau \left[\sum_{jk} \overline{\psi}_j(\tau) \partial_\tau \psi_k(\tau) + H_\mu\left(\overline{\psi}(\tau), \psi(\tau)\right) \right]} \tag{C.72}$$

where the continuum limit $\mathcal{N} \to \infty$ has formally been taken. It is only formal since a concrete calculation (e.g. numerical) needs a discretized version to be definite. The fields $\overline{\psi}_l(\tau)$, $\psi_l(\tau)$ have to fulfill Matsubara boundary conditions $\overline{\psi}(0) = \pm\overline{\psi}(\beta)$.

A source dependent partition sum can be constructed by adding source terms to the action

$$S(\overline{\psi}, \psi; j; \overline{j}) = S(\overline{\psi}, \psi) + \int_0^\beta \mathrm{d}\tau \sum_l \overline{j}_l(\tau)\overline{\psi}_l(\tau) + j_l(\tau)\psi_l(\tau). \tag{C.73}$$

For non-interacting systems the action is at most quadratic in the fields and the path integral is a multidimensional Gaussian integral. The essential formulas were given in Sect. 5.5.3. With these formulas one can reproduce the free propagator formula for $Z_0[j]$ of the foregoing section. Also, one can reproduce the perturbation series. One can use all of the flexible strategies for functional integrals (see Sect. 5.6).

C.4 Exercises

Exercise 1: Susceptibilities
Derive (C.14) by linear imaginary time dependent perturbation theory.
Show that the thermodynamic susceptibility can be written as

$$\chi_{YX} = e^{\beta\Omega} \sum_{\lambda\lambda'} e^{-\beta(\mathcal{E}_\lambda - \mu N_\lambda)} X_{\lambda\lambda'} Y_{\lambda'\lambda} \frac{e^{-\beta(\mathcal{E}_{\lambda'} - \mathcal{E}_\lambda)} - 1}{\mathcal{E}_\lambda - \mathcal{E}_{\lambda'}}$$

and the Kubo-susceptibility as

$$\chi_{YX}(z) = e^{\beta\Omega} \sum_{\lambda\lambda'} \frac{[X_{\lambda\lambda'} Y_{\lambda\lambda'} - Y_{\lambda\lambda'} X_{\lambda\lambda'}]}{\mathcal{E}_{\lambda'} - \mathcal{E}_\lambda + \hbar z} e^{-\beta(\mathcal{E}_\lambda - \mu N_\lambda)}$$

In both expressions Ω follows from

$$\sum_\lambda e^{-\beta(\mathcal{E}_\lambda - \mu N_\lambda)} = e^{-\beta\Omega}$$

Exercise 2: Thermodynamic Potential as Generator
Show that the equilibrium value of $X(F)$ follows from differentiating Ω

$$\langle X(F) \rangle_F = -\partial_F \Omega.$$

References

1. K. Binder, D.W. Heermann, *Monte Carlo Simulation in Statistical Physics. An Introduction*, 4th edn. (Springer, 2002)
2. C.P. Enz, *A Course in Many Body Theory Applied to Solid State Physics* (World Scientific, Singapore, 1992)
3. J.W. Negele, H. Orland, *Quantum Many-particle Systems* (Westview Press, 1998)
4. K. Efetov, *Supersymmetry in Disorder and Chaos* (Cambridge University Press, Cambridge, 1997)

Index

M. Janßen, *Generated Dynamics of Markov and Quantum Processes*,
DOI 10.1007/978-3-662-49696-1