1

Introduction

1.1 Closed time contour

Consider a quantum many-body system governed by a time-dependent Hamiltonian $\hat{H}(t)$. Let us assume that in the distant past $t = -\infty$ the system was in a state specified by a many-body density matrix $\hat{\rho}(-\infty)$. The precise form of the latter is of no importance. It may be, e.g., the equilibrium density matrix associated with the Hamiltonian $\hat{H}(-\infty)$. We shall also assume that the time-dependence of the Hamiltonian is such that at $t = -\infty$ the particles were non-interacting. The interactions are then adiabatically switched on to reach their actual physical strength sometime prior to the observation time. *In addition*, the Hamiltonian may contain *true* time dependence through e.g. external fields or boundary conditions. Due to such true time-dependent perturbations the density matrix is driven away from equilibrium.

The density matrix evolves according to the Von Neumann equation

$$\partial_t \hat{\rho}(t) = -\mathrm{i}\big[\hat{H}(t), \hat{\rho}(t)\big], \tag{1.1}$$

where we set $\hbar = 1$. It is formally solved with the help of the unitary evolution operator as $\hat{\rho}(t) = \hat{\mathcal{U}}_{t,-\infty}\hat{\rho}(-\infty)\big[\hat{\mathcal{U}}_{t,-\infty}\big]^\dagger = \hat{\mathcal{U}}_{t,-\infty}\hat{\rho}(-\infty)\hat{\mathcal{U}}_{-\infty,t}$, where the $\dagger$ denotes Hermitian conjugation. The evolution operator obeys

$$\partial_t \hat{\mathcal{U}}_{t,t'} = -\mathrm{i}\hat{H}(t)\,\hat{\mathcal{U}}_{t,t'}\,; \qquad\qquad \partial_{t'}\hat{\mathcal{U}}_{t,t'} = \mathrm{i}\hat{\mathcal{U}}_{t,t'}\,\hat{H}(t').$$

Notice that the Hamiltonian operators taken at different moments of time, in general, do not commute with each other. As a result, $\hat{\mathcal{U}}_{t,t'}$ must be understood as an infinite product of incremental evolution operators with instantaneous locally constant Hamiltonians

$$\begin{aligned}\hat{\mathcal{U}}_{t,t'} &= \lim_{N\to\infty} \mathrm{e}^{-\mathrm{i}\hat{H}(t-\delta_t)\delta_t}\mathrm{e}^{-\mathrm{i}\hat{H}(t-2\delta_t)\delta_t}\ldots\mathrm{e}^{-\mathrm{i}\hat{H}(t-N\delta_t)\delta_t}\mathrm{e}^{-\mathrm{i}\hat{H}(t')\delta_t} \\ &= \mathbb{T}\exp\left(-\mathrm{i}\int_{t'}^{t}\hat{H}(t)\,\mathrm{d}t\right),\end{aligned} \tag{1.2}$$

where an infinitesimal time-step is $\delta_t = (t-t')/N$ and to shorten the notations the infinite product is abbreviated as the time-ordered, or $\mathbb{T}$-exponent.

One is usually interested to know an expectation value of some observable $\hat{\mathcal{O}}$ (say density or current operator) at a time t.[1] It is defined as

$$\langle\hat{\mathcal{O}}\rangle(t) \equiv \frac{\mathrm{Tr}\{\hat{\mathcal{O}}\hat{\rho}(t)\}}{\mathrm{Tr}\{\hat{\rho}(t)\}} = \frac{1}{\mathrm{Tr}\{\hat{\rho}(t)\}}\ \mathrm{Tr}\big\{\hat{\mathcal{U}}_{-\infty,t}\hat{\mathcal{O}}\hat{\mathcal{U}}_{t,-\infty}\hat{\rho}(-\infty)\big\}, \tag{1.3}$$

where the trace is performed over many-body Hilbert space and in the last equality we cyclically permuted the $\hat{\mathcal{U}}_{-\infty,t}$ operator under the trace sign. The expression under the last trace describes (read from right to left) evolution from $t = -\infty$, where the initial density matrix is specified, toward t, where the observable is calculated, and then back to $t = -\infty$. Therefore calculation of an observable implies evolving the initial state both *forward and backward*.

Such forward–backward evolution is avoided in the equilibrium quantum field theory with a special trick. Let us recall how it works, for example, in the zero-temperature equilibrium formalism [2]. The latter deals with the ground state expectation values of the type $\langle \mathrm{GS}|\hat{\mathcal{O}}|\mathrm{GS}\rangle$, where $|\mathrm{GS}\rangle$ is a ground state of an *interacting* many-body system. It is obtained from the known and simple ground state of the corresponding *non-interacting* system $|0\rangle$ by acting on the latter with the evolution operator $|\mathrm{GS}\rangle = \hat{\mathcal{U}}_{t,-\infty}|0\rangle$. Since we are dealing with the equilibrium situation, the only time dependence allowed for the Hamiltonian is an adiabatic switching of the interactions on and off in the distant past and distant future, respectively. The evolution operator therefore describes the evolution of a simple non-interacting ground state $|0\rangle$ toward $|\mathrm{GS}\rangle$ upon adiabatic switching of the interactions and thus $\langle \mathrm{GS}|\hat{\mathcal{O}}|\mathrm{GS}\rangle = \langle 0|\hat{\mathcal{U}}_{-\infty,t}\hat{\mathcal{O}}\hat{\mathcal{U}}_{t,-\infty}|0\rangle$.

Now comes the trick: one argues that

$$\hat{\mathcal{U}}_{+\infty,-\infty}|0\rangle = \mathrm{e}^{\mathrm{i}L}|0\rangle. \tag{1.4}$$

That is, evolution of the non-interacting ground state upon adiabatic switching of the interactions on and subsequent adiabatic switching them off brings the system back into the state $|0\rangle$, up to a phase factor $\mathrm{e}^{\mathrm{i}L}$. This statement is based on the belief that the adiabatic perturbation keeps the system in its (evolving) ground state at all times. If so, in view of normalization $\langle 0|0\rangle = 1$, the only possible change is the phase of the non-interacting ground state $\mathrm{e}^{\mathrm{i}L} = \langle 0|\hat{\mathcal{U}}_{+\infty,-\infty}|0\rangle$. Similarly $\langle 0|\hat{\mathcal{U}}_{+\infty,-\infty} = \langle 0|\mathrm{e}^{\mathrm{i}L}$. Accepting this, one proceeds as follows:

$$\begin{aligned}\langle \mathrm{GS}|\hat{\mathcal{O}}|\mathrm{GS}\rangle &= \langle 0|\hat{\mathcal{U}}_{-\infty,t}\hat{\mathcal{O}}\hat{\mathcal{U}}_{t,-\infty}|0\rangle = \mathrm{e}^{-\mathrm{i}L}\langle 0|\mathrm{e}^{\mathrm{i}L}\hat{\mathcal{U}}_{-\infty,t}\hat{\mathcal{O}}\hat{\mathcal{U}}_{t,-\infty}|0\rangle \\ &= \mathrm{e}^{-\mathrm{i}L}\langle 0|\hat{\mathcal{U}}_{+\infty,-\infty}\hat{\mathcal{U}}_{-\infty,t}\hat{\mathcal{O}}\hat{\mathcal{U}}_{t,-\infty}|0\rangle = \frac{\langle 0|\hat{\mathcal{U}}_{+\infty,t}\hat{\mathcal{O}}\hat{\mathcal{U}}_{t,-\infty}|0\rangle}{\langle 0|\hat{\mathcal{U}}_{+\infty,-\infty}|0\rangle}\ ,\end{aligned} \tag{1.5}$$

[1] We work in the Schrödinger picture, where observables are t-independent operators, while the wavefunctions and the density matrix evolve.

where in the last equality we used $\hat{\mathcal{U}}_{+\infty,-\infty}\hat{\mathcal{U}}_{-\infty,t} = \hat{\mathcal{U}}_{+\infty,t}$, which is an immediate consequence of Eq. (1.2). The result of this procedure is that one needs to consider only the *forward* evolution. Indeed, the numerator in the last expression (being read from right to left) calls for evolving the non-interacting ground state $|0\rangle$ from the distant past to the observation time, where the observable operator acts, and then proceeding towards the distant future, where the overlap with the same known state $\langle 0|$ is evaluated.

The similar strategy works in the finite-temperature equilibrium formalism [11, 2, 4]. There, one treats the equilibrium density matrix $\mathrm{e}^{-\beta\hat{H}}$, where $\beta = 1/T$ is the inverse temperature, as the evolution operator in the imaginary time τ. The latter is defined on a finite interval $0 \leq \tau < \beta$. The observables (or correlation functions) are also evaluated at imaginary time points $\tau_1, \tau_2, \ldots$ and the result must be analytically continued back to the real-time axis. One may argue that, since the adiabatic switching of interactions does not drive the system out of equilibrium, a statement similar to Eq. (1.4) still holds. As a result one is again left to describe only the forward evolution, albeit along the finite time interval in the imaginary direction.

Let us mention that elimination of the backward evolution comes with a price: the normalization denominator in the last expression in Eq. (1.5). It offsets the phase accumulation $\mathrm{e}^{\mathrm{i}L}$ of the non-interacting ground state $|0\rangle$. In diagrammatic language it amounts to subtracting the so-called disconnected or vacuum loop diagrams. This denominator is a serious liability in the theory of disordered systems. The reason is that the accumulated phase $\mathrm{e}^{\mathrm{i}L}$ sensitively depends on a specific realization of the disorder (which may be thought of as being absent at $t \to \pm\infty$ and adiabatically switched on and off in the process of evolution). Therefore the denominator absolutely must be included in any disorder averaging procedure, which complicates the treatment in a very substantial way.

The much more serious trouble with the outlined procedure is that Eq. (1.4) does *not* work in a non-equilibrium situation. If the Hamiltonian $\hat{H}(t)$ contains non-adiabatic time-dependent external fields, boundary conditions, etc., the evolution drives the system away from equilibrium. Even if all such fields are eventually switched off in the distant future, there is no guarantee that the system returns to its ground (or equilibrium) state. Therefore acting with the operator $\hat{\mathcal{U}}_{+\infty,-\infty}$ on the initial ground (or equilibrium) state results in an unknown superposition of excited states. As a result, the backward evolution, inherent to Eq. (1.3), can't be eliminated.

Nevertheless, it is still convenient to extend the evolution in Eq. (1.3) towards $t = +\infty$ and then back to t. This is achieved with the help of the trivial identity $\hat{\mathcal{U}}_{t,+\infty}\hat{\mathcal{U}}_{+\infty,t} = \hat{1}$. Inserting it into Eq. (1.3) and using $\hat{\mathcal{U}}_{-\infty,t}\hat{\mathcal{U}}_{t,+\infty} = \hat{\mathcal{U}}_{-\infty,+\infty}$, one finds

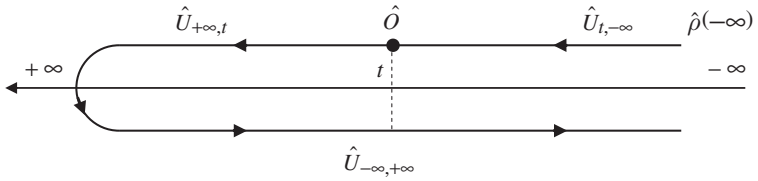

Fig. 1.1 Closed time contour $\mathcal{C}$. Evolution along such a contour is described by Eq. (1.6).

$$\langle\hat{\mathcal{O}}\rangle(t) = \frac{1}{\mathrm{Tr}\{\hat{\rho}(-\infty)\}}\,\mathrm{Tr}\big\{\hat{\mathcal{U}}_{-\infty,+\infty}\hat{\mathcal{U}}_{+\infty,t}\hat{\mathcal{O}}\hat{\mathcal{U}}_{t,-\infty}\hat{\rho}(-\infty)\big\}. \tag{1.6}$$

Here we also used that, according to the Von Neumann equation (1.1), the trace of the initial density matrix is unchanged under the unitary evolution. Equation (1.6) describes evolution along the *closed time contour* $\mathcal{C}$ depicted in Fig. 1.1. The observable $\hat{\mathcal{O}}$ is inserted at time t, somewhere along the forward branch of the contour. Notice that inserting the operator $\hat{\mathcal{U}}_{t,+\infty}\hat{\mathcal{U}}_{+\infty,t} = \hat{1}$ to the right of $\hat{\mathcal{O}}$ in Eq. (1.3), one could equally well arrange to have the observable on the backward branch of the contour. As we shall see, the most convenient choice is to take a half sum of these two equivalent representations.

Evolution along the closed time contour $\mathcal{C}$ is the central subject of this book. The fact that the field theory can be constructed with the time ordering along such a contour was first realized by Schwinger [12] and further developed in [24, 25]. About the same time Konstantinov and Perel' [13] have developed a diagrammatic technique, based on the time contour containing forward and backward branches in the real-time direction along with the imaginary time portion of length β. The formalism was significantly advanced, in particular its utility to derive the kinetic theory, in the seminal book of Kadanoff and Baym [1]. Independently Keldysh [14] (for some of the historic context see [26]) suggested a formulation which does not rely on imaginary time (and thus on the equilibrium density matrix). He also introduced a convenient choice of variables (Keldysh rotation), which made derivation of the kinetic theory particularly transparent. The time contour without the imaginary time piece, along with the Keldysh variables (which we call "classical" and "quantum") appear to be by far the most convenient choices for the functional formulation of the theory presented in this book. For this reason we occasionally refer to the construction as the Keldysh technique (this should by no way diminish the credit deserved by the other authors). Reformulation of the theory for the case of fermions, given later by Larkin and Ovchinnikov [27], became universally accepted. In fact, other theories developed about the same time, while not using the time contour explicitly, appear to be close relatives of

the Schwinger–Kadanoff–Baym–Keldysh construction. Among them are Feynman and Vernon [28], Wyld's [29] diagrammatic technique for fluid dynamics and Martin, Siggia and Rose [30] and DeDominicis' [31] calculus for classical stochastic systems.

The central object of the theory is the evolution operator along the closed contour $\hat{\mathcal{U}}_{\mathcal{C}} = \hat{\mathcal{U}}_{-\infty,+\infty}\hat{\mathcal{U}}_{+\infty,-\infty}$. If the Hamiltonian is the same on the forward and backward branches, then the forward–backward evolution of *any* state brings it back exactly to the original state. (Not even a phase factor is accumulated, indeed, any phase gained on the forward branch is exactly "unwound" on the backward branch.) As a result $\hat{\mathcal{U}}_{\mathcal{C}} = \hat{1}$ and the partition function, defined as $Z \equiv \mathrm{Tr}\{\hat{\mathcal{U}}_{\mathcal{C}}\hat{\rho}(-\infty)\}/\mathrm{Tr}\{\hat{\rho}(-\infty)\}$, is identically equal to unity, $Z = 1$. Nevertheless, the partition function is a convenient object to develop the functional representation and the normalization identity $Z = 1$ is a useful check of its consistency. For this reason we shall use it widely in what follows.

To insert an observable somewhere along the forward (as prescribed by Eq. (1.6)) or backward branches it is convenient to modify the Hamiltonian $\hat{H}(t)$ by adding the source term $\hat{H}^{\pm}_{V}(t) \equiv \hat{H}(t) \pm \hat{\mathcal{O}}V(t)$, where the plus (minus) sign refers to the forward (backward) part of the contour. Now, since the Hamiltonian is different on the two branches, the evolution operator along the contour $\hat{\mathcal{U}}_{\mathcal{C}}[V] \neq \hat{1}$ becomes non-trivial and so does the *generating function*

$$Z[V] \equiv \frac{\mathrm{Tr}\{\hat{\mathcal{U}}_{\mathcal{C}}[V]\,\hat{\rho}(-\infty)\}}{\mathrm{Tr}\{\hat{\rho}(-\infty)\}}. \tag{1.7}$$

The expectation value of the observable $\hat{\mathcal{O}}$, given by Eq. (1.6) (or rather by a half sum of the observable inserted along the forward and backward branches) may be found as $\langle\hat{\mathcal{O}}\rangle(t) = (\mathrm{i}/2)\delta Z[V]/\delta V(t)\big|_{V=0}$. This expression should be compared with the equilibrium technique [2, 4], where the observables are given by variational derivatives of the *logarithm* of the generating (or partition) function. In our case, since $Z = Z[0] = 1$, the presence of the logarithm is optional.[2] Knowledge of the generating function allows thus to find observables of interest. Therefore, after developing the functional formalism for the partition function, we extend it to include the generating function as well.

[2] It is worth mentioning that the denominators in Eqs. (1.5) and (1.7) have very different status. In the latter case $\mathrm{Tr}\{\hat{\rho}(-\infty)\}$ refers entirely to the distant past, when both interactions and disorder are switched off. It is therefore a simple constant, which may be easily evaluated. In the former case $\langle 0|\hat{\mathcal{U}}_{+\infty,-\infty}|0\rangle$ involves evolution of the ground state upon switching on and off the interactions and disorder. It thus depends on both disorder and interactions and requires a separate calculation. The absence of a disorder-dependent denominator makes the closed time contour formalism especially suitable to deal with the averaging over the quenched disorder. The fact that observables do not require the *logarithm* is another manifestation of the absence of the non-trivial denominator.

1.2 The outline of this book

Chapter 2 is devoted to a possibly simplest many-body system of bosonic particles occupying a single quantum state. We briefly develop a second quantization representation and then proceed towards the functional formalism, based on the coherent-state functional integral along the contour $\mathcal{C}$. Here we pay close attention to a fundamental discrete time (see Eq. (1.2)) representation of the evolution operator. The model allows us to expose explicitly the discrete time structure, to verify normalization $Z = 1$ and to explain the meaning and hidden skeletons of the continuous notation. We then introduce Keldysh rotation, "classical/quantum" variables and explain the causality structure. Finally we introduce the generating function in discrete and continuous notations and explain the relation between them.

In Chapter 3 we exploit the analogy between the toy model of Chapter 2 and the harmonic oscillator to formulate the single-particle quantum mechanics as a path integral on the closed time contour. We then use it to investigate a quantum particle coupled to an equilibrium bath of harmonic oscillators. Integrating out the oscillators, degrees of freedom, we derive the real-time version of the celebrated Caldeira–Leggett model. We then use the ideas of time contour to discuss quantum mechanical tunneling in the presence of an external ac field (both with and without coupling to the bath).

In Chapter 4 we pick up the discussion of a particle coupled to a bath, introduced in Chapter 3. In particular we focus on its classical limit, where the corresponding real-time action acquires local (in time) form. We show ultimate relations of the emerging theory to the physics of classical stochastic systems. To this end we derive Langevin and Fokker–Planck equations from the time contour action and explain its connections to the Martin–Siggia–Rose–DeDominicis construction. We then focus on a few examples, which include escape from a metastable state, reaction models, fluctuation theorem and time-dependent perturbations acting on a stochastic system.

All the considerations so far were limited to systems with one (or a few) degrees of freedom, possibly coupled to an external bath. In Chapter 5 we start generalizing the formalism to true many-body systems. We introduce free bosonic fields (both complex and real) and their functional description on the closed contour. We then add interactions (collisions) between the particles and derive diagrammatic technique and the Dyson equation. Following Keldysh [14], we show that the latter contains the kinetic equation for a non-equilibrium distribution function. We demonstrate then how the collision integral emerges from a perturbative treatment of the self-energy.

Chapters 2–5 form the basis of the book. They serve to introduce most of the theoretical apparatus, notations and conventions used throughout the rest of the book. They are absolutely necessary for comprehension of what follows. We then branch into a number of applications, which are to a large extent logically independent of each other. Therefore the subsequent chapters may be read (or omitted) in an arbitrary order, without much damage to the understanding. Yet they share a number of common themes and methods which are developed in a certain sequence. The latter was meant to emphasize the connection between various fields and to reinforce common techniques at every successive encounter of them.

The first example, Chapter 6, is collisionless (i.e. where the particles interact only with a collective electromagnetic field) dynamics of a classical plasma. We derive the Vlasov equations, collective excitations – plasmons, and Landau damping. Though the system is purely classical, we treat it with the quantum formalism. Besides methodological illustration, it allows us to treat fluctuations of the collective electric potential and derive the so-called quasi-linear theory. The latter deals with the coupled kinetic equations for particles and plasmons (while Vlasov theory treats the electric field as fully deterministic, i.e. no fluctuations).

We then go to the essentially quantum system: low temperature weakly interacting Bose gas, in Chapter 7. We derive the Gross–Pitaevskii description of the condensate as a stationary point approximation of the corresponding functional integral. We then consider small fluctuations on top of the stationary field configuration and show that they bring the celebrated Bogoliubov quasiparticle spectrum. We then proceed to a description of a non-equilibrium quasiparticle cloud. To this end we derive a system of equations for the distribution function of quasiparticles coupled to the (modified) Gross–Pitaevskii equation for the condensate wavefunction. Following analogy with the collisionless plasma of Chapter 6, we show that this system contains Langevin forcing of the condensate fluctuations along with their collisionless damping. We then derive various contributions to the collision integral and use them to discuss kinetics of the condensate growth upon evaporative cooling.

Chapter 8 is devoted to the dynamics of phase transitions (mostly classical and only briefly quantum). Following Langer, we first discuss nucleation dynamics of critical droplets in first order transitions. We then switch to dynamics of continuous phase transitions, starting from equilibrium transitions and classification of their dynamic universality classes given by Hohenberg and Halperin. We then turn to essentially non-equilibrium phase transitions. The examples include absorbing state transitions in reaction-diffusion models and Kardar–Parisi–Zhang consideration of the roughening transition on growing interfaces.

The rest of the book, i.e. Chapters 9–14, is devoted to fermions. Chapter 9 presents a fermionic version of the one degree of freedom toy model. It uses a Grassmann functional integral on the closed time contour and is essentially parallel to its bosonic counterpart of Chapter 2. We then introduce fermionic fields and their interactions and derive a diagrammatic technique, the Dyson equation and finally the kinetic equation, again essentially parallel to their bosonic counterparts of Chapter 5. Finally we focus on the spin of the electron and discuss Stoner ferromagnetic transition and the spin part of the kinetic equation.

In Chapter 10 we use fermionic formalism to discuss non-equilibrium quantum transport. In particular we derive the Landauer formula for tunneling conductance, the Lesovik formula for shot-noise, the Levitov's result for the full counting statistics of transmitted charge, the Brouwer formula for adiabatic pumping of charge and, following Nazarov and Tobiska, the exact fluctuation relation and its consequences. We also deal with the spin transport, deriving the Slonczewski–Berger spin-torque term in the Landau–Lifshitz equation along with the spin-torque noise and associated Gilbert damping.

Chapters 11–14 deal with fermionic systems in the presence of a static (quenched) disorder potential. We start in Chapter 11 from the kinetic equation approach, which leads to the diffusive dynamics of density fluctuations and the concept of transport scattering time. The kinetic approximation misses quantum interference and mesoscopic fluctuation effects. To improve upon it we develop a systematic disorder averaging procedure, which takes advantage of the fundamental normalization $Z = 1$ of the closed time contour technique. It leads to the so-called matrix non-linear sigma-model, which we use to rederive the kinetic equation and diffusive density response and supplement it with quantum weak-localization corrections and the scaling theory of Anderson localization.

In Chapter 12 we focus on mesoscopic, i.e. sample-to-sample, fluctuations due to differences in disorder configurations in small metallic samples. We deal with density of states fluctuation and its particular limit, known as Wigner–Dyson statistics. We then proceed to describe universal conductance fluctuations and fluctuations of current–voltage characteristics. Finally we discuss full counting statistics of a disordered quasi-one-dimensional wire and the tunneling action.

We then include electron–electron interactions in disordered systems, which lead to non-trivial singular corrections to the density of states (the so-called zero bias anomaly) and conductivity (Altshuler–Aronov corrections). They also provide collision terms (and thus finite relaxation time) to the diffusive kinetic equation. These effects are the subject of Chapter 13.

Chapter 14 is devoted to the physics of disordered superconductors. We generalize the non-linear sigma-model to include superconducting correlations. Its stationary state condition yields the Usadel equation, which includes equations

for the spectrum of the superconductor under non-equilibrium conditions as well as the kinetic equation for the quasiparticles distribution function. Together with the self-consistency condition they provide a complete framework to study non-equilibrium superconductivity. As examples we work out the spectrum of the collective (Carlson–Goldman) mode of the superconductor, derive the time-dependent Ginzburg–Landau theory and fluctuation corrections to the conductivity above the critical temperature.

2

Bosons

The aim of this chapter is to develop a functional integral representation for the evolution operator along the closed time contour. To this end we use an example of a single quantized level populated by bosonic particles. Notations and structures introduced in this chapter are used throughout the rest of the book.

2.1 Bosonic coherent states

We start by considering a single quantum level occupied by bosonic particles. A *many-body* state with n bosons is denoted by $|n\rangle$. Such *pure number states* form a complete orthonormal basis, meaning $\langle n|n'\rangle = \delta_{nn'}$ and $\sum_n |n\rangle\langle n| = \hat{1}$. It is convenient to introduce bosonic annihilation and creation operators, $\hat{b}$ and $\hat{b}^\dagger$, which operate in the many-body Hilbert space of the system according to the following rules:

$$\hat{b}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,; \qquad \hat{b}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle. \tag{2.1}$$

By acting on an arbitrary basis state, one may check the following relations:

$$\hat{b}^\dagger\hat{b}|n\rangle = n|n\rangle\,; \qquad \hat{b}\hat{b}^\dagger|n\rangle = (n+1)|n\rangle\,; \qquad [\hat{b},\hat{b}^\dagger] = \hat{1}. \tag{2.2}$$

An extremely useful tool for our purposes is the algebra of bosonic coherent states, which we summarize briefly in this section. A coherent state, parametrized by a complex number ϕ, is defined as a right eigenstate of the annihilation operator with the eigenvalue ϕ:

$$\hat{b}\,|\phi\rangle = \phi|\phi\rangle\,; \qquad \langle\phi|\,\hat{b}^\dagger = \bar{\phi}\langle\phi|, \tag{2.3}$$

where the bar denotes complex conjugation. As a result, the matrix elements in the coherent state basis of any *normally ordered* operator $\hat{H}(\hat{b}^\dagger,\hat{b})$ (i.e. such that all the creation operators are to the left of all the annihilation operators) are given by

$$\langle\phi|\hat{H}(\hat{b}^\dagger,\hat{b})|\phi'\rangle = H(\bar{\phi},\phi')\,\langle\phi|\phi'\rangle. \tag{2.4}$$

One may check by direct substitution using Eq. (2.1) that the following linear superposition of the pure number states is indeed the required right eigenstate of the operator $\hat{b}$:

$$|\phi\rangle = \sum_{n=0}^{\infty} \frac{\phi^n}{\sqrt{n!}} |n\rangle = \sum_{n=0}^{\infty} \frac{\phi^n}{n!} \left(\hat{b}^\dagger\right)^n |0\rangle = \mathrm{e}^{\phi \hat{b}^\dagger} |0\rangle, \tag{2.5}$$

where $|0\rangle$ is the vacuum state, $\hat{b}\,|0\rangle = 0$. Upon Hermitian conjugation, one finds $\langle\phi| = \langle 0|\,\mathrm{e}^{\bar{\phi}\hat{b}} = \sum_n \langle n|\bar{\phi}^n/\sqrt{n!}$. The coherent states are not mutually orthogonal and they form an over-complete basis. The overlap of two coherent states is given by

$$\langle\phi|\phi'\rangle = \sum_{n,n'=0}^{\infty} \frac{\bar{\phi}^n \phi'^{n'}}{\sqrt{n!n'!}} \langle n|n'\rangle = \sum_{n=0}^{\infty} \frac{(\bar{\phi}\phi')^n}{n!} = \mathrm{e}^{\bar{\phi}\phi'}, \tag{2.6}$$

where we employed the orthonormality of the pure number states.

One may express resolution of unity in the coherent states basis. It takes the following form:

$$\hat{1} = \int \mathrm{d}[\bar{\phi}, \phi]\; \mathrm{e}^{-|\phi|^2}\, |\phi\rangle\langle\phi|, \tag{2.7}$$

where $\mathrm{d}[\bar{\phi}, \phi] \equiv \mathrm{d}(\mathrm{Re}\,\phi)\,\mathrm{d}(\mathrm{Im}\,\phi)/\pi$. To prove this relation one may employ the Gaussian integral

$$Z[\bar{J}, J] = \int \mathrm{d}[\bar{\phi}, \phi]\, \mathrm{e}^{-\bar{\phi}\phi + \bar{\phi}J + \bar{J}\phi} = \mathrm{e}^{\bar{J}J}, \tag{2.8}$$

where J is an arbitrary complex number. As its consequence one obtains

$$\int \mathrm{d}[\bar{\phi}, \phi]\, \mathrm{e}^{-|\phi|^2}\, \bar{\phi}^n \phi^{n'} = \frac{\partial^{n+n'}}{\partial J^n \partial \bar{J}^{n'}} Z[\bar{J}, J]\bigg|_{\bar{J}=J=0} = n!\,\delta_{n,n'}. \tag{2.9}$$

Substituting Eq. (2.5) and its conjugate into the right hand side of Eq. (2.7) and employing Eq. (2.9) along with the resolution of unity in the number state basis $\hat{1} = \sum_n |n\rangle\langle n|$, one proves the identity (2.7).

The trace of an arbitrary operator $\hat{\mathcal{O}}$, acting in the space of the occupation numbers, is evaluated as

$$\begin{aligned} \mathrm{Tr}\{\hat{\mathcal{O}}\} &\equiv \sum_{n=0}^{\infty} \langle n|\hat{\mathcal{O}}|n\rangle = \sum_{n=0}^{\infty} \int \mathrm{d}[\bar{\phi}, \phi]\, \mathrm{e}^{-|\phi|^2}\, \langle n|\hat{\mathcal{O}}|\phi\rangle\langle\phi|n\rangle \\ &= \int \mathrm{d}[\bar{\phi}, \phi] \mathrm{e}^{-|\phi|^2} \sum_{n=0}^{\infty} \langle\phi|n\rangle\langle n|\hat{\mathcal{O}}|\phi\rangle = \int \mathrm{d}[\bar{\phi}, \phi]\, \mathrm{e}^{-|\phi|^2}\, \langle\phi|\hat{\mathcal{O}}|\phi\rangle, \end{aligned} \tag{2.10}$$

where we have employed resolution of unity first in the coherent state basis and second in the number state basis.

Another useful identity is

$$f(\rho) \equiv \langle \phi | \rho^{\hat{b}^\dagger \hat{b}} | \phi' \rangle = \mathrm{e}^{\bar{\phi}\phi'\rho}. \tag{2.11}$$

The proof is based on the following operator relation: $g(\hat{b}^\dagger \hat{b})\, \hat{b} = \hat{b}\, g(\hat{b}^\dagger \hat{b} - 1)$ valid for an arbitrary function $g(\hat{b}^\dagger \hat{b})$, which is verified by acting on an arbitrary basis vector $|n\rangle$. As a result,

$$\partial_\rho f(\rho) = \langle \phi | \hat{b}^\dagger \hat{b}\, \rho^{\hat{b}^\dagger \hat{b} - 1} | \phi' \rangle = \langle \phi | \hat{b}^\dagger \rho^{\hat{b}^\dagger \hat{b}}\, \hat{b} | \phi' \rangle = \bar{\phi}\phi' f(\rho).$$

Integrating this differential equation with the initial condition $f(1) = \mathrm{e}^{\bar{\phi}\phi'}$, which follows from Eq. (2.6), one proves the identity (2.11).

2.2 Partition function

Let us consider the simplest many-body system: bosonic particles occupying a single quantum state with the energy ω_0. Its secondary quantized Hamiltonian has the form

$$\hat{H}(\hat{b}^\dagger, \hat{b}) = \omega_0\, \hat{b}^\dagger \hat{b}, \tag{2.12}$$

where $\hat{b}^\dagger$ and $\hat{b}$ are bosonic creation and annihilation operators with the commutation relation $[\hat{b}, \hat{b}^\dagger] = \hat{1}$. Let us define the partition function as

$$Z = \frac{\mathrm{Tr}\{\hat{\mathcal{U}}_{\mathcal{C}} \hat{\rho}\}}{\mathrm{Tr}\{\hat{\rho}\}}. \tag{2.13}$$

If one assumes that all external fields are exactly the same on the forward and backward branches of the contour, then $\hat{\mathcal{U}}_{\mathcal{C}} = \hat{1}$ and therefore $Z = 1$. The initial density matrix $\hat{\rho} = \hat{\rho}(\hat{H})$ is some operator-valued function of the Hamiltonian. To simplify the derivations one may choose it to be the equilibrium density matrix, $\hat{\rho}_0 = \exp\{-\beta(\hat{H} - \mu \hat{N})\} = \exp\{-\beta(\omega_0 - \mu)\hat{b}^\dagger \hat{b}\}$, where $\beta = 1/T$ is the inverse temperature and μ is the chemical potential. Since arbitrary external perturbations may be switched on (and off) at a later time, the choice of the equilibrium initial density matrix does not prevent one from treating non-equilibrium dynamics. For the equilibrium initial density matrix one finds

$$\mathrm{Tr}\{\hat{\rho}_0\} = \sum_{n=0}^{\infty} \mathrm{e}^{-\beta(\omega_0 - \mu)n} = [1 - \rho(\omega_0)]^{-1}, \tag{2.14}$$

where $\rho(\omega_0) = \mathrm{e}^{-\beta(\omega_0 - \mu)}$. An important observation is that, in general, $\mathrm{Tr}\{\hat{\rho}\}$ is an interaction- and disorder-independent constant. Indeed, both interactions and disorder are switched on (and off) on the forward (backward) parts of the contour

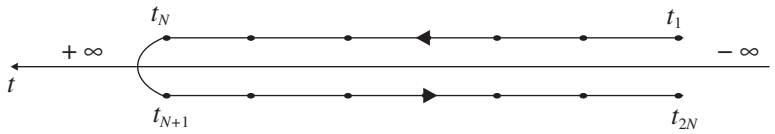

Fig. 2.1 The closed time contour $\mathcal{C}$. Dots on the forward and backward branches of the contour denote discrete time points.

sometime after (before) $t = -\infty$. This constant is therefore frequently omitted without causing confusion.

The next step is to divide the $\mathcal{C}$ contour into $(2N-2)$ time intervals of length δ_t, such that $t_1 = t_{2N} = -\infty$ and $t_N = t_{N+1} = +\infty$, as shown in Fig. 2.1. One then inserts the resolution of unity in the over-complete coherent state basis, Eq. (2.7),

$$\hat{1} = \int \mathrm{d}[\bar{\phi}_j, \phi_j]\, \mathrm{e}^{-|\phi_j|^2} |\phi_j\rangle\langle\phi_j| \tag{2.15}$$

at each point $j = 1, 2, \ldots, 2N$ along the contour. For example, for $N = 3$ one obtains the following sequence in the expression for $\mathrm{Tr}\{\hat{\mathcal{U}}_{\mathcal{C}}\hat{\rho}_0\}$, Eq. (2.10) (read from right to left):

$$\langle\phi_6|\hat{\mathcal{U}}_{-\delta_t}|\phi_5\rangle\langle\phi_5|\hat{\mathcal{U}}_{-\delta_t}|\phi_4\rangle\langle\phi_4|\hat{1}|\phi_3\rangle\langle\phi_3|\hat{\mathcal{U}}_{+\delta_t}|\phi_2\rangle\langle\phi_2|\hat{\mathcal{U}}_{+\delta_t}|\phi_1\rangle\langle\phi_1|\hat{\rho}_0|\phi_6\rangle, \tag{2.16}$$

where $\hat{\mathcal{U}}_{\pm\delta_t}$ is the evolution operator (1.1) during the time interval δ_t in the positive (negative) time direction. Its matrix elements are given by:

$$\begin{aligned}\left\langle\phi_j\left|\hat{\mathcal{U}}_{\pm\delta_t}\right|\phi_{j-1}\right\rangle &\equiv \left\langle\phi_j\left|\mathrm{e}^{\mp\mathrm{i}\hat{H}(b^\dagger,b)\delta_t}\right|\phi_{j-1}\right\rangle \approx \left\langle\phi_j\left|\left(1\mp\mathrm{i}\hat{H}(b^\dagger,b)\delta_t\right)\right|\phi_{j-1}\right\rangle \\ &= \langle\phi_j|\phi_{j-1}\rangle\left(1\mp\mathrm{i}H(\bar{\phi}_j,\phi_{j-1})\delta_t\right) \approx \mathrm{e}^{\bar{\phi}_j\phi_{j-1}}\,\mathrm{e}^{\mp\mathrm{i}H(\bar{\phi}_j,\phi_{j-1})\delta_t},\end{aligned} \tag{2.17}$$

where the approximate equalities are valid up to the linear order in δ_t. Here we have employed expression (2.4) for the matrix elements of a normally-ordered operator along with Eq. (2.6) for the overlap of the coherent states. For the toy example (2.12) one finds $H(\bar{\phi}_j, \phi_{j-1}) = \omega_0\bar{\phi}_j\phi_{j-1}$. However, Eq. (2.17) is not restricted to it, but holds for any *normally-ordered* Hamiltonian. Notice that there is no evolution operator inserted between t_N and t_{N+1}. Indeed, these two points are physically indistinguishable and thus the system does not evolve during this time interval.

Employing the following property of the coherent states (see Eq. (2.11)): $\langle\phi_1|\mathrm{e}^{-\beta(\omega_0-\mu)b^\dagger b}|\phi_{2N}\rangle = \exp\left\{\bar{\phi}_1\phi_{2N}\rho(\omega_0)\right\}$ and collecting all the exponential factors along the contour, one finds for the partition function, Eq. (2.13),

$$Z = \frac{1}{\mathrm{Tr}\{\hat{\rho}_0\}}\int\prod_{j=1}^{2N}\mathrm{d}[\bar{\phi}_j,\phi_j]\,\exp\left(\mathrm{i}\sum_{j,j'=1}^{2N}\bar{\phi}_j\,G^{-1}_{jj'}\,\phi_{j'}\right). \tag{2.18}$$

For $N = 3$ (see Eq. (2.16)), the $2N \times 2N$ matrix $\mathrm{i}G^{-1}_{jj'}$ takes the form

$$\mathrm{i}G^{-1}_{jj'} \equiv \left[\begin{array}{cccc|cccc} -1 & & & & & & & \rho(\omega_0) \\ h_- & -1 & & & & & & \\ & h_- & -1 & & & & & \\ & & 1 & & -1 & & & \\ \hline & & & & h_+ & -1 & & \\ & & & & & h_+ & -1 & \end{array}\right], \tag{2.19}$$

where $h_\mp \equiv 1 \mp \mathrm{i}\omega_0\delta_t$. The main diagonal of this matrix originates from the resolution of unity, Eq. (2.15), while the lower sub-diagonal comes from the matrix elements (2.17). Finally, the upper-right element comes from $\langle\phi_1|\hat{\rho}_0|\phi_{2N}\rangle$ in Eq. (2.16). This structure of the $\mathrm{i}\hat{G}^{-1}$ matrix is straightforwardly generalized to arbitrary N.

To proceed with the multiple integrals appearing in Eq. (2.18), we remind the reader of some properties of the Gaussian integrals.

2.3 Bosonic Gaussian integrals

For any complex $N \times N$ matrix $\hat{A}_{ij}$, where $i, j = 1, \ldots, N$, such that all its eigenvalues, λ_i, have non-negative real parts, $\mathrm{Re}\lambda_i \geq 0$, the following statement holds:

$$Z[\bar{J}, J] = \int \prod_{j=1}^{N} \mathrm{d}[\bar{z}_j, z_j]\ \mathrm{e}^{-\sum\limits_{ij}^{N} \bar{z}_i \hat{A}_{ij} z_j + \sum\limits_{j}^{N} [\bar{z}_j J_j + \bar{J}_j z_j]} = \frac{\mathrm{e}^{\sum\limits_{ij}^{N} \bar{J}_i (\hat{A}^{-1})_{ij} J_j}}{\det\hat{A}}, \tag{2.20}$$

where J_j is an arbitrary complex vector and $\mathrm{d}[\bar{z}_j z_j] = \mathrm{d}(\mathrm{Re}z_j)\mathrm{d}(\mathrm{Im}z_j)/\pi$. This equality is a generalization of the Gaussian integral (2.8), used above. To prove it, one starts from a Hermitian matrix $\hat{A}$, which may be diagonalized by a unitary transformation $\hat{A} = \hat{U}^\dagger \hat{\Lambda} \hat{U}$, where $\hat{\Lambda} = \mathrm{diag}\{\lambda_j\}$. The identity is then proven by a change of variables with a unit Jacobian to $w_i = \sum_j \hat{U}_{ij} z_j$, which leads to

$$Z[\bar{J}, J] = \prod_{j=1}^{N} \int \mathrm{d}[\bar{w}_j, w_j]\ \mathrm{e}^{-\bar{w}_j \lambda_j w_j + \bar{w}_j I_j + \bar{I}_j w_j} = \prod_{j=1}^{N} \frac{\mathrm{e}^{\bar{I}_j \lambda_j^{-1} I_j}}{\lambda_j},$$

where $I_i = \sum_j \hat{U}_{ij} J_j$. Using $\sum_j \bar{I}_j \lambda_j^{-1} I_j = \vec{\bar{J}}^{\mathrm{T}} \hat{U}^\dagger \hat{\Lambda}^{-1} \hat{U} \vec{J} = \vec{\bar{J}}^{\mathrm{T}} \hat{A}^{-1} \vec{J}$, along with $\det\hat{A} = \prod_j \lambda_j$, one obtains the right hand side of Eq. (2.20). Finally, one notices that the right hand side of Eq. (2.20) is an analytic function of both $\mathrm{Re}A_{ij}$ and $\mathrm{Im}A_{ij}$. Therefore, one may continue them analytically to the complex plane to reach an arbitrary complex matrix $\hat{A}_{ij}$. The identity (2.20) is thus valid as long as

the integral is well defined, that is all the eigenvalues of $\hat{A}$ have non-negative real parts.

The Wick theorem deals with the average value of $z_{a_1} \dots z_{a_k} \bar{z}_{b_1} \dots \bar{z}_{b_k}$ weighted with the factor $\exp\big(-\sum_{ij} \bar{z}_i \hat{A}_{ij} z_j\big)$. The theorem states that this average is given by the sum of all possible products of pair-wise averages. For example, with the help of Eq. (2.20) one finds

$$\langle z_a \bar{z}_b \rangle \equiv \frac{1}{Z[0,0]} \frac{\delta^2 Z[\bar{J}, J]}{\delta \bar{J}_a \delta J_b}\bigg|_{J=0} = \hat{A}^{-1}_{ab}, \tag{2.21}$$
$$\langle z_a z_b \bar{z}_c \bar{z}_d \rangle \equiv \frac{1}{Z[0,0]} \frac{\delta^4 Z[\bar{J}, J]}{\delta \bar{J}_a \delta \bar{J}_b \delta J_c \delta J_d}\bigg|_{J=0} = \hat{A}^{-1}_{ac} \hat{A}^{-1}_{bd} + \hat{A}^{-1}_{ad} \hat{A}^{-1}_{bc},$$

etc.

The Gaussian identity for integration over real variables has the form

$$Z[J] = \int \prod_{j=1}^{N} \left(\frac{\mathrm{d}x_j}{\sqrt{2\pi}} \right) \mathrm{e}^{-\frac{1}{2}\sum\limits_{ij}^{N} x_i \hat{A}_{ij} x_j + \sum\limits_{j}^{N} x_j J_j} = \frac{\mathrm{e}^{\frac{1}{2}\sum\limits_{ij}^{N} J_i (\hat{A}^{-1})_{ij} J_j}}{\sqrt{\det \hat{A}}}, \tag{2.22}$$

where $\hat{A}$ is a *symmetric* complex matrix with all its eigenvalues having non-negative real parts. The proof is similar to that in the case of complex variables: one starts from a real symmetric matrix, which may be diagonalized by an orthogonal transformation. The identity (2.22) is then easily proven by a change of variables. Finally, one may analytically continue the right hand side (as long as the integral is well defined) from a real symmetric matrix $\hat{A}_{ij}$ to a *complex symmetric* one.

The corresponding Wick theorem for the average value of $x_{a_1} \dots x_{a_{2k}}$ weighted with the factor $\exp\big(-\frac{1}{2}\sum_{ij} x_i \hat{A}_{ij} x_j\big)$ takes the form

$$\langle x_a x_b \rangle \equiv \frac{1}{Z[0]} \frac{\delta^2 Z[J]}{\delta J_a \delta J_b}\bigg|_{J=0} = \hat{A}^{-1}_{ab}, \tag{2.23}$$
$$\langle x_a x_b x_c x_d \rangle \equiv \frac{1}{Z[0]} \frac{\delta^4 Z[J]}{\delta J_a \delta J_b \delta J_c \delta J_d}\bigg|_{J=0} = \hat{A}^{-1}_{ab} \hat{A}^{-1}_{cd} + \hat{A}^{-1}_{ac} \hat{A}^{-1}_{bd} + \hat{A}^{-1}_{ad} \hat{A}^{-1}_{bc},$$

etc. Notice the additional term in the second line in comparison with the corresponding complex result (2.21). The symmetry of $\hat{A}$ (and thus of $\hat{A}^{-1}$) is necessary to satisfy the obvious relation $\langle x_a x_b \rangle = \langle x_b x_a \rangle$.

2.4 Normalization and continuum notation

Having established the Gaussian identity (2.20), one can apply it to Eq. (2.18) to check the normalization factor. In this case $\hat{A} = -\mathrm{i}\hat{G}^{-1}$ and it is straightforward to evaluate the corresponding determinant employing Eq. (2.19):

$$\det\left[-\mathrm{i}\hat{G}^{-1}\right] = 1-\rho(\omega_0)(h_-h_+)^{N-1} = 1-\rho(\omega_0)\left(1+\omega_0^2\delta_t^2\right)^{N-1}$$
$$\approx 1-\rho(\omega_0)\,\mathrm{e}^{\omega_0^2\delta_t^2(N-1)} \overset{N\to\infty}{\longrightarrow} 1-\rho(\omega_0), \tag{2.24}$$

where one used that $\delta_t^2 N \to 0$ if $N \to \infty$. Indeed, we divide the contour in a way to keep $\delta_t N = \text{const}$ (given by a full extent of the time axis) and as a result $\delta_t^2 \sim N^{-2}$. Employing the fact that the Gaussian integral in Eq. (2.18) is equal to the inverse determinant of the $-\mathrm{i}\hat{G}^{-1}$ matrix, Eq. (2.20), along with Eq. (2.14), one finds

$$Z = \frac{1}{\mathrm{Tr}\{\hat{\rho}_0\}}\,\frac{1}{\det\left[-\mathrm{i}\hat{G}^{-1}\right]} = 1, \tag{2.25}$$

as it should be, of course. Notice that keeping the upper-right element of the discrete matrix, Eq. (2.19), is crucial to maintain this normalization identity.

One may now take the limit $N \to \infty$ and formally write the partition function (2.18) in the continuum notation, $\phi_j \to \phi(t)$, as

$$Z = \int \mathbf{D}[\bar{\phi}(t), \phi(t)]\;\mathrm{e}^{\mathrm{i}S[\bar{\phi},\phi]}, \tag{2.26}$$

where the integration measure is the shorthand notation for $\mathbf{D}[\bar{\phi}(t), \phi(t)] = \prod_{j=1}^{2N} \mathrm{d}[\bar{\phi}_j, \phi_j]/\,\mathrm{Tr}\{\hat{\rho}_0\}$. According to Eqs. (2.18) and (2.19), the action is given by

$$S[\bar{\phi},\phi] = \sum_{j=2}^{2N} \delta t_j \left[\mathrm{i}\bar{\phi}_j\,\frac{\phi_j-\phi_{j-1}}{\delta t_j} - \omega_0\bar{\phi}_j\phi_{j-1}\right] + \mathrm{i}\,\bar{\phi}_1\left[\phi_1 - \mathrm{i}\rho(\omega_0)\phi_{2N}\right], \tag{2.27}$$

where $\delta t_j \equiv t_j - t_{j-1} = \pm\delta_t$ on the forward and backward branches, correspondingly. In continuum notation, $\phi_j \to \phi(t)$, the action acquires the form

$$S[\bar{\phi},\phi] = \int_{\mathcal{C}} \mathrm{d}t\;\bar{\phi}(t)\hat{G}^{-1}\phi(t), \tag{2.28}$$

where the continuum form of the operator $\hat{G}^{-1}$ is (see the first square bracket on the right hand side of Eq. (2.27))

$$\hat{G}^{-1} = \mathrm{i}\partial_t - \omega_0. \tag{2.29}$$

It is extremely important to remember that this continuum notation is only an abbreviation which represents the large discrete matrix, Eq. (2.19). In particular, the upper-right element of the matrix (the last term in Eq. (2.27)), that contains the information about the distribution function, is seemingly absent in the continuum notation, Eq. (2.29). The necessity of keeping the boundary terms originates from the fact that the continuum operator (2.29) possesses the zero mode $\mathrm{e}^{-\mathrm{i}\omega_0 t}$. Its inverse operator $\hat{G}$ is therefore not uniquely defined, unless the boundary terms are included.

To avoid integration along the closed time contour, it is convenient to split the bosonic field $\phi(t)$ into the two components $\phi^+(t)$ and $\phi^-(t)$, which reside on the forward and backward parts of the time contour, respectively. The continuum action may be then rewritten as

$$S[\bar{\phi},\phi]=\int_{-\infty}^{+\infty}\mathrm{d}t\left[\bar{\phi}^+(t)(\mathrm{i}\partial_t-\omega_0)\phi^+(t)-\bar{\phi}^-(t)(\mathrm{i}\partial_t-\omega_0)\phi^-(t)\right], \qquad (2.30)$$

where the relative minus sign comes from the reversed direction of the time integration on the backward part of the contour. Once again, the continuum notation is somewhat misleading. Indeed, it creates an undue impression that the $\phi^+(t)$ and $\phi^-(t)$ fields are completely uncorrelated. In fact, they are connected due to the presence of the non-zero off-diagonal blocks in the discrete matrix, Eq. (2.19). It is therefore desirable to develop a continuum representation that automatically takes into account the proper regularization and mutual correlations. We shall achieve it in the following sections. First the Green functions should be discussed.

2.5 Green functions

According to the basic properties of the Gaussian integrals, see Section 2.3, the correlator of the two complex bosonic fields is given by

$$\left\langle\phi_j\,\bar{\phi}_{j'}\right\rangle\equiv\int\mathbf{D}[\bar{\phi},\phi]\;\phi_j\,\bar{\phi}_{j'}\exp\left(\mathrm{i}\sum_{k,k'=1}^{2N}\bar{\phi}_k\,G^{-1}_{kk'}\,\phi_{k'}\right)=\mathrm{i}G_{jj'}. \qquad (2.31)$$

Notice the absence of the factor Z^{-1} in comparison with the analogous definition in the equilibrium theory [6]. Indeed, in the present construction $Z=1$. This seemingly minor difference turns out to be the major issue in the theory of disordered systems (see further discussion in Chapter 11, devoted to fermions with quenched disorder). Inverting the $2N\times 2N$ matrix (2.19) with $N=3$, one finds

$$\mathrm{i}G_{jj'}=\frac{1}{\det\left[-i\hat{G}^{-1}\right]}\left[\begin{array}{ccc|ccc}
1 & \rho h_+^2 h_- & \rho h_+^2 & \rho h_+^2 & \rho h_+ & \rho \\
h_- & 1 & \rho h_+^2 h_- & \rho h_+^2 h_- & \rho h_+ h_- & \rho h_- \\
h_-^2 & h_- & 1 & \rho h_+^2 h_-^2 & \rho h_+ h_-^2 & \rho h_-^2 \\
\hline
h_-^2 & h_- & 1 & 1 & \rho h_-^2 h_+ & \rho h_-^2 \\
h_-^2 h_+ & h_- h_+ & h_+ & h_+ & 1 & \rho h_-^2 h_+ \\
h_-^2 h_+^2 & h_- h_+^2 & h_+^2 & h_+^2 & h_+ & 1
\end{array}\right], \qquad (2.32)$$

where $\rho\equiv\rho(\omega_0)$. Generalization of the $N=3$ example to an arbitrary N is again straightforward. We switch now to the fields $\phi_j^{\pm}$, residing on the forward (backward) branches of the contour. Hereafter $j=1,\ldots,N$ and thus the $2N\times 2N$

matrix written above is indexed as $1, 2, \ldots, N, N, \ldots, 2, 1$. Then the following correlations may be read out of the matrix (2.32):

$$\langle \phi_j^+ \bar{\phi}_{j'}^- \rangle \equiv \mathrm{i}G^<_{jj'} = \frac{\rho\, h_+^{j'-1} h_-^{j-1}}{\det\big[-\mathrm{i}\hat{G}^{-1}\big]}, \tag{2.33a}$$

$$\langle \phi_j^- \bar{\phi}_{j'}^+ \rangle \equiv \mathrm{i}G^>_{jj'} = \frac{h_+^{N-j} h_-^{N-j'}}{\det\big[-\mathrm{i}\hat{G}^{-1}\big]} = \frac{(h_+h_-)^{N-1} h_+^{1-j} h_-^{1-j'}}{\det\big[-\mathrm{i}\hat{G}^{-1}\big]}, \tag{2.33b}$$

$$\langle \phi_j^+ \bar{\phi}_{j'}^+ \rangle \equiv \mathrm{i}G^{\mathbb{T}}_{jj'} = \frac{h_-^{j-j'}}{\det\big[-i\hat{G}^{-1}\big]} \times \begin{cases} 1, & j \geq j' \\ \rho(h_+h_-)^{N-1}, & j < j' \end{cases}, \tag{2.33c}$$

$$\langle \phi_j^- \bar{\phi}_{j'}^- \rangle \equiv \mathrm{i}G^{\widetilde{\mathbb{T}}}_{jj'} = \frac{h_+^{j'-j}}{\det\big[-i\hat{G}^{-1}\big]} \times \begin{cases} \rho(h_+h_-)^{N-1}, & j > j' \\ 1, & j \leq j' \end{cases}. \tag{2.33d}$$

Here the symbols $\mathbb{T}$ and $\widetilde{\mathbb{T}}$ stand for time ordering and anti-ordering correspondingly, while $<$ $(>)$ is a convenient notation indicating that the first time argument is taken before (after) the second one on the Keldysh contour. Since $h_+^* = h_-$, one notices that

$$\big[G^{<(>)}\big]^\dagger = -G^{<(>)}; \qquad \big[G^{\mathbb{T}}\big]^\dagger = -G^{\widetilde{\mathbb{T}}}, \tag{2.34}$$

where the Hermitian conjugation involves interchange of the two time arguments along with complex conjugation.

Recalling that $h_\mp = 1 \mp \mathrm{i}\omega_0\delta_t$, one can take the $N \to \infty$ limit, keeping $N\delta_t$ a constant. To this end notice that $(h_+h_-)^N = (1+\omega_0^2\delta_t^2)^N \overset{N\to\infty}{\longrightarrow} 1$, while $h_\mp^j \overset{N\to\infty}{\longrightarrow} \mathrm{e}^{\mp\mathrm{i}\omega_0\delta_t j} = \mathrm{e}^{\mp\mathrm{i}\omega_0 t}$, where we denoted $t = \delta_t j$ and correspondingly $t' = \delta_t j'$. Employing also the evaluation of the determinant given by Eq. (2.24), one obtains for the correlation functions in the continuum limit

$$\langle \phi^+(t)\bar{\phi}^-(t')\rangle = \mathrm{i}G^<(t,t') = n_\mathrm{B}\,\mathrm{e}^{-\mathrm{i}\omega_0(t-t')}, \tag{2.35a}$$

$$\langle \phi^-(t)\bar{\phi}^+(t')\rangle = \mathrm{i}G^>(t,t') = (n_\mathrm{B}+1)\,\mathrm{e}^{-\mathrm{i}\omega_0(t-t')}, \tag{2.35b}$$

$$\langle \phi^+(t)\bar{\phi}^+(t')\rangle = \mathrm{i}G^{\mathbb{T}}(t,t') = \theta(t-t')\mathrm{i}G^>(t,t') + \theta(t'-t)\mathrm{i}G^<(t,t'), \tag{2.35c}$$

$$\langle \phi^-(t)\bar{\phi}^-(t')\rangle = \mathrm{i}G^{\widetilde{\mathbb{T}}}(t,t') = \theta(t'-t)\mathrm{i}G^>(t,t') + \theta(t-t')\mathrm{i}G^<(t,t'), \tag{2.35d}$$

where we introduced the *bosonic occupation number* n_B as

$$n_\mathrm{B}(\omega_0) = \frac{\rho(\omega_0)}{1-\rho(\omega_0)}. \tag{2.36}$$

Indeed, to calculate the number of bosons at a certain point in time one needs to insert the operator $\hat{b}^\dagger\hat{b}$ into the corresponding point along the forward or backward branches of the contour. This leads to the correlation function $\langle \phi_{j-1}\bar{\phi}_j\rangle$, or in terms of $\phi^\pm$ fields to either $\langle \phi_{j-1}^+\bar{\phi}_j^+\rangle$ or $\langle \phi_j^-\bar{\phi}_{j-1}^-\rangle$ (notice the reversed indexing along the

backward branch). According to Eqs. (2.33c,d) in the $N \to \infty$ limit both of them equal $n_{\rm B}$.

The step-function $\theta(t)$ in Eqs. (2.35c,d) is defined as $\theta(t-t') = 1$ if $t > t'$ and $\theta(t-t') = 0$ if $t < t'$. There is an ambiguity about equal times. Consulting with the discrete version of the correlation functions, Eqs. (2.33), one notices that in both Eqs. (2.35c) and (2.35d) the first step function should be understood as having $\theta(0) = 1$, and the second as having $\theta(0) = 0$. Although slightly inconvenient, this ambiguity will disappear in the formalism that follows.

In analogy with the definition of the discrete correlation functions as a $2N$-fold integral, Eq. (2.31), it is convenient to write their continuum limit, Eq. (2.35), formally as a *functional* integral

$$\left\langle \phi^{\pm}(t)\, \bar{\phi}^{\pm}(t') \right\rangle = \int \mathbf{D}[\bar{\phi}, \phi]\, \phi^{\pm}(t) \bar{\phi}^{\pm}(t')\, \mathrm{e}^{\mathrm{i}S[\bar{\phi},\phi]}, \tag{2.37}$$

where the action $S[\bar{\phi}, \phi]$ is given by Eq. (2.30). Notice that, despite the impression that the integrals over $\phi^+(t)$ and $\phi^-(t)$ may be split from each other and performed separately, there are non-vanishing cross-correlations between these fields, Eqs. (2.35a,b). The reason, of course, is that the continuum notation (2.37) is nothing but a shorthand abbreviation for the $N \to \infty$ limit of the discrete integral (2.31). The latter contains the matrix (2.19) with non-zero off-diagonal blocks, which are the sole reason for the existence of the cross-correlations. It is highly desirable to develop a continuum formalism, which automatically accounts for the proper cross-correlations without the need to resort to the discrete notations.

This task is facilitated by the observation that not all four Green functions defined above are independent. Indeed, direct inspection shows that

$$G^{\mathbb{T}}(t,t') + G^{\widetilde{\mathbb{T}}}(t,t') - G^{>}(t,t') - G^{<}(t,t') = 0. \tag{2.38}$$

This suggests that one may benefit explicitly from this relation by performing a linear transformation. The Keldysh rotation achieves just that. Notice that, due to the regularization of $\theta(0)$ discussed above, the identity does *not* hold for $t = t'$. Indeed at $t = t'$ the left hand side of Eq. (2.38) is one rather than zero. However, since the $t = t'$ line is a manifold of measure zero, the violation of Eq. (2.38) for most purposes is inconsequential. (Notice that the right hand side of Eq. (2.38) is not a delta-function $\delta(t-t')$. It is rather a Kronecker delta $\delta_{jj'}$ in the discrete version, which disappears in the continuum limit.)

2.6 Keldysh rotation

Let us introduce a new pair of fields according to

$$\phi^{\rm cl}(t) = \frac{1}{\sqrt{2}}\big(\phi^+(t) + \phi^-(t)\big), \qquad \phi^{\rm q}(t) = \frac{1}{\sqrt{2}}\big(\phi^+(t) - \phi^-(t)\big), \tag{2.39}$$

with the analogous transformation for the conjugated fields. The superscripts "cl" and "q" stand for the *classical* and the *quantum* components of the fields, respectively. The rationale for this notation will become clear shortly. First, a simple algebraic manipulation with Eqs. (2.33a)–(2.33d) shows that

$$\left\langle \phi^{\alpha}(t)\,\bar{\phi}^{\,\beta}(t')\right\rangle \equiv \mathrm{i}G^{\alpha\beta}(t,t') = \begin{pmatrix} \mathrm{i}G^{\mathrm{K}}(t,t') & \mathrm{i}G^{\mathrm{R}}(t,t') \\ \mathrm{i}G^{\mathrm{A}}(t,t') & 0 \end{pmatrix}, \tag{2.40}$$

where hereafter $\alpha, \beta = (\mathrm{cl}, \mathrm{q})$. The fact that the (q,q) element of this matrix is zero is a manifestation of the identity (2.38). Superscripts R, A and K stand for the *retarded, advanced* and *Keldysh* components of the Green function, respectively. These three Green functions are the fundamental objects of the Keldysh technique. They are defined as

$$G^{\mathrm{R}}(t,t') = G^{\mathrm{cl,q}}(t,t') = \frac{1}{2}\left(G^{\mathbb{T}} - G^{\widetilde{\mathbb{T}}} + G^{>} - G^{<}\right) = \theta(t-t')\left(G^{>} - G^{<}\right), \tag{2.41a}$$

$$G^{\mathrm{A}}(t,t') = G^{\mathrm{q,cl}}(t,t') = \frac{1}{2}\left(G^{\mathbb{T}} - G^{\widetilde{\mathbb{T}}} - G^{>} + G^{<}\right) = \theta(t'-t)\left(G^{<} - G^{>}\right), \tag{2.41b}$$

$$G^{\mathrm{K}}(t,t') = G^{\mathrm{cl,cl}}(t,t') = \frac{1}{2}\left(G^{\mathbb{T}} + G^{\widetilde{\mathbb{T}}} + G^{>} + G^{<}\right) = G^{>} + G^{<}. \tag{2.41c}$$

As was mentioned after Eq. (2.38), the last equality in each line here holds for $t \neq t'$ only, while the diagonal $t = t'$ is discussed below. Employing Eq. (2.34), one notices that

$$G^{\mathrm{A}} = \left[G^{\mathrm{R}}\right]^{\dagger}, \qquad\qquad G^{\mathrm{K}} = -\left[G^{\mathrm{K}}\right]^{\dagger}, \tag{2.42}$$

where the Green functions are understood as matrices in the time domain. Hermitian conjugation therefore includes complex conjugation along with interchanging of the two time arguments.

The retarded (advanced) Green function is a lower (upper) triangular matrix in the time domain. Since a product of any number of triangular matrices is again a triangular matrix, one obtains the simple rule that the convolution of any number of retarded (advanced) Green functions is also a retarded (advanced) Green function

$$G_1^{\mathrm{R}} \circ G_2^{\mathrm{R}} \circ \cdots \circ G_l^{\mathrm{R}} = G^{\mathrm{R}}, \tag{2.43a}$$

$$G_1^{\mathrm{A}} \circ G_2^{\mathrm{A}} \circ \cdots \circ G_l^{\mathrm{A}} = G^{\mathrm{A}}, \tag{2.43b}$$

where the circular multiplication sign stands for the convolution operation, i.e. multiplication of matrices in the time domain, and subscripts denote all other indices apart from the time.

Both retarded and advanced matrices have non-zero main diagonals, i.e. $t = t'$. The important observation, however, is that

$$G^{\mathrm{R}}(t,t) + G^{\mathrm{A}}(t,t) = 0, \tag{2.44}$$

see Eqs. (2.35c,d) and the discussion of $\theta(0)$ regularization below them. It may be traced back to the fact that $G^{\mathrm{R}} + G^{\mathrm{A}} = G^{\mathbb{T}} - G^{\tilde{\mathbb{T}}}$, and since at the coinciding times the time ordering and anti-ordering are equivalent, the result is zero. This consideration shows that Eq. (2.44) is not restricted to our toy model, but is completely general. In the energy representation Eq. (2.44) takes the form

$$\int \frac{\mathrm{d}\epsilon}{2\pi} \left[G^{\mathrm{R}}(\epsilon) + G^{\mathrm{A}}(\epsilon)\right] = 0, \tag{2.45}$$

and it is tempting to attribute it to the fact the energy integral of a function analytic in the upper (lower) complex half-plane is zero. One should be aware, however, that according to Eqs. (2.41a,b) and (2.35a,b)

$$G^{\mathrm{R}}(t,t) - G^{\mathrm{A}}(t,t) = -\mathrm{i}. \tag{2.46}$$

Once again this expression is not restricted to the toy model, but is very general. Indeed, $G^{\mathrm{R}} - G^{\mathrm{A}} = G^{>} - G^{<} = -\mathrm{i}\langle(bb^{\dagger} - b^{\dagger}b)\rangle = -\mathrm{i}$ since the commutation relation (2.2) at the coinciding times is a generic property of any bosonic system. As a result, $\int \mathrm{d}\epsilon \left[G^{\mathrm{R}}(\epsilon) - G^{\mathrm{A}}(\epsilon)\right] = -2\pi\mathrm{i}$ and therefore $\int \mathrm{d}\epsilon\, G^{\mathrm{R(A)}}(\epsilon) = \mp\pi\mathrm{i}$, which is coming from the integration along the large semicircle closing the integration contour in the upper (lower) complex half-plane. In practical calculations the difference $G^{\mathrm{R}} - G^{\mathrm{A}}$ always comes with the distribution function (see below). The latter usually exhibits poles or branch cuts in both upper and lower energy half-planes and therefore the contour integration is not helpful anyway. Wherever G^{R} or G^{A} show up without the distribution function, they *always* appear in the combination $G^{\mathrm{R}} + G^{\mathrm{A}}$, calling for the contour integration (2.45). We shall thus frequently quote (as a rule of thumb) that $\int \mathrm{d}\epsilon\, G^{\mathrm{R(A)}}(\epsilon) = 0$, or equivalently $G^{\mathrm{R(A)}}(t,t) = 0$, understanding that it is always the sum of the two which matters. This never leads to a confusion and therefore there is no danger in extending Eqs. (2.41a,b) to the diagonal $t = t'$ (with the understanding $\theta(0) = 0$) in the continuum formalism.

It is useful to introduce graphic representations for the three Green functions. To this end, let us denote the classical component of the field by a full line and the quantum component by a dashed line. Then the retarded Green function is represented by a full arrow and dashed line, the advanced by a dashed arrow and full line and the Keldysh by a full arrow and full line, see Fig. 2.2. Notice that the dashed arrow and dashed line, that would represent the $\langle\phi^{\mathrm{q}}\bar{\phi}^{\mathrm{q}}\rangle$ Green function, is absent. The arrow shows the direction from ϕ^{α} towards $\bar{\phi}^{\beta}$.

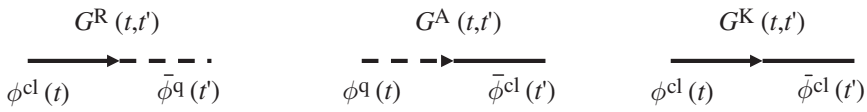

Fig. 2.2 Graphic representation of G^{R}, G^{A} and G^{K}. The full line represents the classical field component ϕ^{cl}, while the dashed line represents the quantum component ϕ^{q}. The arrows are directed from the annihilation operator towards the creation one, i.e. from ϕ^{α} to $\bar{\phi}^{\beta}$.

Employing Eqs. (2.35), one finds for our toy example of the single boson level

$$G^{\mathrm{R}} = -\mathrm{i}\theta(t-t')\,\mathrm{e}^{-\mathrm{i}\omega_0(t-t')} \overset{\mathrm{FT}}{\to} (\epsilon - \omega_0 + \mathrm{i}0)^{-1}, \tag{2.47a}$$

$$G^{\mathrm{A}} = \;\; \mathrm{i}\theta(t'-t)\,\mathrm{e}^{-\mathrm{i}\omega_0(t-t')} \overset{\mathrm{FT}}{\to} (\epsilon - \omega_0 - \mathrm{i}0)^{-1}, \tag{2.47b}$$

$$G^{\mathrm{K}} = -\mathrm{i}\,[2n_{\mathrm{B}}(\omega_0)+1]\,\mathrm{e}^{-\mathrm{i}\omega_0(t-t')} \overset{\mathrm{FT}}{\to} -2\pi\mathrm{i}[2n_{\mathrm{B}}(\epsilon)+1]\delta(\epsilon-\omega_0). \tag{2.47c}$$

The Fourier transforms (FT) with respect to $t - t'$ are given for each of the three Green functions. Notice that the retarded and advanced components contain information only about the spectrum and are independent of the occupation number, whereas the Keldysh component depends on it. In thermal equilibrium $\rho = \mathrm{e}^{-(\omega_0-\mu)/T}$, while $n_{\mathrm{B}} = (\mathrm{e}^{(\omega_0-\mu)/T}-1)^{-1}$ and therefore

$$G^{\mathrm{K}}(\epsilon) = \coth\frac{\epsilon-\mu}{2T}\left[G^{\mathrm{R}}(\epsilon) - G^{\mathrm{A}}(\epsilon)\right], \tag{2.48}$$

where $T = \beta^{-1}$ is the system's temperature, expressed in units of energy.

The last equation constitutes the statement of the *fluctuation–dissipation theorem* (FDT). As we shall see, the FDT is a general property of thermal equilibrium that is not restricted to the toy example considered here. It implies a rigid relation between the response functions and the correlation functions in equilibrium.

In general, it is convenient to parametrize the anti-Hermitian Keldysh Green function, Eq. (2.42), with the help of a Hermitian matrix $F = F^{\dagger}$, as follows:

$$G^{\mathrm{K}} = G^{\mathrm{R}} \circ F - F \circ G^{\mathrm{A}}, \tag{2.49}$$

where $F = F(t,t')$. The Wigner transform (see Section 5.6), $F(t,\epsilon)$, of the matrix F is referred to as the *distribution function*. In thermal equilibrium $F(\epsilon) = \coth((\epsilon-\mu)/2T)$, Eq. (2.48).

2.7 Keldysh action and its structure

One would like to have a continuum action, written in terms of ϕ^{cl}, ϕ^{q}, that properly reproduces the correlators Eqs. (2.40) and (2.47), i.e.

$$\left\langle \phi^{\alpha}(t)\,\bar{\phi}^{\beta}(t')\right\rangle = \mathrm{i}G^{\alpha\beta}(t,t') = \int \mathbf{D}[\phi^{\mathrm{cl}},\phi^{\mathrm{q}}]\;\phi^{\alpha}(t)\,\bar{\phi}^{\beta}(t')\;\mathrm{e}^{\mathrm{i}S[\phi^{\mathrm{cl}},\phi^{\mathrm{q}}]}, \tag{2.50}$$

where the conjugated fields are not listed in the action arguments or the integration measure for brevity. According to the basic properties of Gaussian integrals, Section 2.3, the action should be taken as a quadratic form of the fields with the matrix which is an inverse of the correlator $G^{\alpha\beta}(t,t')$. Inverting the matrix (2.40), one thus finds the proper action

$$S[\phi^{\rm cl},\phi^{\rm q}]=\iint_{-\infty}^{+\infty}{\rm d}t\,{\rm d}t'\,\left(\bar\phi^{\rm cl},\bar\phi^{\rm q}\right)_t\begin{pmatrix}0 & \left[G^{-1}\right]^{\rm A}\\ \left[G^{-1}\right]^{\rm R} & \left[G^{-1}\right]^{\rm K}\end{pmatrix}_{t,t'}\begin{pmatrix}\phi^{\rm cl}\\ \phi^{\rm q}\end{pmatrix}_{t'}. \tag{2.51}$$

The off-diagonal elements are found from the condition $\left[G^{-1}\right]^{\rm R}\circ G^{\rm R}=1$ and the similar one for the advanced component. The right hand side here is the unit matrix, which in the continuum time representation is $\delta(t-t')$. As a result, the off-diagonal components are obtained by the matrix inversion of the corresponding components of the Green functions $\left[G^{-1}\right]^{\rm R(A)}=\left[G^{\rm R(A)}\right]^{-1}$. Such an inversion is most convenient in the energy representation

$$\left[G^{-1}\right]^{\rm R(A)}=\epsilon-\omega_0\pm{\rm i}0\to\delta(t-t')\,({\rm i}\partial_{t'}-\omega_0\pm{\rm i}0)\,, \tag{2.52a}$$

where in the last step we performed the inverse Fourier transform back to the time representation, employing that the Fourier transform of ϵ is $\delta(t-t'){\rm i}\partial_{t'}$.

Although in the continuum limit these matrices look diagonal, it is important to remember that in the discrete regularization $\left[G^{\rm R(A)}\right]^{-1}$ contains $\mp{\rm i}$ along the main diagonal and $\pm{\rm i}-\omega_0\delta_t$ along the lower(upper) sub-diagonal. The determinants of the corresponding matrices are given by the product of all diagonal elements, $\det\left[G^{-1}\right]^{\rm R}\det\left[G^{-1}\right]^{\rm A}=\prod_{j=1}^{N}{\rm i}(-{\rm i})=1$. To obtain this statement without resorting to discretization, one notices that in the energy representation the Green functions are diagonal and therefore $\det\left[G^{-1}\right]^{\rm R}\left[G^{-1}\right]^{\rm A}=\prod_\epsilon\left[G^{\rm R}(\epsilon)G^{\rm A}(\epsilon)\right]^{-1}=\exp\left\{-\int\frac{{\rm d}\epsilon}{2\pi}[\ln G^{\rm R}+\ln G^{\rm A}]\right\}=1$. Here we used the fact that Eq. (2.45) holds not only for the Green functions themselves but, thanks to Eqs. (2.43), also for any function of them. This property is important for maintaining the normalization identity $Z=\int\mathbf{D}[\phi^{\rm cl},\phi^{\rm q}]\,{\rm e}^{{\rm i}S}=1$. Indeed, the integral is equal to minus (due to the factor of i in the exponent) the determinant of the quadratic form, while the latter is (-1) times the product of the determinants of the off-diagonal elements in the quadratic form (2.51).

The diagonal Keldysh component, $[G^{-1}]^{\rm K}$, of the quadratic form (2.51) is found from the condition $G^{\rm K}\circ[G^{\rm A}]^{-1}+G^{\rm R}\circ[G^{-1}]^{\rm K}=0$. Employing the parametrization (2.49), one finds

$$\left[G^{-1}\right]^{\rm K}=-\left[G^{\rm R}\right]^{-1}\circ G^{\rm K}\circ[G^{\rm A}]^{-1}=\left[G^{\rm R}\right]^{-1}\circ F-F\circ\left[G^{\rm A}\right]^{-1}. \tag{2.52b}$$

The action (2.51) should be viewed as a construction devised to reproduce the proper continuum limit of the correlation functions according to the rules of Gaussian integration. It is fully self-consistent in the following senses: (i) it does

not need to appeal to the discrete representation for regularization and (ii) its general structure is intact upon renormalization or "dressing" of its components by the interaction corrections (see Chapter 5).

Here we summarize the main features of the action (2.51), which, for lack of better terminology, we call the *causality structure*.

- The cl $-$ cl component of the quadratic form is zero. It reflects the fact that for a pure classical field configuration ($\phi^{\mathrm{q}} = 0$) the action is zero. Indeed, in this case $\phi^{+} = \phi^{-}$ and the action on the forward part of the contour is canceled by that on the backward part (except for the boundary terms, which are implicit in the continuum limit). The very general statement is, therefore, that

$$S\left[\phi^{\mathrm{cl}}, 0\right] = 0. \tag{2.53}$$

  Obviously this statement is not restricted to the Gaussian action of the form given by Eq. (2.51), but holds for any generic action (see Chapter 5).
- The cl $-$ q and q $-$ cl components are mutually Hermitian conjugated upper and lower (advanced and retarded) triangular matrices in the time domain. This property is responsible for the causality of the response functions as well as for protecting the cl$-$cl component from a perturbative renormalization (see below). Relations (2.44) and (2.45) are crucial for this last purpose and necessary for the consistency of the theory.
- The q $-$ q component is an anti-Hermitian matrix [see Eq. (2.42)]. It is responsible for the convergence of the functional integral and keeps information about the distribution function. In our simple example $\left[G^{\mathrm{K}}\right]^{-1} = 2\mathrm{i}0F$, where F is a Hermitian matrix. The fact that it is infinitesimally small is a peculiarity of the non-interacting model. We shall see in the following chapters that it acquires a finite value, once interactions with other degrees of freedom are included.

2.8 External sources

So far we have been content with the representation of the partition function. The latter does not carry any information in the Keldysh technique, since $Z = 1$. To make the entire construction meaningful one should introduce source fields, which enable one to compute various observables. As an example, let us introduce an external time-dependent potential $V(t)$. It interacts with the bosons through the Hamiltonian $\hat{H}_V = V(t)\hat{b}^{\dagger}\hat{b}$. One can now introduce the generating function $Z[V]$ defined similarly to the partition function (2.13), $Z[V] = \mathrm{Tr}\{\hat{\mathcal{U}}_{\mathcal{C}}[V]\hat{\rho}\}/\mathrm{Tr}\{\hat{\rho}\}$, where the evolution operator $\hat{\mathcal{U}}_{\mathcal{C}}[V]$ includes the source Hamiltonian $\hat{H}_V$ along with the bare one, Eq. (2.12). While any classical external field is the same on both branches of the contour, it is convenient to allow $V^{+}(t)$ and $V^{-}(t)$ to be

distinct and put them equal only at the very end. Repeating the construction of the coherent state functional integral of Section 2.2, one obtains for the generating function

$$Z_{\rm d}[V] = \frac{1}{{\rm Tr}\{\hat\rho_0\}} \int \prod_{j=1}^{2N} {\rm d}[\bar\phi_j, \phi_j] \, \exp\left({\rm i} \sum_{j,j'=1}^{2N} \bar\phi_j \, G^{-1}_{jj'}[V] \, \phi_{j'} \right), \tag{2.54}$$

where the subscript d stands for the discrete representation. The $2N \times 2N$ matrix ${\rm i}G^{-1}_{jj'}[V]$ is similar to the one given by Eq. (2.19) with $h_\mp \to h_\mp[V] = 1 \mp {\rm i}(\omega_0 + V_j)\delta_t$, where $V_j = V(t_j)$. According to Eq. (2.20) the generating function is proportional to the inverse determinant of the $-{\rm i}G^{-1}_{jj'}[V]$ matrix. The latter is calculated in a way very similar to Eq. (2.24), leading to

$$Z_{\rm d}[V] = \frac{1}{{\rm Tr}\{\hat\rho_0\}} \frac{1}{\det\big[-{\rm i}\hat G^{-1}[V]\big]} = \frac{1-\rho(\omega_0)}{1-\rho(\omega_0){\rm e}^{-{\rm i}\int_C {\rm d}t\, V(t)}}. \tag{2.55}$$

It is convenient to introduce classical and quantum components of the source potential $V(t)$ as

$$V^{\rm cl}(t) = \frac{1}{2}\big[V^+(t) + V^-(t)\big]\,; \qquad V^{\rm q}(t) = \frac{1}{2}\big[V^+(t) - V^-(t)\big], \tag{2.56}$$

where $V^\pm(t)$ is the source potential on the forward (backward) branch of the contour. With this notation along with Eq. (2.36) the generating function takes the form

$$Z_{\rm d}[V^{\rm cl}, V^{\rm q}] = \Big[1 - n_{\rm B}(\omega_0)\left({\rm e}^{-2{\rm i}\int {\rm d}t\, V^{\rm q}(t)} - 1\right)\Big]^{-1}. \tag{2.57}$$

The fact that the generating function depends only on the integral of the quantum component of the source and does not depend on its classical component is a peculiarity of our toy model. (Indeed, since $[\hat H, b^\dagger b] = 0$, the number of particles is conserved, making the generating function independent of the classical external potential $V^{\rm cl}$). The very general statement, though, is

$$Z[V^{\rm cl}, 0] = 1. \tag{2.58}$$

Indeed, if $V^{\rm q} = 0$ the source potential is the same on the two branches, $V^+(t) = V^-(t)$, and thus the evolution operator brings the system exactly to its initial state, i.e. $\hat{\mathcal{U}}_C[V^{\rm cl}] = \hat 1$. One crucially needs therefore a fictitious potential $V^{\rm q}(t)$ to generate observables.

Since the source potential is coupled to the number of particles operator $\hat n = \hat b^\dagger \hat b$, differentiation over $V^{\rm q}(t)$ generates an expectation value of $-2{\rm i}\langle \hat n(t)\rangle$ (the factor of two here is due to the fact that we insert $\hat b^\dagger(t)\hat b(t)$ on both branches): $\langle \hat n(t)\rangle = ({\rm i}/2)\delta Z_{\rm d}[V^{\rm q}]/\delta V^{\rm q}(t)|_{V^{\rm q}=0} = n_{\rm B}(\omega_0)$, as was established in Section 2.5. The higher order correlation functions may be obtained by repetitive differentiation

of the generating function. To generate *irreducible* correlators (i.e. cumulants) $\langle\langle \hat{n}^k(t)\rangle\rangle \equiv \langle(\hat{n}(t)-n_{\rm B})^k\rangle$ one needs to differentiate the *logarithm* of the generating function, Eq. (2.57), e.g.

$$\begin{aligned}
\langle\langle \hat{n}^2(t)\rangle\rangle &= \left(\frac{\mathrm{i}}{2}\right)^2 \frac{\delta^2 \ln Z_{\rm d}}{\delta[V^{\rm q}(t)]^2}\bigg|_{V=0} = n_{\rm B}^2 + n_{\rm B};\\
\langle\langle \hat{n}^3(t)\rangle\rangle &= \left(\frac{\mathrm{i}}{2}\right)^3 \frac{\delta^3 \ln Z_{\rm d}}{\delta[V^{\rm q}(t)]^3}\bigg|_{V=0} = 2n_{\rm B}^3 + 3n_{\rm B}^2 + n_{\rm B};\\
\langle\langle \hat{n}^4(t)\rangle\rangle &= \left(\frac{\mathrm{i}}{2}\right)^4 \frac{\delta^4 \ln Z_{\rm d}}{\delta[V^{\rm q}(t)]^4}\bigg|_{V=0} = 6n_{\rm B}^4 + 12n_{\rm B}^3 + 7n_{\rm B}^2 + n_{\rm B};
\end{aligned} \tag{2.59}$$

etc.

Let us see now how these results can be reproduced in the continuum technique, without resorting to discretization. The continuum generating function is defined as

$$Z_{\rm c}[V] = \int \mathbf{D}[\bar{\phi}, \phi]\, \mathrm{e}^{\mathrm{i}S[\bar{\phi},\phi]+iS_V[\bar{\phi},\phi]}, \tag{2.60}$$

where the bare action $S[\bar{\phi}, \phi]$ is given by Eq. (2.30) and

$$S_V[\bar{\phi}, \phi] = -\int_{\mathcal{C}} \mathrm{d}t\; V(t)\bar{\phi}(t)\phi(t) = -\int_{-\infty}^{+\infty} \mathrm{d}t\left[V^+\bar{\phi}^+\phi^+ - V^-\bar{\phi}^-\phi^-\right] \tag{2.61}$$

$$= -\int_{-\infty}^{+\infty} \mathrm{d}t\left[V^{\rm cl}(\bar{\phi}^+\phi^+ - \bar{\phi}^-\phi^-) + V^{\rm q}\,(\bar{\phi}^+\phi^+ + \bar{\phi}^-\phi^-)\right] = -\int_{-\infty}^{+\infty} \mathrm{d}t\, \vec{\bar{\phi}}^{\,\mathrm{T}}\hat{V}\vec{\phi},$$

where $\vec{\phi} = (\phi^{\rm cl}, \phi^{\rm q})^{\rm T}$ and

$$\hat{V}(t) = \begin{pmatrix} V^{\rm q}(t) & V^{\rm cl}(t) \\ V^{\rm cl}(t) & V^{\rm q}(t) \end{pmatrix}. \tag{2.62}$$

As a result, for our example of the single bosonic level the continuum generating function is given by

$$\begin{aligned}
Z_{\rm c}[V^{\rm cl}, V^{\rm q}] &= \int \mathbf{D}[\bar{\phi}, \phi]\; \mathrm{e}^{\mathrm{i}\int \mathrm{d}t\, \vec{\bar{\phi}}^{\,\mathrm{T}}\left(\hat{G}^{-1}-\hat{V}(t)\right)\vec{\phi}} = \frac{1}{\mathrm{Tr}\{\hat{\rho}_0\}}\,\frac{1}{\det\left[-\mathrm{i}\hat{G}^{-1}+\mathrm{i}\hat{V}\right]}\\
&= \frac{1}{\det\left[1-\hat{G}\hat{V}\right]} = \mathrm{e}^{-\mathrm{Tr}\ln\left[1-\hat{G}\hat{V}\right]},
\end{aligned} \tag{2.63}$$

where we have used Eq. (2.25) along with the identity $\ln\det\hat{A} = \mathrm{Tr}\ln\hat{A}$. According to Eqs. (2.40) and (2.47) the matrix Green function is

$$\hat{G}(t,t') = -\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\omega_0(t-t')}\begin{pmatrix} F(\omega_0) & \theta(t-t') \\ -\theta(t'-t) & 0 \end{pmatrix} \tag{2.64}$$

and $F(\omega_0) = 2n_{\mathrm{B}}(\omega_0) + 1$.

The continuum generating function Z_{c} is *not* identical to the discrete one Z_{d}. However, as we shall show, it possesses the same general properties and generates exactly the same statistics of the number operator. First, let us verify Eq. (2.58) by expanding the logarithm in Eq. (2.63). To first order in $\hat{V}$ one finds $-\mathrm{Tr}\ln\left[1-\hat{G}\hat{V}\right] \approx \mathrm{Tr}\hat{G}\hat{V} = \int \mathrm{d}t\,[G^{\mathrm{R}}(t,t) + G^{\mathrm{A}}(t,t)]V^{\mathrm{cl}}(t) = 0$, where we put $V^{\mathrm{q}} = 0$ and employed Eq. (2.44). To second order one encounters $\int \mathrm{d}t\mathrm{d}t' G^{\mathrm{R}}(t,t')V^{\mathrm{cl}}(t')G^{\mathrm{R}}(t',t)V^{\mathrm{cl}}(t)$ and similarly for G^{A}. Since $G^{\mathrm{R}}(t,t') = 0$ if $t < t'$, while $G^{\mathrm{R}}(t',t) = 0$ if $t > t'$, the expression under the integral is non-zero only if $t = t'$. In the continuum limit ($N \to \infty$) this is the manifold of zero measure, making the integral zero. Clearly the same holds in all orders in V^{cl}. This illustrates how the generic feature of the Keldysh technique, Eq. (2.58), works in our simple example.

Consider now $\mathrm{i}\delta Z_{\mathrm{c}}[V]/\delta V^{\mathrm{q}}(t)|_{V=0} = \langle\bar{\phi}^{+}(t)\phi^{+}(t) + \bar{\phi}^{-}(t)\phi^{-}(t)\rangle$; we refer to Eqs. (2.60) and (2.61) to see this relation. The expectation value of which operator is calculated this way? The naive answer is that $\bar{\phi}(t)\phi(t)$ is generated by $\langle\hat{b}^{\dagger}(t)\hat{b}(t)\rangle$ and we deal with the sum of this operator inserted on the forward and backward branches. If this were the case, $\bar{\phi}$ would be taken one time step ahead of the ϕ field, as is indeed the case in the discrete representation. However, our continuum expression indiscriminately places both $\bar{\phi}^{\pm}$ and $\phi^{\pm}$ at the same time t. One can check that such a "democratic" choice of the time arguments corresponds to the expectation value of the symmetric combination $\hat{F}(t) \equiv \hat{b}^{\dagger}(t)\hat{b}(t) + \hat{b}(t)\hat{b}^{\dagger}(t)$. Employing the equal time commutation relation $[\hat{b}(t), \hat{b}^{\dagger}(t)] = \hat{1}$, one finds $\hat{F}(t) = 2\hat{n}(t) + 1$ and $\langle\hat{F}(t)\rangle = \mathrm{i}\,\delta Z_{\mathrm{c}}[V^{\mathrm{cl}}, V^{\mathrm{q}}]/\delta V^{\mathrm{q}}(t)\big|_{V=0} = \mathrm{i}G^{\mathrm{K}}(t,t) = F(\omega_0)$, as it should be, of course. For higher order irreducible correlators one obtains

$$\begin{aligned}
\langle\langle\hat{F}^2(t)\rangle\rangle &= \mathrm{i}^2\,\frac{\delta^2 \ln Z_{\mathrm{c}}}{\delta[V^{\mathrm{q}}(t)]^2}\bigg|_{V=0} = F^2 - 1; \\
\langle\langle\hat{F}^3(t)\rangle\rangle &= \mathrm{i}^3\,\frac{\delta^3 \ln Z_{\mathrm{c}}}{\delta[V^{\mathrm{q}}(t)]^3}\bigg|_{V=0} = 2F^3 - 2F; \\
\langle\langle\hat{F}^4(t)\rangle\rangle &= \mathrm{i}^4\,\frac{\delta^4 \ln Z_{\mathrm{c}}}{\delta[V^{\mathrm{q}}(t)]^4}\bigg|_{V=0} = 6F^4 - 8F^2 + 2;
\end{aligned} \tag{2.65}$$

etc. To see how it works, consider for example the third order term in the expansion of $\ln Z_{\mathrm{c}} = -\mathrm{Tr}\ln[1-\hat{G}\hat{V}]$ in Eq. (2.63) in powers of $V^{\mathrm{q}}(t)$ at $V^{\mathrm{cl}} = 0$:

$$\frac{1}{3}\mathrm{Tr}\{(\hat{G}\hat{V})^3\} = \frac{1}{3}\int \mathrm{d}t\mathrm{d}t'\mathrm{d}t''\mathrm{Tr}\left\{\hat{G}(t,t')V^{\mathrm{q}}(t')\hat{G}(t',t'')V^{\mathrm{q}}(t'')\hat{G}(t'',t)V^{\mathrm{q}}(t)\right\}$$
$$= \mathrm{i}\frac{F^3}{3}\left(\int \mathrm{d}t\, V^{\mathrm{q}}(t)\right)^3 - \mathrm{i}F\int \mathrm{d}t\, V^{\mathrm{q}}(t)\left(\int_t \mathrm{d}t'\, V^{\mathrm{q}}(t')\right)^2 = \mathrm{i}\frac{F^3-F}{3}\left(\int \mathrm{d}t\, V^{\mathrm{q}}(t)\right)^3.$$

To calculate the last integral in the intermediate expression here one introduces $W(t) = \int_t V^{\mathrm{q}}(t)$ and therefore $V^{\mathrm{q}} = -\dot{W}$, and the integral in question is thus $-\int \mathrm{d}t\dot{W}W^2 = -\int \mathrm{d}W W^2 = -(1/3)W^3(t)|_{-\infty}^{\infty} = (1/3)(\int \mathrm{d}t\, V^{\mathrm{q}})^3$. Differentiating over V^{q} three times, one arrives at Eq. (2.65).

Substituting $\hat{F} = 2\hat{n} + 1$ and $F = 2n_{\mathrm{B}} + 1$, it is easy to check that the respective moments (2.59) and (2.65) are exactly equivalent! Therefore, although the generating functions Z_{d} and Z_{c} generate slightly different sets of cumulants, their statistical content is equivalent. From now on we shall always deal with the continuum version, circumventing the tedious discretization procedure.

The generating function $Z[V^{\mathrm{q}}]$ gives access not only to the moments, but to a *full counting statistics* of the operator $\hat{n}(t_0)$, or $\hat{F}(t_0)$. Let us define the probability of measuring n bosons at a time t_0 as $\mathcal{P}(n)$. Then $\langle \hat{n}^k(t_0)\rangle = \int \mathrm{d}n\, n^k \mathcal{P}(n)$. The generating function $Z[\eta] \equiv \int \mathrm{d}n\, \mathrm{e}^{\mathrm{i}\eta n}\mathcal{P}(n) = \sum_k (\mathrm{i}\eta)^k \langle \hat{n}^k(t_0)\rangle/k!$, where η is called the counting "field." Comparing this with $Z_{\mathrm{d}}[V^{\mathrm{q}}]$, one notices that $Z[\eta]$ may be obtained from it by the substitution $V^{\mathrm{q}}(t) = -(\eta/2)\delta(t-t_0)$. Employing Eq. (2.55), one finds

$$Z[\eta] = \frac{1-\rho(\omega_0)}{1-\rho(\omega_0)\,e^{i\eta}} = \big(1-\rho(\omega_0)\big)\sum_{k=0}^{\infty}[\rho(\omega_0)]^k\,\mathrm{e}^{\mathrm{i}k\eta}. \tag{2.66}$$

Performing the inverse Fourier transform and recalling that $\rho(\omega_0) = \mathrm{e}^{-\beta(\omega_0-\mu)}$, one finds

$$\mathcal{P}(n) = \sum_{k=0}^{\infty}\delta(n-k)\left(1-\mathrm{e}^{-\beta(\omega_0-\mu)}\right)\mathrm{e}^{-\beta(\omega_0-\mu)k}. \tag{2.67}$$

That is, one can measure only an integer number of bosons and the corresponding probability is proportional to $\mathrm{e}^{-\beta(E_n-\mu n)}$, where the energy $E_n = n\omega_0$. This is of course a trivial result, which we have already de-facto employed in Eq. (2.14). The important message, however, is that the counting field η is nothing but a particular realization of the quantum source field $V^{\mathrm{q}}(t)$, tailored to generate an appropriate statistics. As opposed to the calculation of the moments (2.59) and (2.65), one should *not* put the quantum source to zero when the *full statistics* is evaluated. We shall employ this lesson in Sections 4.9, 10.3, and 12.4 to discuss less obvious examples of the full counting statistics.

3

Single-particle quantum mechanics

In this chapter we discuss quantum mechanics formulated on the closed time contour. We also derive a real time version of the Caldeira–Leggett model for a quantum particle interacting with a bath of harmonic oscillators. A semiclassical treatment of quantum tunneling on the closed time contour is developed and used to evaluate the tunneling rate through a time-dependent potential barrier with and without coupling to the bath.

3.1 Harmonic oscillator

The simplest many-body system of a single bosonic state, considered above, is equivalent to a quantum harmonic oscillator. To make this connection explicit, consider the Keldysh contour action Eq. (2.28) with the correlator Eq. (2.29) written in terms of the complex field $\phi(t)$. The latter may be parametrized by its real and imaginary parts as

$$\phi(t) = \frac{1}{\sqrt{2\omega_0}} \left(P(t) - \mathrm{i}\,\omega_0\, X(t) \right), \qquad \bar{\phi}(t) = \frac{1}{\sqrt{2\omega_0}} \left(P(t) + \mathrm{i}\,\omega_0\, X(t) \right). \tag{3.1}$$

In terms of the real fields $P(t)$ and $X(t)$ the action, Eq. (2.28), takes the form

$$S[X, P] = \int_{\mathcal{C}} \mathrm{d}t \left[P\,\dot{X} - \frac{1}{2}\,P^2 - \frac{\omega_0^2}{2}\,X^2 \right], \tag{3.2}$$

where the full time derivatives of P^2, X^2 and $P\,X$ were omitted, since they contribute only to the boundary terms, implicit in the continuum notations (they have to be kept for the proper regularization, though). Equation (3.2) is nothing but the action of the quantum harmonic oscillator in the Hamiltonian form. One may perform the Gaussian integration over the real field $P(t)$, with the help of Eq. (2.22), to obtain

$$S[X] = \int_{\mathcal{C}} \mathrm{d}t \left[\frac{1}{2}\,\dot{X}^2 - \frac{\omega_0^2}{2}\,X^2 \right]. \tag{3.3}$$

This is the Feynman Lagrangian action of the harmonic oscillator [32], written on the closed time contour. It may be generalized for an arbitrary single-particle potential $V(X)$:

$$S[X] = \int_{\mathcal{C}} \mathrm{d}t \left[\frac{1}{2}\,\dot{X}^2 - V(X) \right]. \tag{3.4}$$

One may split the $X(t)$ field into two components, $X^+(t)$ and $X^-(t)$, residing on the forward and backward branches of the contour. The Keldysh rotation for real fields is conveniently defined as

$$X^{\mathrm{cl}}(t) = \frac{1}{2}\left[X^+(t) + X^-(t)\right]; \qquad X^{\mathrm{q}}(t) = \frac{1}{2}\left[X^+(t) - X^-(t)\right]. \tag{3.5}$$

In terms of these fields the action takes the form

$$S[X^{\mathrm{cl}}, X^{\mathrm{q}}] = \int_{-\infty}^{+\infty} \mathrm{d}t \left[-2X^{\mathrm{q}}\ddot{X}^{\mathrm{cl}} - V\left(X^{\mathrm{cl}} + X^{\mathrm{q}}\right) + V\left(X^{\mathrm{cl}} - X^{\mathrm{q}}\right) \right], \tag{3.6}$$

where the integration by parts was performed on the term $\dot{X}^{\mathrm{q}}\dot{X}^{\mathrm{cl}}$. This is the Keldysh form of the Feynman path integral. The omitted boundary terms provide a convergence factor of the form $\sim \mathrm{i}0(X^q)^2$.

If the fluctuations of the quantum component $X^{\mathrm{q}}(t)$ are regarded as small, one may expand the potential to first order and find for the action

$$S[X^{\mathrm{cl}}, X^{\mathrm{q}}] = -\int_{-\infty}^{+\infty} \mathrm{d}t \left[2X^{\mathrm{q}} \left(\ddot{X}^{\mathrm{cl}} + V'(X^{\mathrm{cl}}) \right) + O\left[(X^{\mathrm{q}})^3\right] \right], \tag{3.7}$$

where $V'(X) = \partial V(X)/\partial X$. In this approximation the integration over the quantum component, X^{q}, may be explicitly performed, leading to the functional delta-function of the expression in the round brackets. This delta-function enforces the classical Newtonian dynamics of X^{cl}:

$$\ddot{X}^{\mathrm{cl}} = -V'\left(X^{\mathrm{cl}}\right). \tag{3.8}$$

This is the reason the symmetric (over the forward and backward branches) part of the field is called the classical component. One should be careful with this name, though. If the higher order terms in X^{q} are kept in the action, *both* X^{q} and X^{cl} are subject to quantum fluctuations.

Returning to the harmonic oscillator, $V(X) = \omega_0^2 X^2/2$, one may rewrite its Feynman–Keldysh action (3.3) in the matrix form

$$S[\vec{X}] = \frac{1}{2}\int_{-\infty}^{+\infty} \mathrm{d}t\; \vec{X}^{\mathrm{T}}\hat{D}^{-1}\vec{X}, \tag{3.9}$$

where in analogy with the complex field, Eq. (2.51), we introduced

$$\vec{X}(t) = \begin{pmatrix} X^{\mathrm{cl}}(t) \\ X^{\mathrm{q}}(t) \end{pmatrix}; \qquad \hat{D}^{-1} = \begin{pmatrix} 0 & [D^{-1}]^{\mathrm{A}} \\ [D^{-1}]^{\mathrm{R}} & [D^{-1}]^{\mathrm{K}} \end{pmatrix} \tag{3.10}$$

and the superscript T stands for matrix transposition. Here the retarded and advanced components of the quadratic form in the action are given by $\frac{1}{2}[D^{-1}]^{\mathrm{R(A)}} = (\mathrm{i}\partial_t \pm \mathrm{i}0)^2 - \omega_0^2$. As before, one should understand that this expression is simply a continuous abbreviation for the large lower (upper) triangular matrices with $-\delta_t^{-1}$ along the main diagonal, $2\delta_t^{-1} - \omega_0^2\delta_t$ along the lower (upper) sub-diagonal and $-\delta_t^{-1}$ along the second lower (upper) sub-diagonal. This makes the $\hat{D}^{-1}$ matrix symmetric, since its $[D^{-1}]^{\mathrm{K}}$ component must be symmetric by construction (its anti-symmetric part does not enter the action). In continuous notation the Keldysh component $[D^{-1}]^{\mathrm{K}}$ is only a regularization. It is convenient to keep it explicitly, since it suggests the way the matrix $\hat{D}^{-1}$ should be inverted to find the Green function:

$$\left\langle X^{\alpha}(t) X^{\beta}(t') \right\rangle = \int \mathbf{D}[\vec{X}]\, X^{\alpha}(t) X^{\beta}(t')\, \mathrm{e}^{\mathrm{i}S[\vec{X}]} = \mathrm{i}\hat{D}^{\alpha\beta}(t,t'), \tag{3.11}$$

where $\alpha, \beta = (\mathrm{cl}, \mathrm{q})$ and the matrix inverse of Eq. (3.10) is given by

$$\hat{D}^{\alpha\beta}(t,t') = \begin{pmatrix} D^{\mathrm{K}}(t,t') & D^{\mathrm{R}}(t,t') \\ D^{\mathrm{A}}(t,t') & 0 \end{pmatrix}. \tag{3.12}$$

To apply the rules of Gaussian integration for real variables (see Section 2.3), it is crucial that the matrix $\hat{D}^{-1}$ is symmetric. In the Fourier representation components of the equilibrium correlation matrix are given by

$$D^{\mathrm{R(A)}}(\epsilon) = \frac{1}{2}\,\frac{1}{(\epsilon \pm \mathrm{i}0)^2 - \omega_0^2}, \tag{3.13a}$$

$$D^{\mathrm{K}}(\epsilon) = \coth\frac{\epsilon}{2T}\left[D^{\mathrm{R}}(\epsilon) - D^{\mathrm{A}}(\epsilon)\right], \tag{3.13b}$$

where we have assumed an equilibrium thermal distribution with zero chemical potential. One way to check the consistency of the expression for the Keldysh component is to express X^{α} through $\bar{\phi}^{\alpha}$ and ϕ^{α} and employ the correlation functions for the complex fields, derived in Chapter 2. The fact that the chemical potential of a real field *must be zero* follows directly from the symmetry of $D^{\mathrm{K}}(t,t')$ (making $D^{\mathrm{K}}(\epsilon)$ an even function) and the identity $D^{\mathrm{R}}(-\epsilon) = D^{\mathrm{A}}(\epsilon)$.

The normalization identity, $\int \mathbf{D}[\vec{X}]\, \mathrm{e}^{\mathrm{i}S[\vec{X}]} = 1$, is maintained in the following way: (i) first, due to the structure of $\hat{D}^{-1}$ matrix, explained above, $\det[\frac{1}{\mathrm{i}}\hat{D}^{-1}] = -\det[\frac{1}{\mathrm{i}}D^{-1}]^{\mathrm{R}} \det[\frac{1}{\mathrm{i}}D^{-1}]^{\mathrm{A}} = (2/\delta_t)^{2N}$; (ii) the integration measure is understood as $\mathbf{D}[\vec{X}] = \prod_{j=1}^{N} 2\left(\mathrm{d}X_j^{\mathrm{cl}}/\sqrt{2\pi\delta_t}\right)\left(\mathrm{d}X_j^{\mathrm{q}}/\sqrt{2\pi\delta_t}\right)$ (in comparison with Eq. (2.22) there is an additional factor of 2, which originates from the Jacobian of the

transformation (3.5), and factor δ_t^{-1} at each time slice, coming from the integrations over $P_j = P(t_j)$). According to the real Gaussian identity (2.22) this leads exactly to the proper normalization. One can also understand the normalization in the way discussed after Eq. (2.52a), without resorting to the discrete representation.

3.2 Quantum particle in contact with an environment

Consider a quantum particle with coordinate $X(t)$, placed in a potential $V(X)$ and brought into contact with a bath of harmonic oscillators. The bath oscillators are labeled by an index s and their coordinates are denoted by φ_s. They possess a set of frequencies ω_s. The Keldysh action of such a system is given by the three terms $S = S_{\rm p} + S_{\rm bath} + S_{\rm int}$, where

$$S_{\rm p}[X] = \int_{-\infty}^{+\infty} {\rm d}t \left[-2X^{\rm q}\ddot{X}^{\rm cl} - V\left(X^{\rm cl} + X^{\rm q}\right) + V\left(X^{\rm cl} - X^{\rm q}\right)\right], \tag{3.14a}$$

$$S_{\rm bath}[\varphi_s] = \frac{1}{2}\sum_s \int_{-\infty}^{+\infty} {\rm d}t\, \vec{\varphi}_s^{\,\rm T} \hat{D}_s^{-1} \vec{\varphi}_s, \tag{3.14b}$$

$$S_{\rm int}[X, \varphi_s] = \sum_s g_s \int_{-\infty}^{+\infty} {\rm d}t\, \vec{X}^{\rm T}\, \hat{\sigma}_1\, \vec{\varphi}_s, \tag{3.14c}$$

where the symmetric quadratic form $\hat{D}_s^{-1}$ is given by Eq. (3.10) with the frequency ω_s. The interaction term between the particle and the bath oscillators is taken as a product of their coordinates, $\sum_s g_s \int_{\mathcal{C}} {\rm d}t\, X(t)\varphi_s(t) = \sum_s g_s \int {\rm d}t\, (X^+\varphi_s^+ - X^-\varphi_s^-)$. Performing the Keldysh rotation according to Eq. (3.5), one arrives at Eq. (3.14c), where $\hat{\sigma}_1$ is the first Pauli matrix in the Keldysh (cl, q) space. The corresponding coupling constants are denoted by g_s.

One may now integrate out the degrees of freedom of the bath to reduce the problem to the particle coordinate only. Employing Eq. (2.22) for the Gaussian integration over the real variables, one arrives at the so-called dissipative action for the particle:

$$S_{\rm diss} = \frac{1}{2}\iint_{-\infty}^{+\infty} {\rm d}t\, {\rm d}t'\, \vec{X}^{\,\rm T}(t)\, \hat{\mathfrak{D}}^{-1}(t - t')\, \hat{X}(t'), \tag{3.15a}$$

$$\hat{\mathfrak{D}}^{-1}(t - t') = -\hat{\sigma}_1 \left[\sum_s g_s^2 \hat{D}_s(t - t')\right] \hat{\sigma}_1. \tag{3.15b}$$

Straightforward matrix multiplication shows that the dissipative quadratic form $\hat{\mathfrak{D}}^{-1}$ possesses the causality structure as, e.g., Eq. (3.10). For the Fourier transform of its retarded (advanced) components, one finds

$$\left[\mathfrak{D}^{-1}(\epsilon)\right]^{\mathrm{R(A)}} = -\frac{1}{2}\sum_s \frac{g_s^2}{(\epsilon \pm \mathrm{i}0)^2 - \omega_s^2} = \int_0^\infty \frac{\mathrm{d}\omega}{2\pi}\, \frac{\omega J(\omega)}{\omega^2 - (\epsilon \pm \mathrm{i}0)^2}, \tag{3.16}$$

where $J(\omega) = \pi \sum_s (g_s^2/\omega_s)\delta(\omega - \omega_s)$ is the bath spectral density.

We shall assume now that the spectral density behaves as $J(\omega) = 4\gamma\omega$, where γ is a constant at small frequencies. This is the so-called *Ohmic* bath, which is frequently found in more realistic models of the environment (see, e.g., Section 7.8). Substituting it into Eq. (3.16), one finds

$$\left[\mathfrak{D}^{-1}(\epsilon)\right]^{\mathrm{R(A)}} = 4\gamma \int \frac{\mathrm{d}\omega}{2\pi}\, \frac{\omega^2}{\omega^2 - (\epsilon \pm \mathrm{i}0)^2} = \mathrm{const} \pm 2\mathrm{i}\gamma\epsilon, \tag{3.17}$$

where the ϵ-independent real positive constant (the same for R and A components) may be absorbed into the redefinition of the harmonic part of the particle's potential $V(X) = \mathrm{const} \times X^2 + \cdots$ and, thus, may be omitted. If the bath is in equilibrium, the Keldysh component of the correlator is set by FDT,

$$\left[\mathfrak{D}^{-1}(\epsilon)\right]^{\mathrm{K}} = \left(\left[\mathfrak{D}^{\mathrm{R}}\right]^{-1} - \left[\mathfrak{D}^{\mathrm{A}}\right]^{-1}\right) \coth\frac{\epsilon}{2T} = 4\mathrm{i}\gamma\epsilon\, \coth\frac{\epsilon}{2T}, \tag{3.18}$$

where we assumed that the bath is at temperature T and, as explained after Eqs. (3.13), the chemical potential of the real bath oscillators must be zero. Notice that the validity of this expression does *not* rely on the particle being at equilibrium, but only the bath. The Keldysh component is an anti-Hermitian operator with a positive-definite imaginary part, rendering convergence of the functional integral over $\vec{X}(t)$.

In the time representation the retarded (advanced) component of the correlator takes a time-local form: $\left[\mathfrak{D}^{\mathrm{R(A)}}\right]^{-1} = \mp 2\gamma\, \delta(t - t')\, \partial_{t'}$. On the other hand, the Keldysh component is a non-local function that may be found by the inverse Fourier transform of Eq. (3.18):

$$\left[\mathfrak{D}^{-1}(t - t')\right]^{\mathrm{K}} = 4\mathrm{i}\gamma \left[(2T + C)\delta(t - t') - \frac{\pi T^2}{\sinh^2[\pi T(t - t')]}\right], \tag{3.19}$$

where the infinite constant $C = \pi T^2 \int \mathrm{d}t/\sinh^2(\pi T t)$ serves to satisfy the condition $\int dt[\mathfrak{D}^{-1}(t)]^{\mathrm{K}} = [\mathfrak{D}^{-1}(\epsilon = 0)]^{\mathrm{K}} = 8\mathrm{i}\gamma T$. Finally, one obtains for the Keldysh action of the particle connected to the ohmic bath

$$\begin{aligned} S[\vec{X}] = &\int_{-\infty}^{+\infty} \mathrm{d}t \left[-2X^{\mathrm{q}}\left(\ddot{X}^{\mathrm{cl}} + \gamma\dot{X}^{\mathrm{cl}}\right) - V\left(X^{\mathrm{cl}} + X^{\mathrm{q}}\right) + V(X^{\mathrm{cl}} - X^{\mathrm{q}})\right] \\ &+ 2\mathrm{i}\gamma \int_{-\infty}^{+\infty} \mathrm{d}t \left[2T\left(X^{\mathrm{q}}(t)\right)^2 + \frac{\pi T^2}{2}\int_{-\infty}^{+\infty} \mathrm{d}t' \frac{\left(X^{\mathrm{q}}(t) - X^{\mathrm{q}}(t')\right)^2}{\sinh^2[\pi T(t - t')]}\right], \end{aligned} \tag{3.20}$$

where the infinite constant C is absorbed into the two diagonal terms $\sim \left(X^{\mathrm{q}}(t)\right)^2$. This action satisfies all the causality criteria listed in Section 2.7. Notice that in the present case the Keldysh q − q component is not just a regularization, but a finite term, originating from the coupling to the bath and serving to limit fluctuations. This term breaks the symmetry $S[X^{\mathrm{cl}}, -X^{\mathrm{q}}] = -S[X^{\mathrm{cl}}, X^{\mathrm{q}}]$ present in the initial action (3.14). Such a symmetry of the action is a direct consequence of the time reversal symmetry of the problem. Thus the appearance of a finite q − q component of the action is a manifestation of the breaking of the time-reversal symmetry. The latter takes place due to integrating out the continuum of the bath degrees of freedom.

The other manifestation of the bath is the presence of the friction term $\sim \gamma \partial_t$ in the R and the A components. In equilibrium the friction coefficient and fluctuation amplitude are rigidly connected by the FDT. The quantum dissipative action, Eq. (3.20), is a convenient playground to demonstrate various approximations and connections to other approaches. We shall discuss it in detail in Chapter 4. If only linear terms in X^{q} are kept in the action (3.20), the integration over $X^{\mathrm{q}}(t)$ results in the functional delta-function, which enforces the following relation:

$$\ddot{X}^{\mathrm{cl}} = -V'\left(X^{\mathrm{cl}}\right) - \gamma \dot{X}^{\mathrm{cl}}. \tag{3.21}$$

This is the classical Newtonian equation with the viscous friction force. Remarkably, we have obtained the $\dot{X}^{\mathrm{cl}}$ term in the equation of motion from the action principle. It would not be possible, if not for the doubling of the number of fields X^{cl} and X^{q}. Indeed, in any action depending on X^{cl} only, terms linear in the first time derivative may be written as a full time derivative and integrated out, not affecting the equation of motion.

3.3 From Matsubara to Keldysh

Most of the texts dealing with equilibrium systems at finite temperature employ the Matsubara technique [11, 2, 4, 6]. This method is designed to treat the equilibrium density matrix $\mathrm{e}^{-\beta \hat{H}}$ as the evolution operator. To this end one considers an imaginary time quantum mechanics, with the imaginary time τ restricted to the interval $0 \leq \tau < \beta$. When calculating an expectation value of an observable $\hat{\mathcal{O}}(\tau)$, one evaluates a trace of the form $\langle \hat{\mathcal{O}} \rangle = \mathrm{Tr}\{\hat{\mathcal{O}}(\tau)\mathrm{e}^{-\beta \hat{H}}\}$. To this end one divides the imaginary time interval $[0, \beta]$ into N infinitesimal segments and inserts the resolution of unity in the coherent state basis at each segment, similarly to our procedure in Section 2.2. As a result, one ends up with fields, say with coordinate $X(\tau)$ which, in view of the fact that one evaluates the trace, obeys the periodic boundary conditions $X(0) = X(\beta)$. In the Fourier representation it is represented

by a discrete set of components $X_m = \int_0^\beta \mathrm{d}\tau\, X(\tau)\, \mathrm{e}^{\mathrm{i}\epsilon_m \tau}$, where $\epsilon_m = 2\pi m T$ is a set of Matsubara frequencies and m is an integer.

We shall discuss now how to convert an action written with the Matsubara technique into the Keldysh representation. This may be useful, if one wishes to extend treatment of the problem to non-equilibrium or time-dependent conditions. As an example consider the following bosonic Matsubara action:

$$S[X_m] = \frac{\mathrm{i}}{2}\,\gamma T \sum_{m=-\infty}^{\infty} |\epsilon_m| |X_m|^2. \tag{3.22}$$

Due to the absolute value sign $|\epsilon_m| \neq \mathrm{i}\partial_\tau$. In fact, in the imaginary time representation the kernel $K_m = |\epsilon_m|$ acquires the form $K(\tau) = \sum_m |\epsilon_m| \mathrm{e}^{-\mathrm{i}\epsilon_m \tau} = C\delta(\tau) - \pi T \sin^{-2}(\pi T \tau)$, where the infinite constant C is chosen to satisfy $\int_0^\beta \mathrm{d}\tau\, K(\tau) = K_0 = 0$. As a result, in the imaginary time representation the action (3.22) obtains the following non-local form:

$$\begin{aligned} S[X] &= \frac{\mathrm{i}}{2}\,\gamma T \iint_0^\beta \mathrm{d}\tau\, \mathrm{d}\tau' X(\tau)\, K(\tau - \tau')\, X(\tau') \\ &= \frac{\mathrm{i}}{4\pi}\,\gamma \iint_0^\beta \mathrm{d}\tau\, \mathrm{d}\tau' \frac{\pi^2 T^2}{\sin^2[\pi T(\tau - \tau')]} \big(X(\tau) - X(\tau')\big)^2. \end{aligned} \tag{3.23}$$

This action is frequently named after Caldeira and Leggett [33], who used it to investigate the influence of dissipation on quantum tunneling.

To transform to the Keldysh representation one proceeds along the following steps: (i) double the number of degrees of freedom, correspondingly doubling the action, $X \to \vec{X} = (X^{\mathrm{cl}}, X^{\mathrm{q}})^{\mathrm{T}}$ and consider the latter as functions of the real time t or real frequency ϵ; (ii) according to the causality structure, Section 2.7, the general form of the quadratic time translationally invariant Keldysh action is:

$$S\big[\vec{X}\big] = \gamma \int \frac{\mathrm{d}\epsilon}{2\pi} \big(X^{\mathrm{cl}}_\epsilon, X^{\mathrm{q}}_\epsilon\big) \begin{pmatrix} 0 & K^{\mathrm{A}}(\epsilon) \\ K^{\mathrm{R}}(\epsilon) & K^{\mathrm{K}}(\epsilon) \end{pmatrix} \begin{pmatrix} X^{\mathrm{cl}}_\epsilon \\ X^{\mathrm{q}}_\epsilon \end{pmatrix}; \tag{3.24}$$

(iii) the retarded (advanced) component $K^{\mathrm{R(A)}}(\epsilon)$ is the analytic continuation of the Matsubara correlator $K(\epsilon_m) = |\epsilon_m|$ from the *upper* (*lower*) half-plane of the complex variable ϵ_m to the real axis: $\mp\mathrm{i}\epsilon_m \to \epsilon$, see [2]. As a result, $K^{\mathrm{R(A)}}(\epsilon) = \pm\mathrm{i}\epsilon$; (iv) in equilibrium the Keldysh component follows from FDT: $K^{\mathrm{K}}(\epsilon) = \big(K^{\mathrm{R}}(\epsilon) - K^{\mathrm{A}}(\epsilon)\big) \coth(\epsilon/2T) = 2\mathrm{i}\epsilon \coth(\epsilon/2T)$, see Eqs. (3.17) and (3.18). We found thus that $\gamma \hat{K}(\epsilon) = \frac{1}{2}\hat{\mathfrak{D}}^{-1}(\epsilon)$ and therefore the Keldysh counterpart of the Matsubara action, Eq. (3.22) or (3.23), is the already familiar dissipative action (3.20) (without the potential and inertial terms, of course). One may now include external fields and allow the system to deviate from equilibrium.

3.4 Quantum tunneling in a time-dependent potential

We shall discuss here the quasi-classical description of quantum mechanical tunneling. The quasi-classical approach originates from evaluating the Feynman path integral in the stationary path approximation. Taking the variation of the Feynman action, one arrives at the classical Newtonian equation of motion. At first glance the latter fails to describe motion in the classically forbidden under-barrier region. Let us look at it more closely, however. In particular, for a particle with unit mass and energy $E = P^2/2 + V(X)$ one finds

$$P(t) = \frac{\mathrm{d}X}{\mathrm{d}t} = \sqrt{2(E - V(X))}. \tag{3.25}$$

Integrating this equation, one finds for the time t needed to reach infinity starting from a point X,

$$t(X) = \int_X^\infty \frac{\mathrm{d}X'}{\sqrt{2(E - V(X'))}}. \tag{3.26}$$

As long as $X > X_2$, such that $E > V(X)$, the corresponding time is real, see Fig. 3.1. For $X_1 < X < X_2$, where $E < V(X)$, the time changes along the imaginary direction. Finally for $X < X_1$ the time is complex, $t + \mathrm{i}\tau_0$, with a constant imaginary part $\tau_0 = \int_{X_1}^{X_2} \mathrm{d}X/\sqrt{2(V(X) - E)}$. Therefore for a tunneling trajectory, with X going from negative to positive infinity, the time evolves along the $\mathcal{C}^+$ contour depicted in Fig. 3.2.

If one wants the tunneling trajectory to be a solution of the stationary path equation, one has to consider the evolution operator along the contour $\mathcal{C}^+$ in the complex time plane, see Fig. 3.2. The semiclassical approximation for the tunneling amplitude is given by the exponentiated action along the $\mathcal{C}^+$ contour. To calculate the tunneling probability one has to supplement the latter with the conjugated backward contour $\mathcal{C}^-$, see Fig. 3.2. Actually, the locations in time of the vertical parts

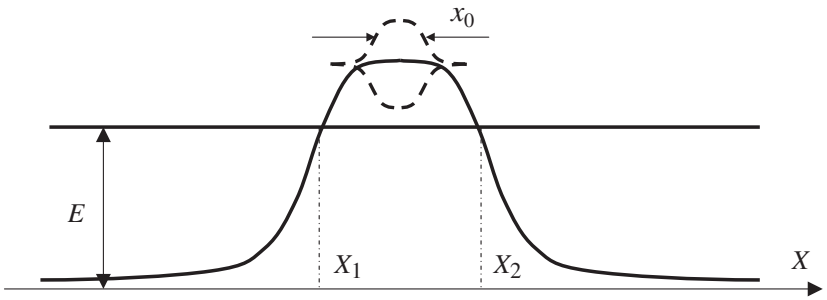

Fig. 3.1 Tunneling potential $V(X)$ and classical turning points X_1 and X_2. Time goes in the imaginary direction for $X_1 < X < X_2$. The dashed lines show a small time-dependent part of the potential, Eq. (3.29).

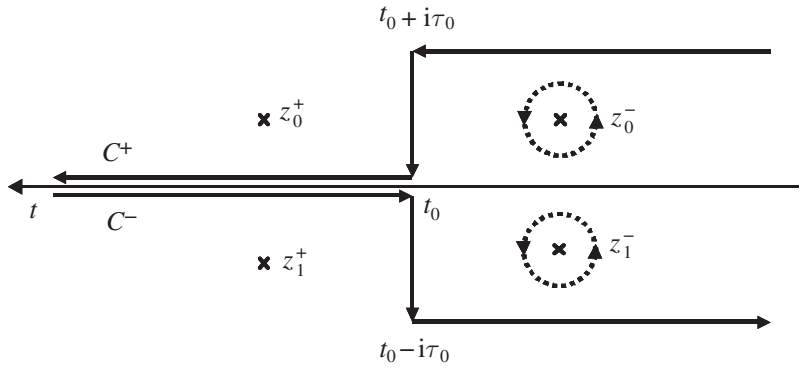

Fig. 3.2 The time contour for semiclassical evaluation of the tunneling probability. The poles at $t = z_n^{\pm}$ appear upon perturbative treatment of a time-dependent potential. After deforming the contour (dotted lines) only the poles at z_0^- and z_1^- contribute to the action.

of the contour are not necessarily the same on the forward and backward branches. This freedom is important for the treatment of multiple tunneling events. Since our immediate goal is to find the probability of a single tunneling event, we can restrict ourselves to the particular contour drawn in Fig. 3.2.

With exponential accuracy the tunneling probability for a particle with energy E is given by

$$P(E) \sim \mathrm{e}^{\,\mathrm{i}\int_{\mathcal{C}^+ + \mathcal{C}^-} \mathrm{d}t \left[\frac{1}{2}\dot{X}^2 - V(X) + E\right]}, \tag{3.27}$$

where $X(t)$ is a solution of the classical equation of motion $\ddot{X} = -V'(X)$ along the contour. The last term in the action, $\int \mathrm{d}t\, E = E(t_\mathrm{f} - t_\mathrm{i})$, where t_f is the final point on $\mathcal{C}^-$ and t_i is the initial point on $\mathcal{C}^+$, serves to fix the energy of the particle. Indeed, demanding stationarity with respect to variations over $t_{\mathrm{f,i}}$ and using [34] $\delta S/\delta t_{\mathrm{f,i}} = \mp H$, one finds that the energy is fixed on both branches of the contour $\dot{X}^2/2 + V(X) = E$. An alternative way of looking at this term is to view it as Fourier transform from the time to the energy representation.

It is easy to see that the action along the horizontal parts of the contour sums up to zero. Indeed, the action of the backward branch cancels exactly that of the forward one. It is therefore the action along the two vertical segments which remains. With the help of the classical equation of motion (3.25) the latter is given by

$$\mathrm{i}S_0 = \mathrm{i}\int_{\mathrm{i}\tau_0}^{-\mathrm{i}\tau_0} \mathrm{d}t\, \dot{X}^2 = 2\mathrm{i}\int_{X_1}^{X_2} \mathrm{d}X\, \dot{X} = -2\int_{X_1}^{X_2} \mathrm{d}X \sqrt{2(V(X) - E)}. \tag{3.28}$$

For the tunneling probability one finds $P(E) \sim \mathrm{e}^{\mathrm{i}S_0}$. This is the well-known WKB result [35], which is in fact obtained by the usual trick [35] of considering the

imaginary time Schrödinger equation (indeed, the horizontal parts of the contour were inconsequential so far).

However, doing the problem the way presented above allows one to consider tunneling in the presence of a time-dependent potential [36]. To be specific, let us consider a potential of the form

$$V(X,t) = -\frac{1}{2}\,\omega_0^2\,X^2 + \frac{\varepsilon\,x_0^2}{X^2+x_0^2}\,\cos\Omega\,t, \tag{3.29}$$

which consists of a parabolic barrier, along with the localized time-dependent potential, oscillating with a frequency Ω. We shall assume that the amplitude of the latter is small and consider a correction to the action linear in ε. To this end we need to find a semi-classical tunneling trajectory $X(t)$ of the unperturbed potential and substitute it into the time-dependent part of the action:

$$\mathrm{i}S_1 = -\mathrm{i}\varepsilon\,x_0^2\int_{\mathcal{C}^+ + \mathcal{C}^-}\mathrm{d}t\;\frac{\cos\Omega\,t}{X^2(t)+x_0^2}. \tag{3.30}$$

The tunneling trajectory of the particle with energy $E<0$ in the unperturbed potential $-\omega_0^2\,X^2/2$ is given by

$$X(t) = X_2\cosh\big(\omega_0(t-t_0)\big), \qquad X_2 = \sqrt{-2E}/\omega_0. \tag{3.31}$$

At time $t=-\infty+\mathrm{i}\tau_0$ the particle starts at $X=-\infty$ and reaches the point $X_1=-X_2$ at time $t=t_0+\mathrm{i}\tau_0$. Then it spends an imaginary time $\mathrm{i}\tau_0=\mathrm{i}\pi/\omega_0$ under the barrier where $X(t_0+\mathrm{i}\tau)=X_2\cos\omega_0\tau$ and finally continues to move in real time from $X=X_2$ towards $X=\infty$. The integral in Eq. (3.30) has poles in the complex time plane at $t=z_n^{\pm}$, where $z_n^{\pm}=t_0\pm\omega_0^{-1}\mathrm{arcsinh}(x_0/X_2)+\mathrm{i}\tau_0(1/2-n)$ and n is an integer. Two of these poles are located inside the contour, z_0^- and z_1^-, see Fig. 3.2. Deforming the contour to run around the poles and evaluating the integral in Eq. (3.30) with the help of the residue theorem, one finds

$$\mathrm{i}S_1 = \frac{2\,\varepsilon\tau_0\,\cos\alpha}{\sqrt{(X_2/x_0)^2+1}}\,\cosh\frac{\Omega\,\tau_0}{2}, \tag{3.32}$$

where $\alpha=\Omega\,t_0-(\Omega/\omega_0)\,\mathrm{arcsinh}(x_0/X_2)$. The tunneling probability is given by $P(E)\sim\mathrm{e}^{\mathrm{i}S_0+iS_1}$, where in the present case $\mathrm{i}S_0=2E\tau_0=2\pi E/\omega_0$ (remember that $E<0$). The correction $\mathrm{i}S_1$ has a random sign, dictated by $\cos\alpha$, which depends on t_0 – the free parameter of the tunneling trajectory (3.31). One should now fix t_0 by maximizing the tunneling probability, i.e. demanding $\cos\alpha=1$. This way one obtains for the tunneling probability in the presence of the oscillating field

$$P(E)\sim\mathrm{e}^{-2|E|\tau_0}\exp\left\{\frac{2\,\varepsilon\tau_0}{\sqrt{(X_2/x_0)^2+1}}\,\cosh\frac{\Omega\tau_0}{2}\right\}. \tag{3.33}$$

Therefore the tunneling probability is exponentially enhanced! The most surprising feature of this result is that at high frequency $\Omega\tau_0 \gg 1$ the enhancement parameter is itself exponentially large $\sim \varepsilon\tau_0 e^{\Omega\tau_0/2}$ [36]. This does not mean that a weak high-frequency field can make the barrier completely transparent. It rather means that there is a surprisingly small scale of the ac modulation amplitude $\varepsilon \sim \omega_0 e^{-\Omega\tau_0/2}$, beyond which the linear correction to the action is not sufficient.

To understand this behavior qualitatively, consider absorption of n quanta of energy Ω. It elevates the energy of an incoming particle to $E + \Omega n$ and therefore changes its tunneling action to $iS_0(E + \Omega n) \approx iS_0 + 2\tau_0\Omega n$, since quite generally $\partial(iS_0)/\partial E = 2\tau_0$, where τ_0 is the (imaginary) time the particle spends under the barrier. The amplitude of the n-quanta absorption process may be estimated as $(\varepsilon/\Omega)^n/n!$. As a result, the probability of tunneling upon absorption of n quanta from the ac field is $e^{iS_0+2\tau_0\Omega n}(\varepsilon/\Omega n)^{2n}$. Optimizing over n one finds $iS_1 \sim (\varepsilon/\Omega)e^{\Omega\tau_0}$, similarly to what we have found above. The difference from the actual result, Eq. (3.33), originates in the overestimated absorption amplitude (the actual one is probably reduced by another factor of $n!$). This consideration shows that the results are applicable as long as $\Omega \ll |E|$.

3.5 Dissipative quantum tunneling

Consider a particle with unit mass moving in a potential

$$V(X) = V_0\left[\delta\left(\frac{X}{a}\right)^2 - \left(\frac{X}{a}\right)^3\right], \tag{3.34}$$

where δ is a dimensionless bifurcation parameter, which governs the shape of the potential. For $\delta > 0$ the potential exhibits a meta-stable minimum at $X = 0$, see Fig. 3.3(a). If $V_0 \gg \delta/a^2$ one may disregard energy quantization in the meta-stable well and consider escape of the particle with zero energy, $E = 0$, initially trapped in the meta-stable minimum. The semiclassical escape trajectory according to Eq. (3.26) is given by

$$X(t) = \frac{\delta a}{\cos^2\frac{\omega_0(t-t_0)}{2}}, \tag{3.35}$$

where $\omega_0 = \sqrt{2V_0\delta/a^2}$. The contour $\mathcal{C}^+$, see Fig. 3.3(b), proceeds along $t + i\tau_0$, where $t \in]-\infty, t_0]$, then goes along the imaginary axis from $t = t_0 + i\tau_0$ to $t = t_0$ and finally goes along the real-time axis from $t = t_0$ to $t = t_0 + \pi/\omega_0$, see Fig. 3.3(b). In the coordinate space the three pieces of the $\mathcal{C}^+$ contour correspond to: (i) the particle staying at $X = 0$; (ii) the particle moving under the barrier, where $X(t_0 + i\tau) = \delta a/\cosh^2(\omega_0\tau/2)$; (iii) the classical motion from the "resurfacing" point $X = \delta a$ towards $X = \infty$. The imaginary time spent under the barrier is

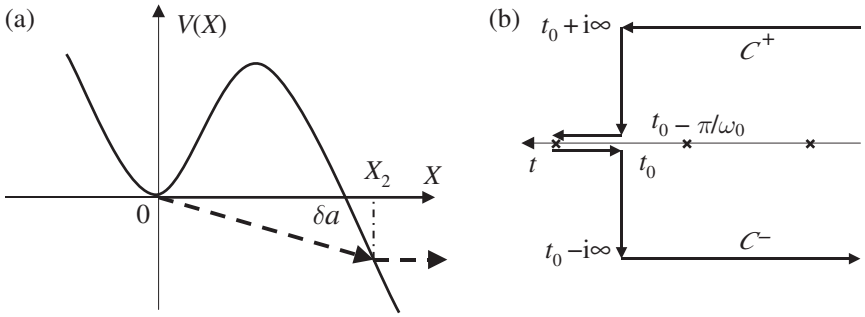

Fig. 3.3 (a) Potential (3.34) with the meta-stable minimum at $X = 0$. If a particle loses energy by exciting the bath, the tunneling trajectory is plotted schematically by the dashed line, with the "resurfacing" point X_2. (b) Contour in the complex time plane. The particle reaches $X = +\infty$ at $t = t_0 + \pi/\omega_0$. There is an infinite set of poles of Eq. (3.35) at $t = t_0 - \pi(1 + 2n)/\omega_0$.

infinite in the present case, $\tau_0 = \infty$. The presence of the poles on the real axis in Eq. (3.35) is an artefact of the too-steep potential drop at $X > \delta a$, allowing the particle to reach $X = \infty$ in a finite time. According to Eq. (3.28), the under the barrier action is given by

$$\mathrm{i}S_0 = -2\int_0^{\delta a} \mathrm{d}X\sqrt{2V(X)} = -\frac{8}{15}\sqrt{2V_0}\, a\, \delta^{5/2}. \tag{3.36}$$

As long as $|\mathrm{i}S_0| \gg 1$, the escape rate from the meta-stable well is $W \propto \omega_0 \mathrm{e}^{\mathrm{i}S_0}$.

We now consider how the coupling to the ohmic bath affects the tunneling escape rate. In this paragraph we restrict ourselves to the purely quantum, i.e. zero temperature scenario, $T = 0$ (the high-temperature case is discussed in Chapter 4). Since all the bath oscillators are in their ground states, they cannot transfer energy to the particle. Therefore one does not expect any activation-like acceleration of the escape. On the other hand, the particle is very far from its ground state and may excite the bath oscillators during its escape. Such processes lead to the particle losing its energy and "sinking" deeper into the barrier, see Fig. 3.3(a). As a result, one expects that the particle emerges from under the barrier somewhere at $X = X_2 > \delta a$ (in fact, we'll see that in the limit of very strong coupling to the bath there is a universal result for such a "resurfacing" point $X_2 = \frac{4}{3}\delta a$). At $X > X_2$ the particle moves in real time, its action is real and cancels between the forward and backward branches of the contour. The finite imaginary part of the action is accumulated during the motion along the imaginary time direction $t = \mathrm{i}\tau$. Taking the limit $T \to 0$ in Eq. (3.23), one finds for the imaginary time action

$$S[X] = \mathrm{i}\int \mathrm{d}\tau \left\{ \frac{1}{2}\left(\partial_\tau X\right)^2 + V(X) + \frac{\gamma}{4\pi}\int \mathrm{d}\tau' \frac{\left(X(t_0 + \mathrm{i}\tau) - X(t_0 + \mathrm{i}\tau')\right)^2}{(\tau - \tau')^2} \right\}. \tag{3.37}$$

Variation of this action with respect to $X(t_0+i\tau)$ leads to the semiclassical equation for under the barrier motion:

$$\partial_\tau^2 X = V'(X) + \frac{\gamma}{\pi}\fint d\tau' \, \frac{X(t_0+i\tau) - X(t_0+i\tau')}{(\tau-\tau')^2}, \tag{3.38}$$

where the integral is understood as a principal value. A general solution of this equation is not known. In the limit of weak dissipation, $\gamma \ll \omega_0$, one may find a correction to the tunneling action using perturbation theory. To this end one needs to substitute the imaginary time tunneling trajectory $X(t_0+i\tau)$, given by Eq. (3.35), into the last term in Eq. (3.37). This way one finds for the small dissipative correction to the bare tunneling action (3.36) that $i\delta S_{\rm diss} = -(12\zeta(3)/\pi^3)\gamma a^2\delta^2$.[1] Notice that this correction, being smaller than the bare tunneling action (3.36), may still result in the exponential suppression of the tunneling rate by the dissipation.

As was first realized by Caldeira and Leggett [33], one may also find a solution of Eq. (3.38) in the opposite limit of strong dissipation $\gamma \gg \omega_0$. In this case the inertia term $\partial_\tau^2 X$ on the left hand side of the equation of motion (3.38) may be neglected. One can check then by direct substitution that the following trajectory is indeed the desired solution:[2]

$$X(t) = \frac{\frac{4}{3}\,\delta a}{1-\omega_1^2(t-t_0)^2}, \tag{3.39}$$

where $t = t_0 + i\tau$ and $\omega_1 = 2V_0\delta/(\gamma a^2) = \omega_0^2/\gamma$. At $t = t_0 + i\infty$ it starts in the meta-stable minimum $X = 0$ and reaches $X_2 = 4\delta a/3$ at $t = t_0 + i0$. Here the particle emerges from under the barrier and continues its motion in real time. The action (3.37) on this trajectory is given by (the inertia term $(\partial_\tau X)^2/2$ is neglected)

$$iS_{\rm diss} = -\frac{2\pi}{9}\,\gamma a^2\delta^2. \tag{3.40}$$

[1] The calculations are easier in the Fourier representation, where the $T = 0$ Matsubara components of the trajectory (3.35) are given by $X_m = 4\pi\delta a\omega_0^{-2}\epsilon_m/\sinh(\pi\epsilon_m/\omega_0)$. Employing the dissipative action in the form of Eq. (3.22) and substituting summation by integration, one finds

$$i\delta S_{\rm diss} = -(\gamma/2)(4\pi\delta a\omega_0^{-2})^2\int (d\epsilon/2\pi)\epsilon^3/\sinh^2(\pi\epsilon/\omega_0) = -(12\zeta(3)/\pi^3)\gamma a^2\delta^2.$$

[2] Indeed, putting $t_0 = 0$ for simplicity,

$$\fint d\tau' \, \frac{X(i\tau)-X(i\tau')}{(\tau-\tau')^2} = \frac{4}{3}\,\delta a\omega_1 \fint \frac{dz'}{(z'-z)^2}\left[\frac{1}{1+z^2} - \frac{1}{1+z'^2}\right] = \frac{4}{3}\,\frac{\delta a\omega_1}{1+z^2}\,{\rm Re}\int \frac{dz'}{z'-z-i0}\,\frac{z'+z}{1+z'^2},$$

where $z = \omega_1\tau$. Evaluating the integral with the help of the residue theorem, one finds

$$\frac{4\pi}{3}\,\frac{\delta a\omega_1}{1+(\omega_1\tau)^2}\,{\rm Re}\,\frac{i+\omega_1\tau}{i-\omega_1\tau} = \frac{4\pi}{3}\,\delta a\omega_1\,\frac{(\omega_1\tau)^2-1}{[1+(\omega_1\tau)^2]^2} = \frac{-\pi V_0}{\gamma}\left[\frac{2\delta X(\tau)}{a^2} - \frac{3X^2(\tau)}{a^3}\right] = \frac{-\pi}{\gamma}\,V'(X).$$

Notice that $S_{\rm diss}/S_0 \sim \gamma/\omega_0 \gg 1$ in the limit of strong dissipation. As a result, the coupling to the bath leads to the exponential suppression of the escape rate $W \sim \mathrm{e}^{\mathrm{i}S_{\rm diss}}$. Remarkably, the scaling of the action with the bifurcation parameter changes from $\delta^{5/2}$ to δ^2. One expects that the Caldeira–Leggett scaling, δ^2, always wins in the immediate vicinity of the bifurcation point, i.e. for $\delta \ll 1$. Indeed, since $\omega_0 \sim \delta^{1/2}$, for $\delta \ll 1$ the dissipation is always strong, i.e. $\omega_0 \ll \gamma$. It may seem paradoxical that the escape rate is independent of the barrier height V_0 (as long as $\delta/a^2 < V_0 < \gamma^2 a^2/\delta$, where the left inequality is needed to disregard level quantization in the meta-stable well and the right one is $\omega_0 \ll \gamma$). In fact, taking the inertia term $(\partial_\tau X)^2/2$ in Eq. (3.37) as a perturbation, i.e. substituting in it the inertia-less solution (3.39), one finds a correction to the action (3.40) $\mathrm{i}\delta S_{\rm inert} = -4\pi V_0 \delta^3/(9\gamma)$. Although smaller than the dissipative action (3.40), this correction still leads to the exponential dependence of the tunneling rate on V_0.

One may notice that the real-time Caldeira–Leggett solution (3.39) does not satisfy Newton's equation with viscous friction, Eq. (3.21). This is because during the imaginary-time part of the trajectory the particle has excited the bath oscillators. The latter also continue to evolve in real time, exerting an additional force on the particle. As discussed in Section 3.3, the real-time counterpart of the dissipative action (3.37) is the Keldysh action (3.20). The corresponding semiclassical equation of motion is given by Eq. (3.21). Combining Eqs. (3.21) and (3.38), one finds the equation of motion for $X(t)$ on the real-time part of the contour, Fig. 3.3b,

$$\ddot{X} = -V'(X) - \gamma\dot{X} - \frac{\gamma}{\pi}\int \mathrm{d}\tau\, \frac{X(t_0 + \mathrm{i}\tau)}{(t - t_0 - \mathrm{i}\tau)^2}, \tag{3.41}$$

where the τ-integration runs along the vertical part of the contour in Fig. 3.3b. It is easy to check that, neglecting the inertia term $\ddot{X}$, the Caldeira–Leggett solution (3.39) satisfies this equation too. Therefore the trajectory (3.39) solves the semiclassical equations of motion along the entire contour! Notice that the tunneling event completed at $t = t_0$ exerts a slowly decaying $\sim (t - t_0)^{-2}$ (for $t - t_0 \gg \omega_1^{-1}$) force, altering the subsequent motion of the particle in real time. This fact may qualitatively change the picture of tunneling between two resonant wells, where multiple tunneling events are important. We shall not develop this theory here, referring the reader to a review [37].

One can use now the analytic form of the tunneling trajectories, Eqs. (3.35) and (3.39), to investigate the influence of an external time-dependent signal on the escape rates. To this end let us consider a weak spatially uniform oscillatory force by adding the following term to the potential (3.34):

$$V(X, t) = \varepsilon\, \frac{X}{a}\, \mathrm{e}^{\nu t}\, \cos \Omega t, \tag{3.42}$$

where ν is an infinitesimal energy scale, which describes an adiabatic switching on of the external time-dependent force. To the first order in ε the change in the tunneling action is evaluated by substituting the trajectory (3.35) or (3.39) into the action $S_1 = -\mathrm{i}\int_{\mathcal{C}^+ + \mathcal{C}^-} \mathrm{d}t\, V(X(t), t)$. Due to the factor $\mathrm{e}^{\nu t}$ (omitted from now on) the $t = -\infty$ part of the contour does not contribute to the action. Deforming the contour, one finds that the integral is reduced to the contribution of the poles of the $X(t)$ function along the $t < t_0$ part of the real-time axis. For the bare tunneling trajectory, Eq. (3.35), the relevant poles are at $t = z_n = t_0 - (\pi + 2\pi n)/\omega_0$, where $n = 0, 1, \ldots$. Summing over all of them and maximizing over the free parameter t_0, one finds [36]

$$\mathrm{i}S_1 = \frac{\varepsilon\Omega}{\omega_0^2}\,\frac{4\pi\delta}{\sin(\pi\Omega/\omega_0)}. \tag{3.43}$$

For $\Omega = \omega_0, 2\omega_0, \ldots$ the external field is in resonance with the small oscillations in the meta-stable minimum and the linear response approach fails. In the limit $\Omega \to 0$ one finds $\mathrm{i}S_1 = 4\delta\varepsilon/\omega_0$. This may be directly obtained from Eq. (3.36) by changing δ^2 to $\delta^2 - 3\varepsilon/V_0$. Indeed, the potential (3.34) is equivalent, up to a trivial shift, to $V(X) = V_0[\delta^2 X/3a - (X/a)^3]$. Therefore, adding to it a static linear term $-\varepsilon X/a$ leads to the aforementioned redefinition of δ^2.

For the case of strong dissipation the only relevant pole of the trajectory (3.39) is at $t = t_0 - 1/\omega_1$, which leads to the following correction to the action:

$$\mathrm{i}S_1 = \frac{4\pi}{3}\,\frac{\varepsilon\delta}{\omega_1} = \frac{2\pi}{9}\,\gamma a^2\,\frac{3\epsilon}{V_0}. \tag{3.44}$$

This is nothing but the adiabatic change of the time-independent result (3.40) by the static reduction of $\delta^2 \to \delta^2 - 3\varepsilon/V_0$. Therefore for not too large frequencies the effect of the ac force on the overdamped tunneling decay is the same as the dc one. At higher frequencies the fact that the $-X^3$ tail of the potential must flatten somewhere becomes important. In this case the particle does not reach infinity in a finite time. This fact translates into the splitting of the poles and moving them away from the real axis by a small imaginary time $\mathrm{i}\tau_\mathrm{s} \sim \mathrm{i}a/\sqrt{V_0}$. Similarly to Section 3.4, it leads to the exponential enhancement of the ac correction at very high frequencies $\mathrm{i}S_1 \propto \varepsilon \mathrm{e}^{\Omega\tau_\mathrm{s}}$ [36].

4

Classical stochastic systems

This chapter is devoted to the classical limit of the quantum dissipative action obtained in Chapter 3. We show how it yields Langevin, Fokker–Planck and optimal path descriptions of classical stochastic systems. These approaches are used to discuss activation escape, fluctuation relation, reaction models and other examples.

4.1 Classical dissipative action

In Section 3.2 we derived the Keldysh action for a quantum particle coupled to an Ohmic environment, Eq. (3.20). If only linear terms in the quantum coordinate $X^{\rm q}(t)$ are kept in this action, it leads to a classical Newtonian equation with a viscous friction force, Eq. (3.21). Such an approximation completely disregards any fluctuations: both quantum and *classical*. Our goal now is to do better than that and to keep classical thermal fluctuations, while still neglecting quantum effects.

To this end it is convenient to restore the Planck constant $\hbar$ in the action and then take the limit $\hbar \to 0$. For dimensional reasons, the factor $\hbar^{-1}$ should stay in front of the entire action. To keep the part of the action responsible for the classical equation of motion (3.21) free from the Planck constant it is convenient to rescale the quantum component as $X^{\rm q} \to \hbar X^{\rm q}$. Indeed, when this is done all terms linear in $X^{\rm q}$ do not contain $\hbar$. Finally, to have the temperature in energy units, one needs to substitute T with $T/\hbar$. As a result, the term $\sim \gamma T\,(X^{\rm q}(t))^2$ does not contain the Planck constant either. The limit $\hbar \to 0$ is now straightforward: (i) one has to expand $\mp V(X^{\rm cl} \pm \hbar X^{\rm q})$ to first order in $\hbar X^{\rm q}$ and neglect all higher order terms; (ii) in the last non-local term in Eq. (3.20) the $\hbar \to 0$ limit is taken with the help of the identity

$$\frac{\pi T^2/(2\hbar)}{\sinh^2(\pi T(t-t')/\hbar)} \xrightarrow{\hbar\to 0} T\delta(t-t'). \tag{4.1}$$

Consequently the non-local term becomes local and drops out in the $\hbar \to 0$ limit. Finally, the classical limit of the dissipative action (3.20) is

$$S[\vec{X}] = \int_{-\infty}^{+\infty} \mathrm{d}t \left\{ -2X^{\mathrm{q}} \left[\ddot{X}^{\mathrm{cl}} + \gamma \dot{X}^{\mathrm{cl}} + V'\big(X^{\mathrm{cl}}\big) \right] + 4\mathrm{i}\gamma T \big(X^{\mathrm{q}}\big)^2 \right\}. \tag{4.2}$$

Notice that this action is local in time. Also, despite its name, the quantum component X^{q} still has a role to play in the classical setting.

Physically the limit $\hbar \to 0$ means that $\hbar\gamma$ and $\hbar\Omega \ll T$, where Ω is a characteristic frequency of the particle's classical motion. These conditions are sufficient for us to neglect both the time non-local term and the higher order expansion of $V(X^{\mathrm{cl}} \pm \hbar X^{\mathrm{q}})$ in Eq. (3.20). Correspondingly, an alternative way to look at the classical expression (4.2) is to view it as a high-temperature limit of the full quantum action (3.20). On the technical level it amounts to substituting $\coth \epsilon/(2T)$ by $2T/\epsilon$ in, e.g., Eq. (3.24). In this chapter we consider some implications of the classical dissipative action (4.2) as well as some of its generalizations.

4.2 Langevin equation

One way to proceed with the classical action (4.2) is to notice that the exponent of its last term (times i) may be rewritten in the following way:

$$\mathrm{e}^{-4\gamma T \int \mathrm{d}t \left(X^{\mathrm{q}}(t)\right)^2} = \int \mathbf{D}[\xi(t)]\ \mathrm{e}^{-\int \mathrm{d}t \left[\frac{1}{4\gamma T}\xi^2(t) - 2\mathrm{i}\xi(t) X^{\mathrm{q}}(t)\right]}. \tag{4.3}$$

This identity is called the Hubbard–Stratonovich transformation, where $\xi(t)$ is an auxiliary Hubbard–Stratonovich field. With the integration measure $\mathbf{D}[\xi(t)]$ normalized such that $\int \mathbf{D}[\xi(t)]\ \mathrm{e}^{-\int \mathrm{d}t\, \xi^2/4\gamma T} = 1$, the identity (4.3) is an immediate consequence of the real Gaussian integral (2.22).

Any observable $\mathcal{O}[X^{\mathrm{cl}}]$ formulated in terms of the classical coordinate (possibly taken in more than one instance of time) may be written as (recall that $Z = 1$ and thus no normalization factor is needed)

$$\begin{aligned}
\langle \mathcal{O}[X^{\mathrm{cl}}] \rangle &= \int \mathbf{D}[X^{\mathrm{cl}}, X^{\mathrm{q}}]\, \mathcal{O}[X^{\mathrm{cl}}]\, \mathrm{e}^{\mathrm{i}S[\vec{X}]} \\
&= \int \mathbf{D}[\xi]\ \mathrm{e}^{-\frac{1}{4\gamma T}\int \mathrm{d}t\, \xi^2} \int \mathbf{D}[X^{\mathrm{cl}}] \mathcal{O}[X^{\mathrm{cl}}] \int \mathbf{D}[X^{\mathrm{q}}]\, \mathrm{e}^{-2\mathrm{i}\int \mathrm{d}t\, X^{\mathrm{q}} \left(\ddot{X}^{\mathrm{cl}} + \gamma \dot{X}^{\mathrm{cl}} + V'(X^{\mathrm{cl}}) - \xi\right)} \\
&= \int \mathbf{D}[\xi]\ \mathrm{e}^{-\frac{1}{4\gamma T}\int \mathrm{d}t\, \xi^2} \int \mathbf{D}[X^{\mathrm{cl}}] \mathcal{O}[X^{\mathrm{cl}}]\, \delta\left(\ddot{X}^{\mathrm{cl}} + \gamma \dot{X}^{\mathrm{cl}} + V'(X^{\mathrm{cl}}) - \xi\right),
\end{aligned} \tag{4.4}$$

where the last line includes the functional delta-function of the expression in the round brackets. This functional delta-function enforces its argument to be zero at

every moment of time. Therefore, among all possible trajectories $X^{\rm cl}(t)$ only those contribute to the observable that satisfy

$$\ddot{X}^{\rm cl} = -\gamma \dot{X}^{\rm cl} - V'(X^{\rm cl}) + \xi(t). \tag{4.5}$$

This is the Newton equation with a friction force $-\gamma \dot{X}$ and a time-dependent external force $\xi(t)$, known also as the Langevin equation.

Equation (4.4) implies the following strategy for finding the expectation value $\langle \mathcal{O}[X^{\rm cl}] \rangle$: (i) choose a particular realization of the force $\xi(t)$; (ii) solve Eq. (4.5) (e.g. numerically); (iii) having its solution, $X^{\rm cl}(t)$, calculate the observable $\mathcal{O}[X^{\rm cl}]$; (iv) average the result over an ensemble of realizations of the random force $\xi(t)$ with the Gaussian weight $\exp\{-\int {\rm d}t\, \xi^2(t)/4\gamma T\}$. The Gaussian statistics of the random force $\xi(t)$ means that only its first and second *irreducible* moments must be specified. In our example $\langle \xi(t) \rangle = 0$ (if the first moment is not zero, it may always be viewed as a part of the deterministic force $-V'$). This means that the Langevin equation (4.5) must be supplemented only with the second moment of the random force, given by

$$\langle \xi(t)\xi(t') \rangle = \int \mathbf{D}[\xi]\, \xi(t)\xi(t')\, {\rm e}^{-\frac{1}{4\gamma T}\int {\rm d}t\, \xi^2} = 2\gamma T \delta(t-t'), \tag{4.6}$$

where we employed the Wick theorem, Eq. (2.23). Since in the frequency representation the right hand side of this equation is a constant, the corresponding random force is often referred to as a *white* noise. It originates from the classical thermal fluctuations of bath oscillators. The fact that the noise amplitude is proportional to the friction coefficient, γ, and temperature T is a manifestation of FDT in its classical limit (i.e. $\coth \epsilon/2T \to 2T/\epsilon$). The latter holds because we assumed the bath to be in thermal equilibrium.

4.3 Multiplicative noise and Martin–Siggia–Rose method

The Langevin equation (4.5) with the white noise force (4.6) provides a convenient way for a numerical treatment of the classical dissipative action (4.2). It is not very useful, though, for analytical approaches. In fact, many problems may be initially formulated as Langevin equations with certain random forces and one would like to have a way to convert them into a proper classical action. Such a procedure, which is in essence an inversion of what was done in the previous section, was formulated by Martin, Siggia and Rose (MSR) [30]. It is presented here in the form suggested by DeDominicis [31] and Janssen [38].

Consider a Langevin equation

$$\dot{X} = A(X) + b(X)\xi(t). \tag{4.7}$$

We have restricted ourselves to the first order differential operator ∂_t. It may be viewed as an overdamped limit (i.e. $\gamma \gg \Omega$, where Ω is a characteristic classical frequency) of the Newton equation (4.5). We shall generalize, however, Eq. (4.7) to more than one variable. This will allow us to treat an arbitrary order operator by representing it as a higher dimensional first order one (see below). The most important difference between Eqs. (4.7) and (4.5) is the fact that the noisy force $\xi(t)$ is modulated in a coordinate-dependent way. This is achieved by multiplying it by a coordinate-dependent function $b(X)$, hence the name *multiplicative* noise. The Gaussian white noise $\xi(t)$ is fully specified by its second moment, which without loss of generality may be normalized as

$$\langle \xi(t)\xi(t')\rangle = 2\delta(t-t'). \tag{4.8}$$

In fact the multiplicative Langevin equation (4.7) is ill-defined unless the regularization of the differential operator is explicitly specified. We shall choose such a regularization in a way to be consistent with the field theoretical treatment of the previous chapters. To this end consider the "partition function"

$$Z[\xi] = \int \mathbf{D}[X(t)]\, \mathcal{J}[X]\, \delta\big(\partial_t X - A(X) - b(X)\xi\big) \equiv 1. \tag{4.9}$$

It is identically equal to unity by virtue of the integration of the delta-function, provided $\mathcal{J}[X]$ is the Jacobian of the operator $\hat{\mathcal{N}}[X] = \partial_t X - A(X) - b(X)\xi$. The way to interpret Eq. (4.9) is to discretize the time axis, introducing N-dimensional vectors $X_j = X(t_j)$ and $\xi_j = \xi(t_j)$, where $j = 1, \ldots, N$. The operator takes the form $\mathcal{N}_j = \mathcal{N}_j^{(0)} + \mathcal{N}_{jl}^{(1)} X_l + \frac{1}{2}\mathcal{N}_{jlk}^{(2)} X_l X_k + \cdots$, where summation is understood over repeated indices. The Jacobian $\mathcal{J}[X]$ in the partition function (4.9) is given by the absolute value of the determinant of the following $N \times N$ matrix: $\mathcal{J}_{jl} \equiv \partial \mathcal{N}_j / \partial X_l = \mathcal{N}_{jl}^{(1)} + \mathcal{N}_{jlk}^{(2)} X_k + \cdots$. It is possible to choose a proper (*retarded*) regularization, where $\mathcal{J}_{jl}$ is the lower triangular matrix with unit main diagonal (coming entirely from the $\mathcal{N}_{jj}^{(1)} = 1$ term). Clearly, in this case $\mathcal{J} = 1$. To this end let us choose the discrete version of the operator as

$$\mathcal{N}_j = X_j - X_{j-1} - \delta_t\big[A(X_{j-1}) + b(X_{j-1})\xi_{j-1}\big]. \tag{4.10}$$

Clearly, in this case $\mathcal{J}_{jj} = 1$ and $\mathcal{J}_{j,j-1} = -1 - \delta_t[A'(X_{j-1}) + b'(X_{j-1})\xi_{j-1}]$, while all other matrix elements $\mathcal{J}_{jl} = 0$. As a result $\mathcal{J}[X] = 1$ for any realization X_j and ξ_j. The regularization (4.10) of the differential operator (4.7) is retarded since the right hand side of Eq. (4.7) is always taken in the "preceding" moment of time $j-1$. Such an understanding of the Langevin equation (4.7) is called *Ito regularization* [39, 40] and it is the most convenient one for field-theoretical treatment.

Although the partition function (4.9) is trivial, it is clear that all meaningful observables and correlation functions may be obtained by inserting a factor $\mathcal{O}[X]$ in the functional integral (4.9). Having this in mind along with the fact that $\mathcal{J}[X]=1$ due to Ito regularization, let us proceed with the partition function. Employing the integral representation of the delta-function with the help of an auxiliary field $X^{\mathrm{q}}(t)$, one obtains:

$$Z[\xi] = \int \mathbf{D}[X] \int \mathbf{D}[X^{\mathrm{q}}]\ \mathrm{e}^{-2\mathrm{i}\int \mathrm{d}t\, X^{\mathrm{q}}(t)\left(\partial_t^{\mathrm{R}} X - A(X) - b(X)\xi(t)\right)}, \tag{4.11}$$

where ∂_t^{R} stays for the retarded (Ito) regularization of the operator. One may average now the partition function over the white noise, Eq. (4.8), by performing the Gaussian integration over $\xi(t)$:

$$Z = \int \mathbf{D}[\xi]\ \mathrm{e}^{-\frac{1}{4}\int \mathrm{d}t\, \xi^2} Z[\xi] = \int \mathbf{D}[X, X^{\mathrm{q}}]\, \mathrm{e}^{\int \mathrm{d}t \left[-2\mathrm{i}\, X^{\mathrm{q}}\left(\partial_t^{\mathrm{R}} X - A(X)\right) - 4(X^{\mathrm{q}})^2 D(X)\right]}, \tag{4.12}$$

where $D(X) \equiv b^2(X) \geq 0$. The exponent on the right hand side is (i times) the MSR action for the Ito–Langevin process (4.7), (4.8). The main difference from the classical limit of the Keldysh action (4.2) is the X-dependent coefficient $D(X)$ in the Keldysh component $\sim (X^{\mathrm{q}})^2$. It clearly originates from the multiplicative nature of the noise term. Notice also that the retarded derivative $\sim X^{\mathrm{q}}\partial_t^{\mathrm{R}} X$ has a correct regularization of the lower triangular matrix with the unit main diagonal. This shows that taking Ito regularization (4.10) of the Langevin process (4.7), is indeed crucial to establishing correspondence with the Keldysh formalism. Let us reiterate thus the discrete form of the MSR action:

$$S[\vec{X}] = \sum_{j=1}^{N} \left[-2X_j^{\mathrm{q}}\left(X_j - X_{j-1} - \delta_t A(X_{j-1})\right) + 4\mathrm{i}\delta_t (X_j^{\mathrm{q}})^2 D(X_{j-1})\right], \tag{4.13}$$

which appears to be *normally ordered* (in a sense that the auxiliary variable X^{q} is taken one time step ahead of the physical variable X, apart from the diagonal term $-2X_j^{\mathrm{q}}X_j$). The MSR method provides a way to go from a classical stochastic problem to its proper functional representation. The latter is useful for analytical analysis. Some examples are discussed below.

One can generalize the above consideration for an M-component vector variable $X_\alpha(t)$, where $\alpha = 1, \ldots, M$. The corresponding Ito–Langevin process reads as

$$\dot{X}_\alpha = A_\alpha(X) + b_{\alpha\beta}(X)\xi_\beta(t); \tag{4.14}$$

$$\langle \xi_\beta(t)\xi_\gamma(t')\rangle = 2\delta_{\beta\gamma}\delta(t-t'), \tag{4.15}$$

where summation over repeated indices is understood. Introducing the corresponding vector of auxiliary fields X_α^{q}, one obtains the following MSR action (in the continuous notation)

$$S[\vec{X}] = \int \mathrm{d}t \left[-2X^{\mathrm{q}}_{\alpha}\big(\dot{X}_{\alpha} - A_{\alpha}(X)\big) + 4\mathrm{i}X^{\mathrm{q}}_{\alpha}X^{\mathrm{q}}_{\beta}D_{\alpha\beta}(X)\right], \tag{4.16}$$

where $D_{\alpha\beta}(X) = \sum_{\gamma=1}^{M} b_{\alpha\gamma}(X)\, b_{\beta\gamma}(X)$ is a symmetric non-negative-definite matrix.[1]

As an example consider the second order Langevin equation (4.5). Renaming the variables as $X_1 = X^{\mathrm{cl}}$ and $X_2 = \dot{X}^{\mathrm{cl}}$, Eq. (4.5) may be brought to the form of Eq. (4.14) with $A_1(X) = X_2$, $A_2(X) = -\gamma X_2 - V'(X_1)$ and $b_{22} = \sqrt{\gamma T}$, while all other components of $b_{\alpha\beta}$ are zero. One may then write the MSR action (4.16) and notice that X^{q}_1 enters the action only linearly. Integrating over X^{q}_1 one thus obtains $\delta(\dot{X}_1 - X_2)$, which allows one now to perform integration over X_2. The resulting action written in terms of $X_1 = X^{\mathrm{cl}}$ and $X^{\mathrm{q}}_2 = X^{\mathrm{q}}$ is exactly the classical dissipative action (4.2). This illustrates that considering the first order Langevin equations is not a real limitation. It also shows that, since the equation $\dot{X}_1 = X_2$ should be understood in the Ito way, i.e. $X_{1,j} - X_{1,j-1} = \delta_t X_{2,j-1}$, the proper regularization of Eq. (4.5) is $X_j - 2X_{j-1} + X_{j-2} = -\delta_t\gamma(X_{j-1} - X_{j-2}) - \delta_t^2 V'(X_{j-2})$. That is, the corresponding quadratic action again has a lower triangular structure with unit diagonal.

4.4 Optimal path approximation

For some applications (most notably associated with rare events) the functional integral in Eq. (4.12) may be evaluated in the stationary path approximation. The corresponding equations are obtained by the variation of the action with respect to $X^{\mathrm{q}}(t)$ and $X(t)$ and have the form

$$\begin{aligned} \dot{X} &= A(X) + 4\mathrm{i}X^{\mathrm{q}}D(X), \\ \mathrm{i}\dot{X}^{\mathrm{q}} &= -\mathrm{i}X^{\mathrm{q}}A'(X) + 2(X^{\mathrm{q}})^2 D'(X). \end{aligned} \tag{4.17}$$

One possible solution of these equations is $X^{\mathrm{q}} = 0$, while $\dot{X} = A(X)$. Clearly this solution corresponds to the noiseless evolution of $X(t)$. Such a noiseless trajectory is by no means the only solution of the stationary path equations (4.17). There are other solutions, which ought to be considered. Since $X(t)$ as well as $A(X)$ and $D(X)$ are all real, one expects that stationary trajectories of the variable X^{q} are purely imaginary. This does not contradict, of course, the fact that $\mathbf{D}[X^{\mathrm{q}}] = \prod_j \mathrm{d}X^{\mathrm{q}}_j$ integrations run along the real axis. What we observed is that the stationary points are located away from the initial integration contour and

[1] Indeed, the eigenvalue equation is $D_{\alpha\beta}s_\beta = b_{\alpha\gamma}b_{\beta\gamma}s_\beta = \lambda s_\alpha$. Multiplying by s_α one finds $\lambda = (b_{\beta\gamma}s_\beta)^2/(s_\alpha)^2 \geq 0$. The zero eigenvalue is possible if the matrix $b_{\alpha\beta}$ possesses a left zero mode, i.e. if $s_\alpha b_{\alpha\beta} = 0$.

therefore the latter must be deformed in the complex planes of X_j^{q} to pass through purely imaginary stationary points (unless $X^{\mathrm{q}} = 0$).

To avoid complex notation it is convenient to rename a *stationary* trajectory $X^{\mathrm{q}}(t)$ as $X^{\mathrm{q}}(t) = P(t)/(2\mathrm{i})$, where $P(t)$ is real on the stationary trajectories. With this notation Eqs. (4.17) acquire the Hamiltonian structure

$$\dot{X} = \partial_P H(P, X)\,, \qquad \dot{P} = -\partial_X H(P, X); \tag{4.18}$$

$$H(P, X) = PA(X) + P^2 D(X). \tag{4.19}$$

Notice that P is not the physical momentum (indeed we deal with the overdamped motion (4.7)). It is rather an auxiliary variable which encodes the noise. Nevertheless it is useful to view it as the canonical pair of the physical variable X. Due to their Hamiltonian nature the stationary path equations possess the integral of motion: the "energy" $H(P, X) = \text{const}$. The corresponding MSR action, acquired along an *optimal trajectory* (i.e. the one satisfying the equations of motion (4.18)), takes the standard form [34]

$$\mathrm{i}S[X, P] = -\int \mathrm{d}t\, \left[P\dot{X} - H(P, X)\right], \tag{4.20}$$

where $H(P, X)$ is a constant along the trajectory. The statistical weight of the corresponding path is given by $\exp\{\mathrm{i}S\}$.

One may visualize solutions of Eqs. (4.18) by plotting the phase portrait, i.e. the curves of constant energy on the phase plane (P, X). The special role is played by the curves of zero energy $H = 0$. Generally (i.e. if $D(X) \neq 0$) there are two of them $P = 0$ and $P = -A(X)/D(X)$. The first one corresponds to the noiseless relaxation according to $\dot{X} = A(X)$, while the second one is responsible for fluctuations. These two intersect at the points where $A(X) = 0$, i.e. at the fixed points of the noiseless dynamics. Along the fluctuation curve $P = -A(X)/D(X)$ the equation of motion reads $\dot{X} = A(X) + 2PD(X) = -A(X)$, i.e. it describes the evolution, which is time reversed compared to that along the noiseless $P = 0$ line. The fact that the fluctuations are time-reversed partners of the relaxation is *not* generic. It is a consequence of the potential nature of the force, see Section 4.12.

As an example consider an overdamped thermal motion in a potential $V(X)$. In this case $A(X) = -V'(X)$ and $D(X) = T$ (we put $\gamma = 1$ for brevity). The fluctuation zero energy curve takes the form $P = V'(X)/T$. Figure 4.1(a) depicts the phase portrait for a potential with a single stable minimum at $X = 0$. The noiseless relaxation drives the system towards the origin $X = 0$ along the $P = 0$ line. If we are interested in a relative weight for finding the system at some $X_0 \neq 0$, we need to identify an optimal trajectory which brings the system to X_0 in a given time. If no time limitations are imposed (i.e. the observation time is unlimited), the

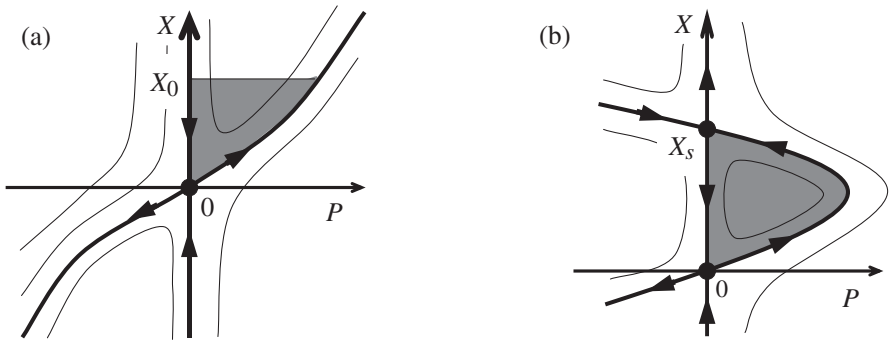

Fig. 4.1 Phase portraits of the Fokker–Planck Hamiltonians: (a) for a potential with a single minimum at $X = 0$; (b) for a potential with a meta-stable minimum at $X = 0$ and unstable maximum at $X = X_s$. Bold lines are curves of zero energy $P = 0$ and $P = V'(X)/T$. The shaded areas give actions of the optimal paths, reaching points X_0 and X_s, respectively.

proper optimal trajectory is the zero energy curve $P = V'(X)/T$. Indeed, it takes an infinite time to depart from the fixed point $X = 0$. Since along the optimal path $H(P, X) = 0$, the accumulated action (4.20) may be written as

$$\mathrm{i}S(X_0) = -\int \mathrm{d}t\, P\dot{X} = -\int_0^{X_0} P\,\mathrm{d}X,$$

i.e. it is given by the geometric area shaded in Fig. 4.1a. Employing that $P = V'(X)/T$, one further obtains

$$\mathrm{i}S(X_0) = -\int_0^{X_0} P\,\mathrm{d}X = -\frac{1}{T}\int_0^{X_0} V'(X)\mathrm{d}X = -\frac{V(X_0) - V(0)}{T}. \tag{4.21}$$

As a result, the relative statistical weight for finding the system at $X = X_0$ is $\propto \exp\{-V(X_0)/T\}$. This is, of course, nothing but the Boltzmann distribution. So far we have found it with exponential accuracy only, i.e. without a pre-exponential factor, which, in principle, could be X_0-dependent. In the next section we'll prove that this is not the case.

Consider now a potential which has a *meta-stable* minimum at $X = 0$ and an unstable maximum at $X = X_s$, see Fig. 3.2. The corresponding phase portrait is depicted in Fig. 4.1b. The fluctuation curve $P = V'(X)/T$ has now two intersections with the relaxation line $P = 0$. The relaxation dynamics in a local vicinity of $X = 0$ is stable (attractive), while at $X = X_s$ it is unstable (repulsive). According to the Liouville theorem of classical mechanics [34], the Hamiltonian motion conserves the area of the phase space. This implies that both fixed points

must be hyperbolic, i.e. have one attractive and one repulsive direction. As a result, the stability of the two fixed points along the fluctuation curve is opposite to that along the relaxation line, i.e. $X = 0$ is repulsive, while $X = X_s$ is attractive, see Fig. 4.1(b). It is clear now that the *activation* escape from the meta-stable fixed point $X = 0$ must proceed along the fluctuation curve $P = V'(X)/T$ until $X = X_s$; starting at the $P = 0$ point and then following the relaxation line $P = 0$. The action is accumulated only along the fluctuation part of the optimal escape trajectory and is given by the shaded area in Fig. 4.1(b). In complete analogy with Eq. (4.21) one finds that the escape rate is proportional to the Boltzmann factor $\propto \exp\{-(V(X_s) - V(0))/T\}$. We shall evaluate the corresponding pre-exponential factor in Section 4.8.

Let us discuss now an overdamped particle in a harmonic potential subject to a multiplicative noise (in the Ito sense), proportional to a certain positive power of $|X|$:

$$\dot{X} = -\kappa X + |X|^{\nu}\xi(t), \tag{4.22}$$

where the Gaussian white noise $\xi(t)$ is specified by Eq. (4.8). The question is whether the particle sticks to the bottom of the well and does not ever leave it, because the noise near the bottom is too weak. The corresponding Hamiltonian reads as $H(P, X) = -\kappa PX + P^2|X|^{2\nu}$ and its phase portrait for the case $\nu > 1/2$ is plotted in Fig. 4.2. Again the relative weight of reaching a point $X_0 \neq 0$ is given by an exponentiated (negative) area enclosed by the curves of zero energy, i.e. $\exp\{-\kappa X_0^{2-2\nu}/(2-2\nu)\}$ for $\nu < 1$. On the other hand, for $\nu \geq 1$ the corresponding area diverges, nullifying the long-time probability of finding the particle away from $X_0 = 0$. As a result, for $\nu \geq 1$ the particle eventually sticks to the bottom and the only steady state distribution is $\delta(X_0)$.

The message of this section is that the stationary path dynamics of *dissipative* stochastic models may be described by the effective Hamiltonian system. The role of momentum is played by the auxiliary MSR variable (times i), which is nothing

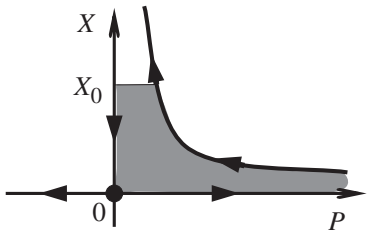

Fig. 4.2 Zero energy lines of the Fokker–Planck Hamiltonian corresponding to Eq. (4.22): $P = 0$, $X = 0$ and $P = \kappa/X^{2\nu-1}$ with $\nu > 1/2$. The action (i.e. the shaded area) diverges for $\nu \geq 1$.

but the classical limit of the Keldysh "quantum" component. A lot of insight in the behavior of the corresponding stochastic model may be gained by an inspection of the phase portrait of the corresponding Hamiltonian. The action (4.20) was written above only for stationary trajectories (i.e. satisfying the equations of motion (4.18)). However, it may be equally well extended to any trajectory $X(t)$ and $P(t)$ and used as a weight in the functional integral, much as the action (4.13) or (4.16). The only thing to remember is that the $\mathbf{D}[P(t)] = \prod_j \mathrm{d}P_j$ integrations run along the *imaginary* axis. Notice that quantities such as the escape rate are determined by the optimal trajectories with some non-zero $X^{\mathrm{q}}(t)$. This means in turn that such trajectories are different along the forward and backward branches of the time contour. The latter is a consequence of the time-reversal invariance being broken by the integration over the bath with a continuous spectrum.

4.5 Fokker–Planck equation

The consideration of the previous section closely resembles the WKB approximation in quantum mechanics. One may take one step forward towards the analogy between the theory of classical stochastic models and quantum mechanics and look for a corresponding "Schrödinger" equation. The latter is derived through the transfer-matrix treatment of the Feynman path integral [32]. To this end one integrates over trajectories which at time $t = t_j$ arrive at the point $X = X_j$ with an arbitrary momentum (i.e. arbitrary X^{q}). From the definition (4.9) it is clear that the corresponding *restricted* partition function $\mathcal{P}(X,t) = Z|_{X(t)=X}$ is proportional to the *probability* (not the amplitude!) of finding the system at the point X at time t. The fact that $\mathcal{P}(X,t)$ is real follows immediately from the form of the action (4.12) and the symmetry $X^{\mathrm{q}} \to -X^{\mathrm{q}}$, while $Z \to Z^*$. In other words, the Keldysh contour provides the product of an amplitude (forward branch) and its complex conjugate (backward branch), resulting in the probability.

We shall formally derive the equation for $\mathcal{P}(X,t)$ below. The result, however, may be anticipated from the Hamiltonian formulation, Eqs. (4.19), (4.20) and analogy with quantum mechanics. The latter states that the required equation has the form $\partial_t \mathcal{P} = \hat{H}\mathcal{P}$. Here the Hamiltonian *operator* $\hat{H}$ is obtained from the *normally ordered* classical Hamiltonian $H(P,X)$ by the substitution of $P \to \hat{P}$, which satisfies the canonical commutation relation $[X, \hat{P}] = 1$ (in our case P runs along the imaginary axis), i.e. $\hat{P} = -\partial_X$. Using Eq. (4.19) for the Hamiltonian, one obtains

$$\partial_t \mathcal{P}(X,t) = -\partial_X \Big[A(X)\mathcal{P}(X,t) - \partial_X \big[D(X)\mathcal{P}(X,t) \big] \Big]. \tag{4.23}$$

This is the Fokker–Planck equation [41] for the evolution of the probability distribution function of the stochastic system (4.7). The normal ordering of the action

(4.13) is crucial to employing the quantum mechanical analogy. Therefore this form of the Fokker–Planck equation is specific to the Ito regularization.

The Fokker–Planck equation has the structure of the continuity relation $\partial_t \mathcal{P} + \partial_X J = 0$, where the probability current is $J = A\mathcal{P} - \partial_X[D\mathcal{P}]$. This fact is responsible for the conservation of probability $\partial_t \int \mathrm{d}X \mathcal{P} = 0$. On the classical level it may be traced back to the observation that $H(P, X) \sim P$, i.e. there are no terms with the zero power of momentum P in the Hamiltonian. Therefore the property of the Hamiltonian

$$H(0, X) = 0 \tag{4.24}$$

is crucial to the conservation of probability. On the other hand, this relation along with expression (4.20) for the action are completely equivalent to the basic Keldysh symmetry $S[X, 0] = 0$, Eq. (2.53) (recall that $P \sim X^{\mathrm{q}}$), the latter follows from the quantum unitarity.

In the case of the additive noise $D(X) = T$ the Fokker–Planck Hamiltonian (4.19) may be transformed into the conventional Schrödinger form. This is achieved by the canonical transformation $x = X$ and $\hat{p} = \hat{P} - V'(X)/(2T)$, which preserves the commutation relation $[x, \hat{p}] = 1$ and thus $\hat{p} = -\partial_x$. With these new variables the Fokker–Planck equation acquires the form of the imaginary-time Schrödinger equation $\partial_t \tilde{\mathcal{P}}(x, t) = \hat{h}(\hat{p}, x)\tilde{\mathcal{P}}(x, t)$, where

$$\hat{h}(\hat{p}, x) = T\hat{p}^2 + W(x)\,; \qquad W(x) = -[V'(x)]^2/(4T) + V''(x)/2, \tag{4.25}$$

while the "wave function" transforms as $\tilde{\mathcal{P}}(x, t) = \mathrm{e}^{V(x)/(2T)}\mathcal{P}(x, t)$. As briefly mentioned below, the effective potential $W(x)$ has some remarkable properties, which originate from the fact that the initial Hamiltonian (4.19) satisfies the normalization identity (4.24).

We turn now to the transfer matrix derivation of the Fokker–Planck equation (4.23). Consider $\mathcal{P}(X_{j-1}, t_{j-1})$, which is obtained from Eq. (4.12) by integration over all X_i with $i = 1, \ldots, j-2$ and all X_i^{q} with $i = 1, \ldots, j-1$. Notice that the X^{q} integration runs one step ahead of the X integration. To find $\mathcal{P} = \mathcal{P}(X, t) = \mathcal{P}(X_j, t_j)$ one needs to perform two more integrations over $\mathrm{d}X_{j-1}\mathrm{d}X_j^{\mathrm{q}}$ with the weight specified by Eq. (4.12):

$$\mathcal{P} = \int \mathrm{d}X_{j-1}\mathrm{d}X_j^{\mathrm{q}}\, \mathrm{e}^{-2\mathrm{i}\,X_j^{\mathrm{q}}\left(X_j - X_{j-1} - \delta_t A(X_{j-1})\right) - 4\delta_t (X_j^{\mathrm{q}})^2 D(X_{j-1})} \mathcal{P}(X_{j-1}, t_{j-1}). \tag{4.26}$$

We now rename the integration variables as $X_j^{\mathrm{q}} = X^{\mathrm{q}}$ and $X_{j-1} = X_j - \delta_X$ and expand the exponent to second order in the small fluctuations δ_X and X^{q}. This leads to the already familiar Keldysh structure

$$\exp\left\{-\begin{pmatrix}\delta_X, X^{\mathrm{q}}\end{pmatrix}\begin{pmatrix}0 & \mathrm{i}\\ \mathrm{i} & 4\delta_t D\end{pmatrix}\begin{pmatrix}\delta_X\\ X^{\mathrm{q}}\end{pmatrix}\right\}. \tag{4.27}$$

From here one concludes that as $\delta_t \to 0$ the fluctuations scale as $X^{\mathrm{q}} \sim \delta_t^{-1/2}$ and $\delta_X \sim \delta_t^{1/2}$. We then approximate $A(X_{j-1}) \approx A - \delta_X A'$, while $D(X_{j-1}) \approx D - \delta_X D' + \delta_X^2 D''/2$ and $\mathcal{P}(X_{j-1}, t_{j-1}) \approx \mathcal{P} - \delta_X \mathcal{P}' + \delta_X^2 \mathcal{P}''/2 - \partial_t \mathcal{P}\delta_t$, where $A = A(X_j)$, $D = D(X_j)$ and $\mathcal{P} = \mathcal{P}(X_j, t_j)$ and primes denote derivatives with respect to X_j. Expanding the exponent up to second order in terms $\delta_X \sim \delta_t^{1/2}$ and up to first order in terms $\delta_X^2 \sim \delta_t$, we find

$$\partial_t \mathcal{P} = -(A'\mathcal{P} + A\mathcal{P}')2\mathrm{i}\langle\delta_X X^{\mathrm{q}}\rangle - (D''\mathcal{P} + 2D'\mathcal{P}')2\langle\delta_X^2 (X^{\mathrm{q}})^2\rangle + \mathcal{P}''\frac{\langle\delta_X^2\rangle}{2\delta_t},$$

where the angular brackets stand for averaging with the Gaussian weight (4.27) and we took into account that, as always, $\langle(X^{\mathrm{q}})^2\rangle = 0$ and also $\langle\delta_X (X^{\mathrm{q}})^3\rangle = \langle\delta_X^2 (X^{\mathrm{q}})^4\rangle = 0$. The remaining non-zero averages are given by $\langle\delta_X X^{\mathrm{q}}\rangle = -\mathrm{i}/2$, $\langle\delta_X^2 (X^{\mathrm{q}})^2\rangle = -1/2$ and $\langle\delta_X^2\rangle = 2\delta_t D$. As a result one obtains the Fokker–Planck equation (4.23), as expected.

The derivation may be straightforwardly extended to the multivariable Ito–Langevin process (4.14), yielding

$$\partial_t \mathcal{P}(X,t) = -\partial_\alpha\Big[A_\alpha(X)\mathcal{P}(X,t) - \partial_\beta\big[D_{\alpha\beta}(X)\mathcal{P}(X,t)\big]\Big], \tag{4.28}$$

where $\partial_\alpha = \partial_{X_\alpha}$ and summation over repeated indices is understood. Again the equation has the structure of the continuity relation $\partial_t \mathcal{P} + \mathrm{div} J = 0$, where the probability current vector $J_\alpha = A_\alpha \mathcal{P} - \partial_\beta[D_{\alpha\beta}(X)\mathcal{P}]$ consists of the drift part and the diffusive part.

For a particular case where the drift is provided by a potential force, i.e. $A_\alpha(X) = -\partial_\alpha V(X)$ and the noise is isotropic and additive, i.e. $D_{\alpha\beta} = \delta_{\alpha\beta} T$, one may look for a stationary solution of Eq. (4.28) by demanding that the current vector is zero: $\partial_\alpha V\mathcal{P} = -T\partial_\alpha \mathcal{P}$. Solving this first order equation, one finds

$$\mathcal{P}(X) = Z^{-1}\,\mathrm{e}^{-V(X)/T}, \tag{4.29}$$

which is a proper stationary probability distribution as long as it can be normalized. This means the normalization constant, also known as the partition function, $Z = \int \prod_\alpha \mathrm{d}X_\alpha\, \mathrm{e}^{-V(X)/T}$ exists.[2] This is, of course, the Boltzmann distribution, which we have already found with exponential accuracy using the optimal path method, see Eq. (4.21). Here we have proved that the pre-exponential factor is an X-independent constant. Notice that if the drift force is not a potential one,

[2] Here Z is not the Keldysh "partition function" normalized to one, but a usual equilibrium statistical mechanics partition function.

the stationary distribution (if it exists) implies, in general, a non-zero divergenceless current, $\mathrm{div} J = 0$, whereas $J_\alpha \neq 0$. The distribution (4.29) is thus not applicable.

The fact that the Fokker–Planck equation has a stationary solution (for the class of normalizable potentials) may be formulated as the presence of a *zero eigenvalue* of the corresponding Hamiltonian operator $\hat{H}(\hat{P}, X)$. Equation (4.29) provides the corresponding eigenfunction, or *zero mode*. In the transformed Schrödinger variables (4.25) the presence of the zero mode follows from the *supersymmetric* nature of the effective potential $W(x)$ [42, 43].

If there is an inertia term $\ddot{X}$ in the Langevin equation (4.5), one needs to consider particle momentum as just another coordinate $X_1 = X$ and $X_2 = \dot{X} = K$. Employing that $A_1(K) = K$, $A_2(X, K) = -\gamma K - V'(X)$ and $D_{22} = \gamma T$ is the only non-zero component of $D_{\alpha\beta}$, one may rewrite Eq. (4.28) for the probability distribution function $\mathcal{P} = \mathcal{P}(X, K, t)$ as

$$\partial_t \mathcal{P} + K\partial_X \mathcal{P} - V'(X)\partial_K \mathcal{P} = \gamma \partial_K \left(K\mathcal{P} + T\partial_K \mathcal{P}\right). \tag{4.30}$$

The left hand side, called the *kinetic* term, may be written as $\partial_t \mathcal{P} - \{E, \mathcal{P}\}$, where the classical Hamiltonian function is $E(K, X) = K^2/2 + V(X)$ and we used standard Poisson brackets. It describes evolution of the distribution function due to the drift of position in the presence of the velocity $K = v_K = \partial_K(K^2/2)$ and the drift of momentum in the presence of the force $-\partial_X V(X)$. The right hand side, also known as the *collision* term, originates from the interaction with the thermal bath. It describes random diffusion in the momentum space superimposed on the drift towards $K = 0$ in the effective "potential" $K^2/2$. The latter is responsible for the particle losing energy and cooling down, if the temperature T is too low.

One may look for a stationary solution of the Fokker–Planck equation (4.30) which separately nullifies the kinetic and the collision terms. From the latter condition one finds that $\mathcal{P}(X, K) = \mathcal{P}(X)\,\mathrm{e}^{-K^2/2T}$. Substituting it into the kinetic term, one finally finds for the corresponding zero mode

$$\mathcal{P}(X, K) = Z^{-1}\,\mathrm{e}^{-V(X)/T}\,\mathrm{e}^{-K^2/2T} = Z^{-1}\,\mathrm{e}^{-E(K,X)/T}, \tag{4.31}$$

where the normalization constant Z, i.e. the partition function, is given by $Z = \int \mathrm{d}X\mathrm{d}K\,\mathrm{e}^{-V(X)/T}\,\mathrm{e}^{-K^2/2T}$. This is the Maxwell–Boltzmann distribution for the particle's potential and kinetic energy in thermal equilibrium.

If the system is out of equilibrium, but all characteristic time scales are much longer than the relaxation time γ^{-1}, one may look for a solution of the Fokker–Planck equation (4.30) in the form

$$\mathcal{P}(X, K, t) = (2\pi T)^{-1/2}\,\mathrm{e}^{-K^2/2T}\left[\mathcal{P}(X, t) + K\mathcal{N}(X, t)\right],$$

where the exponential factor is chosen to nullify the right hand side of Eq. (4.30) and thus to compensate for the large factor γ. We now substitute this trial solution in Eq. (4.30) and (i) integrate over K; (ii) multiply by K and then integrate over K. This way we obtain two coupled equations

$$\partial_t \mathcal{P} + T\,\partial_X \mathcal{N} = 0\,; \qquad T\,\partial_X \mathcal{P} + V'(X)\,\mathcal{P} = -\gamma T \mathcal{N},$$

where in the second equation we neglected the term $T\,\partial_t \mathcal{N}$ as being much smaller than its right hand side. Substituting $\mathcal{N}$ from the second equation into the first one, one finds a closed equation for $\mathcal{P}(X, t)$:

$$\gamma\,\partial_t \mathcal{P} = \partial_X \left[V'(X)\,\mathcal{P} + T\,\partial_X \mathcal{P} \right]. \tag{4.32}$$

This is, of course, the already familiar overdamped Fokker–Planck equation (4.23). The fact that the diffusion coefficient in the coordinate space is $D = T/\gamma$ is known as the *Einstein relation*. Notice that the diffusion coefficient in momentum space, according to Eq. (4.30), is $D_K = \gamma T$. Both of these facts are manifestations of FDT.

Since we are dealing with a classical particle, there is no problem in exactly specifying its coordinate X and momentum K simultaneously. This should be contrasted with the fictitious momentum $P = 2\mathrm{i}X^{\mathrm{q}}$, introduced in Section 4.4. The latter is conjugated to the coordinate X in the sense of the functional integral. It obeys thus the uncertainty principle $\Delta X \Delta P \geq 1$ even in a purely classical setting. One may still discuss trajectories in the phase space (P, X) in the semiclassical (i.e. weak fluctuations, or low temperature) approximation. If the inertia and thus the physical momentum K are taken into account, the semiclassical phase space is four-dimensional: (P, P_2, X, K), where P_2 is conjugate to $K = X_2$.

4.6 Ito vs. Stratonovich

Although Ito regularization of stochastic processes, discussed in Section 4.3, is the most convenient for the field-theoretical representation, one must be aware that there are other regularizations. The one frequently found in physics literature is known as Stratonovich regularization. It appears upon changing variables in stochastic evolution equations. Consider, for example, the Langevin equation (4.7), (4.8) with the additive noise, i.e. $b = 1$. The corresponding Fokker–Planck equation for the probability distribution function $\mathcal{P}(X, t)$ is given by Eq. (4.23) with $D = b^2 = 1$,

$$\dot{X} = A(X) + \xi(t)\,; \qquad \partial_t \mathcal{P} = -\partial_X \big[A\mathcal{P} - \partial_X \mathcal{P} \big]. \tag{4.33}$$

Suppose now we want to change the coordinate $X(t)$ to another coordinate $Y(t)$, such that

$$X = f(Y), \tag{4.34}$$

where f is a monotonic function which provides a one-to-one correspondence between X and Y. We shall assume thus that $f'(Y) = \mathrm{d}X/\mathrm{d}Y > 0$, for convenience. Substituting it in the Langevin equation (4.33), one notices that the corresponding stochastic equation for the new variable $Y(t)$ formally acquires the multiplicative form

$$\dot{Y} = \tilde{A}(Y) + \tilde{b}(Y)\,\xi(t), \tag{4.35}$$

where $\tilde{b}(Y) = 1/f'(Y)$ and $\tilde{A}(Y) = A(f(Y))/f'(Y)$.

Naively one may think that the corresponding Fokker–Planck equation is given by Eq. (4.23) with $D(Y) = \tilde{b}^2(Y) = [1/f'(Y)]^2$. Let us, however, perform the change of variables (4.34) directly in the Fokker–Planck equation (4.33). To maintain normalization of the probability distribution function one has to demand that $\tilde{\mathcal{P}}(Y,t)\,\mathrm{d}Y = \mathcal{P}(X,t)\,\mathrm{d}X$ and thus the proper distribution of the Y variable is $\tilde{\mathcal{P}}(Y,t) = \mathcal{P}(f(Y),t)\,f'(Y)$. Notice also that $\partial_X = (1/f'(Y))\,\partial_Y$. As a result the Fokker–Planck equation (4.33) transforms into

$$\partial_t \tilde{\mathcal{P}}(Y,t) = -\partial_Y\Big[\tilde{A}(Y)\,\tilde{\mathcal{P}}(Y,t) - \tilde{b}(Y)\,\partial_Y\big[\tilde{b}(Y)\tilde{\mathcal{P}}(Y,t)\big]\Big]. \tag{4.36}$$

As before $\tilde{b}(Y) = 1/f'(Y)$. While the drift current is what we expect from the Langevin equation (4.35), the diffusive current is different from that in the Ito–Fokker–Planck equation (4.23). The latter has the form $\partial_Y[\tilde{b}^2\tilde{\mathcal{P}}]$.

The reason for this difference is that the multiplicative noise in Eq. (4.35) does *not* have the Ito retarded regularization. Indeed, the discrete form of the Langevin equation (4.33) is $X_j - X_{j-1} = \delta_t A(X_{j-1}) + \delta_t \xi_{j-1}$. Upon the change of variables given by Eq. (4.34) the left hand side takes the form $f(Y_j) - f(Y_{j-1}) = f(\bar{Y} + \delta_Y/2) - f(\bar{Y} - \delta_Y/2) = f'(\bar{Y})(Y_j - Y_{j-1}) + O(\delta_Y^3)$, where $\delta_Y = Y_j - Y_{j-1}$ and $\bar{Y} = (Y_j + Y_{j-1})/2$. As a result the discrete version of the Langevin equation (4.35) is

$$Y_j - Y_{j-1} = \delta_t \tilde{b}\left(\frac{Y_j + Y_{j-1}}{2}\right) A(Y_{j-1}) + \delta_t \tilde{b}\left(\frac{Y_j + Y_{j-1}}{2}\right)\xi_{j-1}. \tag{4.37}$$

The first term on the right hand side is already $\sim \delta_t$ and therefore may be substituted by $\delta_t \tilde{A}_{j-1} = \delta_t \tilde{b}(Y_{j-1})A(Y_{j-1})$. This is not so with the second term: since $\xi_j \sim \delta_t^{-1/2}$ (indeed the corresponding statistical weight is $\mathrm{e}^{-\delta_t \xi_j^2/4}$), one finds $\delta_t \xi_{j-1} \sim \delta_t^{1/2}$. Therefore it is important to keep the argument of the noise

modulation function as $\tilde{b}\big((Y_j + Y_{j-1})/2\big)$. This is different from the Ito retarded regularization, which assumes $\tilde{b}(Y_{j-1})$ instead. The symmetric regularization of the multiplicative noise as in Eq. (4.37) is known as Stratonovich regularization. It leads to the different form of the diffusion term in the Fokker–Planck equation (4.36).

One may formally bring the Stratonovich diffusion term to the Ito form, by the expense of adding $(\partial_Y \tilde{b})\,\tilde{b}\,\tilde{\mathcal{P}}$ to the drift term. All the considerations may be straightforwardly generalized to an arbitrary dimension M. As a result the Stratonovich–Langevin equation $\dot{X} = A^{(\mathrm{S})} + b\xi$ is equivalent to the Ito–Langevin one $\dot{X} = A^{(\mathrm{I})} + b\xi$ with

$$A_\alpha^{(\mathrm{I})}(X) = A_\alpha^{(\mathrm{S})}(X) + \sum_{\beta,\gamma=1}^{M} \big[\partial_\beta b_{\alpha\gamma}(X)\big]\, b_{\beta\gamma}(X). \tag{4.38}$$

The Ito process may be then used for the field-theoretical treatment via the MSR procedure of Section 4.3.

4.7 Noise with a finite correlation time

Another context where the Stratonovich interpretation appears naturally is stochastic systems with noise which has a short, but finite correlation time τ. Consider Gaussian "colored" noise with the correlation function

$$\langle \eta(t)\eta(t')\rangle = \frac{1}{\tau}\, \mathrm{e}^{-|t-t'|/\tau}, \tag{4.39}$$

known also as the Ornstein–Uhlenbeck process. The white noise (4.8) is obtained in the limit $\tau \to 0$. Such a random function is a result of "filtering" of the white noise force $\xi(t)$, Eq. (4.8), with an overdamped harmonic oscillator (e.g. an RC circuit), having the time constant τ. This means that $\eta(t)$ satisfies

$$\dot{\eta} = \frac{1}{\tau}\big[-\eta + \xi(t)\big]. \tag{4.40}$$

Indeed, the solution of this equation is $\eta(t) = \frac{1}{\tau}\int^t \mathrm{d}t_1\, \xi(t_1)\, \mathrm{e}^{(t_1-t)/\tau}$. Employing Eq. (4.8) one readily establishes the correlation function (4.39).

One may consider the Ornstein–Uhlenbeck process (4.39), (4.40) as a random force term in a multiplicative Langevin equation

$$\dot{X} = A(X) + b(X)\,\eta(t). \tag{4.41}$$

Then in the limit $\tau \ll \Omega^{-1}$ (but still $\tau \gg \delta_t$), where Ω is a characteristic frequency of the deterministic process $\dot{X} = A(X)$, the probability distribution function $\mathcal{P}(X,t)$ obeys the Stratonovich–Fokker–Planck equation (4.36).

To prove this statement let us consider the two evolutionary equations (4.41) and (4.40) as a two-dimensional Langevin process (4.14). In this case $A_X = A(X) + b(X)\,\eta$ and $A_\eta = -\eta/\tau$, while the noise $\xi(t)$ is non-multiplicative with the coupling constant $b_{\eta,1} = 1/\tau$. Because the noise is non-multiplicative, there is no need to specify the regularization. The Fokker–Planck equation for the joint probability distribution $\mathcal{P}(X, \eta, t)$ acquires the form, cf. Eq. (4.28),

$$\partial_t \mathcal{P} = -\partial_X\big[(A(X) + b(X)\,\eta)\mathcal{P}\big] + \partial_\eta\left[\frac{1}{\tau}\,\eta\mathcal{P} + \frac{1}{\tau^2}\,\partial_\eta\mathcal{P}\right]. \tag{4.42}$$

In the absence of coupling, $b = 0$, the η-variable quickly equilibrates to a symmetric Gaussian distribution $\sim \mathrm{e}^{-\eta^2\tau/2}$. One can thus proceed in a way analogous to the one that led from Eq. (4.30) to Eq. (4.32). To this end we look for a solution in the form $\mathcal{P}(X, \eta, t) \sim \mathrm{e}^{-\eta^2\tau/2}\big[\mathcal{P}(X, t) + \eta\mathcal{N}(X, t)\big]$. Substituting it into Eq. (4.42) and then (i) integrating over η and (ii) multiplying by η and then integrating over it, one obtains two equations $\partial_t\mathcal{P} = -\partial_X[A\mathcal{P}] - \partial_X[b\,\mathcal{N}]/\tau$ along with $\mathcal{N}/\tau = -\partial_X[b\mathcal{P}]$, where in the last equation we have neglected $\partial_t\mathcal{N}$ and $\partial_x[A\mathcal{N}]$, as being much less than $\mathcal{N}/\tau$. Substituting the resulting $\mathcal{N}$ into the equation for $\mathcal{P}$, one finds the Stratonovich–Fokker–Planck equation (4.36).

4.8 Kramers problem

We return now to the problem of activation escape of an overdamped particle from a meta-stable potential minimum. It was briefly considered in Section 4.4 in the stationary path approximation. Here we address it employing the Ito–Fokker–Planck equation (4.23). To modify the result for the Stratonovich stochastic process, one can take advantage of the correspondence rule (4.38). The potential $V(X)$ is similar to the one plotted in Fig. 3.3a. Since the Boltzmann distribution (4.29) with such a potential is not normalizable, there is no stationary solution (i.e. zero mode) of the Fokker–Planck equation. One expects, however, that there is a long-lived solution localized in the vicinity of the meta-stable minimum. We shall look for such a solution in the form

$$\mathcal{P}(X, t) = \mathcal{P}(X)\,\mathrm{e}^{-t/\tau_{\mathrm{es}}}, \tag{4.43}$$

where τ_{es} is the escape time, which is expected to be exponentially long. The total probability is not conserved, because there is a probability current J towards $X = \infty$. Substituting this form into Eq. (4.23), one obtains the stationary Fokker–Planck equation for $\mathcal{P}(X)$:

$$\frac{1}{\tau_{\mathrm{es}}}\,\mathcal{P} = \partial_X\big[-V'\mathcal{P} - \partial_X[D\mathcal{P}]\big] = \partial_X J. \tag{4.44}$$

Since the escape rate $1/\tau_{\rm es}$ is expected to be exponentially small, so is $\partial_X J$ everywhere, except near the narrow peak of the meta-stable distribution $\mathcal{P}(X)$ around $X = 0$. As we show below, the latter has the characteristic width $l_0 = \sqrt{D(0)/V''(0)} \ll X_{\rm s}$, if $D(0)$ is small enough (see Fig. 4.1(b)). Therefore the current J out of the meta-stable state is practically a constant for $|X| \gg l_0$. Obviously the current is zero in the negative direction: $J(-\infty) = 0$, while at large positive X it approaches a constant value, which we denote $J(\infty)$. This observation leads to the linear first order differential equation

$$-V'(X)\,\mathcal{P}(X) - \partial_X[D(X)\mathcal{P}(X)] = J(X), \tag{4.45}$$

which may be easily solved to express $\mathcal{P}$ through $J(X)$. The result is

$$\mathcal{P}(X) = \frac{1}{D(X)}\,\mathrm{e}^{-S(X)} \int_X^\infty \mathrm{d}Y\;\; J(Y)\,\mathrm{e}^{\,S(Y)}, \tag{4.46}$$

where S satisfies $S' = V'/D$, i.e.

$$S(X) = \int_{-\infty}^{X} \mathrm{d}Y\,\frac{V'(Y)}{D(Y)}. \tag{4.47}$$

The upper limit of the Y-integration in Eq. (4.46) is basically arbitrary (with exponential accuracy) as long as it is well to the right of the point $Y = X_{\rm s}$. We put it infinite for brevity. One can now integrate the stationary Fokker–Planck equation (4.44) from minus infinity, where the current is zero, to plus infinity (in the same sense as above), where the current is $J(\infty)$. This leads to

$$\tau_{\rm es} = \frac{1}{J(\infty)} \int_{-\infty}^{\infty} \mathrm{d}X\,\mathcal{P}(X) = \int_{-\infty}^{\infty} \frac{\mathrm{d}X}{D(X)}\,\mathrm{e}^{-S(X)} \int_X^\infty \mathrm{d}Y\;\frac{J(Y)}{J(\infty)}\,\mathrm{e}^{\,S(Y)}. \tag{4.48}$$

Notice that adding a constant to S does not change the result. This means that the lower limit of integration in Eq. (4.47) is of no importance.

The X-integral is dominated by the vicinity of the potential minimum, i.e. $|X| \lesssim l_0$. On the other hand, the Y-integral is coming from the vicinity of the maximum i.e. $|X - X_{\rm s}| \lesssim l_{\rm s}$, where the characteristic width of the maximum is $l_{\rm s} = \sqrt{D(X_{\rm s})/|V''(X_{\rm s})|}$. If $l_0 + l_{\rm s} \ll X_{\rm s}$, which is the case for sufficiently small D, one may extend the Y-integral to minus infinity and perform both integrals in the stationary point approximation. The crucial observation is that under the same condition $J(X_{\rm s})/J(\infty) = 1$ with exponential accuracy. As a result one obtains for the escape time, including the pre-exponential factor [44],

$$\tau_{\rm es} = \frac{2\pi}{D(0)}\,\frac{\mathrm{e}^{\,\Delta S}}{\sqrt{S''(0)|S''(X_{\rm s})|}} = \sqrt{\frac{D(X_{\rm s})}{D(0)}}\,\frac{2\pi}{\sqrt{V''(0)|V''(X_{\rm s})|}}\,\mathrm{e}^{\,\Delta S}, \tag{4.49}$$

where we took into account that $S'' = (V'/D)' = V''/D$, since $V'(0) = V'(X_s) = 0$, and

$$\Delta S = S(X_s) - S(0) = \int_0^{X_s} dX \, \frac{V'(X)}{D(X)}. \tag{4.50}$$

This is exactly the action along the zero energy trajectory $P = V'/D$ of the Hamiltonian (4.19), introduced in Section 4.4. The Fokker–Planck equation allowed us to determine the pre-exponential factor. In the case of non-multiplicative noise $D = T = \text{const}$, the exponent is the Boltzmann one, $(V(X_s) - V(0))/T$, while the prefactor is temperature independent, $2\pi[V''(0)|V''(X_s)|]^{-1/2}$. This is the celebrated Kramers result [45]. In the case where the inertia term may not be neglected, the pre-exponential factor was evaluated in [46].

In a vicinity of the bifurcation point, a wide class of problems may be modeled by the cubic potential (3.34) and the additive noise with variance D. According to the Kramers formula the corresponding escape time is

$$\tau_{es} = \frac{\pi a^2}{V_0 \delta} \, e^{\frac{4}{27} \frac{V_0 \delta^3}{D}}. \tag{4.51}$$

The scaling of the action with the bifurcation parameter δ is rather different from both the pure tunneling exponent (3.36) and the dissipative tunneling exponent (3.40).

4.9 Fluctuation relation

Consider an overdamped Langevin dynamics in a time-dependent potential

$$\dot{X} = -\partial_X V(X, t) + \sqrt{T}\, \xi(t), \tag{4.52}$$

where the white noise is normalized according to Eq. (4.8). The time dependence of the potential is limited to a time window $t_i < t < t_f$. Moreover, we shall assume that initially at $t = t_i$ the system is in equilibrium with a bath maintained at temperature T. During the time interval $[t_i, t_f]$ the potential is changing by the action of an external device. Such a device (e.g. a piston) is performing a work W on the system, which may be written as

$$W[X] = \int_{t_i}^{t_f} dt \, \partial_t V(X(t), t). \tag{4.53}$$

The work is a functional of the stochastic trajectory $X(t)$, which the system follows upon a given realization of the random noise $\xi(t)$. As a result, the work W is itself a random quantity, dependent on the noise. One may ask about statistics of the work, for example the work distribution function $\mathcal{P}(W)$. This question probably can't be

answered for an arbitrary potential. There is, however, a particular function of the work, $\mathrm{e}^{-W/T}$, whose average value may be found in a very general form [47, 48].

Employing the MSR method of Section 4.3, one finds for the corresponding average value, cf. Eq. (4.12),

$$\begin{aligned}\left\langle \mathrm{e}^{-W/T}\right\rangle &= \int \mathbf{D}[X,\, X^{\mathrm{q}}]\; \mathrm{e}^{\int \mathrm{d}t\, \left[-2\mathrm{i}\, X^{\mathrm{q}}\left(\dot{X}+\partial_X V(X,t)\right)-4T(X^{\mathrm{q}})^2\right]}\; \mathrm{e}^{-W[X]/T} \\ &= \int \mathbf{D}[X,\, X^{\mathrm{q}}]\; \mathrm{e}^{\int \mathrm{d}t\, \left[-2\mathrm{i}\, X^{\mathrm{q}}\left(\dot{X}+\partial_X V(X,t)\right)-4T(X^{\mathrm{q}})^2-\frac{1}{T}\,\partial_t V(X,t)\right]}. \end{aligned} \tag{4.54}$$

Let us first analyze this expression within the stationary path approximation. Following the procedure of Section 4.4, it is convenient to rename the auxiliary variable as $X^{\mathrm{q}} = P/(2\mathrm{i})$. The action acquires the Hamiltonian form (4.20), where

$$H(P,\, X,\, t) = -P\,\partial_X V(X,\, t) + T\,P^2 - \frac{1}{T}\,\partial_t V(X,\, t). \tag{4.55}$$

Notice that this Hamiltonian does not satisfy the probability conservation condition (4.24), because it includes the specific observable $-W/T$. Since the Hamiltonian is explicitly time dependent, the energy is not conserved and solution of the stationary path equations

$$\dot{X} = \frac{\partial H}{\partial P} = -\partial_X V + 2T\,P\,, \qquad \dot{P} = -\frac{\partial H}{\partial X} = P\,\partial_X^2 V + \frac{1}{T}\,\partial_X \partial_t V \tag{4.56}$$

is not immediately obvious. Remarkably, the activation trajectory of the time-independent problem, i.e. the time-reversed path of the noiseless relaxation $\dot{X} = +\,\partial_X V$ and $P = \partial_X V/T$ still solves the equations of motion. This fact may be checked by direct substitution of this solution into the equations (4.56).[3] Notice that to have such a solution it is crucial to average $\mathrm{e}^{-\eta W}$ with $\eta = 1/T$. It would not work for any other η. The action along this trajectory is given by

[3] This solution may be traced back to the existence of the canonical transformation $(P,\, X,\, H) \to (p,\, x,\, h)$, with the generating function [34] $\Phi = \Phi(x,\, P,\, t) = -xP + V(x,\, t)/T$. Then the following relations hold:

$$X = -\frac{\partial \Phi}{\partial P} = x\,, \qquad p = -\frac{\partial \Phi}{\partial x} = P - \frac{1}{T}\,\partial_x V(x,\, t).$$

The transformed Hamiltonian is

$$\begin{aligned} h = H + \frac{\partial \Phi}{\partial t} &= -\left(p + \frac{1}{T}\,\partial_x V(x,\, t)\right)\partial_x V(x,\, t) + T\left(p + \frac{1}{T}\,\partial_x V(x,\, t)\right)^2 \\ &-\frac{1}{T}\,\partial_t V(x,\, t) + \frac{1}{T}\,\partial_t V(X,\, t) = p\,\partial_x V(x,\, t) + Tp^2. \end{aligned}$$

It is conserved (despite being time dependent), $h = 0$, along the following obvious solution of the equations of motion: $p = 0$, while $\dot{x} = \partial_x V$. Being transformed back to the original variables, it yields the required solution.

$$\mathrm{i}S = -\int \mathrm{d}t\,[P\dot{X} - H] = -\frac{1}{T}\int \mathrm{d}t\,[\partial_X V\dot{X} + \partial_t V] = -\frac{1}{T}\int \mathrm{d}V = \frac{V_\mathrm{i} - V_\mathrm{f}}{T},$$

where $V_{\mathrm{i/f}} = V(X_{\mathrm{i/f}}, t_{\mathrm{i/f}})$ and $\mathrm{e}^{\mathrm{i}S}$ gives the relative weight of a particle moving from X_i to X_f under the action of the time-dependent potential. Since at $t = t_\mathrm{i}$ the system is assumed to be in thermal equilibrium, the initial coordinate is to be weighted with the Boltzmann distribution $\mathrm{e}^{-V_\mathrm{i}/T}/Z(t_\mathrm{i})$. On the other hand, there is no control over the final coordinate X_f and therefore it should be integrated over with the plane measure, resulting in $Z(t_\mathrm{f})$. One thus obtains

$$\left\langle \mathrm{e}^{-W/T}\right\rangle = \frac{\mathrm{e}^{-V_\mathrm{i}/T}}{Z(t_\mathrm{i})}\int \mathrm{d}X_\mathrm{f}\,\mathrm{e}^{(V_\mathrm{i}-V_\mathrm{f})/T} = \frac{Z(t_\mathrm{f})}{Z(t_\mathrm{i})} = \mathrm{e}^{-(F(t_\mathrm{f})-F(t_\mathrm{i}))/T}, \tag{4.57}$$

where $Z(t_{\mathrm{i/f}}) = \int \mathrm{d}X\mathrm{e}^{-V(X,t_{\mathrm{i/f}})/T} \equiv \mathrm{e}^{-F(t_{\mathrm{i/f}})/T}$ are the *equilibrium* partition functions in the potentials $V(X, t_\mathrm{i})$ and $V(X, t_\mathrm{f})$, respectively. Therefore this particular average value of the non-equilibrium work may be expressed through the equilibrium free energies of the system allowed to equilibrate in the initial and final potential configurations. This remarkable statement is known as the Jarzynski fluctuation relation [47, 48]. As a matter of principle, it allows one to measure the equilibrium free energy of the final state, without waiting for the system to equilibrate. To this end one has to accumulate statistics of the work performed to bring the system into final (yet non-equilibrium) states, and average $\mathrm{e}^{-W/T}$.

So far we have derived the fluctuation relation in the stationary path approximation. Let us show now that Eq. (4.57) is actually exact, i.e. there is no pre-exponential factor on its right hand side. To this end we need to derive the Fokker–Planck equation corresponding to the functional integral (4.54) [49]. As explained in Section 4.5 the "quantization" procedure is $\partial_t \mathcal{P}(X, t) = \hat{H}\mathcal{P}(X, t)$, where $\hat{H}$ is obtained from Eq. (4.55) by the substitution $P \to -\partial_X$:

$$\partial_t \mathcal{P} = \partial_X[\partial_X V\,\mathcal{P}] + T\partial_X^2\mathcal{P} - \frac{1}{T}\,\partial_t V\,\mathcal{P}. \tag{4.58}$$

The initial condition is $\mathcal{P}(X, t_\mathrm{i}) = \mathrm{e}^{-V(X,t_\mathrm{i})/T}/Z(t_\mathrm{i})$. Motivated by the stationary path result, we look for the solution of this equation in the following form: $\mathcal{P}(X, t) = \mathrm{e}^{-V(X,t)/T}/Z(t_\mathrm{i})$. It is easy to check that it is indeed the solution, satisfying the initial condition. Notice that having the coefficient $1/T$ in the last term (the observable) is vital to find such a simple solution. By construction of the functional integral (4.54), $\left\langle \mathrm{e}^{-W/T}\right\rangle = \int \mathrm{d}X\mathcal{P}(X, t_\mathrm{f})$, leading directly to Eq. (4.57). This proves that the fluctuation relation (4.57) is not restricted to the stationary path approximation, but is actually exact.

4.10 Reaction models

Another important class of classical stochastic models is provided by reaction systems. These models are formulated in terms of reaction rules which are followed by certain agents. The latter are typically denoted as A, B, etc. and can be atoms, molecules, viruses, organisms, etc. An example of such a reaction rule is $A + A \xrightarrow{\lambda} B$, which states that two agents A may coagulate to form an agent B. A probability for this to happen per unit time (in other words, a reaction rate) is denoted as λ. One would like to have a description which would be able to predict an outcome of many such reactions, provided some initial conditions are specified. It is clear that such a description has to be probabilistic, since there is no way to say with absolute certainty how many and what reactions will happen in a long time span. The other important thing to remember is that the number of agents at any time is always an integer. Therefore a state of the system may be characterized by a time-dependent probability $\mathcal{P}(n, m, \ldots, t)$ of finding n agents A, m agents B, etc. at time t, where $n, m, \ldots$ are integers. Such a probability is normalized as

$$\sum_{n,m,\ldots} \mathcal{P}(n, m, \ldots, t) = 1. \tag{4.59}$$

For any given set of reaction rules one may formulate an evolution equation, also known as a *Master* equation, for probabilities $\mathcal{P}(n, m, \ldots, t)$. For example, for a single species reaction model, the Master equation is

$$\partial_t \mathcal{P}(n, t) = \sum_{n'} \left[W_{n' \to n} \mathcal{P}(n', t) - W_{n \to n'} \mathcal{P}(n, t) \right], \tag{4.60}$$

where $W_{n \to n'}$ is the rate of going from a state with n agents to a state with n' ones. The first term on the right hand side is the rate of *in* processes, i.e. those which lead into the state n from any other state, while the second term is the rate of *out* processes, i.e. those which lead out of the state n into any other state. If, for example, the reaction rules are $A + A \xrightarrow{\lambda} \emptyset$, $A \xrightarrow{\mu} \emptyset$ and $A \xrightarrow{\sigma} 2A$, the corresponding rates are

$$W_{n \to n'} = \lambda \, \delta_{n', n-2} \, n(n-1)/2 + \mu \, \delta_{n', n-1} \, n + \sigma \, \delta_{n', n+1} \, n, \tag{4.61}$$

where $n(n-1)/2$ is the number of pairs which can enter the coagulation reaction, and n is the number of agents amenable to annihilation or branching.

Reaction models may have a stationary state, that is a time-independent solution of the Master equation $\mathcal{P}(n)$. If, in such a stationary state, every term on the right hand side of Eq. (4.60) (i.e. for any integer n') is zero: $W_{n' \to n} \mathcal{P}(n') = W_{n \to n'} \mathcal{P}(n)$, it is said that the reaction scheme satisfies the *detailed balance condition*. If there are no reactions creating agents out of the empty state $\emptyset$, in many cases the only

stationary solution is the complete *extinction* $\mathcal{P}(n) = \delta_{n,0}$. In this case the detailed balance condition is clearly absent.

The Master equation (4.60) may be written as a differential equation. To this end let us formally extend the integer variable n onto the entire real axis. The "in" term of the Master equation includes the shift operation of the function $W_{n\to n+r}\mathcal{P}(n,t)$, where r is an integer, on r units to bring it to the form $W_{n-r\to n}\mathcal{P}(n-r,t)$. Such a shift operation may be written as $\mathrm{e}^{-r\partial_n}$.[4] As a result the Master equation (4.60) acquires the form

$$\partial_t \mathcal{P}(n,t) = \sum_r \left[\mathrm{e}^{-r\partial_n} - 1\right] W_{n\to n+r}\mathcal{P}(n,t). \tag{4.62}$$

It may be thus written as $\partial_t \mathcal{P} = \hat{H}(\hat{p}, n)\,\mathcal{P}$, where the "momentum" operator stands for $\hat{p} = -\partial_n$ and the reaction Hamiltonian is given by [50]

$$H(p,n) = \sum_r \left[\mathrm{e}^{rp} - 1\right] W_{n\to n+r}. \tag{4.63}$$

The reaction Hamiltonian is normally ordered, meaning that all $\hat{p}$ operators stay on the left of the n-dependent functions. It also satisfies the identity (4.24), $H(0,n) = 0$, which is necessary to maintain the conservation of probability (4.59). This way of writing the Master equation brings it into the same category as the Ito–Fokker–Planck equation. The only difference is that the latter has only terms of the first and second power of the $\hat{p}$-operator. For some problems one may expand the exponent in Eq. (4.63) up to second power in rp, reducing the Master equation to the Fokker–Planck equation (4.23). In this case the drift term is $A(n) = \sum_r r W_{n\to n+r}$ while the diffusion coefficient $D(n) = \sum_r r^2 W_{n\to n+r}/2$. Other problems do not allow for such an expansion, nevertheless all the tools developed for the treatment of the Ito–Fokker–Planck dynamics may be directly transferred to the reaction models.

In particular, solution of the Master equation may be formally written through the evolution operator acting on an initial distribution function $\mathcal{P}(n,t) = \int \mathrm{d}n_\mathrm{i}\,\hat{\mathcal{U}}(n,t;n_\mathrm{i},t_\mathrm{i})\,\mathcal{P}(n_\mathrm{i},t_\mathrm{i})$. The evolution operator $\hat{\mathcal{U}}$ may be represented by the Hamiltonian path integral, see Eq. (4.12),

$$\hat{\mathcal{U}}(n,t;n_\mathrm{i},t_\mathrm{i}) = \int \mathbf{D}[n,p]\,\mathrm{e}^{-\int \mathrm{d}t[p\dot{n} - H(p,n)]}, \tag{4.64}$$

where, as explained at the end of Section 4.4, the $\mathbf{D}[p]$ integration runs along the imaginary axis. The trajectories satisfy $n(t_\mathrm{i}) = n_\mathrm{i}$ and $n(t) = n$. We shall first analyze this expression in the stationary path approximation. The corresponding

[4] Indeed, $\mathrm{e}^{-r\partial_n} f(n) = f(n) - rf'(n) + r^2 f''(n)/2 - \cdots = f(n-r)$.

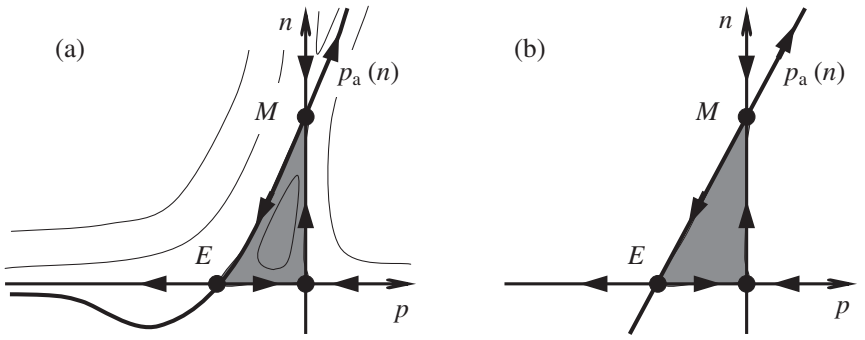

Fig. 4.3 Phase portraits of the reaction Hamiltonians: (a) the one with the reaction rates (4.61); (b) the universal Hamiltonian (4.68) close to the bifurcation point. Bold lines are curves of zero energy, M is the meta-stable point and E the extinction fixed point.

equations of motion are the Hamilton equations $\dot{n} = \partial_p H$ and $\dot{p} = -\partial_n H$. Since they conserve the energy H, one may visualize the solutions by plotting curves of constant energy on the phase plane (p, n), Fig. 4.3(a). As discussed in Section 4.4, the long-time behavior is described by the curves of zero energy $H = 0$. Due to the conservation of probability (4.59) one such line is always $p = 0$. The corresponding stationary path equation is nothing but the *rate* equation

$$\dot{n} = \partial_p H(p, n)\big|_{p=0} = \sum_r r\, W_{n\to n+r} = A(n). \tag{4.65}$$

It provides the mean-field description, which disregards fluctuations and discreteness of the agents. For the reaction scheme of Eq. (4.61) it predicts the stable fixed point at $n = \bar{n} \approx (\sigma - \mu)/\lambda$ and the unstable fixed point at $n = 0$. According to the rate equation (4.65) the population stabilizes at $n \approx \bar{n}$. This is indeed the case at the intermediate time scale (provided $\bar{n} \gg 1$). However, in the long-time limit the only stationary solution of the corresponding Master equation is the extinct state. In the stationary path approximation this fact is reflected in the presence of the $n = 0$ line of constant zero energy, which is thus the invariant line of the Hamiltonian dynamics. This is always the case if $n = 0$ is the *absorbing* state, i.e. $W_{0\to n'} = 0$. As a result all $W_{n\to n'} \sim n$ and therefore $H(p, 0) = 0$.

For a scheme exemplified by Eq. (4.61) one finds, with the help of Eq. (4.63), the following reaction Hamiltonian:

$$H(p, n) = \frac{\lambda}{2}\,(\mathrm{e}^{-2p} - 1)n(n-1) + \mu(\mathrm{e}^{-p} - 1)n + \sigma(\mathrm{e}^{p} - 1)n. \tag{4.66}$$

Its inspection shows that in addition to $p = 0$ and $n = 0$, there is the third curve of zero energy $p = p_a(n)$, which we call the *activation trajectory*, see Fig. 4.3(a).

The activation trajectory intersects the rate equation line $p = 0$ in the meta-stable fixed point $M = (0, \bar{n})$. It also intersects the extinction line $n = 0$ in the extinction fixed point $E = (\bar{p}, 0)$. The large fluctuation, leading to the population extinction, starts at the meta-stable state M and proceeds along the activation trajectory $p_{\rm a}(n)$ until the extinction fixed point E. The rate of such events is $\sim \mathrm{e}^{-S_{\rm ex}}$, where the extinction action is given by (hereafter we absorb the factor $-\mathrm{i}$ into the action, cf. Eq. (4.20))

$$S_{\rm ex} = \int \mathrm{d}t[p\dot{n} - H(p,n)] = \int_{\bar{n}}^{0} p_{\rm a}(n)\,\mathrm{d}n. \tag{4.67}$$

Here we took into account that $H = 0$ along the activation trajectory. The extinction time is thus proportional to the exponentiated area of the shaded triangle in Fig. 4.3(a) [50, 51].

If the two fixed points of the rate equation $n = \bar{n}$ and $n = 0$ are relatively close to each other, the problem may be substantially simplified. For our example (4.61), (4.66) this is the case when $0 < \sigma - \mu \ll \sigma$. One may then disregard the curvature of the activation trajectory between the fixed points M and E and substitute it by a straight line. This leads to the universal reaction Hamiltonian of the form

$$H(p,n) = p\left(\delta - \frac{n}{N} + p\right)n. \tag{4.68}$$

Its three zero-energy lines form the right triangle, Fig. 4.3(b). In terms of our example (4.61) we put $\mu + \sigma = 1$, which fixes units of time, and introduced notations $\delta = (\sigma - \mu)/(\sigma + \mu) \ll 1$ for the so-called bifurcation parameter and $N = (\sigma + \mu)/\lambda \gg 1$ for the effective system size. A large class of models in the vicinity of the bifurcation point may be described by this Hamiltonian. The activation trajectory is given by $p_{\rm a}(n) = n/N - \delta$ and therefore the extinction action (4.67) is $S_{\rm ex} = N\delta^2/2$.

Substituting $p \to -\partial_n$ and keeping the normal ordering in Eq. (4.68), one obtains the universal limit of the Master equation for $\mathcal{P}(n,t)$. Its only true stationary solution is the extinct state $\mathcal{P}(n) = \delta_{n,0}$. There is, however, a long-lived meta-stable solution, which we shall look for in the form $\mathcal{P}(n)\,\mathrm{e}^{-t/\tau_{\rm ex}}$. With the help of the Master equation with the universal Hamiltonian (4.68), one finds $\mathcal{P}/\tau_{\rm ex} = \partial_n\big[(-p_{\rm a}(n) - \partial_n)n\mathcal{P}\big] = \partial_n J$. Since the extinction time $\tau_{\rm ex}$ is expected to be exponentially long, the probability current $J(n)$ is practically a constant away from the narrow peak of the meta-stable distribution around $\bar{n} = N\delta \gg 1$. This constant current is obviously zero for $n \gg \bar{n}$ and is finite, $J(0)$, in the direction of the absorbing boundary at $n = 0$. Integrating the expression for the current, one finds $n\mathcal{P}(n) = -\mathrm{e}^{-S(n)}\int_0^n \mathrm{d}l\, J(l)\,\mathrm{e}^{S(l)}$, where $S(n) = \int^n p_{\rm a}(n)\mathrm{d}n$ and we demanded that $n\mathcal{P} \overset{n\to 0}{\to} 0$. Integrating the equality $\mathcal{P} = \tau_{\rm ex}\partial_n J$ over the entire range of n, one finds

$$\tau_{\rm ex} = -\frac{1}{J(0)}\int_0^\infty {\rm d}n\,\mathcal{P}(n) = \int_0^\infty \frac{{\rm d}n}{n}\,{\rm e}^{-S(n)}\int_0^n {\rm d}l\,\frac{J(l)}{J(0)}\,{\rm e}^{S(l)}. \tag{4.69}$$

The dn integral is dominated by the minimum of the action $S(n)$ i.e. by $n \approx N\delta = \bar{n}$. Under these conditions the dl integral is given by the boundary region $l \approx 0$, where $J(l) \approx J(0)$ with exponential precision. Evaluating the integrals in the stationary/boundary point approximation, one finds

$$\tau_{\rm ex} = \sqrt{\frac{2\pi}{S''(\bar{n})}}\,\frac{1}{\bar{n}}\,\frac{{\rm e}^{S_{\rm ex}}}{|S'(0)|} = \sqrt{\frac{2\pi}{p_{\rm a}'(\bar{n})}}\,\frac{{\rm e}^{S_{\rm ex}}}{\bar{n}|p_{\rm a}(0)|} = \sqrt{\frac{2\pi}{N}}\,\frac{1}{\delta^2}\,{\rm e}^{N\delta^2/2}. \tag{4.70}$$

The result is valid for $N^{-1/2} < \delta \ll 1$. Notice that scaling of the action and the pre-exponential factor with the bifurcation parameter δ is very different from the Kramers activation (4.51). This result, along with pre-exponential factors in more general situations, were found in [52, 53, 54].

4.11 Time-dependent problems

Imagine that the particle's potential or reaction rates are modulated in time. In Sections 3.4 and 3.5 we discussed how such a modulation affects the quantum tunneling. Here we consider its influence on the activation escape time, or the extinction time. In the language of optimal paths these rare events correspond to *instanton* trajectories, which bring the system from e.g. the meta-stable fixed point M to the extinction fixed point E, see Fig. 4.3. In a time-independent setting, such an instanton trajectory may be written $n = n_0(t - t_0)$ and $p = p_0(t - t_0)$, where t_0 is an arbitrary constant which specifies the time of the extinction event. The action does not depend on t_0 and it is therefore said to be a "zero mode". If the Hamiltonian is an explicit function of time, the independence of the action on t_0 is lifted. Indeed, there are more and less preferable instances of undertaking the fluctuation which leads to the extinction. The probabilities of these fluctuations differ exponentially and therefore are largely dominated by the "best chance" t_0, when the extinction is most likely to occur [55].

One can analytically access such an optimal t_0 and the corresponding extinction probability in some limiting cases. The first such case is a *weak* time-dependent modulation of the system's parameters. It leads to a time-dependent reaction (or Fokker–Planck) Hamiltonian

$$H(p, n, t) = H_0(p, n) + \varepsilon H_1(p, n, t), \tag{4.71}$$

where ε is a small parameter. According to the Melnikov theorem of classical mechanics [56, 57], the perturbed Hamiltonian still allows for the optimal

trajectory. This is the case if ε is small enough and another condition, explained below, is satisfied. Such a deformed optimal trajectory may be written as

$$n(t,t_0) = n_0(t-t_0) + \varepsilon n_1(t,t_0)\,, \qquad p(t,t_0) = p_0(t-t_0) + \varepsilon p_1(t,t_0). \quad (4.72)$$

The corresponding action to first order in ε is given by the integral of

$$(p_0+\varepsilon p_1)(\dot n_0+\varepsilon \dot n_1) - H_0 - \partial_n H_0\,\varepsilon n_1 - \partial_p H_0\,\varepsilon p_1 - \varepsilon H_1 = p_0\dot n_0 - \varepsilon H_1,$$

where we employed that $H_0(n_0, p_0) = 0$ along with the equations of motion $\dot n_0 = \partial_p H_0$ and $\dot p_0 = -\partial_n H_0$. We have also disregarded the full time derivative $p_0\dot n_1 + \dot p_0 n_1$. The first term on the right hand side is the unperturbed action $S_{\rm ex}$. Therefore to first order in ε the change of the action (4.20) is

$$S_1(t_0) = -\varepsilon \int \mathrm{d}t\; H_1\big(p_0(t-t_0), n_0(t-t_0), t\big). \quad (4.73)$$

To maximize the extinction (escape) probability $\sim \mathrm{e}^{-(S_{\rm ex}+S_1(t_0))}$, one needs to find minima of $S_1(t_0)$ with respect to the center of the bare instanton t_0. That is, find a t_0 such that $\partial_{t_0} S_1(t_0) = 0$, while the second derivative is positive. This leads to the condition

$$\int \mathrm{d}t\,\big(\partial_p H_1\,\dot p_0 + \partial_n H_1\,\dot n_0\big) = \int \mathrm{d}t\,\big\{H_1, H_0\big\} = 0, \quad (4.74)$$

where $\{\,,\,\}$ denotes classical Poisson brackets [34] and we again employed equations of motion $\dot n_0 = \partial_p H_0$ and $\dot p_0 = -\partial_n H_0$. Existence of simple zeros of this function is the condition of the Melnikov theorem [56, 55, 58].

As an example, consider H_0 given by the universal extinction Hamiltonian (4.68). Its bare instanton trajectory may be easily obtained by putting $p = p_{\rm a}(n) = n/N - \delta$ in the Hamilton equation of motion $\dot n = \partial_p H(p,n)$ and integrating this first order differential equation. The result is

$$n_0(t-t_0) = \frac{N\delta}{1+N\,\mathrm{e}^{\delta(t-t_0)}}\,, \qquad p_0(t-t_0) = -\frac{N\delta\,\mathrm{e}^{\delta(t-t_0)}}{1+N\,\mathrm{e}^{\delta(t-t_0)}}. \quad (4.75)$$

For the time-dependent part we take a weak harmonic modulation of the bifurcation parameter $\delta(t) = \delta(1+\varepsilon\cos\Omega t)$, leading to $H_1(p,n,t) = pn\delta\cos\Omega t$. The resulting correction (4.73) to the action is

$$S_1(t_0) = \varepsilon N^2\delta^3 \int \mathrm{d}t\;\frac{\mathrm{e}^{\delta(t-t_0)}\cos\Omega t}{\big(1+N\,\mathrm{e}^{\delta(t-t_0)}\big)^2} = \frac{\varepsilon\,\pi N\delta\Omega}{\sinh\pi\Omega/\delta}\,\cos\big[\Omega\,(t_0+\delta^{-1}\ln N)\big].$$

Once every period there is the "best chance" t_0, rendering the last cosine to be -1. For such optimal trajectories one finds the negative correction to the extinction action

$$S_1 = -\varepsilon S_{\rm ex}\,\frac{2\pi\Omega/\delta}{\sinh(\pi\Omega/\delta)}, \tag{4.76}$$

where as before $S_{\rm ex} = N\delta^2/2$. The modulation thus leads to the *exponential* reduction of the extinction time (4.69) by the factor $e^{-|S_1|}$. The result is valid as long as $1 < |S_1| \ll S_{\rm ex}$. In the limit $\Omega \ll \delta$ the correction is $-2\varepsilon S_{\rm ex}$, which may be immediately found as the minimizing adiabatic form of the extinction action $S_{\rm ex} = N\delta^2(t)/2$. At large frequency $\Omega > \delta$ the linear correction decays exponentially.[5] This should be compared with the very different frequency dependence for the underdamped, Eq. (3.32), and overdamped, Eq. (3.43), quantum tunneling.

Another example where the optimal path may be explicitly constructed is a sudden temporary change in the system's parameters [60]. We call it a "catastrophic" event. Consider, e.g., the reaction scheme (4.61) and assume that during the time window $-t_c < t < t_c$ the branching rate σ suddenly drops to zero. There is a chance that, after it recovers back to its pre-catastrophic value at $t = t_c$, the population does not recover (provided it was not extinct at the time the catastrophe struck at $t = -t_c$). Our goal is to evaluate the probability that the population goes extinct during the catastrophe or in its immediate aftermath. The corresponding optimal trajectory starts at the meta-stable fixed point M sometime before the catastrophe arrives and ends up in the extinction fixed point E after it ends. Therefore the initial and final pieces of the optimal path follow the *zero energy* activation trajectory $p_a(n)$ of the pre-catastrophic Hamiltonian $H_0(p, n)$. During the time window $|t| < t_c$ the Hamiltonian acquires a different form $H_c(p, n)$, and the optimal path follows one of its *finite energy* trajectories, Fig. 4.4. The latter is selected in such a way that the time elapsed between its two intersections with $p_a(n)$ is exactly $2t_c$.

To be specific, let us model the pre-catastrophic $H_0(p, n)$ by Eq. (4.68), while during the catastrophe $H_c(p, n) = -\mu pn$. The latter corresponds to the pure annihilation reaction $A \xrightarrow{\mu} \emptyset$, where we took into account that $|p| < \delta \ll 1$. Its constant energy H trajectory $p_H(n) = -H/(\mu n)$ intersects the activation trajectory $p_a(n) = n/N - \delta$ in points $n_\pm = (1 \pm \epsilon)N\delta/2$, where $\epsilon = \sqrt{1 - 4H/\mu N\delta^2}$. Since $n(t) \sim e^{-t\mu}$ along $p_H(n)$, the time elapsed between points n_+ and n_- is found to be $e^{-2t_c\mu} = n_-/n_+ = (1-\epsilon)/(1+\epsilon)$. From here one finds the proper energy to be $H = \mu N\delta^2/4\cosh^2(t_c\mu)$. The corresponding extinction action is given by $S(t_c) = \int dt[p\dot{n} - H]$, where the first term is the area shaded in Fig. 4.4, while the second one is $-2t_cH$. Straightforward calculation yields

[5] There is, however, the second order correction to the action $\sim -(\varepsilon\delta/\Omega)^2 S_{\rm ex}$, which decays only as a power law of frequency [59]. The same type of correction is responsible for the Kapitsa pendulum effect. Therefore at $\Omega \gtrsim (\delta/\pi)\ln(1/\varepsilon)$ the linear correction (4.76) may be disregarded.

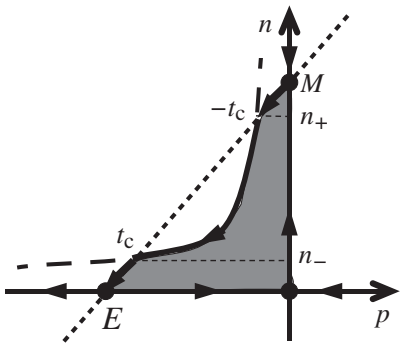

Fig. 4.4 Optimal path to extinction facilitated by the catastrophe – bold line. The dotted line is the activation trajectory of the pre-catastrophic Hamiltonian $p_a(n)$. The dashed line is a finite energy trajectory of the Hamiltonian during the catastrophe, $p_H(n)$. The switches between the two occur at $t = \mp t_c$.

$$S(t_c) = S_{ex}\left[1 - \tanh(t_c\mu)\right] = N\delta^2/(1 + e^{2t_c\mu}). \tag{4.77}$$

The extinction probability in the aftermath of the catastrophe is $\sim e^{-S(t_c)}$. It is of order one if $N\delta^2 e^{-2t_c\mu} \approx 1$. However, according to the rate equation $\dot{n} = -\mu n$, by the time such a catastrophe ends $n(2t_c) = N\delta\, e^{-2t_c\mu} \approx 1/\delta \gg 1$, and one could expect that the population is still in no immediate danger of extinction. The message is that the population may be much less catastrophe-tolerant than a naive expectation based on the rate equations.

4.12 Large deviations in multivariable systems

We discuss now applications of the optimal path approach of Section 4.4 for systems with several degrees of freedom. The ideas touched here were introduced in seminal works of Graham and Tél [61], Dykman and Smelyanskiy [62] and Maier and Stein [63]. Consider, e.g. an overdamped stochastic system with two degrees of freedom X_1 and X_2, i.e. $\dot{X}_\alpha = A_\alpha(X) + \sqrt{T}\,\xi_\alpha(t)$, with the white noise (4.15). Its Fokker–Planck Hamiltonian (4.19) is given by

$$H(P_1, P_2, X_1, X_2) = P_1 A_1(X) + P_2 A_2(X) + T P_1^2 + T P_2^2. \tag{4.78}$$

The corresponding noiseless motion is described by the zero-energy invariant plane of this Hamiltonian $P_1 = P_2 = 0$, indeed $\dot{X}_\alpha = A_\alpha(X) = \partial_{P_\alpha} H\big|_{P=0}$. Let us assume for simplicity that such a noiseless dynamics admits a fixed point at $X_1 = X_2 = 0$, i.e. it is in the origin of the *four*-dimensional phase space. Being the fixed point means $A_\alpha(0) = 0$. Linearizing noiseless equations of motion in the vicinity of this point, one finds $\dot{X}_\alpha = A_{\alpha\beta} X_\beta$, where $A_{\alpha\beta} = \partial_\beta A_\alpha(X)\big|_{X=0}$. The matrix $A_{\alpha\beta}$ may have either two real eigenvalues $\lambda_{1,2}$, or two complex conjugated eigenvalues

$\lambda_{1,2} = \kappa \pm i\omega$. We consider the latter case and assume that $\kappa < 0$, i.e. the fixed point $X = 0$ is a locally stable *focus*. This means that the noiseless relaxation tends to bring the system to the fixed point along a spiral trajectory. In a near vicinity of $X = 0$ the spirals may be characterized in terms of the two right eigenvectors of $A_{\alpha\beta}$, which both belong to the (X_1, X_2) plane of the four-dimensional phase space (analog of the $P = 0$ line in the one degree of freedom example of Fig. 4.1).

Thermal fluctuations take the system out of the fixed point and lead to a certain probability of finding the system at $X_0 \neq 0$. As explained in Section 4.4, such a probability is given by the exponentiated action of an *activation trajectory*, which goes from the origin to a point of the phase space with the coordinates X_0. In case of the single degree of freedom there is only one possible trajectory which departs from the fixed point: the curve of zero energy $P = -A(X)/T$, Fig. 4.1. The situation is much more interesting now. Linearizing the Hamiltonian equations of motion determined by Eq. (4.78) near the origin, one finds

$$\begin{pmatrix} \dot{X}_\alpha \\ \dot{P}_\alpha \end{pmatrix} = \begin{pmatrix} A_{\alpha\beta} & 2T\delta_{\alpha\beta} \\ 0 & -A^T_{\alpha\beta} \end{pmatrix} \begin{pmatrix} X_\beta \\ P_\beta \end{pmatrix}. \tag{4.79}$$

This 4×4 matrix possesses four eigenvalues. Two of them are already familiar eigenvalues of $A_{\alpha\beta}$ denoted as $\lambda_{1,2}$. The corresponding two right eigenvectors have zero components in the P directions. They thus give rise to the relaxation trajectories, which stay entirely within the invariant hyperplane $P = 0$. Two additional eigenvalues $\lambda_{3,4} = -\lambda_{1,2}$ have *positive* real parts and thus describe the activation trajectories which depart from the fixed point. The corresponding right eigenvectors have, in general, non-zero components in all four directions of the phase space. All trajectories which depart from the fixed point along an arbitrary linear superposition of these *two* eigenvectors form the *two-dimensional* Lagrangian manifold of activation trajectories. The energy is still a conserved quantity and therefore all the trajectories forming the Lagrangian manifold have the fixed energy, which is *zero* (indeed, all these trajectories depart from the origin, which has zero energy). The Lagrangian manifold is a generalization of the activation zero energy trajectory of Fig. 4.1. Since for a non-potential force A_α the Lagrangian manifold is *not* given by $P_\alpha(X) = -A_\alpha(X)/T$, [6] the activation trajectories are *not* time-reversed counterparts of the relaxation ones.

[6] Indeed, according to the Hamilton–Jacobi equation [34] the Lagrangian manifold is characterized by $P_\alpha(X) = -\partial_\alpha S(X)$, where S is the action along a trajectory leading to X. Therefore for $P_\alpha(X) = -A_\alpha(X)/T$ to be true one needs to have $\partial_2 A_1 = \partial_1 A_2$, which implies $A_\alpha = -\partial_\alpha V(X)$, i.e. the force is potential (no vorticity). In the language of the Fokker–Planck equation the condition $P_\alpha(X) = -A_\alpha(X)/T$ means that in a stationary state all components of the current vector are zero. Again, this not the case in presence of vorticity – a stationary state does support a finite divergenceless current. The author is indebted to M. Dykman for clarifying this point.

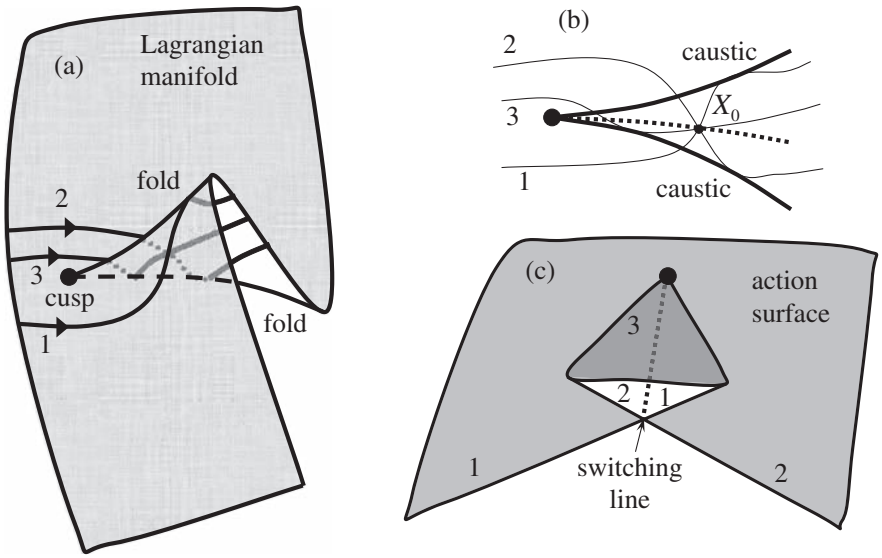

Fig. 4.5 (a) Lagrangian manifold with a cusp singularity and three characteristic trajectories coming from the origin. (b) Projection of the Lagrangian manifold onto the (X_1, X_2) plane. The two folds project onto caustics, while projections of the three trajectories intersect at the point X_0. (c) The action $S(X_0)$ is a three-valued function in between the caustics. Two of its lower branches intersect along the switching line. After [62].

This observation may have dramatic consequences. As shown in [61, 62, 63], for non-potential forces the Lagrangian manifold develops cusp singularities some distance away from the origin, Fig. 4.5(a). The projection of the manifold onto the physical (X_1, X_2) plane exhibits two caustics, emanating from the cusp, Fig. 4.5(b). In between them the projection is three-valued. There are thus three distinct trajectories, whose projections pass through the same point $X_0 = (X_{01}, X_{02})$. Two of them, 1 and 2, reach the point X_0 before being reflected by one of the caustics, i.e. they meet X_0 while being on the top and bottom sheets of the manifold. The projection of 3 passes through X_0 after being reflected once by a caustic, i.e. the corresponding trajectory meets X_0 being on the middle sheet of the Lagrangian manifold. The action $S(X_0)$ calculated along the trajectories is therefore a three-valued function of the physical coordinate in between the two caustics, Fig. 4.5(c). The biggest action is due to trajectories of type 3, which underwent reflection before arriving at the point X_0. The two smaller action branches intersect each other along the *switching line*, which emanates from the projection of the cusp and stays in between the two caustics.

The stationary state probability $\mathcal{P}(X_0)$ of finding the system at point X_0 is given by the exponentiated action, Section 4.4. If the action is multi-valued, one

can observe only its smallest branch, which gives rise to the largest probability. Therefore the large deviation function: $-\lim_{T\to 0}[T \ln \mathcal{P}(X_0)] = T \ \min\{S(X_0)\}$ is a *non-analytic* function of the coordinates along the switching line. Notice that for the potential forces $A_\alpha = -\partial_\alpha V$, this function is simply the potential $V(X_0)$ and thus is perfectly smooth. As a result, the stationary state of non-equilibrium systems (e.g. with non-potential forces) is qualitatively different from equilibrium ones. Strictly speaking, this is only true in the limit of weak noise $T \to 0$, while for a finite noise the singularities are smeared. However, since the action is in the exponent, the change in the derivative across the switching line may be extremely sharp. There is a large mathematical literature devoted to this phenomenon [64, 65].

5

Bosonic fields

In this chapter we generalize the formalism of Chapter 2 for the case of complex and real interacting bosonic fields. We then develop a perturbative diagrammatic technique and use it to derive the quantum kinetic equation.

5.1 Complex bosonic fields

Consider a box of size L filled with bosonic particles of mass m. The single-particle states within the box are labeled by the wavenumber vector $\mathbf{k} = (2\pi/L)\mathbf{n}$, where the vector $\mathbf{n} = (n_x, n_y, n_z)$ has integer components $n_\mu = 0, \pm 1, \pm 2, \ldots$ (we have assumed periodic boundary conditions in all directions). The corresponding energies are given by $\omega_{\mathbf{k}} = \mathbf{k}^2/(2m)$. One may associate bosonic creation and annihilation operators $\hat{b}^\dagger_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}$, obeying the commutation relations $[\hat{b}_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}$, with each of these single-particle states. The kinetic energy part of the Hamiltonian written in terms of such operators takes the form

$$\hat{H}_0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}}. \tag{5.1}$$

Assuming some initial density matrix, e.g. $\hat{\rho}_0 = \exp\{-\beta(\hat{H}_0 - \mu\hat{N})\}$, where the number operator is $\hat{N} = \sum_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}}$, one may write the Keldysh partition function $Z = 1$, see Eq. (2.13), as a functional integral over the closed time contour, Fig. 2.1. The coherent states are parametrized by a set of complex numbers $\phi_j(\mathbf{k})$, labeled by the discrete time index j along with the state index $\mathbf{k}$. Transforming to continuum notation and performing the Keldysh rotation according to Eq. (2.39) for each state $\mathbf{k}$, one obtains the two sets of complex fields $\phi^{\mathrm{cl}}(\mathbf{k}, t)$ and $\phi^{\mathrm{q}}(\mathbf{k}, t)$. The partition function acquires the form

$$Z = \int \mathbf{D}[\phi^{\mathrm{cl}}, \phi^{\mathrm{q}}]\, \mathrm{e}^{\mathrm{i}S_0[\phi^{\mathrm{cl}}, \phi^{\mathrm{q}}]}, \tag{5.2}$$

where the integration measure is given by

$$\mathbf{D}[\phi^{\mathrm{cl}},\phi^{\mathrm{q}}]=\frac{1}{\mathrm{Tr}\{\hat{\rho}_0\}}\prod_{\mathbf{k}}\prod_{j=1}^{N}\frac{\mathrm{d}(\mathrm{Re}\phi_j^{\mathrm{cl}}(\mathbf{k}))\mathrm{d}(\mathrm{Im}\phi_j^{\mathrm{cl}}(\mathbf{k}))}{\pi}\frac{\mathrm{d}(\mathrm{Re}\phi_j^{\mathrm{q}}(\mathbf{k}))\mathrm{d}(\mathrm{Im}\phi_j^{\mathrm{q}}(\mathbf{k}))}{\pi}, \tag{5.3}$$

and the limit $N\to\infty$ is understood. The Keldysh action of the free complex Bose field is written, employing Eqs. (2.51) and (2.52), as

$$S_0[\phi^{\mathrm{cl}},\phi^{\mathrm{q}}]=\sum_{\mathbf{k}}\int_{-\infty}^{\infty}\mathrm{d}t\ (\bar{\phi}^{\mathrm{cl}},\bar{\phi}^{\mathrm{q}})\begin{pmatrix}0 & \mathrm{i}\partial_t-\omega_{\mathbf{k}}-\mathrm{i}0\\ \mathrm{i}\partial_t-\omega_{\mathbf{k}}+\mathrm{i}0 & 2\mathrm{i}0F(\omega_{\mathbf{k}})\end{pmatrix}\begin{pmatrix}\phi^{\mathrm{cl}}\\ \phi^{\mathrm{q}}\end{pmatrix}, \tag{5.4}$$

where $\phi^{\mathrm{cl,q}}=\phi^{\mathrm{cl,q}}(\mathbf{k},t)$. The $\pm\mathrm{i}0$ indicates the retarded/advanced nature of the off-diagonal operators and specifies how the corresponding inverted operators are to be understood. The $\mathrm{q}-\mathrm{q}$ Keldysh component is a pure regularization for the free field. Unlike the $\mathrm{cl}-\mathrm{cl}$ component, it becomes finite (and in general non-local with respect to time and state indices) once the interactions between the particles are included. We kept it explicitly here to remind us that it determines the way the quadratic form in the action is inverted.

The corresponding free (bare) Green function is defined as

$$G_0^{\alpha\beta}(\mathbf{k},\mathbf{k}',t,t')=-\mathrm{i}\int\mathbf{D}[\phi^{\mathrm{cl}},\phi^{\mathrm{q}}]\ \phi^{\alpha}(\mathbf{k},t)\,\bar{\phi}^{\beta}(\mathbf{k}',t')\ \mathrm{e}^{\mathrm{i}S_0[\phi^{\mathrm{cl}},\phi^{\mathrm{q}}]} \tag{5.5}$$

and according to the rules of the Gaussian integration is given by the inverse of the quadratic form in the action

$$G_0^{\alpha\beta}(\mathbf{k},\mathbf{k}',t,t')=\delta_{\mathbf{k},\mathbf{k}'}\begin{pmatrix}G_0^{\mathrm{K}}(\mathbf{k},t-t') & G_0^{\mathrm{R}}(\mathbf{k},t-t')\\ G_0^{\mathrm{A}}(\mathbf{k},t-t') & 0\end{pmatrix}. \tag{5.6}$$

The three non-zero components of the Green function are

$$G_0^{\mathrm{R}}(\mathbf{k},t)=-\mathrm{i}\theta(t)\,\mathrm{e}^{-\mathrm{i}\omega_{\mathbf{k}}t}\overset{\mathrm{FT}}{\to}(\epsilon-\omega_{\mathbf{k}}+\mathrm{i}0)^{-1}; \tag{5.7a}$$

$$G_0^{\mathrm{A}}(\mathbf{k},t)=\mathrm{i}\theta(-t)\,\mathrm{e}^{-\mathrm{i}\omega_{\mathbf{k}}t}\overset{\mathrm{FT}}{\to}(\epsilon-\omega_{\mathbf{k}}-\mathrm{i}0)^{-1}; \tag{5.7b}$$

$$G_0^{\mathrm{K}}(\mathbf{k},t)=-\mathrm{i}F(\omega_{\mathbf{k}})\,\mathrm{e}^{-\mathrm{i}\omega_{\mathbf{k}}t}\overset{\mathrm{FT}}{\to}-2\pi\mathrm{i}F(\epsilon)\,\delta(\epsilon-\omega_{\mathbf{k}}). \tag{5.7c}$$

In equilibrium the distribution function is $F(\epsilon)=\coth(\epsilon-\mu)/(2T)$. Above we also quoted the Fourier transforms with respect to the time argument for all three components.

It is sometimes convenient to perform the linear change of variables in the functional integral to introduce the coordinate space representation for the two complex bosonic fields

$$\phi^{\alpha}(\mathbf{r},t)=\sum_{\mathbf{k}}\phi^{\alpha}(\mathbf{k},t)\,\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{r}}. \tag{5.8}$$

In terms of these fields the bare bosonic action (5.4) takes the form

$$S_0=\int\mathrm{d}\mathbf{r}\int_{-\infty}^{\infty}\mathrm{d}t\;\left(\bar{\phi}^{\mathrm{cl}},\bar{\phi}^{\mathrm{q}}\right)\begin{pmatrix}0 & \mathrm{i}\partial_t+\frac{\nabla_{\mathbf{r}}^2}{2m}-V^{\mathrm{cl}}\\ \mathrm{i}\partial_t+\frac{\nabla_{\mathbf{r}}^2}{2m}-V^{\mathrm{cl}} & 2\mathrm{i}0F\end{pmatrix}\begin{pmatrix}\phi^{\mathrm{cl}}\\ \phi^{\mathrm{q}}\end{pmatrix}, \tag{5.9}$$

where we have added an external classical potential $V^{\mathrm{cl}}=V^{\mathrm{cl}}(\mathbf{r},t)$ in accordance with Eq. (2.61). In the absence of such an external potential, the correlators of the coordinate space bosonic fields are given by the Fourier transform of the Green function (5.6), (5.7)

$$\left\langle\phi^{\alpha}(\mathbf{r},t)\,\bar{\phi}^{\beta}(\mathbf{r}',t')\right\rangle=\mathrm{i}G_0^{\alpha\beta}(\mathbf{r}-\mathbf{r}',t-t')=\mathrm{i}\sum_{\mathbf{k}}G_0^{\alpha\beta}(\mathbf{k},t-t')\mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{r}-\mathbf{r}')}. \tag{5.10}$$

5.2 Interactions

Let us now include interactions between bosonic particles through a pairwise interaction potential $U(\mathbf{r}-\mathbf{r}')$. The corresponding *normally ordered* Hamiltonian takes the form

$$\hat{H}_{\mathrm{int}}=\frac{1}{2}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'}U(\mathbf{q})\,\hat{b}^{\dagger}_{\mathbf{k}}\hat{b}^{\dagger}_{\mathbf{k}'}\hat{b}_{\mathbf{k}'+\mathbf{q}}\hat{b}_{\mathbf{k}-\mathbf{q}}, \tag{5.11}$$

where $U(\mathbf{q})$ is the Fourier transform of the interaction potential. In the case of dilute atomic gases the interaction potential may be thought of as being short-ranged, i.e. momentum-independent, $U(\mathbf{q})=g$, where the interaction constant may be expressed through the s-wave scattering length a_{s} as $g=4\pi a_{\mathrm{s}}/m$ [66]. The corresponding term in the action takes the form

$$S_{\mathrm{int}}=-\frac{g}{2}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'}\int_{\mathcal{C}}\mathrm{d}t\;\bar{\phi}(\mathbf{k},t)\bar{\phi}(\mathbf{k}',t)\phi(\mathbf{k}'+\mathbf{q},t)\phi(\mathbf{k}-\mathbf{q},t).$$

Going to the coordinate space representation, one finds

$$S_{\mathrm{int}}=-\frac{g}{2}\int\mathrm{d}\mathbf{r}\int_{\mathcal{C}}\mathrm{d}t\;(\bar{\phi}\phi)^2=-\frac{g}{2}\int\mathrm{d}\mathbf{r}\int_{-\infty}^{+\infty}\mathrm{d}t\left[(\bar{\phi}^{+}\phi^{+})^2-(\bar{\phi}^{-}\phi^{-})^2\right]. \tag{5.12}$$

It is important to remember that there are no interactions in the distant past, $t=-\infty$ (while they are present in the future, $t=+\infty$). The interactions are supposed to be adiabatically switched on and off on the forward and backward branches correspondingly. Therefore the interactions modify only those matrix elements of the evolution operator, Eq. (2.17), that are away from $t=-\infty$. It is also worth remembering that in the discrete time form the $\bar{\phi}$ fields are taken one time

Fig. 5.1 Graphic representation of the two interaction vertices of the $|\phi|^4$ theory. There are also two complex conjugated vertices with a reversed direction of all arrows.

step δ_t *after* the ϕ fields along the contour $\mathcal{C}$. Performing the Keldysh rotation, Eq. (2.39), one finds

$$S_{\mathrm{int}}[\phi^{\mathrm{cl}},\phi^{\mathrm{q}}] = -\frac{g}{2}\int \mathrm{d}\mathbf{r}\int_{-\infty}^{+\infty}\mathrm{d}t\left[\bar{\phi}^{\mathrm{cl}}\bar{\phi}^{\mathrm{q}}\phi^{\mathrm{cl}}\phi^{\mathrm{cl}}+\bar{\phi}^{\mathrm{cl}}\bar{\phi}^{\mathrm{q}}\phi^{\mathrm{q}}\phi^{\mathrm{q}}+\mathrm{c.c.}\right], \tag{5.13}$$

where c.c. stands for the complex conjugate of the first two terms. The interaction action, Eq. (5.13), obviously satisfies the normalization condition, Eq. (2.53). Diagrammatically, the action (5.13) generates two types of vertex depicted in Fig. 5.1: one with three classical fields (full lines) and one quantum field (dashed line) and the other with one classical field and three quantum fields (as well as two complex conjugated vertices, obtained by reversing the direction of the arrows).

Let us demonstrate that the addition of the interaction term to the action does not violate the normalization identity, $Z = 1$. To this end, one may expand $\exp(\mathrm{i}S_{\mathrm{int}})$ in powers of g and then average term by term with the help of the Gaussian action (5.9). To show that the normalization, $Z = 1$, is intact, one needs to show that $\langle S_{\mathrm{int}}\rangle = \langle S_{\mathrm{int}}^2\rangle = \cdots = 0$. Applying the Wick theorem, Eq. (2.21), one finds for the term linear in g

$$\langle S_{\mathrm{int}}\rangle = -\frac{g}{2}\int \mathrm{d}\mathbf{r}\,\mathrm{d}t\left\langle\bar{\phi}^{\mathrm{cl}}\bar{\phi}^{\mathrm{q}}\phi^{\mathrm{cl}}\phi^{\mathrm{cl}}+\bar{\phi}^{\mathrm{cl}}\bar{\phi}^{\mathrm{cl}}\phi^{\mathrm{cl}}\phi^{\mathrm{q}}+\bar{\phi}^{\mathrm{q}}\bar{\phi}^{\mathrm{cl}}\phi^{\mathrm{q}}\phi^{\mathrm{q}}+\bar{\phi}^{\mathrm{q}}\bar{\phi}^{\mathrm{q}}\phi^{\mathrm{q}}\phi^{\mathrm{cl}}\right\rangle.$$

The first two terms upon application of the Wick theorem lead to diagrams of the type of Fig. 5.2(a):

$$\left\langle\bar{\phi}^{\mathrm{cl}}\bar{\phi}^{\mathrm{q}}\phi^{\mathrm{cl}}\phi^{\mathrm{cl}}+\bar{\phi}^{\mathrm{cl}}\bar{\phi}^{\mathrm{cl}}\phi^{\mathrm{cl}}\phi^{\mathrm{q}}\right\rangle = -2\left[G_0^{\mathrm{R}}(t,t)+G_0^{\mathrm{A}}(t,t)\right]G_0^{\mathrm{K}}(t,t) = 0,$$

where we have suppressed the space arguments and focused only on the time ones and the factor of two originates from the two combinatorial possibilities to make Wick's contractions. This expression vanishes due to the identity (2.44). The last two terms in $\langle S_{\mathrm{int}}\rangle$ trivially vanish because $\left\langle\phi^{\mathrm{q}}\bar{\phi}^{\mathrm{q}}\right\rangle = 0$.

There are two families of terms that are second order in g and contain not more than four quantum fields (terms with six quantum fields unavoidably lead to $\mathrm{q}-\mathrm{q}$ contractions and therefore vanish). They contain

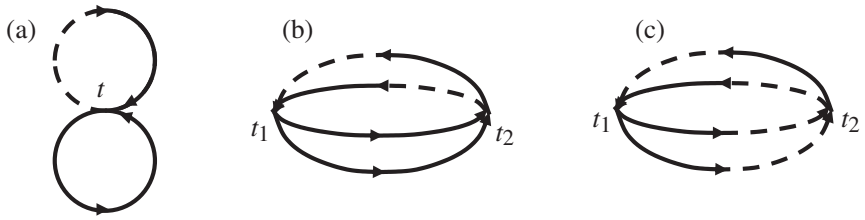

Fig. 5.2 Diagrams for the first (a) and second (b), (c) order interaction corrections to the partition function Z. As explained in the text, they do not change the normalization identity $Z = 1$.

$$\left\langle \bar{\phi}_1^{\mathrm{q}} \bar{\phi}_1^{\mathrm{cl}} \phi_1^{\mathrm{cl}} \phi_1^{\mathrm{cl}} \times \phi_2^{\mathrm{q}} \phi_2^{\mathrm{cl}} \bar{\phi}_2^{\mathrm{cl}} \phi_2^{\mathrm{cl}} \right\rangle = 2 G_0^{\mathrm{R}}(t_2, t_1) G_0^{\mathrm{A}}(t_2, t_1) [G_0^{\mathrm{K}}(t_1, t_2)]^2,$$

Fig. 5.2(b), and

$$\left\langle \bar{\phi}_1^{\mathrm{q}} \bar{\phi}_1^{\mathrm{cl}} \phi_1^{\mathrm{cl}} \phi_1^{\mathrm{cl}} \times \phi_2^{\mathrm{q}} \phi_2^{\mathrm{cl}} \bar{\phi}_2^{\mathrm{q}} \phi_2^{\mathrm{q}} \right\rangle = 2 G_0^{\mathrm{R}}(t_2, t_1) G_0^{\mathrm{A}}(t_2, t_1) [G_0^{\mathrm{R}}(t_1, t_2)]^2,$$

Fig. 5.2(c), where $\phi_{1,2}^{\alpha} = \phi^{\alpha}(\mathbf{r}_{1,2}, t_{1,2})$. Both of these terms are zero, because $G_0^{\mathrm{R}}(t_2, t_1) \sim \theta(t_2 - t_1)$, while $G_0^{\mathrm{A}}(t_2, t_1) \sim G_0^{\mathrm{R}}(t_1, t_2)^* \sim \theta(t_1 - t_2)$ and thus their product has no support in the time domain. One may be concerned that $G_0^{\mathrm{R}}(t_2, t_1)$ and $G_0^{\mathrm{A}}(t_2, t_1)$ are simultaneously non-zero on the diagonal $t_1 = t_2$. The contribution of the diagonal to the double integral over $\mathrm{d}t_1 \mathrm{d}t_2$, however, is of the order $\sim \delta_t^2 N \to 0$, when $N \to \infty$. It is easy to see that, for exactly the same reasons, all higher order terms in g vanish and thus the fundamental normalization is indeed intact (at least in the perturbative expansion). However, the observables and correlation functions are affected by the interactions. We demonstrate it below on the example of the Green functions.

5.3 Dyson equation

We define the full or *dressed* Green function as the correlator of the fields averaged with the weight, which includes both the bare action S_0 and the interaction action:

$$G^{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t') = -\mathrm{i} \int \mathbf{D}[\bar{\phi}\phi]\, \phi^{\alpha}(\mathbf{r}, t)\, \bar{\phi}^{\beta}(\mathbf{r}', t')\ \mathrm{e}^{\mathrm{i}(S_0 + S_{\mathrm{int}})}, \tag{5.14}$$

here $\alpha, \beta = (\mathrm{cl}, \mathrm{q})$ and the action is given by Eqs. (5.9) and (5.13). To evaluate the full Green function one may expand the exponent in powers of S_{int}. The functional integration with the remaining Gaussian action S_0 is then performed using the Wick theorem. This procedure leads to an infinite series of terms which are convenient to represent by Feynman diagrams. Each of these diagrams has two external "legs": an incoming, staying for the contraction $\langle \phi^{\alpha}(x) \bar{\phi}^{\gamma}(x_1) \rangle = \mathrm{i} G_0^{\alpha\gamma}(x, x_1)$, and an outgoing, representing $\langle \phi^{\delta}(x_2) \bar{\phi}^{\beta}(x') \rangle = \mathrm{i} G_0^{\delta\beta}(x_2, x')$, where we introduced a combined notation $x = \mathbf{r}, t$. The interior of a diagram, which is a matrix in Keldysh

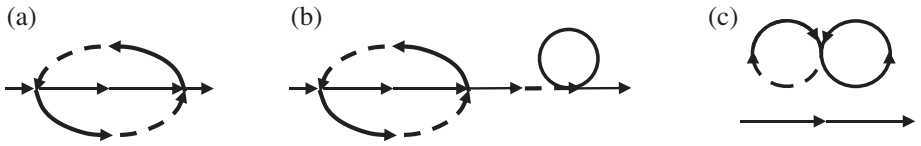

Fig. 5.3 Examples of diagrams for the dressed Green function: (a) an irreducible diagram of second order in g; (b) a reducible diagram of third order, which contains two irreducible blocks; (c) a disconnected diagram of first order.

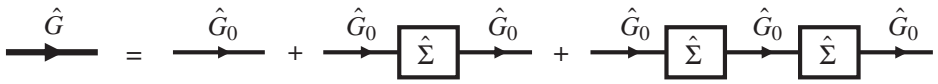

Fig. 5.4 Diagrammatic series for the dressed Green function $\hat{G}$, rearranged into the Dyson series. The self-energy blocks contain the sum of all *irreducible* diagrams.

indices γ, δ as well as in space-time coordinates x_1, x_2, contains a number of internal four-leg vertices, each carrying a factor of $g/2$. Integration over space-time coordinates of all internal vertices as well as summation over Keldysh indices is assumed. Examples of the diagrams are given in Fig. 5.3.

One can now define *irreducible* diagrams as those which can't be cut into two disconnected parts by cutting a single line in the interior of the diagram. The diagram in Fig. 5.3(a) is irreducible, while the one in Fig. 5.3(b) is reducible. The diagram in Fig. 5.3(c) is a disconnected one. The disconnected diagrams contain all the same building blocks as in Fig. 5.2 and thus are zero, as explained above.[1] Rearranging the order of terms in the perturbative expansion, one may formally sum up the inner parts of all irreducible diagrams and call the resulting object the *self-energy* $\Sigma^{\gamma\delta}(x_1, x_2)$. The full series may be written then, Fig. 5.4, as

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \circ \hat{\Sigma} \circ \hat{G}_0 + \hat{G}_0 \circ \hat{\Sigma} \circ \hat{G}_0 \circ \hat{\Sigma} \circ \hat{G}_0 + \cdots = \hat{G}_0 + \hat{G}_0 \circ \hat{\Sigma} \circ \hat{G}, \quad (5.15)$$

where the circular multiplication sign implies convolution of the space-time coordinates as well as a 2×2 Keldysh matrix multiplication. The only difference compared with the standard diagrammatic expansion [2, 4, 6] is the presence of the 2×2 matrix structure. The fact that the series is arranged as a sequence of matrix products is of no surprise. Indeed, the Keldysh index, $\alpha = (\mathrm{cl}, \mathrm{q})$, is just one more index in addition to time, space, spin, etc. Therefore, as with any other index, there is a summation over all of its intermediate values, hence the matrix

[1] Cancelation of disconnected diagrams is a direct consequence of the normalization identity $Z = 1$. Notice that in equilibrium theory the disconnected diagrams are *not* zero and serve to compensate for the denominator e^{iL}, Eq. (1.5), [2, 4].

multiplication. The concrete form of the self-energy matrix, $\hat{\Sigma}$, is specific to the Keldysh technique and is discussed below in some detail.

Multiplying both sides of Eq. (5.15) by $\hat{G}_0^{-1}$ from the left, one obtains an equation for the *exact* dressed Green function, $\hat{G}$,

$$\left(\hat{G}_0^{-1} - \hat{\Sigma}\right) \circ \hat{G} = \hat{1}, \tag{5.16}$$

where $\hat{1}$ is the unit matrix. This equation is named after Dyson. The very non-trivial feature of the Keldysh technique is that the self-energy matrix, $\hat{\Sigma}$, possesses the same causality structure as $\hat{G}_0^{-1}$, Eq. (2.51), namely

$$\hat{\Sigma} = \begin{pmatrix} 0 & \Sigma^{\mathrm{A}} \\ \Sigma^{\mathrm{R}} & \Sigma^{\mathrm{K}} \end{pmatrix}, \tag{5.17}$$

where $\Sigma^{\mathrm{R(A)}}$ are mutually Hermitian conjugated lower (upper) triangular matrices with respect to the two time indices, while Σ^{K} is an anti-Hermitian matrix

$$\Sigma^{\mathrm{R}}(x_1, x_2) = [\Sigma^{\mathrm{A}}(x_2, x_1)]^* \sim \theta(t_1 - t_2)\,; \quad \Sigma^{\mathrm{K}}(x_1, x_2) = -[\Sigma^{\mathrm{K}}(x_2, x_1)]^*. \tag{5.18}$$

This fact will be explicitly demonstrated below. Since both $\hat{G}_0^{-1}$ and $\hat{\Sigma}$ have the same causality structure, one concludes that the dressed Green function, $\hat{G}$, also possesses the causality structure, like Eq. (2.40). As a result, the Dyson equation acquires the form

$$\begin{pmatrix} 0 & \left[G_0^{\mathrm{A}}\right]^{-1} - \Sigma^{\mathrm{A}} \\ \left[G^{\mathrm{R}}\right]_0^{-1} - \Sigma^{\mathrm{R}} & -\Sigma^{\mathrm{K}} \end{pmatrix} \circ \begin{pmatrix} G^{\mathrm{K}} & G^{\mathrm{R}} \\ G^{\mathrm{A}} & 0 \end{pmatrix} = \hat{1}, \tag{5.19}$$

where one took into account that $\left[G_0^{-1}\right]^{\mathrm{K}}$ is a pure regularization ($\sim \mathrm{i}0F$) and thus may be omitted in the presence of a non-zero self-energy component Σ^{K}. Employing the specific form of $\left[G_0^{\mathrm{R(A)}}\right]^{-1}$, Eq. (5.9), one obtains for the retarded (advanced) component

$$\left(\mathrm{i}\partial_t + \frac{1}{2m}\nabla_{\mathbf{r}}^2 - V^{\mathrm{cl}}(\mathbf{r}, t) - \Sigma^{\mathrm{R(A)}}\right) \circ G^{\mathrm{R(A)}}(x, x') = \delta(t - t')\delta(\mathbf{r} - \mathbf{r}'). \tag{5.20}$$

Provided the self-energy component $\Sigma^{\mathrm{R(A)}}$ is known (in some approximation), Eq. (5.20) constitutes a closed equation for the retarded (advanced) component of the dressed Green function.

For the space-time translationally invariant system, $V^{\mathrm{cl}} = 0$, such that $\hat{G}(x, x') = \hat{G}(x - x')$, this equation may be solved explicitly with the help of the Fourier transform, leading to

$$G^{\mathrm{R(A)}}(\mathbf{k}, \epsilon) = \left(\epsilon - \frac{\mathbf{k}^2}{2m} - \Sigma^{\mathrm{R(A)}}(\mathbf{k}, \epsilon)\right)^{-1}. \tag{5.21}$$

Employing Eq. (5.18), one observes that $\mathrm{Re}\Sigma^{\mathrm{R}}(\mathbf{k},\epsilon) = \mathrm{Re}\Sigma^{\mathrm{A}}(\mathbf{k},\epsilon)$ and $\mathrm{Im}\Sigma^{\mathrm{R}}(\mathbf{k},\epsilon) = -\mathrm{Im}\Sigma^{\mathrm{A}}(\mathbf{k},\epsilon) \leq 0$. The real part of the retarded (advanced) self-energy provides renormalization of the particle's dispersion relation. That is, the relation $\epsilon = \mathbf{k}^2/(2m)$ should be substituted by the solution of the equation $\epsilon - \mathbf{k}^2/(2m) - \mathrm{Re}\Sigma^{\mathrm{R(A)}}(\mathbf{k},\epsilon) = 0$. On the other hand, the imaginary part of the self-energy has the meaning of the inverse lifetime a particle spends in a given (renormalized) eigenstate $\mathbf{k}$ of the non-interacting system.

We turn now to the Keldysh component of the Dyson equation. As before, it is convenient to parametrize the Keldysh component of the Green function as

$$G^{\mathrm{K}} = G^{\mathrm{R}} \circ F - F \circ G^{\mathrm{A}} \tag{5.22}$$

(compare with Eq. (2.49)), where $F(x,x')$ is a Hermitian matrix in the space-time domain. The Dyson equation for the Keldysh component then takes the form $\left(\left[G_0^{\mathrm{R}}\right]^{-1} - \Sigma^{\mathrm{R}}\right) \circ \left(G^{\mathrm{R}} \circ F - F \circ G^{\mathrm{A}}\right) = \Sigma^{\mathrm{K}} \circ G^{\mathrm{A}}$. Multiplying it from the right by $\left(\left[G_0^{\mathrm{A}}\right]^{-1} - \Sigma^{\mathrm{A}}\right)$ and employing Eq. (5.20), one finds $F \circ \left(\left[G_0^{\mathrm{A}}\right]^{-1} - \Sigma^{\mathrm{A}}\right) - \left(\left[G_0^{\mathrm{R}}\right]^{-1} - \Sigma^{\mathrm{R}}\right) \circ F = \Sigma^{\mathrm{K}}$. This may be written as

$$F \circ \left[G_0^{\mathrm{A}}\right]^{-1} - \left[G_0^{\mathrm{R}}\right]^{-1} \circ F = \Sigma^{\mathrm{K}} - \left(\Sigma^{\mathrm{R}} \circ F - F \circ \Sigma^{\mathrm{A}}\right). \tag{5.23}$$

Since $\left[G_0^{\mathrm{R}}\right]^{-1}(x',x) = \left[G_0^{\mathrm{A}}\right]^{-1}(x',x) = \delta(x'-x)\left(\mathrm{i}\partial_t + \nabla_{\mathbf{r}}^2/(2m) - V^{\mathrm{cl}}(x)\right)$, where the regularization $\pm\mathrm{i}0$ may be omitted in this context, one finally finds

$$-\left[\left(\mathrm{i}\partial_t + \frac{1}{2m}\nabla_{\mathbf{r}}^2 - V^{\mathrm{cl}}(x)\right) \circ F\right] = \Sigma^{\mathrm{K}} - \left(\Sigma^{\mathrm{R}} \circ F - F \circ \Sigma^{\mathrm{A}}\right), \tag{5.24}$$

where the symbol $[\,\circ\,]$ stands for the commutator. With the help of integration by parts, it may be understood as $[\partial_t \circ F] = (\partial_t + \partial_{t'})F(x,x')$, on the other hand $[\nabla_{\mathbf{r}}^2 \circ F] = (\nabla_{\mathbf{r}}^2 - \nabla_{\mathbf{r}'}^2)F(x,x')$ and $[V \circ F] = (V(x) - V(x'))F(x,x')$. This equation is the quantum kinetic equation for the distribution matrix $F(x,x')$. Schematically, its left hand side forms the *kinetic* term, while the right hand side is the *collision term* or the *collision integral*. In equilibrium the kinetic term vanishes. This implies, in turn, that the self-energy possesses the same structure as the Green function: $\Sigma^{\mathrm{K}} = \Sigma^{\mathrm{R}} \circ F - F \circ \Sigma^{\mathrm{A}}$. The latter is not the case, however, away from equilibrium.

5.4 Real bosonic fields

We briefly repeat now the construction of the interacting field theory for the case of real boson fields, such as, e.g., elastic phonons. To this end we consider a toy model of a d-dimensional "quantum membrane." It is formed by a lattice of quantum particles, where a displacement of an $\mathbf{i}$-th particle from the corresponding lattice point is denoted as $\varphi_{\mathbf{i}}$. For simplicity we consider φ as a scalar,

which may be, e.g., a transversal deformation of the membrane. We assume that the particles interact through some short-ranged potential, which leads to a bending rigidity κ of the membrane. The corresponding contribution to the energy is $U = (\kappa/2a^4)\sum_{\mathbf{i}}(\nabla^2\varphi_{\mathbf{i}})^2$, where ∇ is the lattice gradient operation and a is the lattice constant. In essence, the energy is paid for the *curvature* of the membrane. Furthermore, we also assume that each site experiences a static potential $V(\varphi_{\mathbf{i}})$, created by, e.g., an external substrate. Being expanded around its minimum, such a potential may be written as

$$V(\varphi) = \frac{\omega_0^2}{2}\,\varphi^2 + \frac{\gamma}{6}\,\varphi^3 + \cdots . \tag{5.25}$$

The Keldysh action of an individual quantum particle is given by Eq. (3.4). Generalizing it for the lattice, one finds

$$S[\varphi] = \int_{\mathcal{C}} \mathrm{d}t \sum_{\mathbf{i}} \left(\frac{1}{2}\,\dot{\varphi}_{\mathbf{i}}^{\,2} - \frac{\kappa}{2a^4}\,(\nabla^2\varphi_{\mathbf{i}})^2 - V(\varphi_{\mathbf{i}}) \right), \tag{5.26}$$

where $\varphi_{\mathbf{i}} = \varphi_{\mathbf{i}}(t)$ with t running along the closed time contour. We take now the continuum limit by introducing the displacement density field $\varphi(\mathbf{r}, t)$, where $\mathbf{r}$ is the coordinate in the d-dimensional space of the membrane. In terms of this scalar *real field* the action takes the form

$$S[\varphi] = \int_{\mathcal{C}} \mathrm{d}t \int \mathrm{d}\mathbf{r} \left[\frac{1}{2}\Big(\dot{\varphi}^{\,2} - \kappa\,(\nabla_{\mathbf{r}}^2\varphi)^2 - \omega_0^2\,\varphi^2 \Big) - \frac{\gamma}{6}\,\varphi^3 \right]. \tag{5.27}$$

Performing the Keldysh rotation according to $\varphi^{\mathrm{cl,q}} = (\varphi^+ \pm \varphi^-)/2$, one finds for the quadratic part of the action (5.27)

$$S_0 = \frac{1}{2}\int \mathrm{d}\mathbf{r} \int_{-\infty}^{\infty} \mathrm{d}t\, \left(\varphi^{\mathrm{cl}}, \varphi^{\mathrm{q}}\right) \begin{pmatrix} 0 & -2(\partial_t^2 + \kappa\nabla_{\mathbf{r}}^4 + \omega_0^2) \\ -2(\partial_t^2 + \kappa\nabla_{\mathbf{r}}^4 + \omega_0^2) & -0[\partial_t, F] \end{pmatrix} \begin{pmatrix} \varphi^{\mathrm{cl}} \\ \varphi^{\mathrm{q}} \end{pmatrix}. \tag{5.28}$$

The matrix in the action is the inverse bare Green function $\hat{D}_0^{-1}$. As before its Keldysh q – q component is a pure regularization, showing the way the matrix is to be inverted. Neglecting the cubic non-linearity, the correlator of the real fields is given by the bare Green function

$$D_0^{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t') = -\mathrm{i} \int \mathbf{D}[\varphi^{\mathrm{cl}}, \varphi^{\mathrm{q}}]\; \varphi^{\alpha}(\mathbf{r}, t)\, \varphi^{\beta}(\mathbf{r}', t')\; \mathrm{e}^{\mathrm{i}S_0[\varphi^{\mathrm{cl}}, \varphi^{\mathrm{q}}]}, \tag{5.29}$$

which possesses the standard causality structure

$$D_0^{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t') = \begin{pmatrix} D_0^{\mathrm{K}}(\mathbf{r} - \mathbf{r}', t - t') & D_0^{\mathrm{R}}(\mathbf{r} - \mathbf{r}', t - t') \\ D_0^{\mathrm{A}}(\mathbf{r} - \mathbf{r}', t - t') & 0 \end{pmatrix}. \tag{5.30}$$

As discussed in Section 3.1, the matrix $\hat{D}$ is symmetric (unlike the case of the complex field). The Fourier transforms of the three non-zero components of the bare Green function, according to Eq. (3.13), are

$$D_0^{\mathrm{R(A)}}(\mathbf{k},\epsilon) = \frac{1}{2}\,\frac{1}{(\epsilon \pm \mathrm{i}0)^2 - \omega_{\mathbf{k}}^2}, \tag{5.31a}$$

$$D_0^{\mathrm{K}}(\mathbf{k},\epsilon) = F(\epsilon)\left[D^{\mathrm{R}}(\mathbf{k},\epsilon) - D^{\mathrm{A}}(\mathbf{k},\epsilon)\right], \tag{5.31b}$$

where the dispersion relation for our model is given by $\omega_{\mathbf{k}}^2 = \kappa\mathbf{k}^4 + \omega_0^2$, but the construction may be generalized to accommodate an arbitrary dispersion $\omega_{\mathbf{k}}$. Due to the symmetry of the Green function the distribution function $F(\epsilon)$ must be an *odd* function of energy ϵ. In equilibrium it takes the form $F^{\mathrm{eq}}(\epsilon) = \coth(\epsilon/2T)$.

The cubic non-harmonicity of the action (5.27) after the Keldysh rotation leads to the following non-linear term in the action:

$$S_{\mathrm{int}} = -\int \mathrm{d}\mathbf{r} \int_{-\infty}^{+\infty} \mathrm{d}t \,\left[\gamma\left(\varphi^{\mathrm{cl}}\right)^2\varphi^q + \frac{\gamma}{3}\left(\varphi^{\mathrm{q}}\right)^3\right]. \tag{5.32}$$

The normalization condition (2.53) is again satisfied. Diagrammatically, the cubic non-linearity generates two types of vertex, Fig. 5.5: one with two classical fields (full lines) and one quantum field (dashed line), and the other with three quantum fields. The former vertex carries the factor γ, while the latter has $\gamma/3$. Note that for the real field the lines do not have a direction.

Similarly to the case of the complex field, one may check that addition of the interaction action does not affect the normalization identity $Z = 1$. This property is based on the identity $D_0^{\mathrm{R}}(t,t) + D_0^{\mathrm{A}}(t,t) = 0$ and the rule of thumb $D_0^{\mathrm{R}}(t,t')D_0^{\mathrm{A}}(t,t') = 0$, explained in Section 5.2. The Green function, on the other hand, is affected. The effect of non-linearity on the dressed Green function $\hat{D}(x,x')$ is described by the Dyson equation

$$\left(\hat{D}_0^{-1} - \hat{\Sigma}\right) \circ \hat{D} = \hat{1}, \tag{5.33}$$

where $\hat{\Sigma}(x,x')$ is the self-energy of real bosons, possessing the causality structure, Eq. (5.17), and calculated in the next paragraph to second order in γ. The retarded and advanced components of the Dyson equation take the form

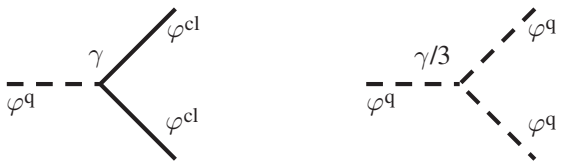

Fig. 5.5 Graphic representation of the two interaction vertices of the φ^3 theory. Note the relative factor of one third between them.

$$-\left(2\partial_t^2 + 2\kappa\,\nabla_{\mathbf{r}}^4 + 2\omega_0^2 + \Sigma^{\mathrm{R(A)}}\right) \circ D^{\mathrm{R(A)}}(x,x') = \delta(t-t')\delta(\mathbf{r}-\mathbf{r}'). \quad (5.34)$$

The Keldysh component of the Green function is again convenient to parametrize as $D^{\mathrm{K}} = D^{\mathrm{R}} \circ F - F \circ D^{\mathrm{A}}$, see Eq. (2.49), where $F(x,x')$ is a Hermitian matrix in the space-time domain. The Dyson equation for the Keldysh component then takes the form of the kinetic equation for the two-point distribution function $F(x,x')$:

$$\left[\left(2\partial_t^2 + 2\kappa\,\nabla_{\mathbf{r}}^4 + 2\omega_0^2\right) \circ ; F\right] = \Sigma^{\mathrm{K}} - \left(\Sigma^{\mathrm{R}} \circ F - F \circ \Sigma^{\mathrm{A}}\right). \quad (5.35)$$

The commutators involved in the kinetic term read $[\partial_t^2 \circ ; F] = (\partial_t^2 - \partial_{t'}^2)F(x,x')$ and $[\nabla_{\mathbf{r}}^4 \circ ; F] = (\nabla_{\mathbf{r}}^4 - \nabla_{\mathbf{r}'}^4)F(x,x')$. Finally $[\omega_0^2 \circ ; F] = 0$; one may allow, though, for some space- and/or time-dependent function $\omega_0(x)$, in the latter case $[\omega_0^2 \circ ; F] = (\omega_0^2(x) - \omega_0^2(x'))F(x,x')$. The self-energy components on the right hand side of Eq. (5.35) are calculated in the following sections.

5.5 Self-energy

Let us demonstrate that the self-energy matrix, $\hat{\Sigma}$, indeed possesses the causality structure, Eq. (5.17). To this end, we consider the real boson field with the $\gamma\varphi^3$ non-linearity, Eq. (5.32), and perform calculations up to second order in the non-linearity γ. Employing the two vertices of Fig. 5.5, one finds the following.

(i) The cl – cl component of the self-energy (i.e. the diagram having two classical external legs) is given by the single diagram, depicted in Fig. 5.6(a). The corresponding analytic expression is

$$\Sigma^{\mathrm{cl-cl}}(x,x') = 4\mathrm{i}\gamma^2 D_0^{\mathrm{R}}(x,x') D_0^{\mathrm{A}}(x,x') = 0.$$

Indeed, the product $D_0^{\mathrm{R}}(t,t')D_0^{\mathrm{A}}(t,t')$ has no support in the time domain (see the discussion in Section 5.2).

(ii) The cl – q (advanced) component is given by the single diagram Fig. 5.6(b). The corresponding expression is

$$\Sigma^{\mathrm{A}}(x,x') = 4\mathrm{i}\gamma^2 D_0^{\mathrm{A}}(x,x') D_0^{\mathrm{K}}(x,x'). \quad (5.36)$$

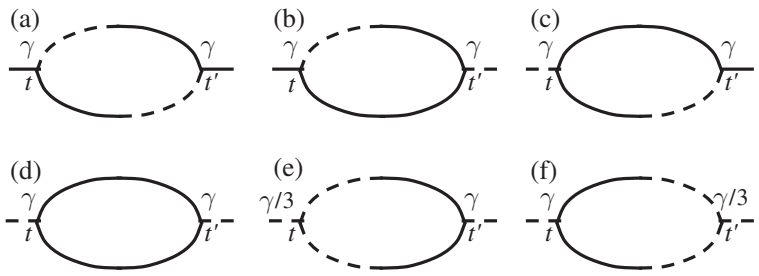

Fig. 5.6 Self-energy diagrams for the φ^3 theory.

Since $\Sigma^{\rm A}(t,t') \sim D_0^{\rm A}(t,t') \sim \theta(t'-t)$, it is, indeed, an advanced (upper triangular) matrix in the time domain. There is a combinatoric factor of 4, associated with the diagram (four ways of choosing external legs $\times$ 2 internal permutations $\times$ 1/(2!) for having two identical vertices).

(iii) The q – cl (retarded) component is given by the diagram of Fig. 5.6(c):

$$\Sigma^{\rm R}(x,x') = 4{\rm i}\gamma^2 D_0^{\rm R}(x,x') D_0^{\rm K}(x,x'), \tag{5.37}$$

which is, in fact, the Hermitian conjugation of Eq. (5.36): $\Sigma^{\rm R} = \left[\Sigma^{\rm A}\right]^\dagger$. Since $\Sigma^{\rm R}(t,t') \sim D_0^{\rm R}(t,t') \sim \theta(t-t')$, it is indeed a retarded (lower triangular) matrix.

(iv) The q – q (Keldysh) component is given by the three diagrams, Fig. 5.6(d)–(f). The corresponding expression (sum of these diagrams) is

$$\begin{aligned}\Sigma^{\rm K}(x,x') &= 2{\rm i}\gamma^2\left[D_0^{\rm K}(x,x')\right]^2 + 6{\rm i}\left(\frac{\gamma}{3}\right)\gamma\left[D_0^{\rm A}(x,x')\right]^2 + 6{\rm i}\gamma\left(\frac{\gamma}{3}\right)\left[D_0^{\rm R}(x,x')\right]^2 \\ &= 2{\rm i}\gamma^2\left(\left[D_0^{\rm K}(x,x')\right]^2 + \left[D_0^{\rm R}(x,x') - D_0^{\rm A}(x,x')\right]^2\right).\end{aligned} \tag{5.38}$$

The combinatoric factors are 2 for diagram (d) and 6 for (e) and (f). In the last equality the fact that $D_0^{\rm R}(t,t')D_0^{\rm A}(t,t') = 0$, due to the absence of support in the time domain, has been used again. Employing the symmetry properties of the Green functions, one finds $\Sigma^{\rm K} = -\left[\Sigma^{\rm K}\right]^\dagger$. This demonstrates that the self-energy $\hat{\Sigma}$ possesses the same structure as $\hat{D}_0^{-1}$. One may check that this statement is not restricted to second order in γ, but holds in higher orders as well.

5.6 Wigner transformation

The distribution matrix $F(x_1,x_2) = F(\mathbf{r}_1,t_1,\mathbf{r}_2,t_2)$ is a function of the two space-time points. It is usually difficult to solve the kinetic equations (5.24) or (5.35) in full generality. One may often take advantage of scale separation between intrinsic microscopic space and time scales and the extrinsic ones, dictated by external perturbations and/or a measurement apparatus. In many instances the latter scales are macroscopic, or at least mesoscopic, and thus are much greater than the former ones. If this is indeed the case, the kinetic theory may be greatly simplified. Most elegantly, it is achieved with the help of the Wigner transformation (WT).

We employ combined notation for space-time $x = \mathbf{r},t$ and momentum-energy $p = \mathbf{k},\epsilon$, with $px = \mathbf{kr} - \epsilon t$. For a two-point function $A(x_1,x_2)$ one may change the variables to the central point coordinate $x = (x_1+x_2)/2$ and the relative coordinate $x' = x_1 - x_2$, such that $x_{1,2} = x \pm x'/2$. One then performs a Fourier transform, going from the relative coordinate x' to its Fourier image p. As a result, the Wigner

transform of the two-point function $A(x_1, x_2)$ is a function of the central coordinate x and the relative momentum p, i.e. $A(x, p)$, defined as

$$A(x, p) = \int \mathrm{d}x' \, \mathrm{e}^{-\mathrm{i}px'} \, A\left(x + \frac{x'}{2}, x - \frac{x'}{2}\right). \tag{5.39}$$

The WT of $A^\dagger(x_1, x_2) = [A(x_2, x_1)]^*$ is simply $[A(x, p)]^*$. The inverse WT takes the form

$$A(x_1, x_2) = \sum_p \mathrm{e}^{\mathrm{i}p(x_1 - x_2)} \, A\left(\frac{x_1 + x_2}{2}, p\right), \tag{5.40}$$

where $\sum_p = \sum_{\mathbf{k}} \int d\epsilon/(2\pi)$.

Let us consider now a two-point function $C = A \circ B$, which means $C(x_1, x_2) = \int \mathrm{d}x_3 \, A(x_1, x_3) B(x_3, x_2)$. According to the above definitions its WT is given by

$$C(x, p) = \int \mathrm{d}x' \mathrm{e}^{-\mathrm{i}px'} \int \mathrm{d}x_3 \sum_{p_1, p_2} \mathrm{e}^{\mathrm{i}p_1(x + x'/2 - x_3) + \mathrm{i}p_2(x_3 - x + x'/2)} \\ A\left(\frac{x + x'/2 + x_3}{2}, p_1\right) B\left(\frac{x_3 + x - x'/2}{2}, p_2\right).$$

We change coordinate variables from x_3, x' to $x_{a,b} = x_3 - x \pm x'/2$ and shift momenta as $p_{a,b} = p_{1,2} - p$ to obtain

$$C(x, p) = \iint \mathrm{d}x_a \mathrm{d}x_b \sum_{p_a, p_b} \mathrm{e}^{\mathrm{i}(p_b x_a - p_a x_b)} A\left(x + \frac{x_a}{2}, p + p_a\right) B\left(x + \frac{x_b}{2}, p + p_b\right).$$

We now formally expand the A and B functions in Taylor series in momenta $p_{a,b}$. The corresponding integrals over momenta may be evaluated employing $\sum_p \mathrm{e}^{\pm \mathrm{i}px} p^n = (\mp \mathrm{i})^n \delta^{(n)}(x)$, where $\delta^{(n)}$ denotes the n-th derivative of the delta-function. Subsequently, the integrals over coordinates $x_{a,b}$ may be also evaluated, leading to the formally exact expression

$$C(x, p) = A(x, p) \, \mathrm{e}^{\frac{\mathrm{i}}{2}\left(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right)} B(x, p), \tag{5.41}$$

where the arrows show the direction of the differentiation, and the scalar products in the exponent are $\partial_x \partial_p = \nabla_{\mathbf{r}} \nabla_{\mathbf{k}} - \partial_t \partial_\epsilon$.

This formally exact result is most useful when the exponential operator on its right hand side may be expanded and only the few lowest order terms kept. It is a legitimate procedure when the operator $\partial_x \partial_p$ may be regarded as small, i.e. if $(\delta x)(\delta p) \gg 1$, where δx and δp are characteristic scales at which the x and p arguments of the WT functions change. This in turn implies that the two-point functions of interest, say $A(x_1, x_2)$, are relatively slow functions of the central coordinate $x = (x_1 + x_2)/2$ and relatively fast functions of the distance between the two points $x' = x_1 - x_2$. The ultimate example is translationally invariant functions, e.g.

$A(x_1 - x_2) = A(x')$, for which $\partial_x = 0$ and therefore only the zeroth order term in the expansion of the exponent in Eq. (5.41) survives, leading to $C(p) = A(p)B(p)$, which is, of course, the well-known convolution theorem of the Fourier analysis. For the case where dependence on the central coordinate x is slow one finds

$$C = AB + \frac{\mathrm{i}}{2}\big(\partial_x A \partial_p B - \partial_p A \partial_x B\big) + \cdots , \tag{5.42}$$

where the arguments of all the functions are (x, p). As a result, WT is a tool to approximately substitute *convolutions* of two-point functions by *algebraic* products of the Wigner transforms and their derivatives. In the same approximation one finds for the commutator of two-point functions

$$[A \circ B] \overset{\mathrm{WT}}{\to} \mathrm{i}\big(\partial_x A \partial_p B - \partial_p A \partial_x B\big) + \cdots , \tag{5.43}$$

i.e. the classical Poisson bracket.

For an algebraic product of two-point functions, as, e.g., in Eqs. (5.36)–(5.38), $C(x_1, x_2) = A(x_1, x_2)B(x_1, x_2)$, one finds after WT

$$C(x, p) = \sum_q A\,(x, p - q)\; B\,(x, q)\,. \tag{5.44}$$

5.7 Kinetic term

A one-point function, such as, e.g., $V^{\mathrm{cl}}(x)$, should be considered as its own WT, which is momentum p independent. We find thus for the commutator in the kinetic term of Eq. (5.24)

$$[V^{\mathrm{cl}} \circ F] \overset{\mathrm{WT}}{\to} \mathrm{i}\partial_x V^{\mathrm{cl}}(x)\partial_p F(x, p) = \mathrm{i}\nabla_{\mathbf{r}} V^{\mathrm{cl}} \nabla_{\mathbf{k}} F - \mathrm{i}\partial_t V^{\mathrm{cl}} \partial_\epsilon F,$$

where $F(x, p) = F(\mathbf{r}, t, \mathbf{k}, \epsilon)$ is the WT of the two-point function $F(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2)$. We turn now to the other commutators in the kinetic terms on the right hand sides of the kinetic equations (5.24) and (5.35). The WT of the translationally invariant operator $\mathrm{i}\partial_t$ is ϵ, as a result $[\mathrm{i}\partial_t \circ F] \overset{\mathrm{WT}}{\to} \mathrm{i}\partial_\epsilon \epsilon \partial_t F = \mathrm{i}\partial_t F$, in a similar way $[-\partial_t^2 \circ F] \overset{\mathrm{WT}}{\to} \mathrm{i}\partial_\epsilon \epsilon^2 \partial_t F = 2\mathrm{i}\epsilon\partial_t F$. Finally, the WT of the operator $-\nabla_{\mathbf{r}}^2$ is $\mathbf{k}^2$ and thus $[-\nabla_{\mathbf{r}}^2 \circ F] \overset{\mathrm{WT}}{\to} -\mathrm{i}\nabla_{\mathbf{k}}\mathbf{k}^2\nabla_{\mathbf{r}} F = -2\mathrm{i}\mathbf{k}\nabla_{\mathbf{r}} F$. For a generic dispersion relation $\omega_{\mathbf{k}}$ one finds $[\omega_{\mathbf{k}}^2 \circ F] \overset{\mathrm{WT}}{\to} -2\mathrm{i}\omega_{\mathbf{k}}\mathbf{v}_{\mathbf{k}}\nabla_{\mathbf{r}} F$, where we introduced the group velocity as $\mathbf{v}_{\mathbf{k}} = \nabla_{\mathbf{k}}\omega_{\mathbf{k}}$. As for the right hand side of Eqs. (5.24) and (5.35), one finds for its WT

$$\Sigma^{\mathrm{K}} - F\Big(\Sigma^{\mathrm{R}} - \Sigma^{\mathrm{A}}\Big) - \mathrm{i}\partial_x\big(\mathrm{Re}\Sigma^{\mathrm{R}}\big)\partial_p F + \mathrm{i}\partial_p\big(\mathrm{Re}\Sigma^{\mathrm{R}}\big)\partial_x F,$$

where we took into account that $\Sigma^{\mathrm{A}}(x, p) = [\Sigma^{\mathrm{R}}(x, p)]^*$.

Combining all the pieces together, one finds for the WT of the kinetic equation (5.24) for the complex boson field

$$\left[\left(1-\partial_\epsilon \mathrm{Re}\Sigma^{\mathrm{R}}\right)\partial_t + (\partial_t \tilde{V})\partial_\epsilon + \tilde{\mathbf{v}}_{\mathbf{k}}\nabla_{\mathbf{r}} - (\nabla_{\mathbf{r}}\tilde{V})\nabla_{\mathbf{k}}\right] F = I^{\mathrm{coll}}[F], \tag{5.45}$$

where

$$\tilde{V}(x,\,p) = V^{\mathrm{cl}}(x) + \mathrm{Re}\left[\Sigma^{\mathrm{R}}(x,\,p)\right]; \quad \tilde{\mathbf{v}}_{\mathbf{k}} = \nabla_{\mathbf{k}}(\omega_{\mathbf{k}} + \mathrm{Re}\Sigma^{\mathrm{R}}) \tag{5.46}$$

and the right hand side, known as the *collision integral*, is

$$I^{\mathrm{coll}}[F] = \mathrm{i}\Sigma^{\mathrm{K}}(x,\,p) + 2F(x,\,p)\,\mathrm{Im}\left[\Sigma^{\mathrm{R}}(x,\,p)\right]. \tag{5.47}$$

Notice that in a static, i.e. $\partial_t = 0$, (including spatially non-uniform) situation *any* function $F(\epsilon)$ which depends on the energy argument only, nullifies the left hand side of the kinetic equation (5.45). As we shall see in the next section, there is one such function $F^{\mathrm{eq}} = \coth(\epsilon-\mu)/2T$, which also nullifies its right hand side. This is the equilibrium solution.

To make progress away from equilibrium, one changes the energy argument of the distribution function as

$$F(\mathbf{r},t,\mathbf{k},\epsilon) = \tilde{F}(\mathbf{r},t,\mathbf{k},\epsilon-\omega_{\mathbf{k}}-\tilde{V}). \tag{5.48}$$

One may check that the distribution function $\tilde{F}$, defined this way, satisfies the equation which differs from Eq. (5.45) only by the absence of the $(\partial_t\tilde{V})\partial_\epsilon$ term on the left hand side. Thus there is no derivative over the last argument in the equation for $\tilde{F}$. *Should* the collision integral depend only on the same local value of the renormalized energy $\tilde{\epsilon} = \epsilon - \omega_{\mathbf{k}} - \tilde{V}$, the kinetic equations for different $\tilde{\epsilon}$s would split and would not talk to each other. Strictly speaking, this is never the case. That is, the collision integral is actually a non-local function of $\tilde{\epsilon} = \tilde{\epsilon}(x,\,p)$ in both the energy and space-time directions. However, in many cases the distribution function $\tilde{F}(\mathbf{r},t,\mathbf{k},\tilde{\epsilon})$ is a much slower function of $\tilde{\epsilon}$ than $G^{\mathrm{R}} - G^{\mathrm{A}}$. The latter is a sharply peaked function at $\tilde{\epsilon} = 0$ with the width given by the inverse quasiparticle lifetime $1/\tau_{\mathrm{qp}}$. As long as the characteristic energy scale $\delta\tilde{\epsilon}$ of the distribution function $\tilde{F}(\mathbf{r},t,\mathbf{k},\tilde{\epsilon})$ is much larger than it, $\delta\tilde{\epsilon} \gg 1/\tau_{\mathrm{qp}}$, one may approximately disregard the $\tilde{\epsilon}$ dependence of $\tilde{F}$ in the collision integral. Indeed, the distribution function, by its definition Eq. (2.49), always shows up in a product with WT of $G^{\mathrm{R}} - G^{\mathrm{A}}$. Since the latter is a sharp function of the renormalized energy at $\tilde{\epsilon} = 0$, one may approximately put that

$$\tilde{F}(\mathbf{r},t,\mathbf{k},\tilde{\epsilon}) \approx \tilde{F}(\mathbf{r},t,\mathbf{k},0) \equiv \tilde{F}(\mathbf{r},t,\mathbf{k}) \tag{5.49}$$

and write down a closed kinetic equation for the *three*-argument, or the *mass-shell restricted* distribution function $\tilde{F}(\mathbf{r},t,\mathbf{k})$.[2] As long as quasiparticles are well

[2] The mass-shell distribution function may be defined as $\tilde{F}(\mathbf{r},t,\mathbf{k}) = \int \mathrm{d}\epsilon\, F(\mathbf{r},t,\mathbf{k},\epsilon)\delta(\epsilon-\omega_{\mathbf{k}}-\tilde{V})$. For free *non-interacting* particles $G^{\mathrm{R}} - G^{\mathrm{A}} = -2\pi\mathrm{i}\delta(\epsilon-\omega_{\mathbf{k}})$, while $G^{\mathrm{K}} = F(G^{\mathrm{R}} - G^{\mathrm{A}})$ and thus this definition is

defined, i.e. $\delta\tilde{\epsilon}\tau_{\rm qp} \gg 1$, the WT of $G^{\rm R} - G^{\rm A}$ remains a sharply peaked function at $\epsilon = \epsilon(\mathbf{r}, t, \mathbf{k})$ satisfying

$$\epsilon - \omega_{\mathbf{k}} - V^{\rm cl}(\mathbf{r}, t) - {\rm Re}\Sigma^{\rm R}(\mathbf{r}, t, \mathbf{k}, \epsilon) = 0, \tag{5.50}$$

cf. Eq. (5.21). As a result, all observables are *approximately* (in the leading order in $(\delta\tilde{\epsilon}\tau_{\rm qp})^{-1}$) determined by $\tilde{F}(\mathbf{r}, t, \mathbf{k})$. Such a "mass-shell" distribution function obeys the following closed kinetic equation:

$$\left[\tilde{Z}^{-1}\,\partial_t + \tilde{\mathbf{v}}_{\mathbf{k}}\nabla_{\mathbf{r}} - (\nabla_{\mathbf{r}}\tilde{V})\nabla_{\mathbf{k}}\right]\tilde{F}(\mathbf{r}, t, \mathbf{k}) = I^{\rm coll}[\tilde{F}], \tag{5.51}$$

where $\tilde{Z}^{-1}(\mathbf{r}, t, \mathbf{k}) = 1 - \partial_\epsilon {\rm Re}\Sigma^{\rm R}$. It is important that velocity and external potential are renormalized according to Eq. (5.46) and the energy argument $\epsilon = \epsilon(\mathbf{r}, t, \mathbf{k})$ of all functions is taken as the solution of Eq. (5.50).

The "mass-shell" distribution function $\tilde{F}(\mathbf{r}, t, \mathbf{k})$ is essentially a classical object. It may be considered as a time-dependent probability of finding a particle at a given point of the classical phase space $(\mathbf{r}, \mathbf{k})$. The quantum mechanics modifies the dispersion relation along with the effective potential and the *quasiparticle weight* $\tilde{Z}$ as well as (possibly) the collision integral. The kinetic equation (5.51) provides thus a semiclassical approximation of the full quantum description. It is instructive to compare the kinetic term (i.e. the left hand side) of Eq. (5.51) with that of the Fokker–Planck equation (4.30). Provided $\tilde{Z} = 1$, both may be written as $\partial_t \ldots - \{E, \ldots\}$, where the curly brackets stand for the classical Poisson brackets and the classical Hamiltonian is $E(\mathbf{k}, \mathbf{r}) = \omega_{\mathbf{k}} + \tilde{V}(\mathbf{r}, \mathbf{k})$. One observes, therefore, that the mass-shell distribution function $\tilde{F}(\mathbf{r}, t, \mathbf{k})$ has basically the same meaning as the classical probability distribution function $\mathcal{P}(\mathbf{R}, \mathbf{K}, t)$. The right hand side of the Fokker–Planck equation (4.30), being linear in $\mathcal{P}$, is different from the collision integral (see Section 5.8). The latter is a non-linear functional of the distribution function $\tilde{F}$. This difference originates from the fact that in the classical problems of Chapter 4 the bath was assumed to be passive and independent of the state of the system. In the present context the many-body system serves as a "bath" for itself.

equivalent to $\tilde{F}(\mathbf{r}, t, \mathbf{k}) = {\rm i}\int({\rm d}\epsilon/2\pi)\, G^{\rm K}(\mathbf{r}, t, \mathbf{k}, \epsilon) = {\rm i}G^{\rm K}(\mathbf{r}, \mathbf{k}, t, t)$. It is therefore frequently stated that the mass-shell distribution function is equivalent to the Keldysh Green function at the coinciding time arguments. As explained in Section 2.8, the latter is given by $2n_{\rm B}(\mathbf{k}) + 1$, where $n_{\rm B}(\mathbf{k})$ is the occupation number of the state $\mathbf{k}$. This latter relation between the equal-time Keldysh function and the occupation number is generic and remains true even in the interacting case. However, the relation between the equal-time Keldysh function and the mass-shell distribution function $\tilde{F}$ is *not*. It is restricted to the non-interacting case, where $G^{\rm R} - G^{\rm A} = -2\pi{\rm i}\delta(\epsilon - \omega_{\mathbf{k}})$. It is therefore important to stress that the kinetic equation is written for the mass-shell distribution function $\tilde{F}(\mathbf{r}, t, \mathbf{k})$ and *not* for the equal-time Keldysh Green function $G^{\rm K}(\mathbf{r}, \mathbf{k}, t, t)$. In particular, in equilibrium $\tilde{F} = \coth(\omega_{\mathbf{k}} - \mu)/2T$ is always a solution of the kinetic equation. On the other hand, the occupation number $n_{\rm B}(\omega_{\mathbf{k}})$ even in equilibrium may be very different from the Bose (or Fermi) distribution. The most famous example probably comes from the fermionic 1d Luttinger model [67], where the occupation number at $T = 0$ is not a Fermi step-function, but rather a power-law non-analytic function. This function is *not* a solution of the kinetic equation; in equilibrium the latter is solved by the Fermi distribution.

This latter "bath", however, is not passive and depends on the local state of the system. Hence the non-linear character of the collision term. Such a non-linearity is still a classical phenomenon (though specific transition rates may, of course, incorporate quantum mechanics in an essential way).

Finally let us formulate the kinetic equation for real boson quasiparticles, such as, e.g., elastic phonons. The Wigner transform of the kinetic term of the real boson Dyson equation (5.35) takes the form

$$\left[\partial_\epsilon\left(2\epsilon^2 - \mathrm{Re}\Sigma^{\mathrm{R}}\right)\partial_t + \partial_t \mathrm{Re}\Sigma^{\mathrm{R}}\partial_\epsilon + \nabla_{\mathbf{k}}\left(2\tilde{\omega}_{\mathbf{k}}^2\right)\nabla_{\mathbf{r}} - \nabla_{\mathbf{r}}(2\tilde{\omega}_{\mathbf{k}}^2)\nabla_{\mathbf{k}}\right] F,$$

where $\tilde{\omega}_{\mathbf{k}}^2 = \omega_{\mathbf{k}}^2 + \mathrm{Re}\Sigma^{\mathrm{R}}/2$. Due to the symmetries of the real boson Green functions, the distribution function F obeys

$$F(\mathbf{r}, t, \mathbf{k}, \epsilon) = -F(\mathbf{r}, t, -\mathbf{k}, -\epsilon). \tag{5.52}$$

Changing the energy argument of the distribution function and acknowledging that $\epsilon \approx \pm\tilde{\omega}_{\mathbf{k}}$, one arrives at the three-argument "mass-shell" distribution function

$$F(\mathbf{r}, t, \mathbf{k}, \epsilon) = s\tilde{F}(\mathbf{r}, t, s\mathbf{k}, \epsilon^2 - \tilde{\omega}_{\mathbf{k}}^2) \to s\tilde{F}(\mathbf{r}, t, s\mathbf{k}, 0), \tag{5.53}$$

where $s = \mathrm{sign}(\epsilon)$. Such a "mass-shell" distribution function obeys the closed kinetic equation

$$\left[\partial_t + \mathbf{v}_{\mathbf{k}}\nabla_{\mathbf{r}}\right]\tilde{F}(\mathbf{r}, t, \mathbf{k}) = I^{\mathrm{coll}}[\tilde{F}], \tag{5.54}$$

where for simplicity we disregarded the dispersion renormalization by the real part of the self-energy. We also took $\epsilon = \omega_{\mathbf{k}} > 0$, that brings the collision integral to the following form:

$$I^{\mathrm{coll}}[\tilde{F}] = \frac{1}{4\omega_{\mathbf{k}}}\left(\mathrm{i}\Sigma^{\mathrm{K}}(x, p) + 2F(x, p)\,\mathrm{Im}\left[\Sigma^{\mathrm{R}}(x, p)\right]\right)\Big|_{\epsilon=\omega_{\mathbf{k}}}. \tag{5.55}$$

Notice that taking $\epsilon = -\omega_{\mathbf{k}} < 0$ is equivalent to making a $\mathbf{k} \to -\mathbf{k}$ substitution in the kinetic equation (5.54).

5.8 Collision integral

We discuss now the collision integral, using real bosons with cubic non-linearity, Section 5.5, as an example. The collision integral for complex bosons is considered in Section 7.7. The proper collision integral is given by Eq. (5.55). To be consistent with the approximations adopted in the derivation of the kinetic term above, we need to restrict ourselves to products of WT only. In particular, $D_0^{\mathrm{K}}(x, p) \approx F(x, p)[D_0^{\mathrm{R}}(x, p) - D_0^{\mathrm{A}}(x, p)]$. Even though the Green functions here are the bare ones, the distribution function F is not determined by the dynamics of the free bosons. We should allow F to be self-consistently determined by

the kinetic part of the Dyson equation. Employing Eqs. (5.36)–(5.38) along with Eq. (5.44), one finds for the corresponding parts of the collision integral

$$\mathrm{i}\Sigma^{\mathrm{K}}(x,\,p) = 8\pi^2\gamma^2 \sum_q \Delta(x,\,p-q)\Delta(x,\,q)\Big[F(x,\,p-q)F(x,\,q)+1\Big], \quad (5.56a)$$

$$2\mathrm{Im}[\Sigma^{\mathrm{R}}(x,\,p)] = -8\pi^2\gamma^2 \sum_q \Delta(x,\,p-q)\Delta(x,\,q)\Big[F(x,\,p-q)+F(x,\,q)\Big], \quad (5.56b)$$

where the right hand side of the last equation is symmetrized with respect to arguments $p-q=\mathbf{k}-\mathbf{q}$, $\epsilon-\omega$ and $q=\mathbf{q}$, ω. Here we defined

$$\Delta(x,\,p) = \frac{\mathrm{i}}{2\pi}\big[D_0^{\mathrm{R}}(x,\,p) - D_0^{\mathrm{A}}(x,\,p)\big] = \frac{1}{4\omega_{\mathbf{k}}}\Big(\delta(\epsilon-\omega_{\mathbf{k}}) - \delta(\epsilon+\omega_{\mathbf{k}})\Big). \quad (5.57)$$

To include the renormalization of the dispersion relation $\omega_{\mathbf{k}}$ by the real part of the self-energy, one may use here the dressed Green functions D. This corresponds to the so-called self-consistent Born approximation, where the self-energy diagram is evaluated using self-consistently defined Green functions. Such an approximation neglects vertex corrections which may lead to a renormalization of the interaction parameter $\gamma \to \Gamma^{\alpha,\alpha',\alpha''}(q,\,p-q)$, where $\alpha = \mathrm{cl}, \mathrm{q}$. In some cases the full Γ may be found from independent considerations, in general one should write an additional equation for the vertex tensor and solve it in an approximation consistent with that for the self-energy.

Employing Eqs. (5.55) and (5.56), one finds for the collision integral

$$I^{\mathrm{coll}}[F] = \frac{2\pi^2\gamma^2}{\omega_{\mathbf{k}}} \sum_q \Delta(x,\,p-q)\Delta(x,\,q) \times \Big[F(x,\,p-q)F(x,\,q)+1-F(x,\,p)\big(F(x,\,p-q)+F(x,\,q)\big)\Big]. \quad (5.58)$$

The combination of the distribution functions in the square brackets is a very general construction, which repeats itself in higher orders in γ. Thanks to the energy delta-functions incorporated in the $\Delta(x,\,p)$ symbols and the "magic" identity:

$$\coth(a)\,\coth(b)+1 = \coth(a+b)\big(\coth(a)+\coth(b)\big), \quad (5.59)$$

the collision integral is identically nullified by the equilibrium Bose distribution $F(\mathbf{r},t,\mathbf{k},\epsilon) = F^{\mathrm{eq}}(\epsilon) = \coth(\epsilon-\mu)/2T$, where T and μ are yet unspecified temperature and chemical potential. For real bosons, due to the requirement that F is an odd function of energy, one has to choose $\mu = 0$. As explained after Eq. (5.47), any function $F = F(\epsilon)$ also nullifies the kinetic term in a stationary situation. As a result, the thermal equilibrium distribution function $F^{\mathrm{eq}}(\epsilon)$ solves the kinetic equation. Such a solution is (locally) stable for any temperature (the

latter is determined either by an external reservoir, or, for a closed system, from the conservation of total energy). Since the equilibrium distribution obviously nullifies both left and right hand sides of Eq. (5.35) the *exact* equilibrium self-energy satisfies $\Sigma^{\mathrm{K}} = \coth(\epsilon/2T)\left[\Sigma^{\mathrm{R}} - \Sigma^{\mathrm{A}}\right]$. Since also the bare Green functions obey the same relation, Eq. (2.48), one concludes that in thermal equilibrium the *exact* dressed Green function satisfies

$$D^{\mathrm{K}}(\mathbf{r}, \mathbf{k}, \epsilon) = \coth \frac{\epsilon}{2\,T} \Big(D^{\mathrm{R}}(\mathbf{r}, \mathbf{k}, \epsilon) - D^{\mathrm{A}}(\mathbf{r}, \mathbf{k}, \epsilon) \Big). \tag{5.60}$$

This is the statement of the *fluctuation–dissipation theorem* (FDT). Its consequence is that in equilibrium the Keldysh component does not contain any additional information with respect to the retarded one. Therefore, the Keldysh technique may be, in principle, substituted by a more compact construction – the Matsubara formalism. The latter does not work, of course, away from equilibrium. Notice that the Green functions may still be space dependent, since the equilibrium implies only stationarity, but *not* translational invariance in space.

To make progress away from equilibrium, one needs to restrict the two-point function F to the mass-shell function $\tilde{F}$ according to Eq. (5.53). This is possible due to the fact that $\Delta(x,\, p-q)$ and $\Delta(x, q)$ are sharply peaked at $\epsilon - \omega = \pm\omega_{\mathbf{k}-\mathbf{q}}$ and $\omega = \pm\omega_{\mathbf{q}}$, while the external argument is to put $\epsilon = \omega_{\mathbf{k}} > 0$. Once the distribution functions are restricted to the "mass-shell," the energy dependence in Eq. (5.58) is explicitly specified by Eqs. (5.53) and (5.57). Thus one can perform the ω-integration explicitly with the help of the delta-functions and find for the collision integral

$$\begin{aligned} I^{\mathrm{coll}}[\tilde{F}(\mathbf{k})] = {} & \frac{\pi\gamma^2}{16\omega_{\mathbf{k}}} \sum_{\mathbf{q}} \frac{1}{\omega_{\mathbf{k}-\mathbf{q}}\omega_{\mathbf{q}}} \\ & \times \Big\{ \delta(\omega_{\mathbf{k}} - \omega_{\mathbf{q}} - \omega_{\mathbf{k}-\mathbf{q}}) \Big[\tilde{F}(\mathbf{k}-\mathbf{q})\tilde{F}(\mathbf{q}) + 1 - \tilde{F}(\mathbf{k})\big(\tilde{F}(\mathbf{k}-\mathbf{q}) + \tilde{F}(\mathbf{q})\big) \Big] \\ & + \delta(\omega_{\mathbf{k}} + \omega_{\mathbf{q}} - \omega_{\mathbf{k}-\mathbf{q}}) \Big[\tilde{F}(\mathbf{k}-\mathbf{q})\tilde{F}(-\mathbf{q}) - 1 + \tilde{F}(\mathbf{k})\big(\tilde{F}(\mathbf{k}-\mathbf{q}) - \tilde{F}(-\mathbf{q})\big) \Big] \\ & + \delta(\omega_{\mathbf{k}} - \omega_{\mathbf{q}} + \omega_{\mathbf{q}-\mathbf{k}}) \Big[\tilde{F}(\mathbf{q}-\mathbf{k})\tilde{F}(\mathbf{q}) - 1 - \tilde{F}(\mathbf{k})\big(\tilde{F}(\mathbf{q}-\mathbf{k}) - \tilde{F}(\mathbf{q})\big) \Big] \Big\}, \end{aligned} \tag{5.61}$$

where we have suppressed slow space-time argument $\mathbf{r}, t$ in the distribution functions $\tilde{F}(\mathbf{r}, t, \mathbf{k}) \to \tilde{F}(\mathbf{k})$. There are three types of process allowed by energy conservation. To appreciate the structure of the corresponding terms it is convenient to express their rates through the boson occupation number $n_{\mathbf{q}}$ related to the distribution function as $\tilde{F}(\mathbf{q}) \approx 2n_{\mathbf{q}} + 1$.[3] Then the rate of the first process is

[3] As discussed in the footnote after Eq. (5.49), this relation is only approximate, valid to the leading order in $(\delta\tilde{\epsilon}\tau_{qp})^{-1}$.

proportional to $[n_{\mathbf{k}-\mathbf{q}}n_{\mathbf{q}} - n_{\mathbf{k}}(n_{\mathbf{k}-\mathbf{q}} + n_{\mathbf{q}} + 1)]$. It states that the state $\mathbf{k}$ may be populated due to the merging of particles from states $\mathbf{q}$ and $\mathbf{k}-\mathbf{q}$ and depopulated due to stimulated emission of $\mathbf{k}-\mathbf{q}$ and $\mathbf{q}$ phonons, or spontaneous emission. The rate of the second process is proportional to $[n_{\mathbf{k}-\mathbf{q}}(n_{-\mathbf{q}} + n_{\mathbf{k}} + 1) - n_{\mathbf{k}}n_{-\mathbf{q}}]$. Here the state $\mathbf{k}$ may be populated due to stimulated or spontaneous decay of a higher energy state $\mathbf{k}-\mathbf{q}$ and depopulated by merging with a particle in a state $-\mathbf{q}$. Finally the rate of the third process is proportional to $[n_{\mathbf{q}}(n_{\mathbf{q}-\mathbf{k}}+n_{\mathbf{k}}+1)-n_{\mathbf{k}}n_{\mathbf{q}-\mathbf{k}}]$ and the physics is the same as in the second process with states $\mathbf{q}$ and $\mathbf{k}-\mathbf{q}$ interchanged.

Within the mass-shell approximation the equilibrium solution of the kinetic equation (5.61) takes the form $\tilde{F}^{\mathrm{eq}}(\mathbf{r},\mathbf{k}) = \coth\omega_{\mathbf{k}}(\mathbf{r})/2T$, which is, in general, a function of coordinates and momenta. Since on the mass-shell $\epsilon = \omega_{\mathbf{k}}(\mathbf{r})$, this is consistent with $F^{\mathrm{eq}}(\mathbf{r},\mathbf{k},\epsilon) = \coth\epsilon/2T$. The latter statement is exact, while the mass-shell one is only an approximation valid for well-defined quasiparticles.

For the dispersion relation of the quantum membrane $\omega_{\mathbf{k}} = \sqrt{\omega_0^2 + \kappa\mathbf{k}^4}$, the energy conservation law $\omega_{\mathbf{k}} = \omega_{\mathbf{q}} + \omega_{\mathbf{k}-\mathbf{q}}$ may be satisfied for $k > k_{\mathrm{c}}$, where $k_{\mathrm{c}}^4 = 4\omega_0^2/\kappa$. For smaller momenta $k < k_{\mathrm{c}}$ the cubic non-linearity alone does not provide relaxation of the distribution function. Therefore it does not lead to thermalization, if the resulting temperature is too small $T \lesssim 2\omega_0$. On the other hand, if a high-energy $k \gg k_{\mathrm{c}}$ mode is excited it decays onto $\mathbf{q}$ and $\mathbf{k}-\mathbf{q}$ modes with almost perpendicular momenta. To find the corresponding relaxation time we restrict the collision integral to the spontaneous emission part in the first term in Eq. (5.61) and find $\partial_t n_{\mathbf{k}} = -n_{\mathbf{k}}/\tau_{\mathbf{k}}$, where

$$\frac{1}{\tau_{\mathbf{k}}} = \frac{\pi\gamma^2}{8\omega_{\mathbf{k}}}\sum_{\mathbf{q}}\frac{\delta(\omega_{\mathbf{k}}-\omega_{\mathbf{q}}-\omega_{\mathbf{k}-\mathbf{q}})}{\omega_{\mathbf{k}-\mathbf{q}}\omega_{\mathbf{q}}} = \frac{3}{128\pi}\,\frac{\gamma^2}{\kappa^2k^5}\,\ln\left(\frac{k}{k_{\mathrm{c}}}\right), \tag{5.62}$$

for $d = 3$.

Finally, let us discuss approximations involved in the Wigner transformations. It is a justified procedure as long as $\delta\mathbf{k}\,\delta\mathbf{r} \gg 1$, where $\delta\mathbf{k}$ is a characteristic microscopic scale of the momentum dependence of the distribution function, while $\delta\mathbf{r}$ is a characteristic scale of its spatial variations. One may ask if there is a similar requirement in the time domain: $\delta\epsilon\,\delta t \gg 1$, with $\delta\epsilon$ and δt being the characteristic energy and the time scale, respectively. Such a requirement is very demanding, since typically $\delta\epsilon \approx T$ and at low temperature it would allow us to treat only very slow processes with $\delta t \gg 1/T$. Fortunately, this is not the case. Because of the peaked structure of $\Delta(\mathbf{k},\epsilon)$, the energy argument ϵ is locked to $\tilde{\omega}_{\mathbf{k}}$ (i.e. to the "mass-shell") and does not have its own dynamics as long as the peak is sharp. The actual criterion is therefore that $\delta\epsilon$ is much larger than the width of the peak in $\Delta(\mathbf{k},\epsilon)$. The latter is the inverse quasiparticle lifetime, $1/\tau_{\mathrm{qp}}$, and therefore the

actual condition is $\tau_{\rm qp} \gg 1/T$. This condition is indeed satisfied in systems with well-defined quasiparticles. Notice that this is exactly the same condition which we employed to justify the restriction of the distribution function to the mass-shell, see Eq. (5.49) and the discussion below it. This is thus a necessary condition for the applicability of the quasi-classical kinetic equation.