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REVIEW ARTICLE

Martingales for physicists: a treatise on stochastic thermodynamics and beyond

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We review the theory of martingales as applied to stochastic thermodynamics and stochastic processes in physics more generally.

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Notations and definitions

We introduce the main notations used in this work (see also the List of Symbols below).

We denote stochastic, physical processes by X_t, where $t \geq 0$ is a discrete ($t = 0, 1, 2, \ldots$) or continuous ($t \geq 0$) time index, and where X_t takes values in the set $\mathcal{X}$, which we call the state space. Depending on the definition of $\mathcal{X}$, the random variable X_t can be scalar or vectorial, and discrete or continuous. For example, if $\mathcal{X} = \mathbb{R}$, then X_t is a one-dimensional process on the real line. We denote the path (trajectory) of X in the time interval $[s, t]$ by $X_{[s,t]} = \{X_u\}_{u \in [s,t]}$.

Elements of the set $\mathcal{X}$ are denoted by $x \in \mathcal{X}$. We use small letters to distinguish them from the stochastic process X. Also, we use $x_{[s,t]} = \{x_u\}_{u \in [s,t]}$ for a deterministic trajectory, in contrast with the stochastic trajectory $X_{[s,t]}$.

Random variables are associated with their probability $\mathcal{P}$. For example, $\mathcal{P}(X_t > 0)$ is the probability that X_t is positive. We also use $\mathcal{P}$ for a probability density of random variable. In particular, when $\mathcal{X}$ is discrete, then the probability density of the trajectory $X_{[0,t]}$ reads

$$\mathcal{P}(x_{[0,t]}) \equiv \mathcal{P}(X_0 = x_0, \ldots, X_t = x_t), \tag{1}$$

for all $x_{[0,t]} \in \mathcal{X}^{t+1}$, and when $\mathcal{X}$ is continuous, then the probability density is defined by

$$\mathcal{P}(x_{[0,t]}) \equiv \mathcal{P}\left(X_0 \in [x_0, x_0 + \mathrm{d}x_0]\,, , \ldots, X_t \in [x_t, x_t + \mathrm{d}x_t]\right), \tag{2}$$

for all $x_0, x_1, \ldots, x_t \in \mathcal{X}$. Probability densities are normalized, i.e.,

$$\sum_{x_0 \in \mathcal{X}} \cdots \sum_{x_t \in \mathcal{X}} \mathcal{P}(x_{[0,t]}) = 1 \tag{3}$$

for discrete-time processes with discrete state space $\mathcal{X}$, and

$$\int_{x_0 \in \mathcal{X}} \cdots \int_{x_t \in \mathcal{X}} \mathcal{P}(x_{[0,t]}) \mathcal{D}x_{[0,t]} = 1, \tag{4}$$

for discrete-time processes with continuous state space $\mathcal{X}$, where we have introduced the notation $\mathcal{D}x_{[0,t]} = \mathrm{d}x_0 \ldots \mathrm{d}x_t$.

We write expected values (averages) with respect to the path probability $\mathcal{P}$ as $\langle \cdot \rangle$. For example, for $\mathcal{X}$ discrete, the expectation (also called "average") value of X_t is given by

$$\langle X_t \rangle = \sum_{x_t \in \mathcal{X}} x_t\, \mathcal{P}(x_{[0,t]}) = \sum_{x \in \mathcal{X}} x\, \rho_t(x). \tag{5}$$

If X_t is continuous, we have

$$\langle X_t \rangle = \int_{x_t \in \mathcal{X}} \mathcal{D}x_{[0,t]} x_t\, \mathcal{P}(x_{[0,t]}) = \int_{x \in \mathcal{X}} \mathrm{d}x\, x\, \rho_t(x). \tag{6}$$

We use $\rho_t(x)$ to denote the instantaneous probability density for both continuous and discrete random variables, see Equations (5) and (6). For discrete X_t, we formally define the instantaneous probability density by

$$\rho_t(x) = \langle \delta_{X_t,x} \rangle \equiv \sum_{x_t \in \mathcal{X}} \mathcal{P}(x_{[0,t]}) \delta_{x_t,x} = \sum_{x_t \in \mathcal{X}} \mathcal{P}(x_t) \delta_{x_t,x}, \tag{7}$$

where $\delta_{i,j}$ is Kronecker's delta. For X_t continuous, we have

$$\rho_t(x) = \langle \delta(X_t - x) \rangle \equiv \int_{x_t \in \mathcal{X}} \mathcal{D}x_{[0,t]} \mathcal{P}(x_{[0,t]}) \delta(x_t - x) = \int_{x_t \in \mathcal{X}} \mathrm{d}x_t \mathcal{P}(x_t) \delta(x_t - x), \tag{8}$$

where $\delta(x)$ is the Dirac delta function. The instantaneous density is normalized as $\sum_{x \in \mathcal{X}} \rho_t(x) = 1$ for discrete X_t and as $\int_{x \in \mathcal{X}} \mathrm{d}x \rho_t(x) = 1$ for continuous X_t, for all $t \geq 0$.

A key concept in martingale theory is the expectation of an observable at a time t conditioned on its history up to a previous time $s \leq t$. A simple example of conditional expectation is that of the physical process X_t itself. If X_t is discrete, such conditional expectation is given by

$$\langle X_t | X_{[0,s]} \rangle = \sum_{x \in \mathcal{X}} x \, \mathcal{P}(X_t = x | X_0, X_1, \ldots, X_s), \tag{9}$$

whereas if X_t is a continuous random variable,

$$\langle X_t | X_{[0,s]} \rangle = \int_{x \in \mathcal{X}} \mathrm{d}x \, x \, \mathcal{P}(X_t \in [x, x + \mathrm{d}x] \, | X_0, X_1, \ldots, X_s). \tag{10}$$

For a discrete random variable Y, we use $\rho_Y(y) = \mathcal{P}(Y = y)$ to denote the probability. For a continuous random variable Y, we denote the probability density by

$$\rho_Y(y) \equiv \frac{\mathcal{P}(Y \in [y, y + \mathrm{d}y])}{\mathrm{d}y}. \tag{11}$$

Analogously, we use the notation $\rho_Y(y|X_0 = x)$ for a conditional probability density, in this case conditioned on $X_0 = x$.

List of symbols

$\mathcal{X}$	State space, continuous or discrete
$\delta(x)$	Dirac's delta function for $\mathcal{X}$ continuous
$\delta_{x,y}$	Kronecker's delta function for $\mathcal{X}$ discrete: $\delta_{x,x} = 1$ and $\delta_{x,y} = 0$ for $y \neq x$
$\mathrm{d}x$	Lebesgue measure (counting measure) for $\mathcal{X}$ continuous (discrete)
t	Time (continuous or discrete)
X_t	Value of the physical process at time t, $X_t \in \mathcal{X}$
$X_{[s,t]}$	Stochastic trajectory $X_{[s,t]}$ in $[s,t]$, with $s \leq t$
$\mathcal{P}(x_{[0,t]}) = \mathcal{P}_{[0,t]}(x_{[0,t]})$	Path probability for the stochastic trajectory $X_{[0,t]}$ to be equal to $x_{[0,t]}$, i.e., path probability for $x_{[0,t]}$ to occur in the interval $[0,t]$
$\mathcal{P}_{[r,s]}(x_{[0,t]})$	Path probability marginal of $\mathcal{P}(x_{[0,t]})$ on the time interval $[r,s]$, with $0 \leq r \leq s \leq t$
$\mathcal{T}$	Stopping time

$\langle \cdot \rangle$ or $\langle \cdot \rangle_{\mathcal{P}}$	Expectation (average) with respect to the path probability $\mathcal{P}$, see Equations (5)–(6) for explicit expressions of the average $\langle X_t \rangle$
$Z_t \equiv Z[X_{[0,t]}]$	Functional of $X_{[0,t]}$ (X-adapted observable)
$\langle Z_u \vert X_{[s,t]} \rangle$	Conditional expectation of Z_u with respect to the filtration generated by $X_{[s,t]}$. For example, $\langle X_t \vert X_{[0,s]} \rangle$ is the average of X_t conditioned on the process tracing a specific trajectory $X_{[0,s]}$ in the interval $[0, s]$, with $0 \leq s \leq t$
$\rho_Y(y)$	Probability density $\rho_Y(y) \equiv \mathcal{P}(Y \in [y, y + \mathrm{d}y])/\mathrm{d}y$ for a continuous random variable Y Probability $\rho_Y(y) \equiv \mathcal{P}(Y = y)$ for a discrete random variable Y
$\rho_t(x)$ or $\rho_t^{\mathcal{P}}(x)$	Instantaneous density (or probability) of the process, given by $\rho_t(x) = \langle \delta(X_t - x) \rangle$ One-point marginal of the path-probability $\mathcal{P}(x_{[0,t]})$
$\rho_{\mathrm{st}}(x)$	Stationary probability density (or probability) of the process
$\mathcal{P}(x_t \vert x_s)$	Conditional probability density for the process to be at $X_t = x_t$ at time t given that at time s the value of the process $X_s = x_s$, with $x_s, x_t \in \mathcal{X}$
$\mathcal{L}_t$	Markovian generator of a generic Markov process
$\mathcal{L}_t^\dagger$	Adjoint of Markovian generator with respect to the canonical scalar product
π_t	Accompanying density, solution of $\mathcal{L}_t^\dagger \pi_t = 0$
T	Temperature of the thermal bath
$k_{\mathrm{B}} = 1$	Boltzmann's constant, set equal to one in this review
$\boldsymbol{\mu}_t(x)$	Mobility matrix
$F_t(x) = -(\nabla V_t)(x) + f_t(x)$	Force vector, with $V_t(x)$ potential and $f_t(x)$ a non-conservative force
$\mathbf{D}_t(x)$	Diffusion matrix
B_t	Wiener process
$\dot{B}_t$	Gaussian white noise
$\dot{X}_t = \nu_t(X_t) + \sqrt{2\mathbf{D}_t(X_t)}\dot{B}_t$	Ito–Langevin equation (overdamped dynamics), with $\nu_t(x) = (\boldsymbol{\mu}_t F_t + \nabla \mathbf{D}_t)(x)$
$\mathbf{D}_t(x) = \frac{T}{2}(\boldsymbol{\mu}_t(x) + [\boldsymbol{\mu}_t(x)]^\dagger)$	Einstein's relation for isothermal processes, with † denoting matrix transposition For symmetric mobility matrix, it reads $\mathbf{D}_t(x) = T\boldsymbol{\mu}_t(x)$
$\omega_t(x, y)$	Transition rate at time t from state x to state y for a Markov-jump process in continuous time
$w_t(x, y)$	Transition probability at time t from state x to state y for a Markov-jump process in discrete time
$J_{t,\rho}(x)$	Instantaneous probability current associated with the density ρ_t For a diffusion process, $J_{t,\rho}(x) = (\boldsymbol{\mu}_t F_t \rho_t)(x) - (\mathbf{D}_t \nabla \rho_t)(x)$ For a jump process, $J_{t,\rho}(x, y) = \rho_t(x)\omega_t(x, y) - \rho_t(y)\omega_t(y, x)$

W_t	Stochastic work done on the system in the time interval $[0,t]$ along a stochastic trajectory $X_{[0,t]}$
Q_t	Stochastic heat absorbed by the system in the time interval $[0,t]$ along a stochastic trajectory $X_{[0,t]}$
$Q_t + W_t = V_t(X_t) - V_0(X_0)$	First law of stochastic thermodynamics along a stochastic trajectory $X_{[0,t]}$
$S_t^{\text{sys}} = -\ln(\rho_t(X_t))$	Stochastic system entropy at time t. The system entropy change along a stochastic trajectory $X_{[0,t]}$ in $[0,t]$ reads $\Delta S_t^{\text{sys}} = S_t^{\text{sys}} - S_0^{\text{sys}} = \ln(\rho_0(X_0)/\rho_t(X_t))$
S_t^{env}	Stochastic environmental entropy change along a stochastic trajectory $X_{[0,t]}$ in $[0,t]$
S_t^{tot}	Stochastic total entropy production along a stochastic trajectory $X_{[0,t]}$ in $[0,t]$
Θ_t	Time reversal operator. In this Review, it is applied to a trajectory $x_{[0,t]}$ as follows: $[\Theta_t(x_{[0,t]})]_s \equiv x_{t-s}$
$\Lambda_t^{\mathcal{P},\mathcal{Q}} = \ln\left[\frac{\mathcal{P}(X_{[0,t]})}{\mathcal{Q}(X_{[0,t]})}\right]$	Λ-entropic functional (associated with a pair of path probabilities $\mathcal{P}$ and $\mathcal{Q}$) evaluated over the stochastic trajectory $X_{[0,t]}$
$\Sigma_t^{\mathcal{P},\mathcal{Q}} = \ln\left[\frac{\mathcal{P}(X_{[0,t]})}{\mathcal{Q}^{(t)}(\Theta_t(X_{[0,t]}))}\right]$	Σ-entropic functional (associated with a pair of path probabilities $\mathcal{P}$ and $\mathcal{Q}$) evaluated over the stochastic trajectory $X_{[0,t]}$
$\Sigma_{[r,s];t}^{\mathcal{P},\mathcal{Q}} = \ln\left[\frac{\mathcal{P}_{[r,s]}(X_{[0,t]})}{\mathcal{Q}^{(t)}_{[t-s,t-r]}(\Theta_t(X_{[0,t]}))}\right]$	Generalized Σ-entropic functional over the subset time interval $[r,s] \subseteq [0,t]$
$D_{\text{KL}}[\rho_X(x)\|\|\sigma_X(x)]$	Kullback–Leibler divergence between the normalized distributions $\rho_X(x)$ and $\sigma_X(x)$ of the random variable $X \in \mathcal{X}$. For the distributions of a random variable with support $\mathcal{X}$ it is given by $D_{\text{KL}}[\rho_X(x)\|\|\sigma_X(x)] = \int_{\mathcal{X}} \mathrm{d}x\, \rho_X(x) \ln\left[\frac{\rho_X(x)}{\sigma_X(x)}\right]$

List of Theorems

Chapter 1. Introduction

Before leaving, M. M. asked me to go to her casino, to take some money and to play, taking her as my partner. I did so. I took all the gold I found, and playing the martingale, doubling my stakes continuously, I won every day during the rest of the carnival. Giacomo Casanova, *History of My Life* (1789).

1.1. *Why this treatise?*

Models based on stochastic processes have proven to be useful in non-equilibrium statistical physics. As a consequence, an extensive set of techniques from stochastic processes have become mainstream in non-equilibrium statistical physics, one notable example being large-deviation theory [1]. Nevertheless, few works in statistical physicists use martingales.

Martingales play a central role in the theory of stochastic processes and find important applications in statistics and mathematical finance. In contrast, applications of martingale theory in physics are limited. This is somewhat surprising, given that unbiased random walks and Brownian motion are martingales. These processes are of paramount importance in physics and many of their important properties can be easily derived using that they are martingales.

An explanation for the absence of martingales in contemporary statistical physics is that martingales are not presented in textbooks and classic references used by physicists to study stochastic processes [2–8]. For physicists, learning martingale theory is a quest, which can be achieved through an exhaustive reading of mathematical textbooks, just like Don Quixote reading cavalric romances, until losing their mind to become a knight errant [9].

This treatise gives an overview of the aspects of martingale theory that we think are important for physics. In particular, we build on recent works that develop martingales in statistical physics [10–16]. We emphasize this work is a treatise rather than a review, inasmuch we discuss a topic in depth by providing a thorough overview of published results but also include extensive novel material. We shall show that martingales are ubiquitous in nonequilibrium physics (i.e., in stochastic thermodynamics), that martingales provide fundamental insights into central concepts in nonequilibrium physics (i.e., on the second law of thermodynamics), and that martingales constitute a powerful tool for mathematical derivations (i.e., for splitting probabilities and extreme value statistics). The review is aimed at readers with a basic knowledge on nonequilibrium statistical mechanics and stochastic processes. It covers mathematical definitions and properties in a comprehensive way, explains how to apply such results to nonequilibrium physics, and discusses applications of martingales in interdisciplinary fields.

1.2. *How to read this treatise*

This treatise is organized as follows. Chapter 1 presents historical remarks on the origin of martingales and provides a few illustrative examples of martingales in physics. Chapter 2 introduces mathematical definitions and key examples of martingales. Chapter 3 revisits the concept of Markov processes and its importance in statistical physics, and discusses its relation with martingales. Chapter 4 presents martingale properties and theorems. Chapter 5 introduces martingale theory in stochastic thermodynamics through paradigmatic examples of stochastic processes. Chapter 6 elaborates advanced knowledge in stochastic thermodynamics; it provides mathematical rigor on how martingales can be identified and applied in the study of a broad class of nonequilibrium processes (stationary and non-stationary), in particular martingales related to path probability ratios. Chapter 7 further elaborates the connection between thermodynamics and martingales by presenting universal properties of entropy production in nonequilibrium stationary states. Chapter 8 reviews recent work that applied martingale theory to non-stationary isothermal processes, revealing fluctuation theorems at stopping times. Chapter 9 presents a tree-like hierarchy of second law that descends from martingale properties of probability ratios. Chapter 10 discusses martingales in the context of progressive quenching in physics. Finally, Chapters 11 and 12 review, respectively, applications of martingales in population dynamics and quantitative finance. Chapter 13 briefly reviews applications of martingales in quantum collapse and presents the conclusion of this review.

Key concepts, results, and theorems that we think are essential in this treatise are highlighted in gray boxes. Sections with advanced content, most of which novel material, and often not recommended for a first read unless for intrepid readers, are highlighted with a superscript$^{\spadesuit}$ at the beginning of their title. We recommend to consult the List of Symbols placed after the Table of Contents. Lengthy mathematical proofs and supplemental material are relegated to the Appendices. As martingales are "fair" games, we do not guarantee potential readers will become wealthy after reading this treatise, but to acquire rich knowledge after a patient and dedicated read.

Depending on the reader's interests and background, it may be preferable to focus on selected chapters of this treatise. Below and in Figure 1.1, we provide possible roadmaps:

- *To know what are martingales and their properties*. We recommend to read Chapter 2 to get a primer on martingales, Chapter 3 to establish connections with Markov processes and Chapter 4 to learn about the key theorems and mathematical relations in martingale theory.
- *To learn foundations of stochastic thermodynamics*. We recommend to first read Chapter 5 and then if sufficiently audacious Chapter 6 (at valiant heart nothing is impossible).
- *For readers with basic notions on stochastic thermodynamics wanting to learn its connection to martingales*. We recommend to first read Chapter 5 to refresh key concepts and learn the martingale structure of the second law in Langevin stationary processes. Further, we recommend to read Chapters 7 and 8 (together with Chapter 4 as a mathematical background) to learn how martingale theory can unveil new universal properties in stochastic thermodynamics.
- *For readers with advanced notions on stochastic thermodynamics wanting to reach the "nirvana" on martingality*. We recommend first to read Chapters 5 and 6 to get the detailed fundamentals on the martingale structure of stochastic thermodynamics, both in stationary and non-stationary setups. Next, we suggest to read Chapters 7 and 8 (with Chapter 4 as a mathematical complement) to learn how martingale theory can unveil new universal properties in stochastic thermodynamics. After this acquired knowledge, the nirvana on martingality can be acquired through a dedicated read of Chapter 9.
- *For fans of the second law of thermodynamics*. We recommend to first read Chapter 5 and then Chapters 7, 8, and 9.
- *For biophysicists wishing to learn the basics of martingales and their applications.* We recommend to start with Chapter 2 to get an informal primer on martingales, Chapter 3.2 to learn basics of continuous-time Markov processes, then Chapter 5 to learn foundations of stochastic thermodynamics and/or Chapter 11 to get familiarized with applications to population dynamics.

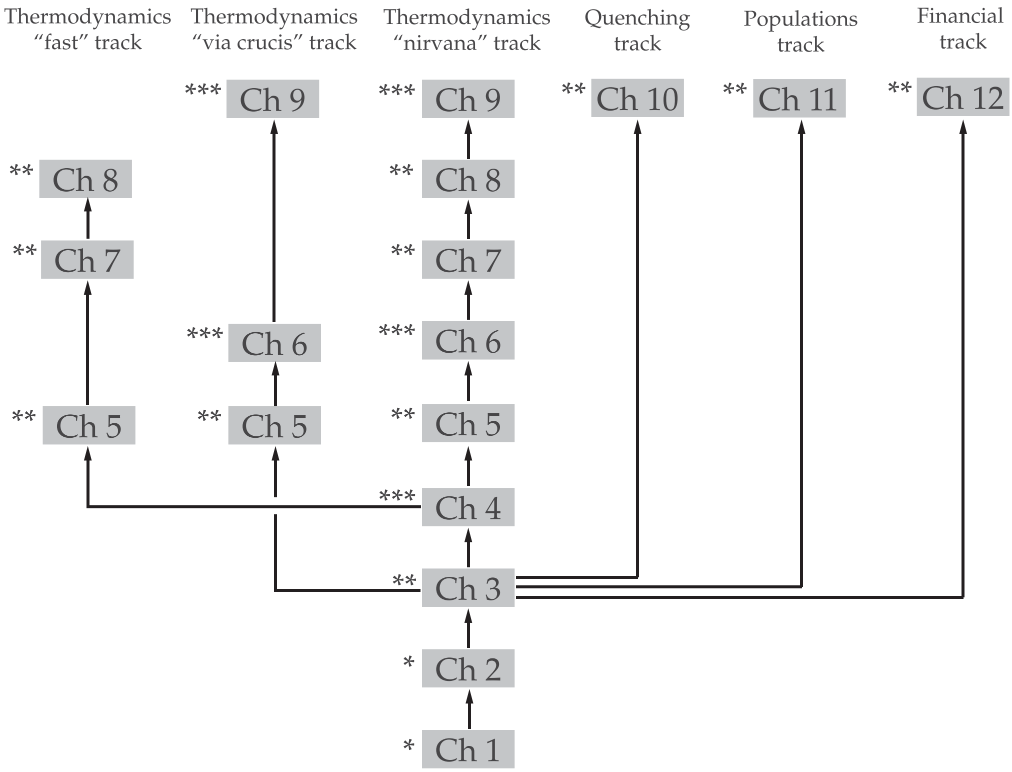

Figure 1.1. Roadmap to this treatise. The branches illustrate different tracks that readers may take when reading this treatise. We classify the each chapter's level of difficulty as * easy, ** normal, and *** advanced.

- *For experts in martingales that want to learn stochastic thermodynamics*. We recommend to first read Chapter 5 and then Chapter 6.
- *To learn applications of martingales other than thermodynamics*. We recommend to read Chapters 2–4 to familiarize with the mathematical properties and examples of martingales, before exploring applications of martingale theory in other domains, in particular progressive quenching (Chapter 10) and population dynamics (Chapter 11).
- *For those looking for arbitrage opportunities in the stock market*. We highly recommend to read Chapter 12 where we revisit how martingale theory is applied in quantitative finance.

1.3. *History of martingales*

1.3.1. *Etymological origin of the word " martingale"*

The word "martingale" presents numerous etymologies that spread across disciplines including: gambling, mathematics, finance, geography, technology and vernacular language [17–19]. The origin of this word dates back to the sixteenth and seventeenth centuries at the foundations of probability theory in France. One of its first appearances in the literature is Casanova's memories from 1754. Its etymology remains obscure; it is mentioned in early French, Spanish and Catalan dictionaries, which highlight the Mediterranean roots of martingales. Some of the usages of the word martingale, in roughly inverse chronological order, are:

- The word “martingale” has a formal meaning in probability theory. Martingales are stochastic processes without drift, i.e., their expected value in the future is given by the last value of a sequence of past observations. Research on the mathematical properties of martingales were mainly developed by Doob in the twentieth century, and applied to derive key results in the theory of stochastic processes, as we discuss in the following chapters.
- In mathematical finance, martingale processes have been used for decades as paradigmatic models of fair markets in which there exists no arbitrage opportunities. Martingale theory has been notoriously boosted in financial research. Krickeberg famously stated:

  > I was never tempted to get involved in the applications of martingales to the theory and, worse, the practice of financial speculations that have contributed in no small measure to the present crisis of the world’s money markets and economy.

- In game theory and gambling, martingales represent fair games of chance in which any player may win or lose with equal probability, irrespective of the previous outcomes of the game. Such “fair” games of chance motivated the origin of probability theory in the seventeenth century. Even earlier, the book of Fra Luca Paccioli (1494) already discussed fair games in the spirit of what today are known as martingales.
- Giacomo Casanova’s memories [20] provide the arguably first literary reference of the word:

  > J’y fus [au casino de Venise], j’ai pris tout l’or que j’ai trouvé, et portant avec la force qu’en terme de jeu on dit à la martingale, j’ai gagné trois et quatre fois par jour pendant tout le rest de carnaval.[1]

  The dictionary of the Académie Française describes Casanova’s gaming strategy as “betting all that was lost”.
- Abbé Prevost describes the martingale as the celebrated playing strategy where the gambler doubles his/her stake at each loss to quit with a sure profit, provided that he/she wins once. In casino’s roulette this is called the “Double Up” strategy. Alexandre Dumas describes this strategy in *La Femme au collier de velours* as “introuvable comme l’âme” (unreachable like the soul) being put at work during the last days of the life of an old gambler who spent all his life looking for the martingale.
- Martingales have also an equestrian meaning, which is in nowadays registered in, i.e., Oxford’s English dictionary as “a strap or set of straps running from the noseband or reins to the girth of a horse, used to prevent the horse from raising its head too high”. Similarly, the Spanish word *almártaga*, which refers also to a horse harness is also considered among one of the possible etymological roots of the word martingales.
- Mistral’s Provençal dictionary cites *martegalo* as the demonym of the residents of Martigues, a French city located northwest of Marseille, currently nested within the Provençe–Alpes–Côte d’Azur region. The isolated location of the Martigues area, at the merger of three boroughs, brought according to Mistral’s dictionary a “proverbial reputation of naivety”. In the same dictionary, we find the Provençal expression *jouga a la martegalo*, which means to play in an absurd – and thus not necessarily fair – way.
- The word *martegalo* is used in sailing as a rope attached above the bowsprit needed to secure the flying jib, and sailors called *martegaux* were famous for net fishing in the south of Italy and Andalusia.
- Cotgrave’s dictionary relates martingales to a sailor’s dance consisting of a repetitive and rough stamping of the ground with the heels. This is mentioned in Charles IX trip to Brignoles (1564) with his court where “the citizens tried to please him through [. . .] the dances of the area [. . .] dances named volte or martingale”.

- In Rabelais' series of novels *Gargantua*, the character Panurge wears the martingale pants, which contain an orifice at the back. In Rabelais' words, "a drawbridge [...] that makes excretion easier".
- Letters from the seventeenth century of a prophetess nicknamed La Martingale have been reported, containing doubtful prophecies (i.e., for the fate of Louis XIV) often accompanied by requests for donations.
- In vernacular language, martingale has been used to refer to prostitutes, courtesans, street-walkers, etc. This meaning can be found in old slang dictionary and also in Scarron's *Virgile Travesti*.
- In Italian language, "martingala" has yet another meaning: a sort of half-belt which tightens the back of a jacket or a coat (Figure 1.2).

1.3.2. *Martingales in probability theory*

The true explosion of the concept of martingales in mathematics dates back to the works by Joseph Leo Doob in the 1940s. Doob proved many fundamental inequalities and limit theorems associated with martingales. These results deeply changed the field of probability theory. In the following years, finding a suitable martingale became the "skeleton key" to solve a challenging new problem in probability theory.

Two important precursors of Doob in martingale theory are:

- Jean Ville, who introduced for the first time the concept of martingale in mathematics in his PhD Thesis "Etude critique de la notion de collectif" (1939) [21]. His thesis includes the first proofs of the so-called Doob's maximal inequality. Doob, who took part to Ville's PhD Thesis committee, recognized that Ville's thesis was a major inspiration for his work.
- Paul Lévy, whose work is in some way, related to martingale theory. For instance, his book "Stochastic Processes and Brownian Motion" (1948) deeply influenced probability theory. Levy's writing style is informal and focused on explanations rather than on mathematical proofs, in contrast with Doob's rigorous and dry mathematical style.

  In 1953, Doob published the influential book "Stochastic Processes" [22], which contains the mathematical foundations of what today is called martingale theory. In the second half of the twentieth century, martingales have provided a new perspective on a plethora of problems in probability theory, for example:
- Stroock and Varadhan introduced in 1969 the "martingale problem" [23], which enable to characterize the distribution of a stochastic process through a martingale condition. In particular, for Markovian processes, this martingale can be expressed in terms of the

Figure 1.2. Some celebrated "Martingales". Left: Rules of game in the roulette of casino in Montecarlo. Middle: Painting of the village of Martigues (France). Right: Joseph L. Doob, mathematician who pioneered the development of martingale processes in probability theory.

infinitesimal generator. This problem is particularly well suited to characterize the limit of a family of Markov processes.

- In stochastic calculus, martingales are stochastic processes that form good integrators. Indeed, the theory of integration with respect to a Wiener process has been extended to integrals that use general martingales as integrators [24].

1.3.3. *Martingales in gambling*

Martingales originated in a class of betting strategies that were popular in the eighteenth-century France. These strategies can be summarized by the principle: "if you lose, double your wager size". Consider a betting involving two gamblers X and Y. Suppose X starts to toss the coin, taken to be fair, with a betting amount of 50. If the outcome is a head, X retains this amount, otherwise loses it to Y. The coin is tossed, and it falls on the tail. Using the martingale strategy, X now increases the betting amount to 100. The coin is tossed, but again it falls on the tail, and so X again doubles the betting amount. So by the time X tosses the coin for the third time, the total amount that X has lost to Y is 350. The coin is tossed, and now, to X's merriment, the coin falls on the head, and so X gets from Y an amount of 400. In the process, X has retained the initial amount of 50. The amount of the winning trade in the above martingale betting strategy exceeds the combined losses of all the previous trades, and the difference is the amount of the original trade. It is evident that the strategy would result in a profit for a gambler, but as we will see in this treatise this assumes that the gambler has infinite (i.e., unbounded) wealth to keep on betting and doubling the betting amount until he wins. Note also that the casino knows that bankruptcy is a possible outcome in case of infinite wealth. To avoid such possibility, a casino often uses table limits to control the maximum bets that a player can play. Most casinos in Las Vegas Strip usually offer tables with a 10,000$ limit. We note, however, that such limits do not exist in financial markets, and investing in the stock market with Casanova's strategy could imply a huge bankruptcy!

The strategy of doubling up on a loss is what had been the betting strategy of Casanova mentioned earlier. Denoting by S_i the total accumulated score up to the ith toss included, and given the outcomes of $i > 1$ tosses, the expectation value of S_{i+1} reads

$$\langle S_{i+1} | S_1, S_2, \ldots, S_i \rangle \geq S_i, \tag{1.1}$$

which makes the stochastic process S_i a *submartingale*, see Ch. 2 for formal definitions.

1.3.4. *Martingales in finance*

Quantitative finance employs mathematical and statistical tools to anticipate the value of financial assets as stocks and options. From early days, physics models such as random walks have been invoked to discuss stock pricing. Jules Augustin Frédéric Regnault, an assistant to a French stock broker, was one of the first to propose a modern theory of stock pricing in his 1863 treatise *Calcul des Chances et Philosophie de la Bourse*, in which he writes "*l'écart des cours est en raison directe de la racine carrée des temps*", which translates as "price deviation is directly proportional to the square root of time". Louis Jean-Baptiste Alphonse Bachelier, a French mathematician who lived at the turn of the twentieth century, was the first to propose as part of his PhD thesis *Théorie de la spéculation* a mathematical model for Brownian motion and how it may be used for discussing stock pricing. His contributions make him arguably the forefather of mathematical theory of finance.

However, it is the American economist Eugene Francis "Gene" Fama whom some people argue is the father of finance, owing to his ground-breaking work in the area, and in particular, for proposing the so-called efficient-market hypothesis. This hypothesis states that in an efficient market, it would not be possible to make definite predictions about future price on the basis of the information available today, so that the best prediction that one can make for the expected future price discounted to the present time is today's price itself. The hypothesis forms a cornerstone of modern financial theory, and in the light of the present review, an implication of the hypothesis is that asset price is a martingale. We will explore this connection in more detail in Chapter 12, in which, among others, we will discuss the very-influential Black–Scholes model used widely by options market participants round the world. This model, named after American economists Fischer Black and Myron Scholes, provides a theoretical estimate of the price of European-style option. The model was introduced in the 1973 paper by Black and Scholes titled "The Pricing of Options and Corporate Liabilities", and published in the *Journal of Political Economy*. Robert C. Merton published his article in this area, "Theory of Rational Option Pricing", in *The Bell Journal of Economics and Management Science*, in which he coined the term "Black–Scholes theory of option pricing". For their work, Black and Merton were awarded the Nobel Prize in Economic Sciences for the year 1997 (Scholes because of his death in 1995 was considered ineligible for the prize).

1.3.5. *Martingales in stochastic thermodynamics*

Stochastic thermodynamics describes the non-equilibrium behavior of mesoscopic systems [25–27]. The application of martingale theory to stochastic thermodynamics has a short yet fruitful history, see, i.e., Refs. [10–16,28–32]. Classical fluctuation relations of stochastic thermodynamics, such as the integral fluctuation relation and Jarzynski's equality, can be understood with martingale theory, and martingale theory generalizes these fluctuation relations, providing a better understanding of fluctuations in mesoscopic systems. In particular, with martingale theory we obtain fluctuation relations at random times and for the extreme values of stochastic processes, while stochastic thermodynamics usually deals with fluctuations at fixed time. Also, martingale theory implies versions of the second law of the thermodynamics for mesoscopic systems that are stronger than those obtained in "standard" stochastic thermodynamics, providing us with a better understanding of the implications of the second law at mesoscopic scales. In particular, the martingale versions of the second law reveal how the observer's knowledge about a system's history affects the second law of thermodynamics. This body of work forms the core of this review (Chapers 5–9), and now we provide some "historical" remarks.

The link between fluctuation relations in stochastic thermodynamics and martingales was first highlighted in Ref. [10]. Reference [11] rediscovered the link between martingales and fluctuation relations in stochastic thermodynamics within the setup of stationary processes, and moreover used the mathematical properties of martingales to derive universal relations for the statistics of extreme-values and stopping-times of entropy production. The results from Ref. [11] were rederived in Ref. [12] within the context of Langevin processes by using Itô calculus and random-time transformations, and Ref. [13] shows how most of the results of Ref. [11] follow readily from one relation, namely, the integral fluctuation relation for entropy production at stopping times. The integral fluctuation relation for entropy production at stopping times is thus a key result of martingale theory for stochastic thermodynamics, and Ref. [13] also introduces the ensuing second law of thermodynamics at stopping times. This latter version of the second law of thermodynamics describes how classical limits in thermodynamics can be overcome by stopping at a cleverly chosen moment. Some of these results have been experimentally verified in single-electron boxes [33] and granular systems [29].

Martingales theory also plays a role for trade-off inequalities between the rate of entropy production, speed, and precision. Reference [34] derives a bound relating first-passage times of

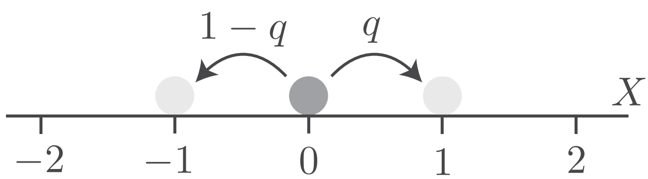

Figure 1.3. Illustration of a discrete-time biased random walk. A particle (gray circle) moves in a one dimensional lattice X (black line). At every (discrete) time step, the particle jumps either forward (positive X direction) with probability q or backward (negative X direction) with probability $1-q$.

current-like observables to the average rate of dissipation. A more in-depth analysis in Ref. [35] shows that this bound can be interpreted as a tradeoff between dissipation, speed, and precision within a first-passage setup, and that the bound is related to the so-called thermodynamic uncertainty relations [36–38]. Moreover, using martingale theory, Ref. [35] shows that the bound is tight for currents proportional to the entropy production, and hence is optimal in this case.

More recently, martingales have been employed to describe fluctuations of generic nonequilibrium Markov process driven by arbitrary external protocols [14,15,28,31,39]. Reference [14] derives in this setup a second law of thermodynamics at stopping times and a Jarzynski equality at stopping times. Reference [15] also provides Jarzynski-like relations and generalized second laws at stopping times, albeit using nonequilibrium free energies instead of equilibrium free energies, and illustrates the result in an experimentally-realized "gambling" demon which stops the dynamics of a process following specific criteria. Further applications of martingales in stochastic thermodynamics have been reported, e.g., in quantum systems [40], molecular motors [41], periodically-driven systems [31], and photoelectric devices [42].

1.4. *"Warm-up" on martingales*

As a first encounter with martingales, we discuss simple random walks, which are possibly the simplest example of martingale processes.

We denote by X_t the position of a one-dimensional, discrete-time, biased, random walk at times $t = 0, 1, 2, \dots$, with initial condition $X_0 = 0$ (see Figure 1.3 for an illustration). For $t \geq 1$, the position of the walker is given by

$$X_t \equiv \sum_{s=1}^{t} \xi_s, \tag{1.2}$$

where ξ_s are independent increments which take the value $+1$ with probability $q < 1$ and -1 with probability $1-q$. The average (expectation) value of X at time t reads $\langle X_t \rangle = \sum_{s=1}^{t} \langle \xi_s \rangle = (2q-1)t$.

What is the expected value of X_t at time $t > 0$ given its history $X_{[0,s]}$ up to a previous time $s < t$? This *conditional expectation* is formally defined as

$$\langle X_t | X_{[0,s]} \rangle = \sum_{x \in \mathcal{X}} x \, \mathcal{P}(X_t = x | X_0, X_1, \dots, X_s), \tag{1.3}$$

where $P(X_t | X_0, X_1, \dots, X_s)$ is the conditional probability of X_t given $X_{[0,s]} = X_0, X_1, \dots, X_s$. For our example,

$$\langle X_t | X_{[0,s]} \rangle = X_s + \sum_{r=s+1}^{t} \langle \xi_r \rangle = X_s + (2q-1)(t-s). \tag{1.4}$$

If $q = 1/2$, then the random walk is unbiased and satisfies the *martingale* property expressed by

$$\langle X_t | X_{[0,s]} \rangle = X_s. \tag{1.5}$$

If $q \geq 1/2$, then X_t is a, so-called, *submartingale* for which $\langle X_t | X_{[0,s]} \rangle \geq X_s$, whereas if $q \leq 1/2$, then X_t is a *supermartingale* $\langle X_t | X_{[0,s]} \rangle \leq X_s$. In words, a martingale is a fair, unbiased process whereas a submartingale (supermartingale) is a biased process with positive (negative) drift.

Interestingly, we can transform a biased random walk (sub or supermartingale) into a martingale. For example, the position of the walker in the comoving frame $Y_t = X_t - vt$, with $v = (2q - 1)$ the net drift, is a martingale.

We can construct infinite martingales from X_t systematically, as we discuss now. A useful trick is to use the multiplicative structure

$$M_t \equiv \prod_{s=1}^{t} \eta_s, \tag{1.6}$$

where η_s are independent random variables with $\langle \eta_s \rangle = 1$, and thus $\langle \eta_s \eta_t \rangle = \langle \eta_s \rangle \langle \eta_t \rangle = 1$ for all $s \neq t$. As one can readily verify, processes of the form (1.6) are martingales, i.e., $\langle M_t | M_{[0,s]} \rangle = M_s$, for any $t \geq s \geq 0$. A possible choice is [43]

$$\eta_s \equiv \frac{\exp(y\xi_s)}{\langle \exp(y\xi_s) \rangle} = \frac{\exp(y\xi_s)}{q \exp(y) + (1-q)\exp(-y)}, \tag{1.7}$$

where $y \in \mathbb{R}$ is a real number. Plugging (1.7) into (1.6), we obtain

$$M_t = \frac{\exp(yX_t)}{[q \exp(y) + (1-q)\exp(-y)]^t}, \tag{1.8}$$

which are martingales for all $y \in \mathbb{R}$. As we motivate later in this treatise, a "popular" choice in stochastic thermodynamics is $y = \ln[(1-q)/q]$, yielding the exponential process

$$M_t = \exp\left[-X_t \ln\left(\frac{q}{1-q}\right)\right] = \left(\frac{1-q}{q}\right)^{X_t}. \tag{1.9}$$

Let us investigate some consequences of the family of martingales M_t, given by Equation (1.8). Expanding M_t in small values of y yields

$$\begin{aligned} M_t &= 1 + \left.\frac{\partial M_t}{\partial y}\right|_{y=0} y + \left.\frac{\partial^2 M_t}{\partial y^2}\right|_{y=0} \frac{y^2}{2!} + O(y^3) \\ &= 1 + y(X_t - vt) + \frac{y^2}{2}[(X_t - vt)^2 - \sigma^2 t] + O(y^3), \end{aligned} \tag{1.10}$$

where

$$v \equiv \langle X_t \rangle / t = (2q - 1) \tag{1.11}$$

and

$$\sigma^2 \equiv 4q(1-q). \tag{1.12}$$

Because M_t is a martingale for all values of $y \in \mathbb{R}$, also $M_t^{(k)} = \frac{\partial^k M_t}{\partial y^k}|_{y=0}$ are martingales, as for any integer $k \geq 1$ they can be written as the difference between two martingales. As a result, all the coefficients in the expansion (1.10) are martingales, in particular,

$$M_t^{(1)} = X_t - vt \tag{1.13}$$

$$M_t^{(2)} = (X_t - vt)^2 - \sigma^2 t, \tag{1.14}$$

and so forth, are martingales. Note that the higher-order derivatives give $M_t^{(k)}$ in terms of powers of X_t up to degree k. The martingale property of $M_t^{(k)}$ can be used to obtain exact expressions for the centered moments of X_t, i.e., $\langle X_t \rangle = vt$ and $\langle (X_t - \langle X_t \rangle)^2 \rangle = \sigma^2 t$.

Martingales are also useful for studying stochastic processes at *stopping times*. Stopping times generalize first-passage times [8]. Put simply, a stopping time is the first time when a process satisfies a certain prescribed condition, provided that the condition is fulfilled at a finite time; otherwise the stopping time is infinite. An example of a stopping time $\mathcal{T}$ is the first time when the biased random walk X_t, starting at $X_0 = 0$, reaches any of two absorbing boundaries located at $L > 0$ and $-L < 0$, i.e., the first exit time from the interval $(-L, L)$. In some cases, such as in the present example of a biased random walk, it is possible to use martingales to determine analytically the absorption probabilities and the mean first-passage time [8,44]. The absorption probabilities P_+ and $P_- = 1 - P_+$ for the walker at the positive and negative boundaries, respectively, are given by

$$P_+ = \frac{1 - \left(\frac{1-q}{q}\right)^L}{1 - \left(\frac{1-q}{q}\right)^{2L}} \quad \text{and} \quad P_- = \frac{\left(\frac{1-q}{q}\right)^L - \left(\frac{1-q}{q}\right)^{2L}}{1 - \left(\frac{1-q}{q}\right)^{2L}}, \tag{1.15}$$

for $q \neq 1/2$ (biased random walk), and

$$P_+ = P_- = 1/2, \tag{1.16}$$

for $q = 1/2$ (unbiased random walk); see Appendix A for an explicit derivation of Equations (1.15)–(1.16). Note that the average value of the "exponential" martingale given by Equation (1.9) evaluated at the first exit time $\mathcal{T}$ out of the $(-L, L)$ reads

$$\langle M_{\mathcal{T}} \rangle = P_- \left(\frac{1-q}{q}\right)^{-L} + P_+ \left(\frac{1-q}{q}\right)^{L} = P_+ + P_- = 1, \tag{1.17}$$

i.e., it is equal to the initial value of the martingale $M_0 = ((1-q)/q)^0 = 1$. In other words, using exit times out of a symmetric interval, the process $M_{\mathcal{T}}$ can on average neither win not lose with respect to the initial wealth $M_0 = 1$, see Eq. (1.9).

The mean first-passage time for $q \neq 1/2$ is given by (see Appendix A)

$$\langle \mathcal{T} \rangle = \frac{L}{1-2q} - \frac{2L}{1-2q} \frac{1 - \left(\frac{1-q}{q}\right)^L}{1 - \left(\frac{1-q}{q}\right)^{2L}} = \frac{L}{1-2q} - \frac{2L}{1-2q} P_+ = \frac{L}{v}(P_+ - P_-), \tag{1.18}$$

where we have used $v = 2q - 1$, and for $q = 1/2$ the mean first-passage time reads

$$\langle \mathcal{T} \rangle = L^2. \tag{1.19}$$

Combining Equations (1.15) and (1.18), and using $v = 2q - 1$ we obtain that

$$\langle M_{\mathcal{T}}^{(1)} \rangle = L(P_+ - P_-) - v \langle \mathcal{T} \rangle = 0, \tag{1.20}$$

which holds for all values of $q \in [0, 1]$. This further illustrates the *fairness* of martingales, as the average value of $M^{(1)}$ at the first exit time equals to its initial value $M_0^{(1)} = 0$.

Perhaps more striking (and less intuitive) is the fact that Equation (1.20) also holds for the mean escape time of the unbiased random walk $M_t^{(1)}$ from *asymmetric* intervals $(-L_-, L_+)$ with $L_+, L_- > 0$ any two integer threshold values, with $L_+ \neq L_-$. In other words, one cannot "win" neither "lose" with the martingale $M_t^{(1)}$ irrespective of the chosen stopping strategy. For example, for $L_- \gg L_+$, the many trajectories that escape the interval through the positive boundary, L_+, are balanced by the few trajectories that escape the interval through the negative boundary, L_-. This points out to the flaw in Casanova's gambling strategy as the wins on most days are balanced by a few big losses.

This result is illustrated in the left panel in Figure 1.4 for the choice $L_+ = 5$ and $-L_- = -10$. Consider a gambler that expects to obtain profit by "stopping" an unbiased random walk whenever it escapes the interval $(-L_-, L_+)$. Let L_+ the wealth gained by the gambler if the random walk first reaches the positive threshold, and $-L_-$ the wealth lost by the gambler if instead the random walk first reaches the negative threshold. The gambler may expect that he/she could get a net profit from the fact that the random walk will reach the positive threshold more often than the negative one, even if the dynamics of the process is unbiased. However, because the unbiased random walk is a martingale, the probability for first reaching the positive threshold $P_+ = L_+/(L_+ + L_-)$ whereas $P_- = L_-/(L_+ + L_-)$ for first reaching the negative one [8]. As a result, the net wealth after many repetitions of this gambling strategy $\langle M_{\mathcal{T}} \rangle = P_+ L_+ - P_- L_- = 0 = M_0$ equals to its initial value, i.e., it is a *fair* strategy that leads to no net win neither to net loss on average. The validity of this property for arbitrary values of the negative threshold value $-L_-$ is further illustrated with numerical simulations in the right panel in Figure 1.4

Equations (1.17) and (1.20) are two examples of the so-called Doob's optional stopping theorem. Loosely said, Doob's optional stopping theorem states that the martingale condition also holds when stopping a process at a clever moment, viz.,

$$\langle M_{\mathcal{T}} \rangle = \langle M_0 \rangle \tag{1.21}$$

holds, where M is a martingale and $\mathcal{T}$ a stopping time. Drawing an analogy with fair games, Equation (1.21) states that it is not possible to win on average with a martingale, as its expected outcome at the end of the game equals to its expected initial value. In this treatise, we will use repeatedly Doob's optional stopping theorem to simplify first-passage-time calculations. For example, as we will show in this treatise, using Doob's optional stopping theorem, Equation (1.17) and (1.20) can be used to shortcut analytical calculations for, i.e., splitting probabilities P_- and P_+ and mean first-passage times.

1.5. *Martingales in biophysics*

We discuss briefly how martingales can be a useful concept in biophysics. For this purpose, we discuss a minimal model of the motion of a molecular machine (motor) on a filament (Figure 1.5).

A molecular motor binds to a linear filament, which provides a periodic, one-dimensional, lattice of binding sites. The filament has a polar asymmetry, which specifies the direction of motion. The motor catalyzes the hydrolysis of a fuel, Adenosinetriphosphate (ATP) to the diphosphate form (ADP), releasing inorganic phosphate (P). This reaction provides an amount $\Delta\mu = \mu_{\mathrm{ATP}} - (\mu_{\mathrm{ADP}} + \mu_P)$ of chemical free energy. As the system is driven out of thermodynamic equilibrium, it will step stochastically from binding site to binding site with a bias in a direction given by the filament polarity. In the presence of an external force $f_{\mathrm{ext},}$ it can perform mechanical work $f_{\mathrm{ext}} a$ per step, where a is the spacing between binding sites.

For simplicity, we describe the molecular motor stepping process as a continuous-time Markov-jump process (a biased random walk), using a discrete position variable $X_t = x \in \mathbb{Z}$ which describes the discrete binding sites. Transitions from site x to $x + 1$ occur at a rate

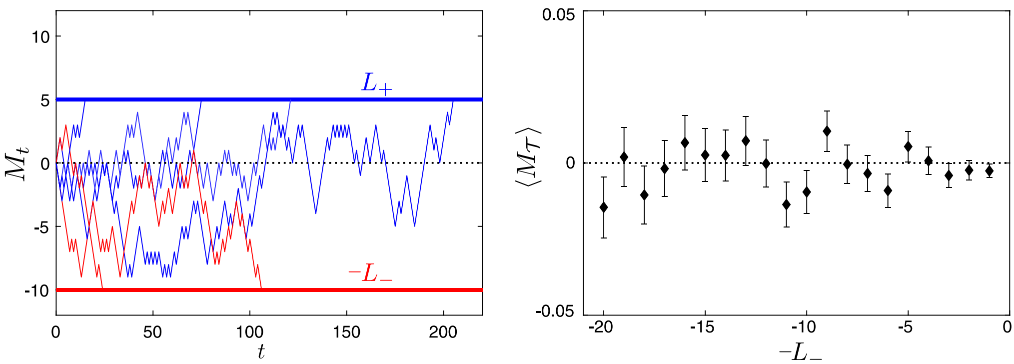

Figure 1.4. Gambling with martingales and stopping conditions. Left: Sample trajectories (lines) of the martingale given by the one-dimensional, discrete-time, random walk described by Equation (1.2), and sketched in Figure 1.3, with equal forward and backward jump probabilities $p = q = 1/2$. Right: Average value $\langle M_{\mathcal{T}} \rangle$ of the random walk evaluated at the stopping time $\mathcal{T}$ given by the first time M_t reaches either $-L_-$ or L_+, for fixed $L_+ = 5$ and different values of $-L_-$. The symbols are obtained from $N = 10^6$ simulations and the error bars from the standard error of the mean. The horizontal dotted lines set to $M_0 = 0$ illustrate Doob's optional stopping theorem $\langle M_{\mathcal{T}} \rangle = M_0 = 0$.

$\omega(x, x+1) = \omega_+$, and transitions in the opposite direction occur at a rate $\omega(x, x-1) = \omega_-$. We can write

$$\omega_\pm = \nu \exp(\pm A/2), \tag{1.22}$$

where

$$\nu = \sqrt{\omega_+ \omega_-} \quad \text{and} \quad A = \ln(\omega_+/\omega_-) \tag{1.23}$$

are the *kinetic* rate and *affinity* of the motor, respectively. In the simplest case of a motor that tightly couples ATP hydrolysis and stepping in a one-to-one manner, thermodynamics requires that the ratio between forward and backward rates is

$$\frac{\omega_+}{\omega_-} = \exp[\beta(\Delta\mu - a f_{\text{ext}})], \tag{1.24}$$

and thus

$$A = \beta(\Delta\mu - a f_{\text{ext}}), \quad \text{with } \beta = T^{-1}. \tag{1.25}$$

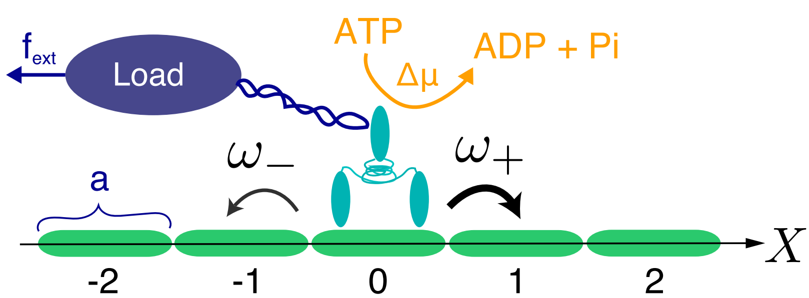

Figure 1.5. Illustration of the minimal stochastic model of molecular motor motion, given by a Markov-jump process in a discrete lattice (a 1D biased random walk). The transition rates are given by $\omega_+ = \nu \exp(A/2)$ and $\omega_- = \nu \exp(-A/2)$, for forward and backward steppings respectively. See text for further details.

We recall readers that we take the Boltzmann constant $k_B = 1$ throughout the treatise. The kinetic rate ν depends on ATP concentration, the external force, and on internal time scales of the motor molecule.

The probability $\rho_t(x)$ to find the motor at position $x = X_t$ at time t obeys the Master equation

$$\frac{\partial \rho_t(x)}{\partial t} = \omega_+ \rho_t(x-1) - (\omega_+ + \omega_-)\rho_t(x) + \omega_- \rho_t(x+1). \tag{1.26}$$

For the initial condition $\rho_0(x) = \delta_{x,0}$, the solution is given by

$$\rho_t(x) = \left(\frac{\omega_+}{\omega_-}\right)^{-x/2} \exp\left[-(\omega_+ + \omega_-)t\right] I_x(2\sqrt{\omega_+\omega_-}t), \tag{1.27}$$

where $I_x(y)$ denotes the modified Bessel function of the first kind. This can be seen using the relations $\mathrm{d}I_x(y)/\mathrm{d}y = I_{x-1}(y) - (x/y)I_x(y)$ and $\mathrm{d}I_x(y)/\mathrm{d}y = I_{x+1}(y) + (x/y)I_x(y)$ which follow from the generating function

$$\sum_{x=-\infty}^{\infty} z^x I_x(y) = \exp\left[y(z+z^{-1})/2\right]. \tag{1.28}$$

The position of the motor is described by the stochastic variable X_t where we choose $X_0 = 0$. Interestingly, the stochastic process [cf. Equation 1.9]

$$M_t = \exp(-AX_t) = \exp\left[-\left(\ln\frac{\omega_+}{\omega_-}\right)X_t\right] \tag{1.29}$$

is a martingale with respect to X_t. This can be proved by noting first that

$$\left\langle M_{t+\mathrm{d}t} \middle| X_{[0,t]}\right\rangle = M_t \left\langle \frac{M_{t+\mathrm{d}t}}{M_t} \middle| X_{[0,t]}\right\rangle = M_t \left\langle \left(\frac{w_-}{w_+}\right)^{X_{t+\mathrm{d}t}-X_t} \middle| X_{[0,t]}\right\rangle. \tag{1.30}$$

Then the central argument here is then that by definition of the transition rate we have the equality

$$\begin{aligned}\left\langle \left(\frac{w_-}{w_+}\right)^{X_{t+\mathrm{d}t}-X_t} \middle| X_{[0,t]}\right\rangle &= \left(\frac{w_-}{w_+}\right) w_+\mathrm{d}t + \left(\frac{w_-}{w_+}\right)^{-1} w_-\,\mathrm{d}t \\ &\quad + \left(\frac{w_-}{w_+}\right)^{0} (1-(w_+ + w_-)\,\mathrm{d}t) + O(\mathrm{d}t^2) \\ &= 1 + O(\mathrm{d}t^2).\end{aligned} \tag{1.31}$$

Combining (1.30) with (1.31), we get $\langle M_{t+\mathrm{d}t}|X_{[0,t]}\rangle = M_t + O(\mathrm{d}t^2)$, therefore using the *tower rule* (Appendix B.2) we have for any $0 \le s < t$:

$$\left\langle M_{t+\mathrm{d}t} \middle| X_{[0,s]}\right\rangle = \left\langle\left\langle M_{t+\mathrm{d}t} \middle| X_{[0,t]}\right\rangle \middle| X_{[0,s]}\right\rangle = \left\langle M_t \middle| X_{[0,s]}\right\rangle + O(\mathrm{d}t^2), \tag{1.32}$$

which implies that $\frac{\mathrm{d}}{\mathrm{d}t}\langle M_t|X_{[0,s]}\rangle = 0$, and then the martingale property

$$\left\langle M_t \middle| X_{[0,s]}\right\rangle = M_s. \tag{1.33}$$

Analogously, one can retrieve the martingale M_t in Equation (1.29) by taking the continuous-time limit of the process (1.8) for the choice $z = A = \ln(\omega_+/\omega_-)$.

We also note that $\exp(-AX_t)$ is not the *only* martingale associated with X_t. In fact, an infinite number of martingales can be defined as functions of X_t and can be constructed similarly as for the discrete-time case in Section 1.4 (see Equation 1.8). The treatise will shed light on how to construct martingales from X_t and why this is useful.

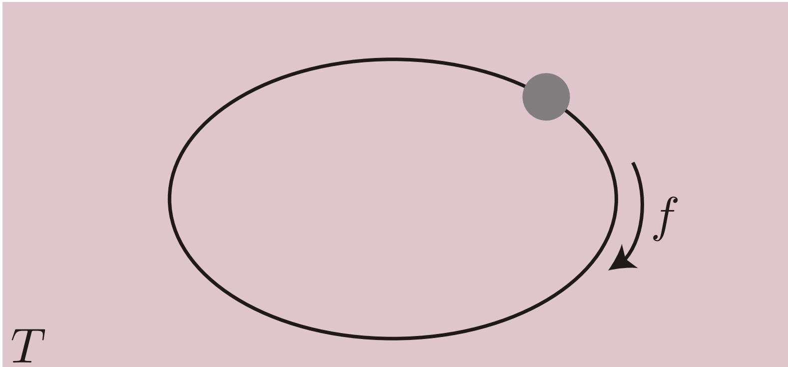

Figure 1.6. Illustration of a minimal stochastic model of nonequilibrium dynamics. A Brownian particle (gray circle) immersed in a thermal bath at temperature T (red box) is subject to move along a ring under the action of an external constant force f.

1.6. *Martingales on a ring*

The martingales given by Equations (1.9) and (1.29) in Sections 1.4 and 1.5, respectively, can be expressed as

$$M_t = \exp(-\text{Entropy production in } [0, t]). \tag{1.34}$$

For a single step of the random walker, the entropy flow into the environment is given by $(X_t - X_{t-1}) \log q/(1-q)$, which measures the degree of irreversibility via the ratio of the probabilities of forward and backward steps, as will be discussed in Chapter 5. In the example of the molecular motor, the entropy flow associated with a step is proportional to $\pm A = \pm\beta(\Delta\mu - af_{\text{ext}})$ which is the heat dissipated to the environment in a forward or backward step. The martingality of the process (1.34) lies at the root of the use of martingales in stochastic thermodynamics, and we discuss this extensively in this treatise.

In this section, we review the connection between stochastic thermodynamics and martingales by discussing the paradigmatic example of a driven particle on a ring. This example, besides its simplicity, is illuminating because it reveals the martingale structure of stochastic entropy production in a simple yet nontrivial way.

We consider the dynamics of a driven overdamped Brownian particle on a ring, see Figure 1.6 for an illustration. A constant, homogeneous external force f is applied to the particle along the ring. The particle moves with mobility μ within a thermal bath that is at temperature T. The dynamics of the position X of the particle is assumed to obey a one-dimensional overdamped Langevin equation

$$\dot{X}_t = \mu f + \sqrt{2\mu T}\dot{B}_t, \tag{1.35}$$

where $\dot{B}_t$ is a zero-mean Gaussian white noise $\langle \dot{B}_t \rangle = 0$ with autocorrelation $\langle \dot{B}_t \dot{B}_s \rangle = \delta(t-s)$, see Section 3.2.3 for further details about this class of processes. Here, and throughout the treatise, we have set the Boltzmann constant equal to 1. We also assume that the initial state is drawn from the stationary distribution in the ring which is here uniform because f is constant.

In a small interval $[t, t + \mathrm{d}t]$ of time, the particle moves by a stochastic amount $\mathrm{d}X_t$. The work done on the particle in $[t, t + \mathrm{d}t]$ by the external force f is stochastic and given by

$$\mathrm{d}W = f\, \mathrm{d}X_t. \tag{1.36}$$

In this example, the particle has no internal degrees of freedom and its internal energy $U = U_0$ is constant and does not change in time, i.e., $\mathrm{d}U_t = 0$. We thus obtain from the first law of stochastic thermodynamics $\mathrm{d}U_t = \mathrm{d}Q_t + \mathrm{d}W_t$ the following expression for the heat absorbed by the particle in $[t, t + \mathrm{d}t]$, viz.,

$$\mathrm{d}Q_t = -\mathrm{d}W_t = -f\,\mathrm{d}X_t. \tag{1.37}$$

Using the Langevin equation (1.35) in Equation (1.37), we obtain a stochastic differential equation for the heat, viz.,

$$-\frac{\dot{Q}_t}{T} = \frac{\mu f^2}{T} + \sqrt{\frac{2\mu f^2}{T}}\dot{B}_t = v^Q + \sqrt{2v^Q}\dot{B}_t, \tag{1.38}$$

where we have defined the expected heat rate

$$v^Q \equiv -\langle \dot{Q}_t \rangle / T = \frac{\mu f^2}{T}. \tag{1.39}$$

Furthermore, changing variables in Equation (1.38) and applying Ito's lemma (see Appendix B.3), we find that the exponential $\exp(\frac{Q_t}{T})$ satisfies the stochastic differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\exp\left(\frac{Q_t}{T}\right) = -\sqrt{2v^Q}\exp\left(\frac{Q_t}{T}\right)\dot{B}_t\,. \tag{1.40}$$

Since the dissipated heat divided by the temperature is the entropy produced in this process, Equation (1.40) reveals that the exponential of the negative entropy production a martingale. This follows from (1.40) which shows that $\exp(Q_t/k_\mathrm{B}T)$ has no drift term, and hence is a martingale. Because $Q_0 = 0$, we find that $\langle \exp(Q_t/k_\mathrm{B}T)\rangle = 1$ at all times, which is often referred to as the "integral fluctuation relation (or theorem)" for the absorbed heat, and this relation is thus closely related to the martingality of $\exp(\frac{Q_t}{T})$.

For the present example, the stochastic heat and its exponential can be determined analytically. Solving (1.38) we get

$$Q_t = -Tv^Q t - T\sqrt{2v^Q}B_t, \tag{1.41}$$

where B_t is the value of the Wiener process at time $t > 0$. Because $v^Q \geq 0$ and $\langle B_t \rangle = 0$, we retrieve the second law of thermodynamics for this example, viz., $\langle Q_t \rangle \leq 0$. In other words, on average the particle dissipates heat into the environment. Moreover, the relation (1.41) implies that the integral of Equation (1.40) is given by

$$\exp\left(\frac{Q_t}{T}\right) = \exp\left(-v^Q t - \sqrt{2v^Q}B_t\right). \tag{1.42}$$

In other words, $\exp(Q_t/T)$ is a geometric Brownian motion with zero drift and volatility $\sqrt{2v^Q}$, a process that has been widely used, i.e., in modelling stock fluctuations in quantitative finance, see Chapter 12.

Chapter 2. Martingales: definitions and examples

The name "supermartingale" was spoiled for me by the fact that every evening the exploits of "Superman" were played on the radio by one of my children.

A conversation with Joe Doob, J. L. Snell, Stat. Sci. **12** (4) (1947).

In this chapter, through examples of martingales, we convince ourselves that martingales are ubiquitous. This chapter is organized into two main parts. Section 2.1 defines and provides examples of martingales in discrete time, and Section 2.2 does the same for martingales in continuous time.

For the sake of clarity, in Chapters 2, 3, and 4 we use the symbol $n \in \mathbb{N} \cup \{0\}$ for a discrete-time index (see Section 2.1) and $t \in \mathbb{R}^+$ for a continuous time index (see i.e., Section 2.2). On the other hand, in the other chapters of this treatise we will use t indiscriminately for both continuous and discrete time.

2.1. *Martingales in discrete time*

2.1.1. *Martingales, submartingales and supermartingales*

Martingales are stochastic processes that have no net drift. Formally, we define discrete-time martingales relative to a stochastic process $X_n \in \mathcal{X}$ as follows.

Let $M_n \in \mathbb{R}$ be a discrete-time stochastic process given by a real-valued function defined on the set of trajectories $X_{[0,n]} = (X_0, X_1, \ldots, X_n)$. We assume that M_n is integrable, i.e., $\langle |M_n| \rangle < \infty$ for all n.

> We say that M_n is a discrete-time **martingale** relative to X_n if M_n has no drift, i.e.,
>
> $$\langle M_n \,|\, X_{[0,m]} \rangle = M_m, \tag{2.1}$$
>
> for all $0 \leq m \leq n$.

Note that conditional expectations are defined as in Equation (1.3). We require that M_n is integrable, as otherwise the conditional expectation is not well defined. See Section 9.7 of Ref. [45] for a list of useful properties of conditional expectations and Figure 2.1 for an illustration of the martingale concept. As done in Figure 2.1, it is often assumed that $X_n = M_n$ and thus $\langle M_n \,|\, M_{[0,m]} \rangle = M_m$ for $0 \leq m \leq n$.

We define submartingales (supermartingales) as processes with a nonnegative (nonpositive) drift. Specifically, consider a real-valued function S_n defined on the set of trajectories $X_{[0,n]}$, and let us assume that S_n is integrable, i.e., $\langle |S_n| \rangle < \infty$. We say that S_n is a **submartingale** (supermartingale) relative to X_n if it has a nonnegative (nonpositive) drift, i.e.,

$$\langle S_n \,|\, X_{[0,m]} \rangle \geq S_m \quad (\langle S_n \,|\, X_{[0,m]} \rangle \leq S_m) \tag{2.2}$$

for all $0 \leq m \leq n$. With these definitions, martingales are particular cases of submartingales. In what follows, when we refer to martingales (or submartingales) we imply that they are defined with respect to a reference stochastic process X_n. See Fig. 2.2 for simple example trajectories of martingale, submartingale, and supermartingale processes.

The condition (2.1) can be complicated to verify in concrete examples of stochastic processes. However, in discrete time there exists a simpler, equivalent condition for martingality, which is a consequence of the **tower property** of conditional expectations, see Appendix B. The tower property states that for any (integrable) functional $Z_p = Z[X_{[0,p]}]$ it holds that

$$\langle \langle Z_p \,|\, X_{[0,n]} \rangle \,|\, X_{[0,m]} \rangle = \langle Z_p \,|\, X_{[0,m]} \rangle, \tag{2.3}$$

for all $0 \leq m \leq n$. Using this tower property, we get the following simpler "one-step-ahead" martingale criterion [46].

One-step-ahead criterion for martingality. The martingale property in discrete time (2.1) is equivalent to the simpler condition

$$\langle M_{n+1} \,|\, X_{[0,n]} \rangle = M_n, \tag{2.4}$$

for all n.

The equivalence between the conditions (2.1) and (2.4) follows from the tower property of conditional expectations. Indeed, for all $m < n$ it holds that

$$\left\langle M_n \,|\, X_{[0,m]} \right\rangle = \left\langle \left\langle M_n \,|\, X_{[0,n-1]} \right\rangle \middle| \, X_{[0,m]} \right\rangle = \left\langle M_{n-1} | \, X_{[0,m]} \right\rangle,$$

which iterates up to

$$\left\langle M_n \,|\, X_{[0,m]} \right\rangle = \left\langle M_m \,|\, X_{[0,m]} \right\rangle = M_m.$$

2.1.2. ♠*Backward martingales, submartingales and supermartingales*

In the definition of the martingale, Equation (2.1), we have that $n \geq m$, and hence the martingale definition uses a part of the trajectory that happened in the past. We can also define martingales conditioned on a part of the trajectory that takes place in the future. In this way, we obtain **backward** martingales, i.e. processes that are martingales backward in time.

Let M_n be a real-valued function defined on the set of trajectories $X_{[n,\infty]} = (X_n, X_{n+1}, \ldots, X_\infty)$. In addition, we assume that M_n is integrable, i.e., $\langle |M_n| \rangle < \infty$ for all $n \in \mathbb{N}$.

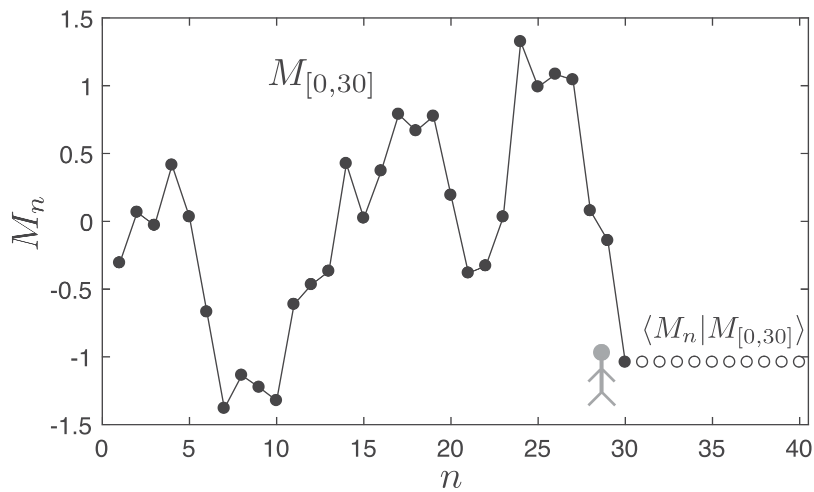

Figure 2.1. Illustration of a martingale process M_n in discrete time $n \in \mathbb{N}$. Here M_n is given by the cumulative sum of n independent Gaussian random numbers with zero mean and standard deviation equal to 1/2. The filled circles with lines illustrate a specific trajectory of the process up to time $m = 30$. The unfilled circles denote the expected values of the martingale $\langle M_n \,|\, M_{[0,m]} \rangle = M_m$ at future times $n > m$, conditioned on the past sequence $M_{[0,m]}$ shown in the figure. The grey cartoon illustrates an observer that collects the values of the sequence $M_{[0,m]}$ and makes predictions about its future expected value.

We say that $M_n \in \mathcal{X}$ is a **backward martingale** relative to X_n if M_n has no drift when conditioned on events in the future, i.e.,

$$\langle M_\ell \,|\, X_{[m,n]} \rangle = M_m, \tag{2.5}$$

for all $0 \leq \ell \leq m \leq n$.

Backward submartingales and backward supermartingales are defined by replacing the equality in Equation (2.5) by $\geq$ and $\leq$, respectively. To distinguish martingales from backward martingales, we sometimes call the former *forward* martingales.

2.1.3. *Examples of martingales in discrete time*

- *Gambler's fortune in a fair game of chance*: A gambler's fortune in a fair game of chance is a martingale [22]. Let us consider the example of a coin toss. The game consists of a series of coin flips with equally likely outcomes $X_n \in \{\text{Head}, \text{Tail}\}$. Each betting round, the gambler guesses the outcome of the coin toss through a betting system. The gambler's guess is denoted by $Y_n \equiv Y(X_{[0,n-1]}) \in \{\text{Head}, \text{Tail}\}$, where $Y(X_{[0,n-1]})$ means that Y_n depends on $X_{[0,n-1]}$; such processes Y_n are called *predictable* processes. If the gambler guesses right, i.e., $Y_n = X_n$, they wins 1 euro, otherwise, if the gambler guesses wrong, i.e., $Y_n \neq X_n$, they loses 1 euro. The gambler's fortune F_n after n betting rounds satisfies

$$F_n \equiv F_0 + \sum_{m=1}^{n} \left(2\delta_{X_m,Y_m} - 1\right), \tag{2.6}$$

  and is a martingale process. Here, $\delta_{i,j}$ denotes the Kronecker delta function. The martingale property $\langle F_n \,|\, X_{[0,m]} \rangle = F_m$ reflects the fairness of this game.
- *Sums of independent random variables*: Let X_i ($i \in \mathbb{N} \cup \{0\}$) be a sequence of independent and identically distributed – denoted **iid** here and in the following – random variables with finite variance. The sum

$$\tilde{X}_n \equiv \sum_{i=0}^{n} X_i \tag{2.7}$$

  has conditional average

$$\langle \tilde{X}_n \,|\, X_{[0,m]} \rangle = \sum_{i=0}^{m} X_i + \sum_{i=m+1}^{n} \langle X_i \rangle. \tag{2.8}$$

  Therefore, $\tilde{X}_n$ is a martingale, submartingale, or supermartingale, if X_i has zero mean, positive mean, or negative mean, respectively. Indeed, it holds that

$$\langle \tilde{X}_n \,|\, X_{[0,m]} \rangle \begin{cases} = \tilde{X}_m, & \text{if } \langle X_i \rangle = 0, \\ \geq \tilde{X}_m, & \text{if } \langle X_i \rangle \geq 0, \\ \leq \tilde{X}_m, & \text{if } \langle X_i \rangle \leq 0. \end{cases} \tag{2.9}$$

Moreover, because the square root is a concave function, we have

$$\langle|\tilde{X}_n|\rangle = \left\langle\sqrt{\tilde{X}_n^2}\right\rangle \leq \sqrt{\langle\tilde{X}_n^2\rangle} < \infty, \tag{2.10}$$

where in the second inequality we used that X_i, and thus also $\tilde{X}_n$, has a finite variance.

The sum $\tilde{X}_n$ also obeys a strong law of large numbers, which states that $\overline{X}_n = \tilde{X}_n/n$ converges almost surely to its mean value $\mu = \langle X_i\rangle$ [44]. In addition, $\tilde{X}_n$ satisfies the central limit theorem, which states that $(\tilde{X}_n - \mu\, n)/\sqrt{n}$ converges in distribution to a standard, normally distributed random variable. In Sections 4.1.4 and 4.1.6, we consider extensions of these properties to martingale processes.

- *Conditional-expectation process (closed Martingale)*: Let X_i ($i \in \mathbb{N}\cup\{0\}$) be a sequence of integrable, possibly correlated, random variables.

  We consider the conditional expectation

$$C^{\ell}_{m,n} \equiv \langle X_\ell\,|\,X_{[m,n]}\rangle, \tag{2.11}$$

which depends on three integers $0 \leq m \leq n$ and $\ell \geq 0$. We can interpret $C^{\ell}_{m,n}$ as a forward martingale or a backward martingale:

  – If we keep ℓ fixed and set $m = 0$, then the process $C^{\ell}_{0,n}$ is a forward martingale for values of n in $0 \leq n \leq \ell$. Indeed,

$$\langle C^{\ell}_{0,n}\,|\,X_{[0,n']}\rangle = C^{\ell}_{0,n'}, \tag{2.12}$$

  for all $0 \leq n' \leq n \leq \ell$. This relation follows from the *tower property* of conditional expectations (see Equation 2.3),

$$\langle C^{\ell}_{0,n}\,|\,X_{[0,n']}\rangle = \langle\langle X_\ell\,|\,X_{[0,n]}\rangle\,|\,X_{[0,n']}\rangle = \langle X_\ell\,|\,X_{[0,n']}\rangle = C^{\ell}_{0,n'}, \tag{2.13}$$

  where we have used the definition (2.11) in the first and third equalities, and the tower property in the second equality. A proof of the tower property can be found in Appendix B.2.

  – Alternatively, for fixed ℓ and n, the process $C^{\ell}_{m,n}$ with m such that $0 \leq \ell \leq m \leq n$, is a backward martingale. Indeed,

$$\langle C^{\ell}_{m,n}\,|\,X_{[m',n]}\rangle = C^{\ell}_{m',n}, \tag{2.14}$$

  for all $0 \leq \ell \leq m \leq m' \leq n$. Also this result follows from the *tower property* of conditional expectations (see Equation 2.3),

$$\langle C^{\ell}_{m,n}\,|\,X_{[m',n]}\rangle = \langle\langle X_\ell\,|\,X_{[m,n]}\rangle\,|\,X_{[m',n]}\rangle = \langle X_\ell\,|\,X_{[m',n]}\rangle = C^{\ell}_{m',n}, \tag{2.15}$$

  where here also we have used the definition (2.11) in the first and third equalities, and the tower property in the second equality.

- *Martingale transform*: Let M_n be a martingale relative to X_n, and let D_n be a process determined by $X_{[0,n]}$. The martingale transform

$$(D \cdot M)_n \equiv D_0 M_0 + \sum_{k=1}^{n} D_{k-1}(M_k - M_{k-1}) \tag{2.16}$$

with $(D \cdot M)_0 = M_0$, is a martingale if $|D_n| \le c$, with c a positive constant. Indeed, it holds that

$$\begin{aligned}\left\langle (D \cdot M)_n \,|\, X_{[0,n-1]} \right\rangle &= \left\langle (D \cdot M)_{n-1} + D_{n-1}\,(M_n - M_{n-1})\,\,|\, X_{[0,n-1]} \right\rangle,\\ &= (D \cdot M)_{n-1} + D_{n-1} \left\langle (M_n - M_{n-1})\,\,|\, X_{[0,n-1]} \right\rangle,\\ &= (D \cdot M)_{n-1} + 0,\\ &= (D \cdot M)_{n-1}.\end{aligned} \tag{2.17}$$

In the second equality, we have used that D_{n-1} is fully determined by $X_{[0,n-1]}$, and the third equality follows from the martingale property of M. By virtue of the one-step-ahead condition (2.4), Equation (2.17) implies that $D \cdot M$ is a martingale. Note that the use of D_{k-1} in the definition (2.16) is important to guarantee the martingality of $(D \cdot M)_n$. In the continuous time limit, martingale transforms take the form of Ito integrals, see Eq. (2.64).

- *Ratios of path probability densities*: Martingales play an important role in stochastic thermodynamics [13], as well as in statistics [47]. One reason is that several quantities of central interest in these fields are expressed as ratios of probability densities, and ratios of probability densities are martingales.

  Specifically, consider two probability densities $\mathcal{P}(x_{[0,n]})$ and $\mathcal{Q}(x_{[0,n]})$, defined on the same set of trajectories $x_{[0,n]} \in \mathcal{X}^n$. We assume that $Q(x_{[0,n]}) = 0$ if $P(x_{[0,n]}) = 0$ for all $n \in \mathbb{N}$, and we say that $\mathcal{Q}$ is locally, *absolutely continuous* with respect of $\mathcal{P}$ when this condition holds. For $\mathcal{Q}$ that are locally, absolutely continuous with respect of $\mathcal{P}$, the process

$$R_n \equiv \frac{\mathcal{Q}(X_{[0,n]})}{\mathcal{P}(X_{[0,n]})}\,, \tag{2.18}$$

with the convention that $0/0 = 0$ exists and is a martingale. Note that in Equation (2.18), we evaluate the probability density $\mathcal{P}(x_{[0,n]})$ on the random realization $X_{[0,n]}$ of the trajectory $x_{[0,n]}$, and analogously for $\mathcal{Q}$.

  The fact that R_n is a martingale can be proven as follows:

$$\begin{aligned}\langle R_n \,|\, X_{[0,m]}\rangle &= \sum_{x_{m+1}} \cdots \sum_{x_n} \mathcal{P}(x_{[m+1,n]} \,|\, X_{[0,m]})\, \frac{\mathcal{Q}(X_{[0,m]}, x_{[m+1,n]})}{\mathcal{P}(X_{[0,m]}, x_{[m+1,n]})}\\ &= \sum_{x_{m+1}} \cdots \sum_{x_n} \frac{\mathcal{P}(X_{[0,m]}, x_{[m+1,n]})}{\mathcal{P}(X_{[0,m]})}\, \frac{\mathcal{Q}(X_{[0,m]}, x_{[m+1,n]})}{\mathcal{P}(X_{[0,m]}, x_{[m+1,n]})}\\ &= \frac{\sum_{x_{m+1}} \cdots \sum_{x_n} \mathcal{Q}(X_{[0,m]}, x_{[m+1,n]})}{\mathcal{P}(X_{[0,m]})}\\ &= \frac{\mathcal{Q}(X_{[0,m]})}{\mathcal{P}(X_{[0,m]})} = R_m,\end{aligned} \tag{2.19}$$

where in the second equality we have used the definition of a conditional probability distribution, and in the last step we have used that $\mathcal{Q}(X_{[0,m]})$ is the marginal probability distribution of $\mathcal{Q}(X_{[0,n]})$ for $m < n$.

If instead R_n is the ratio of a sequence of densities $\mathcal{Q}^{(n)}(X_{[0,n]})$ and $\mathcal{P}^{(n)}(X_{[0,n]})$ that depend explicitly on time n, then the marginalization condition, used in the last step of the derivation of Equation (2.19), does not hold in general, and in this case R_n is in general not a martingale.[2] This observation plays an important role in stochastic thermodynamics, as we discuss in detail in Section 6.2.

- *Random walker on* $\mathbb{Z}$: Let X_n denote the position of a biased random walker on $\mathbb{Z}$ with $X_0 = 0$. The random walker makes one step in the positive direction with a probability q and one step in the negative direction with a probability $1-q$. This model was introduced in Section 1.4, and see Figure 1.3 for an illustration.

The position of the walker relative to its mean, i.e.,

$$M_n \equiv X_n - n(2q-1), \tag{2.22}$$

is a martingale because it is a sum of independent random variables with zero mean, as in Equation (2.7). As shown in Section 1.4 (see Equation (1.8)), the exponential

$$\mathcal{E}_n(y) \equiv \frac{\exp(yX_n)}{[q\exp(y) + (1-q)\exp(-y)]^n} \tag{2.23}$$

is a martingale process for all values of $y \in \mathbb{R}$. This statement is also proven in Appendix B by expressing $\mathcal{E}_n(y)$ as a ratio of two probability densities. Using $y = \ln[(1-q)/q]$, we obtain that

$$\mathcal{E}_n\left(\ln\frac{1-q}{q}\right) = \exp\left[X_n \ln\left(\frac{1-q}{q}\right)\right] = \left(\frac{1-q}{q}\right)^{X_n}, \tag{2.24}$$

which coincides with the martingale given by Equation (1.9).

Since $\mathcal{E}_n(y)$ is a martingale, it holds that

$$\langle \mathcal{E}_n(y)\rangle = \langle \mathcal{E}_0(y)\rangle = 1. \tag{2.25}$$

Therefore, the generating function of X_n is given by

$$g_n(y) = \langle \exp(yX_n)\rangle = (q\exp(y) + (1-q)\exp(-y))^n, \tag{2.26}$$

which can also be verified with a direct computation. Expanding (2.23) in y, we obtain

$$\mathcal{E}_n(y) = 1 + \sum_{j=1}^{\infty} y^j M_n^{(j)}(X_n) \tag{2.27}$$

and hence the processes $M_n^{(j)}(X_n)$ are martingales, viz., the processes

$$M_n^{(1)}(X_n) = X_n - n(2q-1), \tag{2.28}$$

$$M_n^{(2)}(X_n) = (X_n - n(2q-1))^2 - 4nq(1-q), \tag{2.29}$$

$$\dots$$

$$M_n^{(k)}(X_n) = \left.\frac{\partial^{(k)}\mathcal{E}_n(y)}{\partial y^k}\right|_{y=0}, \tag{2.30}$$

and so forth are martingales relative to X_n (cf. Equations 1.13 and 1.14).

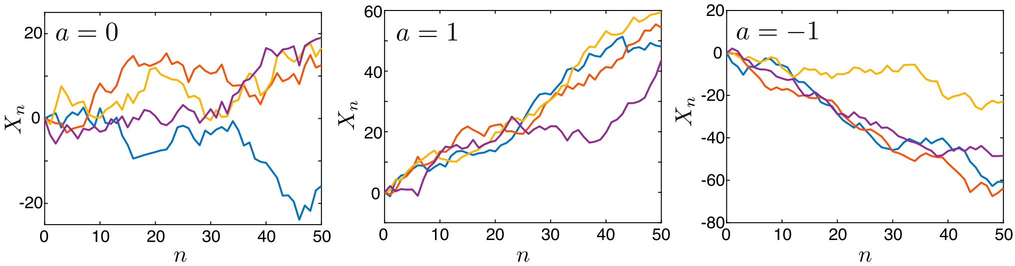

Figure 2.2. Illustration of a martingale (left), submartingale (middle) and supermartingale (right). Sample trajectories of discrete-time random walks on the real line, X_n, as a function of time n, as given by Equation (2.31) with Y_n extracted from a Gaussian distribution with zero mean and standard deviation equal to 2. The different panels are obtained for three different values of the bias parameter a: $a = 0$ (left), $a = 1$ (middle), and $a = -1$ (right), which correspond respectively to martingale, submartingale and supermartingale processes.

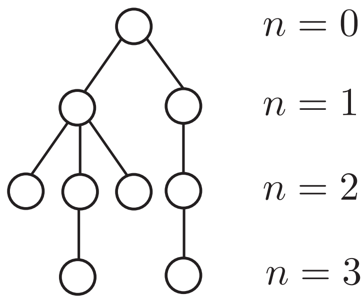

Figure 2.3. An example of one realization of a branching process. In this example, the parent generates a finite population of three generations. For the example shown, $\{Y_{1,0} = 2\}$, $\{Y_{1,1} = 3, Y_{2,1} = 1\}$, $\{Y_{1,2} = 0, Y_{2,2} = 1, Y_{3,2} = 0, Y_{4,2} = 1\}$, and $\{Y_{1,3} = 0, Y_{2,3} = 0\}$.

- *Random walker on* $\mathbb{R}$: We consider a random walker moving on the real line. The position X_n of the random walker satisfies

$$X_n \equiv X_{n-1} + a + Y_n \tag{2.31}$$

for all $n \geq 1$ and $X_0 = 0$. The increments Y_n are iid random variables with zero mean and finite variance, and not necessarily drawn from a Gaussian distribution. If $a = 0$, then X_n is a martingale. On the other hand, if $a > 0$ or $a < 0$, then X_n is a submartingale or a supermartingale, respectively. See Figure 2.2 for illustrations.
- *Martingales in branching processes*: Branching processes are simple models for reproduction [48–50]. Consider a population of constituents, which may be, i.e., nuclei, molecules, viruses, cells, or animals, that multiply themselves. We denote the number of members in the population at time n by $X_n \in \mathbb{N} \cup \{0\}$, with the initial condition $X_0 = 1$. At each time step reproduction takes place, and thus each time step corresponds with one generation. We assume that all members live for exactly one generation. We denote by $Y_{i,n} \in \mathbb{N} \cup \{0\}$ the number of progeny of the ith member of the population at generation n, see Figure 2.3 for an explanation. It holds then that

$$X_n \equiv \sum_{i=1}^{X_{n-1}} Y_{i,n}. \tag{2.32}$$

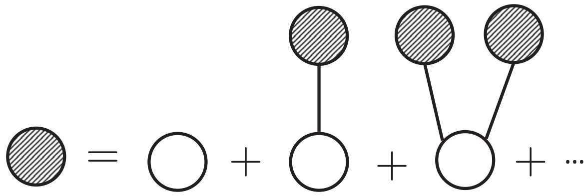

Figure 2.4. A graphical illustration of the self-consistent equation $\eta = g(\eta) = \sum_{y=0} \rho_Y(y)\eta^y$ for the extinction probability of a branching process. The extinction probability η, denoted by the filled circle, is equal to the probability that the parent, denoted by an unfilled circle, has no progeny ($Y = 0$), plus the probability that the parent has one child ($Y = 1$) and this child generates a finite population, plus the probability that the parent has two children ($Y = 2$), both of which generate finite populations, etc.

We assume that the $Y_{i,n}$ are iid drawn random variables from a distribution $\rho_Y(y)$ with $y \in \mathbb{N} \cup \{0\}$. We denote by $\mu = \sum_{y=0}^{\infty} \rho_Y(y)y$ the mean value of Y and by $g(s) = \sum_{y=0}^{\infty} \rho_Y(y)s^y$ the generating function of Y. One can verify that $\langle X_n \rangle = \mu^n$ and that the extinction probability η, which is the probability that the parent generates a finite population, is the smallest nonnegative root of the equation $\eta = g(\eta)$ [49,51]; see Figure 2.4 for a derivation.

The normalized population size

$$W_n \equiv \frac{X_n}{\langle X_n \rangle} \tag{2.33}$$

is a martingale. Indeed,

$$\langle W_n \,|\, X_{[0,n-1]} \rangle = \frac{\langle X_n \,|\, X_{n-1} \rangle}{\langle X_n \rangle} = \frac{\mu X_{n-1}}{\mu^n} = \frac{X_{n-1}}{\langle X_{n-1} \rangle} = W_{n-1}, \tag{2.34}$$

where in the first equality we have used the Markov nature of the process and in the second equality we have used that X_n is the sum of X_{n-1} independent random variables with mean μ. It follows from (2.34) and the tower property of conditional expectations that W_n is a martingale (see discussion around Equation 2.4).

More surprising is that the process [49]

$$V_n \equiv \eta^{X_n}, \tag{2.35}$$

with η the extinction probability, is a martingale. Indeed, it holds that

$$\langle V_n \,|\, X_{[0,n-1]} \rangle = \langle \eta^{\sum_{j=1}^{X_{n-1}} Y_j} \,|\, X_{[0,n-1]} \rangle = \prod_{j=1}^{X_{n-1}} \langle \eta^{Y_j} \rangle = (g(\eta))^{X_{n-1}} = \eta^{X_{n-1}} = V_{n-1},$$

and thus according to the one-step-ahead condition given by Equation (2.34) V_n is a martingale.

- *Martingales in elephant random walks*: So far, we have considered examples of martingales in processes X that are Markovian. We consider now an example of a martingale relative to a non-Markovian process X, namely, the elephant random walk.

  Elephant random walks were introduced in Ref. [52] as examples of non-Markovian processes with long-range memory that can exhibit anomalous diffusion. A diffusing particle exhibits anomalous diffusion when its mean squared displacement grows as a power law, i.e., $\langle X_n^2 \rangle \sim n^{\alpha}$ with an exponent $\alpha \neq 1$ [53]. Anomalous diffusion has been observed, amongst others, in the motion of lipid granules in the cytoplasm [54], in colloidal particles in an optically controlled medium [55] and active particles [56]. Although Markov processes can exhibit anomalous diffusion transiently, i.e., within a finite time window, asymptotically they inevitably transition to a regime with standard diffusion, see Ref. [57]. The elephant random walk describes how superdiffusion emerges in a microscopic random walk model due to the presence of long-range temporal correlations.

References [58,59] identify martingale processes associated with elephant random walks and use these martingales to characterize properties of elephant random walks. Here we review some of their findings in a minimal example.

Let us consider an elephant random walk located at the position $X_n \in \mathbb{Z}$ at time $n = \{0, 1, \dots\}$. The initial position of the walker is $X_0 = 0$. At time $n = 1$ the walker moves to $X_1 = Y_1$, where Y_1 equals $+1$ with probability 1/2 and -1 with probability 1/2. In the next steps, $n \geq 1$, the motion of the walker is as follows:

$$X_{n+1} \equiv X_n + Y_{n+1}, \tag{2.36}$$

where Y_{n+1} is obtained by the following rule. We select uniformly at random an integer (previous time) $k \in \{1, \dots, n\}$ and we then reverse with probability p the sign of the corresponding value at previous time Y_k, i.e.,

$$Y_{n+1} \equiv \begin{cases} Y_k & \text{with probability } p, \\ -Y_k & \text{with probability } 1-p. \end{cases} \tag{2.37}$$

In other words,

$$Y_{n+1} = \sigma_n Y_{\beta_n}, \tag{2.38}$$

where $\sigma_n = 1$ ($\sigma_n = -1$) with probability p ($1-p$) and β_n is drawn from a discrete uniform distribution in $\{1, \dots, n\}$.

The parameter p is called the *memory* parameter of the elephant random walk. For $p \in [0, 3/4)$, a central limit theorem applies, and the elephant random walk is diffusive ($X_n \sim \sqrt{n}$), while for $p \in (3/4, 1)$ the elephant random walk is superdiffusive ($X_n \sim n^\alpha$ with $\alpha > 1/2$). These results can be derived with martingale theory, as we discuss in Chapter 4.

The process X_n is, up to a time-dependent constant, related to a martingale process. Indeed, using Equations (2.36)–(2.38) we find that

$$\begin{aligned} \langle Y_{n+1} \mid Y_{[0,n]} \rangle &= \langle \sigma_n \rangle \langle Y_{\beta_n} \mid Y_{[0,n]} \rangle = \langle \sigma_n \rangle \frac{\sum_{k=1}^n \langle Y_k \mid Y_{[0,n]} \rangle}{n} \\ &= (2p-1) \frac{\sum_{k=1}^n Y_k}{n} = (2p-1) \frac{X_n}{n}, \end{aligned} \tag{2.39}$$

where we have used that $Y_0 = 0$. From Equations (2.36)–(2.39), it follows that the position of the elephant random walker is not a martingale, except for the case $p = 1/2$ when the elephant random walk is a simple random walk. In fact, (2.36) and (2.39) imply that

$$\langle X_{n+1} \mid Y_{[0,n]} \rangle = \frac{n + 2p - 1}{n} X_n = \gamma_n X_n, \tag{2.40}$$

where $\gamma_n = (n + 2p - 1)/n$. Yet, from this result, we obtain a martingale with multiplicative structure. Indeed, let us introduce the quantity

$$a_n \equiv \prod_{k=1}^{n-1} \gamma_k^{-1} = \frac{\Gamma(n+1)\Gamma(2p)}{\Gamma(n+2p)}, \tag{2.41}$$

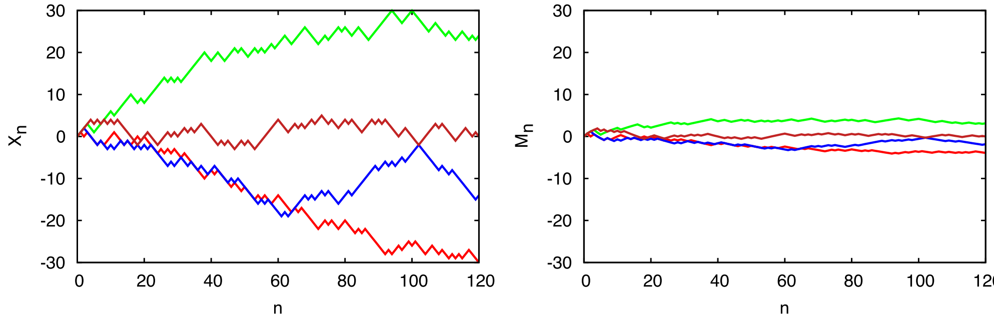

Figure 2.5. Left: Example trajectories of the elephant random walk, X_n, whose dynamics is given by Equations (2.36) and (2.37), as a function of time n, with parameter $p = 0.7$. Right: Martingale process, M_n, constructed using Equation (2.43), and associated with the trajectories in the left panel. The trajectories in the right panel are examples of martingales in a non-Markovian process X. Observe the reduced size of fluctuations in M_n when compared with X_n. Lines are linear interpolation between the discrete values X_n and serve as a guide to the eye.

where Γ is the Gamma function; note that asymptotically,

$$a_n \sim \Gamma(2p)n^{1-2p}. \tag{2.42}$$

Defining

$$M_n \equiv a_n X_n, \tag{2.43}$$

we obtain from the definition (2.43) and Equations (2.39) that

$$\langle M_{n+1} \,|\, Y_{[0,n]} \rangle = a_{n+1} \langle X_{n+1} \,|\, Y_{[0,n]} \rangle = a_{n+1}\gamma_n X_n = a_n X_n = M_n, \tag{2.44}$$

and hence also $\langle M_{n+1} \,|\, X_{[0,n]} \rangle = M_n$. Thus, according to the one-step-ahead condition (2.4), M_n is a martingale. Figure 2.5 shows a couple of trajectories drawn from the elephant random walk X_n and their associated martingale process M_n given in Equation (2.43). As illustrated in Figure 2.5, martingalization not only reduces the persistence of the elephant random walks, rendering them driftless, but also reduces the amplitude of their fluctuations.

- *Run-and-tumble motion:* The run-and-tumble process is an example of a "false friend" of the martingale. This process has zero average drift, but nevertheless is *not* a martingale. The position of a one-dimensional run-and-tumble particle with initial position $X_0 = 0$ may be described as

$$X_n = X_{n-1} + \sigma v_n, \tag{2.45}$$

where the instantaneous normalized velocity $v_n = \{-1, 1\}$ is a Markovian dichotomous noise process, and $\sigma > 0$ the step size. More precisely, the initial value of the normalized velocity is drawn at random $P(\sigma_0 = \pm 1) = 1/2$, and in the subsequent steps it flips its sign ("tumbles") with probability q, i.e., $P(v_n \,|\, v_{n-1}) = q\delta_{v_n,-v_{n-1}} + (1-q)\delta_{v_n,v_{n-1}}$ for all $n \geq 1$. See Refs. [60–62] for generalizations and extensions.

Figure 2.6(a) shows an example trajectory of the position of a run-and-tumble particle described in Equation (2.45), which has a zig-zag-like structure. The unconditioned average $\langle X_n \rangle = X_0 = 0$ vanishes because we have fixed the initial position to $X_0 = 0$ (black line in Figure 2.6 b). On the other hand, the average of the position conditioned over its

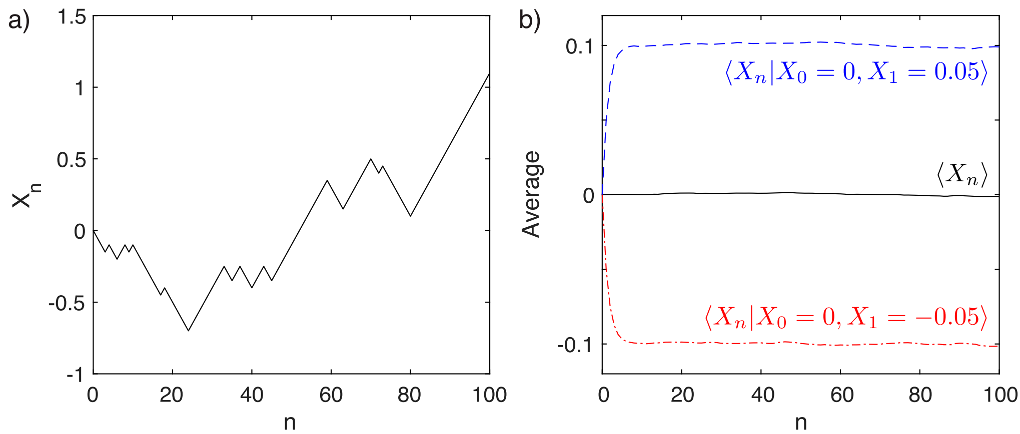

Figure 2.6. Run and tumble motion. (a) Example trajectory of the position of a discrete-time run-and-tumble particle described in Equation (2.45). Lines are linear interpolation between the discrete values X_n and serve as a guide to the eye. (b) Average position as a function time (black solid line), and conditional average of the position over trajectories with a given history X_0, X_1 up to the first jump (blue dashed line, and red dash-dotted line). Results are obtained from numerical simulations with parameters: tumble probability $q = 1/4$; jump amplitude $\sigma = 0.05$, and averages are done over 10^5 numerical simulations.

history $X_{[0,1]} = X_0, X_1$ up to the first step $n = 1$ reveals that X_n is not a martingale. Indeed, $\langle X_n|X_0, X_1\rangle$ for $n > 1$ is time dependent for the two possible values of ($X_0 = 0, X_1 = \sigma$; and $X_0 = 0, X_1 = -\sigma$), see blue dashed line and red dash-dotted line in Figure 2.6(b). Thus we conclude $\langle X_n \,|\, X_0, X_1\rangle \neq X_1$, which implies that X_n is not a martingale.

2.2. *Martingales in continuous time*

2.2.1. *Martingales, submartingales, supermartingales*

We consider martingales M_t in continuous time $t \in \mathbb{R}^+$. Just as for the discrete-time case, martingales in continuous time are processes that have no drift.

Let M_t be a real-valued functional defined on the set of trajectories of $X_{[0,t]} = \{X_s\}_{s\in[0,t]}$. In addition, assume that M_t is integrable, i.e., $\langle |M_t| \rangle < \infty$.

We say that a process M_t is a **martingale** with respect to the process $X_t \in \mathcal{X}$ if M_t has no drift, i.e., it holds with probability 1 that

$$\langle M_t \,|\, X_{[0,s]} \rangle = M_s \tag{2.46}$$

for all $0 \leq s \leq t$.

In continuous time, the condition $\langle M_t \,|\, X_{[0,s]}\rangle = M_s$ holds with probability 1, as we omit events that occur with zero probability. Also, conditional expectations $\langle M_t \,|\, X_{[0,s]}\rangle$ in continuous time should be understood as conditional expectations with respect to the filtration generated by $X_{[0,s]}$, see Appendix B.1 for a brief introduction and further references.

Similarly, we define submartingales (supermartingales) as processes with a nonnegative (nonpositive) drift. We say that S_t is a **submartingale** (supermartingale) relative to X_t if it is

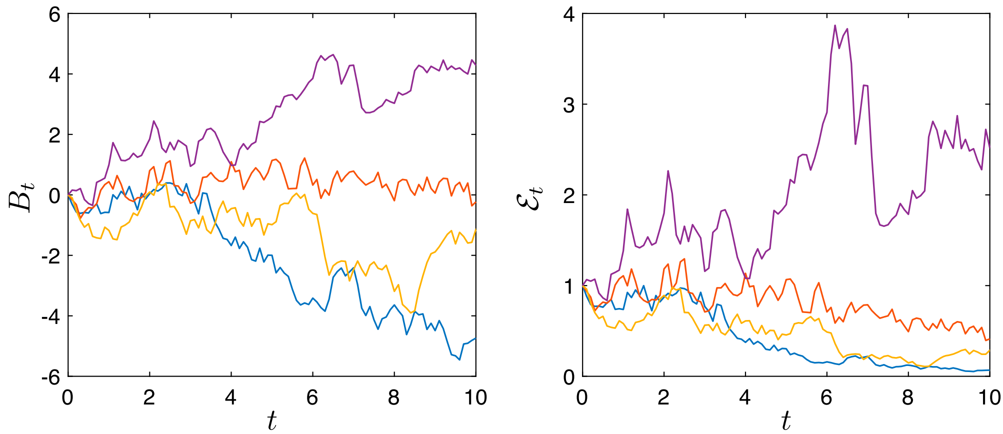

Figure 2.7. Example trajectories for two continuous martingales, namely, the one-dimensional Brownian motion B_t (left panel) and the stochastic exponential $\mathcal{E}_t(zB)$ of zB_t, as defined in Equation (2.59), for the parameter $z = 0.4$ (right panel). Note that B_t can take negative values, whereas $\mathcal{E}_t(zB)$ is a positive martingale. Trajectories have been generated with the Euler numerical integration scheme with time discretization step 0.1.

an integrable stochastic process that has a nonnegative (nonpositive) drift, i.e., it holds with probability 1 that

$$\langle S_t \,|\, X_{[0,s]} \rangle \geq S_s \quad (\langle S_t \,|\, X_{[0,s]} \rangle \leq S_s) \tag{2.47}$$

for all $0 \leq s \leq t$.

We define backward (sub)martingales by conditioning on a future part of the trajectory, analogously to the discrete-time case considered in Section 10.4.1.

2.2.2. *Key examples*

- *The Brownian motion (Wiener process)* B_t: The Brownian motion is a one-dimensional stochastic process that satisfies the following four conditions [63,64]:
  - $B_0 = 0$;
  - the increments $B_t - B_s$ are normally distributed with mean zero and variance $|t - s|$;
  - for $0 \leq t_1 < t_2 < \cdots < t_n < \infty$ it holds that the increments $B_{t_1}, B_{t_2} - B_{t_1}, \ldots, B_{t_n} - B_{t_{n-1}}$ are independent;
  - the process B_t is continuous with probability 1.

  Brownian motion B_t is a paradigmatic physical example of a martingale. The left panel of Figure 2.7 shows a few examples of Brownian trajectories.
- *Counting processes*: Let $N_t \in \mathbb{N}$ be a Poisson process with rate λ, i.e., N_t denotes the number of ticks in the interval $[0, t]$ of a Poisson point process of constant rate λ. N_t is a submartingale. On the other hand, the process

$$M_t \equiv N_t - \lambda t \tag{2.48}$$

  is a martingale. Indeed, since a Poisson process is Markovian and time-homogeneous, it holds that

$$\langle M_t \,|\, N_{[0,s]} \rangle = \langle N_t \,|\, N_{[0,s]} \rangle - \lambda t = \langle N_t \,|\, N_s \rangle - \lambda t = N_s - \lambda s = M_s. \tag{2.49}$$

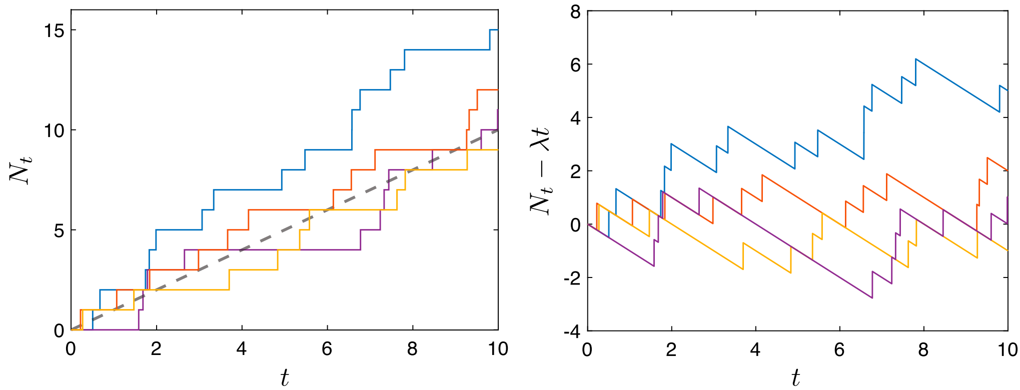

Figure 2.8. Randomly generated trajectories of a Poisson process N_t with rate parameter $\lambda = 1$ (left) and the corresponding trajectories of the martingale $N_t - \lambda t$ (right). The black dashed line in the left panel denotes the deterministic process λt.

Figure 2.8 illustrates four randomly generated trajectories of both the counting (Poisson) process N_t and the corresponding martingale M_t, given by Equation (2.48), as a function of time.

- *Radon–Nikodym density processes* (*a.k.a. path probability ratios*): We consider an extension of the probability ratio (2.18) that applies to processes in continuous time. These processes are martingales and are important for the applications discussed in this review.

  Let X_t be a stochastic process whose statistics are described by one of the two probability measures $\mathcal{P}$ or $\mathcal{Q}$. Probability measures are functions that assign probabilities to measurable sets Φ of trajectories through [65]

$$\mathcal{P}(\Phi) \equiv \langle \mathbf{1}_\Phi(X_{[0,t]}) \rangle_{\mathcal{P}}, \tag{2.50}$$

where

$$\mathbf{1}_\Phi\left(X_{[0,t]}\right) \equiv \begin{cases} 1, & \text{if } X_{[0,t]} \in \Phi, \\ 0, & \text{if } X_{[0,t]} \notin \Phi, \end{cases} \tag{2.51}$$

is the indicator function that equals 1 when $X_{[0,t]} \in \Phi$ and equals 0 otherwise.

We define a density process $R_t \equiv R(X_{[0,t]}) \in \mathbb{R}^+$ such that

$$\langle f(X_{[0,t]}) \rangle_{\mathcal{Q}} = \langle f(X_{[0,t]}) R_t \rangle_{\mathcal{P}}, \tag{2.52}$$

holds for all nonnegative, measurable functions f. We denote the process R_t by

$$R_t = \frac{\mathcal{Q}(X_{[0,t]})}{\mathcal{P}(X_{[0,t]})}, \tag{2.53}$$

and call it the *Radon–Nikodym density process* (a.k.a. *path probability ratio*) of $\mathcal{Q}$ with respect to $\mathcal{P}$, as R_t plays the role of the density of $\mathcal{Q}$ with respect of $\mathcal{P}$. Note that in Equation (2.53) the numerator $\mathcal{Q}(X_{[0,t]})$ does not exist separately from the denominator $\mathcal{P}(X_{[0,t]})$, which distinguishes probability ratios in discrete time, as defined in Equation (2.18), from those in continuous time.

According to the Radon–Nikodym theorem [66], the process R exists as long as $\mathcal{Q}$ is locally, absolutely continuous with respect to $\mathcal{P}$, which means that

$$\mathcal{P}(\Phi) = 0 \Rightarrow \mathcal{Q}(\Phi) = 0 \tag{2.54}$$

for all measurable sets Φ defined on the set of trajectories $X_{[0,t]}$ and for finite t. Provided the absolute continuity conditions are satisfied, the process R_t given by Equation (2.53) is a martingale with respect to $\mathcal{P}$.

An alternative way to represent probability measures $\mathcal{P}$ is through the Onsager–Machlup method, see, i.e., Refs. [67–69]. In this approach, we consider a family of equivalent probability measures $\mathscr{P}$ that are mutually absolutely continuous, i.e., if $\mathcal{P}, \mathcal{Q} \in \mathscr{P}$, then

$$\mathcal{P}(\Phi) = 0 \Leftrightarrow \mathcal{Q}(\Phi) = 0. \tag{2.55}$$

The probability measures in this family, i.e., $\mathcal{P}$ and $\mathcal{Q}$, can be represented as

$$\mathcal{P}\left(x_{[0,t]}\right) = \mathcal{N}^{-1} \exp\left(-\mathcal{A}_{\mathcal{P}}(x_{[0,t]})\right) \tag{2.56}$$

and

$$\mathcal{Q}\left(x_{[0,t]}\right) = \mathcal{N}^{-1} \exp\left(-\mathcal{A}_{\mathcal{Q}}(x_{[0,t]})\right), \tag{2.57}$$

where $\mathcal{A}_{\mathcal{P}}$ and $\mathcal{A}_{\mathcal{Q}}$ are functionals (often called "action" functionals) defined on the trajectories of the process, and $\mathcal{N}$ is a common prefactor. Even though the prefactor $\mathcal{N}$ is ill-defined, the Onsager–Machlup representation is convenient as we obtain Radon–Nikodym density processes between any two probability measures in the equivalence class $\mathscr{P}$ from ratios

$$R_t = \frac{\mathcal{Q}\left(X_{[0,t]}\right)}{\mathcal{P}\left(X_{[0,t]}\right)} = \exp\left(-\mathcal{A}_{\mathcal{Q}}(X_{[0,t]}) + \mathcal{A}_{\mathcal{P}}(X_{[0,t]})\right). \tag{2.58}$$

In other words, the Onsager–Machlup representation allows us to represent the numerator and denominator of R_t independently in terms of the so-called actions $\mathcal{A}_{\mathcal{Q}}$ and $\mathcal{A}_{P}$.

As suggested before, often we will use the physics' slang *path probability* for $\mathcal{P}(x_{[0,t]})$ and *path probability ratio* for R_t, even though $\mathcal{P}$ is not really a probability, but rather a representation of the measure $\mathcal{P}$ in terms of the action.

- The *stochastic exponential of* zB_t: The exponential

$$\mathcal{E}_t(zB) \equiv \exp\left(zB_t - \frac{1}{2}z^2 t\right) \tag{2.59}$$

is a martingale for all $z \in \mathbb{R}$, as shown in Appendix B; see the right panel of Figure 2.7 for an illustration of trajectories of $\mathcal{E}_t(zB)$. Note that (2.59) can be obtained from the continuous-time limit of the martingale (2.23) for $q = 1/2$ by making the substitutions $n = t/\Delta t$, $X_n = B_t/\sqrt{\Delta t}$, and $y = z\sqrt{\Delta t}$, and by subsequently taking the limit $\Delta t \to 0$.

Expanding the exponential (2.59) around $z = 0$, we obtain [63]

$$\exp\left(zx - \frac{1}{2}z^2 t\right) = \sum_{n\geq 0}^{\infty} \frac{z^n}{n!} H_n(t,x). \tag{2.60}$$

Setting $x = B_t$ in Equation (2.60), it follows from the martingale property of the exponential (2.59) that the functions $H_n(t,B_t)$ are martingales for all $n \in \mathbb{N}$. Thus the processes

$$H_1(t,B_t) = B_t, \tag{2.61}$$

$$H_2(t,B_t) = B_t^2 - t, \tag{2.62}$$

$$H_3(t,B_t) = B_t^3 - 3tB_t, \tag{2.63}$$

and so forth, are martingales.

- The *Itô integral*: Let $Z_t = Z(B_{[0,t]})$ be a function defined on the space of trajectories of the Brownian motion. Let $P = [t_1 < t_2 < \ldots < t_n]$, with $t_1 = 0$ and $t_n = t$, be a finite partition of the interval $[0,t]$, and define its norm $\|P\|$ be given by the maximum spacing $t_i - t_{i-1}$ between two consecutive values. The Itô integral is defined by the limit [64,70]

$$I_t = \int_0^t Z_s\, \mathrm{d}B_s = \lim_{\|P\|\to 0} \sum_{i=0}^{n-1} Z_{t_i} \left(B_{t_{i+1}} - B_{t_i}\right), \tag{2.64}$$

where the convergence should be understood in probability. The Brownian motion is recovered as the special case when the diffusion coefficient Z_t is constant. We can also express Itô integrals as stochastic differential equations, i.e.,

$$\frac{\mathrm{d}I_t}{\mathrm{d}t} = Z_t \frac{\mathrm{d}B_t}{\mathrm{d}t}, \tag{2.65}$$

or even more briefly as

$$\dot{I}_t = Z_t \dot{B}_t, \tag{2.66}$$

where the dot represents a derivative towards time. Itô integrals of the form (2.64) are martingales when [64,71]

$$\int_0^t \langle Z_s^2 \rangle\, \mathrm{d}s < \infty. \tag{2.67}$$

Consequently, one has

$$\langle I_t \rangle = 0. \tag{2.68}$$

However, there exist Itô integrals that are not martingales and this leads to the concept of a local martingale, which we introduce later in this review.

Martingales play an important role in the theory of stochastic integration. In fact, Itô integrals also exist when the integrator is a martingale [71], viz.,

$$I_t = \int_0^t Z_s\, \mathrm{d}M_s \equiv \lim_{\|P\|\to 0} \sum_{i=0}^{n-1} Z_{t_i} \left(M_{t_{i+1}} - M_{t_i}\right), \tag{2.69}$$

where M_s is now a martingale process, not necessarily Brownian motion B_s. Note that the Itô integral is the continuous-time version of the martingale transform (2.16). The integral given by Equation (2.64) is a special case of Equation (2.69) for an integrator that is a Brownian motion. In fact, the *martingale representation theorem* states that square integrable, continuous martingales can be written as Itô integrals for which the integrator M_s is a Brownian motion [64], and hence the generic form of the Itô integral equation (2.69) is mainly relevant for martingales that admit jumps. The requisite for martingality (2.67) for the special case of an Itô integral with respect to the Brownian motion, reads for the generic Itô integral equation (2.69) as

$$\int_0^t \langle Z_s^2 \rangle \, \mathrm{d}[M_s, M_s] < \infty, \tag{2.70}$$

where $[M_s, M_s]$ is the quadratic variation process, defined by

$$[M_t, M_t] \equiv \lim_{\|P\| \to 0} \sum_{i=0}^{n-1} \left(M_{t_i} - M_{t_{i-1}}\right)^2. \tag{2.71}$$

For illustration purposes, let us consider two canonical examples of Itô integrals. When the integrator $M_t = B_t$ is a Brownian motion, then

$$[M_t, M_t] = t. \tag{2.72}$$

Note that the quadratic variation can be obtained informally by using the notation $d[Z,Z]_s = (dZ_s)^2$ and the rules of Itô calculus.

Rules of Itô calculus (see Appendix B.3.1):

$$(\mathrm{d}B_t)^2 = \mathrm{d}t, \quad \mathrm{d}B_t\,\mathrm{d}t = 0, \quad \text{and} \quad (\mathrm{d}t)^2 = 0. \tag{2.73}$$

A second canonical example of an integrator is a shifted Poisson process of rate λ, i.e., $M_t = N_t - \lambda t$, for which

$$[M_t, M_t] = N_t. \tag{2.74}$$

Equation (2.74) follows from taking the limit $\|P\| \to 0$ in the right-hand side of Equation (2.71), leading to a sum of three kinds of terms of the form $(M_{t_i} - M_{t_{i-1}})^2$: (i) there are no jumps between t_i and t_{i-1}, in which case $(M_{t_i} - M_{t_{i-1}}) \to 0$ when $\|P\| \to 0$; (ii) there is exactly one jump between t_i and t_{i-1}, in which case $(M_{t_i} - M_{t_{i-1}}) \to 1$ when $\|P\| \to 0$; (iii) there are multiple jumps between t_i and t_{i-1}, in which case $(M_{t_i} - M_{t_{i-1}})^2$ converges to a nontrivial limit. However, the number of such terms converges to zero when $\|P\| \to 0$.

- *Itô process* with nonnegative drift: The stochastic differential equation

$$\dot{J}_t = b_t + \sqrt{2D_t}\dot{B}_t, \tag{2.75}$$

where $b_t \equiv b_t(X_{[0,t]}) \geq 0$ is a drift term and $D_t \equiv D_t(X_{[0,t]}) \geq 0$ satisfying $\int_0^t D_u^2 du < \infty$, is solved by

$$J_t = \int_0^t b_u \, \mathrm{d}u + \int_0^t \sqrt{2D_u}\, \mathrm{d}B_u. \tag{2.76}$$

The process J_t is a submartingale when $b_t \geq 0$.

- The *multidimensional Itô integral*: The multidimensional Itô integral I_t solves

$$\dot{I}_t \equiv \sum_{a=1}^{d} Z_{a,t}\dot{B}_{a,t}, \tag{2.77}$$

where $B_{a,t}$ with $a = 1, 2, \ldots, d$ are a set of d independent Brownian motions and $Z_{a,t} \equiv Z_{a,t}(B_{1,[0,t]}, B_{2,[0,t]}, \ldots, B_{d,[0,t]})$, is a martingale if

$$\sum_{a=1}^{d} \left\langle \int_0^t Z_{a,s}^2 \, \mathrm{d}s \right\rangle < \infty. \tag{2.78}$$

- The Doléans–Dade *stochastic exponential* of an Itô integral I_t: Let X_t be a possibly high dimensional Itô process, and let $S_t \in \mathbb{R}$ be an Itô process that solves

$$\dot{S}_t = D_t + \sqrt{2D_t}\dot{B}_t, \tag{2.79}$$

where $D_t \equiv D(X_{[0,t]})$ is a functional defined on the trajectories of X and B_t is a Brownian motion process that may be correlated with X. Applying Itô's formula for the variable change $S \to \exp(-S)$, see Equation (B14) in Appendix B.3.1 and below in Equation (2.88) for the one-dimensional case, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\exp(-S_t) = -\exp(-S_t)(\dot{S}_t - D_t) = -\exp(-S_t)\sqrt{2D_t}\dot{B}_t, \tag{2.80}$$

and hence $\exp(-S_t)$ is an Itô integral. If we identify in the above equation the Itô integral

$$\dot{I}_t \equiv -\sqrt{2D_t}\dot{B}_t, \tag{2.81}$$

then Equation (2.80) reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\exp(-S_t) = \exp(-S_t)\dot{I}_t. \tag{2.82}$$

We call the solution to an equation of the form (2.82) the *Doléans–Dade stochastic exponential* of I_t, and we denote it by $\mathcal{E}_t(I) = \exp(-S_t)$. Stochastic exponentials play an important role in stochastic thermodynamics and quantitative finance, as we will see in Chapters 5 and 12, respectively.

- *Position of a tagged particle in the symmetric exclusion process*: We present an example in continuous time of a "false friend" of the martingale, i.e., a process with zero average drift that is *not* a martingale. Consider the position of a tagged particle in the symmetric exclusion process (SEP) on $\mathbb{Z}$ [72]. This is a continuous-time random walk of a particle that moves in a crowded environment.

  In the initial configuration, each site of $\mathbb{Z}$ is occupied with probability ρ by a particle, and it is empty with a probability $1-\rho$. Subsequently, each particle moves at a rate 1/2 to its right or with a rate 1/2 to its left neighbor. If the neighboring site is occupied by a particle, then the jump is blocked and the particle stays in its original position.

  Interestingly, although the particle position X_t of a tagged particle is on average driftless, it is not a martingale. Indeed, in Figure 2.9 we plot $\langle X_t \,|\, X_0 = 0, X_{0^+} = 1\rangle$ as a function of time. If it was a martingale, then one would have $\langle X_t \,|\, X_0 = 0, X_{0^+} = 1\rangle = 1$, independent of t. Note that this is indeed approximately the case for small ρ, but for large enough ρ, there is a clear drift towards the left, as the particle leaves a hole in its trail when jumping to the right at time $t = 0$.

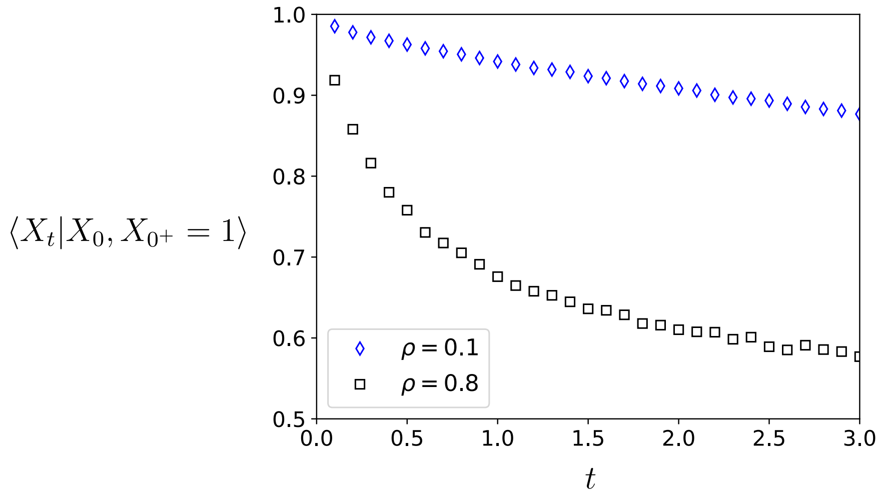

Figure 2.9. The position of a tagged particle in the symmetric exclusion process on $\mathbb{Z}$ is not a martingale. The average position $\langle X_t \,|\, X_0 = 0, X_{0^+} = 1\rangle$ as a function of t, conditioned on the event that X_t makes a jump to the right at time $t = 0$, in the symmetric exclusion process on $\mathbb{Z}$. The total particle occupation probability ρ is given in the legend. Results are empirical means from repeated simulations.

2.2.3. *On stochastic calculus: Itô, Stratonovich, and beyond*

In Section 2.2.2, we have reviewed the prominent role of Itô integrals in martingale theory. In physics, it is often common to use the Stratonovich integral as defined in the books [4,73,74] and the original references [75,76]

$$S_t = \int_0^t Z_s \circ \mathrm{d}B_s = \lim_{\|P\|\to 0} \sum_{i=0}^{n-1} \left(\frac{Z_{t_i} + Z_{t_{i+1}}}{2}\right)\left(B_{t_{i+1}} - B_{t_i}\right), \tag{2.83}$$

where we recall that the limit $\|P\| \to 0$ means the limit of small norm $\|P\|$ of a finite partition $P = [0 = t_1 < t_2 < \cdots < t_n = t]$ of the interval $[0, t]$. The Stratonovich–Fisk convention has the advantage that it allows us to use the standard rules of differential calculus, i.e., the chain rule for derivatives and the fundamental theorem of calculus, see Appendix B.3. However, the Stratonovich integral has the inconvenience of *not* being a martingale as it contains a spurious drift term, see Appendix B.3.4 for details. We recall readers the definition of the Itô integral given in Equation (2.64), copied here for convenience,

$$I_t = \int_0^t Z_s \,\mathrm{d}B_s = \lim_{\|P\|\to 0} \sum_{i=0}^{n-1} Z_{t_i}\left(B_{t_{i+1}} - B_{t_i}\right), \tag{2.84}$$

which differs to the Stratonovich convention on the time point at which the process in the integrand Z is evaluated. The fact that in Itô convention the summation rule is done by evaluating Z at the beginning of each interval of the partition is crucial for Itô processes of the type (2.84) to be martingales.

More generally, we define the α-discretization convention, with $0 \le \alpha \le 1$, via the infinitesimal rules[3]

$$Y_t = \int_0^t Z_s \circ_\alpha \mathrm{d}B_s = \lim_{\|P\|\to 0} \sum_{i=0}^{n-1} \left((1-\alpha) Z_{t_i} + \alpha Z_{t_{i+1}}\right)\left(B_{t_{i+1}} - B_{t_i}\right). \tag{2.85}$$

Apart for the Ito corresponding to $\alpha = 0$, and the Stratonovich–Fisk corresponding to $\alpha = 1/2$, another α-discretization scheme that is widely used in the literature is the anti-Itô convention, corresponding to $\alpha = 1$. However, only in the case of $\alpha = 0$ stochastic integrals are martingales.

In the case of Itô convention, we will omit the $\circ_0$ symbol throughout the treatise. In the following, we use the symbol o to denote the Stratonovich–Fisk convention. As we will show in the subsequent chapters, in physics (i.e., stochastic thermodynamics) it is customary to consider stochastic Itô (Stratonovich) integrals of the type $\int_0^t Z_s \, \mathrm{d}X_s$ ($\int_0^t Z_s \circ \mathrm{d}X_s$) for $Z_s = Z[X_{[0,t]}]$ a functional of the trajectory $X_{[0,t]}$.

2.2.3.1. *Itô's formula.* A useful result in Itô's calculus regards the change of variables, see Appendix B.3.1 for details. Let $X_t \in \mathbb{R}$ be a stochastic process that solves a one-dimensional Itô stochastic differential equation of the form

$$\dot{X}_t = b_t(X_{[0,t]}) + \sigma_t(X_{[0,t]})\dot{B}_t, \tag{2.86}$$

where B_t is the one-dimensional Brownian motion (see Section 2.2.2), and where b_t and σ_t satisfy suitable integrability conditions (see Appendix B.3.1).

Let $g_t(x)$ be a twice continuously differentiable function in $t \in \mathbb{R}^+$ and $x \in \mathbb{R}$ that may depend explicitly on time t. Then the process

$$Y_t = g_t(X_t), \tag{2.87}$$

with X_t described by the Itô stochastic differential equation (2.86), solves the stochastic differential equation [64]

$$\dot{Y}_t = \left(\frac{\partial g_t}{\partial t}\right)(X_t) + \left[\left(\frac{\partial g_t}{\partial x}\right)(X_t)\right]\dot{X}_t + \left[\frac{1}{2}\left(\frac{\partial^2 g_t}{\partial x^2}\right)(X_t)\right]\sigma_t^2(X_{[0,t]}), \tag{2.88}$$

which is known as **Itô's lemma (or Itô's formula)**.

Itô's formula may be understood from a Taylor expansion of $g_{t+\mathrm{d}t}(X_{t+\mathrm{d}t})$, viz.,

$$\begin{aligned} g_{t+\mathrm{d}t}(X_{t+\mathrm{d}t}) - g_t(X_t) = & \left[\left(\frac{\partial g_t}{\partial t}\right)(X_t)\right]\mathrm{d}t + \left[\left(\frac{\partial g}{\partial x}\right)(X_t)\right]\mathrm{d}X_t + \left[\frac{1}{2}\left(\frac{\partial^2 g_t}{\partial t^2}\right)(X_t)\right](\mathrm{d}t)^2 \\ & + \left[\frac{1}{2}\left(\frac{\partial^2 g_t}{\partial x^2}\right)(X_t)\right](\mathrm{d}X_t)^2 + \left[\frac{1}{2}\left(\frac{\partial^2 g_t}{\partial t \partial x}\right)(X_t)\right]\mathrm{d}t\,\mathrm{d}X_t + \cdots \end{aligned} \tag{2.89}$$

Using $\mathrm{d}X_t = \dot{X}_t \, \mathrm{d}t$, the rules of Itô calculus (Equations 2.73), and neglecting contributions of orders higher than $\mathrm{d}t$, we get Equation (2.88). Similarly, one can show that if instead one has a Stratonovich stochastic differential equation

$$\dot{X}_t = b_t(X_{[0,t]}) + \sigma_t(X_{[0,t]}) \circ \dot{B}_t, \tag{2.90}$$

the process $Y_t = g_t(X_t)$ obeys the standard "chain rule"

$$\dot{Y}_t = \left(\frac{\partial g_t}{\partial t}\right)(X_t) + \left[\left(\frac{\partial g_t}{\partial x}\right)(X_t)\right] \circ \dot{X}_t. \tag{2.91}$$

Indeed, this follows from using

$$\left[\left(\frac{\partial g}{\partial x}\right)(X_t)\right]\mathrm{d}X_t + \left[\frac{1}{2}\left(\frac{\partial^2 g_t}{\partial x^2}\right)(X_t)\right](\mathrm{d}X_t)^2 = \frac{1}{2}\left[\left(\frac{\partial g_t}{\partial x}\right)(X_t) + \left(\frac{\partial g_t}{\partial x}\right)(X_{t+\mathrm{d}t})\right]\mathrm{d}X_t$$
$$= \left(\frac{\partial g_t}{\partial x}\right)(X_t)\circ \mathrm{d}X_t. \tag{2.92}$$

We refer readers to Appendix B.3 for further details, generalizations and extensions to, i.e., $d > 1$ dimensions.

2.2.3.2. *From Itô to Stratonovich and back.* As we will show in the subsequent chapters, in statistical physics it is important to convert Itô integrals of the type $\int_0^t g_s(X_s)\,\mathrm{d}X_s$ into Stratonovich integrals of the type $\int_0^t g_s(X_s)\circ\mathrm{d}X_s$, and vice versa. The theorem below provides a rigorous answer for such conversions in the case when X_t is a one-dimensional stochastic process and $g_t(x)$ a smooth function.

THEOREM 1 (**Conversion from Stratonovich to Itô integrals in one dimension**) *Let $X_t \in \mathbb{R}$ be the solution of the Itô stochastic differential equation*

$$\dot{X}_t = b_t(X_t) + \sigma_t(X_t)\dot{B}_t, \tag{2.93}$$

with B_t the one-dimensional Brownian motion and b_t and σ_t two functions satisfying suitable integrability conditions (see Appendix B.3.1). Then the following identity between the Stratonovich and Itô products holds:

$$g_t(X_t)\circ\mathrm{d}X_t = g_t(X_t)\,\mathrm{d}X_t + \frac{\sigma_t^2(X_t)}{2}\left[\left(\frac{\partial g_t}{\partial x}\right)(X_t)\right]\mathrm{d}t, \tag{2.94}$$

which is valid for any function $g_t(x)$ that may depend explicitly on time and is continuously differentiable function in $t \in \mathbb{R}^+$ and $x \in \mathbb{R}$.

The relation (2.94) implies that under the assumptions of Theorem 1, one has the following rule to convert a Stratonovich integral into an Itô integral:

$$\int_0^t g_s(X_s)\circ\dot{X}_s\,\mathrm{d}s = \int_0^t g_s(X_s)\dot{X}_s\,\mathrm{d}s + \int_0^t \frac{\sigma_s^2(X_s)}{2}[(\partial_x g_s)(X_s)]\,\mathrm{d}s, \tag{2.95}$$

which holds for any $t \geq 0$. Equations (2.94) and (2.94) can be generalized to, i.e., processes X_t following $(d > 1)$-dimensional stochastic differential equations, see Equation (3.72).

Chapter 3. Martingales and Markov processes

Time, dear friend, time brings round opportunity; opportunity is the martingale of man. The more we have ventured the more we gain, when we know how to wait.
The three musketeers, A. Dumas (1844).

As discussed in Chapter 2, not all martingales are defined in Markov processes. Nevertheless, in this chapter we focus on martingales associated with Markov processes, as they play a central role in physics. In fact, most mesoscopic, physical processes, whether they are an object in a fluid, transport processes, or chemical reactions, are described by Markov processes.

This chapter is organized into two main parts. Section 3.1 is devoted to martingales in discrete-time Markov processes, and Section 3.2 reviews the theory of martingales in continuous-time Markov processes.

3.1. *Markov processes and martingales in discrete time*

We review the theory of discrete-time martingales M_n defined with respect to Markov chain X_n. First, in Section 3.1.1 we revisit the definition of Markov chains. Next, in Section 3.1.2, we consider the martingale problem, which is one of the central results in the theory of Markov processes. Subsequently, we consider important examples of martingales in Markov processes. In Section 3.1.3, we define Dynkin's martingales (also referred to Lévy's Martingales [77]). Then, in Section 3.1.4 we define multiplicative martingales, which are simple examples of martingales that are not Dynkin's martingales. In Section 3.1.5, we consider martingales that are ratios of path probability densities of Markov chains, which play a prominent role in physics, in particular, in nonequilibrium thermodynamics (see Chapters 5–9).

3.1.1. *Definition of Markov chains*

A **discrete-time Markov chain** is a stochastic process such that its future values conditioned on its current value are statistically independent of its past values. For processes on discrete state space $\mathcal{X}$ this implies

$$\mathcal{P}\left(X_n = x_n \,|\, X_{[0,n-1]}\right) = \mathcal{P}\left(X_n = x_n \,|\, X_{n-1}\right), \tag{3.1}$$

which motivates us to introduce the **transition matrix** of a time-homogeneous discrete-time Markov chain X_n in discrete state space $\mathcal{X}$ as

$$w(x,y) \equiv \mathcal{P}\left(X_n = y \,|\, X_{n-1} = x\right), \quad \forall\, x, y \in \mathcal{X}. \tag{3.2}$$

For processes in continuous state space $\mathcal{X}$, we define their transition matrix as

$$w(x,y) \equiv \frac{\mathcal{P}\left(X_n \in [y, y+\mathrm{d}y] \,|\, X_{n-1} = x\right)}{\mathrm{d}y}, \quad \forall\, x, y \in \mathcal{X}. \tag{3.3}$$

Equations (3.1)–(3.3) imply that the probability (density) for a sequence $x_{[0,n]} = (x_0, x_1, \ldots, x_n)$ to occur in the discrete-time Markov chain is given by

$$\mathcal{P}(x_{[0,n]}) = \rho_0(x_0) \prod_{j=1}^{n} w(x_{j-1}, x_j), \tag{3.4}$$

where $\rho_0(x)$ is the probability (density) of the initial state X_0.

In general, Markov chains are inhomogeneous, i.e., their transition probabilities $w_n(x,y)$ may depend explicitly on time n. However, for clarity we postpone the discussion of time-inhomogeneous Markov processes to Section 3.2 on Markov processes in continuous time, while in discrete time we focus on time-homogeneous processes, i.e., we use $w_n(x,y) = w(x,y)$ throughout Section 3.1.

3.1.2. *Constructing martingales from Markov processes*

Martingales play a prominent role in the theory of Markov processes [78,79]. One reason is due to the following theorem (Theorem 4.1.3. in [78]):

THEOREM 2 (**Characterization of Markov processes with martingales**) *Let X_n be a stochastic process that takes values in $\mathcal{X}$. The following two statements are equivalent:*

- *X_n is a Markov chain with transition matrix $w(x,y)$;*
- *for all real-valued, bounded functions f defined on $\mathcal{X}$ it holds that the process*

$$M_n = f(X_n) - f(X_0) - \sum_{m=0}^{n-1}\sum_{x\in\mathcal{X}}\left(w(X_m,x) - \delta_{x,X_m}\right)f(x) \tag{3.5}$$

is a martingale with respect to X_n.

Taken together, Equation (3.5) implies that M_n is a martingale if and only if X_n is Markovian.

Theorem 2 follows from the identity $M_{n+1} - M_n = f(X_{n+1}) - \sum_{x\in\mathcal{X}} w(X_n,x)f(x)$, which implies

$$\left\langle M_{n+1}|\,X_{[0,n]}\right\rangle = M_n + \left\langle f\,(X_{n+1})|\,X_{[0,n]}\right\rangle - \sum_{x\in\mathcal{X}} w\,(X_n,x)\,f\,(x).$$

Due to this last relation, we obtain

$$\left\langle M_{n+1}|\,X_{[0,n]}\right\rangle = M_n \iff \left\langle f\,(X_{n+1})|\,X_{[0,n]}\right\rangle = \sum_{x\in\mathcal{X}} w\,(X_n,x)\,f\,(x). \tag{3.6}$$

The right-hand side of the second equality of the equivalence (3.6) is a function of X_n only, which implies that X_n is a Markov chain with transition matrix w.

3.1.3. *Dynkin's martingales*

Processes of the form (3.5) are called Dynkin's additive martingales, and we can also express them as

$$M_n = \sum_{m=0}^{n-1}\left(f\,(X_{m+1}) - \sum_{x\in\mathcal{X}} w(X_m,x)f\,(x)\right). \tag{3.7}$$

Put simply, Dynkin's additive martingales, as defined by Equation (3.7), are the cumulative differences between the function $f\,(X_{m+1})$ evaluated on the process X at time $m+1$ minus the expected value of f at time $m+1$ when conditioned on its value at the previous time step. In what follows, we discuss two key examples of Dynkin's martingales.

3.1.3.1. *Processes without memory.* Let us consider the case when X_n is an i.i.d. sequence. This is the particular case of a Markov chain with transition probability $w(y,x) = \mathcal{P}(x)$, where $\mathcal{P}(x)$ is the law of the variables in an i.i.d. sequence. In this case, Dynkin's martingale takes the form

$$M_n = \sum_{m=0}^{n-1} \left(f(X_{m+1}) - \langle f(X_m)\rangle\right). \tag{3.8}$$

Specializing to the case $f(x) = \ln(x)$, we obtain the martingale

$$M_n = \sum_{m=0}^{n-1} (\ln(X_{m+1}) - \langle \ln(X_m)\rangle) = \ln\left(\prod_{m=0}^{n-1} X_{m+1}\right) - n\langle \ln X_0\rangle. \tag{3.9}$$

On the other hand, for the choice $f(x) = x$ we obtain the additive martingale

$$M_n = \sum_{m=0}^{n-1} X_{m+1} - n\langle X_0\rangle, \tag{3.10}$$

which coincides with the martingale (2.7) when $X \in \{1, -1\}$ with probabilities $\mathcal{P}(1) = q$ and $\mathcal{P}(-1) = 1 - q$.

3.1.3.2. *Harmonic functions.* We say that $h(x)$ is a *harmonic* function if it is a bounded function for which

$$\sum_{x\in\mathcal{X}} w(y,x)h(x) = h(y), \quad \forall\, y \in \mathcal{X}. \tag{3.11}$$

Hence, harmonic functions are the right eigenvectors associated with the Perron root of w; note that these are different from the left eigenvectors of the Perron root, which represent the stationary probability distributions. For an unbiased random walk, Equation (3.11) is a discrete version of the equation $\partial_x^2 h(x) = 0$, which clarifies why we call h a harmonic function. Analogously, we say that $s(x)$ is a *subharmonic* function if it is a bounded function for which

$$\sum_{x\in\mathcal{X}} w(y,x)s(x) \geq s(y), \quad \forall\, y \in \mathcal{X}. \tag{3.12}$$

Theorem 2 implies that processes of the form $h(X_n)$, with h a harmonic function, are martingales. Indeed, plugging Equation (3.11) in Equation (3.5), Theorem 2 implies that $h(X_n)$ is a martingale. We can also prove this result directly:

$$\langle h(X_n) \,|\, X_{[0,n-1]}\rangle = \langle h(X_n) \,|\, X_{n-1}\rangle = \sum_{x\in\mathcal{X}} w(X_{n-1}, x)h(x) = h(X_{n-1}), \tag{3.13}$$

where the first equality follows from the Markov property, the second from the definition of the transition matrix (3.2), and the third equality from the definition of harmonic functions (3.11). Analogously, processes of the form $s(X_n)$ with s a subharmonic function are submartingales [77].

For ergodic Markov processes, the trivial function $h(x) = 1$ is the only harmonic function [77]. Indeed, for ergodic processes, the Perron root of the operator $w(x, y)$ is nondegenerate, and hence the left eigenvector of $w(x, y)$ associated with the Perron root is unique. On the other hand, for nonergodic processes, the Perron root is degenerate, and we can construct nontrivial harmonic functions.

As an example of a nontrivial harmonic function, consider the process X_n with initial condition $X_0 \in \mathcal{X} \setminus (\mathcal{X}_1 \cup \mathcal{X}_2)$ that "stops" as soon as X_n reaches the absorbing set $\mathcal{X}_1 \cup \mathcal{X}_2$. In other words, the transition matrix is given by

$$\widetilde{w}(y, x) = \begin{cases} \delta_{x,y}, & \text{if } y \in \mathcal{X}_1 \cup \mathcal{X}_2, \\ w(y, x), & \text{if } y \in \mathcal{X} \setminus (\mathcal{X}_1 \cup \mathcal{X}_2) \, . \end{cases} \tag{3.14}$$

We assume that $\mathcal{X}_1 \cap \mathcal{X}_2 = \phi$. In this case, the process is nonergodic as the states in the sets $\mathcal{X}_1$ and $\mathcal{X}_2$ are absorbing. Let

$$\mathcal{T}_{\mathcal{X}_1} = \min \{n \geq 0 : X_n \in \mathcal{X}_1\} \quad \text{and} \quad \mathcal{T}_{\mathcal{X}_2} = \min \{n \geq 0 : X_n \in \mathcal{X}_2\} \tag{3.15}$$

be the first-passage times when X_n hits the sets $\mathcal{X}_1$ or $\mathcal{X}_2$, respectively. Let us now define the splitting probability that the process X_t hits the set $\mathcal{X}_1$ before hitting the set $\mathcal{X}_2$ given that the state at time k was $X_k = x$,

$$h_{\mathcal{X}_1,\mathcal{X}_2}(x) = \mathcal{P}\left(\mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2} \,|\, X_k = x\right). \tag{3.16}$$

Note that, because the transition rates are considered to be time homogeneous, the splitting probabilities (3.16) are independent of k. It holds that the splitting probability $h_{\mathcal{X}_1,\mathcal{X}_2}(x)$ is a harmonic function related of $\widetilde{w}(y, x)$ [80]. Indeed, using the Markovianity of X, we find iteration

$$\mathcal{P}\left(\mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2} \,|\, X_0 = x\right) = \sum_{y \in \mathcal{X}} \tilde{w}(x, y) \mathcal{P}\left(\mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2} \,|\, X_0 = y\right), \tag{3.17}$$

and hence $h_{\mathcal{X}_1,\mathcal{X}_2}(x)$ solves the Dirichlet problem

$$h_{\mathcal{X}_1,\mathcal{X}_2}(x) = \begin{cases} 1, & \text{if } x \in \mathcal{X}_1, \\ 0, & \text{if } x \in \mathcal{X}_2, \\ \displaystyle\sum_{y \in \mathcal{X}} w(x, y) h_{\mathcal{X}_1,\mathcal{X}_2}(y), & \text{if } x \in \mathcal{X} \setminus (\mathcal{X}_1 \cup \mathcal{X}_2). \end{cases} \tag{3.18}$$

Consequently, the splitting probability $h_{\mathcal{X}_1,\mathcal{X}_2}(x)$ is an example of a nontrivial harmonic function, and it is a martingale.

3.1.3.3. *Doob's h-transform.* An interesting application of positive harmonic functions h is the construction of path probability ratios associated with h through the, so-called, Doob's h-transform, which we introduce below.

Let X be a Markov process, and let h be a positive and harmonic function. Then there exists a Markov process with path probability density $\mathcal{P}_h$ such that

$$\langle f(X_{[0,n]}) \,|\, X_0 \rangle_h = \frac{1}{h(X_0)} \langle h(X_n) f(X_{[0,n]}) \,|\, X_0 \rangle, \tag{3.19}$$

for all $n \in \mathbb{N} \cup \{0\}$, where $\langle \cdot \rangle_h$ denotes the expectation with respect to $\mathcal{P}_h$. We call $\mathcal{P}_h$ the Doob h-transform of $\mathcal{P}$.

THEOREM 3 (**Doob's h-transform**) *Let $\mathcal{P}$ be the path probability density of a Markov chain with transition matrix $w(y,x)$. If h is a non-negative harmonic function associated with this Markov chain, then there exists a Markov chain $\mathcal{P}_h$ with transition matrix $w_h(y,x)$ such that*

$$\frac{\mathcal{P}_h(x_{[0,n]}\,|\,x_0)}{\mathcal{P}(x_{[0,n]}\,|\,x_0)} = \frac{h(x_n)}{h(x_0)}. \tag{3.20}$$

Proof Since h is a positive and harmonic function, it holds that

$$w_h(y,x) = \frac{h(x)}{h(y)}w(y,x) \tag{3.21}$$

is a transition matrix. Indeed, $w_h(y,x) \geq 0$ and

$$\sum_{x\in\mathcal{X}} w_h(y,x) = \sum_{x\in\mathcal{X}} \frac{h(x)}{h(y)}w(y,x) = 1. \tag{3.22}$$

Using that

$$\mathcal{P}_h(X_{[0,n]}\,|\,X_0) = \prod_{j=1}^{n} w_h(X_{j-1},X_j), \quad \mathcal{P}(X_{[0,n]}\,|\,X_0) = \prod_{j=1}^{n} w(X_{j-1},X_j), \tag{3.23}$$

we obtain

$$\frac{\mathcal{P}_h(X_{[0,n]}\,|\,X_0)}{\mathcal{P}(X_{[0,n]}\,|\,X_0)} = \prod_{j=1}^{n} \frac{w_h(X_{j-1},X_j)}{w(X_{j-1},X_j)} = \frac{h(X_n)}{h(X_0)}, \tag{3.24}$$

which completes the proof. ■

Doob's h-transform can be used to map the statistics of a conditioned process, provided by the measure $\mathcal{P}_h$, on the statistics provided by an unconditioned process, given by $\mathcal{P}$, see Refs. [81,82] for some explicit examples. For example, if h is the splitting probability (3.16), $h(x) = h_{\mathcal{X}_1,\mathcal{X}_2}(x)$, then

$$\begin{aligned} w_h(y,x) &= \frac{h(x)}{h(y)}w(y,x) \\ &= \frac{h_{\mathcal{X}_1,\mathcal{X}_2}(x)}{h_{\mathcal{X}_1,\mathcal{X}_2}(y)}w(y,x) \\ &= \frac{\mathcal{P}\left(\mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2}\,|\,X_n = x\right)}{\mathcal{P}\left(\mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2}\,|\,X_{n-1} = y\right)}\mathcal{P}\left(X_n = x\,|\,X_{n-1} = y\right) \\ &= \frac{\mathcal{P}\left(X_n = x, \mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2}\,|\,X_{n-1} = y\right)}{\mathcal{P}\left(\mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2}\,|\,X_{n-1} = y\right)} \\ &= \mathcal{P}\left(X_n = x\,|\,X_{n-1} = y, \mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2}\right). \end{aligned} \tag{3.25}$$

Hence, $\mathcal{P}_h$ is the probability distribution of a Markov process that describes the statistics conditioned on the event $\mathcal{T}_{\mathcal{X}_1} < \mathcal{T}_{\mathcal{X}_2}$.

3.1.4. *Multiplicative martingales*

Given a real-valued, bounded function f, the product

$$M_n = \prod_{j=0}^{n-1} \frac{f(X_{j+1})}{\sum_{x\in\mathcal{X}} w(X_j, x) f(x)} \tag{3.26}$$

is martingale. The martingality of M_n follows from the identity

$$M_{n+1} = M_n \frac{f(X_{n+1})}{\sum_{x\in\mathcal{X}} w(X_n, x) f(x)}, \tag{3.27}$$

together with

$$\langle f(X_{n+1}) \,|\, X_{[0,n]} \rangle = \sum_{x\in\mathcal{X}} w(X_n, x) f(x). \tag{3.28}$$

For the particular case of i.i.d. sequences with transition probability $w(y,x) = \mathcal{P}(x)$, the multiplicative martingale (3.26) takes the form

$$M_n = \frac{\prod_{j=0}^{n-1} f(X_{j+1})}{\langle f(X_0) \rangle^n}. \tag{3.29}$$

Setting $f(x) = \exp(yx)$ and assuming that $X = \{1, -1\}$ is a binary random variable with $\mathcal{P}(1) = q$, we recover the martingale given by Equation (1.8).

3.1.5. *Ratios of path probability densities*

We consider the ratio R_n (see Equation 2.18) of two path probability densities $\mathcal{P}$ and $\mathcal{Q}$ of two time-homogeneous Markov processes in discrete time. To obtain an explicit expression for R_n, we denote $\mathcal{P}(x_{[0,n]})$ as in Equation (3.4), and we write

$$\mathcal{Q}\left(x_{[0,n]}\right) = \rho^{\mathcal{Q}}(x_0) \prod_{j=1}^{n} w^{\mathcal{Q}}(x_{j-1}, x_j). \tag{3.30}$$

When (i) $w^{\mathcal{Q}}(y,x) = 0$ for all $x, y \in \mathcal{X}$ for which $w(y,x) = 0$ and (ii) $\rho^{\mathcal{Q}}(x) = 0$ for all $x \in \mathcal{X}$ for which $\rho(x) = 0$, then the probability density $\mathcal{Q}$ is locally absolutely continuous with respect of $\mathcal{P}$, such that the ratio

$$R_n = \frac{\rho^{\mathcal{Q}}(X_0)}{\rho(X_0)} \prod_{j=1}^{n} \frac{w^{\mathcal{Q}}(X_{j-1}, X_j)}{w(X_{j-1}, X_j)} \tag{3.31}$$

exists and is a $\mathcal{P}$-martingale.

3.2. *Martingales in continuous-time Markov processes*

The second section of this chapter deals with martingales that are defined relative to a Markov process X_t that runs in continuous time. These are arguably the most important examples of martingales for physics, as the lion's share of models that describe physical processes at the mesoscopic scale are continuous time Markov processes, see [25,26,83].

The present section is organized as follows. In Section 3.2.1, we introduce the mathematical quantities defining Markov processes in continuous time. In the following two sections, we define two main classes of Markov processes in continuous time, namely, Markov jump processes in Section 3.2.2 and diffusion processes in Section 3.2.3. In Section 3.2.4, we formulate the martingale problem for Markov processes in continuous time. The last three sections are devoted to examples of martingales that are defined relative to a continuous-time Markov process, namely, Dynkin's martingales in Section 3.2.5, exponential martingales in Section 3.2.6, and Radon–Nikodym derivative processes in Section 3.2.7.

3.2.1. *Markov processes in continuous time: three definitions*

We discuss three complementary ways to define Markov processes [78]. The first approach is based on the path probabilities $\mathcal{P}(x_{[0,t]})$. The second approach is based on the observation that for Markov processes on a discrete state space $\mathcal{X}$

$$\mathcal{P}(X_t = y \,|\, X_{[0,s]}) = \mathcal{P}(X_t = y \,|\, X_s) \tag{3.32}$$

for any $t \geq s \geq 0$, and therefore to determine a Markov process it is sufficient to define the transition function $\mathcal{P}(X_t = y \,|\, X_s = x)$ that gives the transition probability between two states X_s and X_t at times s and t, respectively. A third way to define Markov processes is with the generator or adjoint generator of the process; the former determines the evolution with respect of time s with $t \geq s \geq 0$ of the transition function $\mathcal{P}(X_t = y \,|\, X_s = x)$, and the latter determines the evolution in time of the instantaneous probability density of X.

3.2.1.1. *Path probabilities.* Let us start with a description of Markov processes through path probabilities.

> The **measures** $\mathcal{P}(x_{[0,t]})$ specify the probability to observe sets of paths $x_{[0,t]}$ in the time window $[0,t]$. In general, it is not possible to present an explicit expression for $\mathcal{P}(x_{[0,t]})$. However, we can express the density of $\mathcal{P}(x_{[0,t]})$ relative to another equivalent measure $\mathcal{Q}(x_{[0,t]})$ through the Radon–Nikodym derivative process, see Equation (2.52), or we can use the Onsager–Machlup approach to represent each member $\mathcal{P}$ of an equivalence class $\mathscr{P}$ of mutually absolutely continuous measures in terms of the action functional $\mathcal{A}_{\mathcal{P}}(x_{[0,t]})$, see Equations (2.56)–(2.58). At the end of this section, we present a couple of examples of Radon–Nikodym derivatives of jump processes and diffusions.

3.2.1.2. *Transition functions.* According to Equation (3.32), Markov processes can also be specified with their transition function (again, for discrete state space $\mathcal{X}$)

$$\mathcal{P}_{s,t}(x,y) \equiv \mathcal{P}(X_t = y \,|\, X_s = x), \tag{3.33}$$

for $t \geq s \geq 0$, see Refs. [84,85]. For continuous state space $\mathcal{X}$, we define transition function as

$$\mathcal{P}_{s,t}(x,y) \equiv \frac{\mathcal{P}(X_t \in [y, y+\mathrm{d}y] \;|\, X_s = x)}{\mathrm{d}y}. \tag{3.34}$$

The **transition function** operates on bounded, real-valued functions ϕ defined on $\mathcal{X}$ through

$$\mathcal{P}_{s,t}[\phi](x) \equiv \langle \phi(X_t) \,|\, X_s = x \rangle = \int_{\mathcal{X}} \mathrm{d}y \mathcal{P}_{s,t}(x,y)\phi(y). \tag{3.35}$$

The transition function satisfies the Chapman–Kolmogorov condition

$$\int_{\mathcal{X}} \mathrm{d}y \mathcal{P}_{s,t}(x,y)\mathcal{P}_{t,t'}(y,z) = \mathcal{P}_{s,t'}(x,z), \tag{3.36}$$

for all $s \leq t \leq t'$.

3.2.1.3. *Generators.* A third approach to define a Markov process is through either its generator $\mathcal{L}_t$ or the adjoint generator $\mathcal{L}_t^\dagger$ that describes the evolution in time of the instantaneous probability density ρ_t. Since the latter is used more often in physics, we introduce it first.

The **instantaneous density** of a continuous-time Markov process $X_t \in \mathcal{X}$ is defined as

$$\rho_t(x) \equiv \langle \delta(X_t - x) \rangle, \tag{3.37}$$

where $\langle \cdot \rangle$ is the average over repeated realizations of the Markov process X. The instantaneous density ρ_t is the solution of the Fokker–Planck or Master equation

$$\partial_t \rho_t = \mathcal{L}_t^\dagger \rho_t, \tag{3.38}$$

where $\mathcal{L}_t^\dagger$ is the adjoint of the generator $\mathcal{L}_t$ that expresses the evolution in time of the transition function,

$$\partial_t \mathcal{P}_{s,t} = \mathcal{P}_{s,t}\mathcal{L}_t. \tag{3.39}$$

The explicit time dependence in $\mathcal{L}_t^\dagger$ is relevant for Markov processes with time-dependent, external driving. An invariant density $\rho_{\mathrm{st}}(x)$ is a time-independent distribution that solves for all $t \geq 0$

$$0 = \mathcal{L}_t^\dagger \rho_{\mathrm{st}} \tag{3.40}$$

and we say that ρ_{st} is a **stationary probability density** if in addition to Equation (3.40) one has the normalization condition

$$\int_{\mathcal{X}} \rho_{\mathrm{st}}(x)\,\mathrm{d}x = 1. \tag{3.41}$$

For the special the case of time-homogeneous dynamics, we have $\mathcal{L}_t^\dagger = \mathcal{L}^\dagger$.

Let us clarify some of the mathematical notation used in Equations (3.38)–(3.40):

- The generator $\mathcal{L}_t$ is a linear operator that acts on the Hilbert space $L^2(\mathcal{X})$ of functions $\phi : \mathcal{X} \to \mathbb{R}$ with finite norm $\int_{x\in\mathcal{X}} \mathrm{d}x\phi^2(x)$ and endowed with the inner product

$$(\phi_1, \phi_2) = \int_{x\in\mathcal{X}} \mathrm{d}x\phi_1(x)\phi_2(x). \tag{3.42}$$

In Equation (3.42), dx refers to the Lebesgue measure if the space $\mathcal{X}$ is continuous and to the counting measure if $\mathcal{X}$ is discrete. For the latter, integrals are finite sums, i.e.,

$$\int_{x\in\mathcal{X}} \mathrm{d}x\phi_1(x)\phi_2(x) = \sum_{x\in\mathcal{X}} \mathrm{d}x\phi_1(x)\phi_2(x), \tag{3.43}$$

and operators $\mathcal{L}_t$ are matrices. We will follow this convention throughout this treatise.
- The operator $\mathcal{L}_t^\dagger$ can be seen as the adjoint of the operator $\mathcal{L}_t$ on the Hilbert space $L^2(\mathcal{X})$. In other words, the $\mathcal{L}_t^\dagger\phi_2$ is the function such that

$$(\phi_2, \mathcal{L}_t\phi_1) = \left(\mathcal{L}_t^\dagger\phi_2, \phi_1\right) \tag{3.44}$$

for all functions ϕ_1 in the domain of $\mathcal{L}_t$. Consequently, the right-hand side of Equation (3.38) is the function

$$\left(\mathcal{L}_t^\dagger\rho_t\right)(x) = \int_{\mathcal{X}} \mathrm{d}y\rho_t(y)\mathcal{L}_t(y, x). \tag{3.45}$$

In the particular case where $\mathcal{X}$ is finite, $\mathcal{L}_t^\dagger$ is the matrix transpose of $\mathcal{L}_t$.
- We underline that the left-hand side of Equation (3.39) should be understood as acting on scalar functions $\phi(x)$ as in Equation (3.35), as for the right-hand side

$$(\mathcal{P}_{s,t}[\mathcal{L}_t\phi])(x) = \int_{\mathcal{X}} \mathrm{d}y\mathcal{P}_{s,t}(x, y)\int_{\mathcal{X}} \mathrm{d}z\mathcal{L}_t(y, z)\phi(z). \tag{3.46}$$

- Note that time-homogeneous and stationary Markov processes are, in general, not equivalent. Indeed, a time-homogeneous Markov processes is nonstationary when its distribution ρ_t is nonstationary, and a stationary Markov process is time-inhomogeneous when the generator $\mathcal{L}_t$ depends on time t. Indeed, a Markov process may obey detailed balance with a certain potential $V(x)$ and have time-dependent rates.

Although the most general Markov process consists of a mixture of diffusions and random jumps [86,87], in this treatise, we will focus on two paradigmatic classes of Markov processes in nonequilibrium physics, namely pure jump processes (for which the continuous part is absent) and pure diffusion processes (for which the jump part is absent).

3.2.2. *Markov jump processes*

Markov jump processes are Markov processes for which the process X_t changes its state in a purely discontinuous manner. Figure 3.1 shows an example of a minimal model of a continuous-time Markov jump process in a discrete set of states together with an illustration of a single trajectory of the process.

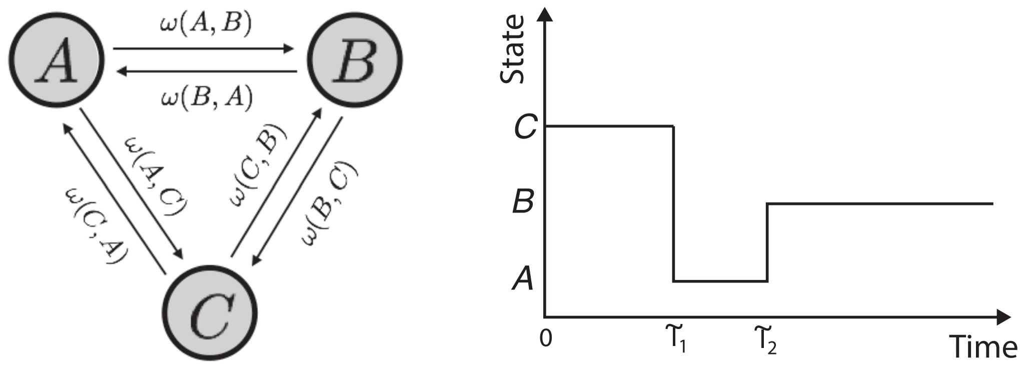

Figure 3.1. Left: Illustration of a three-state continuous-time Markov jump process between the states (gray circles) A, B, and C. The transition rate values between each pair of states are indicated on the arrows. Right: Example trajectory of the process, where the system jumps at a random time $\mathcal{T}_1$ from the initial state C to state A and at a later time $\mathcal{T}_2$ from state A to state B. See text for further details.

3.2.2.1. *Mathematical form.* The trajectories of a Markov jump process are piecewise constant functions, with jump times $\mathcal{T}_i$, with $\mathcal{T}_0 = 0$ and with $i \in \{1, 2, \ldots, N_t\}$, and where N_t is the number of times the process has jumped in the time interval $[0, t]$. In between two jump times, the process X_t does not change its value. We denote the value of X_t right before the ith jump by

$$X_{\mathcal{T}_i^-} = \lim_{\epsilon \to 0, \epsilon > 0} X_{\mathcal{T}_i - \epsilon} \tag{3.47}$$

and right after the ith jump by

$$X_{\mathcal{T}_i^+} = \lim_{\epsilon \to 0, \epsilon > 0} X_{\mathcal{T}_i + \epsilon}, \tag{3.48}$$

so that

$$X_t = X_{\mathcal{T}_{i-1}^+} = X_{\mathcal{T}_i^-} \quad \text{if } t \in [\mathcal{T}_{i-1}, \mathcal{T}_i). \tag{3.49}$$

The *transition rate* $\omega_t(x, y)$ of the jump process is the rate for the transition $x \to y$ at time t, i.e., the average number of jumps from state x to state y occurring in the time interval $[t, t + dt]$.

Other observables that we often use for Markov jump processes are the number of times $N_t(x, y)$ that X_t has jumped form x to y in the time window $[0, t]$ and the residence time $\tau_t(x)$ that the process X_t has spent in the xth state. For discrete sets $\mathcal{X}$, these quantities are formally defined as

$$N_t(x, y) \equiv \sum_{j=1}^{N_t} \delta_{X_{\mathcal{T}_j^-}, x} \delta_{X_{\mathcal{T}_j^+}, y} \tag{3.50}$$

and

$$\tau_t(x) \equiv \int_0^t \delta_{X_s, x} \, \mathrm{d}s, \tag{3.51}$$

where δ is here the Kronecker delta function; analogous definitions can be written down for continuous sets $\mathcal{X}$. Occasionally, we also use $\dot{N}_t(x, y)$, for which it should be understood that

$$N_t(x, y) = \int_0^t \dot{N}_s(x, y) \, \mathrm{d}s. \tag{3.52}$$

The **Markov generator** associated with the Fokker–Planck equation (3.38) is given by

$$(\mathcal{L}_t\phi)\,(x) \equiv \int_{\mathcal{X}} \mathrm{d}y\omega_t(x,y)\,(\phi(y) - \phi(x))\,, \tag{3.53}$$

where $\mathcal{X}$ can be either discrete or continuous. If $\mathcal{X}$ is discrete, the integral in (3.53) must be read as a sum.

When X_t has no explosions [78], i.e., the total number of jumps $\sum_{x\neq y} N_t(x,y)$ is with probability 1 finite, then the generator $\mathcal{L}_t$ uniquely defines the Markov jump process.

The **Fokker–Planck equation** (3.38) associated with a Markov jump process reads

$$\partial_t \rho_t(x) = -\int_{\mathcal{X}} \mathrm{d}y J_{t,\rho}(x,y), \tag{3.54}$$

where the **probability current** reads

$$J_{t,\rho}(x,y) = \rho_t(x)\omega_t(x,y) - \rho_t(y)\omega_t(y,x). \tag{3.55}$$

The Fokker–Planck equation (3.54) can be also written as

$$\partial_t \rho_t(x) = \int_{\mathcal{X}} \mathrm{d}y\,[\rho_t(y)\omega_t(y,x) - \rho_t(x)\omega_t(x,y)]\,, \tag{3.56}$$

which for $\mathcal{X}$ discrete reads

$$\partial_t \rho_t(x) = \sum_{y\in\mathcal{X}} [\rho_t(y)\omega_t(y,x) - \rho_t(x)\omega_t(x,y)]\,. \tag{3.57}$$

Equation (3.57) provides the familiar form for the Master equation of a continuous-time Markov chain where we identify the first term in the right-hand side as probability influxes to state x and the second term as probability outfluxes from state x.

3.2.2.2. *Physical setup: isothermal case.* To add physical content to the dynamics of a Markov jump process, we use the principle of local detailed balance [26,88]. Consider a mesoscopic system, say a molecular motor, that is pushed by an external force of magnitude f_t and is in contact with one thermal bath at temperature T, and m particle reservoirs characterized by the chemical potentials $\mu^{(a)}$, where $a = 1, 2, \ldots, m$. We assume that all particle reservoirs are at temperature T. For isothermal processes, the principle of local detailed balance implies that the ratio of transition rates satisfies

$$\frac{\omega_t(x,y)}{\omega_t(y,x)} = \exp\left(\frac{-(V_t(y) - V_t(x)) + f_t r(x,y) + \sum_{a=1}^{n} \mu^{(a)} n_a(x,y)}{T}\right), \tag{3.58}$$

where $V_t(x)$ is a thermodynamic potential, $r(x,y)$ is the distance moved when the system jumps from x to y, and $n_a(x,y)$ is the number of particles exchanged with the ath particle reservoir when the system jumps from x to y. The plus sign in front of f_t indicates that a negative force opposes forward motion, and the plus sign in front of $\mu^{(a)}$ indicates that $n_a > 0$ when the system binds particles and $n_a < 0$ when the system releases particles. Generalization to particle reservoirs at different temperatures can be found in [89].

3.2.3. *Diffusion processes*

A continuous-time Markov process is a diffusion process if its trajectories X_t are continuous functions of t [90]. We determine diffusion processes through stochastic differential equations, which we first discuss in their mathematical form, and subsequently, we discuss their physical interpretation.

> A d-dimensional **Itô process** $X_t = (X_t^1, X_t^2, \ldots, X_t^d) \in \mathbb{R}^d$ solves the stochastic differential equation
>
> $$\dot{X}_t = b_t(X_t) + \sigma_t(X_t)\dot{B}_t, \tag{3.59}$$
>
> where $b_t = (b_t^1, b_t^2, \ldots, b_t^d)^\dagger \in \mathbb{R}^d$ is a smooth, vectorial function; σ_t is a smooth matrix – not necessarily square – defined on $\mathcal{X}$ with size $d \times n$, and n arbitrary which is the number of noises. In other words, $B_t = (B_t^1, B_t^2, \ldots, B_t^n)^\dagger \in \mathbb{R}^n$ is a vector of n independent Brownian processes. We call
>
> $$D_t(x) = \frac{\sigma_t(x)\sigma_t^\dagger(x)}{2} \tag{3.60}$$
>
> the *diffusion matrix* which is nonnegative and of size $d \times d$.

3.2.3.1. *Mathematical form.*

The generator associated with the diffusion process given by Equation (3.59) takes the form

$$\mathcal{L}_t = b_t \nabla + \mathbf{D}_t \nabla \nabla, \tag{3.61}$$

where $\nabla = (\partial_{x^1}, \partial_{x^2}, \ldots, \partial_{x^d})^\dagger$ is the gradient vector. On a scalar function ϕ, the generator equation (3.61) acts as

$$(\mathcal{L}_t\phi)(x) = b_t(x)(\nabla\phi) + \mathbf{D}_t(x)(\nabla\nabla\phi). \tag{3.62}$$

> The *Fokker–Planck* equation (3.38) associated with a d-dimensional Itô process (3.59) takes the form
>
> $$\partial_t \rho_t + \nabla \cdot J_{t,\rho} = 0, \tag{3.63}$$
>
> where the probability current
>
> $$J_{t,\rho}(x) = b_t(x)\rho_t(x) - \nabla \cdot (\mathbf{D}_t(x)\rho_t(x)). \tag{3.64}$$

3.2.3.2. *Physical setup: Langevin equations.* In physics, Equation (3.59) is often written in a different form that highlights physically relevant quantities, such as the potential and external forces, which is commonly called the *Langevin equation* [4,25,73]. The Langevin equations are mathematically equivalent to (3.59), and when describing multi-dimensional diffusions in a physics context we consider Langevin equations, as these equations are useful for describing physical process, i.e., the dynamics of a set of interacting mesoscopic systems moving in multi-dimensions under external driving.

The **Langevin equation** is the Itô process equation (3.59) for $d = n$ written in terms of physical meaningful quantities [4,25,73]. In particular, we write

$$\dot{X}_t = \boldsymbol{\mu}_t(X_t)F_t(X_t) + (\nabla\,\mathbf{D}_t)\,(X_t) + \sqrt{2\mathbf{D}_t(X_t)}\dot{B}_t, \tag{3.65}$$

where $\boldsymbol{\mu}_t(x)$ is the mobility matrix that may depend on time and space, and is not necessarily symmetric. The force vector $F_t(x)$ can be decomposed as

$$F_t(x) \equiv -\,(\nabla V_t)\,(x) + f_t(x), \tag{3.66}$$

where $V_t(x)$ is a time-dependent potential and $f_t(x)$ is a non-conservative force. The potential is controlled by an external agent through a deterministic protocol λ_t, such that $V_t(x) = V(x, \lambda_t)$. The **Markovian generator** (3.61) associated with the Langevin equation (3.65) takes the form

$$\mathcal{L}_t = (\boldsymbol{\mu}_t F_t)\nabla + \nabla\,\mathbf{D}_t\,\nabla, \tag{3.67}$$

and the *probability current* equation (3.64) takes the form

$$J_{t,\rho}(x) \equiv (\boldsymbol{\mu}_t F_t)(x)\rho_t(x) - \mathbf{D}_t(x)\nabla\rho_t(x). \tag{3.68}$$

The noise vector B_t in the Langevin equation (3.65) consists of d independent standard Brownian motions. The d-dimensional vector X_t may contain both position and momentum variables, such as *underdamped Langevin equations*, in which case the diffusion matrix $\mathbf{D}_t$ is singular; this is the reason why in Equation (3.59) the matrix $\mathbf{D}_t(x)$ is nonnegative instead of positive. The term $(\nabla\,\mathbf{D}_t)^i(x) = \sum_{j=1}^{d}(\partial_j \mathbf{D}_t(x))^{ij}$ is a spurious drift term which comes from the x dependence of the diffusion matrix; its physical origin is discussed below.

In many physical situations, the mobility matrix $\boldsymbol{\mu}_t$ and the diffusion matrix $\mathbf{D}_t$ depend on space. Examples are, among others, the Landau–Lifshitz–Bloch dynamics of a Brownian spin [91] and the diffusion of water molecules near soft-matter phase boundaries [92]. For simplicity, we provide in Figure 3.2 three paradigmatic examples of diffusions that are relevant to physics.

For isothermal systems, the mobility matrix $\boldsymbol{\mu}_t(x)$ is related to the diffusion matrix $\mathbf{D}_t(x)$ by *Einstein's relation*

$$\mathbf{D}_t(x) = \frac{T}{2}\left(\boldsymbol{\mu}_t(x) + \left[\boldsymbol{\mu}_t(x)\right]^{\dagger}\right), \tag{3.69}$$

where T is the temperature of the environment and we have used units for which the Boltzmann constant is equal to one. Einstein's relation (3.69) states that friction (dissipation) and

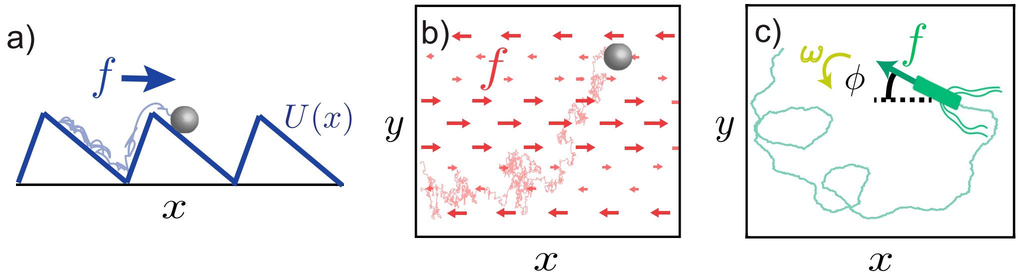

Figure 3.2. Illustration of three diffusion processes described by a Langevin equation of the type (3.65). (a) A Brownian particle moves in a tilted periodic 1D sawtooth potential, $\dot{X}_t = \mu[f - \partial_X V(X_t)] + \sqrt{2D}\dot{B}_t$, with $V(x) = (U_0 x)/x^*$ for $x \in [0, x^*]$ and $V(x) = U_0(1-x)/(1-x^*)$ for $x \in [x^*, 1]$. (b) Motion of a colloid in a 2D force field: $\dot{X}_t = \mu f \cos(2\pi Y_t) + \sqrt{2D}\dot{B}_{x,t}$ and $\dot{Y}_t = \sqrt{2D}\dot{B}_{x,t}$. (c) Chiral active Brownian motion described by the position coordinates $\dot{X}_t = \mu f \cos(\phi_t) + \sqrt{2D}\dot{B}_{x,t}$, $\dot{Y}_t = \mu f \sin(\phi_t) + \sqrt{2D}\dot{B}_{y,t}$ and the orientation angle $\dot{\phi}_t = \mu_\phi \omega + \sqrt{2D_\omega}\dot{B}_{\phi,t}$. See Ref. [12] for further details.

noise (fluctuation) are two conjugated effects of the interaction with the thermal bath. For this reason, Equation (3.69) is also called *fluctuation–dissipation* theorem [93]. When the Einstein relation (3.69) holds, we say that Equation (3.65) is an *isothermal* Langevin equation, and when in addition the mobility matrix is symmetric, i.e., $\boldsymbol{\mu}_t = [\boldsymbol{\mu}_t]^\dagger$, then one retrieves

$$\mathbf{D}_t(x) = T\boldsymbol{\mu}_t(x) \tag{3.70}$$

and we say that Equation (3.65) is an *isothermal overdamped* Langevin. Note that Einstein's relations do not apply if the system interacts with multiple thermal reservoirs at different temperatures, or if the system interacts with a thermal reservoir that is not at equilibrium.

The presence of the "spurious" drift[4]term $(\nabla \mathbf{D}_t)(X_t)$ in Equation (3.65) may appear exotic to readers, however, we note that this term ensures *thermodynamic consistency* in the following sense: if we consider a time-independent potential $V_t = V$ and if we assume that the Einstein relation holds, then in the absence of a non-conservative force ($f = 0$), the term $(\nabla \mathbf{D}_t)(X_t)$ ensures that the stationary distribution of Equation (3.40) is the Boltzmann distribution

$$\rho_{\rm st}(x) = \frac{\exp(-V(x)/T)}{Z}, \tag{3.71}$$

where Z is the partition function, see Refs. [94,95] for details. Note that if the diffusion matrix $\mathbf{D}_t$ depends explicitly on time, then the process is stationary but time-inhomogeneous.

In the following chapters, it will be useful to consider the following identity relating Stratonovich and Ito integrals associated with

$$\int_0^t g_s(X_s) \circ \dot{X}_s \, \mathrm{d}s = \int_0^t g_s(X_s)\dot{X}_s \, \mathrm{d}s + \int_0^t \mathbf{D}_s(X_s) \left[(\nabla g_s)(X_s)\right] \mathrm{d}s, \tag{3.72}$$

which is valid for any function $g_t(x)$ that is smooth on x and t. This relation is a generalization of Equation (2.95) (see also Theorem 1) to d dimensions.

3.2.4. ♠*Stroock–Varadhan martingale problem*

Martingales play a prominent role in the theory of continuous-time Markov processes because, among others, it is possible to characterize Markov processes using martingales [23,79]. This is proved rigorously in the Theorem on page 182 in Ref. [80]. Here we give an informal version of the theorem:

Theorem 4 (**Characterization of Markov processes with martingales**) *Let X_t be a continuous-time stochastic process that takes values in $\mathcal{X}$. The following two statements are equivalent:*

- *X_t is a Markov process with generator $\mathcal{L}_t$, i.e., its instantaneous density obeys $\partial_t \rho_t = \mathcal{L}_t^\dagger \rho_t$, see Equation (3.38).*
- *The process*

$$M_t = g_t(X_t) - g_0(X_0) - \int_0^t \mathrm{d}s \, (\partial_s g_s + \mathcal{L}_s g_s)\,(X_s) \tag{3.73}$$

is a martingale with respect to X_t for all family of real-valued bounded functions $g_t(x)$ defined on $\mathcal{X}$.

The martingale M_t in Equation (3.73) is called *Dynkin's martingale* associated with the function g. Written in an infinitesimal way, the relation (3.73) gives the *generalized Itô formula*

$$d\,(g_t(X_t)) = (\partial_t g_t + \mathcal{L}_t g_t)\,(X_t)\,\mathrm{d}t + \mathrm{d}M_t. \tag{3.74}$$

Theorem 4 is useful in at least two ways. First, given a Markov process X_t, we can construct an arbitrary number of martingales by using different choices of the function g in Equation (3.73). Second, if one proves that the right-hand side of (3.73) is a martingale for all bounded functions g, then it is guaranteed that X_t is a Markov process with generator $\mathcal{L}_t$. Despite its simplicity, Theorem 4 is one of the most important results of probability theory, as it has no counterpart in the theory of ordinary or partial differential equations. It was introduced in the late 1960s by D.W. Stroock and S.R.S. Varadhan, and it contributed to the boost of martingales in modern probability theory.

We sketch the proof of the equivalence in the first direction, i.e., we show that M_t given by Equation (3.73) is a martingale when X_t is a Markov process. Indeed, starting from Equation (3.73), we obtain

$$M_t - M_s = g_t(X_t) - g_s(X_s) - \int_s^t \mathrm{d}u \, (\partial_u g_u + \mathcal{L}_u g_u)\,(X_u). \tag{3.75}$$

Taking the expectation value of Equation (3.75) conditioned on $X_{[0,s]}$ yields

$$\begin{aligned}\left\langle (M_t - M_s) | \, X_{[0,s]} \right\rangle &= \left\langle g_t(X_t) | \, X_{[0,s]} \right\rangle - g_s(X_s) - \int_s^t \mathrm{d}u \left\langle (\partial_u g_u + \mathcal{L}_u g_u)\,(X_u) | \, X_{[0,s]} \right\rangle \\ &= \langle g_t(X_t) | \, X_s \rangle - g_s(X_s) - \int_s^t \mathrm{d}u \,\langle (\partial_u g_u + \mathcal{L}_u g_u)\,(X_u) | \, X_s \rangle\end{aligned}$$

$$
\begin{aligned}
&= \left(\mathcal{P}_{s,t}\left[g_t\right] - g_s - \int_s^t \mathrm{d}u \mathcal{P}_{s,u}\left[(\partial_u + \mathcal{L}_u)\, g_u \right] \right) (X_s) \\
&= \left(\mathcal{P}_{s,t}\left[g_t\right] - g_s - \int_s^t \mathrm{d}u \partial_u \left(\mathcal{P}_s^u [g_u] \right) \right) (X_s) \\
&= 0.
\end{aligned} \tag{3.76}
$$

The second equality of Equation (3.76) follows from the Markov property, the third equality comes from the definition equation (3.35) of the transition function. In particular, in this equality, we have used for the first term the relation

$$
\langle g_t(X_t) | X_s \rangle = \int \mathrm{d}y \mathcal{P}_{s,t}(X_s, y) g_t(y) = \mathcal{P}_{s,t}[g_t](X_s), \tag{3.77}
$$

which follows from the convention given by Equation (3.46), and we have proceeded analogously for the third term. Finally, the fourth equality follows from the forward Kolmogorov equation (3.39) $\partial_u \mathcal{P}_{s,u} = \mathcal{P}_{s,u}\mathcal{L}_u$, fulfilled by the transition probability.

3.2.5. *Dynkin's martingales*

For each function g_t, Equation (3.73) provides us a recipe to construct a martingale M_t associated with a given Markov process X_t. Hence we can use Equation (3.73) to either systematically construct martingales in Markov processes, or to show whether a given process $g_t(X_t)$ is a martingale or not. We call martingales of the form (3.73) *Dynkin's additive martingales*. Note that g_t does not necessarily need to be a bounded function to be a martingale, but it is sufficient to guarantee that $\langle |M_t| \rangle < \infty$. We illustrate some examples below.

3.2.5.1. *Dynkin's martingales associated with jump processes.* If X_t is a Markov jump process, as defined in Section 3.2.2 with generator given in Equation (3.53), then Dynkin's martingales (3.73) take the expression

$$
M_t = g_t(X_t) - g_0(X_0) - \int_0^t \mathrm{d}s \left((\partial_s g_s)(X_s) + \int_{\mathcal{X}} \mathrm{d}y\, \omega_s(X_s, y) \left(g_s(y) - g_s(X_s) \right) \right), \tag{3.78}
$$

where we recall that $g_t(x)$ here is an arbitrary real function of $t \geq 0$ and of $x \in \mathcal{X}$. To illustrate how martingales can be constructed with Dynkin's formula (3.73), we give some explicit examples.

(1) *A Dynkin Martingale associated with the Poisson process.* For a Poisson process N_t with time-dependent transition rate λ_t, i.e., $\mathcal{X} = \mathbb{N}$, $N_0 = 0$, and $\omega_t(n, n+1) = \lambda_t$ with $n \in \mathbb{N}$, the associated Dynkin's martingale is given by

$$
M_t = g_t(N_t) - g_0(0) - \int_0^t \mathrm{d}s \left((\partial_s g_s)(N_s) + \lambda_s \left(g_s(N_s + 1) - g_s(N_s) \right) \right). \tag{3.79}
$$

In particular, the Dynkin martingale associated with the function $g_t(n) = n$ takes the simple expression

$$
M_t = N_t - \int_0^t \mathrm{d}s \lambda_s, \tag{3.80}
$$

which is a generalization of the martingale equation (2.48) for time-independent rates $\lambda_t = \lambda$. Analogously, using $g_t(n) = n^2$, we obtain the martingale

$$
M_t = N_t^2 - \int_0^t \mathrm{d}s \lambda_s \left(2N_s + 1 \right). \tag{3.81}
$$

(2) *A Dynkin Martingale associated with a three-state model.* Let X_t be a three-state continuous-time Markov jump process defined on $\mathcal{X} = \{A, B, C\}$ and with time-independent transition rates $\omega(X, Y)$ between states $X \in \mathcal{X}$ and $Y \in \mathcal{X}$ (see Figure 3.1 for an illustration). For $X_0 = A$, and for the choice $g_t(x) = \delta_{C,x}$, with $\delta_{i,j}$ the Kronecker delta, the associated Dynkin martingale is given by

$$M_t = \delta_{C,X_t} - \int_0^t \mathrm{d}s\omega(X_s, C) + (\omega(C,B) + \omega(C,A)) \int_0^t \mathrm{d}s\delta_{C,X_s}. \quad (3.82)$$

The second term in (3.82) is the accumulated *inflow probability* [96] to state C. On the other hand, the third term in (3.82) depends on the escape rate from state C, $\lambda(C) = \omega(C,B) + \omega(C,A)$, and also on the empirical occupation probability $(1/t)\int_0^t \mathrm{d}s\delta_{\cdot}(X_s)$ of state C.

3.2.5.2. *Dynkin's martingales associated with Langevin dynamics.* If X_t is a Markov diffusion process defined by the Langevin equation (3.65), then using the explicit expression (3.67) of the generator, we obtain Dynkin's martingales of the form:

$$M_t = g_t(X_t) - g_0(X_0) - \int_0^t \mathrm{d}s \left(\partial_s g_s + (\boldsymbol{\mu}_s F_s)\nabla g_s + \nabla\left(\mathbf{D}_s \nabla g_s\right)\right)(X_s). \quad (3.83)$$

We now provide few illuminating physical examples of the Martingales (3.83).

(1) *Martingales associated with Brownian motion.* For a Wiener process $X_t = B_t$ with $B_0 = 0$, Dynkin's martingales are given by

$$M_t = g_t(B_t) - g_0(0) - \int_0^t \mathrm{d}s \left(\partial_s g_s + \frac{1}{2}\partial_{xx} g_s\right)(B_s). \quad (3.84)$$

For example, the Dynkin martingale associated to the functions $g_t(x) = x$, $g_t(x) = x^2$ and $g_t(x) = x^3$ are, respectively, the martingales B_t, $B_t^2 - t$ and $B_t^3 - 3tB_t$ given by, respectively, Equations (2.61), (2.62) and (2.63), the key examples presented in Section 2.2.2 of martingales associated with the Wiener process.

(2) *Martingales associated with Brownian motion in two dimensions.* For $X_t = (B_{x,t}, B_{y,t})^T$ a two-dimensional Brownian motion with $B_{x,t}$ and $B_{y,t}$ two independent Wiener processes, and initial condition $X_0 = (0,0)^T$, Dynkin's martingales are given by

$$M_t = g_t(B_{x,t}, B_{y,t}) - g_0(0,0) - \int_0^t \mathrm{d}s \left(\partial_s g_s + \frac{1}{2}\partial_{xx} g_s + \frac{1}{2}\partial_{yy} g_s\right)(B_{x,t}, B_{y,t}). \quad (3.85)$$

For example, Dynkin's martingale associated with the function $g_t(x,y) = x^2y^2$ is given by

$$M_t = B_{x,t}^2 B_{y,t}^2 - \int_0^t \mathrm{d}s \left(B_{x,s}^2 + B_{y,s}^2\right). \quad (3.86)$$

3.2.5.3. *Dynkin's martingales associated with harmonic functions.* Dynkin's martingale construction implies that processes of the form $h_t(X_t)$, with $h_t(x)$ a harmonic function are martingales, for generic Markovian X_t. We say that $h_t(x)$ is a space–time *harmonic* function if

$$\partial_s h_s + \mathcal{L}_s h_s = 0. \quad (3.87)$$

As a key example, consider the one-dimensional Brownian motion B_t (Wiener process), whose Markovian generator is $\mathcal{L} = \frac{1}{2}\partial_{xx}$. An example of a space–time harmonic function associated with this generator is $h_t(x) = x^2 - t$. Then we recover again that $h_t(B_t) = B_t^2 - t$ is a martingale with respect to the Wiener process.

Similarly, $h_t(x) = \exp(zx - \frac{1}{2}z^2 t)$ is an space–time harmonic function for z any real number. From this result, we recover that the stochastic exponential of B_t introduced in (2.59), $h_t(B_t) = \exp(zB_t - \frac{1}{2}z^2 t)$, is a martingale with respect to the Wiener process for all values of z.

The harmonic martingale $h_t(X_t)$, with $h_t(x)$ a space–time harmonic function, plays a crucial role in Doob's conditioning theory, which has applications in control theory [82].

3.2.6. *Exponential martingales*

For all real-valued, bounded functions g, the continuous version of the discrete time multiplicative martingale (3.26) is the exponential martingale

$$M_t = (g_0(X_0))^{-1} \exp\left[-\int_0^t \mathrm{d}s \left(g_s^{-1} (\partial_s g_s) + g_s^{-1} \mathcal{L}_s [g_s] \right) (X_s) \right] g_t(X_t). \tag{3.88}$$

A canonical example of an exponential martingale is the stochastic exponential (2.59), corresponding to the choices $g_t(x) = \exp(zx)$ and $X_t = B_t$ the Wiener process. Multiplicative martingales (3.88) have important applications in nonequilibrium physics. As a matter of fact, it was shown in [10] that the martingale condition $\langle M_t \,|\, X_{[0,s]} \rangle = M_s$ for the martingales (3.88) is a nonperturbative version of the fluctuation–dissipation theorem. Notably, these martingales are also related to the conditioning theory on rare events [82,97,98].

To prove that M_t in Equation (3.88) is a martingale we first differentiate the process

$$\mathrm{d}M_t = -M_t \left(f_t^{-1} (\partial_t f_t) + f_t^{-1} L_t [f_t] \right) (X_t) \ \mathrm{d}t + M_t f_t^{-1} (X_t) \, d \left(f_t (X_t) \right). \tag{3.89}$$

Next, we apply the generalized Itô formula (3.74) to the function $f_t(X_t)$, which reads

$$d \left(f_t(X_t) \right) = \left(\partial_t g_t + \mathcal{L}_t g_t \right) (X_t) \, \mathrm{d}t + \mathrm{d}M_t^g, \tag{3.90}$$

where we note that M_t^g is the Dynkin's martingale associated with g_t see Equation (3.73). Combining Equations (3.89)–(3.90), we obtain

$$\mathrm{d}M_t = M_t g_t^{-1} (X_t) \, \mathrm{d}M_t^g. \tag{3.91}$$

Equation (3.91) implies that M_t is a martingale because M_t^g is a martingale and M_t is an Itô integral of the form (2.69), or equivalently because M_g is the stochastic exponential that we will introduce later in Section 4.2.5.

3.2.7. *Path probability ratios*

As a last step in our "world tour" on the relation between Markov processes and martingales in continuous time, we present explicit expressions for the path probability ratios R_t, as defined in Equations (2.52)–(2.53). To this aim, we use the Onsager–Machlup approach that represents measures $\mathcal{P}$ that belong to a class $\mathscr{P}$ of mutually absolutely continuous measures with action functionals $\mathcal{A}(X_{[0,t]})$ (see the discussion around Equations 2.56–2.58).

3.2.7.1. *Markov jump processes.* We consider a Markov jump process with transition rates $\omega_t(x, y)$ that determine its generator through Equation (3.53). In addition, we assume that the initial distribution is $\rho_0(x)$. Recall that the trajectories $X_{[0,t]}$ of Markov Jump processes are piecewise constant functions with consecutive states X_i and jump times $\mathcal{T}_i$, see Equation (3.49).

The action functional associated with a Markov jump process is

$$\mathcal{A}(X_{[0,t]}) = -\ln\left(\rho_0(X_0)\right) - \sum_{j=1}^{N_t} \ln\left(\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})\right) + \int_0^t \mathrm{d}s \lambda_s(X_s), \tag{3.92}$$

where we have used

$$\lambda_t(x) = \int_{y\in\mathcal{X}} \mathrm{d}y \omega_t(x,y), \tag{3.93}$$

for the exit rate from state x.

3.2.7.2. *Diffusion processes.* We consider diffusion processes $X_t \in \mathbb{R}^d$ defined through their generator, given in Equation (3.67) with mobility matrix $\boldsymbol{\mu}_t \in \mathbb{R}^{d^2}$, force vector $F_t \in \mathbb{R}^d$, and diffusion matrix $\boldsymbol{D}_t \in \mathbb{R}^{d^2}$, all of which are time dependent. Also, we consider initial distributions $\rho_0(x)$. Note that absolute continuity of the measures $\mathcal{P}$ in $\mathscr{P}$ requires, among others, that all measures have the same diffusion matrix $\boldsymbol{D}_t$.

If the diffusion matrix $\mathbf{D}_t$ is independent of X, then the action takes the form [99,100]

$$\begin{aligned}\mathcal{A}(X_{[0,t]}) = {} & -\ln\rho_0(X_0) - \frac{1}{2}\int_0^t \left(\mathbf{D}_s^{-1}\boldsymbol{\mu}_s F_s\right)(X_s) \circ \dot{X}_s \,\mathrm{d}s \\ & + \frac{1}{4}\int_0^t \left(\boldsymbol{\mu}_s F_s\right)\cdot\left(\mathbf{D}_s^{-1}\boldsymbol{\mu}_s F_s\right)(X_s)\,\mathrm{d}s + \frac{1}{2}\int_0^t \nabla\cdot\left(\boldsymbol{\mu}_s F_s\right)(X_s)\,\mathrm{d}s,\end{aligned} \tag{3.94}$$

where the last term in Equation (3.94) appears due to the Stratonovich convention used in the first integral. We use the Stratonovich convention here as this convention will prove to be useful in physics because of its properties under time reversal. An alternative form of the action $\mathcal{A}$, more commonly used in physics, reads

$$\begin{aligned}\mathcal{A}(X_{[0,t]}) = {} & -\ln\rho_0(X_0) + \int_0^t \frac{1}{4}\left(\dot{X}_s - \boldsymbol{\mu}_s(X_s)F_s(X_s)\right)\mathbf{D}_s^{-1}\left(\dot{X}_s - \boldsymbol{\mu}_s(X_s)F_s(X_s)\right)\,\mathrm{d}s \\ & + \frac{1}{2}\int_0^t \nabla\cdot\left(\boldsymbol{\mu}_s F_s\right)(X_s)\,\mathrm{d}s,\end{aligned} \tag{3.95}$$

which is equivalent to Equation (3.94), as in Equation (2.56) the $\dot{X}_s\mathbf{D}_s^{-1}\dot{X}_s$ can be absorbed into the normalization constant $\mathcal{N}$; note that this is possible as $\mathbf{D}_t$ is the same for all measures $\mathcal{P} \in \mathscr{P}$. However, a complication with Equation (3.95) is that the mathematical meaning of $\dot{X}_s\mathbf{D}_s^{-1}\dot{X}_s$ is not clear, even though this term, whatever it signifies, disappears when taking the ratio between $\mathcal{P}$ and another measure $\mathcal{Q} \in \mathscr{P}$.

The action can also be expressed as

$$\mathcal{A}(X_{[0,t]}) = -\ln\rho_0(X_0) + \int_0^t \mathrm{d}s \mathscr{L}_s(X_s, \dot{X}_s), \tag{3.96}$$

in terms of a Lagrangian

$$\mathscr{L}_s(X_s, \dot{X}_s) \equiv \frac{1}{4}\left(\dot{X}_s - \boldsymbol{\mu}_s(X_s)F_s(X_s)\right)\mathbf{D}_s^{-1}\left(\dot{X}_s - \boldsymbol{\mu}_s(X_s)F_s(X_s)\right) + \frac{1}{2}\nabla\cdot\left(\boldsymbol{\mu}_s F_s\right)(X_s). \tag{3.97}$$

If $\boldsymbol{D}_t$ depends on X_t, then the mathematical meaning of the action $\mathcal{A}$ is less simple [95,100,101]. In this case, we directly consider the Radon–Nikodym derivative process R_t of $\mathcal{Q}$ with respect to

$\mathcal{P}$ that reads [23,85]

$$R_t = \frac{\mathcal{Q}(X_{[0,t]})}{\mathcal{P}(X_{[0,t]})} = \frac{\rho_0^{\mathcal{Q}}(X_0)}{\rho_0^{\mathcal{P}}(X_0)} \exp\left(\frac{1}{2}\int_0^t \left((\boldsymbol{\mu}_s^{\mathcal{Q}} F_s^{\mathcal{Q}} - \boldsymbol{\mu}_s^{\mathcal{P}} F_s^{\mathcal{P}})\right)(X_s)\cdot \mathbf{D}_s^{-1}(X_s)\circ \dot{X}_s\right),$$
$$\times \exp\left(-\int_0^t \frac{1}{4}(\boldsymbol{\mu}_s^{\mathcal{Q}} F_s^{\mathcal{Q}} - \boldsymbol{\mu}_s^{\mathcal{P}} F_s^{\mathcal{P}})(X_s)\cdot \mathbf{D}_s^{-1}(X_s)\left(\boldsymbol{\mu}_s^{\mathcal{Q}} F_s^{\mathcal{Q}} + \boldsymbol{\mu}_s^{\mathcal{P}} F_s^{\mathcal{P}} - 2\nabla\cdot \mathbf{D}_s\right)(X_s)\,\mathrm{d}s\right)$$
$$\times \exp\left(-\int_0^t \frac{1}{2}\nabla\cdot\left[\boldsymbol{\mu}_s^{\mathcal{Q}} F_s^{\mathcal{Q}} - \boldsymbol{\mu}_s^{\mathcal{P}} F_s^{\mathcal{P}}\right](X_s)\,\mathrm{d}s\right). \tag{3.98}$$

Here, it should be understood that $\rho_0^{\mathcal{P}}$ ($\rho_0^{\mathcal{Q}}$), $\mathbf{D}_s^{\mathcal{P}}$ ($\mathbf{D}_s^{\mathcal{Q}}$), $\boldsymbol{\mu}_s^{\mathcal{P}}$ ($\boldsymbol{\mu}_s^{\mathcal{Q}}$), and $F_s^{\mathcal{P}}$ ($F_s^{\mathcal{Q}}$) determine $\mathcal{P}$ ($\mathcal{Q}$).

Chapter 4. Martingales: Mathematical properties

There exist only two kinds of modern mathematics books: one which you cannot read beyond the first page and one which you cannot read beyond the first sentence.
Cheng Ning Yang. Physics Nobel prize (1957).

The properties of martingales are rich, encompassing various branches of mathematics, see, e.g., the textbooks [45,63,66]. Instead of giving a complete overview of martingale theory, we focus on those properties that we think are important for physics. To this aim, we are guided by recent works on martingales in physics, which we review in later chapters.

This chapter is divided into two main sections: Section 4.1 deals with martingales in discrete time and Section 4.2 deals with martingales in continuous time.

4.1. *Discrete time*

4.1.1. *Relating submartingales to martingales*

If M_n is a positive martingale, then $-\ln M_n$ is a submartingale. This is because $-\ln(x)$ is convex (its second-order derivative is nonnegative), and a convex function of a submartingale is a submartingale, as formulated by the following theorem:

THEOREM 5 (**Convex nondecreasing functions of submartingales**) *Let S_n be a submartingale and let $f(x)$ be a real-valued function defined on $\mathbb{R}$ that is nondecreasing, convex, and $\langle |f(S_n)|\rangle < \infty$ for all $n \in \mathbb{N}$. Then the process $f(S_n)$ is a submartingale.*

Proof We verify condition (2.2) that appears in the definition of the submartingale. First, we apply Jensen's inequality to the average of the convex function f, leading to

$$\langle f(S_n)|X_{[0,m]}\rangle \geq f\left(\langle S_n|X_{[0,m]}\rangle\right). \tag{4.1}$$

Subsequently, we use that S_n is a submartingale,

$$\langle S_n|X_{[0,m]}\rangle \geq S_m \tag{4.2}$$

and that f is nondecreasing

$$f\left(\langle S_n | X_{[0,m]}\rangle\right) \geq f(S_m). \tag{4.3}$$

Relation (4.1) together with (4.3) implies that $f(S_n)$ has a nonnegative drift and is thus a submartingale. ■

We will use Theorem 5 in Chapters 5 and 7 to derive the submartingale property of entropy production and the second law of thermodynamics.

If S is a submartingale and its mean value is a constant independent of time, i.e.,

$$\langle S_t \rangle = c, \tag{4.4}$$

then S_t is a martingale. Indeed, the process

$$\langle S_t | X_{[0,s]}\rangle - S_s, \quad t \geq s, \tag{4.5}$$

for fixed s, is a nonnegative process with zero expectation, and thus

$$\langle S_t | X_{[0,s]}\rangle = S_s. \tag{4.6}$$

4.1.2. *Doob's decomposition theorem*

We call a stochastic process A_n *predictable* if A_n is a function of $X_{[0,n-1]}$ and we say that a process is *increasing* if with probability one, $0 = A_0 \leq A_1 \leq A_2 \cdots$.

It is always possible to decompose a submartingale into a martingale and an increasing process that is predictable, and this decomposition is unique (see Theorem 2.13 in Ref. [66]).

THEOREM 6 (**Doob's decomposition**) *Let Y_n be a discrete-time process that is a function of the set of trajectories $X_{[0,n]} = (X_0, X_1, \ldots, X_n)$, and integrable (i.e., $\langle |Y_n| \rangle < \infty$ for all n). Then it can be uniquely decomposed as*

$$Y_n = Y_0 + M_n + \underbrace{\sum_{k=0}^{n-1} v_k}_{A_n}, \tag{4.7}$$

where we have introduced the conditional velocity

$$v_k = \left\langle (Y_{k+1} - Y_k) \, | X_{[0,k]} \right\rangle. \tag{4.8}$$

The predictable process A_n is called the compensator and M_n, defined as

$$M_{n+1} - M_n = Y_{n+1} - Y_n - v_n, \tag{4.9}$$

is a martingale with respect to the underlying process X_n, i.e., $\langle M_n | X_{[0,m]}\rangle = M_m$, for $m \leq n$.

If Y_n is a submartingale (supermartingale), then $v_k \geq 0$ ($v_k \leq 0$), and the compensator A_n is increasing (decreasing). In Theorem 6 "unique" means that if there exist two Doob decompositions $S_n = M_n + A_n$ and $S_n = M'_n + A'_n$, then for all $n \in \mathbb{N}$ one has $\mathcal{P}(M_n = M'_n, A_n = A'_n) = 1$.

Example 1 Doob decomposition for the square of a stochastic process We consider the Doob decomposition of the square $Y_n = Z_n^2$ of a discrete-time process Z_n, namely,

$$Z_n^2 = Z_0^2 + M_n + \sum_{k=0}^{n-1} v_k, \tag{4.10}$$

where

$$\begin{cases} v_k \equiv \left\langle \left(Z_{k+1}^2 - Z_k^2\right) |X_{[0,k]}\right\rangle, \\ M_{n+1} \equiv M_n + Z_{n+1}^2 - Z_n^2 - v_n. \end{cases} \tag{4.11}$$

The velocity v_n is called the *angle bracket* process of Z_n. Now, if additionally Z_n is a martingale with respect to X_n, then the angle bracket process satisfies

$$v_k = \left\langle \left(Z_{k+1}^2 - Z_k^2\right) |X_{[0,k]}\right\rangle \tag{4.12}$$

$$= \left\langle (Z_{k+1} - Z_k)^2 \, |X_{[0,k]}\right\rangle + 2\left\langle Z_{k+1}Z_k|X_{[0,k]}\right\rangle - 2\left\langle Z_k^2|X_{[0,k]}\right\rangle \tag{4.13}$$

$$= \left\langle (Z_{k+1} - Z_k)^2 \, |X_{[0,k]}\right\rangle, \tag{4.14}$$

where we have used the martingale property of Z_n in the third equality. Processes of the type $\langle (Z_{k+1} - Z_k)^2 | X_{[0,k]}\rangle$ are often called *sharp bracket* processes and the associated compensator, which is also called the *conditional variance* of Z_n, reads

$$V_n = \sum_{k=0}^{n-1} v_k = \sum_{k=0}^{n-1} \left\langle (Z_{k+1} - Z_k)^2 \, |X_{[0,k]}\right\rangle. \tag{4.15}$$

Note that if Z_n is a martingale, then by virtue of Theorem 5 Z_n^2 is a submartingale with respect to X_n.

Example 2 Doob decomposition for a function of a Markov chain X_n Theorem 2 directly gives the Doob decomposition of $f(X_n)$ for all real-valued bounded functions f, viz.,

$$f(X_n) = f(X_0) + M_n + \underbrace{\sum_{m=0}^{n-1} \sum_{x \in \mathcal{X}} \left(w(X_m, x) - \delta_{x,X_m}\right) f(x)}_{A_n}, \tag{4.16}$$

where M_n is Dynkin's additive martingale, as defined in (3.5), and $w(x, y)$ is the transition matrix of the Markov chain X_n.

4.1.3. *Extreme values*

4.1.3.1. *Doob's maximum inequality.* Let A be a positive random variable. Markov's inequality states that

$$\mathcal{P}\left(A \geq \lambda\right) \leq \frac{\langle A \rangle}{\lambda}. \tag{4.17}$$

Doob's maximum inequality is a refinement of Markov's inequality that involves the supremum of a submartingale. More precisely the following theorem holds:

THEOREM 7 (**Doob's maximum inequality**) *Let S_n be a submartingale. Then*

$$\mathcal{P}\left(\sup_{m\leq n} S_m \geq \lambda\right) \leq \frac{\langle \max\{S_n, 0\}\rangle}{\lambda}, \tag{4.18}$$

where $\lambda \geq 0$.

Proof We consider the sequence of sets

$$\Phi_1 = \{S_1 > \lambda\}, \tag{4.19}$$

$$\Phi_2 = \{S_1 \leq \lambda, S_2 > \lambda\}, \tag{4.20}$$

$$\vdots$$

$$\Phi_k = \{S_1 \leq \lambda, S_2 \leq \lambda, \ldots S_{k-1} \leq \lambda, S_k > \lambda\}, \tag{4.21}$$

with $\lambda > 0$ and $k \geq 2$. Doob's maximum inequality follows from the following inequalities:

$$\langle S_n \rangle \geq \sum_{k=1}^{n} \mathcal{P}\left(\Phi_k\right) \langle S_n | \Phi_k \rangle \tag{4.22}$$

$$\geq \sum_{k=1}^{n} \mathcal{P}\left(\Phi_k\right) \langle S_k | \Phi_k \rangle \tag{4.23}$$

$$\geq \lambda \sum_{k=1}^{n} \mathcal{P}\left(\Phi_k\right) = \lambda\, \mathcal{P}\left(\sup_{n'\leq n} S_{n'} \geq \lambda\right). \tag{4.24}$$

The first inequality (4.22) follows from the fact that S_n is nonnegative. The second inequality (4.23) holds because S is a submartingale. Finally, the last inequality is a consequence of the definition of the sets Φ_k. ■

Note that in discrete time, the supremum can be replaced by the maximum, whereas in continuous time this will not be the case.

In Chapter 7, we use Doob's maximum inequality to derive the infimum law for entropy production.

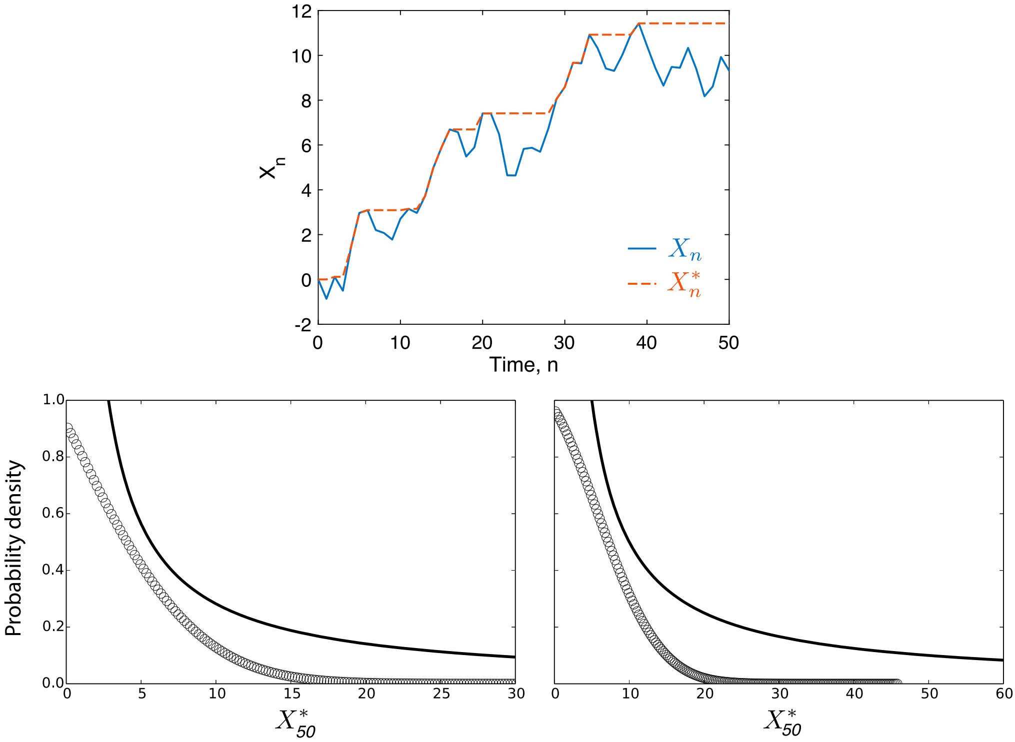

Figure 4.1. Top: Example trajectory X_n (blue line) of a discrete-time random walker on $\mathbb{R}$ given by $X_n = X_{n-1} + a + Y_n$, with $X_0 = 0$, $a = 0.1$, and Y_n ($n \geq 1$) a Gaussian random number with zero mean and unit standard deviation. The red dashed line is the running maximum $X_n^* = \max_{n' \leq n} X_{n'}$ associated with the trajectory, see Equation (4.25). Bottom: Distributions $\rho_{X_n^*}$ of the maximum X_n^* of a random walker on the real line with parameters $n = 50$, $a = 0$ (bottom left) and $a = 0.1$ (bottom right) and with Y a Gaussian random variable with zero mean and unit variance. Markers are the numerical results of the distribution $\rho_{X_n^*}$ and the solid line is the martingale bound given in Equation (4.18) with $\langle \max\{X_n, 0\} \rangle = \sqrt{n/2\pi}$ (left) and $\langle \max\{X_n, 0\} \rangle = an + O(\sqrt{n} \exp(-a^2 n/2))$ (right).

4.1.3.2. *Application: extreme values of random walkers.* Doob's maximum inequality can be used to bound the cumulative distribution of extreme values of stochastic processes, which have attracted considerable attention in various scientific disciplines such as statistical physics [102–105], climate science [106,107], and finance [108]. Here, for illustrative purposes, we consider the discrete-time random walk $X_n = X_{n-1} + a + Y_n$, as defined in Equation (2.31), for different values of a and with the noise variable Y_n a random variable with zero mean and finite variance, see Figure 4.1.

It is in general difficult to obtain an exact expression for the cumulative distribution of the finite-time maximum

$$X_n^* = \max_{n' \leq n} X_{n'}. \tag{4.25}$$

For example, for the special case of $a = 0$ the cumulative distribution of the maximum is described by the Pollaczek–Spitzer formula [109–112]. The quantity $q_n(\lambda) = 1 - \mathcal{P}\left[X_n^* \geq \lambda\right]$ denotes the probability that the process stays below the threshold λ, and therefore we call it the survival probability. The Pollaczek–Spitzer formula provides a formula for the double inverse Laplace transform of the survival probability in terms of the Fourier transform

$\phi(k) = \int_{-\infty}^{\infty} \rho_Y(y) \exp(iky)\, dy$ of the distribution ρ_Y of the increment [112], viz.,

$$\int_0^\infty \left[\sum_{n=0}^{\infty} q_n(x_0) s^n\right] \exp(-p x_0)\, dx_0 = \frac{1}{p\sqrt{1-s}} \exp\left(-\frac{p}{\pi}\int_0^\infty \frac{\ln(1 - s\phi(k))}{p^2+k^2}\, dk\right). \quad (4.26)$$

Although it is in general difficult to take the inverse of the double Laplace transform in Equation (4.26), one can readily bound the distribution of the maximum of a random walker with the martingale bound equation (4.18). Indeed, it is often easy to determine $\langle \max\{X_n, 0\}\rangle$, as illustrated in Figure 4.1. In Figure 4.1, we compare numerically obtained results for the distribution of X_n^* with analytical results from the martingale bound $\langle \max\{X_n, 0\}\rangle / x^*$ in Theorem 7. In particular, we consider the case when Y is a random variable drawn from a standard Gaussian distribution with $a = 0$ (left) and with $a > 0$ (right).

4.1.4. *Convergence theorems*

A fundamental result in martingale theory is that, under a set of conditions specified in the martingale convergence theorems, the fluctuations in the trajectories of a martingale decrease as a function of n, yielding the convergence to an asymptotic limit, i.e.,

$$\lim_{n\to\infty} M_n = M_\infty. \quad (4.27)$$

The martingale convergence theorem is a fundamental property of martingales that follows from the fact that martingales represent a gambler's fortune in a fair game of chance. Consequently, a martingale process cannot keep fluctuating as otherwise a gambler could exploit a buy low and sell high strategy to make profit out of a fair game of chance. Note that this is more than a simple analogy as the martingale convergence theorem is proved with Doob's upward crossing lemma, which precisely bounds the profit a gambler can make out of the buy low and sell high strategy.

There exist two versions of the martingale convergence theorem, one that holds for submartingales bounded from above and another that holds for uniformly integrable martingales.

Now, let us get to the specifics. Let x_n, with $n \in \mathbb{N}$, be a nondecreasing deterministic sequence of real numbers that is bounded from above (i.e., $\sup_n x_n < \infty$), then elementary math gives $\lim_{n\to\infty} x_n = x_\infty \in \mathbb{R}$. The following theorem (Theorem 2.6 in Ref. [66]) generalizes the previous result to submartingale processes.

THEOREM 8 (**Submartingale convergence theorem**) *Let S_n be a submartingale for which*

$$\sup_n \langle \max\{S_n, 0\}\rangle < \infty. \quad (4.28)$$

Then there exists a S_∞ for which

$$\langle \max\{S_\infty, 0\}\rangle < \infty, \quad (4.29)$$

such that

$$\mathcal{P}\left(\lim_{n\to\infty} S_n = S_\infty\right) = 1. \quad (4.30)$$

Next we discuss the second version of the martingale convergence theorem that holds for uniformly integrable processes. We say that a stochastic process A_n is *uniformly integrable* if

$$\lim_{m\to\infty} \sup_{n\in\mathbb{N}\cup\{0\}} \langle |A_n|\, 1_{|A_n|\geq m}\rangle = 0. \tag{4.31}$$

Note that because m in Equation (4.31) is independent of n, Equation (4.31) implies that A_n cannot escape to infinity. Uniform integrability is important since it allows us to swap expectation values with limits, i.e.,

$$\left\langle \lim_{n\to\infty} A_n \right\rangle = \lim_{n\to\infty} \langle A_n\rangle, \tag{4.32}$$

if $\lim_{n\to\infty} A_n$ exists with probability 1.

The properties of uniformly integrable martingales can be characterized with the following theorem (Theorem 2.7 in Ref. [66]), which states that uniformly integrable martingales and conditional expectations processes are equivalent:

THEOREM 9 (**Convergence theorem for uniformly integrable martingales**) *Let M_n be a martingale defined on $n \in \mathbb{N}\cup\{0\}$. The following conditions are equivalent:*

- *the process M_n is uniformly integrable;*
- $\sup_n\langle |M_n|\rangle < \infty$ *and thus* $M_\infty = \lim_{n\to\infty} M_n$ *exists. In addition, M_n is regular, which means that with probability 1 it holds that*

$$M_n = \langle M_\infty | X_{[0,n]}\rangle. \tag{4.33}$$

- $M_\infty = \lim_{n\to\infty} M_n$ *exists and*

$$\lim_{n\to\infty} \langle |M_\infty - M_n|\rangle = 0. \tag{4.34}$$

Uniform integrability extends thus the martingale sequence from the natural numbers $\mathbb{N}$ to the natural numbers extended with infinity $\mathbb{N}\cup\{\infty\}$.

Several fundamental results in probability theory can be derived from Doob's martingale convergence theorem. A notable example is *Lévy's upwards theorem*, which states that

$$\lim_{n\to\infty} \langle A|X_{[0,n]}\rangle = \langle A|X_{[0,\infty)}\rangle \tag{4.35}$$

holds for integrable random variables A, where convergence should be understood either with probability 1 or in the L^1 norm. In addition, Lévy's upwards theorem implies *Kolmogorov's zero-one law*, which states that tail events Φ, which are events independent of any finite sequence $X_1, X_2, \ldots, X_n$, i.e.,

$$\mathbb{P}\left[\Phi, X_{[0,n]} = x_{[0,n]}\right] = \mathbb{P}[\Phi]\,\mathbb{P}\left[X_{[0,n]} = x_{[0,n]}\right] \tag{4.36}$$

occur either with probability 1, $\mathbb{P}[\Phi] = 1$, or with probability 0, $\mathbb{P}[\Phi] = 0$. This law is used, i.e., in percolation theory [113], to show that an infinite, percolating cluster exists either with probability 0 or 1 [114].

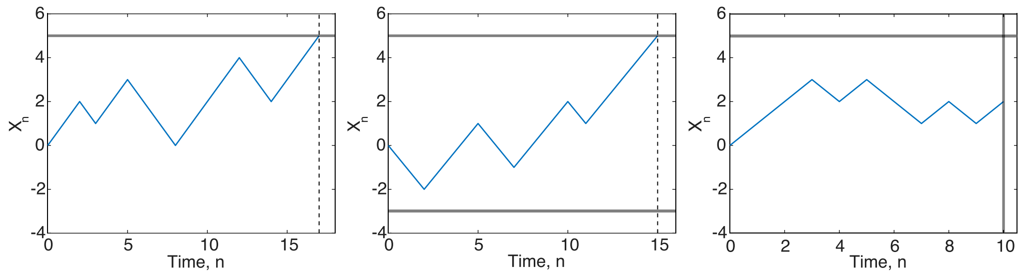

Figure 4.2. Three examples of stopping times evaluated over trajectories of a discrete-time biased random walk on $\mathbb{Z}$, with forward jump probability $q = 0.7$ and backward jump probability $1 - q = 0.3$. Left: First passage time to reach the absorbing boundary $\ell_+ = 5$. Middle: First escape time from the interval $[-3, 5]$. Right: $\min(\mathcal{T}_1, 10)$ with $\mathcal{T}_1$ the first passage time to reach the absorbing boundary $\ell_+ = 5$. In the three examples, the blue zigzag lines are a linear interpolation between the discrete values X_n and a guide to the eye, the thick horizontal lines illustrate the boundaries of the stopping-time problem, and the dashed vertical lines denote the time when the stopping condition takes place.

4.1.5. *Stopping times*

Martingales can be used to study stochastic processes at random times, and this has been up to now one of its main uses in stochastic thermodynamics. Therefore, in this section we introduce the concept of a stopping time.

4.1.5.1. *Definition and examples.* Put simply, a stopping time is the time when a specific criterion is met for the first time. Importantly, the stopping criterion obeys causality, and this makes stopping times suitable for modelling physical processes.

> A **stopping time** is a nonnegative random variable $\mathcal{T} = \mathcal{T}(X_{[0,\infty)}) \in \mathbb{N} \cup \{0, \infty\}$ that is statistically independent of the part of the trajectory $X_{[\mathcal{T}+1,\infty)}$ that comes after the stopping time.

Note that this definition can be generalized to continuous time. Examples of stopping times are:

- The mth time a stochastic process visits a subset of $\mathcal{X}$. In the particular case of $m = 1$, we obtain first-passage times.
- The first time a functional $f(X_{[0,n]}) \in \mathbb{R}$ defined on the trajectories of X exits an interval $(-\ell_-, \ell_+)$. Since the main observables of stochastic thermodynamics are functionals, this example is of particular importance. In the specific case of $f(X_{[0,n]}) = X_n$, this stopping time equals the first escape time of X_n from the interval $(-\ell_-, \ell_+)$.
- $\mathcal{T}_1 \wedge n = \min(\mathcal{T}_1, n)$, where $\mathcal{T}_1$ is the first time that a prescribed condition is met for the stochastic process of interest, and $n \in \mathbb{N}$ determines a finite time horizon.

On the other hand, the following quantities *are not* stopping times:

- The time when a random walker leaves indefinitely a subset of $\mathcal{X}$
- The time a stochastic process attains a minimum or maximum value (which may be a local minimum or maximum)
- The occupation time spent in a given subset of $\mathcal{X}$ (Figure 4.2).

4.1.5.2. *Doob's optional stopping theorems.* Consider a gambler who participates in a fair game of chance. Can (s)he make on average profit by leaving the game at an intelligently chosen moment $\mathcal{T}$? In other words, is it possible that $\langle M_{\mathcal{T}} \rangle > \langle M_0 \rangle$?

The optional stopping theorem states that $\langle M_{\mathcal{T}} \rangle = \langle M_0 \rangle$, given certain conditions on the stopping time $\mathcal{T}$ and the martingale M. Loosely said, these conditions impose that the gambler does not have access to an infinite budget. Indeed, if the gambler has access to an infinite budget, then strategies to make profit out of a fair game of chance exist, and this leads to paradoxes, the most well known being the St. Petersburg paradox [115].

We illustrate the optional stopping theorem with the example of a gambler's wealth F_n in a fair coin toss game, see Equation (2.6). We assume that $F_0 = f_{\rm init}$. If

$$\mathcal{T}^{(1)} = \min\{n \geq 0 : F_n = f_{\rm init} + m_+\} \tag{4.37}$$

with $m_+ \in \mathbb{N}$, then

$$\langle F_{\mathcal{T}^{(1)}} \rangle = f_{\rm init} + m_+ \geq f_{\rm init} = F_0, \tag{4.38}$$

which implies that the gambler is earning money on average and that the optional stopping theorem does not apply. However, if

$$\mathcal{T}^{(2)} = \min\{n \geq 0 : F_n = f_{\rm init} + m_+ \text{ or } F_n = f_{\rm init} - m_-\} \tag{4.39}$$

with $m_+, m_- \in \mathbb{N}$, then

$$\langle F_{\mathcal{T}^{(2)}} \rangle = f_{\rm init} = F_0. \tag{4.40}$$

The difference between the stopping times $\mathcal{T}^{(1)}$ Equation (4.37) and $\mathcal{T}^{(2)}$ Equation (4.39) is that in the first case the gambler has access to an infinite budget (F_n can take arbitrary large negative values) whereas in the second case the gambler has a finite budget (F_n is bounded between $f_{\rm init} - m_-$ and $f_{\rm init} + m_+$).

In what follows, we consider several versions of Doob's optional stopping theorem. Amongst Doob's theorems, the first important result that we review is the following (Theorem 2.1, chapter VII in Ref. [22]).

THEOREM 10 (**Doob's optional sampling theorem**) *Let M_n be a martingale (submartingale) and let $\mathcal{T}$ be a stopping time, both with respect to the process X_n. Then the stopped process $M_{\mathcal{T}\wedge n}$, with $\mathcal{T} \wedge n = \min\{\mathcal{T}, n\}$ a finite stopping time, is also a martingale (submartingale), i.e.,*

$$\langle M_{\mathcal{T}\wedge n} | X_{[0,m]} \rangle = M_{\mathcal{T}\wedge m} \quad \left(\langle M_{\mathcal{T}\wedge n} | X_{[0,m]} \rangle \geq M_{\mathcal{T}\wedge m} \right), \tag{4.41}$$

for $0 \leq m \leq n$.

Proof The process $M_{\mathcal{T}\wedge n}$ is integrable, since it is a finite sum of integrable random variables. Because of the tower property of conditional expectations, it is sufficient to show that

$$\langle M_{\mathcal{T}\wedge n} | X_{[0,n-1]} \rangle = M_{\mathcal{T}\wedge(n-1)}. \tag{4.42}$$

It holds that

$$\langle M_{\mathcal{T}\wedge n} | X_{[0,n-1]} \rangle = M_{\mathcal{T}\wedge(n-1)} + \langle (M_n - M_{n-1}) \mathbf{1}_{\mathcal{T}\geq n} | X_{[0,n-1]} \rangle \tag{4.43}$$

$$= M_{\mathcal{T}\wedge(n-1)} + \mathbf{1}_{\mathcal{T}\geq n} \langle (M_n - M_{n-1}) | X_{[0,n-1]} \rangle = M_{\mathcal{T}\wedge(n-1)}, \tag{4.44}$$

where we used the indicator function Equation (2.51) for

$$\Phi = \left\{ X_{[0,\infty]} : \mathcal{T}(X_{[0,\infty]}) \geq n \right\}. \tag{4.45}$$

The proof in the case of submartingales is analogous. ■

Applying the optional sampling theorem to uniform integrable martingales, see definition (4.31), we obtain Doob's optional stopping theorem (Theorem 2.9 in [66]).

Theorem 11 (**Doob's Optional stopping, version I**) *Let M_n be a uniformly integrable martingale and let $\mathcal{T}_1$ and $\mathcal{T}_2$ be two stopping times with $P(\mathcal{T}_2 \geq \mathcal{T}_1) = 1$, then*

$$\langle M_{\mathcal{T}_2} | X_{[0,\mathcal{T}_1]} \rangle = M_{\mathcal{T}_1}. \tag{4.46}$$

For the particular case of $\mathcal{T}_1 = 0$ and $\mathcal{T}_2 = \mathcal{T}$, we obtain

$$\langle M_{\mathcal{T}} | X_0 \rangle = M_0, \tag{4.47}$$

i.e., the average of a uniformly integrable martingale conditioned on the initial state X_0 equals its initial value M_0.

For simplicity, we give here the proof of the particular case (4.47).

Proof According to Theorem 10, it holds that

$$\lim_{n\to\infty} \langle M_{\mathcal{T}\wedge n}|X_0\rangle = M_0. \tag{4.48}$$

Since $M_{\mathcal{T}\wedge n}$ is a uniformly integrable, it holds that

$$\lim_{n\to\infty} \langle M_{\mathcal{T}\wedge n}|X_0\rangle = \langle \lim_{n\to\infty} M_{\mathcal{T}\wedge n}|X_0\rangle. \tag{4.49}$$

In addition,

$$\langle \lim_{n\to\infty} M_{\mathcal{T}\wedge n}|X_0\rangle = \langle M_{\mathcal{T}\wedge\infty}|X_0\rangle = \langle M_{\mathcal{T}}|X_0\rangle. \tag{4.50}$$

Equations (4.48)–(4.50) imply (4.47), which is what we meant to prove. ■

An alternative version of Doob's optional stopping theorem corresponds to the case of a gambler that has a finite budget (Theorem 4.1.1 in [78]).

THEOREM 12 (**Doob's optional stopping, version II**) *Let M_n be a martingale and let $\mathcal{T}$ be a stopping time. If $\mathcal{P}(\mathcal{T} < \infty) = 1$ and if there exists a constant m such that $|M_n| \leq m$ for all $n \leq \mathcal{T}$, then*

$$\langle M_{\mathcal{T}}\rangle = \langle M_0\rangle. \tag{4.51}$$

The two versions of Doob's optional stopping theorem are related to each other, and in fact one can derive Theorem 12 from Theorem 11, see for example the proofs in the appendix of Ref. [13].

The optional stopping theorem is one of the key properties that characterize martingales, and in fact, it is a defining property of martingales [90]. Indeed, as we will show, the condition equation (2.1) can be written in terms of the stopping time

$$\mathcal{T} = m\mathbf{1}_{\Phi}(X_{[0,m]}) + n\mathbf{1}_{\Phi^c}(X_{[0,m]}), \tag{4.52}$$

where Φ is a measurable subset of the set of trajectories $x_{[0,m]}$, where Φ^c is the complement of Φ, where $\mathbf{1}_{\Phi}(x_{[0,m]})$ is the indicator function that returns the value 1 when $x_{[0,m]} \in \Phi$ and 0 when $x_{[0,m]} \notin \Phi$, and where $m \leq n$.

THEOREM 13 *A stochastic process $M_n = M[X_{[0,n]}]$ is a martingale if and only if for every bounded stopping time $\mathcal{T}$,*

$$\langle |M_{\mathcal{T}}|\rangle < \infty \tag{4.53}$$

and

$$\langle M_{\mathcal{T}}\rangle = \langle M_0\rangle. \tag{4.54}$$

Proof We show the if part, as the only if part readily follows from the optional stopping theorem.

Applying the optional stopping theorem to the stopping time $\mathcal{T}$ defined in Equation (4.52) yields

$$\langle M_0 \rangle = \langle M_{\mathcal{T}} \rangle = \langle M_n \mathbf{1}_{\Phi^c}(X_{[0,m]}) \rangle + \langle M_m \mathbf{1}_{\Phi}(X_{[0,m]}) \rangle, \tag{4.55}$$

and applying Equation (4.54) to the stopping time n yields,

$$\langle M_0 \rangle = \langle M_n \rangle = \langle M_n \mathbf{1}_{\Phi^c}(X_{[0,m]}) \rangle + \langle M_n \mathbf{1}_{\Phi}(X_{[0,m]}) \rangle. \tag{4.56}$$

Equations (4.55) and (4.56) imply that

$$\langle M_n \mathbf{1}_{\Phi}(X_{[0,m]}) \rangle = \langle M_m \mathbf{1}_{\Phi}(X_{[0,m]}) \rangle \tag{4.57}$$

for all subsets Φ of the set of trajectories $x_{[0,m]}$. By the tower property of conditional expectations, we can rewrite this equation as

$$\langle \langle M_n | X_{[0,m]} \rangle \mathbf{1}_{\Phi}(X_{[0,m]}) \rangle = \langle M_m \mathbf{1}_{\Phi}(X_{[0,m]}) \rangle, \tag{4.58}$$

for all subsets Φ of the set of trajectories $x_{[0,m]}$, and therefore by the definition of conditional expectations it holds with probability 1 that

$$\langle M_n | X_{[0,m]} \rangle = M_m. \tag{4.59}$$

■

4.1.5.3. *First-passage problems of random walks with martingales.* We use the optional stopping theorem to derive the statistics of first-passage times in a stochastic process. We consider the random-walk example X_n discussed in Section 2.1.3. Here, X_n is a discrete-time, biased random walker on $\mathbb{Z}$ with $X_0 = 0$; it moves one step in the positive (negative) direction with probability q $(1-q)$. We consider the first-passage time

$$\mathcal{T}^{(2)} = \min \{ n \geq 0 : X_n = -x_- \text{ or } X_n = x_+ \}, \tag{4.60}$$

where the constants $x_-, x_+ \in \mathbb{N}$, such that $-x_-$ and x_+ are absorbing sites. In other words, $\mathcal{T}^{(2)}$ is the first escape time of the walker from the interval (x_-, x_+). Using Doob's optional stopping theorem, version II, we derive exact results for the statistics of $\mathcal{T}^{(2)}$. Let us consider the martingale (2.24), denoted here as

$$M_n = \eta^{X_n} \text{ with } \eta = (1-q)/q. \tag{4.61}$$

Applying Theorem 12 to the martingale M_n given by Equation (4.61), we obtain

$$\langle M_{\mathcal{T}^{(2)}} \rangle = P_+ \eta^{x_+} + (1 - P_+) \eta^{-x_-} = 1, \tag{4.62}$$

where $P_+ = \mathcal{P}(X_{\mathcal{T}^{(2)}} = x_+)$, and we have used the fact that $P_- = \mathcal{P}(X_{\mathcal{T}^{(2)}} = -x_-) = 1 - P_+$ (i.e., X_n escapes the interval at finite time with probability 1). Solving Equation (4.62) towards

P_+ we obtain

$$P_+ = \frac{1-\eta^{-x_-}}{\eta^{x_+}-\eta^{-x_-}}. \tag{4.63}$$

Second, we apply Theorem 12 to the martingale $X_n - (2q-1)n$, see Equation (2.28), obtaining

$$\langle \mathcal{T}^{(2)} \rangle = \frac{\langle X_{\mathcal{T}^{(2)}} \rangle}{(2q-1)}. \tag{4.64}$$

Using

$$\langle X_{\mathcal{T}^{(2)}} \rangle = P_+ x_+ - (1-P_+)x_- = \frac{1-\eta^{-x_-}}{\eta^{x_+}-\eta^{-x_-}} x_+ - \frac{\eta^{x_+}-1}{\eta^{x_+}-\eta^{-x_-}} x_- \tag{4.65}$$

in (4.66), we obtain the following explicit expression for the mean first-passage time:

$$\langle \mathcal{T}^{(2)} \rangle = \frac{1}{2q-1} \left(\frac{1-\eta^{-x_-}}{\eta^{x_+}-\eta^{-x_-}} x_+ - \frac{\eta^{x_+}-1}{\eta^{x_+}-\eta^{-x_-}} x_- \right). \tag{4.66}$$

Analogously, the optional stopping theorem can be used to derive an explicit expression for the second moment $\langle (\mathcal{T}^{(2)})^2 \rangle$ of the first-passage time and its generating function, see , e.g., the appendices of Ref. [35].

4.1.6. ♠*Martingale central limit theorem*

Central limit theorems refer to a collection of results that describe how the sum of a large number of random variables converges to a normal distribution. The study of central limit theorems initiated in the beginning of the nineteenth century with the work of Pierre–Simon Laplace, who was the first to observe the universal character of the Gaussian distribution [116]. The central limit theorem has been extended and refined in various ways ever since, see Ref. [117] for an overview of the history of central limit theorems. The idea underlying the different central limit theorems is however the same, viz., the statistics of the sum of a large number of variables converges to a normal distribution if the variables are weakly correlated and the sum is not dominated by a few large outliers.

Let us consider a sum of n real-valued random variables Y_j given by

$$\tilde{X}_n = \sum_{j=1}^{n} Y_j. \tag{4.67}$$

Central limit theorems determine under which conditions the statistics of a rescaled and shifted version of $\tilde{X}_n$ are described by the normal distribution, i.e.,

$$\lim_{n\to\infty} \left\langle \delta\left(\frac{\tilde{X}_n - \mu_n}{\sigma_n} - x \right) \right\rangle = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2), \tag{4.68}$$

where $\delta(x)$ is the Dirac delta distribution, μ_n is the average shift, and σ_n determines the scaling of $\tilde{X}_n - \mu_n$ with n.

The version of the central limit theorem that is best known holds for sums $\tilde{X}_n$ of iid random variables Y_j with fixed mean μ and finite variance σ^2, as defined in Equation (2.7). This central limit theorem states that Equation (4.68) holds for the standard "norming" (see Theorem 27.1 of Ref.[118])

$$\mu_n = \mu\, n, \quad \text{and} \quad \sigma_n = \sigma\sqrt{n}. \tag{4.69}$$

A natural extension of the central limit theorem for iid random variables considers sums of random variables Y_j that are independent, but not identically, distributed, random variables. Assuming that Y_j are independent random variables with mean μ_j and finite variance σ_j, then Equation (4.68) applies for (see Theorem 27.2 of Ref. [118])

$$\mu_n = \sum_{j=1}^{n} \mu_j \quad \text{and} \quad \sigma_n^2 = \sum_{j=1}^{n} \sigma_j^2, \tag{4.70}$$

as long as the Lindeberg condition

$$\lim_{n\to\infty} \frac{1}{\sigma_n^2} \sum_{j=1}^{n} \int_{|y_j|\geq \epsilon\sigma_n} \mathrm{d}y_j\, y_j^2\, \rho_Y\left(y_j\right) = 0 \tag{4.71}$$

holds for all $\epsilon > 0$. Note that the Lindeberg condition compares the total accumulated variance σ_n^2, which is a measure for the number of variables contained in the sum, with the statistical weight accumulated in the tails of the distribution determined by $\sum_{j=1}^{n} \int_{|y_j|\geq\epsilon\sigma_n} \mathrm{d}y_j\, y_j^2\, \rho_Y(y_j)$. The central limit theorem holds as long as the former is infinitely larger than the latter.

Martingales are natural candidates to extend the central limit theorem to the case of dependent, albeit uncorrelated, random variables Y_j. Indeed, a martingale M_n can be written as the sum of martingale differences

$$Y_j = M_j - M_{j-1}. \tag{4.72}$$

The martingale condition implies that

$$\langle Y_{i_1} Y_{i_2} \ldots Y_{i_k} \rangle = 0 \tag{4.73}$$

holds for any k-tuple of distinct indices $(i_1, i_2, \ldots, i_k)$. Therefore, M_n is a sum $\tilde{X}_n$ of n random variables Y_j with vanishing autocorrelation function.

Central limit theorems for martingales have been derived originally by Lévy [119,120], and many extensions has been derived since, see [121] for an overview. We consider here the version of the martingale central limit theorem of Ref. [122], as for clarity we do not want to deal with the more general case of double indexed sequences considered in Ref. [121].

THEOREM 14 (**Martingale central limit theorem**) *Let $M_n = \sum_{j=1}^{n} Y_j$ be a zero mean martingale, and let V_n be its conditional variance, as defined in Equation (4.15). Assume that for all $\epsilon > 0$,*

$$\lim_{n\to\infty} \mathcal{P}\left(\left|V_n - \sigma_n^2\right| > \epsilon\right) = 0, \tag{4.74}$$

where $\sigma_n^2 = \langle V_n \rangle$, and assume that the Lindeberg condition equation (4.71) holds. Then the central limit theorem equation (4.68) applies for $\tilde{X}_n = M_n$, $\mu_n = 0$, and σ_n^2 given by the expected value of the conditional variance.

Note that the martingale central limit theorem also relies on the Lindeberg condition, but now the expected value $\langle V_n \rangle$ of the conditional variance plays the role of σ_n, instead of the sum of the variance equation (4.70) as was the case for independent random variables.

Just as is the case for sums of iid random variables, in the continuous-time limit a properly rescaled martingale process converges to a Wiener process, see Theorem 3 in Ref. [122]. In addition, martingales obey a law of iterated logarithm, which determines that the absolute value of the maximum of M_n grows as $\sqrt{2\sigma_n^2 \log\log \sigma_n^2}$ [121].

4.1.7. *Elephant random walks: convergence and central limit theorem*

We apply the martingale convergence theorem 8 to the martingale M_n of Equation (2.43), associated with the elephant random walk X_n defined in (2.36). As shown in Ref. [58], the conditional variance V_n of the martingale M_n, as defined in Equation (4.15), is bounded from above by

$$\nu_n = \sum_{k=1}^{n} a_n^2 > V_n. \tag{4.75}$$

The asymptotic behavior of the sequence ν_n depends on the memory parameter p, namely,

$$\nu_n \sim \begin{cases} \dfrac{(\Gamma(2p))^2}{3-4p} n^{3-4p}, & \text{if } p \in [0, 3/4), \\ \dfrac{\pi}{4} \log n, & \text{if } p = 3/4, \\ b, & \text{if } p \in (3/4, 1], \end{cases} \tag{4.76}$$

where b is a finite number that can be expressed in terms of a generalized hypergeometric function [58].

It follows from Equation (4.76) that $\sup_n \langle M_n \rangle$ is finite, as $\sup_n \langle M_n \rangle \le \sup_n \sqrt{\langle M_n^2 \rangle} = \sup_n \sqrt{\sum_{k=0}^{n-1} \langle (M_{k+1} - M_k)^2 \rangle} \sim b$, where we have used (4.10) and (4.15). Therefore, Theorem 8 applies and the martingale M_n converges almost surely to a finite random variable M_∞ when $p > 3/4$. As shown in Ref. [58], M_∞ has a sub-Gaussian distribution with a p-dependent kurtosis $\mathcal{K}(p)$ that decreases monotonically as a function of p, such that $\mathcal{K}(3/4) = 3$ and $\mathcal{K}(1) = 1$. Consequently, according to Equations (2.42) and (2.43), the elephant random walk process converges almost surely to

$$X_n \sim n^{2p-1} \frac{M_\infty}{\Gamma(2p)}, \tag{4.77}$$

which is superdiffusive for $p > 3/4$. Note that for $p \to 3/4$ it approaches the diffusive regime $p \in [0, 3/4)$. We refer the reader to Figure 4.3 where we plot example trajectories of X_n for $p = 0.5, p = 0.7$, and $p = 0.8$.

We discuss the implications of the martingale central limit, Theorem 14, on the elephant random walk. The martingale M_n, given by Equation (2.43), satisfies the martingale central limit theorem when $p \le 3/4$ [58,123,124]. Indeed, as indicated by Equation (4.76), the conditional variance V_n grows indefinitely for $p \le 3/4$. This argument can be made rigorous, and in [58] Bercu has shown that the martingale M_n satisfies the martingale central limit if $p \le 3/4$. Using Equations (2.42) and (2.43), it follows that also X_n obeys a central limit theorem with $\mu_n = 0$ and $\sigma_n = \sqrt{n/(3-4p)}$ or $\sigma_n = \sqrt{n \log(n)}$ for $p \in [0, 3/4)$ or $p = 3/4$, respectively. For $p > 3/4$, the conditional variance V_n converges to a finite limit, and hence the Lindeberg condition is not

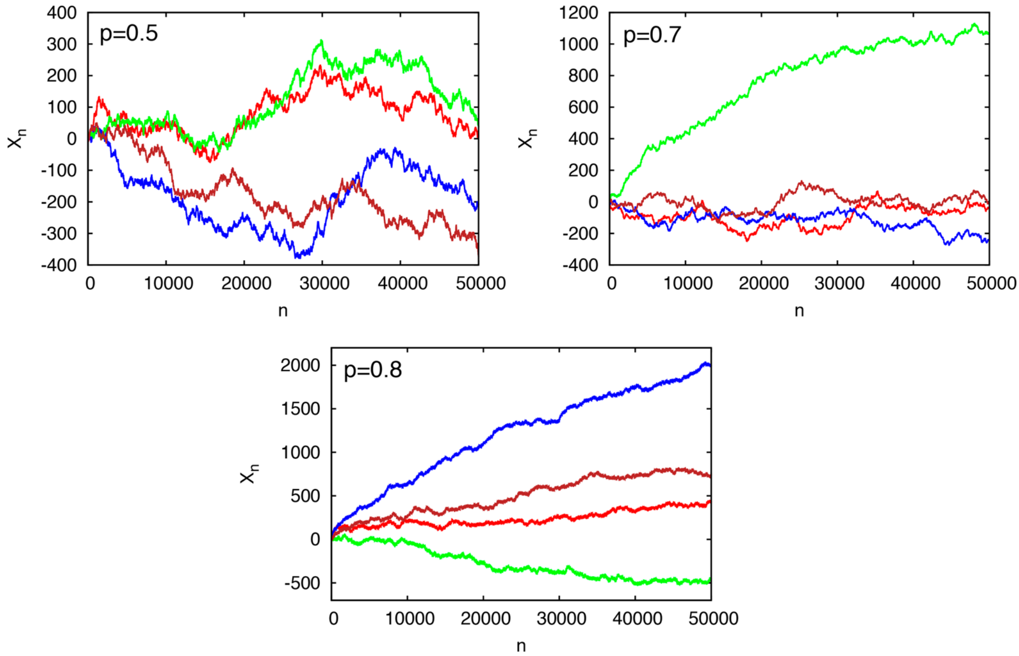

Figure 4.3. Illustration of the implication of the martingale central limit theorem for the trajectories of the elephant random walk X_n with memory parameter p. Plots show four trajectories of the elephant random walk for three values of p. Upper left panel: $p = 0.5$, corresponding to a simple random walk without memory. The standard central limit theorem applies, and in the asymptotic (or continuum) limit X_n converges to a standard Brownian motion with $\langle X_n X_m \rangle = m$ for $m < n$. Upper right panel: $p = 0.7$, corresponding to a diffusive random walk with memory. The martingale central limit theorem applies, and in the asymptotic limit X_n converges to a Brownian motion with a nontrivial memory kernel, such that $\langle X_n X_m \rangle = 5n^{0.6}m^{0.4}$ for $m < n$. Lower panel: $p = 0.8$, corresponding with the superdiffusive regime. The martingale central limit theorem does not apply, and the asymptotic limit takes the form $X_n \sim Yn^{0.6}$ with Y a time-independent random variable.

satisfied. In this case, the correlations in the process are too strong to generate enough data in the process, as quantified by V_n. The distinction between the diffusive regime, where the central limit theorem applies, and the superdiffusive regime, with strong memory effects, is also apparent in the continuum limit of the model [123]. For $p \in [0, 3/4)$, $X_{\lfloor nt \rfloor}/\sqrt{n}$, with $\lfloor a \rfloor$ the floor function, converges for large n to a Wiener process B_t with zero mean and autocovariance $\langle B_t B_s \rangle = s(t/s)^{2p-1}/(3-4p)$ for $0 < s \leq t$, while in the superdiffusive regime, $X_{\lfloor nt \rfloor}/n^{2p-1}$ converges to $t^{2p-1}Y$ with Y a real-valued random variable independent of time.

4.2. *Continuous time*

4.2.1. *Properties of continuous-time martingales that carry over from discrete time*

Fundamental properties of martingales, such as Doob's optional stopping theorems and Doob's maximum inequality, carry over to the continuous-time case if we assume that the trajectories of the martingale are right continuous, i.e., the process is continuous with occasional jumps. Fortunately, according to Doob's regularity theorem, see Theorem 3.1 in Ref. [66], (sub)martingales can be considered right-continuous when the mean value $\langle S_t \rangle$ is right continuous, i.e., $\lim_{\epsilon \to 0^+} \langle S_{t+\epsilon} \rangle = \langle S_t \rangle$. Indeed, in this case there exists a process $\tilde{S}_t$ that is right continuous and for which $\mathcal{P}(\tilde{S}_t = S_t) = 1$ for all $t \geq 0$. So, Doob's regularity theorem implies that when working with martingales or submartingales we can assume that we work on its right continuous modification, and hence Doob's optional stopping theorems and maximum inequality apply to this modification.

4.2.2. ♠*Local martingales*

A notable distinction between martingale theory in continuous time and martingale theory in discrete time is that in continuous time there exist processes that are not martingales, even though they are locally driftless. Such processes are called *local martingales*, and just as martingales they play an important role in the theory of stochastic processes in continuous time.

The formal definition for a local martingale goes as follows:

> We say that a process L_t is a **local martingale** if there exists a sequence of nondecreasing stopping times $\mathcal{T}_n$ with $n \in \mathbb{N}$ such that [125]
>
> - with probability 1, $\lim_{n\to\infty} \mathcal{T}_n = \infty$;
> - the stopped process $L(t \wedge \mathcal{T}_n)$ is a uniform integrable martingale for each n.

A martingale is a local martingale, since we can set $\mathcal{T}_n = n$. We speak of a *strict local martingale* if a stochastic process is a local martingale but not a martingale [126]. In discrete time, local martingales are martingales, see Theorem VII.1 in [127], and hence *strict local martingales* are a distinct feature of continuous-time processes.

One way to realize the sequence of stopping times $\mathcal{T}_n$ is through a random time transformation. A **random time** $\tau(X_{[0,t]})$ is a nonnegative and increasing process in t, and it can be used to define a sequence of stopping times by

$$\mathcal{T}_n = \inf\left\{t \geq 0 : \tau(X_{[0,t]}) > n\right\}. \tag{4.78}$$

This yields the following alternative characterization of local martingales.

> For local martingales L_t, there exists a **random-time transformation**
>
> $$t \to \tau(X_{[0,t]}),$$
>
> such that L_τ is a martingale.

4.2.2.1. *Itô-integrals and random time transformations.* The importance of local martingales follows from the fact that Itô integrals of Equation (2.64), copied here for convenience

$$I_t = \int_0^t Z_s \, \mathrm{d}B_s,$$

are local martingales. Indeed, Itô integrals exist for integrands D_s that obey

$$\mathcal{P}\left(\int_0^t Z_s^2 \, \mathrm{d}s < \infty\right) = 1, \tag{4.79}$$

which is a weaker condition than Equation (2.67), that for convenience we copy here as well,

$$\int_0^t \langle Z_s^2 \rangle \, \mathrm{d}s < \infty.$$

While the latter condition implies that I_t is a martingale, the previous condition (4.79) implies that I_t is a local martingale, see Ref. [64]. Indeed, consider a general Itô integral

$$\frac{\mathrm{d}I_t}{\mathrm{d}t} = Z_t \frac{\mathrm{d}B_t}{\mathrm{d}t}, \tag{4.80}$$

with $Z_t = Z(I_{[0,t]}, t) \geq 0$ and B_t a Brownian motion. Define the random time

$$\frac{\mathrm{d}\tau_t}{\mathrm{d}t} = Z_t^2, \tag{4.81}$$

with time change rate Z_t^2. It then holds that [64]

$$\frac{\mathrm{d}I_{\zeta_\tau}}{\mathrm{d}\tau} = \frac{\mathrm{d}\tilde{I}_\tau}{\mathrm{d}\tau} = \frac{\mathrm{d}B_\tau}{\mathrm{d}\tau}, \tag{4.82}$$

with $\tau \in \mathbb{R}^+$ the time parameter, and where

$$\zeta_\tau = \inf \left\{ s \geq 0 : \tau_s(I_{[0,s]}) \geq \tau \right\} \tag{4.83}$$

is the functional inverse of $\tau_t(I_{[0,t]})$. Note that according to Equations (4.80)–(4.82) a rescaling of the form $Z_t \, \mathrm{d}B_t = \mathrm{d}B_\tau$ requires that $\mathrm{d}\tau = Z_t^2 \, \mathrm{d}t$, which follows from the fundamental property $\langle B_t^2 \rangle = t$ of the Brownian motion. In physics notation, we drop the tilde, writing $\tilde{I}_\tau = I_\tau$ and understanding that this is I expressed in the time τ. Hence, according to Equation (4.82), I_τ is a Brownian motion and thus a martingale, and therefore I_t is a local martingale.

4.2.2.2. *Sufficient conditions for martingality of a local martingale.* We discuss here a few criteria to determine whether a local martingale is a martingale. If the local martingale L_t is bounded, i.e., $\langle \sup_{s \leq t} |L_s| \rangle < \infty$, then it will be martingale (see Theorem 51 in chapter I page 38 of [70]). Another criterion uses the quadratic variation (Corollary 3 of Theorem 27 in chapter II of [70]).

THEOREM 15 (**Condition for a local martingale to be a martingale**) *A local martingale L_t is a martingale with $\langle L_t^2 \rangle < \infty$ for all $t \geq 0$ if and only if $\langle [L, L]_t \rangle < \infty$ for all $t \geq 0$. Moreover, it holds that*

$$\langle L_t^2 \rangle = \langle [L, L]_t \rangle. \tag{4.84}$$

The formula (4.84) is called the Itô isometry. Theorem 15 implies that the Itô isometry is a fundamental property of square integrable martingales. Finally, if M is a nonnegative, local martingale with $\langle M_0 \rangle < \infty$, then M is a supermartingale (Lemma 14.3 in section IV.14 of [63]). This clarifies why in the panel (b) of Figure 4.4 the mean value $\langle X_t \rangle$ is a decreasing function.

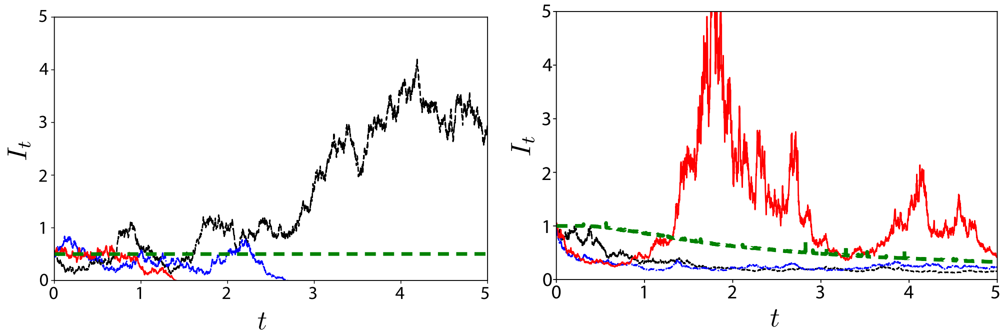

Figure 4.4. Illustration of a martingale (left) and a strict local martingale (right). We show three realizations of the process (4.85) for $k = 0.5$ (left) and $k = 1.5$ (right). The dotted green curve is an estimate of the average $\langle I_t \rangle$ based on an empirical average over 10^6 realizations of the process. If $k = 0.5$, then $\langle I_t \rangle = 1$ and the process is driftless, whereas for $k = 1.5$ the mean value $\langle I_t \rangle$ decreases as a function of t.

4.2.2.3. *Example of a local martingale.* We consider an example of a strict local martingale, i.e., a local martingale that is not a martingale. Consider the Itô unidimensional stochastic differential equation [128,129]:

$$\dot{I}_t = I_t^k \dot{B}_t, \tag{4.85}$$

with $I_0 = 1$, k a real number, and B_t a Brownian motion as before.

The physical picture is as follows: the process I_t is nonnegative and it has an absorbing state at $I_t = 0$. If $k > 1$, then the diffusion constant gets small enough for $I_t \to 0$, such that I_t gets trapped near the origin. As a consequence, $\langle I_t \rangle$ decreases as a function of t and the Itô integral I_t is not a martingale. On the other hand, when $k < 1$, then the diffusion constant does not decay fast enough for $X_t \to 0$ and the process reaches the origin in a finite time. In other words, if $\mathcal{T}_0 = \inf\{t > 0 : X_t = 0\}$, then $\mathcal{P}(\mathcal{T}_0 < \infty) = 1$. In this case, the process $X_{t \wedge \mathcal{T}_0}$ is a martingale as shown in Ref. [128] and illustrated in Figure 4.4.

4.2.3. *Doob–Meyer decomposition*

Local martingales appear in the decomposition of a process into a martingale and a predictable process, which extends the Doob decomposition theorem, given by Theorem 6, to processes in continuous time (Theorem 16 in chapter III on page 116 in [70]). In continuous time, a stochastic process A_t is *predictable* if $\langle A_t | X_{[0,t-\mathrm{d}t]} \rangle = A_t + O(\mathrm{d}t)$.

THEOREM 16 (**Doob–Meyer decomposition**) *Let Y_t be a right-continuous stochastic process function of the set of trajectories $X_{[0,t]}$ and integrable (i.e., $\langle |Y_t| \rangle < \infty$ for all t). Then it can be uniquely decomposed as*

$$Y_t = Y_0 + L_t + \underbrace{\int_0^t v_s \, \mathrm{d}s}_{A_t}, \tag{4.86}$$

where we have introduced the conditional velocity

$$v_s = \lim_{h\to 0^+} \left\langle \frac{Y_{s+h} - Y_s}{h} \middle| X_{[0,s]} \right\rangle$$

The predictable process A_t is called compensator and L_t is a local martingale with respect to the underlying process X_t.

We now give some remarks about Doob–Meyer decomposition theorem.

- If Y_t is a submartingale (supermartingale), then $v_s \geq 0$ ($v_s \leq 0$) and then the compensator A_t is increasing (decreasing).
- The compensator of the square X_t^2 of a stochastic process is denoted by $\langle X_t, X_t\rangle$ and called the *predictable quadratic variation* or sharp bracket of X [70]. For continuous processes, the predictable quadratic variation equals the quadratic variation defined in Equation (2.71), but for processes with jumps these are in general different. Take for example the counting process N_t of example (2.48). In this case, $[N_t, N_t] = N_t$, whereas $\langle N_t, N_t\rangle = \lambda_t$. On the other hand, for the Brownian motion, $[B_t, B_t] = \langle B_t, B_t\rangle = t$.
- Theorem 4 directly gives the Doob–Meyer decomposition for a real-valued bounded function $f_t(X_t)$ evaluated on a Markovian process X_t, viz.,

$$f_t(X_t) = f(X_0) + M_t + \underbrace{\int_0^t \mathrm{d}s\, (\partial_s f_s + \mathcal{L}_s f_s)\,(X_s)}_{A_t}, \tag{4.87}$$

  where M_t is the Dynkin's additive martingale, as defined in (3.73), and $\mathcal{L}_s$ is the generator of X_t.

4.2.4. *Continuous martingales*

We consider the case of continuous martingales, i.e., martingales with trajectories that are continuous functions of time. The main result we discuss here is the martingale representation theorem, which states that for square integrable, continuous martingales the integrator dM_s in the Itô integral can be assumed to be a Brownian motion.

As discussed before, an Itô integral $I_t = \int_0^t Z_s\, \mathrm{d}B_s$, as defined in Equation (2.64), with an integrand Z_t that obeys Equation (2.67), i.e., $\int_0^t \langle Z_s^2\rangle\, \mathrm{d}s < \infty$, is a martingale. In addition, it is square integrable. Indeed, from Itô's formula, see Appendix B.3, it follows that

$$I_t^2 = 2\int_0^t I_s Z_s\, \mathrm{d}B_s + \int_0^t Z_s^2\, \mathrm{d}s \tag{4.88}$$

and since $\langle \int_0^t I_s Z_s\, \mathrm{d}B_s\rangle = 0$,

$$\langle I_t^2\rangle = \left\langle \int_0^t Z_s^2\, \mathrm{d}s \right\rangle, \tag{4.89}$$

which is finite, as assumed with Equation (2.67).

Remarkably, the converse is also true, i.e., a square integrable martingale with respect to the Brownian motion $B_{[0,t]}$ is an Itô integral. This constitutes the martingale representation theorem (Theorem 4.3.4 in [64]).

THEOREM 17 (**Martingale representation theorem**) *Suppose M_t is a martingale relative to B_t and suppose that $\langle M_t^2 \rangle < \infty$ for all $t \geq 0$. Then there exists a unique Z_t evaluated on the trajectories $X_{[0,t]}$ that satisfies $\int_0^t \langle Z_s^2 \rangle \, \mathrm{d}s < \infty$ and that satisfies with probability 1,*

$$M_t = \langle M_0 \rangle + \int_0^t Z_s \, \mathrm{d}B_s \tag{4.90}$$

for all $t \geq 0$.

As an illustrative example, consider the martingale $B_t^2 - t$, see Equation (2.62), which can be expressed as an Itô integral as follows:

$$M_t = B_t^2 - t = 2 \int_0^t B_s \, \mathrm{d}B_s, \tag{4.91}$$

where the second equation follows from applying Itô's lemma, see Equation (2.88).

4.2.5. ♠*Stochastic exponential*

As we will see in the next chapter, the exponentiated, negative, fluctuating, entropy production of a nonequilibrium stationary process is a stochastic exponential. For this reason, we discuss here stochastic exponentials in more detail.

Let $X_t \in \mathbb{R}^d$ be a possibly multidimensional càdlàg process, i.e., a process with right-continuous trajectories ($X_{t_+} = X_t$) that have left limits everywhere (X_{t^-} exists), and let $Y_t(X_{[0,t]}) \in \mathbb{R}$ be a stochastic process defined on X_t. The stochastic (Dolé ans–Dade) exponential [130] associated with Y is the solution of the stochastic differential equation [70]

$$\dot{\mathcal{E}}_t(Y) = \mathcal{E}_{t-}(Y)\dot{Y}_t, \tag{4.92}$$

where $\mathcal{E}_{t-} = \lim_{\epsilon \to 0^+} \mathcal{E}_{t-\epsilon}$ and with $\mathcal{E}_0 = 1$.

The stochastic exponential is specified by the process Y_t and therefore we denote it by $\mathcal{E}_t(Y)$; sometimes we drop Y because it is clear which process is meant. We remark that the notation $\mathcal{E}_t(Y)$ is done in analogy with exponentials, yet the process $\mathcal{E}_t(Y)$ in Equation (4.92) is a functional of the trajectory $Y_{[0,t]}$. For the particular case of $Y_t = B_t$ we recover, using Equation (4.92), the stochastic exponential associated with the Wiener process, whose solution is given in Equation (2.59) with $z = 1$, i.e.,

$$\mathcal{E}_t(B) = \exp\left(B_t - \frac{t}{2}\right). \tag{4.93}$$

Note that interpreting Equation (4.92) in Stratonovich, we would obtain the solution $\exp(Y_t - Y_0)$. However, the stochastic exponential use this equation in the Itô interpretation, leading to a different stochastic process.

If $Y_t = L_t$, a local martingale, then also $\mathcal{E}(L)$ is a local martingale, and hence the stochastic exponential inherits the local martingale property. In addition, if $\mathcal{E}_t(L) > 0$, then it is a positive supermartingale [70,90]. If $\mathcal{E}_t(L) > 0$, then a necessary and sufficient condition for the martingality of a stochastic exponential is that

$$\langle \mathcal{E}_t(L) \rangle = 1 \tag{4.94}$$

holds for all t, which is reminiscent of the integral fluctuation relation, see below. Equation (4.94) follows from the fact that $\mathcal{E}_t(L)$ is a supermartingale with constant expectation, see the discussion around Equation (4.4). In the present case, for which $\mathcal{E}_t(L) > 0$ and (4.94) holds, we can define the path probability

$$\mathcal{Q}(X_{[0,t]}) \equiv \mathcal{E}_t(L)\mathcal{P}(X_{[0,t]}) \tag{4.95}$$

so that

$$\mathcal{E}_t(L) = R_t = \frac{\mathcal{Q}(X_{[0,t]})}{\mathcal{P}(X_{[0,t]})}. \tag{4.96}$$

Hence, not all stochastic exponentials are Radon–Nikodym derivative processes, but if $\mathcal{E}_t$ is a positive, martingale, then it is.

On the other hand, unlike for the local-martingale property, the stochastic exponential does not inherit the martingale property. Indeed, if $Y_t = M_t$, a martingale process, then it is not guaranteed that $\mathcal{E}_t(M)$ is a martingale. Instead, one needs to verify some additional conditions that we discuss below.

Let us consider a few examples of stochastic exponentials:

4.2.5.1. *Stochastic exponential of a differentiable function.* If $I_t = f_t$, with $f_t \in \mathbb{R}$ a differentiable function evaluated on t, then we obtain the differential equation

$$\dot{\mathcal{E}}_t(f) = \mathcal{E}_t(f)\dot{f}_t \tag{4.97}$$

with solution

$$\mathcal{E}_t(f) = \exp(f_t - f_0). \tag{4.98}$$

Note that this is because Itô and Stratonovich calculus are the same for differentiable functions.

4.2.5.2. *Stochastic exponential of a continuous process.* Let X be a possibly multidimensional process, and let $Y_t(X_{[0,t]}) \in \mathbb{R}$ be a continuous càdlàg process. Equation (4.92) then reads

$$\dot{\mathcal{E}}_t = \mathcal{E}_t \dot{Y}_t \tag{4.99}$$

and is solved by

$$\mathcal{E}_t(Y) = \exp\left(Y_t - Y_0 - \frac{1}{2}[Y, Y]_t\right), \tag{4.100}$$

where $[Y, Y]_t$ is the quadratic variation defined in Equation (2.71).[5]

As an example of stochastic exponential of a continuous process, consider the case of Equation (2.82), copied here for convenience,

$$\frac{\mathrm{d}}{\mathrm{d}t}\underbrace{\exp(-S_t)}_{\mathcal{E}_t(Y)} = -\underbrace{\exp(-S_t)}_{\mathcal{E}_t(Y)}\sqrt{2D_t}\dot{B}_t. \tag{4.101}$$

In this case, $Y_t = -\int_0^t \mathrm{d}s\sqrt{2D_s}\dot{B}_s$ and the quadratic variation

$$[Y,Y]_t = 2\int_0^t D_s\,\mathrm{d}s, \tag{4.102}$$

so that

$$\mathcal{E}_t(Y) = \exp\left(Y_t - Y_0 - \int_0^t D_s\,\mathrm{d}s\right) = \exp(-S_t). \tag{4.103}$$

We now give some remarks about the martingale structure of the stochastic exponential of continuous stochastic processes.

- If $Y_t = L_t$ is a local martingale, then $\mathcal{E}(L)$ is a local martingale, and the converse is also true, i.e., a strictly positive, continuous, local martingale takes the form of stochastic exponential $\mathcal{E}_t(L)$ [90].
- If $Y_t = M_t$ is a continuous martingale, then $\mathcal{E}_t(M)$ is a martingale when Novikov's condition [131],

$$\left\langle \exp\left(\frac{1}{2}[M,M]_t\right)\right\rangle < \infty, \tag{4.104}$$

  holds for all $t \geq 0$. Note that the Novikov condition is a sufficient, and not a necessary condition for martingality. However, this condition is often not very practical as we will see in the next chapter on thermodynamics.
- Another necessary condition for martingality is the Kazamaki condition [132], which states that if $\exp(L_t/2)$ is a submartingale, then $\mathcal{E}_t(L)$ is a martingale. These conditions have been refined [133,134].
- See Ref. [135] for a generalization of the stochastic exponential $\mathcal{E}_t(Y)$ to the case of processes with jumps.

Chapter 5. Martingales in stochastic thermodynamics I: Introduction

Voudriez-vous bien passer vos jours
A faire le Sardanapale,
Et servir une martingale?
(Would you like to spend your days
To do the Sardanapale,
And serve a martingale?)
Paul Scarron, Le Virgile travesti, Chapter IV (1648).

Since the origins of thermodynamics in the nineteenth century, physicists have been intrigued by the implications of the second law of thermodynamics at the mesoscopic level. One of the first references to thermodynamics at the mesoscopic scale appeared in Tait's *Sketch of Thermodynamics* (1878), on which J. C. Maxwell commented

> a finite number of molecules [⋯] are still and every now and then still deviating very considerably from the theoretical mean of the whole system [they belong to]. [...] Hence the second law of thermodynamics is continually being violated, and that to a considerable extent, in any sufficiently small group of molecules belonging to a real body [136,137].

The pioneering thoughts of Tait and Maxwell illustrate the puzzle of formulating a second law of thermodynamics for mesoscopic systems. This puzzle has, to a large extent, been resolved in the past decades with proper definitions of heat and entropy production based on the theory of stochastic processes. According to stochastic thermodynamics, entropy production can be transiently negative, but is on average positive. Moreover, the fluctuations of negative entropy production are constrained by fluctuation relations.

Several of the standard results of stochastic thermodynamics can be understood and improved with martingale theory. In the present chapter, we provide an introduction to martingale theory in stochastic thermodynamics. After briefly reviewing key definitions and results, we show how martingales naturally appear in the theory of stochastic thermodynamics. In particular, with two examples of stochastic processes, namely, one-dimensional overdamped Langevin processes and Markov jump processes, we show that for stationary processes the exponentiated negative entropy production is a martingale, which is the central result in martingale theory for stochastic thermodynamics. Through the study of two simple examples, the present chapter sets the stage for the next three chapters that discuss the theory in a more general setup (see Chapter 6) and provide a detailed analysis of the implications of martingale theory (see Chapters 7 and 8).

This chapter is structured as follows: in Section 5.1, we introduce the setup of an overdamped, one-dimensional, isothermal, Langevin process, and subsequently we review the basic thermodynamics results for this setup. In Section 5.2, we show for this setup that if the process is stationary, then the exponential of the negative entropy production is a martingale. Subsequently, in Section 5.3, we review thermodynamics for Markov jump processes, and in Section 5.4 we discuss the thermodynamics of Markov jump processes with martingale theory.

5.1. *Introduction: Langevin equation and thermodynamics*

Before embarking on a journey through thermodynamics with martingales, we derive the "standard" first and second laws of thermodynamics for nonequilibrium isothermal processes described by a one-dimensional, overdamped, isothermal, Langevin equation. Note that since the focus of this paper is on martingales, and since there exist already several textbooks and review papers on stochastic thermodynamics, we review here the essentials of stochastic thermodynamics, referring the interested reader to Refs. [25–27,138] for further details.

5.1.1. *System setup*

Consider a particle with mass m that moves with homogeneous mobility μ (or equivalently, friction coefficient $\gamma = 1/\mu$) in a homogeneous thermal bath in equilibrium and at a constant temperature T, as illustrated in Figure 5.1. The particle is subject to a potential $V_t(x) \equiv V(x, \lambda_t)$ whose shape is controlled by a time-dependent deterministic protocol λ_t. Moreover, a non-conservative force $f_t(x)$ (i.e., solenoidal) is exerted on the particle. The dynamics of the particle is described by the underdamped Langevin equation

$$\begin{cases} \dot{X}_t = P_t/m, \\ \dot{P}_t = -\dfrac{\gamma}{m}P_t - (\partial_x V_t)(X_t) + f_t(X_t) + \sqrt{2T\gamma}\dot{B}_t, \end{cases} \tag{5.1}$$

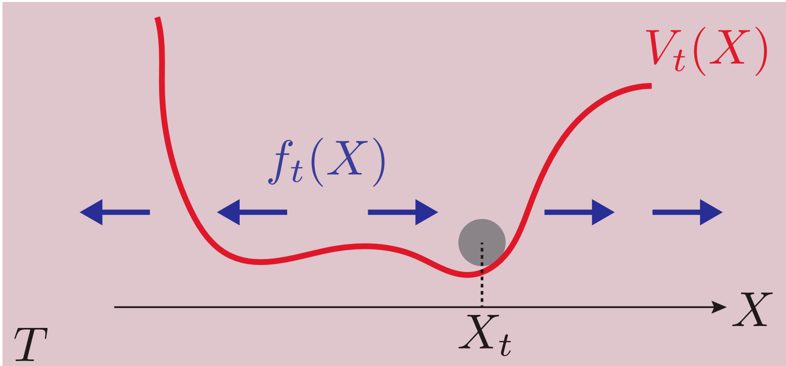

Figure 5.1. Illustration of the paradigmatic model discussed in Section 5.1. A Brownian particle (gray circle) confined in a one-dimensional potential that may be time dependent ($V_t(X)$, red line) is subject to an external force that may depend on time and space ($f_t(X)$, blue arrows). The position X_t of the particle at time t evolves according to Equation (5.3). In this model, the particle fluctuates moving along the potential and under the action of the external force field – the blue arrows illustrate the direction of the external force and the length of the arrows its magnitude (note that the external force $f_t(x)$ is in general different from minus the instantaneous value of the slope of the potential $-\partial_x V_t(x)$).

where B_t is a Brownian noise, P_t is the momentum of the particle at time t, and X_t is its position. The first-order equations (5.1) can be written equivalently as the one-dimensional second-order equation

$$m\ddot{X}_t = -\gamma \dot{X}_t - (\partial_x V_t)(X_t) + f_t(X_t) + \sqrt{2T\gamma}\,\dot{B}_t. \tag{5.2}$$

For simplicity, in stochastic thermodynamics it is customary to consider the overdamped limit, which we introduce in the following.

In the overdamped limit, $m\mu \ll 1$, the position X_t of the particle is described by the **overdamped, isothermal Langevin equation**

$$\dot{X}_t = -\mu(\partial_x V_t)(X_t) + \mu f_t(X_t) + \sqrt{2\mu T}\,\dot{B}_t, \tag{5.3}$$

where we have used the notation $-(\partial_x V_t)(X_t) = -\partial_x V_t(x)|_{x=X_t}$ for the value of the conservative force evaluated at X_t.

Notice that Equation (5.3) is the one-dimensional version ($d = 1$) of Equation (3.65) with a homogeneous diffusion constant $D = \mu T$ determined by Einstein's relation equation (3.69). Despite its simplicity, the Langevin equation (5.3) contains all the minimal ingredients of stochastic thermodynamics, namely fluctuations (thermal noise), energy (potential), and nonequilibrium forces (a time-dependent potential and external forces).

5.1.2. *First law of stochastic thermodynamics*

We follow the conventional route in thermodynamics [136,137]: we first define the work done on the system, and consequently we obtain the heat from the first law of thermodynamics.

The work done on the system in the time interval $[t, t + \mathrm{d}t]$ consists of two contributions, namely, the work due to a changing potential $(\partial_t V_t)(X_t, t)$ and the work due to a nonconservative force f_t. Adding the two contributions, we obtain that the power exerted on the system in $[t, t + \mathrm{d}t]$ is [139,140]

$$\dot{W}_t \equiv (\partial_t V_t)(X_t) + f_t(X_t) \circ \dot{X}_t, \tag{5.4}$$

where $\circ$ denotes the Stratonovich product (see Section 2.2.3 for a reminder on stochastic calculus).

Integrating over time, we find the **stochastic work** $W_t = \int_0^t \dot{W}_s\,\mathrm{d}s$ done on the system along a stochastic trajectory $X_{[0,t]}$, which using Equation (5.4) reads

$$W_t = \int_0^t [(\partial_s V_s)(X_s)\,\mathrm{d}s + f_s(X_s) \circ \mathrm{d}X_s]\,. \tag{5.5}$$

Note that in Equations (5.4)–(5.5) we have used a Stratonovich integral to define the work done by a non-conservative force on the system, and not an Itô integral, and this will prove to be important for developing a thermodynamically consistent picture.

Given the work W_t, we use the first law of thermodynamics to obtain an explicit expression for the heat.

The **first law of stochastic thermodynamics** reads [139,140]

$$Q_t + W_t = V_t(X_t) - V_0(X_0), \tag{5.6}$$

which we assume to hold along any trajectory $X_{[0,t]}$ traced by a nonequilibrium system described by the isothermal Langevin equation (5.3).

The first law of thermodynamics, Equation (5.6), defines the heat Q_t. In rate form, Equation (5.6) reads

$$\dot{Q}_t + \dot{W}_t = \dot{V}_t = (\partial_t V_t)(X_t) + (\partial_x V_t)(X_t) \circ \dot{X}_t. \tag{5.7}$$

Substituting Equation (5.4) in Equation (5.7), we find

$$\dot{Q}_t = -F_t(X_t) \circ \dot{X}_t, \tag{5.8}$$

where the total force

$$F_t(X_t) = -(\partial_x V_t)(X_t) + f_t(X_t) \tag{5.9}$$

contains, in general, conservative (first) and non-conservative (second) terms; this is the one-dimensional version of the more general expression (3.66). Note that the heat absorbed per unit of time in $[t, t + \mathrm{d}t]$, given by Equation (5.8), can also be expressed by

$$\dot{Q}_t = (-\gamma \dot{X}_t + \sqrt{2\gamma T}\dot{B}_t) \circ \dot{X}_t, \tag{5.10}$$

which was the original expression for the stochastic heat in overdamped Langevin systems obtained by Sekimoto [139].

Integrating $\dot{Q}_s$ over the interval $s \in [0, t]$, we obtain the **stochastic heat** $Q_t = \int_0^t \dot{Q}_s \, \mathrm{d}s$ absorbed by the system along a stochastic trajectory $X_{[0,t]}$ [139,140],

$$Q_t = -\int_0^t F_s(X_s) \circ \mathrm{d}X_s. \tag{5.11}$$

Note that the Stratonovich rule implies that for time-homogenous total forces, $F_s(x) = F(x)$, Q_t changes sign under time reversal.

The formalism presented here has been extended to underdamped Langevin systems for which the kinetic energy change leads to an additional term in the stochastic heat [25,138,141].

5.1.3. *Second law of stochastic thermodynamics*

Consider the Fokker–Planck equation

$$\partial_t \rho_t(x) = -\partial_x J_{t,\rho}(x) \tag{5.12}$$

for the instantaneous density $\rho_t(x) = \langle \delta(X_t - x) \rangle$, which is the one-dimensional version of Equation (3.63). According to Equation (3.64), the hydrodynamic current is given by

$$J_{t,\rho}(x) = \mu F_t(x)\rho_t(x) - \mu T \partial_x \rho_t(x). \tag{5.13}$$

Given a state X_t, Shannon's instantaneous information content is given by [142,143]

$$S_t^{\mathrm{sys}} \equiv -\ln \rho_t(X_t), \tag{5.14}$$

which we identify as the **nonequilibrium system entropy** for the system in state X_t at time t. The (nonequilibrium) system entropy change associated with $X_{[0,t]}$ is thus given by

$$\Delta S_t^{\mathrm{sys}} \equiv S_t^{\mathrm{sys}} - S_0^{\mathrm{sys}} = \ln \frac{\rho_0(X_0)}{\rho_t(X_t)}. \tag{5.15}$$

Now, we review the notion of stochastic environmental entropy change, as commonly used in the stochastic thermodynamics of isothermal systems.

Since the environment is in a state of thermal equilibrium at temperature T, the **entropy change of the environment** is given by Clausius' statement

$$S_t^{\mathrm{env}} = -\frac{Q_t}{T}, \tag{5.16}$$

where we recall that Q_t is the stochastic heat given by Equation (5.11). Equation (5.16) thus provides the definition for the stochastic environmental entropy change along a trajectory of an isothermal, overdamped, Langevin equation.

To obtain a balance equation for entropy, we determine the rate of change of the nonequilibrium system entropy. An explicit calculation yields

$$\dot{S}_t^{\rm sys} = \frac{\mathrm{d}\left(-\ln\left(\rho_t\left(X_t\right)\right)\right)}{\mathrm{d}t} \tag{5.17}$$

$$= -\frac{\left(\partial_t \rho_t\right)\left(X_t\right)}{\rho_t\left(X_t\right)} - \frac{\left(\partial_x \rho_t\right)\left(X_t\right)}{\rho_t\left(X_t\right)} \circ \dot{X}_t \tag{5.18}$$

$$= \underbrace{-\frac{\left(\partial_t \rho_t\right)\left(X_t\right)}{\rho_t\left(X_t\right)} + \frac{J_{t,\rho}(X_t)}{\mu T \rho_t\left(X_t\right)} \circ \dot{X}_t}_{\dot{S}_t^{\rm tot}} - \underbrace{\frac{F_t(X_t)}{T} \circ \dot{X}_t}_{\dot{S}_t^{\rm env}}. \tag{5.19}$$

The steps we have used in Equations (5.17)–(5.19) are the following: in Equation (5.17), we have used the definition of stochastic system entropy (5.14). In Equation (5.18), we have used Stratonovich rules of calculus, which are formally identical to those of standard calculus. In Equation (5.19) we have used the definition of the probability current (5.13). Lastly, in Equation (5.19), we have identified the second term as the change of the environmental entropy $\dot{S}_t^{\rm env} = -\dot{Q}_t/T$, taking into account the expression (5.8) for the stochastic heat $\dot{Q}_t = -F(X_t, t) \circ \dot{X}_t$.

The first two terms in the right-hand side of Equation (5.19) are changes in the system's entropy that do not involve environmental entropy changes, thus we identify them as the stochastic entropy production rate in $[t, t + \mathrm{d}t]$

$$\dot{S}_t^{\rm tot} = -\frac{\left(\partial_t \rho_t\right)\left(X_t\right)}{\rho_t\left(X_t\right)} + \frac{J_{t,\rho}(X_t)}{\mu T \rho_t\left(X_t\right)} \circ \dot{X}_t. \tag{5.20}$$

Note that the definition (5.20) is consistent with Prigogine's balance equation [144]

$$\dot{S}_t^{\rm tot} \equiv \dot{S}_t^{\rm sys} + \dot{S}_t^{\rm env}, \tag{5.21}$$

with $\dot{S}_t^{\rm sys}$ given by Equation (5.14) and $\dot{S}_t^{\rm env}$ given by Equation (5.16).

The **stochastic entropy production** associated with a trajectory $X_{[0,t]}$ of an overdamped Langevin equation (5.3) equals the sum of the system entropy change plus the environmental entropy change,

$$S_t^{\rm tot} = \Delta S_t^{\rm sys} - \frac{Q_t}{T}. \tag{5.22}$$

Integrating Equation (5.20) over time, we get the explicit expression [143]

$$S_t^{\rm tot} = \int_0^t \left[-\frac{\left(\partial_s \rho_s\right)\left(X_s\right)}{\rho_s\left(X_s\right)} + \frac{J_{s,\rho}(X_s)}{\mu T \rho_s\left(X_s\right)} \circ \dot{X}_s\right] \mathrm{d}s. \tag{5.23}$$

Note that the stochastic entropy production $S_t^{\rm tot}$ is a stochastic process that thus fluctuates in time, and as we show below it can take negative values. On the other hand, a second law is recovered for the average of $S_t^{\rm tot}$. Here and in the following, we use the interpretation $\langle \dot{Z}_t \rangle \equiv (\mathrm{d}/\mathrm{d}t)\langle Z_t \rangle$ for all functionals $Z_t = Z[X_{[0,t]}]$.

Indeed, averaging Equation (5.20) over many realizations of the process, we find that the average rate of entropy production is non-negative

$$\langle \dot{S}_t^{\mathrm{tot}} \rangle = \frac{1}{\mu T} \int_{\mathcal{X}} \frac{\left(J_{t,\rho}(x)\right)^2}{\rho_t(x)} \, \mathrm{d}x \geq 0. \tag{5.24}$$

Thus we call Equation (5.24) the **second law of thermodynamics** for overdamped Langevin equations. Integrating over time and using $S_0^{\mathrm{tot}} = 0$ we obtain

$$\langle S_t^{\mathrm{tot}} \rangle \geq 0. \tag{5.25}$$

See Section 6.1.5.4 for a detailed derivation of Equation (5.24) in a more general setting beyond the unidimensional case.

If we call the system together with its environment the *universe*, then the second law of thermodynamics states that on average the total entropy of the universe increases.

To derive the second law of thermodynamics, given in Equation (5.24), for overdamped Langevin equations, we convert the Stratonovich integral in Equation (5.20) into an Itô integral and use the Langevin equation (5.3) for $\dot{X}_t$, yielding (see Appendix C.1)

$$\dot{S}_t^{\mathrm{tot}} = -2\frac{(\partial_t \rho_t)\,(X_t)}{\rho_t(X_t)} + \underbrace{\frac{1}{\mu T}\left(\frac{J_{t,\rho}(X_t)}{\rho_t(X_t)}\right)^2}_{v_t^S(X_t)} + \underbrace{\left(\sqrt{\frac{2}{\mu T}}\,\frac{J_{t,\rho}(X_t)}{\rho_t(X_t)}\right)}_{\sqrt{2v_t^S(X_t)}} \dot{B}_t, \tag{5.26}$$

where v_t^S is the time-dependent *entropic drift* [12], which we discuss further in Section 5.2.2.1. Averaging Equation (5.26) over the noise, the first and third terms in (5.26) vanish. Indeed, the first term has zero average due to conservation of probability and the third term because it is a martingale. The average of the second term yields precisely the right-hand side in Equation (5.24). In Section 6.1.5.4, we generalize Equation (5.26) to the case of $d > 1$ dimensions.

5.1.4. *Stratonovich and Ito formulations: recap*

We provide here for readers' ease a short recap on the formulation of the first and second laws of thermodynamics in Stratonovich and Ito formulations. To this aim, we collect results from the previous sections 5.1.2 and 5.1.3 and provide the stochastic rates of heat, work, energy, and entropy production in $[t, t + \mathrm{d}t]$ associated with the overdamped Langevin dynamics (5.3).

Stratonovich formulation. The work and heat exchanges read

$$\dot{W}_t = (\partial_t V_t)(X_t) + f_t(X_t) \circ \dot{X}_t, \tag{5.27}$$

$$\dot{Q}_t = (\partial_x V_t)(X_t) \circ \dot{X}_t - f_t(X_t) \circ \dot{X}_t, \tag{5.28}$$

which leads to the first law

$$\dot{V}_t = (\partial_t V_t)(X_t) + (\partial_x V_t)(X_t) \circ \dot{X}_t. \tag{5.29}$$

Note that Equation (5.29) could be retrieved from standard rules of calculus (chain rule for differentiation) that apply in the Stratonovich convention. The rate of stochastic entropy production reads

$$\dot{S}_t^{\text{tot}} = -\frac{(\partial_t \rho_t)(X_t)}{\rho_t(X_t)} + \left[\frac{J_{t,\rho}}{\mu T \rho_t}\right](X_t) \circ \dot{X}_t, \tag{5.30}$$

which leads to the second law at the average level $\langle \dot{S}_t^{\text{tot}} \rangle \geq 0$.

Ito formulation. The work and heat exchanges can be retrieved by applying to Equations (5.27) and (5.28) the rules of conversion between Stratonovich and Ito products (Theorem 1)

$$\dot{W}_t = [\partial_t V_t + \mu T (\partial_x f_t)](X_t) + f_t(X_t)\dot{X}_t, \tag{5.31}$$

$$\dot{Q}_t = \mu T [\partial_x^2 V_t - (\partial_x f_t)](X_t) + [\partial_x V_t - f_t](X_t)\dot{X}_t, \tag{5.32}$$

which leads to the first law

$$\dot{V}_t = (\partial_t V_t)(X_t) + (\partial_x V_t)(X_t)\dot{X}_t + \mu T (\partial_x^2 V_t)(X_t), \tag{5.33}$$

which can be retrieved directly applying Ito rules of calculus, i.e. Ito's lemma (see Equation 2.88). On the other hand, the rate of stochastic entropy production reads

$$\dot{S}_t^{\text{tot}} = \left[-\frac{(\partial_t \rho_t)}{\rho_t} + \partial_x \frac{J_{t,\rho}}{\rho_t}\right](X_t) + \left[\frac{J_{t,\rho}}{\mu T \rho_t}\right](X_t)\,\dot{X}_t, \tag{5.34}$$

which follows from applying to Equation (5.30) Theorem 1 for conversion of Stratonovich to Ito product. Next, replacing $\dot{X}_t$ in Equation (5.34) by the Langevin dynamics (6.39), one finds

$$\dot{S}_t^{\text{tot}} = \left[-2\frac{(\partial_t \rho_t)}{\rho_t} + v_t^S\right](X_t) + \left[\sqrt{2 v_t^S}\right](X_t)\dot{B}_t, \tag{5.35}$$

which reveals the martingale structure of $\exp(-S_t^{\text{tot}})$ in time-homogeneous stationary states, as we will show in Section 5.2.

Taken together, the results in this section illustrate the fact that Stratonovich convention provides a more simple mathematical formulation of the first law of thermodynamics, whereas the Ito convention is more suitable to discuss the second law. Generalizations of Equations (5.27)–(5.35) to d-dimensional overdamped Langevin dynamics can be found in Ref. [12].

5.2. *Martingale theory for stationary 1D isothermal Langevin processes*

A central result of martingale theory for stochastic thermodynamics is that in nonequilibrium stationary processes the exponentiated negative entropy production is a martingale. We first derive this result, and subsequently, we discuss some interesting implications. Notably, we discuss here some of the universal fluctuation properties of entropy production that can be derived from martingale theory. A more extensive overview of the implications of martingale theory for thermodynamics is presented in Chapters 6–9, which includes the martingale fluctuation relations and the martingale version of the second law of thermodynamics.

For reasons of clarity, we restrict ourselves to the simplest case of one-dimensional, stationary, overdamped, Langevin processes. Nevertheless, martingale theory for thermodynamics is general and applies also to nonstationary, underdamped, or multidimensional Langevin processes, see Refs. [10,12,14,15,28] or Chapter 6. Therefore, we encourage the reader, based on the derivations below, to derive the corresponding results for, i.e., the multidimensional, underdamped, or nonstationary cases (this is fun!).

5.2.1. *Stationary overdamped Langevin processes*

A Langevin process is *stationary* when the initial distribution obeys

$$\rho_t(x) = \rho_{\rm st}(x), \tag{5.36}$$

for all $t \geq 0$ and $x \in \mathcal{X}$, where $\rho_{\rm st}$ is the stationary probability distribution solving Equation (3.40). Analogously, the stationary current is defined as the hydrodynamic current (5.13) associated with the stationary distribution (5.36), i.e.,

$$J_{t,{\rm st}}(x) \equiv J_{t,\rho_{\rm st}}(x) = \mu F_t(x)\rho_{\rm st}(x) - \mu T \partial_x \rho_{\rm st}(x). \tag{5.37}$$

Note that the stationary distribution solves $\partial_x J_{t,{\rm st}}(x) = 0$, see Equation (5.12).

We say that the Langevin equation (5.3) is *time homogeneous* when the conditions

$$f_t = f \quad \text{and} \quad V_t = V \tag{5.38}$$

are satisfied, and this is a necessary condition for stationarity when the mobility matrix is independent of time; note that this is not the case with time-dependent mobilities. When (5.38) holds, then also the total force is time independent,

$$F(x) = F_t(x) = (\partial_x V)(x) + f(x). \tag{5.39}$$

Throughout this section, we assume *stationarity and time homogeneity*, in other words, we assume that X_t obeys the Langevin equation (5.3)

$$\dot{X}_t = -\mu F(X_t) + \sqrt{2T\mu}\dot{B}_t, \tag{5.40}$$

and $\rho_0(x) = \rho_{\rm st}(x)$. Following Equation (5.37), the stationary current is time independent and reads

$$J_{\rm st}(x) = \mu F(x)\rho_{\rm st}(x) - \mu T\partial_x \rho_{\rm st}(x). \tag{5.41}$$

5.2.2. *Martingality of the exponentiated negative entropy production*

We show that for stationary processes X_t, described in Equation (5.3) with the stationarity condition given in Equation (5.36), the exponentiated negative entropy production $\exp(-S^{\rm tot}_t)$ is a martingale. To this aim, we use three distinct, but equivalent, approaches, namely, we show that $\exp(-S^{\rm tot}_t)$ is (a) an Itô integral of the form (2.64); (b) a Radon–Nikodym derivative process (or path-probability ratio) of the form (2.53); and (c) a Dynkin's martingale of the form (3.73). Note that the latter approach (Dynkin's) is new to our knowledge and thus first shown here. While initially we will not bother too much with the distinction between local martingales and martingales, we will come back on this point at the end of the section.

5.2.2.1. *Itô-integral approach.* As discussed in Section 2.2.2, Itô integrals of the form (2.64) that satisfy Equation (2.67) are martingales. Here, we show that $\exp(-S^{\rm tot}_t)$ is an Itô integral.

For time-homogeneous stationary processes for which $\partial_t \rho_t(x) = 0$ for all x, the Itô stochastic differential equation for S_t^{tot}, given in (5.26), simplifies into the compact form

$$\dot{S}_t^{\text{tot}} = v^S(X_t) + \sqrt{2v^S(X_t)}\dot{B}_t, \tag{5.42}$$

where $v^S(X_t)$ is the so-called **entropic drift** [12] defined by

$$v^S(X_t) \equiv \frac{1}{\mu T}\left(\frac{J_{\text{st}}(X_t)}{\rho_{\text{st}}(X_t)}\right)^2 \geq 0, \tag{5.43}$$

and where the noise $\dot{B}_t$ is the same noise as in the Langevin equation (5.3) for the dynamics of the particle.

Since $v_t^S \geq 0$, it follows readily from Equation (5.42) that S_t^{tot} is a submartingale. Note that according to Equation (5.42) the drift and diffusion coefficients of S_t^{tot} are identical, which are reminiscent of the Einstein relation (3.69).

The equality of the drift and diffusion coefficients of S_t^{tot} determines the martingality of $\exp(-S_t^{\text{tot}})$. Indeed, applying Itô's formula, see Equation (B14) in Appendix B.3.1, to the variable change $S_t^{\text{tot}} \to \exp(-S_t^{\text{tot}})$, and using Equation (5.42), we obtain

$$\frac{\mathrm{d}\exp(-S_t^{\text{tot}})}{\mathrm{d}t} = -\sqrt{2v^S(X_t)}\,\exp(-S_t^{\text{tot}})\dot{B}_t, \tag{5.44}$$

and hence $\exp(-S_t^{\text{tot}})$ is an Itô integral; note the formal analogy between Equations (5.44) and (4.101). In addition, Equation (5.44) shows that $\exp(-S_t^{\text{tot}})$ is the stochastic exponential $\mathcal{E}_t(M)$ of the martingale

$$M_t = -\int_0^t \mathrm{d}s\sqrt{2v^S(X_s)}\dot{B}_s; \tag{5.45}$$

the latter process is a martingale according to Equation (2.67) as $\langle v^S(X)\rangle = \langle \dot{S}^{\text{tot}}\rangle < \infty$.

5.2.2.2. *Path-probability-ratio approach.* We show that $\exp(-S_t^{\text{tot}})$ takes the form of a path-probability ratio by identifying a suitable measure $\mathcal{Q}$ for which $\exp(-S_t^{\text{tot}})$ can be written as a Radon–Nikodym derivative process of the form (2.53) [10,11,138,145–147].

To this purpose, we introduce the time-reversal map Θ_t that acts on the trajectories $x_{[0,t]}$ through

$$\left[\Theta_t\left(x_{[0,t]}\right)\right]_s \equiv x_{t-s} \quad \text{for } s \leq t. \tag{5.46}$$

Subsequently, we show one of the central results in stochastic thermodynamics, namely

$$S_t^{\text{tot}} = \ln\frac{\mathcal{P}\left(X_{[0,t]}\right)}{(\mathcal{P}\circ\Theta_t)\left(X_{[0,t]}\right)}, \tag{5.47}$$

or equivalently,

$$\exp(-S_t^{\text{tot}}) = \frac{(\mathcal{P} \circ \Theta_t)\left(X_{[0,t]}\right)}{\mathcal{P}\left(X_{[0,t]}\right)}. \tag{5.48}$$

For time-homogeneous stationary processes, the measure $\mathcal{P} \circ \Theta_t$ appearing in the numerator of Equation (5.48) is independent of t, see Refs. [84,98,148], and hence the measure $\mathcal{Q}$ in Equation (2.53) is in this case $\mathcal{P} \circ \Theta_t$. This can be understood heuristically as follows. The map Θ_t is a time-reversal map that mirrors trajectories around the reflection point $t/2$. Since by assumption $\mathcal{P}$ is a stationary measure, the location of the reflection point does not alter the statistics determined by $\mathcal{P}$. We come back to this point at the end of the derivation.

5.2.2.3. *Proof of relation between stochastic entropy production and path-probability ratio.* Let us now prove the relation (5.47). Using the Onsager–Machlup path-integral approach, see Equations (2.56)–(2.58) and Equations (3.94), we can write explicit expressions for the conditional path probabilities,[6] viz.,

$$\mathcal{P}(X_{[0,t]}|X_0) = \frac{1}{\mathcal{N}} \exp\left(-\frac{1}{4\mu T}\int_0^t \left\{\left[\dot{X}_s - \mu F(X_s)\right]^2 + \frac{\mu}{2}(\partial_x F)(X_s)\right\} \mathrm{d}s\right), \tag{5.49}$$

and analogously,

$$\mathcal{P}(\Theta_t(X_{[0,t]})|X_t) = \frac{1}{\mathcal{N}} \exp\left(-\frac{1}{4\mu T}\int_0^t \left\{\left[-\dot{X}_s - \mu F(X_s)\right]^2 + \frac{\mu}{2}(\partial_x F)(X_s)\right\} \mathrm{d}s\right). \tag{5.50}$$

Taking the ratio of Equations (5.49) and (5.50), we obtain the so-called local detailed balance condition,

$$\frac{\mathcal{P}(\Theta_t(X_{[0,t]})|X_t)}{\mathcal{P}(X_{[0,t]}|X_0)} = \exp\left(-\frac{1}{T}\int_0^t F(X_s) \circ \dot{X}_s \, \mathrm{d}s\right) = \exp\left(\frac{Q_t}{T}\right) = \exp\left(-S_t^{\text{env}}\right) \tag{5.51}$$

that relates the stochastic heat Q_t to the path probabilities. Lastly, multiplying Equation (5.51) by $\exp(S_0^{\text{sys}} - S_t^{\text{sys}}) = \rho_{\text{st}}(X_t)/\rho_{\text{st}}(X_0)$ (see (5.14)), we obtain

$$\frac{\mathcal{P}(\Theta_t(X_{[0,t]}))}{\mathcal{P}(X_{[0,t]})} = \frac{\mathcal{P}(\Theta_t(X_{[0,t]})|X_t)\rho_{\text{st}}(X_t)}{\mathcal{P}(X_{[0,t]}|X_0)\rho_{\text{st}}(X_0)} = \exp(-S_t^{\text{env}} - \Delta S_t^{\text{sys}}) = \exp(-S_t^{\text{tot}}), \tag{5.52}$$

which is Equation (5.48) that we were meant to show.

As promised, we now show that $\mathcal{P}[\Theta_t(X_{[0,t]})] = \mathcal{Q}[X_{[0,t]}]$, and hence there is no explicit time dependence on t. For this, we show that the Lagrangian of $\mathcal{P}[\Theta_t(X_{[0,t]})]$ contains no explicit time dependency on t – see Equation (3.97) for the definition of a Lagrangian. Equation (5.50) can be rewritten as

$$\begin{aligned}
\mathcal{P}\left(\Theta_t\left(X_{[0,t]}\right)\right) &= \rho_{\text{st}}\left(X_t\right)\frac{1}{\mathcal{N}}\exp\left(-\frac{1}{4\mu T}\int_0^t \left\{\left(\dot{X}_s + \mu F\left(X_s\right)\right)^2 + \frac{\mu}{2}\left(\partial_x F\right)\left(X_s\right)\right\}\mathrm{d}s\right)\\
&= \rho_{\text{st}}\left(X_0\right)\frac{1}{\mathcal{N}}\exp\left(-\int_0^t \left[\begin{array}{c}\frac{1}{4\mu T}\left\{\left(\dot{X}_s + \mu F\left(X_s\right)\right)^2 + \frac{\mu}{2}\left(\partial_x F\right)\left(X_s\right)\right\}\\ -\partial_x\left(\ln\rho_{\text{st}}\right)\left(X_s\right)\dot{X}_s\end{array}\right]\mathrm{d}s\right).
\end{aligned}$$

Hence, the Lagrangian transforms under reversal as

$$(\Theta_t \mathcal{L}) \left[X_s, \dot{X}_s\right] = \frac{1}{4\mu T} \left(\left(\dot{X}_s + \mu F\left(X_s\right)\right)^2 + \frac{\mu}{2} \left(\partial_x F\right)\left(X_s\right) \right) - \partial_x \left(\ln \rho_{st}\right)\left(X_s\right) \dot{X}_s. \tag{5.53}$$

The absence of an explicit t-dependence in the right-hand side of the last relation shows that the measure $\mathcal{P} \circ \Theta_t$ is not explicitly dependent on t, as claimed before. This allows us to conclude that $\exp(-S_t^{\rm tot})$ is a martingale.

In Section 6.2.2, we give an alternative proof of the martingality of $(\mathcal{P} \circ \Theta_t)(X_{[0,t]})/\mathcal{P}(X_{[0,t]})$ in stationary processes. In addition, in Section 6.1, we extend the path-probability ratio formula (5.48) to the non-stationary and/or time-inhomogeneous set up. In this non-stationary and/or time-inhomogeneous set up, the explicit time dependency of the measure $\mathcal{Q}^{(t)}$ in the numerator prevents us from proving that $\mathcal{Q}^{(t)}(X_{[0,t]})/\mathcal{P}(X_{[0,t]})$ is a martingale, as done for discrete time in (2.19); the latter is developed in Section 6.2.2.

We end this section with a comment on the second law of thermodynamics.

> The second law of thermodynamics is recovered when averaging the stochastic entropy production over the probability $\mathcal{P}(X_{[0,t]})$, as this yields the Kullback–Leibler divergence between the forward and reverse path probabilities [149]:
>
> $$\langle S_t^{\rm tot} \rangle = \int \mathcal{D}x_{[0,t]} \mathcal{P}(x_{[0,t]}) \ln \frac{\mathcal{P}(x_{[0,t]})}{\mathcal{P}(\Theta_t(x_{[0,t]}))} = D_{\rm KL}[\mathcal{P}(x_{[0,t]}) || \mathcal{P}(\Theta_t(x_{[0,t]}))] \geq 0. \tag{5.54}$$

5.2.2.4. ♠*Dynkin's martingale approach.* According to Theorem 4 and Equation (3.87), harmonic functions of the generator of a Markov process define martingales. We show here that $\exp(-s)$ is a harmonic function of the corresponding generator. This provides a third derivation of the martingale property of $\exp(-S_t^{\rm tot})$, which to the best of our knowledge has not appeared before in the literature.

Consider the two-dimensional joint process $\mathscr{X}_t = (S_t^{\rm tot}, X_t)^{\rm T}$ which according to Equations (5.3) and (5.42) solves the stochastic differential equations

$$\begin{cases} \dot{S}_t^{\rm tot} = v^S(X_t) + \sqrt{2v^S(X_t)}\dot{B}_t, \\ \dot{X}_t = \mu F(X_t) + \sqrt{2\mu T}\dot{B}_t, \end{cases} \tag{5.55}$$

with common noise $\dot{B}_t$. The Markovian generator associated with the two-dimensional diffusion process $\mathscr{X}_t$ given in Equation (5.55) is (see Equation 3.67)

$$\mathcal{L} = v^S(x)\partial_s + \mu F(x)\partial_x + v^S(x)\partial_s^2 + \mu T \partial_x^2 + 2\sqrt{T\mu v^S(x)}\partial_x\partial_s. \tag{5.56}$$

We readily verify that

$$\mathcal{L}\left[\exp(-s)\right](s,x) = 0, \tag{5.57}$$

and hence $\exp(-s)$ is a harmonic function of the generator $\mathcal{L}$, implying, according to Theorem 4 and Equation (3.87), that $\exp(-S_t^{\rm tot})$ is a martingale. We also find that

$$\mathcal{L}[s](s,x) = v^S(x) \geq 0, \tag{5.58}$$

and thus s is a subharmonic function of the generator, which implies that $S_t^{\rm tot}$ is a submartingale [77].

Now, we write the two-dimensional stochastic differential equation (5.55) in the Langevin form (3.65) associated with the joint process $\mathscr{X}_t = (S_t^{\text{tot}}, X_t)^{\text{T}}$,

$$\dot{\mathscr{X}}_t = -(D\nabla\mathscr{V})(\mathscr{X}_t) + (\nabla\cdot D)(\mathscr{X}_t) + \sigma(\mathscr{X}_t)\dot{B}_t, \tag{5.59}$$

where ∇ is in this case the gradient in (x,s)-space with components $\nabla_1 = \partial_s$ and $\nabla_2 = \partial_x$. In Equation (5.59), we have also introduced

$$\sigma(s,x) = \begin{pmatrix} \sqrt{2v^S(x)} \\ \sqrt{2T\mu} \end{pmatrix}, \tag{5.60}$$

the generalized diffusion matrix

$$D(s,x) = \frac{\sigma(x,s)\sigma^{\dagger}(x,s)}{2} = \begin{pmatrix} v^S & \sqrt{T\mu v^S(x)} \\ \sqrt{T\mu v^S(x)} & T\mu \end{pmatrix}, \tag{5.61}$$

and the generalized time homogeneous potential

$$\mathscr{V}(s,x) = -s - \ln\rho_{\text{st}}(x). \tag{5.62}$$

We remark that Equation (5.59) has a mobility matrix equal to the diffusion matrix, which is reminiscent of Einstein's relation. The form of Equation (5.59) readily implies that the generalized Boltzmann distribution

$$\rho_{\text{st}}(s,x) = \exp(-\mathscr{V}(s,x)) = \rho_{\text{st}}(x)\exp(s) \tag{5.63}$$

is the invariant measure. Note that this measure is not normalizable, which follows from the fact that the generalized potential $\mathscr{V}(s,x)$ given by Equation (5.62) is not confining. Physically, the latter statement means that S_t^{tot} is extensive in time. Note also that the factorization property, revealed in Equation (5.63), suggests an asymptotic independence between X_t and S_t^{tot}.

5.2.2.5. ♠*Martingale or strict local martingale?*. Is the exponentiated negative entropy production a martingale ($\langle\exp(-S_t^{\text{tot}})\rangle = 1$) or a strict local martingale ($\langle\exp(-S_t^{\text{tot}})\rangle < 1$)?

Formally, Equation (5.44) implies that $\exp(-S_t^{\text{tot}})$ is a local martingale, and to prove martingality we need to show that Equation (2.67) holds. Alternatively, according to Equation (5.44), $\exp(-S_t^{\text{tot}})$ is the stochastic exponential

$$\exp(-S_t^{\text{tot}}) = \mathcal{E}(M_t), \tag{5.64}$$

as defined in Equation (4.92), of the martingale

$$M_t = -\int_0^t \sqrt{2v^S(X_u)}\dot{B}_u\,\mathrm{d}u. \tag{5.65}$$

Hence $\exp(-S_t^{\text{tot}})$ is a martingale when Novikov's condition equation (4.104) holds, which here reads

$$\left\langle \exp\left(\int_0^t v^S(X_s)\,\mathrm{d}s\right)\right\rangle < \infty \tag{5.66}$$

for all $t \geq 0$.

In the Radon–Nikodym derivative approach, we also need Novikov's condition equation (5.66) to guarantee that $\exp(-S_t^{\rm tot})$ is a martingale. Indeed, the Onsager–Machlup path integral method, widely used in physics [26], assumes that $\mathcal{P} \circ \Theta_t$ is absolutely continuous with respect to $\mathcal{P}$. However, there is no guarantee that this is actually the case, and we need an additional condition, such as the Novikov condition[7] to demonstrate this.

Note that Novikov's condition is a mathematical requirement for martingality, but currently we are not aware of physical examples for which $\exp(-S_t^{\rm tot})$ is a local martingale but not martingales.

5.2.2.6. *On the non-submartingality of the environmental entropy change.* In general, the stochastic heat and environmental entropy change are not martingales. In particular, for time-homogeneous stationary states, we obtain from Equations (5.16), (5.8), (5.3), and (5.37) the following stochastic differential equation for the environmental entropy change:

$$\dot{S}_t^{\rm env} = v^E(X_t) + \sqrt{2v^E(X_t)} \circ \dot{B}_t, \text{ where } \quad v^E(X_t) \equiv \frac{\mu F^2(X_t)}{T} \geq 0. \tag{5.67}$$

Note that in Equation (5.67), B_t is the same noise that enters in the Langevin equation for X_t (5.3), and that the equation should be interpreted in the Stratonovich sense. On the other hand, using Itô's convention, we get

$$\dot{S}_t^{\rm env} = \mu\,(\partial_x F)\,(X_t) + v^E(X_t) + \sqrt{2v^E(X_t)}\dot{B}_t. \tag{5.68}$$

This implies that for a generic F it does not hold, in general, that $S_t^{\rm env}$ has positive drift, even though v^E is non-negative. Nevertheless, if $\partial_x F(x) + F^2(x)/T \geq 0$ holds for all x, then $\dot{S}_t^{\rm env}$ is a submartingale. This is the case, among others, when $\partial_x F(x) = 0$, such that $F(x)$ is homogeneous and independent of x (see, e.g., the example in Chapter 1.6). In such a case, $v^E(X_t) = v^E$ is independent of X_t and Equation (5.68) is equivalent to $\dot{S}_t^{\rm env} = v^E + \sqrt{2v^E}\dot{B}_t$, similar to Equation (5.70) for $S_t^{\rm tot}$ in time-homogeneous stationary processes.

5.2.2.7. *Non-stationary processes.* We consider the dynamics of $S_t^{\rm tot}$ for non-stationary and/or non time-homogeneous processes X. The Itô stochastic differential equation for $S_t^{\rm tot}$ (5.26) reads then

$$\dot{S}_t^{\rm tot} = -2\,(\partial_t \ln \rho_t)\,(X_t) + v_t^S(X_t) + \sqrt{2v_t^S(X_t)}\dot{B}_t, \tag{5.69}$$

which is the Doob–Meyer decomposition of $S_t^{\rm tot}$ (see Theorem 16). We recall readers the definition of time-dependent entropic drift $v_t^S(X_t)$ given in Equation (5.26). Since for nonstationary processes $\partial_t \rho_t \neq 0$, the first term in Equation (5.69) does not vanish and can be negative, which implies that the predictable process in the Doob–Meyer decomposition is not increasing, and as a consequence $S_t^{\rm tot}$ is not a submartingale. In addition, the drift and diffusion constants in Equation (5.69) are not equal as in Equation (5.70) for stationary processes, and as a consequence the statistical properties (i.e., global infimum) described above are not universal for non-stationary overdamped Langevin processes. In Chapter 6, we elaborate further on stochastic thermodynamics in nonstationary processes, and in particular we discuss thermodynamic martingale processes for this case.

Note that the fact that a process is not stationary does not preclude other thermodynamic quantities whose negative exponential is an Itô integral. Indeed, Refs. [28,39] showed that the so-called housekeeping entropy production obeys an equation analogous to Equation (5.44) (and is thus an Itô integral) for any Markovian process that may be non-stationary. We refer the readers to Equation (6.68) and Refs. [150–152] for further details on the concept of housekeeping (also called adiabatic [152]) entropy production.

5.2.3. *Universal properties for the fluctuations of the stochastic entropy production*

The (local) martingale property of $\exp(-S_t^{\rm tot})$ together with the continuity of the process $S_t^{\rm tot}$ as a function of time implies that several fluctuation properties of $S_t^{\rm tot}$ are universal. Here, following Ref. [12], we derive the universal properties of $S_t^{\rm tot}$ directly from the evolution equation (5.42) for entropy production, while in the next chapter we use Doob's theorems, as reviewed in Chapter 4, to derive these results.

5.2.3.1. *Entropic random-time change.* Our starting point is the Itô stochastic differential equation for $S_t^{\rm tot}$ in time-homogeneous stationary states, see Equations (5.42)–(5.43) and copied here for convenience (Figure 5.2),

$$\dot{S}_t^{\rm tot} = v^S(X_t) + \sqrt{2v^S(X_t)}\dot{B}_t, \quad \text{with } v^S(X_t) \equiv \frac{1}{\mu T}\left(\frac{J_{\rm st}(X_t)}{\rho_{\rm st}(X_t)}\right)^2. \tag{5.70}$$

Now, consider the following time reparametrization:

$$\mathrm{d}t \to \mathrm{d}\tau_t(X_t) \equiv v^S(X_t)\,\mathrm{d}t, \tag{5.71}$$

such that $\mathrm{d}\tau_t$ quantifies the expected entropy production in $[t, t+\mathrm{d}t]$ given that the system was at state X_t at time t. This is an example of a *random-time* transformation (see Section 4.2.2 and also Section 8.5 in [64]) of a stochastic process, in which a "clock" ticks faster (slower) whenever the system passes by a state of large (small) local entropy production. Following a single realization

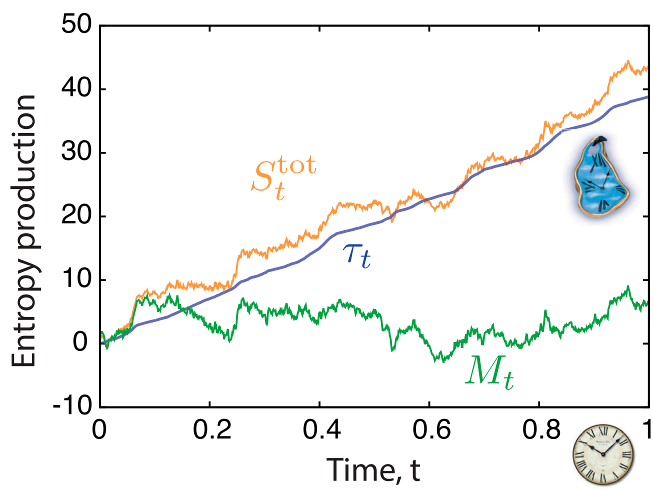

Figure 5.2. Illustration of the Doob–Meyer decomposition of entropy production (Equation 5.73). In time-homogeneous nonequilibrium stationary states, the stochastic entropy production $S_t^{\rm tot}$ (orange line) can be decomposed as the sum of the entropic time τ_t (blue line) plus a martingale M_t (green line). The white clock in the x-axis illustrates the regular passage of time t whereas the blue *Dalinean* clock illustrates the irregular passage of entropic time τ which depends on the states visited by the system. Figure adapted from Ref. [12].

of duration t its associated entropic random time is given by

$$\tau_t = \int_0^t \mathrm{d}\tau_s(X_s) = \int_0^t v^S(X_s)\,\mathrm{d}s, \tag{5.72}$$

which highlights the fact that τ_t is a functional of the trajectory $X_{[0,t]}$. Because $\langle \dot{S}^{\mathrm{tot}}_{\mathrm{s}} | X_{[0,t]} \rangle = v^S(X_t)$, see Equation (5.70), the entropic time can be interpreted as the expected entropy production given that the system has traced a specific trajectory $X_{[0,t]}$. Integrating Equation (5.70) over time, we get

$$S^{\mathrm{tot}}_t = \tau_t + M_t, \tag{5.73}$$

where $M_t = \int_0^t \sqrt{2v^S(X_s)}\dot{B}_s ds$ is a martingale and $\tau_t \geq 0$ is a monotonously nondecreasing process, as $v^S(x) \geq 0$ for all t and x. In martingale theory, this decomposition of entropy production (a submartingale) in the sum of the entropic time (a predictable process) and a noise process (martingale) is known as the *Doob–Meyer decomposition*, see Theorem 16 in Chapter 4. Applying the entropic random-time change given in Equations (5.71)–(5.73), we get

$$\dot{S}^{\mathrm{tot}}_\tau = 1 + \sqrt{2}\,\dot{B}^{\mathrm{S}}_\tau, \tag{5.74}$$

where $\dot{B}^{\mathrm{S}}_\tau$ is a Gaussian white noise with $\langle \dot{B}^{\mathrm{S}}_\tau \rangle = 0$ and $\langle \dot{B}^S_\tau \dot{B}^S_{\tau'} \rangle = \delta(\tau - \tau')$; note that here the dot stands for the derivative with respect to τ.

5.2.3.2. *Universal properties in stationary states.* Equation (5.74) reveals that, for any Langevin model described by Equation (5.3), S_{tot} obeys a drift-diffusion equation with both drift and diffusion coefficient equal to 1 when measuring time in units of τ. This means that any statistical property of S_{tot} that is independent of τ is universal in this class of models. For example, even though the distribution of $\rho_{S^{\mathrm{tot}}_t}(s)$ at a fixed time t is model dependent, the distribution of S^{tot}_τ evaluated at entropic times is universal and given by

$$\rho_{S^{\mathrm{tot}}_\tau}(s) = \frac{\exp\left(-(s-\tau)^2/4\tau\right)}{\sqrt{4\pi\tau}}. \tag{5.75}$$

The universality of entropy production revealed here extends to multidimensional overdamped Langevin systems, for which S^{tot}_t also obeys an Itô stochastic differential equation of the form (5.42) with an entropic drift that is generalized to $d > 1$ dimensions – see Equations (6.56) and (6.57). We illustrate this universality principle in Figure 5.3 where we plot the distributions of stochastic entropy production for a driven colloidal particle ($d = 1$-dimensional Langevin equation), a 2D diffusion in a space-dependent velocity field ($d = 2$), and an active Brownian chiral swimmer ($d = 3$).

Furthermore, Equation (5.74) reveals that any statistical property of S^{tot}_t that is independent of time contractions and dilations falls in the universality class of the standard one-dimensional drift diffusion process with unit drift and diffusion constant. For example, the global infimum of entropy production, defined as the minimum value that S^{tot} can

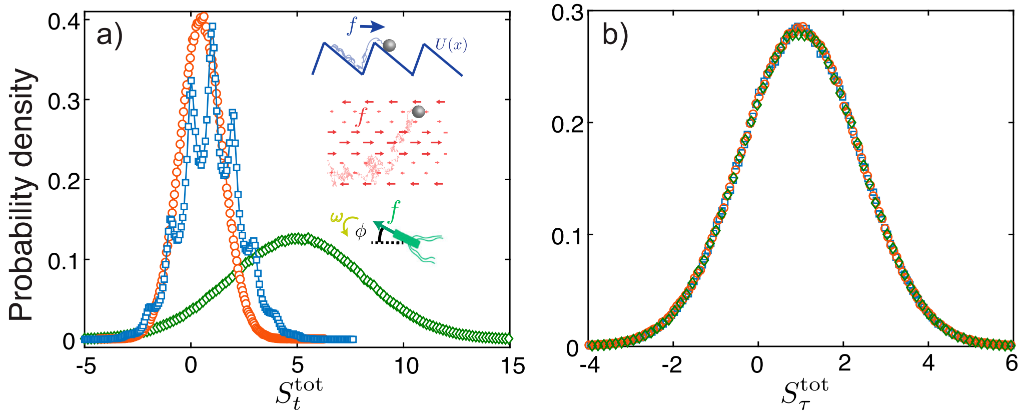

Figure 5.3. Universality of entropy production at entropic times. Distributions of stochastic entropy production obtained from numerical simulations at fixed time $t = 1$ (a) and at fixed entropic time $\tau = 1$ (b). The three different symbols are obtained from numerical simulations of the three models sketched in the caption in (a), see Figure 3.2 for further details and Ref. [12] for details and parameter values of the simulations.

take at any time, i.e.,

$$S^{\text{inf}} = \inf_{t \geq 0} S_t^{\text{tot}} \tag{5.76}$$

is a universal property for overdamped Langevin systems. This is because the value of S^{inf} associated with a given trajectory is independent of when it occurs, and thus on the value of τ. As a result, its probability distribution can be found from that of the minimum of the 1D drift diffusion process,

$$\rho_{S^{\text{inf}}}(s) = \exp(s), \text{ with } s \in \mathbb{R}^-, \tag{5.77}$$

i.e., it is an exponential distribution with mean $\langle S^{\text{inf}} \rangle = -1$. One may also consider the finite-time entropy-production infimum

$$S_t^{\text{inf}} = \inf_{0 \leq t' \leq t} S_t^{\text{tot}}, \tag{5.78}$$

that is, the minimum value that entropy production takes over a finite time interval $[0, t]$. The random variable $S_t^{\text{inf}} \leq 0$ is always larger than its long-time limit $S_t^{\text{inf}} \geq S^{\text{inf}}$, which together with (5.77) implies for Langevin systems the so-called infimum law

$$\langle S_t^{\text{inf}} \rangle \geq -1. \tag{5.79}$$

As shown below in Section 7.4.2, the **infimum law** (5.79) extends for a broader class of nonequilibrium stationary processes.

Other universal properties that can be identified from the entropy-production random-time change are as follows (see Figure 3 in [12]):

- The maximum value that entropy production attains before reaching its global infimum

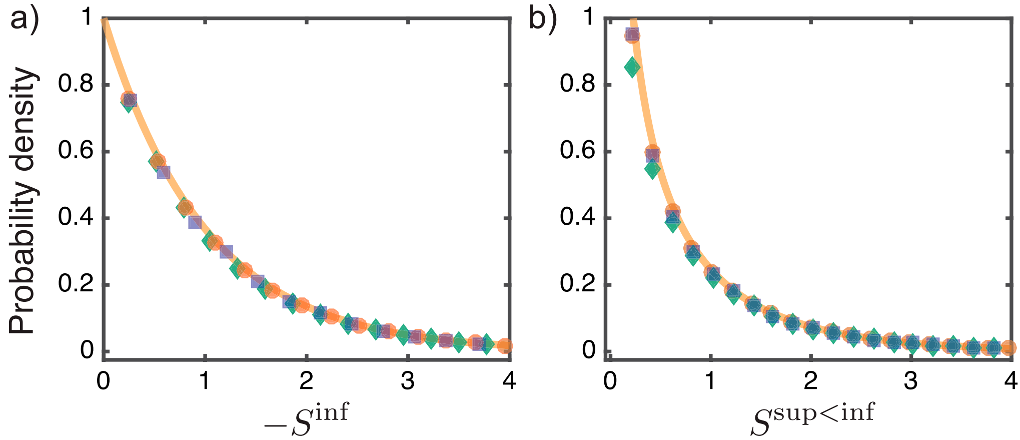

Figure 5.4. Universal properties of entropy production at entropic times in time-homogeneous stationary states. Distributions of minus the infimum $-S^{\text{inf}}$ (a) and supremum before the infimum $S^{\text{sup<inf}}$ (b) associated with the stochastic entropy production S_t^{tot} obtained for the model examples sketched in Figure 5.3(a). The different symbols correspond to results from numerical simulations done for each model: particle in a periodic potential (blue squares), particle in a 2D force field (red circles), active Brownian chiral swimmer (green diamonds). The orange lines are given by the analytical distributions obtained from the drift-diffusion process with unit drift and diffusivity $\dot{X}_t = 1 + \sqrt{2}\dot{B}_t$: $\rho_{S^{\text{inf}}}(s) = \exp(s)$, with $s \in \mathbb{R}^-$ (a), and $\rho_{S^{\text{sup<inf}}}(s) = 2\exp(s)\text{acoth}(2\exp(s) - 1) - 1$, with $s \in \mathbb{R}^+$ (b). See Ref. [12] for further details.

- The number of crossings that entropy production crosses from $-s_0$ to s_0 with $s_0 > 0$ a positive real number
- The number of "record breaking" events before reaching the global supremum/infimum.

Notably, one can identify an *infinite* number of universal properties from the random-time stochastic differential equation for entropy production. Moreover, the distribution of such universal quantities can be retrieved from the one-dimensional drift-diffusion process with both drift velocity and diffusion coefficient equal to 1, such as the distribution of the global infimum given in Equation (5.77). See Figure 5.4 for two examples of such universal properties. On the other hand, statistical properties that depend on the measurement of time, i.e., the first-passage time to reach a positive threshold, are not necessarily universal, and thus their distribution depends, in principle, on the model details.

5.3. *Thermodynamics of isothermal Markov jump processes*

As a second example, we revisit the thermodynamics of isothermal Markov jump processes $X_t \in \mathcal{X}$, as defined in Section 3.2.2, for which $\mathcal{X}$ is a discrete phase space. We assume that the transition rates satisfy the local detailed balance condition given in Equation (3.58), copied here for convenience

$$\frac{\omega_t(x,y)}{\omega_t(y,x)} = \exp\left(\frac{-(V_t(y) - V_t(x)) + f_t\, r(x,y) + \sum_{a=1}^{m} \mu^{(a)}\, n_a(x,y)}{T}\right). \tag{5.80}$$

First, we derive the first and second laws of thermodynamics within this setup, see Refs. [25–27] for more details, and then we revise martingale theory for the thermodynamics of Markov jump processes.

5.3.1. *First law of stochastic thermodynamics*

We define work at the level of a single trajectory, $X_{[0,t]}$, and subsequently use the first law of thermodynamics to obtain an expression for the heat.

Recall that for Markov jump processes, trajectories are piecewise constant functions of the form (3.49). The work done by an external agent on the system is

$$W_t = \int_0^t \mathrm{d}s\,(\partial_s V_s)\,(X_s) + \sum_{j=1}^{N_t} f_{\mathcal{T}_j}\, r(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+}), \tag{5.81}$$

where the first term represents the energy change of the system due to a protocol that changes the shape of the potential V_t and the second term represents the work done on the system by the nonconservative force f_t. For example, f_t could be an external mechanical force and $r(x,y)$ the distance travelled by the system in the jump from x to y.

The first law of thermodynamics reads

$$Q_t + W_t = V_t(X_t) - V_0(X_0), \tag{5.82}$$

which holds at the level of individual trajectories $X_{[0,t]}$.

Using Equation (5.81) in Equation (5.82), we obtain the heat

$$Q_t = \sum_{j=1}^{N_t} \left(V_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}) - V_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}) \right) - \sum_{j=1}^{N_t} f_{\mathcal{T}_j}\, r(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+}). \tag{5.83}$$

Note that the heat can be expressed in terms of the individual contributions

$$\Delta Q_{\mathcal{T}_j}(X_{\mathcal{T}_j}, X_{\mathcal{T}_{j+1}}) = V_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}) - V_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}) - f_{\mathcal{T}_j}\, r(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_{j+1}^+}) \tag{5.84}$$

for each jump in the trajectory $X_{[0,t]}$.

5.3.2. *Second law of stochastic thermodynamics*

The derivation is analogous to the one presented for Langevin processes in Section 5.14, and hence we will follow it closely here.

We define the system entropy as in Equation (5.14), viz.,

$$S_t^{\mathrm{sys}} - S_0^{\mathrm{sys}} = -\ln\left(\frac{\rho_t\,(X_t)}{\rho_0\,(X_0)}\right) \tag{5.85}$$

$$= -\int_0^t \mathrm{d}s\,(\partial_s\,(\ln \rho_s))\,(X_s) - \sum_{i=1}^{N_t} \ln\left(\frac{\rho_{\mathcal{T}_i}(X_{\mathcal{T}_i^+})}{\rho_{\mathcal{T}_i}(X_{\mathcal{T}_i^-})}\right). \tag{5.86}$$

Subsequently, we use the fact that the environment consists of a thermal reservoir at temperature T plus n particle reservoirs with chemical potentials $\mu^{(a)}$, and hence the environment entropy change according to standard thermodynamics is [153]

$$S_t^{\rm env} = \frac{-Q_t + \sum_{j=1}^{N_j} \sum_{a=1}^{n} \mu^{(a)} n_a(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}{T}. \tag{5.87}$$

Substituting the heat, given by Equation (5.83), in the above equation, we obtain

$$\begin{aligned} S_t^{\rm env} &= \sum_{j=1}^{N_t} \frac{-\left(V_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}) - V_{\mathcal{T}_j}(X_{\mathcal{T}_j^-})\right) - f_{\mathcal{T}_j}\, r(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+}) + \sum_{a=1}^{n} \mu^{(a)} n_a(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}{T} \\ &= \sum_{j=1}^{N_t} \ln\left(\frac{\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}{\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}, X_{\mathcal{T}_j^-})}\right), \end{aligned} \tag{5.88}$$

where the last line follows from the local detailed balance formula (5.80). Lastly, adding Equations (5.86) and (5.88), and using the balance equation (5.21), we find

$$S_t^{\rm tot} = -\int_0^t {\rm d}s (\partial_s \ln \rho_s)(X_s) - \sum_{j=1}^{N_t} \ln\left(\frac{\rho_{\mathcal{T}_j}(X_{\mathcal{T}_j^+})\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}, X_{\mathcal{T}_j^-})}{\rho_{\mathcal{T}_j}(X_{\mathcal{T}_j^-})\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}\right). \tag{5.89}$$

Taking the ensemble average of the above equation, we obtain

$$\langle \dot{S}_t^{\rm tot} \rangle = \sum_{(x,y)\in\mathcal{X}^2} \rho_t(x)\omega_t(x,y) \ln\left(\frac{\rho_t(x)\omega_t(x,y)}{\rho_t(y)\omega_t(y,x)}\right) \geq 0, \tag{5.90}$$

which is the second law of thermodynamics for Markov jump processes. To pass from Equation (5.89) to Equation (5.90), we proceeded as follows. The average of the first term in Equation (5.89) vanishes because of the conservation of probability

$$\begin{aligned} \left\langle \int_0^t {\rm d}s\, (\partial_s \ln \rho_s)\, (X_s) \right\rangle &= \int_0^t {\rm d}s \int_{\mathcal{X}} {\rm d}x \rho_s(x)\, (\partial_s \ln \rho_s)\, (x) \\ &= \int_0^t {\rm d}s \int_{\mathcal{X}} {\rm d}x\, (\partial_s \rho_s)\, (x) \\ &= \int_0^t {\rm d}s \partial_s \int_{\mathcal{X}} {\rm d}x \rho_s\, (x) = 0. \end{aligned} \tag{5.91}$$

On the other hand, using the definition of transition rates one gets that the average of the second term in the right-hand side of Equation (5.89) yields the right-hand side of Equation (5.90). Moreover, we derive the inequality in Equation (5.90) in Appendix C.2. We have used the convention $\ln 0/0 = 0$. For stationary processes, the average rate of entropy production and the second law simplify into

$$\langle \dot{S}_t^{\rm tot} \rangle = \sum_{(x,y)\in\mathcal{X}^2} \rho_{\rm st}(x)\omega(x,y) \ln\left(\frac{\rho_{\rm st}(x)\omega(x,y)}{\rho_{\rm st}(y)\omega(y,x)}\right) \geq 0. \tag{5.92}$$

5.4. *Martingale theory for stationary Markov jump processes*

We show that $\exp(-S_t^{\text{tot}})$ is a martingale within the context of stationary Markov jump processes. However, we show that universal properties that apply to Langevin processes do not necessarily apply to the Markov jump processes, as the latter are not continuous. In this section, we assume that the dynamics is time-homogeneous ($\omega_t(x,y) = \omega(x,y)$ for all t) and stationary ($\rho_0(x) = \rho_{\text{st}}(x)$ and $\partial_t \rho_t(x) = 0$). For stationary Markov jump processes,

$$\sum_{x\in\mathcal{X}} \rho_{\text{st}}(x)\omega(x,y) = \sum_{y\in\mathcal{X}} \rho_{\text{st}}(y)\omega(y,x). \tag{5.93}$$

5.4.1. *The martingality of the exponentiated negative entropy production*

We show, using three approaches, that the exponentiated negative entropy production is a martingale.

5.4.1.1. ♠*Dynkin's martingale approach.* We show that $\exp(-s)$ is a harmonic function of the generator of the join process $\mathscr{X}(t) = (S_{\text{tot}}(t), X(t))^{\text{T}}$, and hence, and according to Theorem 4 $\exp(-S_t^{\text{tot}})$ is a martingale. Moreover, we show that s is a subharmonic function of this generator, and thus a submartingale.

From Equations (5.89) and (3.53), we find the following expression for the generator of the joint process that acts on functions $\phi(x,s)$ as

$$\mathcal{L}\left[\phi\right](s,x) = \int_{\mathbb{R}} \mathrm{d}\tilde{s} \sum_{y\in\mathcal{X}} \omega(x,y)\left(\phi(\tilde{s},y) - \phi(s,x)\right)\delta\left(\tilde{s} - s - \ln\left(\frac{\rho_{\text{st}}(x)\omega(x,y)}{\rho_{\text{st}}(y)\omega(y,x)}\right)\right), \tag{5.94}$$

where δ is the Dirac delta distribution.

The generator acting on $\exp(-s)$ gives

$$\begin{aligned}\mathcal{L}\left[\exp(-s)\right] &= \exp(-s)\sum_{y\in\mathcal{X}} \omega(x,y)\left(\frac{\rho_{\text{st}}(y)\omega(y,x)}{\rho_{\text{st}}(x)\omega(x,y)} - 1\right)\\ &= \frac{\exp(-s)}{\rho_{\text{st}}(x)}\sum_{y\in\mathcal{X}} \left(\rho_{\text{st}}(y)\omega(y,x) - \rho_{\text{st}}(x)\omega(x,y)\right) = 0,\end{aligned} \tag{5.95}$$

where in the last step we have used the stationarity condition (5.93). Equation (5.95) states that for stationary Markov jump processes $\exp(-s)$ is a harmonic function of the generator $\mathcal{L}$, and hence $\exp(-S_t^{\text{tot}})$ is a martingale. Also,

$$\mathcal{L}\left[s\right] = \sum_{y\in\mathcal{X}} \omega(x,y)\ln\left(\frac{\rho_{\text{st}}(x)\omega(x,y)}{\rho_{\text{st}}(y)\omega(y,x)}\right) \geq 0, \tag{5.96}$$

where the last inequality follows from the stationarity condition (5.93) and s is thus a subharmonic function. Indeed, the positivity comes from writing

$$\mathcal{L}\left[s\right] = \frac{1}{\rho_{\text{st}}(x)}\sum_{y\in\mathcal{X}} \rho_{\text{st}}(x)\omega(x,y)\ln\left(\frac{\rho_{\text{st}}(x)\omega(x,y)}{\rho_{\text{st}}(y)\omega(y,x)}\right) \tag{5.97}$$

and the elementary convexity relation $a\ln(a/b) - a + b \geq 0$ for all $a \neq b \geq 0$. Indeed, we can identify $a(x,y) = \rho_{\text{st}}(x)\omega(x,y)$ and $b(x,y) = \rho_{\text{st}}(y)\omega(y,x)$, and the stationarity condition (5.93) implies $\sum_{y\in\mathcal{X}}(a(x,y) - b(x,y)) = 0$.

5.4.1.2. *Path-probability-ratio approach.* We use the path-probability-ratio approach to show that $\exp(-S_t^{\mathrm{tot}})$ is a martingale. The rationale goes as follows: (i) we demonstrate that Equation (5.48) also holds for Markov jump processes; (ii) we show that $\mathcal{P} \circ \Theta_t \equiv \mathcal{Q}$ does not depend explicitly on t; (iii) the martingality of $\exp(-S_t^{\mathrm{tot}})$ is concluded following the derivation (2.19) that holds for all ratios of the form (2.53).

First, we show that Equation (5.48) also holds for Markov jump processes. To this aim, we use the Onsager–Machlup approach. Assuming that $\mathcal{P}$ and $\mathcal{P} \circ \Theta$ are mutually absolutely continuous, we can use the action $\mathcal{A}(X_{[0,t]})$ given in Equation (3.92). The corresponding action of the time-reversed process is

$$\mathcal{A}[\Theta_t(X_{[0,t]})] = -\ln\left(\rho_{\mathrm{st}}(X_t)\right) - \sum_{i=1}^{N_t} \ln\left(\omega(X_{\mathcal{T}_i^+}, X_{\mathcal{T}_i^-})\right) + \int_0^t \mathrm{d}s \lambda(X_s). \tag{5.98}$$

Taking the ratio

$$\begin{aligned}\frac{(\mathcal{P} \circ \Theta_t)[X_{[0,t]}]}{\mathcal{P}[X_{[0,t]}]} &= \exp\left(-\mathcal{A}[\Theta(X_{[0,t]})] + \mathcal{A}[X_{[0,t]}]\right) \\ &= \exp\left(\ln\left(\frac{\rho_{st}(X_t)}{\rho_{st}(X_0)}\right) + \sum_{i=1}^{N_t} \ln\left(\frac{\omega(X_{\mathcal{T}_i^+}, X_{\mathcal{T}_i^-})}{\omega(X_{\mathcal{T}_i^-}, X_{\mathcal{T}_i^+})}\right)\right) = \exp(-S_t^{\mathrm{tot}}).\end{aligned} \tag{5.99}$$

Second, in Appendix C.3 we show that $\mathcal{P} \circ \Theta_t$ is not t explicitly dependant.

Finally, the martingality of $\exp(-S_t^{\mathrm{tot}})$ is concluded from the derivation in Equation (2.19).

In Section 6.2.2, we give an alternative proof that $(\mathcal{P} \circ \Theta_t)(X_{[0,t]})/\mathcal{P}(X_{[0,t]})$ is a martingale in the stationary setup.

5.4.1.3. ♠*Itô's integral approach.* The exponentiated negative entropy production, $\exp(-S_t^{\mathrm{tot}})$, is a stochastic exponential $\mathcal{E}_t(M)$ of a martingale M, just as was the case for Langevin processes, see Section 5.2.2.1. Indeed, as we show in Appendix C.4 that the stochastic exponential solves Equation (4.92), i.e.,

$$\frac{\mathrm{d}\exp(-S_t^{\mathrm{tot}})}{\mathrm{d}t} = \exp(-S_{t-}^{\mathrm{tot}})\dot{M}_t \tag{5.100}$$

with M_t the martingale

$$M_t = \sum_{x,y \in \mathcal{X}^2} \left(\frac{\rho_{\mathrm{st}}(y)\omega(y,x)}{\rho_{\mathrm{st}}(x)\omega(x,y)} - 1\right)(N_t(x,y) - \tau_t(x)\omega(x,y)), \tag{5.101}$$

and where we have used $N_t(x, y)$ for the total number of times X has jumped from x to y in the interval $[0, t]$, and $\tau_t(x)$ for the total amount of time the process X has spent in the state x in the interval $[0, t]$, see Equations (3.50) and (3.51) for definitions. Note that M_t is a martingale as it is the sum of martingales of the form (2.48), which can be derived with Dynkin's martingales, see Equation (3.80).

5.4.1.4. ♠*Novikov's condition for Markov jump processes.* Just as was the case for Section 5.2.2, the three approaches presented above demonstrate that $\exp(-S_t^{\mathrm{tot}})$ is a local martingale, and to confirm martingality we need to consider Novikov's condition. Using Novikov's condition for the stochastic exponential of a jump process, we derive in Appendix C.5 the condition

$$\left\langle \exp\left(\sum_{x,y\in\mathcal{X}} \left(\frac{\rho_{\rm st}(y)\omega(y,x)}{\rho_{\rm st}(x)\omega(x,y)} - 1\right)^2 \omega(x,y)\tau_t(x)\right)\right\rangle < \infty, \quad \forall t \geq 0. \tag{5.102}$$

Three shades of martingality

We conclude that there are three (equivalent) ways of representing the martingality of $\exp(-S_t^{\rm tot})$ in time-homogeneous nonequilibrium stationary processes:

- The exponentiated negative entropy production is the stochastic exponential of a martingale M_t,

$$\frac{{\rm d}\exp\left(-S_t^{\rm tot}\right)}{{\rm d}t} = \exp\left(-S_{t^-}^{\rm tot}\right)\dot{M}_t. \tag{5.103}$$

- The function $\exp(-s)$ is a harmonic function of the generator $\mathcal{L}$ of the joint process $(S_t^{\rm tot}, X_t)$,

$$\mathcal{L}[\exp(-s)] = 0. \tag{5.104}$$

- The exponentiated negative entropy production is a path-probability ratio

$$\exp\left(-S_t^{\rm tot}\right) = \frac{(\mathcal{P}\circ\Theta_t)[X_{[0,t]}]}{\mathcal{P}(X_{[0,t]})}, \tag{5.105}$$

where $\mathcal{P}\circ\Theta_t$ has no explicit dependency on time t.

5.4.2. *Non-universal properties for the fluctuations of the stochastic entropy production*

Unlike for Langevin processes where we showed in Section 5.2.3 that a random-time change renders the fluctuations of $S_t^{\rm tot}$ universal, such property is not inherited by Markov-jump processes, even when their continuum limit is a Langevin process. However, as we show in Chapter 7, for processes with jumps there exist universal bounds on the fluctuation properties of entropy production, i.e., bounds that are valid for all time-homogeneous stationary processes. Here, we anticipate and illustrate some of these results on a paradigmatic model of a discrete process, namely, a biased random walk, and in Chapter 7 we review results in a generic setup.

Let us consider a biased random walk given by a continuous-time Markov jump process in one dimension, with periodic boundary conditions. We also assume a homogeneous bias, i.e., transitions from site x to $x+1$ occurring at a space-independent rate $\omega(x,x+1) = \omega_+$, and transitions in the opposite direction to at a space-independent rate $\omega(x,x+1) = \omega_-$. Following Section 1.5, we introduce an "affinity" bias parameter A through the local detailed balance condition

$$\frac{\omega_+}{\omega_-} = \exp(A), \tag{5.106}$$

and a kinetic rate $\nu = \sqrt{\omega_+\omega_-}$, such that $\omega_\pm = \nu\exp(\pm A/2)$, see also Ref. [154]. For the case of molecular motors, A can be related to the hydrolysis free energy of ATP hydrolyzation, the work done by an external force, and the temperature of the environment, see Equation (1.24) in Section 1.5. The homogeneous bias together with the periodic boundary conditions induces a homogeneous stationary density, which implies that $\Delta S_t^{\text{sys}} = -\ln[\rho_{\text{st}}(X_t)/\rho_{\text{st}}(X_0)] = 0$, and thus

$$S_t^{\text{tot}} = S_t^{\text{env}} = \ln\left(\left(\frac{\omega_+}{\omega_-}\right)^{X_t - X_0}\right). \tag{5.107}$$

In Equation (5.107), we have used Equation (5.88) for the environmental entropy change of a Markov-jump process and the fact that $X_t - X_0$ equals to the net number of jumps in the positive direction up to time t. Using Equations (5.106) and (5.107) yields the martingale

$$\exp(-S_t^{\text{tot}}) = \exp[-A(X_t - X_0)]. \tag{5.108}$$

The martingality of $\exp(-S_t^{\text{tot}})$ implies integral fluctuation relations at stopping times. Let us consider the stopping time

$$\mathcal{T} = \inf\{t \geq 0 \,|\, (X_t - X_0) \notin (-x_-, x_+)\}, \tag{5.109}$$

i.e., the first escape time of the position (relative to its initial value) from the interval $(-x_-, x_+)$ with x_- and x_+ two finite positive integers. For the stopping time (5.109), we have that $\langle|\exp(-S_{\mathcal{T}}^{\text{tot}})|\rangle < \exp[-A\min(x_-, x_+)] < \infty$ and $\mathcal{P}(T < \infty) < 1$ ($\mathcal{T}$ is finite), and we can thus readily apply Doob's optional stopping Theorem 4.51

$$\langle\exp(-S_{\mathcal{T}}^{\text{tot}})\rangle = \langle\exp(-S_0^{\text{tot}})\rangle = 1, \tag{5.110}$$

which follows from $S_0^{\text{tot}} = 0$. Furthermore, we can unfold the average at the stopping time (5.109) as

$$\langle\exp(-S_{\mathcal{T}}^{\text{tot}})\rangle = P_+(x_+, x_-)\exp(-Ax_+) + P_-(x_+, x_-)\exp(Ax_-), \tag{5.111}$$

where $P_+(x_+, x_-)$ and $P_-(x_+, x_-)$ denote the absorption probabilities at x_+ and $-x_-$, respectively. Using $P_+(x_+, x_-) + P_-(x_+, x_-) = 1$ together with Equations (5.110)–(5.111), we find

$$P_-(x_+, x_-) = \frac{1 - \exp(-Ax_+)}{\exp(Ax_-) - \exp(-Ax_+)}. \tag{5.112}$$

For $x_+ \to \infty$, we have the absorption probability at position $-x < 0$

$$P_-(x) = \exp(-Ax), \tag{5.113}$$

which gives the probability that the relative position with respect to the initial value $X_t - X_0$ ever reaches the value $-x$. When $\omega_+ > \omega_-$, $A > 0$ and thus $P_-(x) < 1$, i.e., if the drift is positive, the probability to ever reach a negative threshold is smaller or equal than 1. Similarly, for $x_- \to \infty$ and absorption at position $x > 0$, we have $P_+(x) = 1$ for $A > 0$, i.e. the walker reaches with probability 1 a single absorbing positive boundary when the drift is positive.

In what follows, we assume $\omega_+ > \omega_-$, i.e., $A > 0$ (positive average velocity) without loss of generality. The analytical expression (5.113) for the absorption probability in a negative boundary can be used to obtain the statistics of extremal values of position

$$\Delta X_t^{\min} \equiv \min_{s\in[0,t]} (X_s - X_0), \tag{5.114}$$

$$\Delta X_t^{\max} \equiv \max_{s\in[0,t]} (X_s - X_0), \tag{5.115}$$

as well as of entropy production $S_t^{\min} = A\Delta X_t^{\min}$ and $S_t^{\max} = A\Delta X_t^{\max}$. We first consider the long-time limit $\Delta X^{\min} \equiv \lim_{t\to\infty} \Delta X_t^{\min}$. The probability that the global minimum is at $-x < 0$ is

$$\rho_{\Delta X^{\min}}(-x) = P_-(x) - P_-(x+1), \tag{5.116}$$

and therefore

$$\rho_{\Delta X^{\min}}(-x) = \rho_{S^{\min}}(-Ax) = \exp(-Ax)(1 - \exp(-A)). \tag{5.117}$$

The averages of minima of position and entropy production are then given by

$$\langle S_{\min}\rangle = \frac{-A}{\exp A - 1} \tag{5.118}$$

and

$$\langle X_{\min}\rangle = \frac{-1}{\exp A - 1}. \tag{5.119}$$

The global minimum of entropy production (5.118) therefore satisfies the infimum law $\langle S_{\min}\rangle \geq -1$. Note, however, that in the case of continuous processes the infimum law at infinite time imposes precisely $\langle S_{\min}\rangle = -1$, which is, as we have derived here, not obeyed for the biased random walk. Instead for the model discussed here, the average global infimum of entropy production is *not universal* as it depends on the model parameter A, see Equation (5.118).

The limit of a continuous process is reached when taking the diffusion limit where the Peclet number $\mathrm{Pe} = v/D = 2\tanh(A)$ is small, $\mathrm{Pe} \ll 1$, where $v = (\omega_+ - \omega_-) = 2\nu\sinh(A/2)$ and $D = (\omega_+ + \omega_-)/2$ is the effective diffusion coefficient. This diffusion limit therefore corresponds to the regime of small A. In this limit, Equation (5.118) approaches indeed the infimum law of entropy production for continuous stochastic processes $\langle S_{\min}\rangle = -1$. Interestingly, in this limit the velocity v is small and the motor close to stall. However the fluctuations become large for small A which is reflected in a divergence of the average minimum $\langle X_{\min}\rangle$ according to Equation (5.119). Numerical and analytical illustrations of the non-universal feature of the global infimum of entropy production are provided in Figure 5.5 [41].

Lastly, we would like to point to an interesting symmetry between the extrema of entropy production $S_t^{\min}$ and $S_t^{\max}$ during the time interval $[0, t]$ during which the entropy production changes from $S_0^{\mathrm{tot}} = 0$ to S_t^{tot}. Indeed, the reduction of entropy $S_0^{\mathrm{tot}} - S_t^{\min} \geq 0$ between start and minimum obeys the same statistics as the reduction of entropy $S_t^{\max} - S_t^{\mathrm{tot}} \geq 0$. This follows from considering the time reversed process with trajectories $\tilde{X}_{[0,t]} = \{X_{t-u}\}_{u=0}^{t}$ with path distribution $\mathcal{Q}(\Theta_t X_{[0,t]}) = \mathcal{P}(X_{[0,t]})$. This statistics of $\tilde{X}$ is generated by the same hopping process but with rates ω_+ and ω_- exchanged or equivalently with $A \to -A$. The entropy production of the time reversed process therefore is $\tilde{S}_u^{\mathrm{tot}} = A(X_t - \tilde{X}_u)$, where $\tilde{X}_u = X_{t-u}$. Note that extrema of X_t and its time reverse are the same, $\tilde{X}_t^{\max} = X_t^{\max}$ and $\tilde{X}_t^{\min} = X_t^{\min}$. The extrema of entropy production of the time reversed process are therefore $\tilde{S}_t^{\min} = S_t^{\mathrm{tot}} - S_t^{\max}$ and $\tilde{S}_t^{\max} = S_t^{\mathrm{tot}} - S_t^{\min}$. Because

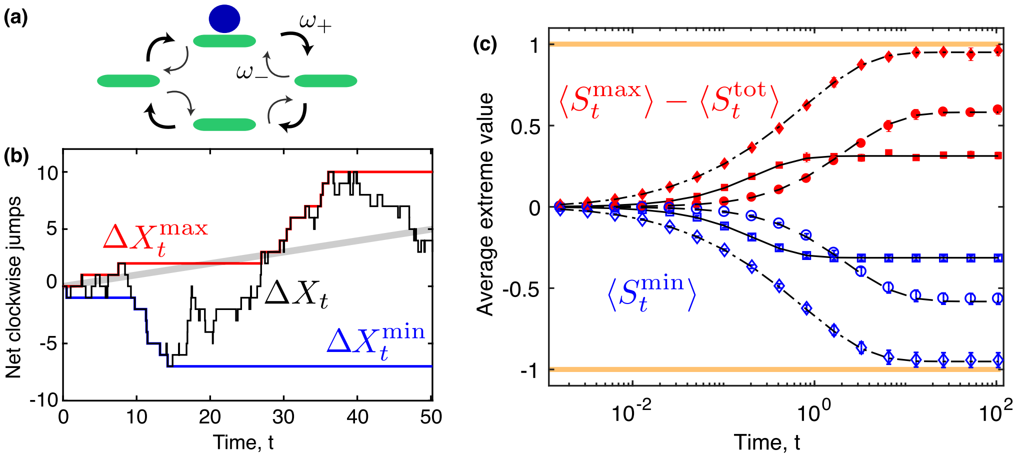

Figure 5.5. (a) Illustration of the minimal stochastic model of molecular motor motion, given by a continuous-time biased random walk in a discrete lattice with periodic boundary conditions. The transition rates are given by $\omega_+ = \omega(x,x+1) = \nu\exp(A/2)$ and $\omega_- = \omega(x,x-1) = \nu\exp(-A/2)$, for forward (clockwise) and backward (counterclockwise) steppings respectively. (b) Net number of clockwise jumps as a function of time in an example trajectory of the model ($X_t - X_0$, black line), together with the average value over many realizations $\langle \Delta X_t\rangle$ (thick black line). The finite-time maximum $\Delta X_t^{\max} = \max_{s\in[0,t]}(X_s - X_0)$ and minimum of the trajectory $\Delta X_t^{\min} = \min_{s\in[0,t]}(X_s - X_0)$ are displayed with red and blue lines, respectively. (c) Averages of the finite-time minimum $\langle S_t^{\min}\rangle$ (blue symbols) and $\langle S_t^{\max}\rangle - \langle S_t^{\rm tot}\rangle$ with $S_t^{\max}$ the finite-time maximum of entropy production (red symbols) as a function of time t. Different symbols are obtained for different degrees of nonequilibrium: $A=1, \nu=0.5$ (squares), $A=2, \nu=2$ (circles), and $A=1, \nu=100$ (diamonds). The horizontal lines are set to ± 1. In (c), symbols are obtained from numerical simulations and the lines are obtained from analytical calculations, see [41] for further details.

$\mathcal{Q}(\tilde{X}_{[0,t]}) = \mathcal{P}(X_{[0,t]})$, the statistics of $\{\tilde{X}_u - X_t\}_{u=0}^t$ and $\{X_u - X_0\}_{u=0}^t$ are the same. Therefore the statistics of $\tilde{S}_s^{\rm tot}$ and $S_s^{\rm tot}$ are also the same as well as those of minima $\tilde{S}_t^{\min}$, $S_t^{\min}$ and those of maxima $\tilde{S}_t^{\max}$, $S_t^{\max}$. As a consequence, the distributions of minima and maxima of entropy production obey the symmetry relation

$$\rho_{S_0^{\rm tot}-S_t^{\min}}(s) = \rho_{S_t^{\max}-S_t^{\rm tot}}(s), \tag{5.120}$$

i.e., the reduction of entropy from time $t=0$ until the minimum value $S_t^{\min}$ has the same statistics as the reduction of entropy from the maximum value $S_t^{\max}$ until it reaches $S_t^{\rm tot}$ at time t. A special case of the general statement (5.120) is that the averages are the same

$$\langle S_t^{\max} - \langle S_t^{\rm tot}\rangle\rangle = -\langle S_7^{\min}7t\rangle. \tag{5.121}$$

The definitions of $\tilde{S}_t^{\rm tot}$ and $S_t^{\rm tot}$ further imply that $\exp(-\tilde{S}_t^{\rm tot})$ and $\exp(S_t^{\rm tot})$ are both martingales with respect to the distribution $\mathcal{Q}$, while $\exp(\tilde{S}_t^{\rm tot})$ and $\exp(-S_t^{\rm tot})$ are both martingales with respect to $\mathcal{P}$.

Chapter 6. Martingales in stochastic thermodynamics II: Formal foundations

As far as I see, all a priori statement in Physics have their origin in symmetry.
Herman Weyl (1952).

After the works of the founding fathers of thermodynamics, among others, Clausius, Maxwell, and Boltzmann, the concept of entropy has become the cornerstone of the second law of thermodynamics. Entropy is a source of continuous discussion with a common theme: there does not exist a unique fully satisfactory notion of entropy and the different definitions of entropy introduced in the literature are interesting for different applications/perspectives [146,155–160]. In the present chapter, we review different notions of entropy as they have been used in stochastic thermodynamics and discuss their relation with martingale theory.

The present chapter builds further on Chapter 5, where we have developed martingale theory for stationary processes in two simple examples, namely, the one-dimensional overdamped Langevin process and Markov jump processes. The aim of the present chapter is to extend martingale theory in thermodynamics for general processes that may be nonstationary. To this aim, we use path-probability ratios, which provide a versatile tool to construct martingales in stochastic thermodynamics, and which will correspond to different notions of entropy.

This chapter is organized into three sections. In the first Section 6.1, we introduce the entropic functionals, which are a generic classes of functionals defined through path-probability ratios. Furthermore, we provide examples of entropic functionals that play a central role in stochastic thermodynamics, such as the entropy production, work, heat, and we illustrate these on specific models, such as Langevin processes and jump processes. In the second Section 6.2, we derive rigorously the martingale structure for the functionals introduced in Section 6.1. In the last Section 6.3, we introduce the generalized entropic functionals and discuss their relevance for stochastic thermodynamics and martingale theory.

To develop formal foundations in this chapter, unless specified otherwise, the physical process X_t with associated path probability $\mathcal{P}$ is a *generic stochastic process*, which can be both in discrete or continuous time, and is not necessarily stationary and/or Markovian.

6.1. *Stochastic entropic functionals and fluctuation relations*

6.1.1. *Notations and preliminaries*

We review the notation that we use for the path probability of a trajectory $x_{[0,t]}$ of a process X_t for discrete time and space, even though we apply it throughout this section in continuous time and space. We denote the path probability to observe a trajectory $x_{[0,t]}$ in the observation time window $[0, t]$ by

$$\mathcal{P}(x_{[0,t]}) \equiv \mathcal{P}(X_0 = x_0, X_1 = x_1, \ldots, X_{t-1} = x_{t-1}, X_t = x_t), \tag{6.1}$$

where $t \in \mathbb{N}$ are natural numbers and $x_s \in \mathcal{X}$ for all values of $s \in [0, t]$. An analogous definition can be formulated for continuous time and/or space, which is nota bene the typical setup for physics.

Since $\mathcal{P}$ denotes the path probability of the physical process X of interest, we often use the simplified notation

$$\langle \cdot \rangle \equiv \langle \cdot \rangle_{\mathcal{P}} \tag{6.2}$$

for averages over the physical path probability $\mathcal{P}$. In this chapter, an important quantity is the path probability $\mathcal{P}$ evaluated on the stochastic process $X_{[0,t]}$, which we denote by $\mathcal{P}(X_{[0,t]})$. We emphasize that $\mathcal{P}(X_{[0,t]})$ is itself a stochastic process.

We often consider a second stochastic process $\mathcal{Q}(X_{[0,t]})$, which is the path probability $\mathcal{Q}$ evaluated on the same stochastic trajectory $X_{[0,t]}$. The path probability $\mathcal{Q}$ may correspond to another physical process, called the *auxiliary process*. Note that in general $\mathcal{P}(X_{[0,t]}) \neq \mathcal{Q}(X_{[0,t]})$. Throughout this chapter, we assume that the path probabilities $\mathcal{P}$ and $\mathcal{Q}$ are mutually *absolutely* *continuous*, which in the discrete case means that for all trajectories $x_{[0,t]}$ for which $\mathcal{Q}(x_{[0,t]}) = 0$, also $\mathcal{P}(x_{[0,t]}) = 0$, and vice versa. We also assume the *microreversibility*, i.e., $\mathcal{P}$ and $\mathcal{Q}$ are mutually absolutely continuous when $\mathcal{Q}$ is evaluated on a time-reversed trajectory.

The time-reversed trajectory denoted by $\Theta_t(x_{[0,t]})$ is the time-reversed path of $x_{[0,t]}$ whose value at time $s \leq t$ is given by

$$\left[\Theta_t\left(x_{[0,t]}\right)\right]_s \equiv x_{t-s}. \tag{6.3}$$

In general, the time-reversed trajectory could also include spatial involution of $\mathcal{X}$, i.e.,

$$\left[\Theta_t\left(x_{[0,t]}\right)\right]_s \equiv x^\star_{t-s}, \tag{6.4}$$

where the involution $x^\star$ has the property $(x^\star)^\star = x$. In particular, for general Kramers–Einstein–Smoluchowski equation (5.2) X_t may contain both position and momenta variables, and the time reversal operation involves a change of sign of all the momentum degrees of freedom. However, for simplicity, we do not consider momentum-like degrees of freedom in this chapter, and we refer the reader to Refs. [98,138] for further analyses.

We also consider families of path probabilities denoted by

$$\mathcal{P}^{(u)}(x_{[0,t]}) \equiv \mathcal{P}^{(u)}\left(X_0 = x_0, X_1 = x_1, \ldots, X_{t-1} = x_{t-1}, X_t = x_t\right), \tag{6.5}$$

where $u, t \geq 0$, and analogously for $\mathcal{Q}^{(u)}$.

Lastly, let us discuss an important choice of $\mathcal{Q}^{(t)}$ that appears in the Markovian context. In the Markovian context, when $\mathcal{P}$ is the path probability of a process X with Markovian generator $\mathcal{L}_t$, the most important choice for $\mathcal{Q}^{(t)}$ corresponds with the *time-reversed protocol*, which we denote by $\tilde{\mathcal{P}}^{(t)}$ (see Figure 6.1 for an illustration). In this case, for each fixed t the auxiliary process is the Markov process with time-reversed Markovian generator

$$\tilde{\mathcal{L}}^{(t)}_s \equiv \mathcal{L}_{t-s}, \tag{6.6}$$

for all $0 \leq s \leq t$, and with a given *arbitrary* initial density

$$\tilde{\rho}^{(t)}_0 \equiv \rho_0^{\tilde{\mathcal{P}}^{(t)}}. \tag{6.7}$$

Analogously, we denote the instantaneous density of X associated with $\tilde{\mathcal{P}}^{(t)}$ by

$$\tilde{\rho}^{(t)}_s \equiv \rho_s^{\tilde{\mathcal{P}}^{(t)}}, \tag{6.8}$$

for all $0 \leq s \leq t$. Note that this is not the time-reversal process that appears often in probabilistic literature [84,98,148] in which, differently to as in Figure 6.1, the instantaneous density is the time reversal of the original.

Meet the entropic functionals. As shown in Chapter 5, key quantities in stochastic thermodynamics are expressed as *functionals* that take a specific value when evaluated over stochastic trajectories $X_{[0,t]}$. These *entropic* functionals (i.e., stochastic entropy production, stochastic environmental entropy change, etc.) take the form of path-probability ratios. In this chapter, we present some of the most relevant entropic functionals in stochastic thermodynamics and discuss their martingale properties from both mathematical and physical viewpoints. To guide the

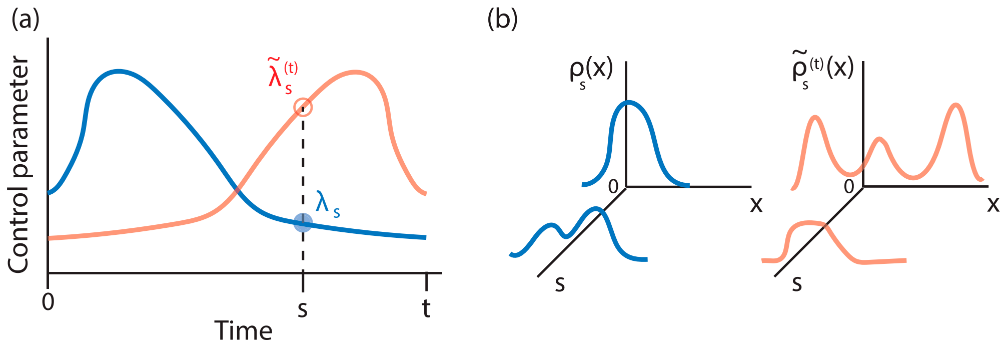

Figure 6.1. Panel (a): Illustration of a physical process through the evolution of a control parameter λ as a function of time (blue line) and of the backward, time-reversed protocol associated with the forward physical process (red line). We highlight the value of the forward (blue filled circle) and backward (red open circle) protocols at a time s smaller than the time t with respect which the time reversal is applied. Note that for $s \leq t$, the reversed protocol is defined as $\tilde{\lambda}_s = \lambda_{t-s}$, i.e., in general $\tilde{\lambda}_s \neq \lambda_s$. Panel (b) Left: Illustration of the time evolution of an initial probability density in the forward process. Right: Illustration of the evolution of an arbitrary probability density in the backward process.

reader in this journey through the almanac of probability ratios, we provide here a quick summary of the entropic functionals that we define later in this chapter:

- The Λ-stochastic entropic functionals involve the statistics of the physical process $\mathcal{P}(X_{[0,t]})$ and that of an arbitrary auxiliary process $\mathcal{Q}^{(t)}(X_{[0,t]})$, both evaluated over the trajectories of X. A physical example of a Λ-stochastic entropic functional is the housekeeping entropy production S_t^{hk}.
- The Σ-stochastic entropic functionals involve the statistics of the physical process $\mathcal{P}(X_{[0,t]})$ evaluated over $X_{[0,t]}$, and that of an arbitrary auxiliary process $\mathcal{Q}^{(t)}(\Theta_t(X_{[0,t]}))$ evaluated over the time-reversal $\Theta_t(X_{[0,t]})$ of $X_{[0,t]}$. Two physical examples of Σ-stochastic entropic functionals are the Σ^{tot}-stochastic entropic functional, which is a stochastic process proportional to the fluctuating work dissipated in an isothermal system, and the $\mathcal{Q}$-stochastic entropy production, which we discuss in the next bullet point.
- The $\mathcal{Q}$-stochastic entropy production is a Σ-stochastic entropic functional for which the initial distribution of auxiliary process $\mathcal{Q}^{(t)}$ equals the instantaneous density ρ_t of the process $X_{[0,t]}$. Physical examples of the $\mathcal{Q}$-stochastic entropy production are the total stochastic entropy production S_t^{tot} and the excess stochastic entropy production S_t^{ex}.
- The generalized Σ-stochastic entropic functionals have an analogous structure to the Σ-stochastic entropic functionals, except that they involve probability ratios over arbitrary intervals $[r, s] \subseteq [0, t]$. As we show in Chapter 9, the generalized Σ-stochastic entropic functionals yield a plethora of different formulations of the second law, some of which are well known, and Others that we derive in this treatise for the first time.

6.1.2. *Definitions of Σ- and Λ-stochastic entropic functionals*

Key quantities in stochastic thermodynamic quantities, such as work, heat, entropy, and energy, are formally functionals of stochastic trajectories. Here we introduce the Σ-stochastic and Λ-stochastic entropic functionals as two classes of functionals that involve two (different) path probabilities, generalizing the formulae (5.51), (5.52), and (5.99) of the previous chapter.

We define the Σ-**stochastic entropic functionals** and the Λ-**stochastic entropic functionals**, both associated with a generic stochastic process X_t, by

$$\Sigma_t^{\mathcal{P},\mathcal{Q}} \equiv \Sigma_t^{\mathcal{P},\mathcal{Q}}\left(X_{[0,t]}\right) \equiv \ln\left[\frac{\mathcal{P}\left(X_{[0,t]}\right)}{\mathcal{Q}^{(t)}\left(\Theta_t\left(X_{[0,t]}\right)\right)}\right] \tag{6.9}$$

and

$$\Lambda_t^{\mathcal{P},\mathcal{Q}} \equiv \Lambda^{\mathcal{P},\mathcal{Q}}\left(X_{[0,t]}\right) \equiv \ln\left[\frac{\mathcal{P}\left(X_{[0,t]}\right)}{\mathcal{Q}^{(t)}\left(X_{[0,t]}\right)}\right], \tag{6.10}$$

where $\mathcal{P}$ is the path probability describing the statistics of the physical process of interest, X_t, and $\mathcal{Q}^{(t)}$ is a sequence of path probabilities describing the statistics of auxiliary processes.

Now, we discuss a few key properties related to Σ-stochastic entropic and Λ-stochastic entropic functionals:

- The Σ-stochastic entropic functional is also known as the *action functional* [145,161].
- The role of the time index t in the superscript of $\mathcal{Q}^{(t)}$ is different from the one that appears in the subscript of $X_{[0,t]}$. Indeed, the t in the subindex $[0,t]$ of $X_{[0,t]}$ determines the time window over which the path probability $\mathcal{Q}$ is evaluated; $\mathcal{Q}(X_{[0,t]})$ is obtained through marginalization of $\mathcal{Q}(X_{[0,\infty)})$. On the other hand, the superindex (t) in $\mathcal{Q}^{(t)}$ indicates a supplementary dependency on time that represents a sequence of path probabilities. Note that the supplementary dependency on t is not related to nonstationarity or time-inhomogeneity of the process X, as both $\mathcal{P}$ and $\mathcal{Q}^{(t)}$ for fixed t can represent time-inhomogeneous processes. In stochastic thermodynamics, the supplementary dependence on t in $\mathcal{Q}^{(t)}$ originates from reversing the direction of time relative to time t. For example, in Markov processes $\mathcal{Q}^{(t)}$ represents often a time-reversed Markov process determined by a reversed protocol (6.6) $\tilde{\mathcal{L}}_s^{(t)} = \mathcal{L}_{t-s}$, which depends on the time-reversal reflection point t. For a first reading of this chapter, we advice to focus on the particular case of $\mathcal{Q}^{(t)} = \mathcal{Q}$. Note that it is unnatural to consider the analogous case $\mathcal{P}^{(t)}$, because $\mathcal{P}$ is the path probability of the physical process X, and hence there is no reason to have an additional dependency on t.
- The mathematical properties of $\Sigma_t^{\mathcal{P},\mathcal{Q}}$ and $\Lambda_t^{\mathcal{P},\mathcal{Q}}$ are similar (see below). Moreover, $\Sigma_t^{\mathcal{P},\mathcal{Q}}$ functionals can be written as $\Lambda_t^{\mathcal{P},\mathcal{Q}'}$ functionals (and reciprocally) by using a suitable choice for the path probability $\mathcal{Q}'$, which is called time reversal of $\mathcal{Q}$ in the probability theory literature [84,98,148].

  Therefore, it is natural to ask why there is a need to introduce the two entropic functionals Σ and Λ? The answer is *blowin' in the wind* of martingales: as we show in Section 6.2, $\exp(-\Lambda_t^{\mathcal{P},\mathcal{Q}})$ can be a martingale with respect to $\mathcal{P}$ even if $\mathcal{Q}$ is nonstationary, whereas $\exp(-\Sigma_t^{\mathcal{P},\mathcal{Q}})$ requires in general a stationary $\mathcal{Q}$ to be a martingale. An intuitive idea behind this result is that the sequence $\mathcal{Q}'^{(t)}$ that satisfies $\Sigma_t^{\mathcal{P},\mathcal{Q}} = \Lambda_t^{\mathcal{P},\mathcal{Q}'^{(t)}}$ depends in general explicitly on t, even when $\mathcal{Q}$ is a nonstationary path probability without explicit t-dependence.

- Let us illustrate the difference between the two t-dependencies in $\mathcal{Q}^{(t)}(X_{[0,t]})$ on the example of a Langevin process.[8] For a sequence of path probabilities $\mathcal{Q}^{(t)}$, the corresponding sequence $\mathscr{L}_s^{(t)}$ of Lagrangians reads, see Equation (3.94)

$$\mathscr{L}_s^{(t)}(X_s, \dot{X}_s) \equiv \frac{1}{4}\left(\dot{X}_s - \boldsymbol{\mu}_s^{(t)}(X_s)F_s^{(t)}(X_s)\right)\left(\mathbf{D}_s^{(t)}\right)^{-1}\left(\dot{X}_s - \boldsymbol{\mu}_s^{(t)}(X_s)F_s^{(t)}(X_s)\right) + \frac{1}{2}\nabla\cdot\left(\boldsymbol{\mu}_s^{(t)}F_s^{(t)}\right)(X_s). \tag{6.11}$$

We recall readers Equation (3.96) for the definition of Lagrangian L in this context. The corresponding actions defining $\mathcal{Q}^{(t)}$ are, see Equations (2.56)–(2.57)

$$\mathcal{A}^{(t)}(X_{[0,t]}) = -\ln(\rho_0(X_0)) + \int_0^t \mathrm{d}s L_s^{(t)}(X_s, \dot{X}_s). \tag{6.12}$$

Note that the explicit t-dependency of $\mathcal{Q}^{(t)}$, denoted by the superscript in $\mathcal{Q}^{(t)}$, is due to the second t-dependency in the mobility matrix $\boldsymbol{\mu}_s^{(t)}$, diffusion matrix $\mathbf{D}_s^{(t)}$, and total force $F_s^{(t)}$. Nevertheless, for each fixed value of t, the Lagrangian $\mathscr{L}_s^{(t)}$ describes time-inhomogeneous Langevin processes, as $\boldsymbol{\mu}_s^{(t)}$, $\mathbf{D}_s^{(t)}$, and $F_s^{(t)}$ depend explicitly on s.
- A key feature of Σ-stochastic entropic functionals (6.9) (resp., Λ-stochastic entropic functionals) is the duality relations

$$\Sigma_t^{\mathcal{P},\mathcal{Q}}\left(\Theta_t(X_{[0,t]})\right) = -\Sigma_t^{\mathcal{Q},\mathcal{P}}(X_{[0,t]}) \tag{6.13}$$

and

$$\Lambda^{\mathcal{P},\mathcal{Q}}\left(X_{[0,t]}\right) = -\Lambda^{\mathcal{Q},\mathcal{P}}(X_{[0,t]}). \tag{6.14}$$

In words, Σ changes sign under the simultaneous reversal of time and the exchange of the measures $P \leftrightarrow Q$, whereas Λ changes sign under exchange of the measures $P \leftrightarrow Q$.
- Unlike the entropy production of the macroscopic second law of thermodynamics, see Refs. [144,162], both the Σ-stochastic entropic functional $\Sigma_t^{\mathcal{P},\mathcal{Q}}$ and the Λ-stochastic entropic functional $\Lambda_t^{\mathcal{P},\mathcal{Q}}$ can take negative values. However, average values of entropic functionals are positive (see below).
- The existence of $\Sigma_t^{\mathcal{P},\mathcal{Q}}$ and $\Lambda_t^{\mathcal{P},\mathcal{Q}}$ requires that $\mathcal{P}$ is *absolutely continuous* with respect to $\mathcal{Q}^{(t)}\Theta_t$ and $\mathcal{Q}^{(t)}$, respectively (see Chapter 2 for a discussion of the continuous case). For example, in discrete space $\Sigma_t^{\mathcal{P},\mathcal{Q}}$ and $\Lambda_t^{\mathcal{P},\mathcal{Q}}$ are well defined if for all trajectories $X_{[0,t]}$ for which $\mathcal{Q}^{(t)}(\Theta_t(X_{[0,t]})) = 0$ or $\mathcal{Q}^{(t)}(X_{[0,t]}) = 0$ it holds that also $\mathcal{P}_{[0,t]}(X_{[0,t]}) = 0$. These conditions ensure that the Σ-stochastic entropic and Λ-stochastic entropic functionals, respectively, do not diverge when evaluated along a stochastic trajectory.
- In Section 6.3, we will introduce the *generalized* Σ-*stochastic entropic functionals*, which will provide martingales that lead to refinements of the second law of thermodynamics in Chapter 9.

The average values with respect to $\mathcal{P}$ of both the Σ-stochastic entropic and Λ-stochastic entropic functionals are Kullback–Leibler divergences, viz.,

$$\left\langle \Sigma_t^{\mathcal{P},\mathcal{Q}} \right\rangle = D_{\mathrm{KL}} \left[\mathcal{P}\left(X_{[0,t]}\right) || \mathcal{Q}^{(t)}\left(\Theta_t\left(X_{[0,t]}\right)\right)\right] \tag{6.15}$$

and

$$\left\langle \Lambda_t^{\mathcal{P},\mathcal{Q}} \right\rangle = D_{\mathrm{KL}} \left[\mathcal{P}\left(X_{[0,t]}\right) || \mathcal{Q}^{(t)}\left(X_{[0,t]}\right)\right]. \tag{6.16}$$

As $\mathcal{P}$, $\mathcal{Q}$, and $\mathcal{Q}^{(t)}\Theta_t$ are normalized path probabilities, the Kullback–Leibler divergences in the right-hand side of Equations (6.15)–(6.16) are greater or equal than zero, which imply the *"second laws"*

$$\left\langle \Sigma_t^{\mathcal{P},\mathcal{Q}} \right\rangle \geq 0 \quad \text{and} \quad \left\langle \Lambda_t^{\mathcal{P},\mathcal{Q}} \right\rangle \geq 0. \tag{6.17}$$

6.1.3. *Fluctuation relations for stochastic entropic functionals*

Fluctuation relations follow readily from the definitions (6.9) and (6.10), as can be seen from the following central equations:

The **"mother" fluctuation relations** for an arbitrary functional $Z(X_{[0,t]})$ read [138]

$$\left\langle Z\left(\Theta_t(X_{[0,t]})\right)\right\rangle_{\mathcal{Q}^{(t)}} = \left\langle \exp\left(-\Sigma_t^{\mathcal{P},\mathcal{Q}}\right) Z\left(X_{[0,t]}\right)\right\rangle \tag{6.18}$$

and

$$\left\langle Z\left(X_{[0,t]}\right)\right\rangle_{\mathcal{Q}^{(t)}} = \left\langle \exp\left(-\Lambda_t^{\mathcal{P},\mathcal{Q}}\right) Z\left(X_{[0,t]}\right)\right\rangle. \tag{6.19}$$

Notably, Equations (6.18)–(6.19) hold for any functional Z and any pair $\mathcal{P}$ and $\mathcal{Q}^{(t)}$ of absolutely continuous path probabilities.

Setting $Z(X_{[0,t]}) = \delta(\Sigma_t^{\mathcal{P},\mathcal{Q}} - \sigma)$ and $Z(X_{[0,t]}) = \delta(\Lambda_t^{\mathcal{P},\mathcal{Q}} - \lambda)$ in the first and second lines of Equations (6.19), respectively, and using the duality relations (6.13)–(6.14), we obtain the following *generalized Crooks fluctuation relations* [163]:

$$\left\langle \delta(\Sigma_t^{\mathcal{Q},\mathcal{P}} + \sigma)\right\rangle_{\mathcal{Q}^{(t)}} = \exp(-\sigma)\left\langle \delta(\Sigma_t^{\mathcal{P},\mathcal{Q}} - \sigma)\right\rangle \tag{6.20}$$

and

$$\left\langle \delta(\Lambda_t^{\mathcal{P},\mathcal{Q}} - \lambda)\right\rangle_{\mathcal{Q}^{(t)}} = \exp(-\lambda)\left\langle \delta(\Lambda_t^{\mathcal{P},\mathcal{Q}} - \lambda)\right\rangle. \tag{6.21}$$

Using Equation (6.14), one can rewrite Equation (6.21) as

$$\left\langle \delta(\Lambda_t^{\mathcal{Q},\mathcal{P}} + \lambda)\right\rangle_{\mathcal{Q}^{(t)}} = \exp(-\lambda)\left\langle \delta(\Lambda_t^{\mathcal{P},\mathcal{Q}} - \lambda)\right\rangle. \tag{6.22}$$

Equations (6.20) and (6.22) can also be written as

$$\frac{\rho^{\mathcal{P}}_{\Sigma_t^{\mathcal{P},\mathcal{Q}}}(\sigma)}{\rho^{\mathcal{Q}^{(t)}}_{\Sigma_t^{\mathcal{Q},\mathcal{P}}}(-\sigma)} = \exp(\sigma), \quad \text{and} \quad \frac{\rho^{\mathcal{P}}_{\Lambda_t^{\mathcal{P},\mathcal{Q}}}(\lambda)}{\rho^{\mathcal{Q}^{(t)}}_{\Lambda_t^{\mathcal{Q},\mathcal{P}}}(-\lambda)} = \exp(\lambda). \tag{6.23}$$

In the first relation of Equation (6.23), the numerator (denominator) denotes the probability density of $\Sigma_t^{\mathcal{P},\mathcal{Q}}$ ($\Sigma_t^{\mathcal{Q},\mathcal{P}}$) under the probability law $\mathcal{P}$ ($\mathcal{Q}^{(t)}$), and analogously for the Λ-stochastic entropic functional in the second equation. For the choice $Z(X_{[0,t]}) = 1$, Equation (6.19) become the *generalized integral fluctuation relations* given by

$$\left\langle \exp\left(-\Sigma_t^{\mathcal{P},\mathcal{Q}}\right)\right\rangle = 1 \quad \text{and} \quad \left\langle \exp\left(-\Lambda_t^{\mathcal{P},\mathcal{Q}}\right)\right\rangle = 1. \tag{6.24}$$

Note that the generalized integral fluctuation relations hold for any (normalized) path probability $\mathcal{Q}^{(t)}$ that is absolutely continuous with respect to $\mathcal{P}$.

In the following, by considering specific choices for the path probability $\mathcal{Q}^{(t)}$ of the auxiliary process, we discuss examples of Σ-stochastic entropic functionals and Λ-stochastic entropic functionals that are relevant for physics.

6.1.4. *$\mathcal{Q}$-stochastic entropy production*

We review the $\mathcal{Q}$-stochastic entropy production, which is a Σ-stochastic entropic functional for a specific choice of $\mathcal{Q}^{(t)}$ that is widely used in stochastic thermodynamics [26,138,145,164,165]. In particular, we assume that

$$\rho_0^{\mathcal{Q}^{(t)}}(x) \equiv \langle \delta(X_0 - x)\rangle_{\mathcal{Q}^{(t)}} = \langle \delta(X_t - x)\rangle \equiv \rho_t(x), \tag{6.25}$$

where $\rho_t(x)$ is the probability density of X_t under its native dynamics, determined by $\mathcal{P}$.

When specializing the Σ-stochastic entropic functional (6.9) to $\mathcal{Q}^{(t)}$ that satisfy Equation (6.25), we obtain the so-called **$\mathcal{Q}$-stochastic entropy production**, which we denote by $S_t^{\mathcal{P},\mathcal{Q}}$ [26,138,145,164,165]

$$S_t^{\mathcal{P},\mathcal{Q}} \equiv \Sigma_t^{\mathcal{P},\mathcal{Q}} = \ln\left(\frac{\mathcal{P}\left(X_{[0,t]}\right)}{\mathcal{Q}^{(t)}\left(\Theta_t(X_{[0,t]})\right)}\right), \quad t \in \mathbb{R}^+. \tag{6.26}$$

Using Bayes' law, the $\mathcal{Q}$-stochastic entropy production (6.26) can be split into two parts, namely, a system entropy change $\Delta S_t^{\rm sys}$ and an environmental $\mathcal{Q}$-stochastic entropy change $S_t^{{\rm env},\mathcal{P},\mathcal{Q}}$, viz.,

$$S_t^{\mathcal{P},\mathcal{Q}} = \underbrace{\ln\left(\frac{\rho_0(X_0)}{\rho_t(X_t)}\right)}_{\Delta S_t^{\rm sys}} + \underbrace{\ln\left(\frac{\mathcal{P}\left(X_{[0,t]}\,|\,X_0\right)}{\mathcal{Q}^{(t)}\left(\Theta_t(X_{[0,t]})\,|\,X_t\right)}\right)}_{\equiv S_t^{{\rm env},\mathcal{P},\mathcal{Q}}}, \tag{6.27}$$

where for consistency with Equation (5.51), we have omitted the superscript $\mathcal{P}$ in the system entropy $\rho_t^{\mathcal{P}}$, and where the conditioning in the numerator and the denominator of the environment entropy change is on the respective initial state. More generally, we have for a Σ-stochastic entropic functional

$$\Sigma_t^{\mathcal{Q},\mathcal{P}} = \ln\left(\frac{\rho_0(X_0)}{\rho_0^{\mathcal{Q}^{(t)}}(X_t)}\right) + \underbrace{\ln\left(\frac{\mathcal{P}\left(X_{[0,t]}\,|\,X_0\right)}{\mathcal{Q}^{(t)}\left(\Theta_t\left(X_{[0,t]}\right)\,|\,X_t\right)}\right)}_{\equiv S_t^{\mathrm{env},\mathcal{P},\mathcal{Q}}}, \tag{6.28}$$

where the conditioning in the numerator and the denominator is again initial conditioning.

The decomposition (6.27) is one of the cornerstones of stochastic thermodynamics; it is the fluctuating version of the second law for open systems

$$\langle S_t^{\mathcal{P},\mathcal{Q}}\rangle = \langle \Delta S_t^{\mathrm{sys}}\rangle + \langle S_t^{\mathrm{env},\mathcal{P},\mathcal{Q}}\rangle \geq 0, \tag{6.29}$$

which was introduced for a specific choice of $\mathcal{Q}$ by Prigogine et al. in the 1950s [166,167]. Of course, we should keep in mind that the appropriate choice of $\mathcal{Q}^{(t)}$ leading to an environment entropy change $S_t^{\mathrm{env},\mathcal{P},\mathcal{Q}}$ with physical content depends on the physical context.

The choice of the initial density $\rho_0^{\mathcal{Q}^{(t)}} = \rho_t$ in (6.26) is not arbitrary. In particular, this choice of $\rho_0^{\mathcal{Q}^{(t)}}$ minimizes the average value of $\Sigma_t^{\mathcal{P},\mathcal{Q}}$. Indeed, taking the average of the difference between Equations (6.28) and (6.9) we obtain

$$\langle \Sigma_t^{\mathcal{P},\mathcal{Q}}\rangle - \langle S_t^{\mathcal{P},\mathcal{Q}}\rangle = \int \mathrm{d}x \rho_t(x) \ln \frac{\rho_t(x)}{\rho_0^{\mathcal{Q}^{(t)}}(x)} = D_{\mathrm{KL}}[\rho_t(x)||\rho_0^{\mathcal{Q}^{(t)}}(x)] \geq 0. \tag{6.30}$$

This result justifies the name "$\mathcal{Q}$-entropy production", as the Σ-entropic functional contains an additional cost resulting from the initial density of the auxiliary process, while for the $\mathcal{Q}$-entropy production the cost from the initial state vanishes on average, and hence the average "$\mathcal{Q}$-entropy production" is determined by the dynamics described by $\mathcal{Q}$.

In the following, we show that for specific choices of $\mathcal{Q}$, the Σ-entropic functional $\Sigma_{[0,t]}^{\mathcal{P},\mathcal{Q}}$, the $\mathcal{Q}$-entropy production $S_t^{\mathcal{P},\mathcal{Q}}$, and the environmental $\mathcal{Q}$-stochastic entropy change $S_t^{\mathrm{env},\mathcal{P},\mathcal{Q}}$ identify with usual quantities which are commonly introduced in stochastic thermodynamics. We refer to Refs. [10,91,96,138,168] for other interesting choices of $\mathcal{Q}$, such as those leading to universal fluctuations relations for phase-space contraction and/or multiplicative fluctuation relations for the finite-time Lyapunov exponents.

6.1.5. *Total Σ-stochastic entropic functionals and stochastic entropy production for Markovian processes*

We define the total Σ-stochastic entropic functional Σ_t^{tot} as the Σ-stochastic entropic functional, given in (6.9), specialized to the following choices of $\mathcal{P}$ and $\mathcal{Q}$:

- The statistics $\mathcal{P}$ of the physical process X are generated by a generic, Markovian, non-equilibrium process with Markov generator $\mathcal{L}$.
- The statistics $\mathcal{Q}^{(t)}$ of the auxiliary process are determined by the time-reversed Markov process defined in (6.6).

The **total Σ-stochastic entropic** functional (6.9) is defined by

$$\Sigma_t^{\text{tot}} \equiv \Sigma_t^{\mathcal{P},\tilde{\mathcal{P}}^{(t)}} = \ln\left(\frac{\mathcal{P}(X_{[0,t]})}{\tilde{\mathcal{P}}^{(t)}(\Theta_t(X_{[0,t]}))}\right). \tag{6.31}$$

Following analogous steps as in Section 6.1.4, we can split Σ_t^{tot} into a system and an environment entropy changes during the time interval $[0,t]$, see also Equation (6.28),

$$\Sigma_t^{\text{tot}} = \ln\left(\frac{\rho_0(X_0)}{\tilde{\rho}_0^{(t)}(X_t)}\right) + \underbrace{\ln\left(\frac{\mathcal{P}\left(X_{[0,t]}\,|\,X_0\right)}{\tilde{\mathcal{P}}^{(t)}\left(\Theta_t\left(X_{[0,t]}\right)\,|X_t\right)}\right)}_{\equiv S_t^{\text{env}}}. \tag{6.32}$$

The second term in the right-hand side of (6.32) is the so-called *stochastic environmental entropy flow*, which has a similar structure as the environmental entropy change S_t^{env} given in (5.51). The first term in (6.32) is a generalized system entropy change, which involves the initial density of the physical process and the probability density $\tilde{\rho}_0^{(t)}(X_t)$, which is the initial density of the auxiliary process evaluated at final state of the trajectory $X_{[0,t]}$.

If $\tilde{\rho}_0^{(t)} = \rho_t$ in Equation (6.32), then Σ_t^{tot} is also called the **stochastic entropy production**, denoted by S_t^{tot}, i.e.,

$$S_t^{\text{tot}} \equiv \underbrace{\ln\left(\frac{\rho_0(X_0)}{\rho_t(X_t)}\right)}_{\Delta S_t^{\text{sys}}} + \underbrace{\ln\left(\frac{\mathcal{P}\left(X_{[0,t]}\,|\,X_0\right)}{\tilde{\mathcal{P}}^{(t)}\left(\Theta_t\left(X_{[0,t]}\right)\,|\,X_t\right)}\right)}_{S_t^{\text{env}}}. \tag{6.33}$$

In Chapter 5, we have studied S^{tot} for one-dimensional Langevin processes and Markov jump processes. In Sections 6.1.5.1 and 6.1.5.2, we provide for illustrative purposes explicit expressions of Σ_t^{tot} and S_t^{tot} for Markov jump processes and diffusion processes in arbitrary dimensions.

6.1.5.1. *Markov-jump processes.* For a Markov jump process defined by time-dependent, transition rates $\omega_t(x,y)$ for all $x,y \in \mathcal{X}$ (see Section 3.2.2), the total Σ-stochastic entropic functional (6.32) is given by

$$\Sigma_t^{\text{tot}} = \ln\left(\frac{\rho_0(X_0)}{\tilde{\rho}_0^{(t)}(X_t)}\right) + \sum_{j=1}^{N_t} \ln\left[\frac{\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}{\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}, X_{\mathcal{T}_j^-})}\right], \tag{6.34}$$

where $\mathcal{T}_j$ in the right-hand side are the times when X jumps between different states, with $0 \leq \mathcal{T}_1 \leq \mathcal{T}_2 \leq \cdots \mathcal{T}_{N_t} \leq t$, and N_t is the total number of jumps in the trajectory $X_{[0,t]}$. Note that it is also possible to write analogous explicit expressions for the general Markovian $\mathcal{Q}$ in Σ-stochastic entropic functionals, given in (6.9), and the Λ-stochastic entropic functionals, given in (6.10), associated to such pure jump processes.

Note that Σ_t^{tot} in (6.34) exists if the so-called *microreversibilty* condition holds, viz., for all $x, y \in \mathcal{X}$, $\omega_t(x,y) > 0$ implies $\omega_t(y,x) > 0$; these conditions are equivalent to the assumed absolute continuity between $\mathcal{P}$ and $\tilde{\mathcal{P}}\Theta_t$.

For a microreversible Markov jump process, the total stochastic entropy production S_t^{tot} (6.33) is given by

$$S_t^{\text{tot}} = \underbrace{\ln\left(\frac{\rho_0(X_0)}{\rho_t(X_t)}\right)}_{\Delta S_t^{\text{sys}}} + \underbrace{\sum_{j=1}^{N_t} \ln\left[\frac{\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}{\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}, X_{\mathcal{T}_j^-})}\right]}_{S_t^{\text{env}}}, \tag{6.35}$$

where we decomposed S_t^{tot} in terms of system entropy change ΔS_t^{sys} and the environment entropy change S_t^{env}. Rewriting the first term in Equation (6.35), S_t^{tot} can be expressed in its alternative form (5.89)

$$S_t^{\text{tot}} = -\int_0^t \mathrm{d}s (\partial_s \ln \rho_s)(X_s) + \sum_{j=1}^{N_t} \ln\left[\frac{\rho_{\mathcal{T}_j}(X_{\mathcal{T}_j^-})\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}{\rho_{\mathcal{T}_j}(X_{\tau_j^+})\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}, X_{\mathcal{T}_j^-})}\right], \tag{6.36}$$

For a system in equilibrium, $S_t^{\text{tot}} = 0$, as $\rho_s = \rho_{st}$ is independent of time and the detailed balance relation $\rho_{\text{st}}(x)\omega_s(x,y) = \rho_{\text{st}}(y)\omega_s(y,x)$ holds for all $x, y \in \mathcal{X}$ and $s \geq 0$. On the other hand, for a nonequilibrium system the average total entropy production reads (see also Equations 5.90 and 5.91)

$$\langle S_t^{\text{tot}} \rangle = \int_0^t \mathrm{d}s \int_{\mathcal{X}} \mathrm{d}x \int_{\mathcal{X}} \mathrm{d}y \rho_s(x)\omega_s(x,y) \ln\left[\frac{\rho_s(x)\omega_s(x,y)}{\rho_s(y)\omega_s(y,x)}\right] \tag{6.37}$$

$$= \frac{1}{2}\int_0^t \mathrm{d}s \int_{\mathcal{X}} \mathrm{d}x \int_{\mathcal{X}} \mathrm{d}y J_{s,\rho}(x,y) \ln\left[\frac{\rho_s(x)\omega_s(x,y)}{\rho_s(y)\omega_s(y,x)}\right], \tag{6.38}$$

where in the second equality we have used the definition of the instantaneous probability current $J_{s,\rho}(x,y) = \rho_s(x)\omega_s(x,y) - \rho_s(y)\omega_s(y,x)$, with $s \in [0,t]$. Equation (6.38) is the celebrated Schnakenberg formula for the entropy production of Markovian systems [83], which was derived two decades before the origins of stochastic thermodynamics.

6.1.5.2. *Multidimensional overdamped Langevin processes.* We consider a multidimensional Langevin process described in Equation (3.65), and which we rewrite here for convenience,

$$\dot{X}_t = (\boldsymbol{\mu}_t F_t)(X_t) + (\nabla \mathbf{D}_t)(X_t) + \sqrt{2\mathbf{D}_t(X_t)}\dot{B}_t. \tag{6.39}$$

Recall that $F_t(x) = -\nabla V_t(x) + f_t(x)$ is a generic force which has a conservative part $-\nabla V_t(x)$ and a non-conservative $f_t(x)$ part, and both contributions can depend explicitly on time, see Equation (3.66).

The total Σ-stochastic entropic functionals associated with trajectories generated by the overdamped Langevin equation (6.39) are given by [138,161]

$$\Sigma_t^{\text{tot}} = \ln\left(\frac{\rho_0(X_0)}{\tilde{\rho}_0^{(t)}(X_t)}\right) + \underbrace{\int_0^t \left((\boldsymbol{\mu}_s F_s)\,\mathbf{D}_s^{-1}\right)(X_s) \circ \dot{X}_s \,\mathrm{d}s}_{S_t^{\text{env}}}. \tag{6.40}$$

Here, $\mathbf{D}_t$ needs to be invertible, which implies that this result does not hold for underdamped Langevin equations. Note that it is possible to write analogous explicit expressions for the general Σ-stochastic entropic functional (6.9) associated to Markovian $\mathcal{Q}$ and Λ-stochastic entropic functional (6.10) associated to multidimensional Langevin equations [138].

The total stochastic entropy production of a multidimensional Langevin process is given by

$$S_t^{\rm tot} = \underbrace{\ln\left(\frac{\rho_0(X_0)}{\rho_t(X_t)}\right)}_{\Delta S_t^{\rm sys}} + \underbrace{\int_0^t \left(\left(\boldsymbol{\mu}_s F_s\right)\mathbf{D}_s^{-1}\right)(X_s)\circ \dot{X}_s\,\mathrm{d}s}_{S_t^{\rm env}}\,. \tag{6.41}$$

Using the definition of the probability current equation (3.64)

$$J_{t,\rho}(x) \equiv \left(\left(\boldsymbol{\mu}_t F_t\right)\rho_t\right)(x) - (\mathbf{D}_t\nabla\rho_t)(x), \tag{6.42}$$

and using the Stratonovich (i.e., standard) rules of calculus, we can rewrite Equation (6.41) as

$$S_t^{\rm tot} = -\int_0^t (\partial_s \ln\rho_s)(X_s)\,\mathrm{d}s + \int_0^t (J_{s,\rho}\,(\rho_s\mathbf{D}_s)^{-1})(X_s)\circ\dot{X}_s\,\mathrm{d}s, \tag{6.43}$$

which generalizes Equation (5.20) to the multidimensional case. To pass from Equations (6.41) – (6.43) we used the relation

$$\ln\left(\frac{\rho_0\,(X_0)}{\rho_t\,(X_t)}\right) = -\int_0^t \mathrm{d}\,(\ln(\rho_s\,(X_s))) = -\int_0^t \left((\partial_s\ln\rho_s)\,(X_s)\,\,\mathrm{d}s + (\nabla\ln\rho_s)\,(X_s)\circ\dot{X}_s\,\mathrm{d}s\right). \tag{6.44}$$

For equilibrium processes, the total stochastic entropy production vanishes, even at the stochastic level. This is because equilibrium dynamics satisfy $\rho_t = \rho_{\rm st}$ and the "detailed balance" condition $J_{s,\rho_{\rm st}} = 0$, and hence the two terms in (6.43) vanish. On the other hand, for nonequilibrium processes $S_t^{\rm tot}$ can take any value (positive or negative), yet its average is positive. Indeed, the average total stochastic entropy production is a quadratic form of the probability current, viz.,

$$\langle S_t^{\rm tot}\rangle = \int_0^t \mathrm{d}s\int_{\mathcal{X}} \mathrm{d}x\left(J_{s,\rho}\,(\rho_s\mathbf{D}_s)^{-1}\,J_{s,\rho}\right)(x) \geq 0, \tag{6.45}$$

and the positivity follows from $(J_{s,\rho}(\rho_s\mathbf{D}_s)^{-1}J_{s,\rho}))(x) \geq 0$ for all values of $x \in \mathcal{X}$; we refer to Section 6.1.5.4 for a derivation of Equation (6.45).

6.1.5.3. *Overdamped isothermal Langevin equation.* Consider now the Langevin dynamics described in Equation (6.39) with the Einstein relation (3.69) fulfilled, i.e., $\mathbf{D}_t(x) = T\boldsymbol{\mu}_t(x)$, with $\boldsymbol{\mu}_t(x)$ a symmetric mobility matrix. We call this the *overdamped isothermal Langevin equation*. For overdamped isothermal Langevin processes, the stochastic environmental entropy change (6.41) is given by

$$S_t^{\rm env} = \frac{1}{T}\int_0^t F_s(X_s)\circ\dot{X}_s\,\mathrm{d}s = -\frac{Q_t}{T}, \tag{6.46}$$

where in the second equality we have used the relation (5.11) for the stochastic heat absorbed by the system. Equation (6.46) shows that the Clausius relation between environmental entropy change and heat also holds for isothermal multidimensional Langevin system.

Now, we explicit $\Sigma_t^{\rm tot}$ in an important physical example. Suppose that the potential V is determined by a deterministic protocol λ_s $(s \in [0,t])$, and that the system is initially described by an equilibrium ensemble with initial density

$$\rho_0(x) = \exp\left(-\frac{(V_0(x) - G_0^{\mathrm{eq}})}{T}\right), \tag{6.47}$$

where

$$G_t^{\mathrm{eq}} \equiv -T\ln\left(\int_{\mathcal{X}} \mathrm{d}x \exp\left(-\frac{V_t(x)}{T}\right)\right), \tag{6.48}$$

is the equilibrium free energy at time $t \geq 0$. Note that if an external force is present, $\rho_0(x)$ is not a steady state, even if the potential is constant. Consider now as auxiliary reference process with initial density equal to

$$\rho_0^{\mathcal{Q}}(x) = \exp\left(-\frac{(V_t(x) - G_t^{\mathrm{eq}})}{T}\right), \tag{6.49}$$

which coincides with the stationary equilibrium distribution that the system may have if the driving is stopped at time t (i.e., for $s \geq t$ we have $f_s = 0$ and $V_s = V_t$). Moreover, we assume that the driving of the auxiliary process is the "time-reversal" $\lambda_s^{\mathcal{Q}} = \lambda_{t-s}$ for $s \in [0, t]$. The associated Σ^{tot}-entropic functional given in Equation (6.40) reads

$$\begin{aligned}\Sigma_t^{\mathrm{tot}} &= \frac{V_t(X_t) - V_0(X_0) + G_0^{\mathrm{eq}} - G_t^{\mathrm{eq}} + \int_0^t F_s(X_s) \circ \dot{X}_s\,\mathrm{d}s}{T},\\ &= \frac{G_0^{\mathrm{eq}} - G_t^{\mathrm{eq}} + \int_0^t \left(f_s(X_s) \circ \dot{X}_s\,\mathrm{d}s + (\partial_s V_s)(X_s)\,\mathrm{d}s\right)}{T},\end{aligned} \tag{6.50}$$

where in the second equality we used the Stratonovich (i.e., standard) rules of calculus and Equation (3.66) for the total force $F_s(X_s) = -\partial_x V_s(X_s) + f_s(X_s)$ for this particular dynamics. As shown below, Equation (6.50) together with the martingale properties of Σ_t^{tot} allows us to derive the celebrated Jarzynski's equality [169] and Crooks' fluctuation relation [163] involving the fluctuating work done and the equilibrium free energy changes in driven overdamped isothermal systems.

For isothermal overdamped Langevin systems that are driven away by a time-dependent deterministic protocol from an initial, thermal state (6.47), Equation (6.50) relates Σ_t^{tot} to the fluctuating work done on the system and to the equilibrium free energy change in the interval $[0, t]$, viz.,

$$\Sigma_t^{\mathrm{tot}} = \frac{W_t - (G_t^{\mathrm{eq}} - G_0^{\mathrm{eq}})}{T}. \tag{6.51}$$

Equation (6.51) follows from identifying the integral in the right-hand side of Equation (6.50) as the stochastic work exerted on the system, see Equation (5.5) for the expression of the stochastic work W_t for the one-dimensional case. Here, we have also used that G_t^{eq} is the **equilibrium free energy** defined in (6.48). Specializing the integral fluctuation relation for Σ-entropic functionals (6.120) to the choice (6.51), we obtain **Jarzynki's**

equality [169]

$$\left\langle \exp\left(-\frac{W_t}{T}\right)\right\rangle = \exp\left(-\frac{(G_t^{\rm eq} - G_0^{\rm eq})}{T}\right). \tag{6.52}$$

We remark that the average in the left-hand side in Equation (6.52) is done over all trajectories starting from the initial canonical distribution given in Equation (6.47).

We note that the relation (6.51) can also be derived from the expression (6.34) for $\Sigma^{\rm tot}$ associated with isothermal Markov-jump processes (3.58). Moreover, for general underdamped isothermal Langevin systems (5.2), the stochastic work exerted on the system on the time interval $[0, t]$ can still be related to a Σ-entropic functional, see relations (7.16)–(7.17) in [138].

6.1.5.4. *Martingale structure of the stochastic entropy production for Langevin processes.* Now, we study in more detail the martingale structure of $\exp(-S_t^{\rm tot})$ for multidimensional Langevin equations.

The explicit expression for $S_t^{\rm tot}$, given in Equation (6.43) in the Stratonovich form, can be rewritten as follows in the Itô form,

$$\begin{aligned} S_t^{\rm tot} = &- \int_0^t {\rm d}s\, (\partial_s \ln \rho_s)\,(X_s) + \int_0^t (J_{s,\rho}\,(\rho_s \mathbf{D}_s)^{-1})(X_s)\dot{X}_s\, {\rm d}s \\ &+ \int_0^t {\rm d}s \left[\mathbf{D}_s \nabla \left(J_{s,\rho}\,(\rho_s \mathbf{D}_s)^{-1}\right)\right](X_s). \end{aligned} \tag{6.53}$$

The conversion of $S^{\rm tot}$ from Stratonovich (Equation 6.43) to Itô (Equation 6.53) follows from Equation (3.72), copied here for convenience

$$\int_0^t g_s(X_s) \circ \dot{X}_s\, {\rm d}s = \int_0^t g_s(X_s)\dot{X}_s\, {\rm d}s + \int_0^t \mathbf{D}_s(X_s)\,[(\nabla g_s)\,(X_s)]\, {\rm d}s,$$

which is valid for any function $g_t(x)$ that is smooth on t and x. Plugging the Langevin equation (6.39) in Equation (6.53), we obtain

$$\begin{aligned} S_t^{\rm tot} = &\int_0^t \left[-(\partial_s \ln \rho_s) + \mathbf{D}_s \nabla\left(J_{s,\rho}\,(\rho_s \mathbf{D}_s)^{-1}\right) + J_{s,\rho}\,(\rho_s \mathbf{D}_s)^{-1}\,\boldsymbol{\mu}_s F_s\right](X_s)\, {\rm d}s \\ &+ \int_0^t \left[J_{s,\rho}\,(\rho_s \mathbf{D}_s)^{-1}\,(\nabla \mathbf{D}_s)\right](X_s)\, {\rm d}s + \int_0^t \left[J_{s,\rho}\,(\rho_s \mathbf{D}_s)^{-1}\sqrt{2\mathbf{D}_s}\right](X_s)\dot{B}_s\, {\rm d}s. \end{aligned}$$

Expanding the second term of the first line, and simplifying some terms, we find

$$\begin{aligned} S_t^{\rm tot} = &\int_0^t \left[\left(-(\partial_s \ln \rho_s) + \frac{\nabla J_{s,\rho}}{\rho_s} - \frac{J_{s,\rho} \nabla \rho_s}{\rho_s^2} + J_{s,\rho}\,(\rho_s \mathbf{D}_s)^{-1}\,\boldsymbol{\mu}_s F_s\right)(X_s)\right] {\rm d}s \\ &+ \int_0^t \left[(J_{s,\rho}\,(\rho_s \mathbf{D}_s)^{-1}\sqrt{2\mathbf{D}_s})(X_s)\dot{B}_s\right] {\rm d}s. \end{aligned} \tag{6.54}$$

Lastly, using the Fokker–Planck equation (3.63), and the definition of the probability current (3.68), we get

$$S_t^{\text{tot}} = \int_0^t \left[\left(-2\left(\partial_s \left(\ln \rho_s\right)\right) + \frac{J_{s,\rho}\mathbf{D}_s^{-1}J_{s,\rho}}{(\rho_s)^2} \right)(X_s) + J_{s,\rho}(X_s)\left(\rho_s\mathbf{D}_s\right)^{-1}(X_s)\sqrt{2\mathbf{D}_s(X_s)}\dot{B}_s \right] \mathrm{d}s. \tag{6.55}$$

Taking the average of Equation (6.55) over the Brownian noise yields the second law equation (6.45). In addition, Equation (6.55) together with the rules of Itô calculus allows us to uncover the martingale structure of $\exp(-S_t^{\text{tot}})$.

Itô stochastic differential equation for stochastic entropy production in multidimensional Langevin processes and martingality. Deriving Equation (6.55) with respect to time we get

$$\dot{S}_t^{\text{tot}} = \left[-2\partial_t \ln \rho_t + \frac{J_{t,\rho}\mathbf{D}_t^{-1}J_{t,\rho}}{(\rho_t)^2} \right](X_t) + \left(\sqrt{2}\frac{J_{t,\rho}}{\rho_t}\mathbf{D}_t^{-1/2} \right)(X_t)\,\dot{B}_t. \tag{6.56}$$

We can define a new scalar white noise $\dot{B}_t^S$, with zero mean $\langle \dot{B}_t^S \rangle = 0$ and autocorrelation $\langle \dot{B}_t^S \dot{B}_s^S \rangle = \delta(t-s)$, such that Equation (6.56) takes the form

$$\dot{S}_t^{\text{tot}} = -2\left(\partial_t \ln \rho_t\right)(X_t) + \underbrace{\left(\frac{J_{t,\rho}\mathbf{D}_t^{-1}J_{t,\rho}}{(\rho_t)^2} \right)(X_t)}_{\equiv v_t^S(X_t)} + \underbrace{\sqrt{\left(2\frac{J_{t,\rho}\mathbf{D}_t^{-1}J_{t,\rho}}{(\rho_t)^2} \right)(X_t)}}_{\equiv\sqrt{2v_t^S(X_t)}}\,\dot{B}_t^S. \tag{6.57}$$

Averaging over many realizations, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle S_t^{\text{tot}} \rangle = \int_{\mathcal{X}} \mathrm{d}x \left(J_{s,\rho}\left(\rho_s\mathbf{D}_s\right)^{-1} J_{s,\rho} \right)(x) \geq 0, \tag{6.58}$$

which is equivalent to Equation (6.45).

Equation (6.57) has an analogous structure to the unidimensional case (5.42), but with an entropic drift

$$v_t^S(x) = \left(\frac{J_{t,\rho}\mathbf{D}_t^{-1}J_{t,\rho}}{\rho_t^2} \right)(x). \tag{6.59}$$

Applying the multidimensional Itô formula, see Appendix (B.3.2), to the change of variable $S_t^{\text{tot}} \to \exp(-S_t^{\text{tot}})$, we obtain from (6.56) the stochastic differential equation

$$\frac{d\exp(-S_t^{\text{tot}})}{\mathrm{d}t} = -2\exp(-S_t^{\text{tot}})\left(\partial_t \ln \rho_t\right)(X_t) - \exp(-S_t^{\text{tot}})\left(\sqrt{2}\frac{J_{t,\rho}}{\rho_t}\mathbf{D}_t^{-1/2} \right)(X_t)\,\dot{B}_t. \tag{6.60}$$

Note that this is not a closed set of stochastic differential equations because it is not autonomous in $\exp(-S_t^{\rm tot})$, but the joint process $(X_t, \exp(-S_t^{\rm tot}))$ admits a closed set of stochastic differential equations. Equations (6.57) and (6.60) extend Equations (5.42) and (5.44) to the multidimensional context and with space–time inhomogeneous mobility.

Because of the presence of a non-vanishing drift in Equation (6.60), $\exp(-S_t^{\rm tot})$ **is not a martingale in general**. Instead, $\exp(-S_t^{\rm tot})$ is a martingale **if and only if** $\partial_t \rho_t = 0$, i.e., in a stationary state (which can be an equilibrium state or nonequilibrium steady state). Thus for time-homogeneous nonequilibrium stationary processes, the exponentiated, negative, total entropy production is an exponential martingale and the martingale fluctuation relation

$$\langle \exp(-S_t^{\rm tot}) \,|\, X_{[0,s]} \rangle = \exp(-S_s^{\rm tot}) \tag{6.61}$$

holds, which implies a conditional second law (submartingale property) for the total entropy production in steady state

$$\langle S_t^{\rm tot} \,|\, X_{[0,s]} \rangle \geq S_s^{\rm tot}, \tag{6.62}$$

for any $0 \leq s \leq t$.

In Section 6.2, we will come back to this martingale properties in more fundamental way, and for a more generic setup that includes also other entropic functionals and jump processes.

6.1.6. ♠*Excess and housekeeping entropy production for Markovian processes*

Now, we review the notions of excess and housekeeping entropy production as introduced by Oono and Paniconi [150] and further explored in Refs. [138,151,152,164,170,171] in the context of fluctuation relations within stochastic thermodynamics. We choose here to keep the original terminology used by Oono and Paniconi [150] for isothermal Markovian processes despite the setup that we consider is more general. We also note that a popular alternative terminology was introduced by Esposito and Van den Broeck [152,171], where they substitute the word "excess" by "non-adiabatic" and the word "housekeeping" by "adiabatic" in the context of non-isothermal environments.

For a nonequilibrium Markovian stochastic process X_t with arbitrary Markovian generator $\mathcal{L}_t$, the fluctuating total entropy production $S_t^{\rm tot}$ given in Equation (6.33) can be decomposed as the sum of two terms:

$$S_t^{\rm tot} = S_t^{\rm ex} + S_t^{\rm hk}, \tag{6.63}$$

where $S_t^{\rm ex}$ and $S_t^{\rm hk}$ are respectively the so-called excess stochastic entropy production and housekeeping stochastic entropy production which are defined below.

The **excess stochastic entropy production** $S_t^{\rm ex}$ is a $\mathcal{Q}$-stochastic entropy production of the form (6.26) specialized to the choice $\mathcal{Q}^{(t)} = \mathcal{P}^{{\rm ex},(t)}$ (see Ref. [98] for details),

$$S_t^{\rm ex} \equiv S_t^{\mathcal{P},\mathcal{P}^{{\rm ex},(t)}} = \ln\left(\frac{\mathcal{P}\left(X_{[0,t]}\right)}{\mathcal{P}^{{\rm ex},(t)}\left(\Theta_t\left(X_{[0,t]}\right)\right)}\right)$$
$$= -\ln\left(\frac{\rho_t}{\pi_t}(X_t)\right) + \ln\left(\frac{\rho_0}{\pi_0}(X_0)\right) - \int_0^t {\rm d}s(\partial_s \ln \pi_s)(X_s). \quad (6.64)$$

Here, the path probability $\mathcal{P}^{{\rm ex},(t)}$ is associated with the dynamics generated by "dual" time-reversed generator [98] given for all $0 \le s \le t$ by

$$\mathcal{L}_s^{{\rm ex},(t)} \equiv \pi_{t-s}^{-1} \circ \mathcal{L}_{t-s}^{\dagger} \circ \pi_{t-s}, \quad (6.65)$$

where $\circ$ denotes here the composition operator, and π_t is the so-called *accompanying density* [6] which obeys

$$\mathcal{L}_t^{\dagger}\pi_t = 0, \quad (6.66)$$

for all values of time $t \ge 0$.

Note that π_t would be the stationary density of the process if the external parameters are constant and equal to those at time t. We give below further remarks and clarifications about the accompanying density, which is not equal to the instantaneous density of the process generating X_t. To further clarify the notation in (6.65), we note that $\mathcal{L}_s^{{\rm ex},(t)}$ acts on a function $f(x)$ as follows:

$$(\mathcal{L}_s^{{\rm ex},(t)} f)(x) = \frac{(\mathcal{L}_{t-s}^{\dagger}(\pi_{t-s} f))(x)}{\pi_{t-s}(x)}. \quad (6.67)$$

From (6.63), the **housekeeping stochastic entropy production** $S_t^{\rm hk} = S_t^{\rm tot} - S_t^{\rm ex}$ is defined as the difference between the total and excess stochastic entropy production, which, after some cumbersome algebra given in Section 10.5.2 in [98], can be written for generic Markov processes in the form of a Λ-entropic functional

$$S_t^{\rm hk} = \Lambda_t^{\mathcal{P},\mathcal{P}^{\rm hk}} = \ln\left(\frac{\mathcal{P}\left(X_{[0,t]}\right)}{\mathcal{P}^{\rm hk}\left(X_{[0,t]}\right)}\right). \quad (6.68)$$

Here, $\mathcal{P}^{\rm hk}$ is the path probability associated with the same initial density ρ_0 and with the "dual" Markovian generator given for all $s \ge 0$ by

$$\mathcal{L}_s^{\rm hk} \equiv \pi_s^{-1} \circ \mathcal{L}_s^{\dagger} \circ \pi_s. \quad (6.69)$$

Let us now give some important remarks concerning the definition of housekeeping and excess entropy production.

- The fact that, $S_t^{\text{tot}} - S_t^{\text{ex}}$, a difference of two Σ-stochastic entropic functionals can be expressed as S_t^{hk}, a Λ-entropic functional, is a special property that does not hold in general for arbitrary Σ-stochastic functionals.
- A key insight often overlooked in the literature is that the accompanying density π_t given by the solution of Equation (6.66) is *not* in general a solution of the Fokker–Planck equation (3.38) associated with the dynamics of the process X_t, i.e., in general

$$\partial_t \pi_t \neq \mathcal{L}_t^{\dagger} \pi_t. \tag{6.70}$$

On the other hand, π_t satisfies $\mathcal{L}_t^{\dagger}\pi_t = 0$ at all times t, i.e., it coincides with the stationary density of a process on which Markov generator would be frozen for at its value at time t. In other words, π_t is the instantaneous density of the process if and only if the dynamics is either stationary or quasistatic at all times.
- The average value of the excess entropy production (6.64) reads

$$\langle S_t^{\text{ex}} \rangle = D_{\text{KL}}\left[\rho_0 || \pi_0\right] - D_{\text{KL}}\left[\rho_t || \pi_t\right] - \int_0^t \mathrm{d}s \int_{\mathcal{X}} \mathrm{d}x \rho_s(x) (\partial_s \ln \pi_s)(x). \tag{6.71}$$

Choosing $\rho_0 = \pi_0$, the positivity of $\langle S_t^{\text{ex}} \rangle$ given in (6.17) allows one to derive the result by Vaikuntanathan and Jarzynski [172] $-\int_0^t \mathrm{d}s \int_{\mathcal{X}} \mathrm{d}x \rho_s(x)(\partial_s \ln \pi_s)(x) \geq D_{\text{KL}}[\rho_t||\pi_t]$.

Moreover, the formulae (6.71) can also be written as [98]

$$\langle S_t^{\text{ex}} \rangle = \int_0^t \mathrm{d}s \int_{\mathcal{X}} \mathrm{d}x \left(\partial_s \rho_s(x)\right) \left(\ln \frac{\pi_s}{\rho_s}\right)(x). \tag{6.72}$$

Equation (6.72) implies that $\langle S_t^{\text{ex}} \rangle$ is close to zero for adiabatic processes, i.e., when $\rho_s \simeq \pi_s$.
- *Physical interpretation of housekeeping and excess entropy production*. Note that if instantaneous detailed balance holds, i.e., $\pi_s \circ \mathcal{L}_s \equiv \mathcal{L}_s^{\dagger} \circ \pi_s$, then $\mathcal{L}_s^{\text{hk}} = \mathcal{L}_s$ and $S_t^{\text{hk}} = 0$, see Equation (6.68), yielding $S_t^{\text{tot}} = S_t^{\text{ex}}$. This clarifies the adjective "housekeeping" from the fact that it corresponds to the entropy production that results from the violation of instantaneous detailed balance, even if the process is stationary. On the other hand, the excess entropy production vanishes on average (see Equation 6.72) for stationary processes and otherwise it is non-zero, even when instantaneous detailed balance holds.

Two important paradigmatic examples are as follows: (i) a nonequilibrium stationary state ($\rho_0 = \rho_t = \rho_{\text{st}}$) with time-independent driving, one has $\pi_t = \rho_{st}$, which implies $S_t^{\text{tot}} = S_t^{\text{hk}}$; (ii) a nonstationary relaxation with instantaneous detailed balance with respect to π, i.e., $\pi_s \circ \mathcal{L}_s \equiv \mathcal{L}_s^{\dagger} \circ \pi_s$, of a system from an arbitrary initial distribution to a final state, for which one gets $S_t^{\text{tot}} = S_t^{\text{ex}}$. For most nonequilibrium process, however, S_t^{hk} and S_t^{ex} may both be nonzero fluctuating quantities.
- The expression (6.64) for S_t^{ex} and (6.68) for S_t^{hk} are generic for Markovian processes, without the need to restrict to pure Jump or diffusion processes, i.e., it holds also for Markovian stochastic equation with Gaussian and Poissonian white noise. We provide in Appendix D alternative explicit expressions for the excess (6.64) and housekeeping (6.68) stochastic entropy production when process is restricted to Markov-jump and to multidimensional Langevin processes.
- Because S_t^{ex} and S_t^{hk} are examples of Σ-stochastic entropic and Λ-stochastic entropic functionals respectively, they obey mother fluctuation theorems (6.19), which imply

Crooks-like (6.23) and Jarzynski-like (6.120) fluctuation relations for both quantities. The latter are given by

$$\langle \exp\left(-S_t^{\text{ex}}\right)\rangle = 1, \quad \langle \exp\left(-S_t^{\text{hk}}\right)\rangle = 1, \tag{6.73}$$

where the first equality is often known as the Hatano–Sasa relation [151] (see also [173,174] for previous derivations of similar results) and the second equality as the integral fluctuation relation for the housekeeping entropy production, which for the case of one-dimensional Langevin equations with additive noise is known as the Speck–Seifert relation [170]. A corollary of these fluctuation relations is the second laws

$$\langle S_t^{\text{ex}}\rangle \geq 0, \quad \langle S_t^{\text{hk}}\rangle \geq 0, \tag{6.74}$$

which hold for arbitrary nonequilibrium processes. The inequality $\langle S_t^{\text{ex}}\rangle \geq 0$ has been found to be crucial to define the efficiency of active-matter heat engines [175]. Finally, the relation (6.74) together with the Oono–Paniconi decomposition (6.63) implies the "refinement" of the second law for S_t^{tot} :

$$\langle S_t^{\text{tot}}\rangle \geq \sup\left(\langle S_t^{\text{ex}}\rangle, \langle S_t^{\text{hk}}\rangle\right) \geq 0, \tag{6.75}$$

which is the main result of this theory. Note that other approaches to the Oono–Paniconi decompositions are available even for quantum systems, where the positivity of the adiabatic entropy is not guaranteed at discrete times [176].

6.2. *Martingale structure of entropic functionals*

In this section, we identify martingales with respect to a physical stochastic process X_t that play an important role in stochastic thermodynamics. The martingales that we identify are exponentials of specific examples of Σ-stochastic entropic and Λ-stochastic entropic functionals, as introduced in Section 6.1, multiplied by minus one.

For simplicity, we consider in the proofs of this section that time is discrete, so that $t \in \mathbb{N}$. In this case, $\mathcal{P}(X_{[0,t]})$ and $\mathcal{Q}^{(t)}(X_{[0,t]})$ are normalized path probabilities. Nevertheless, the results obtained below are also valid for the continuous-time setup, which is the usual setup of stochastic thermodynamics.

6.2.1. *When are exponentiated, negative Λ-stochastic entropic functionals exponential martingales?*

Assume that the path probability $\mathcal{Q}$ has no supplemental t dependence, i.e., $\mathcal{Q}^{(t)} = \mathcal{Q}$. It holds then that the Λ-stochastic entropic functional

$$\Lambda_t^{\mathcal{P},\mathcal{Q}} = \ln[\mathcal{P}\left(X_{[0,t]}\right) / \mathcal{Q}\left(X_{[0,t]}\right)] \tag{6.76}$$

is a **submartingale** and the process $\exp(-\Lambda_t^{\mathcal{P},\mathcal{Q}})$ is a **martingale**, both with respect to $X_{[0,t]}$. In particular, for all $t \geq s \geq 0$ it holds that

$$\left\langle \exp\left(-\Lambda_t^{\mathcal{P},\mathcal{Q}}\right) \middle| X_{[0,s]}\right\rangle = \exp\left(-\Lambda_s^{\mathcal{P},\mathcal{Q}}\right) \tag{6.77}$$

and

$$\langle \Lambda_t^{\mathcal{P},\mathcal{Q}} \,|\, X_{[0,s]} \rangle \geq \Lambda_s^{\mathcal{P},\mathcal{Q}}. \tag{6.78}$$

Hence, all Λ-stochastic entropic functionals of the form (6.10) with the additional condition $\mathcal{Q}^{(t)} = \mathcal{Q}$ increase conditionally with respect to time.

For $\mathcal{Q}^{(t)} = \mathcal{Q}$, the martingale property in (6.77) follows from a derivation similar to the one presented in Equation (2.19) of Chapter 2, viz.,

$$\left\langle \exp\left(-\Lambda_t^{\mathcal{P},\mathcal{Q}}\right) \middle| X_{[0,s]} \right\rangle = \int \mathcal{D}x_{[s+1,t]} \frac{\mathcal{Q}(X_{[0,s]}, x_{[s+1,t]})}{\mathcal{P}(X_{[0,s]}, x_{[s+1,t]})} \mathcal{P}(x_{[s+1,t]} \,|\, X_{[0,s]}) \tag{6.79}$$

$$= \int \mathcal{D}x_{[s+1,t]} \frac{\mathcal{Q}(X_{[0,s]}, x_{[s+1,t]})}{\mathcal{P}(X_{[0,s]}, x_{[s+1,t]})} \frac{\mathcal{P}(X_{[0,s]}, x_{[s+1,t]})}{\mathcal{P}(X_{[0,s]})} \tag{6.80}$$

$$= \frac{\int \mathcal{D}x_{[s+1,t]} \mathcal{Q}(X_{[0,s]}, x_{[s+1,t]})}{\mathcal{P}(X_{[0,s]})} \tag{6.81}$$

$$= \frac{\mathcal{Q}(X_{[0,s]})}{\mathcal{P}(X_{[0,s]})} = \exp\left(-\Lambda_s^{\mathcal{P},\mathcal{Q}}\right). \tag{6.82}$$

In Equation (6.79), we have used the definition (6.10) of the Λ-entropic functional; in Equation (6.80) we have used Bayes' theorem; in Equation (6.81) we have used the fact that $\mathcal{P}(X_{[0,s]})$ is independent of $X_{[s+1,t]}$; and in Equation (6.82) we have marginalized $\mathcal{Q}$. The marginalization step from Equation (6.81) to Equation (6.82) is crucial for the proof of martingality, which in this case follows immediately from the fact that $\mathcal{Q}$ is a path probability, i.e.,

$$\int \mathcal{D}x_{[s+1,t]} \mathcal{Q}(X_{[0,s]}, x_{[s+1,t]}) = \int \mathrm{d}x_{s+1} \cdots \int \mathrm{d}x_t \mathcal{Q}(X_0, \ldots, X_s, x_{s+1}, \ldots, x_t)$$
$$= \mathcal{Q}(X_0, \ldots, X_s) = \mathcal{Q}(X_{[0,s]}). \tag{6.83}$$

For path probabilities with supplementary t-dependence, denoted by $\mathcal{Q}^{(t)}$, martingality requires the marginalization property (see last step of previous proof):

$$\int \mathcal{D}x_{[s+1,t]} \mathcal{Q}^{(t)}(x_{[0,t]}) = \mathcal{Q}^{(s)}(x_{[0,s]}). \tag{6.84}$$

Relevant examples of (sequences) of path probabilities $\mathcal{Q}^{(t)}$ that contain a supplementary t-dependence are: $\mathcal{Q} = \mathcal{P}^{\mathrm{ex},(t)}$ with $\mathcal{P}^{\mathrm{ex},(t)}$ the Markovian path probability associated with the generator (6.65) and $\mathcal{Q} = \tilde{\mathcal{P}}^{(t)}$ with $\tilde{\mathcal{P}}^{(t)}$ the Markovian path probability associated with the generator (6.6). Moreover, as we show in the next paragraph, when the path probability $\mathcal{Q}$ involves time-reversal maps Θ_t, then $\mathcal{Q}$ has a supplementary t-dependence.

Moreover, for any functional Λ_t that obeys the following two conditions it holds that $\exp(-\Lambda_t)$ is a martingale: (i) the Λ_t functional is additive in time, i.e., $\Lambda_t = \Lambda_s + \Lambda_{[s,t]}$ for any $0 \leq s \leq t$ and (ii) the Λ_t functional obeys the Jarzynski-like equality $\langle \exp(-\Lambda_{[s,t]}) \,|\, X_{[0,s]} \rangle = 1$ for any $t \geq s \geq 0$.[9] These two conditions imply that $\langle \exp(-\Lambda_t) \,|\, X_{[0,s]} \rangle = \exp(-\Lambda_s) \langle \exp(-\Lambda_{[s,t]}) \,|\, X_{[0,s]} \rangle = \exp(-\Lambda_s)$, and hence $\exp(-\Lambda_t)$ is a martingale. Note that the additive structure $\Lambda_t = \Lambda_s + \Lambda_{[s,t]}$ is not a generic property for Λ-stochastic entropic functionals. However, the additive structure is fulfilled by Λ-stochastic functionals of

Equation (6.10) for which both $\mathcal{P}$ and $\mathcal{Q}$ are by path probabilities of Markovian processes. As shown below, conditions (i) and (ii) are sufficient but not necessary conditions for $\exp(-\Lambda_t)$ to be an exponential martingale.

6.2.1.1. *Example: Housekeeping entropy production of a Markovian process.* The housekeeping entropy production $S_t^{\rm hk}$, as defined in Equation (6.68), is an example of a Λ-stochastic entropy functional that results from the choice $\mathcal{Q} = \mathcal{P}^{\rm hk}$, where $\mathcal{P}^{\rm hk}$ the Markovian path probability associated with the "dual" t-independent generator, defined in Equation (6.69).

Therefore, Equation (6.77) implies that $\exp(-S_t^{\rm hk})$ is a martingale, i.e.,

$$\langle \exp(-S_t^{\rm hk}) \,|\, X_{[0,s]} \rangle = \exp(-S_s^{\rm hk}), \tag{6.85}$$

which holds for any $t \geq s \geq 0$ and any $X_{[0,s]}$.

Applying Jensen's inequality to Equation (6.85), we obtain a **conditional second law** for the **housekeeping entropy production**, viz.,

$$\langle S_t^{\rm hk} \,|\, X_{[0,s]} \rangle \geq S_s^{\rm hk}, \tag{6.86}$$

for any $t \geq s \geq 0$. In other words, $S_t^{\rm hk}$ is a submartingale, and the housekeeping entropy production is **conditionally increasing** with time.

Specializing Equation (6.85) to $s = 0$ and taking the average over the initial state, we obtain as a corollary the integral fluctuation relation

$$\begin{aligned}\langle \exp(-S_t^{\rm hk}) \rangle &= \int_{\mathcal{X}} {\rm d}x_0 \rho_0(x_0) \langle \exp(-S_t^{\rm hk}) \,|\, X_0 = x_0 \rangle \\ &= \int_{\mathcal{X}} {\rm d}x_0 \rho_0(x_0) \left\langle \exp(-S_0^{\rm hk}) \right\rangle \\ &= 1. \end{aligned} \tag{6.87}$$

The second equality in Equation (6.87) comes from the martingale condition (6.85), and the third equality comes from Equation (6.85) for $t = 0$ and $S_0^{\rm hk} = 0$. Similarly, using the submartingale condition (6.86), the second-law like inequality $\langle S_t^{\rm hk} \rangle \geq 0$ follows, which in fact holds for any initial density ρ_0. Further details about the martingale structure of the exponentiated negative housekeeping entropy production can be found in Refs. [28,39].

6.2.2. ♠*When are exponentiated, negative, Σ-stochastic entropic functionals exponential martingales?*

Contrarily to Λ-stochastic functionals, it holds that $\exp(-\Sigma_t^{\mathcal{P},\mathcal{Q}})$ is in general not a martingale even when the path probability $\mathcal{Q}$ has no supplemental t dependence. Indeed, following similar steps as for the Λ-stochastic entropic functional in the previous section, we find that the martingale condition is, in general, not fulfilled:

$$\left\langle \exp\left(-\Sigma_t^{\mathcal{P},\mathcal{Q}}\right) \middle| X_{[0,s]} \right\rangle = \int \mathcal{D}x_{[s+1,t]} \frac{\mathcal{Q}^{(t)}_{[0,t]}(\Theta_t(X_{[0,s]}, x_{[s+1,t]}))}{\mathcal{P}_{[0,t]}(X_{[0,s]}, x_{[s+1,t]})} \mathcal{P}(x_{[s+1,t]} \mid X_{[0,s]}) \tag{6.88}$$

$$= \int \mathcal{D}x_{[s+1,t]} \frac{\mathcal{Q}^{(t)}_{[0,t]}(\Theta_t(X_{[0,s]}, x_{[s+1,t]}))}{\mathcal{P}_{[0,t]}(X_{[0,s]}, x_{[s+1,t]})} \frac{\mathcal{P}_{[0,t]}(X_{[0,s]}, x_{[s+1,t]})}{\mathcal{P}_{[0,s]}(X_{[0,s]})} \tag{6.89}$$

$$= \frac{\int \mathcal{D}x_{[s+1,t]} \mathcal{Q}^{(t)}_{[0,t]}(\Theta_t(X_{[0,s]}, x_{[s+1,t]}))}{\mathcal{P}_{[0,s]}(X_{[0,s]})} \tag{6.90}$$

$$\neq \frac{\mathcal{Q}^{(s)}_{[0,s]}(\Theta_s X_{[0,s]})}{\mathcal{P}_{[0,s]}(X_{[0,s]})} = \exp\left(-\Sigma_s^{\mathcal{P},\mathcal{Q}^{(s)}}\right). \tag{6.91}$$

Here, the key step is the inequality (6.91), which can be written more explicitly as

$$\int \mathcal{D}x_{[s+1,t]} \mathcal{Q}^{(t)}_{[0,t]}(\Theta_t(X_{[0,s]}, x_{[s+1,t]})) = \int \mathrm{d}x_{s+1} \cdots \int \mathrm{d}x_t \mathcal{Q}^{(t)}_{[0,t]}(x_t, \ldots, x_{s+1}, X_s, \ldots, X_0)$$
$$= \mathcal{Q}^{(t)}_{[t-s,t]}(X_s, \ldots, X_0) \tag{6.92}$$

$$= \mathcal{Q}^{(t)}_{[t-s,t]}(\Theta_s X_{[0,s]}) \neq \mathcal{Q}^{(s)}_{[0,s]}(\Theta_s X_{[0,s]}). \tag{6.93}$$

Note that for bookkeeping purposes, we have used the subindices $[0,t]$, $[0,s]$, and $[t-s,t]$ to denote marginalized path probabilities of $\mathcal{P}$ and $\mathcal{Q}^{(t)}$. For example, $\mathcal{P}_{[0,t]}(x_{(0,t)})$ denotes the marginal of $\mathcal{P}(x_{[0,\infty]})$ for which all variables $x_{[t,\infty]}$ have been integrated out. Analogously, $\mathcal{Q}^{(t)}_{[0,s]}(x_{[0,s]})$ denote the marginal of $\mathcal{Q}^{(t)}(x_{[0,\infty]})$ for which all variables $x_{[s,\infty]}$ have been integrated out, and so forth.

Hence, Equations (6.88)–(6.91) imply that for general driven nonequilibrium processes

$$\left\langle \exp\left(-\Sigma_t^{\mathcal{P},\mathcal{Q}}\right) \middle| X_{[0,s]} \right\rangle = \exp\left(-\Sigma_s^{\mathcal{P},\mathcal{Q}}\right) \frac{\mathcal{Q}^{(t)}_{[t-s,t]}(\Theta_s X_{[0,s]})}{\mathcal{Q}^{(s)}_{[0,s]}(\Theta_s X_{[0,s]})}, \tag{6.94}$$

any $0 \leq s \leq t$.

Consequently, in general, $\exp(-\Sigma_t^{\mathcal{P},\mathcal{Q}})$ are *not* martingales, i.e.,

$$\left\langle \exp\left(-\Sigma_t^{\mathcal{P},\mathcal{Q}}\right) \middle| X_{[0,s]} \right\rangle \neq \exp\left(-\Sigma_s^{\mathcal{P},\mathcal{Q}}\right). \tag{6.95}$$

In special cases, the equality

$$\mathcal{Q}^{(t)}_{[t-s,t]}(\Theta_s X_{[0,s]}) = \mathcal{Q}^{(s)}_{[0,s]}(\Theta_s X_{[0,s]}) \tag{6.96}$$

required for the martingality of $\exp(-\Sigma_t^{\mathcal{P},\mathcal{Q}})$ holds. In particular, Equation (6.96) holds when the following conditions are met: (i) $\mathcal{Q}^{(t)}$ is independent of (t), i.e., $\mathcal{Q}^{(t)} = \mathcal{Q}$; (ii) $\mathcal{Q}$ is a stationary measure; and (iii) $\mathcal{Q}$ is time homogeneous, i.e., $\mathcal{Q}^{(t)} = \mathcal{Q}^{\mathrm{st}}$. If conditions (i) –(iii) hold, then $\exp(-\Sigma_t^{\mathcal{P},\mathcal{Q}})$ is a martingale. A notable example is the process $\exp(-S_t^{\mathrm{tot}})$, where S_t^{tot} is the entropy production of a time-homogeneous, stationary process X, as discussed in Section 6.1.5.4 (see also below for details).

Hence, $\exp(-\Sigma^{\mathcal{P},\mathcal{Q}})$ is a *martingale* when $\mathcal{Q}^{(t)} = \mathcal{Q}^{\mathrm{st}}$ is a t-independent , stationary, and time homogeneous path probability. In this case, $\mathcal{Q}^{(t)}_{[t-s,t]} = \mathcal{Q}^{st}_{[0,s]}$, and the martingale property of $\exp(-\Sigma^{\mathcal{P},\mathcal{Q}}))$ is restored, viz.,

$$\langle \exp(-\Sigma_t^{\mathcal{P},\mathcal{Q}^{\mathrm{st}}}) \,|\, X_{[0,s]}\rangle = \exp(-\Sigma_s^{\mathcal{P},\mathcal{Q}^{\mathrm{st}}}), \tag{6.97}$$

for all $0 \leq s \leq t$.

Using Jensen's inequality on Equation (6.97), we find that

$$\langle \Sigma_t^{\mathcal{P},\mathcal{Q}^{\mathrm{st}}} \,|\, X_{[0,s]}\rangle \geq \Sigma_s^{\mathcal{P},\mathcal{Q}^{\mathrm{st}}}, \tag{6.98}$$

and hence for t-independent , stationary, and time homogeneous path probabilities $\mathcal{Q}^{(t)} = \mathcal{Q}^{\mathrm{st}}$, the process $\Sigma_t^{\mathcal{P},\mathcal{Q}^{\mathrm{st}}}$ is a *submartingale*.

Note that the martingale property (6.97) does not require that $\mathcal{P}$ is stationary and/or Markovian.

If $\mathcal{P}$ and/or $\mathcal{Q}$ are nonnormalized, then Equation (6.97) does not hold due to breaking of marginalization property. A notable example is the environmental $\mathcal{Q}$-stochastic entropy change $S_t^{\mathrm{env},\mathcal{P},\mathcal{Q}}$, as defined in Equation (6.28), for which $\exp(-S_t^{\mathrm{env},\mathcal{P},\mathcal{Q}})$ is not a martingale (see also Section 5.2.2.5). This in spite of the fact that, according to the decomposition (6.27), $S_t^{\mathrm{env},\mathcal{P},\mathcal{Q}}$ is a Σ-stochastic entropic functional when $\rho_0(x) = \rho_0^{\mathcal{Q}}(x) = 1$. However, in this case, $\mathcal{P}$ and $\mathcal{Q}$ are not normalized, and therefore $\exp(-S_t^{\mathrm{env},\mathcal{P},\mathcal{Q}})$ is not a martingale.

We further discuss two examples of Σ-stochastic entropic functionals that are important for stochastic thermodynamics:

- For Markovian processes, the condition $\mathcal{Q}^{(t)} = \mathcal{Q}^{\mathrm{st}}$ is equivalent to the three conditions:
  (1) The family $\mathcal{Q}^{(t)}$ has no supplementary dependence on the final time t, i.e., $\mathcal{Q}^{(t)} = \mathcal{Q}$ for a certain path probability $\mathcal{Q}$.
  (2) In addition to Condition 1, the Markovian generator of $\mathcal{Q}$ is time homogeneous.
  (3) In addition to Condition 1, the initial density of $\mathcal{Q}$ is the associated stationary density, i.e., $\rho_0^{\mathcal{Q}} = \rho_{st}^{\mathcal{Q}} = \rho_t^{\mathcal{Q}}$ for all $t \geq 0$.

  In one side, conditions (1), (2), and (3) together are sufficient conditions for the martingale property (6.97). But from another side, in Section 6.1.5.4, we have shown that for stationary, multidimensional Langevin processes $\exp(-S_t^{\mathrm{tot}})$ is a martingale, even when condition (2) does not hold.[10] Hence, Conditions (1)–(3) are sufficient but not necessary. An another interesting example is the excess entropy S_t^{ex}, as defined in (6.64), which is also a Σ-stochastic entropic functional. In this case, $\exp(-S_t^{\mathrm{ex}})$ is not a martingale, and S_t^{ex} does not satisfy any of the conditions 1, 2, and 3, except in the trivial case where $S_t^{\mathrm{ex}} = 0$ for all t.
- In the case where the path measure $\mathcal{Q}$ satisfies Conditions 1 and 2 of the previous item, and not Condition 3, i.e., when $\mathcal{Q}$ represents a time-homogeneous system that relaxes to its stationary state, then the bulk term in the ratio $\mathcal{Q}^{(t)}_{[t-s,t]}/\mathcal{Q}^{(s)}_{[0,s]}$ cancels out, and Equation (6.94)

takes the form

$$\left\langle \exp\left(-\Sigma_t^{\mathcal{P},\mathcal{Q}}\right) \middle| X_{[0,s]} \right\rangle = \exp\left(-\Sigma_s^{\mathcal{P},\mathcal{Q}}\right) \frac{\rho_{t-s}^{\mathcal{Q}}}{\rho_0^{\mathcal{Q}}}(X_s). \tag{6.99}$$

In this case, it is possible to "martingalize" Equation (6.99) by eliminating the border term as follows:

$$\langle \exp(-\Sigma_t^{\mathcal{P},\mathcal{Q}} - \alpha_t^{\mathcal{Q},(t)}) \,|\, X_{[0,s]} \rangle = \exp(-\Sigma_s^{\mathcal{P},\mathcal{Q}} - \alpha_s^{\mathcal{Q},(t)}), \tag{6.100}$$

for all $0 \leq s \leq t$, and where

$$\alpha_s^{\mathcal{Q},(t)} = \ln\left(\frac{\rho_0^{\mathcal{Q}}(X_s)}{\rho_{t-s}^{\mathcal{Q}}(X_s)}\right). \tag{6.101}$$

6.2.2.1. *Example of total entropy production for Markovian processes.* As shown in Section 6.1.5.4, for stationary processes X_t the exponential $\exp(-S_t^{\mathrm{tot}})$ of the total stochastic entropy production S_t^{tot} is a martingale. Otherwise, if X_t (and thus $\mathcal{P}$) is a non-stationary process, then Equation (6.94) for $\mathcal{Q}^{(t)} = \tilde{\mathcal{P}}^{(t)}$, where $\tilde{\mathcal{P}}^{(t)}$ is the path probability associated with a protocol that has been reversed at time t, yields

$$\left\langle \exp\left(-S_t^{\mathrm{tot}}\right) \middle| X_{[0,s]} \right\rangle = \exp\left(-S_s^{\mathrm{tot}}\right) \frac{\tilde{\mathcal{P}}_{[t-s,t]}^{(t)}(\Theta_s X_{[0,s]})}{\tilde{\mathcal{P}}_{[0,s]}^{(s)}(\Theta_s X_{[0,s]})}. \tag{6.102}$$

Simplifying the ratio $\tilde{\mathcal{P}}_{[t-s,t]}^{(t)}/\tilde{\mathcal{P}}_{[0,s]}^{(s)}$ in Equation (6.102), we obtain the relation

$$\left\langle \exp\left(-S_t^{\mathrm{tot}}\right) \middle| X_{[0,s]} \right\rangle = \exp\left(-S_s^{\mathrm{tot}}\right) \frac{\rho_{t-s}^{\tilde{\mathcal{P}}^{(t)}}(X_s)}{\rho_s(X_s)}, \tag{6.103}$$

where $\rho_{t-s}^{\tilde{\mathcal{P}}^{(t)}} = \tilde{\rho}_{t-s}^{(t)}$ is the instantaneous density at time $t-s$ resulting from the evolution of the initial density $\rho_0^{\tilde{\mathcal{P}}^{(t)}} = \tilde{\rho}_0^{(t)} = \rho_t$ by the dynamics with the protocol that has been time-reversed at time t. This comes from the fact that in this case the initial density of $\tilde{\mathcal{P}}_{[t-s,t]}^{(t)}$ in (6.102) is $\rho_{t-s}^{\tilde{\mathcal{P}}^{(t)}} = \tilde{\rho}_{t-s}^{(t)}$ and the initial density of $\tilde{\mathcal{P}}_{[0,s]}^{(s)}$ in (6.102) is $\rho_0^{\tilde{\mathcal{P}}^{(s)}} = \tilde{\rho}_0^{(s)} = \rho_s$, see Figure 6.2 for an illustration.

Equation (6.103) implies that we can "martingalize" $\exp(-S_t^{\mathrm{tot}})$ in generic nonequilibrium Markovian processes, as we discuss now.

Indeed, for all $0 \leq s \leq t$ it holds that

$$\langle \exp(-S_t^{\mathrm{tot}} - \delta_t^{(t)}) \,|\, X_{[0,s]} \rangle = \exp(-S_s^{\mathrm{tot}} - \delta_s^{(t)}), \tag{6.104}$$

with

$$\delta_s^{(t)} = \ln\left(\frac{\rho_s(X_s)}{\tilde{\rho}_{t-s}^{(t)}(X_s)}\right); \tag{6.105}$$

note that $\delta_t^{(t)} = 0$.

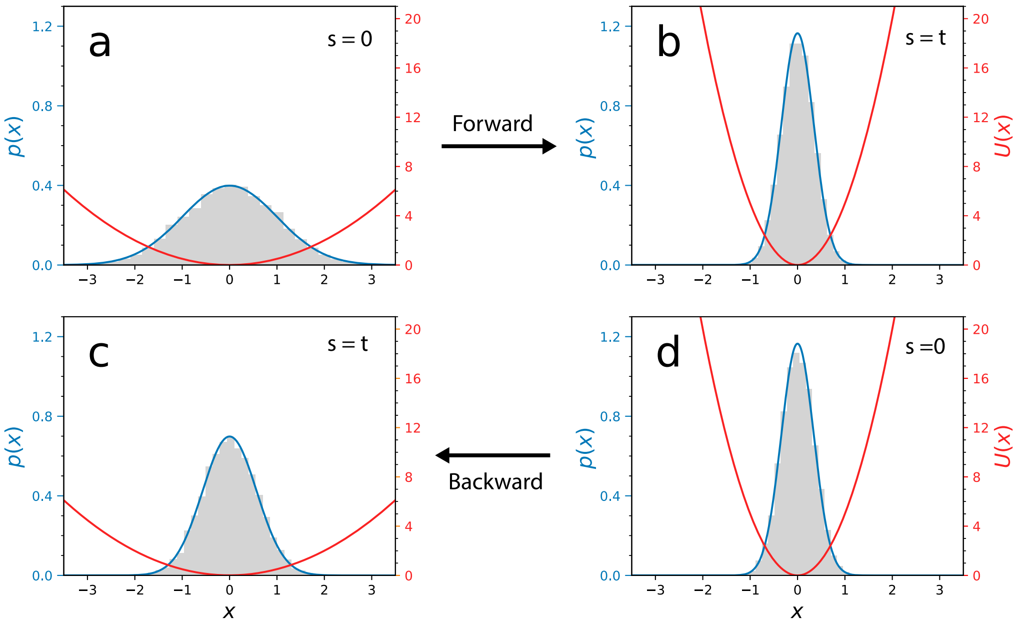

Figure 6.2. Distributions $\rho(x)$ (blue lines) of the position of a particle x in a time-dependent harmonic potential $U(X)$ (red lines), obtained from samples at different times $s = 0, t$ (see legends) during forward (a→b) and backward (d→c) processes, with the latter initialized with the final distribution of the forward process. The results are obtained for a system described by the Langevin equation $\dot{X}_s = -\mu\kappa_t X_s + \sqrt{2D}\dot{B}_s$, with $\kappa_s = \kappa_0 + rs$ in the forward process, and $\tilde{\kappa}_s = \kappa_{t-s}$ in the backward process. The gray bars are obtained from numerical simulations and the blue line from analytical calculations. Values of the parameters: $\mu = 10$, $\kappa_0 = 1$, $r = 9/t$, $t = 0.05$, $D = 1$, simulation time step 5×10^{-5}, 10^4 realizations. Figure courtesy of Tarek Tohme.

The relations (6.103)–(6.105) are extension in general set-up of the martingale integral fluctuation relation (6.61). The term $\delta_s^{(t)}$ is the so-called *stochastic distinguishability* between conjugate times in the forward and backward processes, and $\delta_s^{(t)}$ vanishes for (possibly nonequilibrium) stationary states – for which ρ_s and $\tilde{\rho}_s^t$ are independent on time – where one recovers the martingale condition (6.61). For non-stationary states, one has in general $\rho_s(x) \neq \tilde{\rho}^{(t)}_{t-s}(x)$ (see Figure 6.2 a,d), and $\delta_s^{(t)}$ fluctuates in time s. See also Ref. [10] for the appearance of the stochastic distinguishability, but for the generalized Σ-stochastic entropic functional introduced in the next section.

Note that by the tower property of condition expectations (see Equations 2.3) and (6.103) implies for all $0 \leq u \leq s \leq t$ that

$$\begin{aligned}\langle \exp(-S_s^{\text{tot}} - \delta_s^{(t)}) \,|\, X_{[0,u]}\rangle &= \langle\langle \exp(-S_t^{\text{tot}} - \delta_t^{(t)}) \,|\, X_{[0,s]}\rangle \,|\, X_{[0,u]}\rangle \\ &= \langle \exp(-S_t^{\text{tot}} - \delta_t^{(t)}) \,|\, X_{[0,u]}\rangle \\ &= \exp(-S_u^{\text{tot}} - \delta_u^{(t)}). \end{aligned} \tag{6.106}$$

Thus we conclude that $\exp(-S_s^{\text{tot}} - \delta_s^{(t)})$ are Martingales.

Applying Doob's optional stopping theorem (Theorem 12) to a stopping time $\mathcal{T}$ with $\mathcal{T} \leq t$, we obtain (6.104) (see Ref. [15] for the original proof)

$$\langle \exp(-S^{\rm tot}_{\mathcal{T}} - \delta^{(t)}_{\mathcal{T}}) \rangle = \langle \exp(-S^{\rm tot}_0 - \delta^{(t)}_0) \rangle = \int {\rm d}x \rho_0(x) \left[\frac{\tilde{\rho}^{(t)}_t(x)}{\rho_0(x)} \right] = \int {\rm d}x \tilde{\rho}^{(t)}_t(x) = 1. \quad (6.107)$$

The third equality uses that $S^{\rm tot}_0 = 0$. The last equality is the normalization of $\tilde{\rho}^{(t)}_t(x)$.

6.3. ♠ *Generalized* **Σ**-*stochastic entropic functional*

As shown in the previous section, a $\Sigma^{\mathcal{P},\mathcal{Q}}_t$ functional may obey an integral fluctuation relation $\langle \exp(-\Sigma^{\mathcal{P},\mathcal{Q}}_t) \rangle = 1$, even though $\exp(-\Sigma^{\mathcal{P},\mathcal{Q}}_t)$ is not a martingale. This follows from the "mother" fluctuation relation (6.120); a notable example is when $\Sigma^{\mathcal{P},\mathcal{Q}}_t = S^{\rm ex}_t$, the excess entropy production. To rationalize this fact, and find the lost martingale behind this integral fluctuation relation, we introduce in this section the *generalized* Σ-stochastic entropic functionals introduced in Ref. [10]. With these functionals, we can disentangle the connection between integral fluctuation relation and the martingality of a stochastic process.

6.3.1. *Definition of generalized* Σ*-stochastic entropic functionals*

Just as was the case for Σ-stochastic entropic functionals, *generalized* Σ-stochastic entropic functionals involve two path probabilities, viz., the path probability $\mathcal{P}$ evaluated on the trajectory $X_{[0,t]}$, and a second $\mathcal{Q}$ evaluated on the time-reversed trajectory $\Theta_t(X_{[0,t]})$. The difference between Σ-stochastic entropic functionals and *generalized* Σ-stochastic functionals lies in the fact that generalized Σ-stochastic entropic functionals are evaluated over *subset* intervals $[r, s] \subseteq [0, t]$, as described below.

The **generalized Σ-stochastic entropic functionals** are functions defined on the paths $X_{[r,s]}$ associated with subsets $[r, s] \subseteq [0, t]$ of the time interval $[0, t]$, which is the time interval to which the time reversal operation Θ_t applies. The generalized Σ-stochastic entropic functionals are defined by

$$\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t} \equiv \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}\left(X_{[r,s]}\right) \equiv \ln\left[\frac{\mathcal{P}_{[r,s]}(X_{[0,t]})}{\mathcal{Q}^{(t)}_{[t-s,t-r]}\left(\Theta_t X_{[0,t]}\right)} \right], \quad (6.108)$$

with $0 \leq r \leq s \leq t$, and where $\mathcal{P}_{[r,s]}(X_{[0,t]})$ is the marginal of $\mathcal{P}_{[0,t]}(X_{[0,t]})$ defined on the time window $[r, s]$, and hence $\mathcal{P}_{[r,s]}(X_{[0,t]})$ depends only on $X_{[r,s]}$; for discrete time and space, we can write

$$\mathcal{P}_{[r,s]}(x_{[0,t]}) \equiv \mathcal{P}(X_r = x_r, X_{r+1} = x_{r+1}, \ldots, X_{s-1} = x_{s-1}, X_s = x_s). \quad (6.109)$$

Analogously, $\mathcal{Q}^{(t)}_{[t-s,t-r]}(\Theta_t X_{[0,t]})$ is the marginal of $\mathcal{Q}^{(t)}_{[0,t]}(\Theta_t X_{[0,t]})$ on the time window $[t - s, t - r]$, and also only depends on $X_{[r,s]}$; for discrete time and space,

$$\mathcal{Q}^{(t)}_{[t-s,t-r]}(\Theta_t x_{[0,t]}) \equiv \mathcal{Q}^{(t)}(X_{t-s} = x_s, X_{t-s+1} = x_{s-1}, \ldots, X_{t-r-1} = x_{r-1}, X_{t-r} = x_r). \quad (6.110)$$

Note that the Σ-stochastic entropic functional, given in Equation (6.10), is a generalized Σ-stochastic entropic functional of Equation (6.108) for the choice $r = 0$ and $s = t$:

$$\Sigma^{\mathcal{P},\mathcal{Q}}_{[0,t];t} = \Sigma^{\mathcal{P},\mathcal{Q}}_{t}. \tag{6.111}$$

Also, when $Q^{(t)} = Q_{\rm st}$ is t-independent and stationary, then (see p.168 in [98])

$$\Sigma^{\mathcal{P},\mathcal{Q}_{\rm st}}_{[0,s];t} = \Sigma^{\mathcal{P},\mathcal{Q}_{\rm st}}_{s}. \tag{6.112}$$

for all $0 \leq s \leq t$.

The choice of the time window $[t-s, t-r]$ for $\mathcal{Q}^{(t)}$ leads to path probabilities in the numerator and denominator of the generalized Σ-stochastic entropic functional, as given in Equations (6.109) and (6.110), respectively, that are evaluated on the same part of the trajectory $x_{[0,t]}$. Indeed, if instead we would have used

$$\mathcal{Q}^{(t)}_{[r,s]}(\Theta_t x_{[0,t]}) = \mathcal{Q}^{(t)}(X_r = x_{t-r+1}, X_{r+1} = x_{t-r}, \ldots, X_{s-1} = x_{t-s}, X_s = x_{t-s+1}), \tag{6.113}$$

then the denominator would not be compatible with Equation (6.109).

Similar to the case of Σ-stochastic entropic functionals in Chapter 6.1, it holds that:

- The *generalized* Σ-stochastic entropic functionals verify the duality relation [10]

$$\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}\left(\Theta_t(X_{[0,t]})\right) = -\Sigma^{\mathcal{Q},\mathcal{P}}_{[t-s,t-r];t}(X_{[0,t]}), \tag{6.114}$$

  for all $0 \leq r \leq s \leq t$.
- The average values with respect to $\mathcal{P}$ of generalized Σ-stochastic entropic functionals are Kullback–Leibler divergences [10], viz.,

$$\left\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t} \right\rangle = D_{\rm KL}\left[\mathcal{P}_{[r,s]}(X_{[0,t]}) || \mathcal{Q}^{(t)}_{[t-s,t-r]}\left(\Theta_t X_{[0,t]}\right)\right]. \tag{6.115}$$

  As both $\mathcal{P}$ and $\mathcal{Q}$ are normalized path probabilities, the Kullback–Leibler divergence in the right-hand side of Equations (6.115) is greater or equal than zero, which implies the *"second laws"* [10]

$$\left\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t} \right\rangle \geq 0, \tag{6.116}$$

  for all $0 \leq r \leq s \leq t$.

6.3.2. *Fluctuation relation for generalized Σ-stochastic entropic functionals*

Following similar steps as in Chapter 6.1 for Σ-stochastic entropic functionals, we derive fluctuation relations for the generalized Σ-stochastic entropic functionals, as defined in Equation (6.108).

The **"mother" fluctuation relation** [10] for arbitrary functionals $Z[X_{[r,s]}]$ reads

$$\langle Z[\Theta_t(X_{[r,s]})] \rangle_{\mathcal{Q}^{(t)}} = \left\langle \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}\right) Z\left[X_{[r,s]}\right] \right\rangle, \tag{6.117}$$

for all $0 \leq r \leq s \leq t$.

Setting $Z[X_{[r,s]}] = \delta(\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t} - \sigma)$ and using the duality relations (6.114), we obtain the *generalized Crooks fluctuation relation* [10]

$$\left\langle \delta(\Sigma^{\mathcal{Q},\mathcal{P}}_{[t-s,t-r];t} + \sigma) \right\rangle_{\mathcal{Q}^{(t)}} = \exp(-\sigma) \left\langle \delta(\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t} - \sigma) \right\rangle, \tag{6.118}$$

for all $0 \le r \le s \le t$. This can also be expressed as

$$\frac{\rho^{\mathcal{P}}_{\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}}(\sigma)}{\rho^{\mathcal{Q}^{(t)}}_{\Sigma^{\mathcal{Q},\mathcal{P}}_{[t-s,t-r];t}}(-\sigma)} = \exp(\sigma), \tag{6.119}$$

for all $0 \le r \le s \le t$.

With the choice $Z[X_{[r,s]}] = 1$, Equation (6.117) becomes the *generalized integral fluctuation theorems* given in

$$\left\langle \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}\right) \right\rangle = 1, \tag{6.120}$$

for all $0 \le r \le s \le t$. Note that the generalized integral fluctuation relation holds for any (normalized) path probability $\mathcal{Q}^{(t)}$ that is absolutely continuous with respect to $\mathcal{P}$.

6.3.3. *Exponentiated, negative, generalized Σ-stochastic entropic functional are martingales*

Exponentiated, negative, generalized Σ-stochastic entropic functionals $\exp(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t})$ with $[r,s] \subseteq [0,t]$ are **martingales** with respect to the final time s when r and t are fixed. Indeed, it holds that

$$\left\langle \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s'];t}\right) \middle| X_{[r,s]} \right\rangle = \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}\right), \tag{6.121}$$

for all $0 \le r \le s \le s' \le t$. Applying Jensen's inequality to Equation (6.121) we get that $\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}$ are *submartingales* with respect to the final time s when r and t are fixed. More precisely,

$$\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s'];t} \,|\, X_{[r,s]} \rangle \ge \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}, \tag{6.122}$$

for all $0 \le r \le s \le s' \le t$.

Now, we derive Equation (6.121). For all $0 \le r \le s \le s' \le t$, it holds that

$$\begin{aligned} &\left\langle \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s'];t}\right) \middle| X_{[r,s]} \right\rangle \\ &= \int \mathcal{D}x_{[s+1,s']} \frac{\mathcal{Q}^{(t)}_{[t-s',t-r]}(\Theta_t\left(X_{[0,s]}, x_{[s+1,s']}, X_{[s',t]}\right))}{\mathcal{P}_{[r,s']}(X_{[0,s]}, x_{[s+1,s']}, X_{[s',t]})} \mathcal{P}_{[r,s']}(x_{[s+1,s']} \,|\, X_{[r,s]}) \end{aligned} \tag{6.123}$$

$$= \int \mathcal{D}x_{[s+1,s']} \frac{\mathcal{Q}^{(t)}_{[t-s',t-r]}(\Theta_t\left(X_{[0,s]},x_{[s+1,s']},X_{[s',t]}\right))}{\mathcal{P}_{[r,s']}(X_{[0,s]},x_{[s+1,s']},X_{[s',t]})} \frac{\mathcal{P}_{[r,s']}(X_{[0,s]},x_{[s+1,s']},X_{[s',t]})}{\mathcal{P}_{[r,s']}(X_{[r,s]})} \tag{6.124}$$

$$= \frac{\int \mathcal{D}x_{[s+1,s']}\mathcal{Q}^{(t)}_{[t-s',t-r]}(\Theta_t\left(X_{[0,s]},x_{[s+1,s']},X_{[s',t]}\right))}{\mathcal{P}_{[r,s]}(X_{[0,t]})} \tag{6.125}$$

$$= \frac{\mathcal{Q}^{(t)}_{[t-s,t-r]}(\Theta_t X_{[0,t]})}{\mathcal{P}_{[r,s]}(X_{[0,t]})} = \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}\right). \tag{6.126}$$

The relation (6.123) follows from the fact that the left-hand side of Equations (6.109) and (6.110) is independent of $x_{[0,r-1]}$ and $x_{[s+1,t]}$. We also use this property to obtain the denominator of the last term of Equation (6.124). Then, to obtain Equation (6.125), we use the marginalization $\mathcal{P}_{[r,s']}(X_{[r,s]}) = \mathcal{P}_{[r,s]}(X_{[r,s]})$ for all $0 \le s \le s'$, and the previous independence property to obtain $\mathcal{P}_{[r,s']}(X_{[r,s]}) = \mathcal{P}_{[r,s]}(X_{[r,s]}) = \mathcal{P}_{[r,s]}(X_{[0,t]})$. Finally, the first equality in (6.126) follows from the integration of (6.110) which yields

$$\int \mathcal{D}x_{[s+1,s']}\mathcal{Q}^{(t)}_{[t-s',t-r]}(\Theta_t x_{[0,t]}) = \mathcal{Q}^{(t)}(X_{t-s} = x_s, X_{t-s+1} = x_{s-1}, \ldots, X_{t-r} = x_r)$$
$$\equiv \mathcal{Q}^{(t)}_{[t-s,t-r]}(\Theta_t x_{[0,t]}). \tag{6.127}$$

It may appear surprising that the quantity $\exp(-\Sigma^{\mathcal{P},\mathcal{Q}^{(t)}}_{[r,s];t})$, which is a martingale with respect to the final time s, contains as a particular case (6.111) the exponentials of Σ-stochastic entropic functionals $\exp(-\Sigma^{\mathcal{P},\mathcal{Q}^{(t)}}_t)$, that are not martingales. This comes from the fact that by choosing $r = 0, s' = t$ the forward martingale property (6.121) becomes, for all $0 \le s \le t$,

$$\left\langle \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_t\right) \middle| X_{[0,s]} \right\rangle = \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[0,s];t}\right) \neq \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_s\right), \tag{6.128}$$

except for t independent and stationary $\mathcal{Q}$, when we have the relation (6.112).

Moreover, in [10,98], it is shown that the generalized Σ-stochastic entropic functionals $\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}$ do not only have an exponential martingale structure as a function of the final time s when conditioning over the past, but they also have a backward martingale structure as a function of the initial time r when conditioning on the future.

The exponentiated, negative, generalized Σ-stochastic entropic functionals $\exp(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t})$ with $[r,s] \subseteq [0,t]$ are **backward martingales** with respect to the initial time r when s and t are fixed. Indeed, it holds that [98]

$$\left\langle \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}\right) \middle| X_{[r',s]} \right\rangle = \exp\left(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r',s];t}\right), \tag{6.129}$$

for all $0 \le r \le r' \le s \le t$. Applying Jensen's inequality to Equation (6.129), we find that $\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t}$ are **backward submartingales** with respect to the initial time r when s and t are fixed. In particular,

$$\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t} \,|\, X_{[r',s]} \rangle \ge \Sigma^{\mathcal{P},\mathcal{Q}}_{[r',s];t}, \tag{6.130}$$

for all $0 \le r \le r' \le s \le t$.

Note that in Equations (6.129)–(6.130), the conditional expectation is done over trajectories which have a *future* constraint, as $[r', s]$ comes after $[r, r']$. In other words, the generalized Σ-stochastic entropic functionals *conditionally increase backwards in time* when looking at the initial time of the scanned interval $[r, s]$. As we will show below in Section 9.1.4, the backward martingale structure of $\exp(-\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s];t})$ is instrumental to recover some traditional formulations of the second law of thermodynamics and derive also new universal principles.

Taken all together, we conclude that the generalized Σ-entropic functionals on $[r, s] \subseteq [0, t]$ have a "two-faced" martingale structure. They are *forward submartingales* with respect to the final time s and *backward submartingales* with respect to the initial time r. In other words, $\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s]}$ conditionally increases with respect to s and conditionally decreases with respect to r.

6.3.4. *Generalized Σ-stochastic entropic functional for Markovian processes*

We discuss generalized Σ-stochastic entropic functionals for Markovian processes. The Markov property implies:

- First, a decomposition of the generalized Σ-stochastic entropic functional in terms of the environmental $\mathcal{Q}$-stochastic entropy change, as defined in (6.27), and a boundary term:

$$\Sigma^{\mathcal{P},\mathcal{Q}}_{[0,s],t} = \ln\left(\frac{\rho_0\left(X_0\right)}{\rho^{\mathcal{Q}^{(t)}}_{t-s}\left(X_s\right)}\right) + S^{\mathrm{env},\mathcal{P},\widehat{\mathcal{Q}}^{(t,s)}}_s, \tag{6.131}$$

for all $0 \le s \le t$. In this relation, the environment entropy change $S^{\mathrm{env},\mathcal{P},\widehat{\mathcal{Q}}^{(t,s)}}_s$ is (6.27)

$$S^{\mathrm{env},\mathcal{P},\widehat{\mathcal{Q}}^{(t,s)}}_s = \ln\left(\frac{\mathcal{P}_{[0,s]}\left(X_{[0,s]}\middle| X_0\right)}{\left[\widehat{\mathcal{Q}}^{(t,s)}\right]_{[0,s]}\left(\Theta_s X_{[0,s]}\middle| X_s\right)}\right), \tag{6.132}$$

with the path probability $\widehat{\mathcal{Q}}^{(t,s)}$ is defined by iterating the reversed protocol, see Equation (6.6), twice, viz.,

$$\widehat{\mathcal{Q}}^{(t,s)} \equiv \widetilde{\widetilde{\mathcal{Q}^{(t)}}^{(t)}}^{(s)}, \tag{6.133}$$

where we recall that in Section 6.1, we defined the measure $\widetilde{\mathcal{Q}}^{(t)}$ as time-reversed protocol of the path measure $\mathcal{Q}$ with respect to the reference time t. This apparently-complicated object $\widehat{\mathcal{Q}}^{(t,s)}$ is in fact the path probability of a Markovian process with generator

$$\left(\mathcal{L}^{\widehat{\mathcal{Q}}^{(t,s)}}\right)_u = \left(\mathcal{L}^{\left(\widetilde{\mathcal{Q}}^{(t)}\right)}\right)_{s-u} = \mathcal{L}_{t-s+u}, \tag{6.134}$$

for all $0 \le u \le s \le t$. In other words, the iteration of two reversed protocols is just a time translation.

The relation (6.131) follows from the equality

$$\mathcal{Q}^{(t)}_{[t-s,t]}\left(\Theta_t X_{[0,t]}\right) = \rho^{\mathcal{Q}^{(t)}}_{t-s}\left(X_s\right)\left[\widehat{\mathcal{Q}}^{(t,s)}\right]_{[0,s]}\left(\Theta_s X_{[0,s]}\middle| X_s\right), \tag{6.135}$$

which holds for all $0 \le r \le s \le t$. We advice readers to prove the relation (6.135) for Langevin systems with additive noise by using the Lagrangian given by Equation (3.97).

- Second, the factorization of the path probability resulting from Markov property permits to obtain for all $0 \leq r \leq s \leq t$ the decomposition formulae of generalized Σ-stochastic entropic functional [11]:

$$\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t} = \ln\left(\frac{\rho_r\,(X_r)}{\rho^{\mathcal{Q}^{(t)}}_{t-r}\,(X_r)}\right) + \Sigma^{\mathcal{P},\mathcal{Q}}_{[0,s],t} - \Sigma^{\mathcal{P},\mathcal{Q}}_{[0,r],t}. \tag{6.138}$$

Combining Equations (6.131) and (6.138), we obtain the general formulae

$$\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t} = \ln\left(\frac{\rho_r\,(X_r)}{\rho^{\mathcal{Q}^{(t)}}_{t-s}\,(X_s)}\right) + S^{env,\mathcal{P},\widehat{\mathcal{Q}}^{(t,s)}}_s - S^{env,\mathcal{P},\widehat{\mathcal{Q}}^{(t,r)}}_r. \tag{6.139}$$

Moreover, using the decomposition (6.27) of the $\mathcal{Q}$-stochastic entropy production, the relation (6.139) can also be written as a $\mathcal{Q}$-stochastic entropy production

$$\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t} = \ln\left(\frac{\rho_s\,(X_s)}{\rho^{\mathcal{Q}^{(t)}}_{t-s}\,(X_s)}\right) + S^{\mathcal{P},\widehat{\mathcal{Q}}^{(t,s)}}_s - S^{\mathcal{P},\widehat{\mathcal{Q}}^{(t,r)}}_r. \tag{6.140}$$

Equations (6.139) and (6.140) provide an interpretation of the generalized Σ-stochastic entropic functional for Markovian processes. Moreover, the forward and backward martingale properties of $\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t}$ proven in this chapter imply that the right-hand side of (6.139) and (6.140) have the same martingale structure.

Specializing the relation (6.55) to the particular case $\mathcal{Q}^{(t)} = \widetilde{\mathcal{P}}^{(t)}$ gives that $\widehat{\mathcal{Q}}^{(t,s)} = \widetilde{\mathcal{P}}^{(s)}$ and $\widehat{\mathcal{Q}}^{(t,r)} = \widetilde{\mathcal{P}}^{(r)}$, and then Equation (6.139) yields

$$\Sigma^{\mathcal{P},\widetilde{\mathcal{P}}^{(t)}}_{[r,s],t} = \underbrace{\ln\left(\frac{\rho_r\,(X_r)}{\widetilde{\rho}^{(t)}_{t-s}\,(X_s)}\right)}_{\equiv \alpha^{(t)}_{r,s}} + S^{\rm env}_s - S^{\rm env}_r, \tag{6.141}$$

for all $0 \leq r \leq s \leq t$, where S^{env}_s is the environment entropy change defined in Equation (6.32), and where

$$\alpha^{(t)}_{r,s} \equiv \ln\left(\frac{\rho_r\,(X_r)}{\widetilde{\rho}^{(t)}_{t-s}\,(X_s)}\right). \tag{6.142}$$

The martingale property of $\exp(-\Sigma^{\mathcal{P},\widetilde{\mathcal{P}}^{(t)}}_{[r,s],t})$ allows us to retrieve the theory of Ref. [14] (see Chapter 8.2) within the general context of generalized Σ-stochastic entropic functionals. The generalized integral fluctuation relations (6.120) read here

$$\left\langle \exp\left(-S^{\rm env}_s + S^{\rm env}_r - \alpha^{(t)}_{s,r}\right)\right\rangle = 1, \tag{6.143}$$

for all $0 \leq r \leq s \leq t$.

Lastly, by using the decomposition (6.33) of total entropy production, the relation (6.141) can also be written for all $0 \leq r \leq s \leq t$.

$$\Sigma^{\mathcal{P},\widetilde{\mathcal{P}}^{(t)}}_{[r,s];t} = \underbrace{\ln\left(\frac{\rho_s(X_s)}{\tilde{\rho}^{(t)}_{t-s}(X_s)}\right)}_{\delta^{(t)}_s} + S^{\rm tot}_s - S^{\rm tot}_r, \tag{6.144}$$

where the stochastic distinguishability $\delta^{(t)}_s$ was defined in relation (6.105). This time, the induced martingality property of the right-hand side allows to retrieve the results (6.104) and (6.105) (see also Ref. [15]). Moreover, the generalized integral fluctuation theorems (6.120) become here

$$\left\langle \exp\left(-S^{\rm tot}_s + S^{\rm tot}_r - \delta^{(t)}_s\right)\right\rangle = 1, \tag{6.145}$$

for all $0 \leq r \leq s \leq t$.

To give examples, the relation (6.141) for the case of multidimensional Langevin process described by Equation (3.65) reads

$$\Sigma^{\mathcal{P},\widetilde{\mathcal{P}}^{(t)}}_{[r,s],t} = \underbrace{\ln\left(\frac{\rho_r\,(X_r)}{\tilde{\rho}^{(t)}_{t-s}\,(X_s)}\right)}_{\alpha^{(t)}_{r,s}} + \underbrace{\int_r^s \left(\left(\boldsymbol{\mu}_u F_u\right)\mathbf{D}_u^{-1}\right)(X_u) \circ \dot{X}_u\,\mathrm{d}u}_{S^{\rm env}_s - S^{\rm env}_r}. \tag{6.146}$$

In Section 8.2, we will give another proof of the martingale property of $\exp(-\Sigma^{\mathcal{P},\widetilde{\mathcal{P}}^{(t)}}_{[r,s],t})$ in this setup. For general jump processes, the relation (6.141) becomes

$$\Sigma^{\mathcal{P},\widetilde{\mathcal{P}}^{(t)}}_{[r,s];t} = \underbrace{\ln\left(\frac{\rho_r\,(X_r)}{\tilde{\rho}^{(t)}_{t-s}(X_s)}\right)}_{\alpha^{(t)}_{r,s}} + \underbrace{\sum_{j|r\leq\mathcal{T}_j\leq s} \ln\left(\frac{\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}{\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}, X_{\mathcal{T}_j^-})}\right)}_{S^{\rm env}_s - S^{\rm env}_r}. \tag{6.147}$$

Chapter 7. Martingales in stochastic thermodynamics III: Stationary states

As far as we know today, there is no automatic, permanently effective perpetual motion machine, in spite of the molecular fluctuations, but such a device might, perhaps, function regularly if it were appropriately operated by intelligent beings..

Smoluchowski, Vorträge über die kinetische Theorie der Materie u. Elektrizitat, (1914, p.89).

In this chapter, we show how several classical results of stochastic thermodynamics can be significantly improved with martingale theory. In particular, we derive more general versions of the second law of thermodynamics and fluctuation relations. Moreover, using the powerful technology of martingales, as discussed in Chapters 2, 3, and 4, we exactly describe certain fluctuation properties of entropy production, notably, for their infima, first-passage times, and splitting probabilities. Lastly, we discuss how these results can be used to (apparently) overcome classical thermodynamic limits by cleverly exploiting the fluctuations in a stochastic process.

7.1. *Setup: nonequilibrium stationary states*

Throughout this chapter, we focus on time-homogeneous, stationary processes. Figure 7.1 depicts two paradigmatic examples of such processes. Figure 7.1(a) shows a Brownian particle that moves in a periodic potential under the action of a constant, non-conservative force. The non-conservative force induces a net current along the ring, which results in a net dissipation of heat to the environment. Since the process is stationary, we assume that the initial distribution of the system is given by its nonequilibrium, stationary distribution.

Further examples of physical systems belonging to this class are, e.g., systems described by multidimensional Langevin equations and stationary Markov-jump processes. See Figure 7.1(b) for a many-particle example relevant in the study of active matter systems [175] and the inset in Figure 5.3(a) for sketches of some other multidimensional overdamped Langevin models.

The general philosophy of the chapter goes as follows: we assume from the get-go that X is a stationary, stochastic process for which the exponentiated, negative, total entropy production during $[0, t]$ takes the form (6.33)

$$\exp(-S_t^{\mathrm{tot}}) = \frac{(\mathcal{P} \circ \Theta_t)(X_{[0,t]})}{\mathcal{P}(X_{[0,t]})}. \tag{7.1}$$

Consequently, as shown in Chapters 5 and 6, $\exp(-S_t^{\mathrm{tot}})$ is a martingale (because of stationarity), which is a fundamental fact in nonequilibrium thermodynamics. Subsequently, we derive various results based on the martingality of $\exp(-S_t^{\mathrm{tot}})$.

Note that Equation (7.1) could also describe the thermodynamics of active matter systems, as long as X describes the trajectories of all degrees of freedom that are driven out of equilibrium (in the example of Panel(b) in Figure 7.1, this involves the dynamics of both the gray and white spheres).

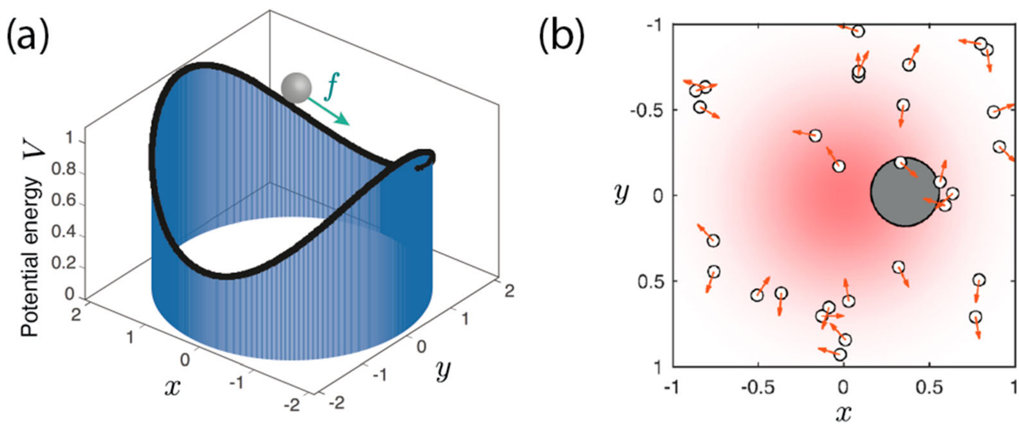

Figure 7.1. Panel (a): Illustration of a paradigmatic, single-particle model for a nonequilibrium, time-homogeneous, stationary process. A Brownian particle (gray sphere) moves on top of a “rollercoaster” potential under the action of an external, constant, force *f*. Figure adapted from Ref. [11]. For the special case of a flat potential, this model is equivalent to a driven particle on a ring, as illustrated in Figure 1.6. Panel (b): Illustration of a many-particle model for a nonequilibrium, time-homogeneous, stationary process. An overdamped Brownian particle (gray sphere) immersed in a fluid with periodic boundary conditions is trapped within a potential (red). The particle interacts with an ensemble of $N > 1$ overdamped “active” Brownian particles (white circles) that are self-propelled in randomly-varying directions (red arrows); see Ref. [175] for a study of thermodynamics in active matter systems.

We start this chapter with Section 7.2 that summarizes results in conventional stochastic thermodynamics, and which forms a useful point of reference for the more general results that follow from martingale theory and are derived in the later sections of this chapter. Subsequently, in Section 7.3, following Refs. [10,11,13,28,98], we review some of the central results from martingale theory for thermodynamics, namely, the martingale versions of the fluctuation relations and the ensuing versions of the second law of thermodynamics. In Section 7.4, we review results on splitting probabilities, and the statistics of first-passage times, and extreme values of entropy production, taken mainly from Refs. [11,13]. Next we review thermodynamic bounds on first-passage times of dissipative currents, taken from Refs. [32,34,35,177,178]. Section 7.5 discusses an application, namely how to overcome classical limits on thermodynamic processes by stopping a stochastic process at a cleverly chosen moment [13].

7.2. *Conventional fluctuation relations*

Fluctuation relations are mathematical relations that constrain the statistics of stochastic thermodynamic quantities. These results were introduced in the 1990s and are also referred to as fluctuation theorems, see Refs. [26,27,139,141,152,161,168] for some classical references. Here we review some celebrated fluctuation relations that are generic for time-homogeneous, nonequilibrium, stationary states.

The detailed fluctuation relation,

$$\frac{\rho_{S_t^{\rm tot}}(s)}{\rho_{S_t^{\rm tot}}(-s)} = \exp(s), \tag{7.2}$$

states that in a stationary process the probability density of the stochastic entropy production evaluated at $S_t^{\rm tot} = s > 0$ is exponentially larger than the probability density evaluated at $S^{\rm tot} = -s < 0$; note that this is a special case of Equation (6.23) valid for the total, stochastic, entropy production of a nonequilibrium stationary state. The mathematical derivation of fluctuation relations can be found in Chapter 6 of this treatise, see Equation (6.23) with (6.31) and (6.33).

From Equation (7.2) follows the integral fluctuation relation

$$\langle \exp(-S_t^{\rm tot}) \rangle = \int_{-\infty}^{\infty} {\rm d}s \rho_{S_t^{\rm tot}}(s) \exp(-s) = \int_{-\infty}^{\infty} {\rm d}s\, \rho_{S_t^{\rm tot}}(-s) = 1. \tag{7.3}$$

Applying Jensen's inequality

$$\langle \exp(-X) \rangle \geq \exp(-\langle X \rangle) \tag{7.4}$$

to $X = S_t^{\rm tot}$, we obtain the second law of stochastic thermodynamics

$$\langle S_t^{\rm tot} \rangle \geq 0, \tag{7.5}$$

which is illustrated in Figure 7.2. For stationary systems, the stronger version

$$\langle \dot{S}_t^{\rm tot} \rangle \geq 0, \tag{7.6}$$

of the second law holds, because $\langle \dot{S}_t^{\rm tot} \rangle = \langle \dot{S}_0^{\rm tot} \rangle = \langle S_t^{\rm tot} \rangle / t \geq 0$.

Another interesting consequence of the integral fluctuation relation is that negative fluctuations of entropy must exist in nonequilibrium processes. Applying Markov's inequality

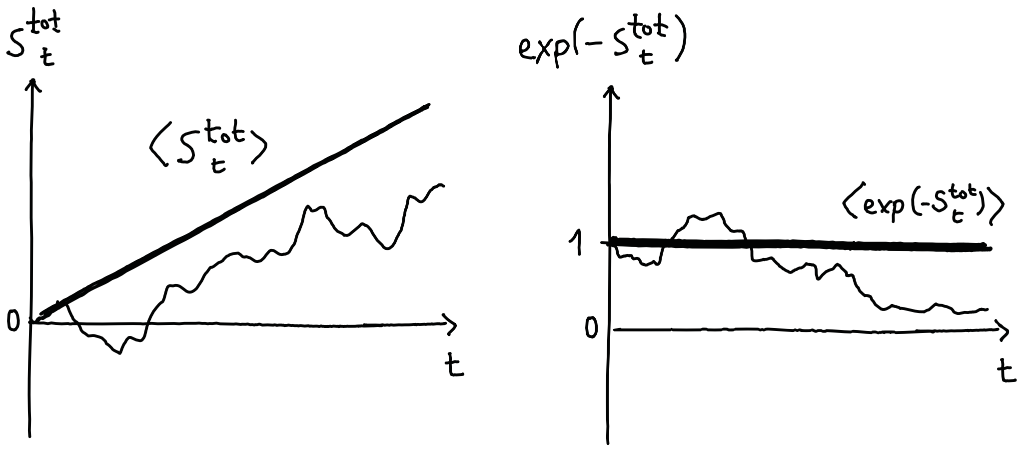

Figure 7.2. Illustration of the (classic) second law of thermodynamics $\langle S_t^{\text{tot}}\rangle \geq 0$ and the (classic) integral fluctuation relation $\langle \exp(-S_t^{\text{tot}})\rangle = 1$. We sketch a single trajectory of the stochastic entropy production S_t^{tot} (left, thin lines) and of its negative exponential $\exp(-S_t^{\text{tot}})$ (right, thin line) in nonequilibrium stationary states. The thick lines in both panels illustrate the values of S_t^{tot} (left panel) and $\exp(-S_t^{\text{tot}})$ (right panel) averaged over many different realizations.

equation (4.17) to $A = \exp(-S_t^{\text{tot}})$ and using the integral fluctuation relation, we obtain the constraint [26]

$$\mathcal{P}\left(S_t^{\text{tot}} \leq -s\right) \leq \exp(-s), \quad \text{for} \quad s \geq 0, \tag{7.7}$$

on negative fluctuations of entropy production.

In what follows, we use martingales to significantly extend these classical results from stochastic thermodynamics, i.e., the second law of thermodynamics (7.5), the integral fluctuation relation (7.3), and the bound on negative fluctuations of entropy (7.7).

7.3. *Martingale fluctuation relations and martingale versions of the second law*

7.3.1. *Martingale integral fluctuation relations*

We derive extensions for the integral fluctuation relation (7.3) that follow from martingale theory [13].

As the exponentiated, negative, entropy production is a martingale, the relation (6.61) implies that [10,11]

$$\langle \exp(-S_t^{\text{tot}}) \,|\, X_{[0,s]} \rangle = \exp(-S_s^{\text{tot}}), \tag{7.8}$$

which is known as the **martingale integral fluctuation relation**.

We provide an illustration of the martingale integral fluctuation relation (7.8) in Figure 7.3.

According to Theorem 13, the martingale integral fluctuation relation (7.8) is equivalent to the following integral fluctuation relation at *stopping times*.

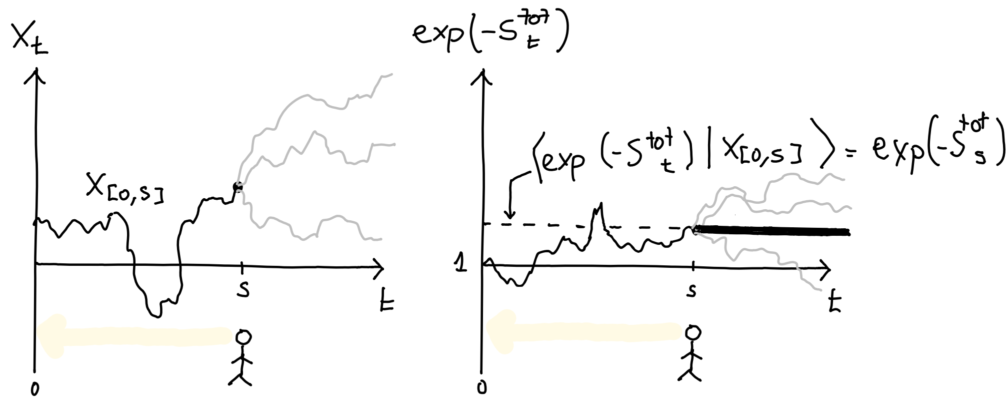

Figure 7.3. Sketch of the martingale integral fluctuation relation given in Equation (7.8). Left: An observer tracks the evolution of a process up to time s, recording a stochastic trajectory $X_{[0,s]}$ (black line). The evolution of the process at later times, given $X_{[0,s]}$, is stochastic and can have different outcomes (gray lines). Right: Given $X_{[0,s]}$, the value of the exponentiated negative entropy production is known up to time s. The martingale condition (7.8) implies that future average values of $\exp(-S_t^{\rm tot})$ for $t \geq s$, given $X_{[0,s]}$, remain constant and equal to the value $\exp(-S_s^{\rm tot})$ (black thick horizontal line).

Applying Doob's optional stopping theorems (see Section 4.1.5) to $\exp(-S_t^{\rm tot})$, we obtain the **integral fluctuation relations at stopping times**

$$\langle \exp(-S_{\mathcal{T}}^{\rm tot})\rangle = 1, \tag{7.9}$$

which holds when either the stopping time $\mathcal{T}$ is bounded or $\mathcal{T}$ is with probability 1 finite and $S_t^{\rm tot}$ is bounded for all $t < \mathcal{T}$.

The integral fluctuation relations at stopping times reveal a new level of universality, as they hold for stopping times satisfying one of the following two conditions:

- $\mathcal{T} \in [0, t_0]$ for a fixed time $t_0 \in \mathbb{R}^+$;
- $\mathcal{P}(\mathcal{T} < \infty) = 1$ and $|S_t^{\rm tot}| < c$ for all $t \in [0, \mathcal{T}]$.

Later in this chapter, we determine the statistics of extreme values of entropy production and the splitting probabilities of entropy production by specializing the integral fluctuation relation at stopping times (7.9) to specific classes of stopping times. But, first we use in the next section the martingale fluctuation relations to derive martingale versions of the second law of thermodynamics.

7.3.2. *Martingale versions of the second law of thermodynamics*

Although the second law of thermodynamics (7.6) implies that on average the entropy of the universe increases, this result is not entirely satisfactory. Indeed, since for mesoscopic systems negative fluctuations of entropy production exist, as implied in Equation (7.3), it is not excluded that an intelligent being, say a demon, can anticipate when entropy decreases, and this question has puzzled physicists [179,180]. However, the following two martingale versions of the second law of thermodynamics state that negative fluctuations of entropy cannot be anticipated.

Since S_t^{tot} is a submartingale, the relation (6.62) implies the **conditional strong second law** of thermodynamics, i.e.,

$$\langle S_t^{\text{tot}} \,|\, X_{[0,s]} \rangle \geq S_s^{\text{tot}}. \tag{7.10}$$

Taking the average over $X_{[0,s]}$ in Equation (7.10), we readily obtain the "classical" second law of stochastic thermodynamics given in Equation (7.5).

Applying Jensen's inequality (7.4) for $X = S_{\mathcal{T}}^{\text{tot}}$ to Equation (7.9), we obtain the **second law of thermodynamics at stopping times**, viz.,

$$\langle S_{\mathcal{T}}^{\text{tot}} \rangle \geq 0. \tag{7.11}$$

Note that the martingale version of the second law, Equation (7.10), implies the second law (7.5) and is a significantly stronger result. Even though in stochastic processes negative fluctuations of entropy production exist, according to the martingale second law, Equation (7.10), an observer cannot anticipate those so-called transient "violations" of the second law based on the past history $X_{[0,s]}$ of the process! Hence, Equation (7.10) is a stochastic version of the second law of thermodynamics, in the same way that (5.6) is a stochastic version of the first law of thermodynamics.

The second law of thermodynamics at stopping times provides a different, but equivalent, perspective: an observer cannot reduce entropy by stopping the processes at a cleverly chosen moment.

We illustrate the second law at stopping times (7.11) in Figure 7.4 for the example of non-interacting colloidal particles moving in a two-dimensional fluid under the influence of a force field. In this example, the stopping time is the first exit time of a particle from a circle centered at the initial position of the particles and with a fixed positive radius.

7.4. *Statistics of stopping times and extreme values*

We review several results on stopping times and extreme values in stationary processes.

7.4.1. *Splitting probabilities for entropy production*

In the present section, the stopping time $\mathcal{T}$ determines the stopping problem

$$\mathcal{T} \equiv \left\{ t \geq 0 : S_t^{\text{tot}} \notin (-s_-, s_+) \right\}, \tag{7.12}$$

where $s_-, s_+ \geq 0$, and we denote the corresponding splitting probabilities by

$$P_+(s_+, s_-) \equiv \mathcal{P}\left(S_{\mathcal{T}}^{\text{tot}} \geq s_+\right) \quad \text{and} \quad P_-(s_+, s_-) \equiv \mathcal{P}\left(S_{\mathcal{T}}^{\text{tot}} \leq -s_-\right). \tag{7.13}$$

The stopping problem equation (7.12) is illustrated in Figure 7.5. Following [11,13], we derive now explicit expressions for P_+ and P_-.

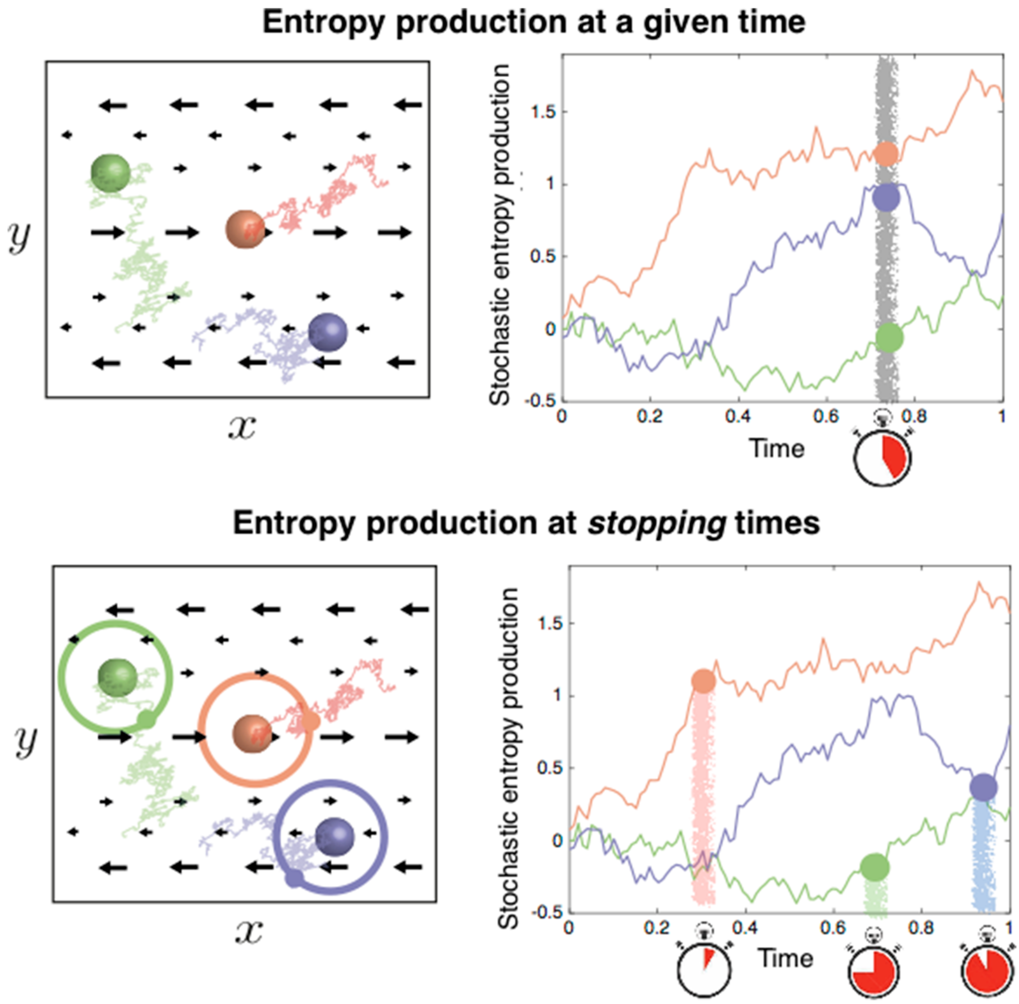

Figure 7.4. Illustration of the implications of the second law of thermodynamics at fixed times and stopping times. Top left: Illustration of three stochastic trajectories drawn from a nonequilibrium stationary state (force field in black arrows). Top right: Stochastic entropy production associated with the three trajectories. Their value at a fixed time (clock) is, according to the second law $\langle S_t^{\rm tot}\rangle \geq 0$, on average positive. Bottom left: Illustration of three trajectories that are "stopped" when they cross a circle of a given radius centered at their initial position (rings). Bottom right: The stochastic entropy production along the stopped trajectories. We highlight in filled circles the values that $S_T^{\rm tot}$ takes when the particles cross the circle. Their average over many trajectories obeys the second law at stopping times $\langle S_T^{\rm tot}\rangle \geq 0$.

For nonequilibrium stationary states, $S_t^{\rm tot}$ grows indefinitely, and hence

$$P_+(s_+, s_-) + P_-(s_+, s_-) = 1. \tag{7.14}$$

Moreover, using the integral fluctuation relation at stopping times, Equation (7.9), on the stopping time (7.12) we obtain

$$P_+(s_+, s_-)\langle \exp(-S_T^{\rm tot})\rangle_+ + P_-(s_+, s_-)\langle \exp(-S_T^{\rm tot})\rangle_- = 1. \tag{7.15}$$

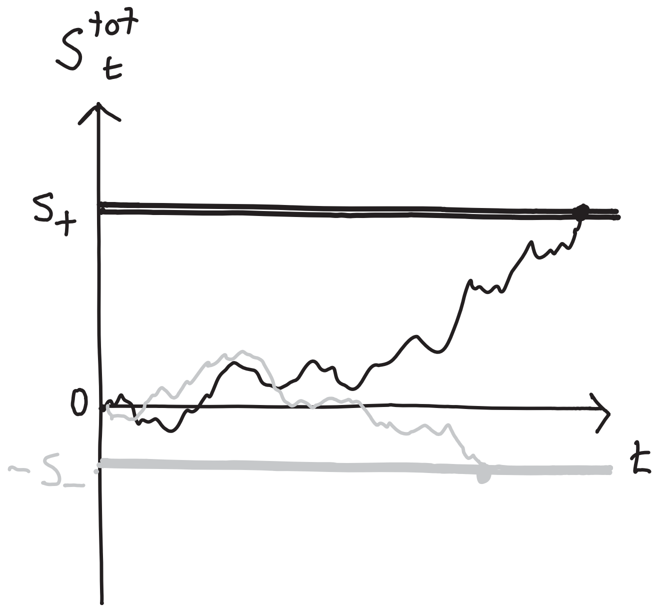

Figure 7.5. Illustration of two trajectories of stochastic entropy production escaping from the interval $(-s_-, s_+)$ through the positive threshold (black line) and through the negative threshold (gray line).

Here, we have introduced the conditional averages

$$\langle\cdot\rangle_+ = \langle\cdot|S_{\mathcal{T}}^{\text{tot}} \geq s_+\rangle, \text{ and } \langle\cdot\rangle_- = \langle\cdot|S_{\mathcal{T}}^{\text{tot}} \leq -s_-\rangle. \tag{7.16}$$

Solving the set of Equations (7.14)–(7.15), we obtain the solution

$$P_+(s_+, s_-) = \frac{\langle\exp(-S_{\mathcal{T}}^{\text{tot}})\rangle_- - 1}{\langle\exp(-S_{\mathcal{T}}^{\text{tot}})\rangle_- - \langle\exp(-S_{\mathcal{T}}^{\text{tot}})\rangle_+} \tag{7.17}$$

and

$$P_-(s_+, s_-) = \frac{1 - \langle\exp(-S_{\mathcal{T}}^{\text{tot}})\rangle_+}{\langle\exp(-S_{\mathcal{T}}^{\text{tot}})\rangle_- - \langle\exp(-S_{\mathcal{T}}^{\text{tot}})\rangle_+}. \tag{7.18}$$

For time-homogeneous, stationary states with $S_{\mathcal{T}}^{\text{tot}} \in \{-s_-, s_+\}$, which includes diffusion processes for which S_t^{tot} is continuous in t, we obtain the following **universal** expressions for the **splitting probabilities of entropy production**,

$$P_+(s_+, s_-) = \frac{\exp(s_-) - 1}{\exp(s_-) - \exp(-s_+)} \tag{7.19}$$

and

$$P_-(s_+, s_-) = \frac{1 - \exp(-s_+)}{\exp(s_-) - \exp(-s_+)}. \tag{7.20}$$

Remarkably, the splitting probabilities are independent of the finite-time moments of entropy production, such as the rate of entropy production; the universality of splitting probabilities can also be understood with the random time transformation discussed in Section 5.2.3.

Note that the **splitting-probability fluctuation relation**

$$\frac{P_-(s_+, s_-)}{P_+(s_-, s_+)} = \exp(-s_-) \tag{7.21}$$

holds, which is reminiscent of the detailed fluctuation relation (7.2). However, contrarily to the detailed fluctuation relation, the splitting probability fluctuation relation compares the splitting probabilities P_- and P_+ in two different stopping problems, except when $s_- = s_+ = s$ in which case we obtain

$$\frac{P_-(s, s)}{P_+(s, s)} = \exp(-s). \tag{7.22}$$

For processes with jumps, we do not obtain universal expressions for P_- and P_+, in correspondence with the results in Section 5.4.2. Nevertheless, we can derive universal bounds on P_- and P_+.

Using that $\langle \exp(-S^{\text{tot}}_{\mathcal{T}}) \rangle_+ \leq \exp(-s_+)$ and $\langle \exp(-S^{\text{tot}}_{\mathcal{T}}) \rangle_- \geq \exp(s_-)$, we obtain from Equations (7.17) and (7.18) the following **universal bounds on splitting probabilities**:

$$P_+(s_+, s_-) \geq 1 - \frac{1}{\exp(s_-) - \exp(-s_+)} \tag{7.23}$$

and

$$P_-(s_+, s_-) \leq \frac{1}{\exp(s_-) - \exp(-s_+)}, \tag{7.24}$$

which hold for time-homogeneous, stationary states.

Another interesting quantity is the survival probability $P_{\text{surv}}(\tau)$ for S^{tot} to stay below a positive threshold $s_+ > 0$ in a finite time $\tau \geq 0$. This survival probability can be tackled by specializing the integral fluctuation theorem at stopping times for $T_{\text{surv}} = \mathcal{T} \wedge \tau = \min(\mathcal{T}, \tau)$, with $\mathcal{T}$ the first-passage time to reach the threshold s_+ with $s_- \gg 1$. Following analogous steps as for $\mathcal{T}$, we get

$$P_{\text{surv}}(\tau) = \frac{\langle \exp(-S^{\text{tot}}_{\mathcal{T}}) \rangle - 1}{\langle \exp(-S^{\text{tot}}_{\mathcal{T}}) \rangle - \langle \exp(-S^{\text{tot}}_{\tau}) \rangle_{\text{surv}}}, \tag{7.25}$$

where $\langle \cdot \rangle_{\text{surv}}$ denotes an average over all the trajectories that did not cross the threshold in the finite-time interval of duration τ.

7.4.2. *Extreme-value statistics of entropy production*

The results obtained in Section 7.4.1 for the splitting probabilities can be used to determine the extreme-value statistics of entropy production.

The global infimum of entropy production, defined by

$$S^{\text{inf}} \equiv \inf_{t \geq 0} S_t^{\text{tot}}, \tag{7.26}$$

is the largest lower bound of entropy production along a trajectory. Because $S_0^{\text{tot}} = 0$, S^{inf} can only take nonpositive values, i.e., $S^{\text{inf}} \leq 0$. We use martingale theory to determine the statistical properties of the global infimum of entropy production.

First we tackle the cumulative distribution of S^{inf}. The probability $\mathcal{P}(S^{\text{inf}} \leq -s)$ that the infimum S^{inf} is smaller or equal than $-s$, with $s > 0$, equals the probability that entropy production crosses at any time $t \geq 0$ an absorbing boundary located at $-s$.

> Taking the limit $s_- \to s$ and $s_+ \to \infty$ in the right-hand side of Equation (7.24), gives the **universal bound**
>
> $$P(S^{\text{inf}} \leq -s) \leq \exp(-s), \quad \text{for} \quad s \geq 0, \tag{7.27}$$
>
> on **extreme negative fluctuations of entropy production**.

The bound equation (7.27) from martingale theory should be compared with the weaker bound equation (7.7) from "classical" stochastic thermodynamics [26]. In this regard, note that Equation (7.27) is a stronger result as $S^{\text{inf}} \leq S_t$ for all values of t. Moreover, for stationary diffusion processes the equality in the bound equation (7.27) is attained, and the bound is thus as good as it gets. Indeed, taking the limit $s_- \to s$ and $s_+ \to \infty$ of the right-hand side in Equation (7.20), we obtain

$$P(S^{\text{inf}} \leq -s) = \exp(-s). \tag{7.28}$$

Equation (7.28) implies that the entropy-production global infimum in a continuous stochastic process follows an exponential distribution with mean equal to -1, i.e.,

$$\rho_{S^{\text{inf}}}(s) = \exp(s), \quad \forall s \leq 0. \tag{7.29}$$

From the bound equation (7.27), we obtain a second-law-like relation on the infimum of entropy production that was coined the infimum law in Ref. [11].

> The inequality equation (7.27) implies the **infimum law**
>
> $$\langle S^{\text{inf}} \rangle \geq -1, \tag{7.30}$$
>
> where the equality is attained for driven diffusion processes (i.e., when X_t is a continuous process in t).

The bound equations (7.27) on extreme negative fluctuations of entropy production and the infimum law (7.30) are illustrated in Figure 7.6 for the one-dimensional Langevin process of Equation (5.3) with periodic boundary conditions, potential $V(x) = T \ln(\cos(x) + 2)$, and constant external force $f_t = f$.

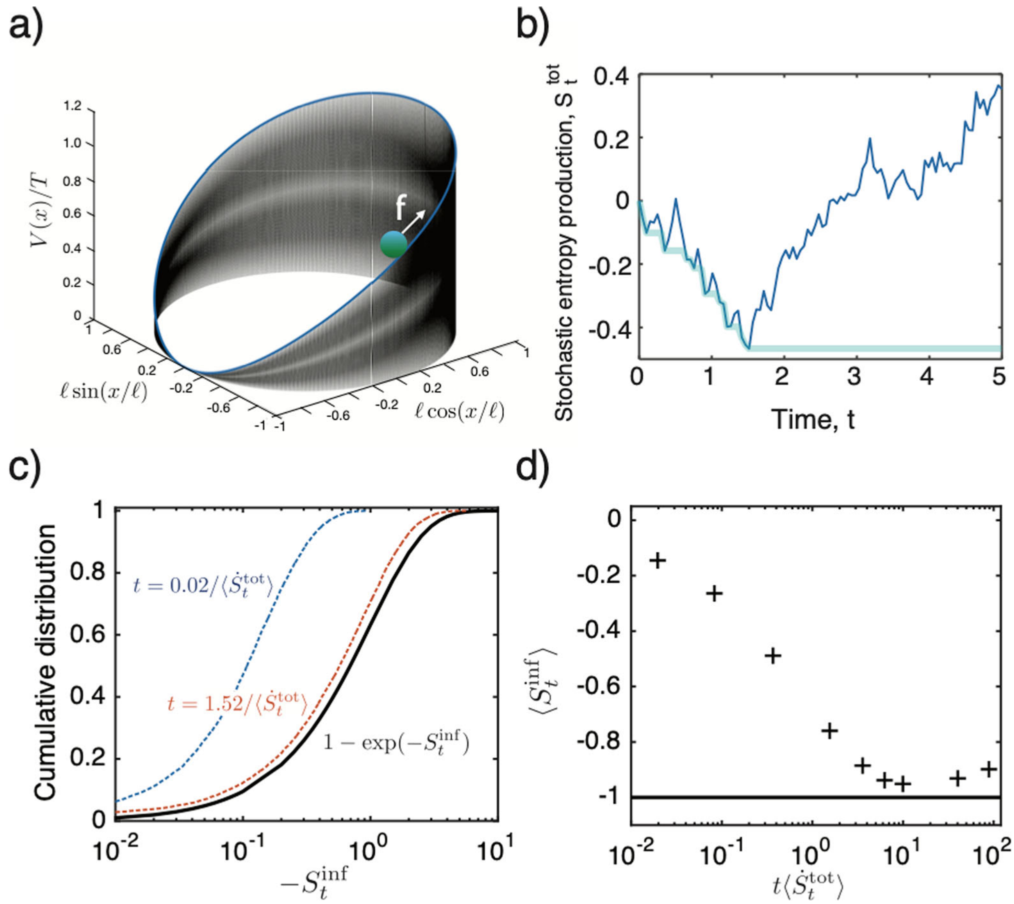

Figure 7.6. Illustration of the universal bounds on the statistics of extreme values of entropy production in the one-dimensional Langevin process described in Equation (5.3) with periodic boundary conditions, constant external force f, and potential $V(x) = T\ln(\cos(x) + 2)$. Panel (a): Graphical illustration of the model. Panel (b): Example trajectory of the stochastic entropy production S_t^{tot} associated with a stochastic trajectory of the particle position (blue thin line). The finite time infimum S_t^{inf} of entropy production associated with the stochastic trajectory of S_t^{tot} is shown in thick cyan line. Panel (c): Cumulative distribution of the entropy production finite-time infimum S_t^{inf} for different values of t (in units of the rate of entropy production $\langle \dot{S}^{tot}\rangle$) obtained from simulations, see legend. The dashed lines are obtained from numerical simulations of the model shown in (a) and compared with the right-hand side of the universal bound from the infimum law (black thick line), Equation (7.32). Panel (d): Entropy production finite-time infimum S_t^{inf} averaged over many simulations, as a function of time t. See Ref. [11] for further details.

The universal bounds for the statistics of the global infimum of S_t^{tot} serve to tackle the statistics of the finite-time infimum of entropy production (also called *running minimum* in the random-walk literature [181]), defined as

$$S_t^{inf} \equiv \inf_{s\in[0,t]} S_s^{tot}, \tag{7.31}$$

and illustrated in Figure 7.7. Because the finite-time infimum is greater or equal than the global infimum $S_t^{\rm inf} \geq = \lim_{t\to\infty} S_t^{\rm inf} \equiv S^{\rm inf}$, Equations (7.27) and (7.30) imply respectively the universal bounds

$$P(S_t^{\rm inf} \leq -s) \leq \exp(-s), \quad \text{for} \quad s \geq 0, \tag{7.32}$$

and

$$\langle S_t^{\rm inf} \rangle \geq -1. \tag{7.33}$$

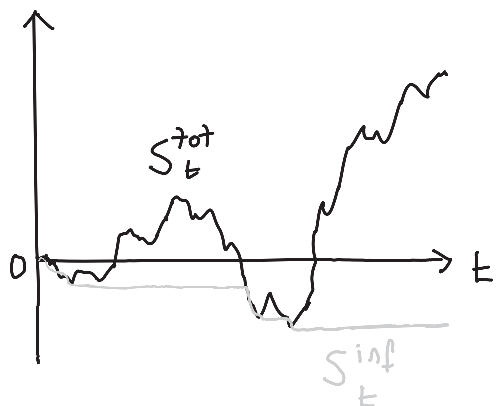

Figure 7.7. Illustration of a trajectory of stochastic entropy production $S_t^{\rm tot}$ (black line) and its finite-time infimum given in Equation (7.31).

Experimental tests of Equation (7.32) and the infimum law (7.33) have been reported in electronic double dots [33] and in a Brownian motor immersed in a granular gas [29]. In recent papers [32,182], the present arguments for the extreme values of entropy production have been extended to the case of arbitrary edge currents in a Markov jump process, and it was proven that the statistics of extreme values of a generic edge current are described by a geometric distribution characterized by an effective affinity. Moreover in Ref. [42], bounds tighter than the infimum law have been derived using Doob's L^p inequalities [45], and applied to bound the survival statistics of the work in steady-state heat engines.

7.4.2.1. *Negative fluctuations of entropy production on a ring.* With an illustrative example, we show that infima of entropy production are more effective in probing negative fluctuations of entropy production and testing fluctuation relations than classical results based on fixed time observables. For this, let us consider the unidimensional drift-diffusion process on a ring introduced in Equation (1.35), i.e.,

$$\dot{X}_t = \mu f + \sqrt{2\mu T}\dot{B}_t \tag{7.34}$$

This is in fact a particular example of Equation (5.3) for a conservative force that is homogeneous in time and space, i.e., $f_t(x) = f$. The entropy production solves Equation (5.42), i.e.,

$$\dot{S}_t^{\rm tot} = v^S + \sqrt{2v^S}\dot{B}_t, \tag{7.35}$$

with the homogeneous entropic drift given by

$$v^S = \frac{\mu f^2}{T}. \tag{7.36}$$

Thus for this example, $S_t^{\rm tot}$ is a drift-diffusion process with the distribution

$$\rho_{S_t^{\rm tot}}(s) = \frac{1}{\sqrt{4\pi v^S}} \exp\left(-\frac{(s - v^S t)^2}{4v^S}\right) \tag{7.37}$$

and with the cumulative distribution

$$\mathcal{P}\left(S_t^{\rm tot} \leq -s\right) = \frac{1}{2}\left(1 + {\rm erf}\left(\frac{s - v^S t}{2\sqrt{v^S}}\right)\right), \tag{7.38}$$

where ${\rm erf}(x) = (2/\sqrt{\pi}) \int_0^x \exp(-y^2) dy$ is the error function. On the other hand, the cumulative distribution of the entropy-production infimum is given by

$$\mathcal{P}\left(S_t^{\rm inf} \leq -s\right) = \frac{1}{2}\left(1 + {\rm erf}\left(\frac{s - v^S t}{2\sqrt{v^S t}}\right)\right) + \frac{\exp(s)}{2}\left(1 - {\rm erf}\left(\frac{-s - v^S t}{2\sqrt{v^S t}}\right)\right), \tag{7.39}$$

which follows from the exact expression for the infimum distribution of a 1D drift diffusion process [11].

Figure 7.8 shows the two cumulative distributions $\mathcal{P}(S_t^{\rm tot} \leq -s)$ and $\mathcal{P}(S_t^{\rm inf} \leq -s)$ and compares them with the exponential bounds (7.7) and (7.32), respectively. From Figure 7.8, it is apparent that Equation (7.7) is a loose bound for all values of t, while Equation (7.32) is tight in the limit of large t, as predicted by martingale theory. Also, note that the quality of the bound (7.7) worsens as a function of t.

7.4.3. *First-passage-time fluctuation relation for Langevin processes*

We review the first-passage-time fluctuation relations for entropy production in stationary Langevin processes [11]. This fluctuation relation considers the statistics of the first-passage-time equation (7.12) for symmetric thresholds $s_+ = s_- = s$.

To state the first-passage-time fluctuation relation, we define the following stopping times for entropy production (see Figure 7.9 for an illustration)

- $\mathcal{T}_+$ is the first time when $S_t^{\rm tot}$ reaches the positive threshold $s > 0$, given that $S_t^{\rm tot}$ did not pass below $-s_- = -s$ at earlier times $t' < t$; if $S_t^{\rm tot}$ escapes first through the negative threshold, then we set $\mathcal{T}_+ = \infty$.
- $\mathcal{T}_-$ is the first time when $S_t^{\rm tot}$ reaches the negative $-s < 0$, given that $S_t^{\rm tot}$ did not go above $s > 0$ at earlier times $t' < t$; if $S_t^{\rm tot}$ first escapes through the positive threshold, then $\mathcal{T}_- = \infty$.

Remarkably, the cumulative probabilities for $\mathcal{T}_+$ and $\mathcal{T}_-$ obey the relation

$$\frac{\mathcal{P}(\mathcal{T}_+ \leq t)}{\mathcal{P}(\mathcal{T}_- \leq t)} = \exp(s), \tag{7.40}$$

which holds for all $t \geq 0$ and for all $s \geq 0$.

We sketch a proof of Equation (7.40):

$$\mathcal{P}(\mathcal{T}_+ \leq t) = \langle \theta(t - \mathcal{T}_+) \rangle \tag{7.41}$$

$$= \int \mathcal{D}x_{[0,t]} \mathcal{P}(x_{[0,t]}) \theta(t - \mathcal{T}_+[x_{[0,t]}]) \tag{7.42}$$

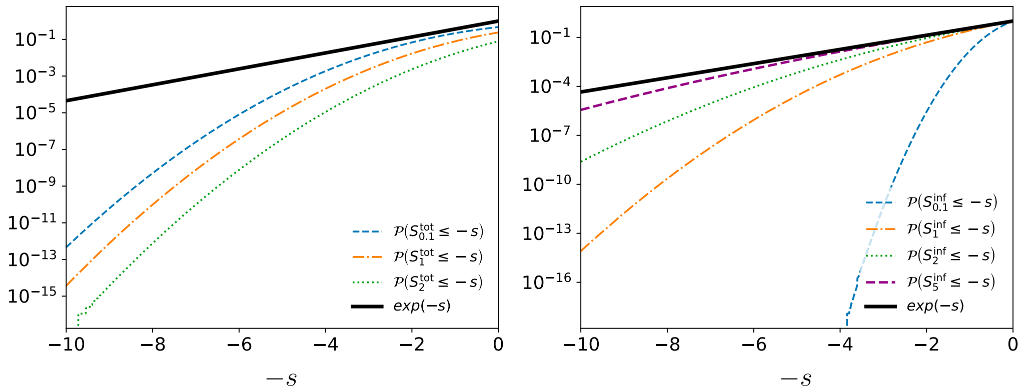

Figure 7.8. Comparison between the upper bounds on negative fluctuations of entropy production from classical stochastic thermodynamics (7.7) (left) and from martingale stochastic thermodynamics (7.27) (right) on the example of the drift-diffusion process on a ring described by Equation (7.34). Left: Plot of $\mathcal{P}(S_t^{\rm tot} \leq -s)$ from Equation (7.38) as a function of $-s < 0$ for $v^S = 1$ and given values of t, and comparison with the upper bound $\exp(-s)$. Right: Plot of $\mathcal{P}(S_t^{\rm inf} \leq -s)$ from Equation (7.39) as a function of $-s < 0$ for the same values of v^S and t as in the left panel, and comparison with the upper bound $\exp(-s)$ from thermodynamics with martingales, see Equation (7.32).

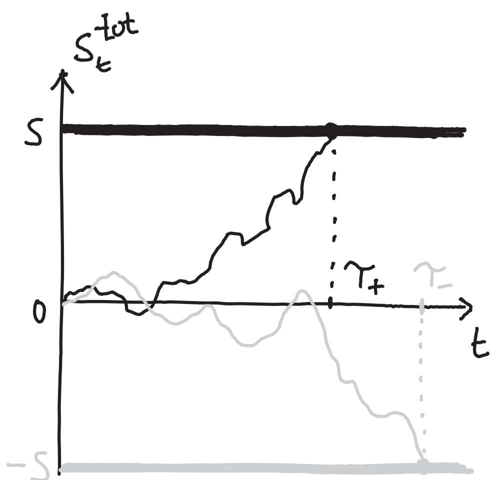

Figure 7.9. Illustration of the stopping times $\mathcal{T}_+$ and $\mathcal{T}_-$ for entropy production to first escape the interval $(-s, s)$ from its positive and negative boundaries, respectively.

$$= \int \mathcal{D}x_{[0,t]} \exp(S^{\text{tot}}(x_{[0,t]}))\mathcal{P}(\Theta_t x_{[0,t]})\theta(t - \mathcal{T}_+(x_{[0,t]})) \tag{7.43}$$

$$= \int \mathcal{D}x_{[0,t]} \exp(-S^{\text{tot}}(\Theta_t x_{[0,t]}))\mathcal{P}(\Theta_t x_{[0,t]})\theta(t - \mathcal{T}_-(\Theta_t x_{[0,t]})) \tag{7.44}$$

$$= \int \mathcal{D}x_{[0,t]} \exp(-S^{\text{tot}}(x_{[0,t]}))\mathcal{P}(x_{[0,t]})\theta(t - \mathcal{T}_-(x_{[0,t]})) \tag{7.45}$$

$$= \langle \exp(-S_t^{\text{tot}})|\mathcal{T}_- \leq t\rangle \mathcal{P}(\mathcal{T}_- \leq t) \tag{7.46}$$

$$= \langle \exp(-S_{\mathcal{T}_-}^{\text{tot}})\rangle \mathcal{P}(\mathcal{T}_- \leq t) \tag{7.47}$$

$$= \exp(s)\mathcal{P}(\mathcal{T}_- \leq t). \tag{7.48}$$

We provide details on the most involved steps in the derivation shown above. In Equation (7.44), we have used that $S^{\text{tot}}(x_{[0,t]}) = -S^{\text{tot}}(\Theta_t(x_{[0,t]}))$ and $\mathcal{T}_+(x_{[0,t]}) = \mathcal{T}_-(\Theta_t(x_{[0,t]}))$. In Equation (7.44), we have used the fact that the Jacobian of the transformation $x_{[0,t]} \to \Theta_t x_{[0,t]}$ is one. In Equation (7.46), we have used the martingality of $\exp(-S_t^{\text{tot}})$ and Equation (4.46) of Doob's optional stopping Theorem 11 for $\mathcal{T}_1 = \mathcal{T}_-$, $\mathcal{T}_2 = t$, and for the uniformly integrable martingales $\exp(-S_{t'\wedge t}^{\text{tot}})$ that are defined at fixed values of $t \geq 0$ and for $t' \in [0, t]$. Lastly, in Equation (7.47) we have used the fact that X_t is a diffusion process. We have also used here θ for the Heaviside theta function, not to be confused with the time-reversal operator Θ_t.

Equation (7.40) implies that the first-passage densities obey the **first-passage-time fluctuation relation** for the stochastic entropy production in nonequilibrium stationary processes [11,183], viz.,

$$\frac{\rho_{\mathcal{T}_+}(t)}{\rho_{\mathcal{T}_-}(t)} = \exp(s). \tag{7.49}$$

Note that the s-dependency on the left-hand side of Equation (7.49) is hidden in the boundary conditions of the stopping times $\mathcal{T}_\pm$.

Note that $\rho_{\mathcal{T}_+}(t)\mathrm{d}t$ and $\rho_{\mathcal{T}_-}(t)\mathrm{d}t$ are defined by $\rho_{\mathcal{T}_\pm}(t) \equiv \mathcal{P}(\mathcal{T}_\pm \in [t, t + dt])/dt$, but we remark that these are unnormalized densities because the splitting probabilities obey $\mathcal{P}(\mathcal{T}_\pm \leq \infty) = P_\pm(s, s) < 1$. This motivates us to define the conditional (normalized) densities

$$\hat{\rho}_{\mathcal{T}_\pm}(t) \equiv \frac{\mathcal{P}(\mathcal{T}_\pm \in [t, t + dt]|\mathcal{T}_\pm < \infty)}{dt} = \frac{\rho_{\mathcal{T}_\pm}(t)}{P_\pm(s, s)}. \tag{7.50}$$

From Equation (7.49), and the fluctuation relation for the splitting probabilities $P_+(s, s)/P_-(s, s) = \exp(s)$ (see Equation (7.22)), we find the **first-passage-time symmetry**

$$\hat{\rho}_{\mathcal{T}_+}(t) = \hat{\rho}_{\mathcal{T}_-}(t). \tag{7.51}$$

In words, Equation (7.51) states that it takes the same amount of time to increase entropy production by s as it takes to reduce entropy production by $-s$.

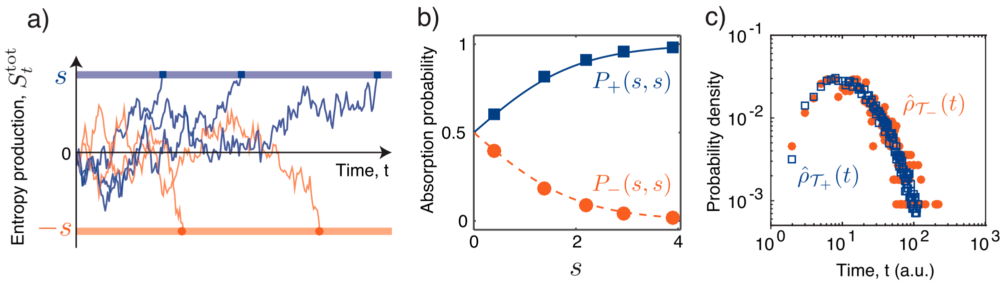

Figure 7.10. The escape problem for entropy production out of a symmetric interval $(-s, s)$. Panel (a): Example trajectories of $S_t^{\rm tot}$ as a function of time. We highlight in blue three trajectories that first reach s before $-s$ (at stochastic times $\mathcal{T}_+$), and in red two trajectories that first reach $-s$ before s (at stochastic times $\mathcal{T}_-$). Panel (b): Splitting probabilities $P_+(s, s)$ that $S_t^{\rm tot}$ goes above s before it (possibly) passes below $-s$ (blue squares), and $P_-(s, s)$ for $S_t^{\rm tot}$ to first pass below $-s$ before it goes above s (red circles). Markers are obtained from numerical simulations, and the lines denote the analytical expressions (7.19) $[P_+(s, s)$, blue solid line] and (7.20) $[P_+(s, s)$, red dashed line] for $s_+ = s_- = s$. (c) Conditional normalized densities for $\mathcal{T}_+$ (blue open squares) and for $\mathcal{T}_-$ (red filled circles) obtained from numerical simulations. Results illustrate the symmetry relation given in Equation (7.51). All numerical results are obtained for the model sketched in Figure 7.6(a) (see Ref. [11] for further details).

Relations analogous to the remarkable symmetry given in Equation (7.51) have been derived in the context of Haldane equalities in enzyme kinetics [184] and for first-passage-time dualities in diffusion processes [185]. Figure 7.10 shows a numerical test for the symmetry relation (7.51) for first-passage times and the fluctuation relation (7.22) for splitting probabilities.

7.4.4. *Trade-offs between speed, uncertainty, and dissipation*

A recurrent theme in nonequilibrium thermodynamics is that processes far from thermal equilibrium are governed by a trade-off between speed, uncertainty, and dissipation. Indeed, concrete examples of this thermodynamic trade-off have been found in kinetic proof reading [186–188], sensory adaptation [189], and microscopic heat engines [190]. Even though speed and uncertainty are quantified differently in these examples, they are suggestive of universal inequalities describing a trade-off between speed, uncertainty, and dissipation in nonequilibrium systems.

In recent years, universal inequalities expressing trade-offs in generic, nonequilibrium, stationary states have been derived for Markov jump processes and overdamped Langevin processes. We revisit here two inequalities based on first-passage times, namely, the speed-uncertainty-dissipation trade-off relation [34,35,178] and the thermodynamic uncertainty relation [177].

As discussed in Section 4.1.5, martingale theory provides a powerful set of tools to study processes at stopping times, and we will use this here to study nonequilibrium trade-off relations involving first-passage times. In particular, we use martingale theory to show that the speed-uncertainty-dissipation trade-off relation is optimal in a specific sense that we discuss below, and we also use martingale theory to evaluate the trade-off relations in a simple example of a nonequilibrium process.

7.4.4.1. *Setup: empirical current and stopping time.* Let J_t be an empirical integrated current in a stochastic process X_t that is either a stationary Markov jump process or an overdamped Langevin process, and assume without loss of generality that $\langle J_t \rangle > 0$. In a Markov jump process, an empirical current takes the form

$$J_t = \sum_{(x,y)} c(x,y) J_t(x,y), \tag{7.52}$$

where $J_t(x,y) = N_t(x,y) - N_t(y,x)$ is the difference between the number of jumps $N_t(x,y)$ from x to y minus the number of jumps $N_t(y,x)$ from y to x counted in the time interval $[0,t]$ (see definition in Equation 3.50), and $c(x,y) \in \mathbb{R}$ quantifies the "resource" transported when the process jumps from x to y. The stochastic entropy production, defined in Equation (6.35), takes here the form

$$S_t^{\rm tot} = \frac{1}{2} \sum_{x,y} \ln \left(\frac{\rho_{\rm st}(x)\omega(x,y)}{\rho_{\rm st}(y)\omega(y,x)} \right) J_t(x,y), \tag{7.53}$$

and is a particular example of empirical current, where we identify $c(x,y)$ in this case as the total entropy change in a jump. An analogous formalism applies to Langevin processes in which case empirical currents are Stratonovich integrals, viz.,

$$J_t = \int_0^t c(X_s) \circ dX_s. \tag{7.54}$$

In what follows, and throughout this Section 7.4.4, we rely on the first-passage time

$$\mathcal{T} \equiv \inf\{t \geq 0 : J_t \notin (-\ell_-, \ell_+)\} \tag{7.55}$$

for the current J_t to exit the open interval defined by the thresholds $\ell_-, \ell_+ > 0$, and we consider the limit $\ell_{\rm min} \gg 1$, where $\ell_{\rm min} = \min\{\ell_-, \ell_+\}$.

7.4.4.2. *Trade-off relations based on first-passage times.* We review thermodynamic, trade-off relations between speed, uncertainty, and dissipation that are based on first-passage processes.

The **nonequilibrium, thermodynamical trade-off** relations we consider take the form

$$a\, \epsilon_{\rm unc} \langle \dot{S}_t^{\rm tot} \rangle \langle \mathcal{T} \rangle (1 + o_{\ell_{\rm min}}(1)) \geq 1, \tag{7.56}$$

where $a \in \mathbb{R}^+$ is a constant, where $\langle \dot{S}_t^{\rm tot} \rangle$ is the average entropy production rate that quantifies **dissipation**, $\langle \mathcal{T} \rangle$ is the mean first-passage time that quantifies **speed**, and where $\epsilon_{\rm unc}$ is a dimensionless observable that quantifies **uncertainty** in the process. Later when considering specific examples of such trade-off relations, we define a and $\epsilon_{\rm unc}$.

The factor $1 + o_{\ell_{\rm min}}(1)$ represents an arbitrary function that converges to one when $\ell_{\rm min} \gg 1$ and implies that Equation (7.56) is an asymptotic relation that holds in the limit of large values of the first-passage thresholds ℓ_+ and ℓ_-. Dissipation $\langle \dot{S}_t^{\rm tot} \rangle$ is given in (6.38) for Markov jump processes and in (6.45) for Langevin processes. The trade-off relation equation (7.56) states that processes that are fast, have a small amount of fluctuations, and dissipate little, are physically nonpermissible, see Panel (a) of Figure 7.11 for an illustration.

Below we review two examples of trade-off relations that take the form of Equation (7.56), but differ in the way that uncertainty $\epsilon_{\rm unc}$ is quantified.

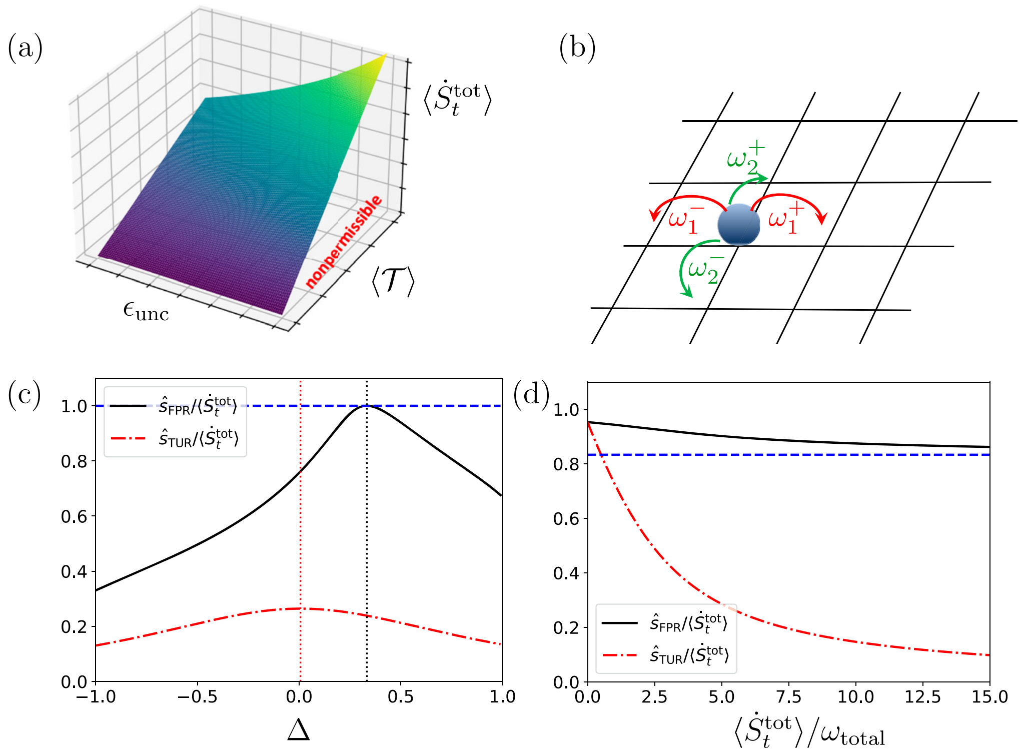

Figure 7.11. Trade-off between speed, uncertainty, and dissipation. Panel (a): Illustration of the trade-off relation equation (7.56). Processes under the plotted surface are nonpermissible. These processes are fast, fluctuate little, and dissipate little. Panel (b): Illustration of the random walk model on a two-dimensional lattice, as defined in Section 7.4.4.4. Panel (c): Plot of the ratios $\hat{s}_{\rm FPR}/\langle \dot{S}_t^{\rm tot} \rangle$ and $\hat{s}_{\rm TUR}/\langle \dot{S}_t^{\rm tot} \rangle$ for the model illustrated in Panel (b) as a function of the parameter Δ that defines the current, see Equation (7.66). Parameters $\omega_1^+ = \exp(2.5)/[4\cosh(2.5)]$, $\omega_1^- = \exp(-2.5)/[4\cosh(2.5)]$, $\omega_2^+ = \exp(5)/[4\cosh(5)]$, and $\omega_2^- = \exp(-5)/[4\cosh(5)]$. Vertical dashed lines denote the locations of the maxima of $\hat{s}_{\rm FPR}$ and $\hat{s}_{\rm TUR}$, the former corresponding with Equation (7.67). Panel (d): Similar plot as in Panel (c), but now the ratios are plot as a function of $\langle \dot{S}_t^{\rm tot} \rangle/\omega_{\rm total}$, where $\omega_{\rm total} = \omega_1^- + \omega_1^+ + \omega_2^- + \omega_2^+$. To this aim, the model parameters are set to $\omega_1^+ = \exp(\nu/2)/[4\cosh(\nu/2)]$, $\omega_1^- = \exp(-\nu/2)/[4\cosh(\nu/2)]$, $\omega_2^+ = \exp(\nu)/[4\cosh(\nu)]$, and $\omega_2^- = \exp(-\nu)/[4\cosh(\nu)]$ and ν is varied. All figures are taken from Refs. [35,178].

The first relation we discuss is the **speed-uncertainty-dissipation trade-off relation** [34,35,178], which is the inequality equation (7.56) for

$$\epsilon_{\rm unc} \equiv \frac{1}{|\ln P_-|}, \quad \text{and} \quad a \equiv \frac{\ell_-}{\ell_+}, \tag{7.57}$$

where

$$P_- \equiv \mathcal{P}\left[J(\mathcal{T}) \leq -\ell_-\right], \tag{7.58}$$

is the probability that J_t leaves for the first time the interval $(-\ell_-, \ell_+)$ through the lower threshold.

The measure $\epsilon_{\text{unc}} \in [0, 1/|\ln 2|]$ takes the value $\epsilon_{\text{unc}} = 0$ for processes without fluctuations ($P_- = 0$) and takes the value $\epsilon_{\text{unc}} = 1/|\ln 2|$ for processes with a large amount of fluctuations ($P_- = 1/2$).

The second relation we consider is the **thermodynamic uncertainty relation** [177], which is the inequality equation (7.56) for

$$\epsilon_{\text{unc}} \equiv \frac{\langle \mathcal{T}^2 \rangle - \langle \mathcal{T} \rangle^2}{\langle \mathcal{T} \rangle^2} \quad \text{and} \quad a \equiv \frac{1}{2}. \tag{7.59}$$

In the thermodynamic uncertainty relation, uncertainty is determined by the variance of the first-passage time; an equivalent uncertainty relation holds at fixed times [36–38]. It should be emphasized that both the speed-uncertainty-dissipation trade-off relation and the thermodynamic uncertainty relation are generically valid for nonequilibrium stationary states of Markov jump processes and Langevin processes.

7.4.4.3. *Comparing the quality of different trade-off relations.* To compare the quality of the two trade-off relations, we evaluate the following estimates:

$$\hat{s}_{\text{FPR}} \equiv \frac{\ell_+}{\ell_-} \frac{|\ln P_-|}{\langle \mathcal{T} \rangle} \le \langle \dot{S}^{\text{tot}}_t \rangle \quad \text{and} \quad \hat{s}_{\text{TUR}} \equiv 2 \frac{\langle \mathcal{T} \rangle}{\langle \mathcal{T}^2 \rangle - \langle \mathcal{T} \rangle^2} \le \langle \dot{S}^{\text{tot}}_t \rangle \tag{7.60}$$

of dissipation based on first-passage times. The ratios $\hat{s}_{\text{FPR}}/\langle \dot{S}^{\text{tot}}_t \rangle$ and $\hat{s}_{\text{TUR}}/\langle \dot{S}^{\text{tot}}_t \rangle$ determine the fraction of the average rate of dissipation $\langle \dot{S}^{\text{tot}}_t \rangle$ captured by the estimators of dissipation $\hat{s}_{\text{FPR}}$ and $\hat{s}_{\text{TUR}}$ based on the trade-off relation between speed, uncertainty and dissipation or the thermodynamic uncertainty relation, respectively. The closer the ratios $\hat{s}_{\text{FPR}}/\langle \dot{S}^{\text{tot}}_t \rangle$ and $\hat{s}_{\text{FPR}}/\langle \dot{S}^{\text{tot}}_t \rangle$ are to one, the tighter are the inequalities in Equation (7.60), and hence the better is the quality of the trade-off relation.

Using martingale methods, we show that for currents that are proportional to the entropy production, viz.,

$$J_t = c S^{\text{tot}}_t, \tag{7.61}$$

where c is a constant, it holds that

$$\hat{s}_{\text{FPR}} = \langle \dot{S}^{\text{tot}}_t \rangle, \tag{7.62}$$

and hence the speed-uncertainty-dissipation trade-off relation is optimal in this case. Indeed, Equation (7.18) in the limit of $\ell_-, \ell_+ \gg 1$ implies

$$P_- = \exp(-\ell_-/c(1 + o_{\ell_{\min}}(1))). \tag{7.63}$$

In addition, since in this case [35],

$$\langle \mathcal{T} \rangle = \frac{\ell_+}{c \langle S^{\text{tot}}_t \rangle}(1 + o_{\ell_{\min}}(1)), \tag{7.64}$$

we obtain from Equations (7.63) and (7.64) the equality

$$\hat{s}_{\text{FPR}} = \langle \dot{S}^{\text{tot}}_t \rangle \tag{7.65}$$

for currents that are proportional to S^{tot}_t.

7.4.4.4. *Comparing $\hat{s}_{\rm FPR}$ with $\hat{s}_{\rm TUR}$ in a simple example of a nonequilibrium process.* Let us now compare $\hat{s}_{\rm FPR}$ with $\hat{s}_{\rm TUR}$ for the general case of currents J_t that are not necessarily proportional to $S_t^{\rm tot}$ in a simple model of a nonequilibrium process X, as done in Ref. [178].

We consider the process $X = (X_t^{(1)}, X_t^{(2)})$ describing the position of a particle that jumps on a two-dimensional lattice at rates ω_1^+, ω_1^-, ω_2^+, and ω_2^-, for which we assume that $\omega_1^+ > \omega_1^-$ and $\omega_2^+ > \omega_2^-$, see Panel (b) of Figure 7.11 for an illustration. In this example, empirical currents take the form

$$J_t = (1-\Delta)X_t^{(1)} + (1+\Delta)X_t^{(2)}, \tag{7.66}$$

and when

$$\Delta = \frac{\ln(\omega_2^+/\omega_2^-) - \ln(\omega_1^+/\omega_1^-)}{\ln(\omega_2^+/\omega_2^-) + \ln(\omega_1^+/\omega_1^-)}, \tag{7.67}$$

the current J_t is proportional to $S_t^{\rm tot}$.

The mean rate of dissipation is, from definition Equation (5.92), given by

$$\langle \dot{S}_t^{\rm tot} \rangle = (\omega_1^+ - \omega_1^-)\ln\frac{\omega_1^+}{\omega_1^-} + (\omega_2^+ - \omega_2^-)\ln\frac{\omega_2^+}{\omega_2^-}. \tag{7.68}$$

Note that here we have applied Equation (5.92) and assumed periodic boundary conditions in the two-dimensional lattice which leads to a homogeneous steady-state density, i.e., $\rho_{\rm st}(x)$ to be independent of x.

To determine $\hat{s}_{\rm FPR}$ and $\hat{s}_{\rm TUR}$, we use in Appendix E.2 martingales and the technology of Doob's optional stopping theorems, as discussed in Section 4.1.5, to determine an explicit expression for the splitting probability P_-, the mean first-passage time $\langle \mathcal{T} \rangle$, and the variance $\langle \mathcal{T}^2 \rangle - \langle \mathcal{T} \rangle^2$, yielding

$$\hat{s}_{\rm FPR} = |z^*|\left((1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)\right)(1 + o_{\ell_{\rm min}}(1)), \tag{7.69}$$

where z^* is the nonzero solution to

$$\begin{aligned} 0 = {} & [1 - \exp(z^*(1-\Delta))]\omega_1^+ + [1 - \exp(-z^*(1-\Delta))]\omega_1^- \\ & + [1 - \exp(z^*(1+\Delta))]\omega_2^+ + [1 - \exp(-z^*(1+\Delta))]\omega_2^-, \end{aligned} \tag{7.70}$$

and

$$\hat{s}_{\rm TUR} = 2\frac{[(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)^2(\omega_2^+ - \omega_2^-)]^2}{(1-\Delta)^2(\omega_1^+ + \omega_1^-) + (1+\Delta)^2(\omega_2^+ + \omega_2^-)}. \tag{7.71}$$

In Panel (c) of Figure 7.11, we use Equations (7.68), (7.69), and (7.71), to plot $\hat{s}_{\rm FPR}/\langle \dot{S}_{\rm tot}\rangle$ and $\hat{s}_{TUR}/\langle \dot{S}_{\rm tot}\rangle$ as a function of Δ. Observe that for Δ given in Equation (7.67), as indicated by the vertical dotted line in Figure 7.11, the inequality for $\hat{s}_{\rm FPR}$ is tight, as predicted by martingale theory. In addition, for all values of Δ it holds that $\langle \dot{S}_t^{\rm tot}\rangle \geq \hat{s}_{\rm FPR} \geq \hat{s}_{\rm TUR}$, and hence $\hat{s}_{\rm FPR}$ is in this example a better estimator of dissipation.

In Panel (d) of Figure 7.11, we plot $\hat{s}_{\rm FPR}$ and $\hat{s}_{\rm TUR}$, as a function of $\langle \dot{S}_{\rm tot}\rangle$. This figure reveals that $\hat{s}_{\rm FPR} = \hat{s}_{\rm TUR}$ near equilibrium ($\langle \dot{S}_{\rm tot}\rangle \approx 0$), whereas in the opposing nonequilibrium limit it holds that $\hat{s}_{\rm TUR}/\langle \dot{S}_t^{\rm tot}\rangle \to 0$, whereas $\hat{s}_{\rm FPR}/\langle \dot{S}_t^{\rm tot}\rangle$ converges to a finite nonzero value for increasing values of $\langle \dot{S}_t^{\rm tot}\rangle$, which is indicated by the blue dashed line in the figure. Hence, far from equilibrium $\hat{s}_{\rm TUR}$ captures a negligible fraction of the dissipation, while $\hat{s}_{\rm FPR}$ captures a finite fraction of the dissipation.

7.5. Overcoming classical thermodynamic limits by stopping at a clever moment

The second law of thermodynamics at stopping times, given in Equation (7.11), states that it is not possible to reduce entropy by stopping at a clever moment. This law applies to the total entropy production $S_t^{\rm tot}$ and implies that a demon cannot reduce entropy, not even when it is infinitely smart and has complete knowledge of the past.

However, there exist observables $Y_t(X_{[0,t]})$ that obey a classic second law of thermodynamics, in the sense that

$$\langle Y_t \rangle \geq 0, \tag{7.72}$$

but do not obey a second law at stopping times, in the sense that

$$\langle Y_{\mathcal{T}} \rangle \ngeq 0, \tag{7.73}$$

i.e., its average at stopping times is *not necessarily* greater than or equal to zero. A notable example of such an observable is the heat dissipated $-Q_t$, as defined in Equation (5.8), for stationary, isothermal, overdamped, unidimensional Langevin processes given in Equation (5.3). In this case, the second law of thermodynamics implies that the heat decreases on average, but nevertheless, a demon can use stopping times $\mathcal{T}$ to overcome this classical thermodynamic limit. More generally, for generic stationary processes the environment entropy change $S_t^{\rm env}$, defined in (6.33), obeys, on one hand[12]

$$\langle S_t^{\rm env} \rangle \geq 0, \tag{7.74}$$

even though $S_t^{\rm env}$ is not a submartingale. On the other hand,

$$\langle S_{\mathcal{T}}^{\rm env} \rangle \geq -\langle \Delta S_{\mathcal{T}}^{\rm sys} \rangle \ngeq 0, \tag{7.75}$$

i.e., the average environmental entropy change at stopping times is not necessarily greater than or equal to zero. Equation (7.75) implies that a demon can overcome the classical limit equation (7.74) by stopping a process at a cleverly chosen moment $\mathcal{T}$, as anticipated by Maxwell [180]. Note that the operation of such a demon relies crucially on (i) the possibility to stop a process at a random time and (ii) the fact that we ignore changes in the entropy of the demon itself.

In what follows, we discuss two examples of cases for which a demon can use stopping times to overcome the classical limit (7.74) in isothermal (Section 7.5.1) and non-isothermal (Section 7.5.2) conditions.

7.5.1. *Heat extraction from stopping at a cleverly chosen moment*

Let X be the position of a colloidal particle described by the one-dimensional Langevin process (Equation 5.3). As already anticipated in the introduction of this section, the negative heat $-Q_t$ obeys the classical second law

$$-\langle Q_t \rangle \geq 0, \tag{7.76}$$

which follows from inserting Equation (5.22) into Equation (5.25) and using that for stationary systems $\langle \Delta S_t^{\rm sys} \rangle = 0$; $S_t^{\rm sys}$ is the system entropy as defined in Equation (5.14). On the other hand, from the second law at stopping times (Equation 7.11) it follows that

$$-\langle Q_{\mathcal{T}} \rangle \geq -T\langle S_{\mathcal{T}}^{\rm sys} \rangle + T\langle S_0^{\rm sys} \rangle. \tag{7.77}$$

Since the right-hand side of Equation (7.77) can be negative, the negative heat does not satisfy a second law at stopping times, and a colloidal particle can in principle absorb heat from a thermal reservoir by stopping at a time $\mathcal{T}$ defined by a suitable prescribed criterion.

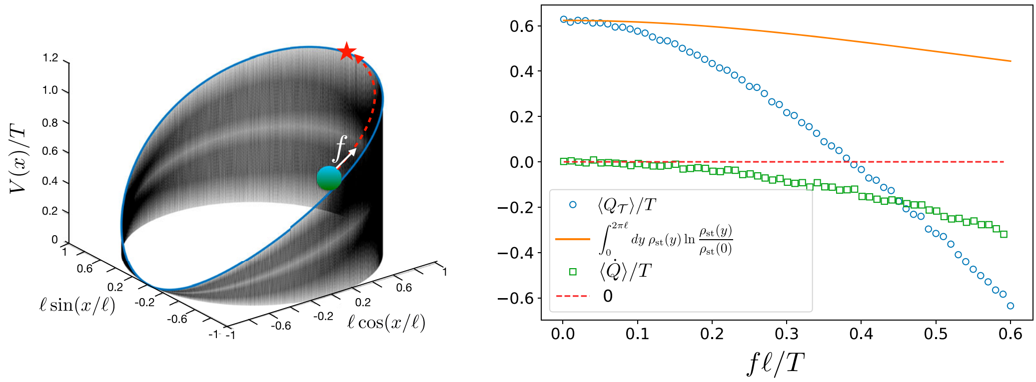

Figure 7.12. Heat extraction by a colloidal particle from an reservoir at temperature T. Left panel: Illustration of the model used in the right panel, viz., a colloidal particle on a ring. The position of the particle is described in Equation (5.3) with potential $V(x) = T\ln(\cos(x/\ell)+2)$ and constant force f. Right panel: The average heat $\langle Q_{\mathcal{T}}\rangle$ at the stopping time $\mathcal{T}$, defined in Equation (7.78) and illustrated in the Left Panel by a star, and the average heat rate $\langle\dot{Q}\rangle$, both plotted as a function of the forcing $f\ell/T$. Here, we estimate the average heat rate as $\langle\dot{Q}\rangle \simeq \langle Q_t\rangle/t$ using empirical averages and t sufficiently large, which leads to $\langle\dot{Q}\rangle \leq 0$ by virtue of $\langle Q_t\rangle = -T\langle S_t^{\rm env}\rangle \leq 0$, see Equation (7.74). Simulation results are in agreement with the classical second law $\langle Q_t\rangle \leq 0$ (Equation (7.76)) and the second law at stopping times (Equation (7.77)), specialized for this example as $\langle Q_{\mathcal{T}}\rangle \leq T\int_0^{2\pi} {\rm d}y\rho_{\rm st}(y)\ln[\rho_{\rm st}(y)/\rho_{\rm st}(0)]$ (Equation (7.79)). In the simulations, the parameters were set to $T=1$, $\mu=1$, and $\ell=1$. Figures taken from Ref. [13].

In Figure 7.12, we illustrate heat extraction for a colloidal particle that moves in a nonconstant potential on a ring under the influence of a nonconservative force. The position of the colloidal particle is described in Equation (5.3) with periodic boundary conditions, a constant, nonconservative force f, and a potential $V(x) = T\ln(\cos(x/\ell)+2)$, as considered before in Figure 7.6. The stopping criterion we implement is shown in the left panel of Figure 7.12: we stop the process as soon as the colloidal particle reaches the peak of the potential located at $x=0$, i.e.,

$$\mathcal{T} = \inf\{t \geq 0 : X_t = 0\}\,. \tag{7.78}$$

As shown in the right panel of Figure 7.12, as long as f is small enough, the system extracts on average heat from the thermal reservoir at the stopping time $\mathcal{T}$, i.e., $\langle Q_{\mathcal{T}}\rangle \geq 0$ (see blue squares in the right panel in Figure 7.12), and the amount of heat that can be extracted is upper bounded by the second law at stopping times given in Equation (7.77). More precisely, in this example the system's dynamics is initialized in the stationary state $\rho_{\rm st}(x)$ whereas $\rho_{\rm st}(X_{\mathcal{T}}) = \rho_{\rm st}(0)$. Thus the average system entropy change up to the stopping time (7.78) reads $\langle S^{\rm sys}_{\mathcal{T}}\rangle - \langle S^{\rm sys}_0\rangle = \int_0^{2\pi} {\rm d}y\rho_{\rm st}(y)\ln \rho_{\rm st}(y)/\rho_{\rm st}(0)$. As a result, the second law at stopping times (7.77), copied here for convenience

$$-\frac{\langle Q_{\mathcal{T}}\rangle}{T} + [\langle S^{\rm sys}_{\mathcal{T}}\rangle - \langle S^{\rm sys}_0\rangle] \geq 0,$$

is specialized for this example as an upper bound for the averaged absorbed heat up to the stopping time $\mathcal{T}$ given in Equation (7.78), i.e.,

$$\frac{\langle Q_{\mathcal{T}}\rangle}{T} \leq \int_0^{2\pi} {\rm d}y\rho_{\rm st}(y)\ln\frac{\rho_{\rm st}(y)}{\rho_{\rm st}(0)}. \tag{7.79}$$

We provide a numerical verification of the inequality (7.79) in the right panel of Figure 7.12, which shows that such second law at stopping times is tight when the system is near equilibrium, i.e., when $f \approx 0$.

7.5.2. *Super Carnot efficiency at stopping times*

Steady-state heat engines are thermal machines that are permanently in contact with two thermal reservoirs, one at hotter $T_{\rm h}$ and another at a colder $T_{\rm c} \leq T_{\rm h}$ temperature. After a transient, the engine achieves an average stationary heat flow from the hot to the cold reservoir that can be used to extract power. A key example of a steady-state heat engine is *Feynman's ratchet* where a ratchet and a pawl are immersed in two gas containers held at different temperatures. As shown earlier [191,192], the nonequilibrium constraint $T_{\rm c} \neq T_{\rm h}$ results in a net extraction of work which can be used, i.e., to lift a weight against the gravitational pull.

It is well known the key role of fluctuations in determining the thermodynamic performance of steady-state heat engines [26,193]. However, only very recently thermodynamic insights of such machines at stopping times have been unveiled with the help of martingales [13,42]. For example, an important question is what is the average heat transfer between two "main events" corresponding to two consecutive passages in the teeth of Feynman's ratchet wheel?

The average thermodynamic fluxes in steady-state heat engines over a fixed time interval $[0, t]$ obey $\langle W_t \rangle \leq 0$ (work extraction), $\langle Q_{\rm h} \rangle \geq 0$ (absorption of heat from the hot bath), and $\langle Q_{\rm c} \rangle \leq 0$ (dissipation of heat in the cold bath). The first law of thermodynamics implies

$$\langle \dot{W} \rangle + \langle \dot{Q}_{\rm c} \rangle + \langle \dot{Q}_{\rm h} \rangle = 0 \tag{7.80}$$

and the second law for steady-state heat engines

$$\langle \dot{S}_t^{\rm tot} \rangle = -\langle \dot{Q}_{\rm c} \rangle / T_{\rm c} - \langle \dot{Q}_{\rm h} \rangle / T_{\rm h} \geq 0, \tag{7.81}$$

which follows from stationarity. Combining Equations (7.80) and (7.81), one finds that the long-time efficiency (defined analogously as in classical heat engines) of the engine is always smaller or equal than Carnot efficiency, i.e.,

$$\eta = \frac{-\langle \dot{W} \rangle}{\langle \dot{Q}_{\rm h} \rangle} \leq \underbrace{1 - \frac{T_{\rm c}}{T_{\rm h}}}_{\equiv \eta_C}. \tag{7.82}$$

We now ask the question: what are the implications of the second law of thermodynamics at stopping times (7.11) concerning the efficiency achieved by a steady-state heat engine cleverly stopped at a stochastic time $\mathcal{T}$? To this aim, we consider the *stopping-time efficiency* $\eta_{\mathcal{T}}$ associated with the stopping time $\mathcal{T}$ as

$$\eta_{\mathcal{T}} \equiv \frac{-\langle W_{\mathcal{T}} \rangle / \langle \mathcal{T} \rangle}{\langle Q_{{\rm h},\mathcal{T}} \rangle / \langle \mathcal{T} \rangle} = \frac{-\langle W_{\mathcal{T}} \rangle}{\langle Q_{{\rm h},\mathcal{T}} \rangle}, \tag{7.83}$$

where $-\langle W_{\mathcal{T}} \rangle$ and $\langle Q_{{\rm h},\mathcal{T}} \rangle$ are respectively the average work extracted and the average heat absorbed from the hot bath in the time interval $[0, \mathcal{T}]$. In general, trajectories $X_{[0,\mathcal{T}]}$ are not cyclic, i.e., $\rho_{\mathcal{T}} \neq \rho_0$. This implies that the first law averaged over many trajectories $X_{[0,\mathcal{T}]}$ stopped at a stochastic time $\mathcal{T}$ reads

$$\langle W_{\mathcal{T}} \rangle + \langle Q_{{\rm c},\mathcal{T}} \rangle + \langle Q_{{\rm h},\mathcal{T}} \rangle = \langle \Delta V_{\mathcal{T}} \rangle. \tag{7.84}$$

Here, $\Delta V_{\mathcal{T}} = V(X_{\mathcal{T}}) - V(X_0)$ is the energy change in $[0, \mathcal{T}]$, which one cannot simply neglect with respect to the average heat and work done up to the stopping time – as in the traditional first law (7.80). Similarly, the second law of thermodynamics at stopping times (7.11) reads in this case

$$\langle S^{\rm tot}_{\mathcal{T}}\rangle = \langle \Delta S^{\rm sys}_{\mathcal{T}}\rangle - \langle Q_{{\rm c},\mathcal{T}}\rangle/T_{\rm c} - \langle Q_{{\rm h},\mathcal{T}}\rangle/T_{\rm h} \geq 0, \tag{7.85}$$

with $\Delta S^{\rm sys}_{\mathcal{T}}$ the system entropy change in $[0,\mathcal{T}]$. The second law (7.85) reveals something interesting, namely, the stopping time carries an additional system entropy term with respect to the traditional second law (7.81). We also note that $Y_t = -Q_c/T_{\rm c} - Q_h/T_{\rm h}$ satisfies a second law of thermodynamics at fixed times but not at stopping times, and this is a key property that allows us to overcome classical limits. In particular, combining Equations (7.83),(7.84) and (7.85) we obtain

$$\eta_T \leq \eta_C - \frac{\langle \Delta G^{\rm ne}_{{\rm c},\mathcal{T}}\rangle}{\langle Q_{{\rm h},\mathcal{T}}\rangle}, \tag{7.86}$$

where

$$G^{\rm ne}_{{\rm c},\mathcal{T}} = V(X_{\mathcal{T}}) \; - T_{\rm c} S^{\rm sys}_{\mathcal{T}}, \tag{7.87}$$

is the nonequilibrium free energy of the system at stopping times with respect to the cold thermal bath. Notably, the second term in the right-hand side of (7.86) may be positive for specific “clever” choices of stopping times. Therefore, the second law of thermodynamics at stopping times does not prevent stopping-time efficiencies $\eta_{\mathcal{T}}$ to surpass the Carnot efficiency.

For illustrational purposes, we borrow from Ref. [13] the illustration of the bound (7.86) applied to a paradigmatic model of a steady-state engine, namely the Brownian gyrator which was introduced in Ref. [194] and realized experimentally in [195], see also Refs. [190,196,197] for theoretical insights. The model is described by a two-dimensional Langevin equation describing the motion of an overdamped Brownian particle in an elliptical confining potential that is subject to two nonequilibrium constraints: (i) two thermal baths at temperatures $T_{\rm h}$ and $T_{\rm c} < T_{\rm h}$ each acting only along the x and y axes, respectively; and (ii) an external torque generated by external, non-conservative forces. See Figure 7.13(a) for an illustration of the Brownian gyrator. The equations of motion of the model read (cf. Equation (3.59))

$$\begin{pmatrix} \dot{X}_t \\ \dot{Y}_t \end{pmatrix} = -\mu \begin{pmatrix} \partial_x V(X_t,Y_t) \\ \partial_y V(X_t,Y_t) \end{pmatrix} + \mu \begin{pmatrix} f_x(X_t,Y_t) \\ f_y(X_t,Y_t) \end{pmatrix} + \begin{pmatrix} \sqrt{2\mu T_h} & 0 \\ 0 & \sqrt{2\mu T_c} \end{pmatrix} \begin{pmatrix} \dot{B}_x \\ \dot{B}_y \end{pmatrix}. \tag{7.88}$$

In Equation (7.88), the potential

$$V(x,y) = \frac{1}{2}\left(u_1 x^2 + u_2 y^2 + cxy\right), \tag{7.89}$$

with $u_1, u_2 > 0$, and $0 < c < \sqrt{u_1 u_2}$ [190]. Furthermore, the two components of the external non-conservative force are

$$f_x(x,y) = ky, \quad f_2(x,y) = -kx, \tag{7.90}$$

and B_x and B_y are two independent Wiener processes,

Amongst the infinite possible choices of stopping strategies, Ref. [13] considered the stopping time of first occurrence of the “main event”

$$\mathcal{T} = \inf\{t > 0 : \varphi_{t^-} > \pi/2, \varphi_{t^+} \leq \pi/2\}, \tag{7.91}$$

where we assume that at $t = 0$ the system is initialized in its stationary state (see green circles in Figure 7.13 a). In Equation (7.91), the variable $\varphi_t = \tan^{-1}(Y_t/X_t) \in [-\pi,\pi]$ is the phase associated with the state (X_t, Y_t), thus $\mathcal{T}$ corresponds to the first crossing from the second quadrant

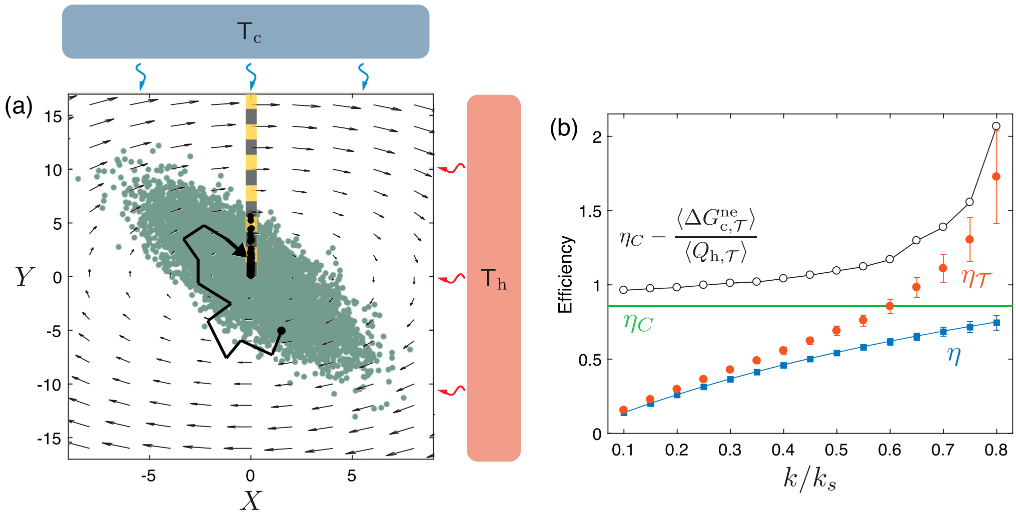

Figure 7.13. Efficiency of a gyrator that stops at a cleverly chosen time. (a) Illustration of the model: An overdamped Brownian particle moves in one dimension, X and Y, trapped in an elliptical potential (7.89), under the action of an external, non-conservative force field (7.90) (black arrows) and subject to thermal fluctuations of different temperatures T_h and $\mathsf{T}_c < \mathsf{T}_h$ along the X and Y coordinates, respectively. The thick black arrow illustrates a single trajectory stopped at $\mathcal{T}$ given in Equation (7.91) being the first time at which the "barrier" (thick line with black and orange stripes) is crossed by crossing from the second to the first quadrant. The green filled circles show the initial state of 100 independent realizations drawn from the stationary state, whereas the black filled circles are their value at the stopping time $\mathcal{T}$. (b) Efficiencies as a function of the stiffness k of the non-conservative force (in units of the "stalling" stiffness $k_s \equiv c\eta_C/(2-\eta_C)$ at which the net current vanishes), viz., the long-time efficiency η (Equation 7.82, blue squares, simulations; blue solid line, theory), the stopping-time efficiency $\eta_{\mathcal{T}}$ (Equation 7.83, red circles), and the upper bound to the stopping time efficiency dictated by the second law of thermodynamics at stopping times (right-hand side in Equation 7.86, black open circles). The horizontal green line is set at Carnot efficiency $\eta_C = 1 - (\mathsf{T}_c/\mathsf{T}_h) = 7$. Parameter values: $\mu = 1$, $u_1 = 1$, $u_2 = 1.2$, $\mathsf{T}_c = 1$, $\mathsf{T}_h = 7$, $c = 0.9$, 10^4 independent realizations, and simulation time step $\Delta t = 10^{-3}$, see [13] for further details.

to the first quadrant. The distribution at stopping times $\rho_{X_{\mathcal{T}},Y_{\mathcal{T}}}$ is concentrated near the positive y axis (black circles in Figure 7.13a) and is less broad than the initial distribution (green circles in Figure 7.13a). Thus the system entropy change in $[0,\mathcal{T}]$, $\Delta S^{\mathrm{sys}}_{\mathcal{T}} = S^{\mathrm{sys}}_{\mathcal{T}} - S^{\mathrm{sys}}_0$, is often negative for this example and this choice of stopping time. This result, together with the fact that the system energy change in $[0,\mathcal{T}]$, $\Delta V_{\mathcal{T}} = V_{\mathcal{T}} - V_0$, is often smaller than $-T_c \Delta S^{\mathrm{sys}}_{\mathcal{T}}$, leads to positive free energy changes $\langle \Delta G^{\mathrm{ne}}_{\mathrm{c},\mathcal{T}} \rangle$, which opens up the possibility for stopping time efficiencies above the Carnot limit, see Equation (7.86). Readers are referred to Ref. [13] for details on the calculations of the free energy change at stopping times. We show in Figure 7.13(b) with results obtained from numerical simulations, that the stopping-time efficiency associated with the stopping time $\mathcal{T}$ (red circles), which satisfies the bound (7.86), can surpass the Carnot efficiency near equilibrium, a result that is inaccessible by stopping trajectories at a fixed time (blue squares).

Chapter 8. Martingales in stochastic thermodynamics IV: Non-stationary processes

La martingale est introuvable comme l'âme.
(The martingale is as elusive as the soul.)
Alexandre Dumas, La Femme au collier de velours, Chapter XVIII (1850).

We use martingales to further extend classical results in stochastic thermodynamics, but this time for nonstationary processes.

To this purpose, we use the generalized Σ-stochastic entropic functionals, as defined in Equation (6.108), for the special case of $r = 0$ and $\mathcal{Q}^{(t)} = \widetilde{\mathcal{P}}^{(t)}$, where $\widetilde{\mathcal{P}}^{(t)}$ is a sequence of probability measures associated with the time-reversed protocol. For simplicity, we denote here such generalized Σ-stochastic entropic functionals by $\hat{\Sigma}_s$. Note that in Section 6.3 we have shown that $\hat{\Sigma}_s$ can be decomposed in terms of a stochastic environmental entropy flow, given in Equation (6.32), or equivalently, in terms of a stochastic total entropy production, given in Equation (6.33), viz.,

$$\hat{\Sigma}_s = \ln\left(\frac{\rho_0\left(X_0\right)}{\tilde{\rho}^{(t)}_{t-s}\left(X_s\right)}\right) + S^{\text{env}}_s = \ln\left(\frac{\rho_s(X_s)}{\tilde{\rho}^{(t)}_{t-s}(X_s)}\right) + S^{\text{tot}}_s, \tag{8.1}$$

which holds for $0 \leq s \leq t$. Here, $\tilde{\rho}^{(t)}$ is the instantaneous density associated with the time-reversed protocol for a specified initial distribution $\tilde{\rho}^{(t)}_0 = \rho_t$ (see Equation (6.8) for its definition).

Importantly, as shown in Section 6.3, the process $\exp(-\hat{\Sigma}_s)$ is a martingale with respect to $X_{[0,s]}$. In this chapter, we use the martingale property of $\exp(-\hat{\Sigma}_s)$ to derive fluctuation relations at stopping times for nonstationary nonequilibrium processes.

We initiate this chapter with Section 8.1 that reviews Jarzynski's equality. Subsequently, following Refs. [10,14], in Section 8.2 we extend Jarzysnki's equality to an equality that applies at stopping times and discuss applications of this result. In Section 8.3, we review another extension of Jarzynski's equality for non-stationary processes, which is then used to design *gambling demons* that can extract on average more work than the free energy difference at the stopping time.

8.1. *Jarzynski's equality*

Jarzynski's celebrated equality, introduced in Ref. [169], provides an equality between the statistics of the stochastic work done on the system and the (deterministic) equilibrium free energy change between the initial and final states of a nonequilibrium protocol. As reviewed in Section 6.1.5.3 (see Equation 6.52), Jarzynski's equality is given by

$$\left\langle \exp\left(-\frac{W_t - \Delta G^{\text{eq}}}{T}\right)\right\rangle = 1, \tag{8.2}$$

where the average $\langle\cdot\rangle$ is taken over the trajectories $X_{[0,t]}$ of a mesoscopic process that is initially at time $s = 0$ in an equilibrium state and is for $s \in [0,t]$ driven away from equilibrium by an external protocol (after which it can be assumed to relax again to an equilibrium state). The ΔG^{eq} in Equation (8.2) denotes the free energy difference between the final and initial states. Equation (8.2) was first derived for a Hamiltonian system in [169] and was later extended with a Master equation approach to stochastic processes, including Langevin processes in Refs. [165,198,199]; in Section 6.1.5.3 we have rederived the Jarzynski equality for overdamped isothermal Langevin processes. The Jarzynski equality implies the second law

$$\langle W_t\rangle \geq \Delta G^{\text{eq}}, \tag{8.3}$$

which states that the work done on a system must on average be larger than the free energy difference between the final and initial states.

8.2. *Jarzynski equality at stopping times*

Events in mesoscopic systems can happen at random times. Hence to address questions of the sort "*how much work is needed on average for a particle to escape a metastable state?*" or "*how much work is required to stretch a polymer to a certain predefined fixed length?*", we need a formulation of the second law of thermodynamics that holds at random times [14].

We further detail the latter example, which serves as a canonical example in this section. Consider a polymer with one end attached to an anchor fixed at position $x = 0$, and the second (dangling) end attached by a spring to a molecular motor positioned at $\lambda_0 = \lambda_{\rm i}$, as shown in the upper panel of Figure 8.1. At time $t = 0$, the motor starts moving forwards. Our event of interest is the binding of the second endpoint of the polymer to an anchor located at $x = \ell$, as shown in the bottom panel of Figure 8.1. How much work does the motor perform on average on the polymer to complete this event of interest, and what is the corresponding second law of thermodynamics?

Since the polymer is a mesoscopic system the position of its end point is a stochastic process, and therefore the time $\mathcal{T}$ when the event of interest happens is a random variable. Consequently, the classical second law of thermodynamics, Equation (8.3), does not apply. Instead, following Refs. [10,14] we present a generalization of the second law of thermodynamics that applies at random times.

8.2.1. *System setup*

For simplicity, we focus here on the one-dimensional Langevin process

$$\dot{X}_s = -\mu \partial_x V(X;\lambda_s) + \sqrt{2\mu T}\, \dot{B}_s, \tag{8.4}$$

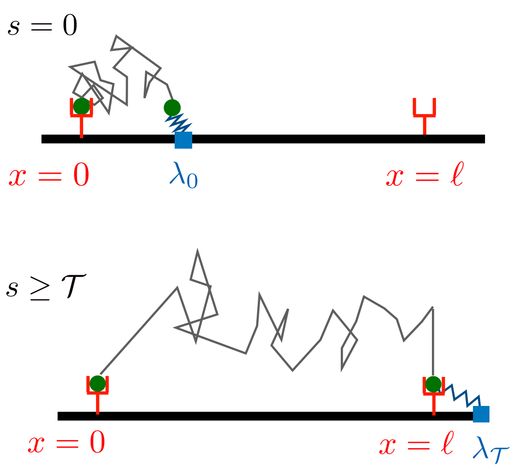

Figure 8.1. How much work is required to stretch a polymer to a certain fixed length ℓ? A polymer (gray zigzag line) has one end point (green circle) bound to an anchor point (red symbol) located at $x = 0$ and has another end point coupled to a spring representing a molecular motor located initially located at λ_0 (blue zigzag line). At times $s > 0$, the motor moves forward and when the dangling end point of the polymer reaches the anchor point located at $x = \ell$, it binds to it. Since the dangling end point of the polymer is fluctuating, also the time $\mathcal{T}$ of arrival at $x = \ell$ is random, and hence for this event the second law of thermodynamics at stopping times Equation (8.30) applies. Figure taken from [14].

where $s \geq 0$ is the time index, and

$$\lambda_s \equiv \begin{cases} \lambda_{\rm i} & \text{if } s \leq 0, \\ \lambda_s & \text{if } s \in [0, \tau], \\ \lambda_{\rm f} & \text{if } s \geq \tau, \end{cases} \tag{8.5}$$

denotes a protocol that runs over a time interval $s \in [0, \tau]$ of finite duration τ; note that we use here s as a time index instead of t to have a notation consistent with Section 6.3 on generalized entropic functionals, as it will turn out that the central quantity of interest is a generalized Σ-stochastic entropic functional. Equation (8.4) equals Equation (5.3) in the absence of a nonconservative force $f_s = 0$ and for $V_s(x) = V(x; \lambda_s)$. We assume that the initial state

$$\rho_0(x) = \rho^{\rm eq}(x; \lambda_{\rm i}), \tag{8.6}$$

where

$$\rho^{\rm eq}(x; \lambda) = \exp\left(-\frac{V(x;\lambda) + G^{\rm eq}(\lambda)}{T}\right), \quad \forall x \in \mathcal{X}, \tag{8.7}$$

is the Boltzmann distribution, and

$$G^{\rm eq}(\lambda) = T \ln\left(\int_{\mathcal{X}} {\rm d}x \exp\left(-\frac{V(x;\lambda)}{T}\right)\right) \tag{8.8}$$

is the equilibrium free energy for a given value of the parameter λ.

8.2.2. *Martingale associated with X*

We identify a martingale, which we denote by $\exp(-\hat{\Sigma}_s)$, associated with the process X_s.

Consider the process

$$\hat{\Sigma}_s = -\frac{Q_s}{T} + \ln\left(\rho^{\rm eq}(X_0; \lambda_{\rm i})\right) - \ln\left(\tilde{\rho}^{(\tau)}_{\tau-s}(X_s)\right), \tag{8.9}$$

where

$$\dot{Q}_s = \partial_x V(X; \lambda_s) \circ \dot{X}_s \tag{8.10}$$

is the rate of heat absorbed by the system, as defined in Equation (5.11) or (6.46), and where $\tilde{\rho}^{(\tau)}_{\tau-s}$ is the solution to the Fokker–Planck equation

$$\partial_s \tilde{\rho}^{(\tau)}_s + \partial_x \tilde{J}_{s,\tilde{\rho}^{(\tau)}} = 0 \tag{8.11}$$

with the probability current

$$\tilde{J}_{s,\tilde{\rho}^{(\tau)}} = -\mu \partial_x V(x; \tilde{\lambda}_s) \tilde{\rho}^{(\tau)}_s(x) - \mu T \partial_x \tilde{\rho}^{(\tau)}_s(x), \tag{8.12}$$

with the time-reversed protocol

$$\tilde{\lambda}_s \equiv \begin{cases} \lambda_{\rm f} & \text{if } s \leq 0, \\ \lambda_{\tau-s} & \text{if } s \in [0, \tau], \\ \lambda_{\rm i} & \text{if } s \geq \tau, \end{cases} \tag{8.13}$$

and with the initial state

$$\tilde{\rho}_0^{(\tau)}(x) = \rho^{\text{eq}}(x; \lambda_{\text{f}}). \tag{8.14}$$

The constant term $\ln(\rho_{\text{eq}}(X_0; \lambda_i))$ in the expression (8.9) of $\hat{\Sigma}_s$ assures that

$$\langle \exp(-\hat{\Sigma}_0) \rangle = \int_{\mathcal{X}} \mathrm{d}x \tilde{\rho}_\tau^{(\tau)}(x) = 1. \tag{8.15}$$

As suggested by the notation, the process $\hat{\Sigma}_s$ given in Equation (8.9) is a particular case of the generalized Σ-stochastic entropic functional (8.1) for $t = \tau$, for $\tilde{\rho}_0^{(t)}$ given in Equation (8.6), and for S^{env} given by Claussius' statement equation (6.46).

In Appendix F.1, we use the Itô integral approach from Section 5.2.2.1 to derive a compact Itô stochastic differential equation for $\hat{\Sigma}_s$, viz.,

$$\frac{\mathrm{d}}{\mathrm{d}s} \hat{\Sigma}_s = v_s^S(X_s) + \sqrt{2 v_s^S(X_s)} \dot{B}_s, \tag{8.16}$$

where

$$v_s^S = \frac{1}{\mu T} \left(\frac{\tilde{J}_{\tau - s, \tilde{\rho}^{(\tau)}}(X_s)}{\tilde{\rho}_{\tau - s}^{(\tau)}(X_s)} \right)^2. \tag{8.17}$$

Note that Equation (8.16) has the same form as Equation (5.42), albeit with an entropic drift v_s^S that exhibits an explicit dependence on time s.

Applying Itô's formula (see Appendix B.3.1) to the variable transformation $\hat{\Sigma}_s \to \exp(-\hat{\Sigma}_s)$ and using Equation (8.16), we obtain

$$\frac{\mathrm{d} \exp(-\hat{\Sigma}_s)}{\mathrm{d}s} = -\sqrt{2 v_s^S(X_s)} \exp(-\hat{\Sigma}_s) \dot{B}_s, \tag{8.18}$$

and hence $\exp(-\hat{\Sigma}_s)$ is an Itô integral. Hence, according to Equation (8.18) $\exp(-\hat{\Sigma}_s)$ is the stochastic exponential $\mathcal{E}_s(M)$ of the martingale

$$M_s = \int_0^s \mathrm{d}u \sqrt{2 v_u^S(X_u)} \dot{B}_u. \tag{8.19}$$

Hence, we have "rediscovered" (see previous Section 5.2.2.1 and Section 5.2.2.4) in an explicit way that $\exp(-\hat{\Sigma}_s)$ is a martingale provided Novikov's condition is satisfied, which we assume to be the case in what follows. Moreover, since $v_s^S \geq 0$, it holds that $\hat{\Sigma}_s$ is a submartingale, and it satisfies a conditional strong second law

$$\langle \hat{\Sigma}_s | X_{[0,u]} \rangle \geq \hat{\Sigma}_u \tag{8.20}$$

for all $0 \leq u \leq s$.

Note that this example has the appealing property that the origin of time reversal $t = \tau$ is immaterial. Indeed, the same process $\hat{\Sigma}_s$ is obtained for all $t \geq \tau$, as we show in Appendix F.2. This is because the initial state is given in Equation (8.14) and the protocol has finite duration.

8.2.2.1. ♠*Note on uniform integrability.* An important distinction between the process $\exp(-S_t^{\rm tot})$ for stationary X, as defined in Chapter 5, and the process $\exp(-\hat{\Sigma}_s)$ defined in (8.1)–(8.9) for nonstationary X, is that $\exp(-\hat{\Sigma}_s)$ is (in general) a uniformly integrable for $s \in \mathbb{R}^+$, while $\exp(-S_t^{\rm tot})$ is not uniformly integrable for $t \in \mathbb{R}^+$. This can be understood as follows.

Both $\exp(-S_t^{\rm tot})$ and $\exp(-\hat{\Sigma}_s)$ are bounded from below, and hence according to the martingale convergence theorem, Theorem 8, limits

$$\exp(-S_\infty^{\rm tot}) = \lim_{t\to\infty} \exp(-S_t^{\rm tot}) \tag{8.21}$$

and

$$\exp(-\hat{\Sigma}_\infty) = \lim_{s\to\infty} \exp(-\hat{\Sigma}_s) \tag{8.22}$$

exist. According to condition equation (4.34), if in addition $\langle \exp(-S_\infty^{\rm tot})\rangle = 1$ and $\langle \exp(-\hat{\Sigma}_\infty)\rangle = 1$, then $\exp(-S_t^{\rm tot})$ and $\exp(-\hat{\Sigma}_s)$ are, respectively, uniformly integrable processes.

However, for stationary processes

$$0 = \langle \exp(-S_\infty^{\rm tot})\rangle \neq \langle \exp(-S_t^{\rm tot})\rangle = 1, \tag{8.23}$$

and hence $\exp(-S_t^{\rm tot})$ is not uniformly integrable. This is because with probability 1, $\lim_{t\to\infty} S_t^{\rm tot} = +\infty$.

On the other hand,

$$\langle \exp(-\hat{\Sigma}_\infty)\rangle = \langle \exp(-\hat{\Sigma}_s)\rangle = 1, \tag{8.24}$$

as with probability 1, $\lim_{s\to\infty} \hat{\Sigma}_s \in \mathbb{R}^+$.

8.2.3. *Derivation of the Jarzynski equality at stopping times*

To obtain a Jarzynski equality at stopping times, we rewrite the process $\hat{\Sigma}_s$ in terms of the stochastic work W_t done on the system and the equilibrium free energy $G^{\rm eq}(\lambda_s)$, given in Equation (8.8). Using the first law of thermodynamics equation (5.6) and the Boltzmann distribution equation (8.7), we obtain

$$\hat{\Sigma}_s = \frac{W_s - \Delta G^{\rm eq}(\lambda_s)}{T} - \pi_s, \tag{8.25}$$

where the *equilibrium* free energy difference between the final and initial states reads (8.9)

$$\Delta G^{\rm eq}(\lambda_s) = G^{\rm eq}(\lambda_s) - G^{\rm eq}(\lambda_{\rm i}), \tag{8.26}$$

and where the remainder term

$$\pi_s \equiv \ln\left(\frac{\tilde{\rho}^{(\tau)}_{\tau-s}(X_s)}{\rho^{\rm eq}(X_s;\lambda_s)}\right). \tag{8.27}$$

Since for finite τ the process $\exp(-\hat{\Sigma}_s)$ is a uniformly integrable martingale, see note on uniform integrability in Section 8.2.2, Doob's optional stopping theorem, Theorem 11, applies, yielding the **Jarzynski equality at stopping times** [14], i.e.,

$$\left\langle \exp\left(-\frac{W_{\mathcal{T}} - \Delta G^{\mathrm{eq}}(\lambda_{\mathcal{T}})}{T} + \pi_{\mathcal{T}}\right)\right\rangle = 1. \tag{8.28}$$

Equation (8.28) is reminiscent of Jarzynski's equality equation (8.2), except for the presence of the remainder term $\pi_{\mathcal{T}}$ that includes the nontrivial contributions to $\hat{\Sigma}_s$ due to the fact that we stopped the process X at a random time $\mathcal{T}$. Nevertheless, it is justified to call Equation (8.28) a Jarzynski equality at stopping times as in several limiting cases it holds that $\pi_{\mathcal{T}} = 0$ yielding the good-looking equality

$$\left\langle \exp\left(-\frac{W_{\mathcal{T}} - \Delta G^{\mathrm{eq}}(\lambda_{\mathcal{T}})}{T}\right)\right\rangle = 1, \tag{8.29}$$

which is Equation (8.2) for $t \to \mathcal{T}$.

Equation (8.29) applies in the following limiting cases for which it holds that $\pi_{\mathcal{T}} = 0$:

(i) $\mathcal{T} = \tau$: indeed, in this case $\tilde{\rho}_0^{(\tau)}(x) = \rho^{\mathrm{eq}}(x;\lambda_{\mathrm{f}})$ and thus $\pi_\tau = 0$. In this case, equation (8.28) is identical to the Jarzynski equality equation (8.2) as $\mathcal{T} = \tau$.
(ii) The stopping time $\mathcal{T}$ is larger or equal than τ: indeed, $\tilde{\rho}_{\tau-\mathcal{T}}^{(\tau)}(x) = \rho^{\mathrm{eq}}(x;\lambda_{\mathrm{f}})$ for $\mathcal{T} > \tau$ and thus $\pi_s = 0$ for $s > \tau$.
(iii) The driving λ_s is quasi-static: in this case, $\tilde{\rho}_{\tau-s}^{(\tau)}(x) = \rho^{\mathrm{eq}}(x;\lambda_s)$ for all s, such that $\pi_s = 0$.
(iv) The protocol is quenched (i.e., $\lambda_s = \lambda_{\mathrm{f}}$ for $s > 0$) and the stopping time is with probability 1 greater than 0 (i.e., $\mathcal{P}(\mathcal{T} > 0) = 1$): this is a special case of (iii).

We derive now a second law of thermodynamics at stopping times based on the Jarzynski equality at stopping times.

Jensen's inequality equation (7.4) applied to $X = S_s$, together with Jarzynski's equality at stopping times, Equation (8.28), yields the **second law of thermodynamics at stopping times** [14]

$$\langle W_{\mathcal{T}}\rangle - \langle \Delta G^{\mathrm{eq}}(\lambda_{\mathcal{T}})\rangle + T\langle \pi_{\mathcal{T}}\rangle \geq 0. \tag{8.30}$$

Although here, for reasons of simplicity we have derived Equations (8.28) and (8.30) for one-dimensional, overdamped Langevin processes, these relations are generally valid for multidimensional overdamped Langevin processes and Markov jump processes [14].

Note that for the special cases where $\pi_{\mathcal{T}} = 0$, as discussed below Equation (8.29), we obtain the appealing bound

$$\langle W_{\mathcal{T}}\rangle \geq \langle \Delta G^{\mathrm{eq}}(\lambda_{\mathcal{T}})\rangle. \tag{8.31}$$

In other words, the average amount of work we need to perform on a system in order for a certain event of interest to happen, as determined by the stopping time $\mathcal{T}$, must be greater or equal than the average increase in free energy. This second law of thermodynamics holds for quenched protocols for which the event happens with probability 1 at nonzero times and for quasistatic protocols.

Although the remainder term $\pi_{\mathcal{T}}$ in Equation (8.30) spoils in general the more practical inequality equation (8.31), the remainder is at the origin of interesting phenomena, such as events in which on average an agent increases the free energy of a system more than the work it does on it.

In what follows, we illustrate the second law of thermodynamics Equation (8.30), as well as Equation (8.31), on the canonical example of the polymer in Figure 8.1, and we discuss the role of the remainder term $\pi_{\mathcal{T}}$.

8.2.4. *Canonical example illustrating the second law of thermodynamics*

We illustrate the second law at stopping times, Equation (8.30), on the example of Figure 8.2.

We assume that the position X of the dangling end point is well described in Equation (8.4) with the thermodynamic potential

$$V(x;\lambda_s) = \frac{\kappa_{\rm p}}{2}\,x^2 + \frac{\kappa_{\rm m}}{2}\,(x-\lambda_s)^2\,, \tag{8.32}$$

which is the sum of the potential $\kappa_{\rm p}x^2/2$ of a polymer with one of its end points anchored to the substrate at $x = 0$, and the potential $\kappa_{\rm m}(x-\lambda_s)^2/2$, of the spring that connects the dangling end point of the polymer to the molecular motor with its center of mass located at λ_s. At time $s = 0$, this motor-polymer system is in thermal equilibrium with its surroundings, and at time $s > 0$ the motor starts moving forwards. The dynamics of the center of mass of the molecular motor is

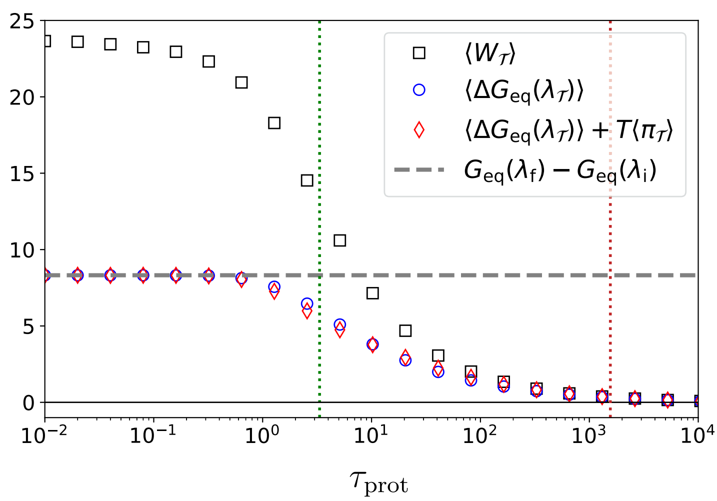

Figure 8.2. Simulation results demonstrating the second law of thermodynamics at stopping times (Equation (8.30)), for the model defined in Section 8.2.4 and illustrated in Figure 8.1. The parameters used in simulations are $\ell = 2.2$, $\mu = 0.1$, $T = \kappa_{\rm p} = 1$, $\kappa_{\rm m} = 2$, $\lambda_{\rm i} = 0.2$, $\lambda_{\rm f} = 5$, and $\tau = 10^6$. The vertical dotted lines denote the relaxation time $\tau_{\rm rel} = 10/3$ of the polymer towards equilibrium and the mean first-passage time $\tau_{\rm fp} = 1560$ for the polymer to reach the dangling end point from the initial point in the absence of a driving protocol. The black solid line indicates zero and is a guide to the eye. Figures are taken from Ref. [14].

described by

$$\lambda_s = \lambda_\mathrm{i} + (\lambda_\mathrm{f} - \lambda_\mathrm{i}) \frac{1 - \exp\left(-s/\tau_\mathrm{prot}\right)}{1 - \exp\left(-t/\tau_\mathrm{prot}\right)}, \quad s \in [0, t], \tag{8.33}$$

where $\tau_\mathrm{prot} > 0$ is the time scale determining the protocol speed. The polymer relaxes over a time scale $\tau_\mathrm{rel} = 1/(\mu(\kappa_\mathrm{m} + \kappa_\mathrm{p}))$. If $\tau_\mathrm{prot} \ll \tau_\mathrm{rel}$, then the molecular motor quenches the polymer, whereas if $\tau_\mathrm{prot} \gg \tau_\mathrm{rel}$, then the motor stretches the polymer in a quasi-static manner.

We determine the average work $\langle W_\mathcal{T} \rangle$ that the motor performs on the polymer to bring the second end point of the polymer to the location $X(t) = \ell$. Hence, the stopping time is defined by

$$\mathcal{T} = \inf\{s \geq 0 : X_s = \ell\}. \tag{8.34}$$

Simulation results in Figure 8.2 show numerically that the second law of thermodynamics at stopping times, Equation (8.30), holds. We observe two regimes, viz., the quenched regime for $\tau_\mathrm{prot} < \tau_\mathrm{rel}$, in which case the dissipated work $\langle W_\mathcal{T} \rangle - \langle \Delta G^\mathrm{eq}(\lambda_\mathcal{T}) \rangle$ is large, and the opposing quasi-static limit of $\tau_\mathrm{prot} > \tau_\mathrm{fp}$, for which $\langle W_\mathcal{T} \rangle - \langle \Delta G^\mathrm{eq}(\lambda_\mathcal{T}) \rangle \approx 0$. Another relevant time scale for this problem is the mean first-passage time τ_fp that X needs to reach $X = \ell$ when $\lambda_\mathrm{f} = \lambda_\mathrm{i}$. If $\tau_\mathrm{prot} > \tau_\mathrm{fp}$, then $\langle W_\mathcal{T} \rangle \approx 0$.

An interesting feature of the second law, which becomes evident from Figure 8.2, is that $\langle \pi_\mathcal{T} \rangle \approx 0$, and hence the appealing bound equation (8.31) ensues. The approximation $\langle \pi_\mathcal{T} \rangle \approx 0$ follows from the fact that $\langle \pi_\mathcal{T} \rangle = 0$ in the two limiting cases $\tau_\mathrm{prot} \gg \tau_\mathrm{rel}$ and $\tau_\mathrm{prot} \ll \tau_\mathrm{rel}$, for which the protocol is quasistatic and quenched, respectively. As discussed in Equation (8.29), in these two limiting cases $\pi_\mathcal{T} = 0$. In the intermediate regime $\pi_\mathcal{T} \neq 0$, but simulation results in Figure 8.2 show that nevertheless $\langle \pi_\mathcal{T} \rangle \approx 0$.

Taken together, it often holds that $\langle \pi_\mathcal{T} \rangle \approx 0$ and hence the practical inequality equation (8.31) applies. This inequality states that also at random times on average the free energy of a system cannot increase more than the average work done on it, in accordance with the classical result equation (8.3).

8.2.5. *Overcoming classical limits by stopping at a clever moment:* $\langle W_\mathcal{T} \rangle \leq \langle \Delta G^\mathrm{eq}(\lambda_\mathcal{T}) \rangle$

As discussed in Section 7.5, it is possible to (apparently) overcome classical limits by stopping a process at a clever moment. We consider now this question from the perspective of a nonstationary process, which is significantly more subtle than the stationary case.

It is the remainder term $\pi_\mathcal{T}$ in the second law equation (8.30) that describes the possibility to increase on average the free energy of a system more than the work put into it. To achieve this, we need a large enough positive value of $\langle \pi_\mathcal{T} \rangle$ as the dissipated work is lower bounded by $-T\langle \pi_\mathcal{T} \rangle$, viz.,

$$\langle W_\mathcal{T} \rangle - \langle \Delta G^\mathrm{eq}(\lambda_\mathcal{T}) \rangle \geq -T\langle \pi_\mathcal{T} \rangle. \tag{8.35}$$

To have $\langle W_\mathcal{T} \rangle$ small enough we need a large enough value of $\langle \pi_\mathcal{T} \rangle$, which as discussed in the previous section can be attained when $\mathcal{P}(\mathcal{T} = 0) > 0$.

We illustrate this in Figure 8.3 for the same model for X as considered in Figure 8.2, i.e., the Langevin equation (8.4) with potential equation (8.32). A notable difference is that the stopping event is defined by

$$\mathcal{T} = \min\{s \geq 0 : X_s \leq \ell\} \tag{8.36}$$

so that $\mathcal{P}(\mathcal{T} = 0) > 0$. The numerical results in Figure 8.3 show that there exists a region at intermediate protocol speeds τ_prot for which $\langle W_\mathcal{T} \rangle < \langle \Delta G^\mathrm{eq}(\lambda_\mathcal{T}) \rangle$, demonstrating that the classical limit $\langle W_t \rangle > \Delta G^\mathrm{eq}$ can be overcome by stopping a process at a cleverly chosen moment.

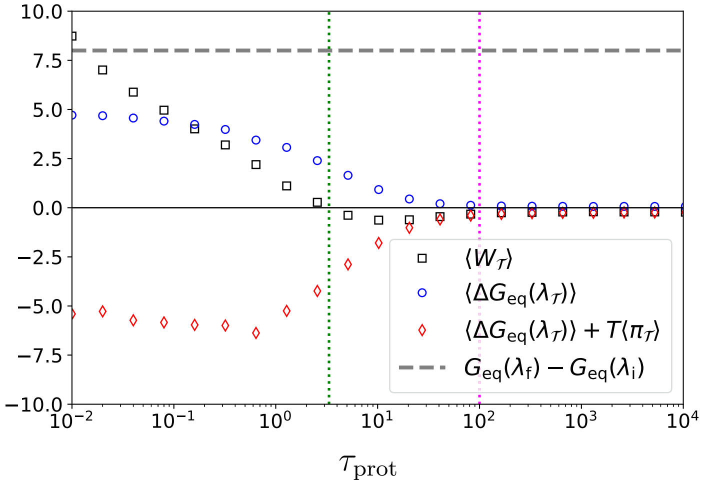

Figure 8.3. Overcoming classical limits by stopping at a clever moment, viz. $\langle W_{\mathcal{T}}\rangle \leq \langle \Delta G^{\rm eq}(\lambda_{\mathcal{T}})\rangle$. The model used in the one of Figure 8.1 and defined in Section 8.2.4. The parameters used in simulations are $\ell = 0.2$, $\mu = 0.1$, $T = 10$, $\kappa_{\rm p} = 1$ $\kappa_{\rm m} = 2$, $\lambda_{\rm i} = 1$, $\lambda_{\rm f} = 5$, and $\tau = 50$. The stopping time used is $\mathcal{T} = \min\{s \geq 0 : X_s \leq \ell\}$. The black solid line indicates zero and is a guide to the eye. Figures are taken from [14].

8.3. *Second law at stopping times and gambling demons*

The objects of interest in this section will be the generalized stochastic entropic functional given in Equation (8.1):

$$\hat{\Sigma}_s = \underbrace{\ln\left(\frac{\rho_s(X_s)}{\tilde{\rho}^{(t)}_{t-s}(X_s)}\right)}_{\delta^{(t)}_s} + S^{\rm tot}_s, \tag{8.37}$$

where the first term is denoted as the **stochastic distinguishability** between conjugate times in the forward and backward processes [15]; it is given in Equation (6.105), copied here for convenience

$$\delta^{(t)}_s = \ln\left(\frac{\rho_s(X_s)}{\tilde{\rho}^{(t)}_{t-s}(X_s)}\right). \tag{8.38}$$

We recall that here the stochastic total entropy production $S^{\rm tot}_s$ is given in (6.31)–(6.33)

$$S^{\rm tot}_s = \ln\left[\frac{\mathcal{P}\left(X_{[0,s]}\right)}{\widetilde{\mathcal{P}}^{(s)}\left(\Theta_s(X_{[0,t]})\right)}\right], \tag{8.39}$$

and we will consider $0 \leq s \leq t$ throughout this section. Here, the path probabilities $\mathcal{P}$ and $\tilde{\mathcal{P}}^{(t)}$ are defined as follows:

- Forward process is a nonequilibrium Markovian process with initial state drawn from $\rho_0(x)$ and driven through a deterministic protocol λ_u to a final state with distribution $\rho_t(x)$. In the forward process, a given trajectory $x_{[0,t]}$ is produced with probability $\mathcal{P}(x_{[0,t]})$.

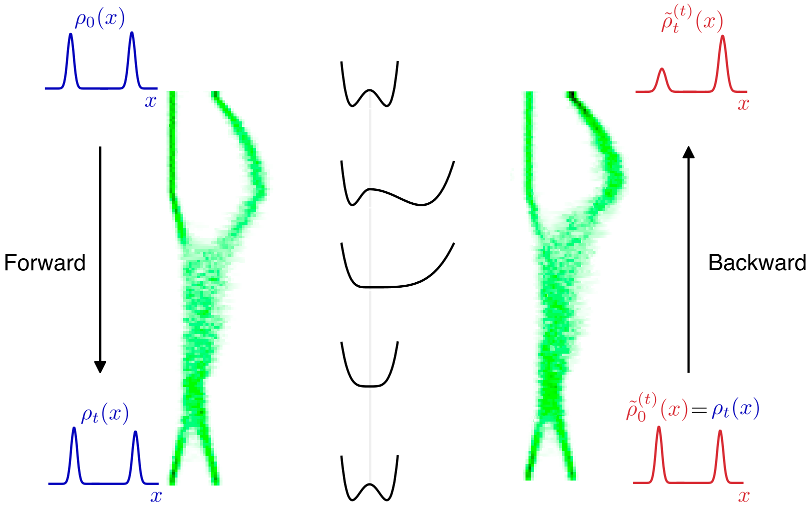

Figure 8.4. Illustration of forward and backward processes used in Section 8.3, where a Brownian particle immersed in a fluid is externally controlled with a feedback trap creating a time-dependent potential (black line in the central column). In the forward (backward) process, the particle is initially drawn from the distribution $\rho_0(x)$ ($\rho_0^{(t)}(x)$) and the potential evolves as in the central column from top to bottom (bottom to top), reaching a final state characterized by the distribution $\rho_t(x)$ ($\rho_t^{(t)}(x)$). The green dots illustrate histograms of the particle position taken during the evolution of the forward (left) and backward (right) processes, revealing the time-reversal asymmetry in the statistics of X, i.e., in general $\rho_s(x) \neq \tilde{\rho}_{t-s}^{(t)}(x)$ for $s \in (0, t]$, see Equation (8.38). Figure adapted from [200] with permission.

- Auxiliary backward process starts from state drawn from the final distribution of the forward process $\tilde{\rho}_0^{(t)}(x) = \rho_t(x)$. It is driven by a protocol that is the time-reversal mirror of the forward protocol $\tilde{\lambda}_s = \lambda_{t-s}$. In the backward auxiliary process, a given trajectory $x_{[0,t]}$ is produced with probability $\widetilde{\mathcal{P}}^{(t)}(x_{[0,t]})$. See Figure 8.4 for an illustration of forward and backward processes.

In the following, we make use of the mathematical power of the martingales to extract knowledge about entropy production at stopping times for Markovian processes that are in general non-stationary. First, we report recent results (see Refs. [14,15]) that revealed the stochastic total entropy production S_t^{tot} is not an exponential martingale in generic non-stationary nonequilibrium processes.

For generic non-stationary Markovian processes, the stochastic entropy production S_t^{tot} given in Equation (8.39) **is not an exponential martingale**, i.e., in general $\langle \exp(-S_t^{\text{tot}}) \,|\, X_{[0,s]} \rangle \neq \exp(-S_s^{\text{tot}})$. However, as we saw in two different ways – in equation (6.104) in Section 6.2.2 and in relation (6.144) in Section 6.3.4 – it is possible to "martingalize" S_t^{tot} in non-stationary nonequilibrium processes, i.e., find a process related to S_t^{tot} that is an exponential martingale. In particular, it follows that for generic (even non-stationary) nonequilbrium processes, for $0 \leq u \leq s \leq t$, it holds that (6.129)

$$\langle \exp(-S_s^{\text{tot}} - \delta_s^{(t)}) \,|\, X_{[0,u]} \rangle = \exp(-S_u^{\text{tot}} - \delta_u^{(t)}). \tag{8.40}$$

Note that $\delta_t^{(t)} = 0$ for all t and that the superindex in $\delta_s^{(t)}$ denotes the time with respect one does the time-reversal operation, t. The stochastic distinguishability vanishes at all times for (possibly nonequilibrium) stationary states – for which ρ_s and $\rho_s^{\tilde{\mathcal{P}}^{(t)}}$ are independent on time s. For non-stationary processes, $\delta_s^{(t)}$ fluctuates and can in principle take any value.

Applying Jensen's inequality to the "martingale property" (8.40), we obtain that for any $0 \le s \le t$ we have the sub-Martingale relation

$$\langle S_t^{\rm tot} + \delta_t^{(t)} \,|\, X_{[0,s]} \rangle \ge S_s^{\rm tot} + \delta_s^{(t)}. \tag{8.41}$$

Specializing the "submartingale" condition (8.41) to $s = 0$, noting that $S_0^{\rm tot} = 0 = \delta_t^{(t)}$, and averaging with respect to X_0, we get the refined second law for non-stationary Markovian processes (6.116)

$$\langle S_t^{\rm tot} \rangle \ge \langle \delta_0^{(t)} \rangle, \tag{8.42}$$

where (8.38)

$$\langle \delta_0^{(t)} \rangle = \int_{\mathcal{X}} {\rm d}x \rho_0(x) \ln \left[\frac{\rho_0(x)}{\tilde{\rho}_t^{(t)}(x)} \right] \ge 0, \tag{8.43}$$

is the Kullback–Leibler divergence between the distribution ρ_0 and $\tilde{\rho}_t^{(t)}$. It is equal to zero for $t = 0$ and it is positive otherwise. We will generalize this second law in Section 9.2.1 within the context of deterministic refinements of the second law.

The fact that for any $0 \le s \le t$, $S_s^{\rm tot} + \delta_s^{(t)}$ is an exponential martingale has other important consequences for stochastic thermodynamics, which can be found applying Doob's optional stopping theorems. Similarly to the integral fluctuation theorem (7.9) at stopping times for stationary processes, $\langle \exp(-S_{\mathcal{T}}^{\rm tot}) \rangle = 1$, for non-stationary processes one can show (see Section 6.2.2) that an integral fluctuation theorem holds.

Integral fluctuation relation at stopping times for driven Markovian processes that may not be stationary. For a stopping time $\mathcal{T} \le t$,

$$\langle \exp(-(S_{\mathcal{T}}^{\rm tot} + \delta_{\mathcal{T}}^{(t)})) \rangle = 1, \tag{8.44}$$

see Equation (6.107) and mathematical derivation in Section 6.2.2. Note that here, it is crucial to note that the quantity $\delta_{\mathcal{T}}^{(t)} = \ln(\rho_s(X_s)/\tilde{\rho}_{t-s}^{(t)}(X_s))|_{s=\mathcal{T}}$ results from evaluating the instantaneous densities $\rho_s(X_s)$ and $\tilde{\rho}_{t-s}^{(t)}(X_s)$ at (stochastic) stopping times $s = \mathcal{T}$ that are extracted from the forward process. For stationary processes $\delta_{\mathcal{T}}^{(t)} = 0$, and thus one recovers $\langle \exp(-S_{\mathcal{T}}^{\rm tot}) \rangle = 1$, see Equation (7.9).

The fact that the stochastic distinguishability can in principle take any value at stopping times has implications regarding the extension of the second law for $S_t^{\rm tot}$ in generic Markovian nonequilibrium processes, as we show below, in terms of the so-called second law at stopping times.

Second law at stopping times for driven Markovian processes that may not be stationary. Applying Jensen's inequality to (8.44), we find that for any stopping time $\mathcal{T} \leq t$, one has

$$\langle S^{\text{tot}}_{\mathcal{T}} \rangle \geq -\langle \delta^{(t)}_{\mathcal{T}} \rangle, \tag{8.45}$$

where

$$\langle \delta^{(t)}_{\mathcal{T}} \rangle = \int_0^t \mathrm{d}s \int_{\mathcal{X}} \mathrm{d}x \; \rho_{X_{\mathcal{T}},\mathcal{T}}(x,s) \ln \left[\frac{\rho_s(x)}{\tilde{\rho}^{(t)}_{t-s}(x)} \right]. \tag{8.46}$$

Here $\rho_{X_{\mathcal{T}},\mathcal{T}}$ is the joint probability density for the stopping time to take the value $\mathcal{T} = s$ and for the system to be at state $X_{\mathcal{T}} = x$ when the stopping condition happens. On the other hand, the densities $\rho_s(x)$ and $\tilde{\rho}^{(t)}_{t-s}(x)$ denote the instantaneous density of the forward and backward process evaluated at times s and $t - s$, respectively.

Note that, using Bayes' formula, we have in Equation (8.46) that $\rho_{X_{\mathcal{T}},\mathcal{T}}(x,s) = \rho_{\mathcal{T}}(s)\rho_{X_{\mathcal{T}}|\mathcal{T}}(x|s)$, however, in general $\rho_{X_{\mathcal{T}}|\mathcal{T}}(x|s) \neq \rho_s(x)$. This highlights the fact that the right-hand side of Equation (8.46) is not a Kullback–Leibler divergence, hence it is not obvious the sign of the term $\langle \delta^{(t)}_{\mathcal{T}} \rangle$. In the following, we present a physical example of a system in which using stopping strategies one can find negative average stochastic entropy production at stopping times, i.e., $\langle S^{\text{tot}}_{\mathcal{T}} \rangle < 0$, a feature that is not forbidden by the second law at stopping times (8.45).

Experimental implementation with single electron transistors. We now discuss a recent application of the second law at stopping times given in Equation (8.45) in the context of information demons, see Ref. [15] for details. Maxwell's demon thought experiment is considered the cornerstone of information thermodynamics. Such a "demon" is able to, i.e., induce a net heat flow from a cold to a hot reservoir by using information acquired from the bath molecules in a clever way. In Maxwell's original proposal, an external controller ("demon") is allowed to open and close a tiny gate separating two gas containers that are held at different temperatures. Such demon acts at stochastic times, it opens the gate only when a particle get sufficiently close to the gate. Moreover, it applies a feedback protocol, as it opens the gate only to particles coming from the cold bath than are colder than the average, and to particles coming from the hot reservoir that are hotter than the average. This way, the demon applies feedback control on the entire system by changing the concentration of particles in each of the baths, which results in a net heat flow from the cold to hot bath, in an apparent violation of the second law. Such conundrum have been thoroughly studied within the framework of information thermodynamics [201], which established the minimal energetic costs and the entropy production associated with measurement and feedback, which led to the derivation of second laws in the presence of information processing (Figure 8.5).

We now ask the question: what is the entropy production associated with a demon that is only able to stop the dynamics of a physical process at stochastic times using suitable *gambling* strategies? Such scenario may result from considering a Maxwell-like demon that is able to terminate a process at a random time (open/close a gate) but does not apply feedback control after taking such action. We exemplify this question on an experiment in which an isothermal system at temperature T is driven out of equilibrium through a time-dependent protocol of a fixed finite duration t. By varying this protocol, the potential of the system is switched from $V_0(x)$ to $V_t(x)$. When averaging over many repetitions of the same protocol, the second law of thermodynamics

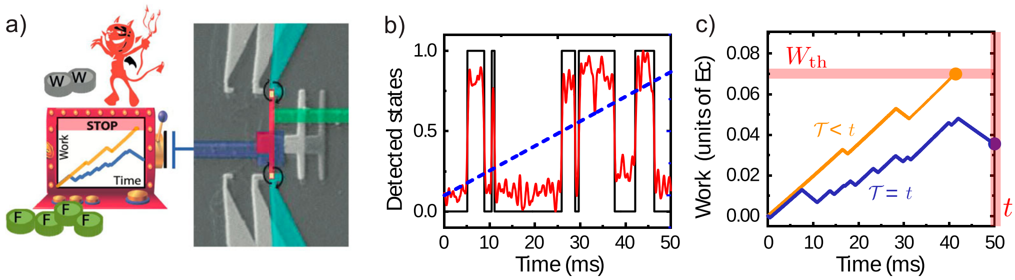

Figure 8.5. Experimental realization of a Gambling demon. (a) Sketch of the gambling demon and experimental setup. An external controller ("demon") monitors the fluctuations of a mesoscopic system that is driven out of equilibrium by a deterministic protocol of a prefixed duration t. The demon gambles with the information retrieved from the system, by stopping its evolution when a specific criterion is first met. In this case, it stops the external driving if the work done on the system exceeds a threshold value (orange line) or in the contrary at time t (blue line). As a result of this procedure, the demon expects to extract on average more free energy (gold coins) than the work invested (silver coins), an outcome that is inacessible without using gambling strategies (i.e., stopping the dynamics always at time t). Such idea was realized in [15] with an electronic system in which individual electrons can tunnel (black arrows) into a metallic island (red) whose voltage is controlled in time. (b) The experimental value of the detected state of the island (red line) is digitized (black line) and used for gambling. The blue line shows the expected value of the state of the electron averaged over many trajectories in the absence of gambling. (c) Experimental values of the work done on the electron until the stopping event of the gambling protocol takes place in two example trajectories that stop at $\mathcal{T} < t$ (orange) and at $\mathcal{T} = t$. Figure adapted from Ref. [15].

implies that

$$\langle W_t \rangle - \langle \Delta G_t^{\rm ne} \rangle \geq 0, \tag{8.47}$$

where $\Delta G_t^{\rm ne} = G_t^{\rm ne} - G_0^{\rm ne}$ is the nonequilibrium free energy difference between the final and initial states of the system.[13]

A relevant question in this context is the following. Can one find a suitable stopping strategy – in particular a bounded stopping time $\mathcal{T} \leq t$ – that results on an average work extracted that is above the free energy difference $\langle \Delta G_{\mathcal{T}}^{\rm ne} \rangle$ averaged over all stopped trajectories? Note that here, $\langle \Delta G_{\mathcal{T}}^{\rm ne} \rangle = G_{\mathcal{T}}^{\rm ne} - G_0^{\rm ne}$ is calculated between the state at the stopping time and the initial state, therefore it involves trajectories of *stochastic* duration $[0, \mathcal{T}]$. From the second law at stopping times (8.45) and noting that [202] $S_s^{\rm tot} = (W_s - \Delta G_s^{\rm ne})/T$ for isothermal systems, one has

$$\langle W_{\mathcal{T}} \rangle - \langle \Delta G_{\mathcal{T}}^{\rm ne} \rangle \geq -T \langle \delta_{\mathcal{T}}^{(\tau)} \rangle, \tag{8.48}$$

where the stochastic distinguishability term $\langle \delta_{\mathcal{T}}^{(t)} \rangle$ is given as in Equation (8.46). Equation (8.48) opens the possibility for average work extraction beyond the nonequilibrium free energy change using stopping times.

In Ref. [15], a gambling demon was proposed theoretically and realized with a single-electron transistor (SET) experimental setup. Briefly, the dynamics of an electron hopping in an out of metallic island was tracked in time. The energy of the island was externally controlled through a deterministic protocol that was repeated many times to extract sufficient statistics. The stochastic dynamics of the electron resembles that of a two level system with states 0 and 1 and time-dependent transition rates. Under the assumption of local detailed balance, the transition rates between the two states obey

$$\omega(0,1)/\omega(1,0) = \exp(-\Delta V/T) \tag{8.49}$$

where ΔV is the energy difference between the two levels at time $s \in [0, t]$. A useful choice of gambling strategy is given by the family of stopping times

$$\mathcal{T} = \min(\mathcal{T}_{\text{wth}}, t), \tag{8.50}$$

where $\mathcal{T}_{\text{wth}}$ is the first passage time of the work done on the system to reach a predefined threshold value $W_{\text{th}} \geq 0$. For the two-level model system considered here, the work done up to time $s \leq t$ reads

$$W_s = V_s(X_s) - V_0(X_0) - \sum_{j=1}^{N_s} \left[V_{\mathcal{T}_j}(X_{\mathcal{T}_j^+}) - V_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}) \right], \tag{8.51}$$

which follows from Equation (5.81). We recall here that the second term in (8.51) is the heat absorbed by the system, which involves the energy change of the system at the j-th jump between states $X_{\mathcal{T}_j^-} \to X_{\mathcal{T}_j^+}$, and that N_t is the total number of jumps in the trajectory $X_{[0,t]}$. We recognize in the right-hand side of (8.51) the first term as the energy change and the second term as the heat absorbed by the system up to time t. Note also that here $X_t \in \{0, 1\}$ for all t and time is assumed to be continuous. The gambling strategy resulting from executing the stopping condition (8.50) is such that it satisfies $\mathcal{T} \leq t$, as required by the second law at stopping times (8.48). It is important to remark that other strategies involving stopping times would also satisfy the same constraint. The strategy defined in (8.50) is such that the work at the end of the gambling protocol $W_{\mathcal{T}}$ is a random variable which takes the value

$$W_{\mathcal{T}} = \begin{cases} W_{\text{th}} & \text{if } \mathcal{T} < t, \\ W_t \leq W_{\text{th}} & \text{if } \mathcal{T} = t. \end{cases} \tag{8.52}$$

Because W_t is a random variable, $W_{\mathcal{T}}$ is also a random variable whose distribution depends crucially on the threshold value W_{th}.

Experimental results in Ref. [15] explored the fluctuations of $W_{\mathcal{T}}$, with $\mathcal{T}$ defined in Equation (8.50), for different values of the work threshold W_{th}, see Figure 8.6.

Figure 8.6(a) shows that the fluctuations of the work done up to the stopping time $\mathcal{T}$ defined in Equation (8.50) does not satisfy Jarzynski's equality, i.e.,

$$\langle \exp(-(W_{\mathcal{T}} - \Delta G^{\text{ne}}_{\mathcal{T}})/T) \rangle \neq 1. \tag{8.53}$$

Notably, one recovers $\langle \exp(-(W_{\mathcal{T}} - \Delta G^{\text{ne}}_{\mathcal{T}})/T) \rangle = 1$ for the case of W_{th} large, which corresponds to the case in which no gambling is executed at all, and all trajectories have the same duration $\mathcal{T} = t$, as in Jarzynski's setup. The experimental results are however in excellent agreement, see Figure 8.6(a), for all threshold values W_{th} with the integral fluctuation relation at stopping times

$$\langle \exp(-(W_{\mathcal{T}} - \Delta G^{\text{ne}}_{\mathcal{T}})/T) \exp(-\delta^{(t)}_{\mathcal{T}}) \rangle = 1, \tag{8.54}$$

which is a special case of Equation (8.44) for isothermal systems. Consistent with Equation (8.54), the average work done on the system by gambling along trajectories of stochastic duration $\mathcal{T}$ obeys the second law at stopping times $\langle W_{\mathcal{T}} \rangle - \langle \Delta G^{\text{ne}}_{\mathcal{T}} \rangle \geq -T \langle \delta^{(t)}_{\mathcal{T}} \rangle$, see

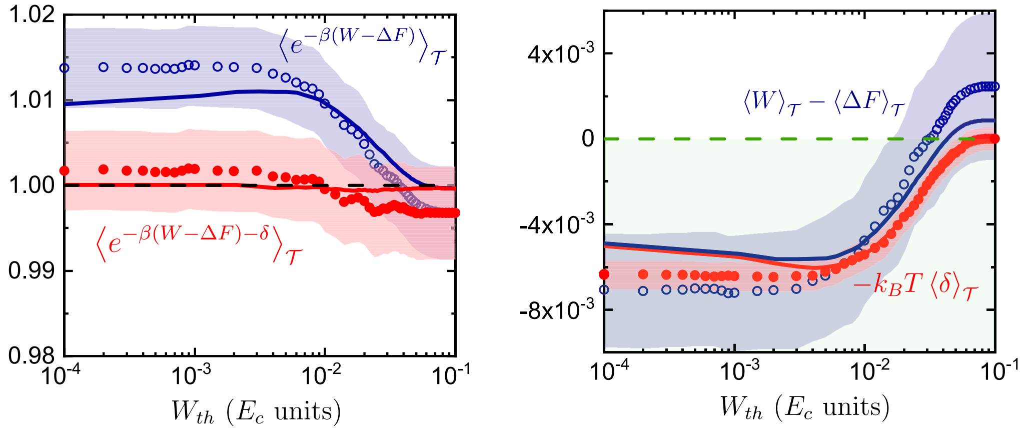

Figure 8.6. Experimental verification of the integral fluctuation theorem at stopping times (8.54) (left) and of the second law at stopping time (8.48) (right) for the gambling demon setup: experimental values (circles) and theoretical predictions (lines). In both panels, we plot the results obtained as a function of the work threshold value W_{th} used in the stopping rule given in Equation (8.50). Here $E_c = 109\mu$eV is the charging energy of the island. For large threshold values, Jarzynski's equality (top) and the standard second law (bottom) are recovered, as expected. See Ref. [15] for details.

Equation (8.48) which follows from applying Jensen's inequality to (8.54). For the experimental conditions used in [15], the term $\langle \delta_{\mathcal{T}}^{(t)} \rangle$ was positive for all the choices of the work threshold W_{th}, see Figure 8.6(b) (red circles). Moreover, the second law at stopping times (8.48) provides a tight bound in this system, which leads to values of work extraction at stopping times beyond the free energy change along the stopped trajectories, i.e., $\langle W_{\mathcal{T}} \rangle \leq \langle \Delta G_{\mathcal{T}}^{\text{ne}} \rangle$, a result that is forbidden by the standard second law, i.e., without using gambling or feedback control. Moreover as it was shown in [15] that the extent at which the "traditional" second law is violated, measured by how negative can $\langle W_{\mathcal{T}} \rangle - \langle \Delta G_{\mathcal{T}}^{\text{ne}} \rangle$ be, depends on the degree of time-asymmetry induced by the external protocol, which can be rationalized as follows. When the system is driven slowly (fast), the statistics of the forward and backward protocols are similar (fast) at stopping times, which makes the stochastic distinguishability term to be small (large).

Chapter 9. Martingales in stochastic thermodynamics V: the "tree" of second laws

Hänggi's Law: The more trivial your research, the more people will read it and agree. You write a nontrivial paper and you likely will be the only one who will remember it.

Arthur Bloch, Murphy's Law: Book three (1985).

This chapter provides different formulations of the second law of thermodynamics descending from the martingale properties unveiled in Chapter 6. As fruits of the martingale theory of stochastic thermodynamics, we derive a plethora of second-law-like inequalities from the submartingale conditions of Chapter 6, from which the second laws Equations (7.10), (8.20) and (8.41) from Chapters 7 and 8 are specific examples.

The "classical" second law of thermodynamics that appears in stochastic thermodynamics takes the form

$$\langle Z(X_{[0,t]}) \rangle \geq 0, \tag{9.1}$$

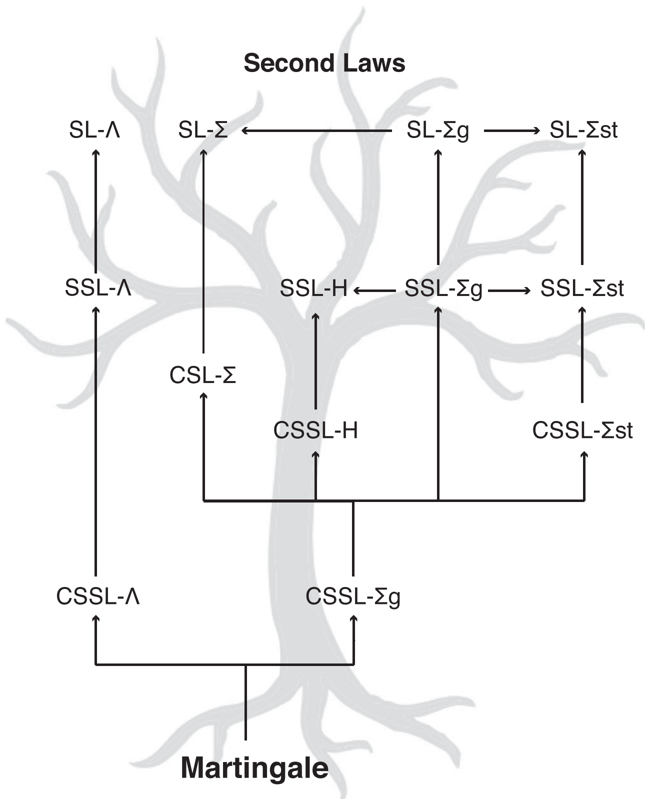

Figure 9.1. A "tree" of second laws emerge with its root at the martingale property of the entropic functionals introduced in Sections 6.1,6.2, and 6.3. The second laws are arranged in a hierarchical structure with the arrows denoting which laws follow as specific examples of more general results. The different acronyms stand for different formulations of the second law introduced below. See Section 9.1 for the definitions of the conditional strong second laws (CSSL). See Section 9.2 for the definitions of the conditional second laws (CSL). See Section 9.3 for strong second laws (SSL). See Section 9.4 for second laws (SL).

where Z is a functional evaluated over stochastic trajectories $X_{[0,t]}$. Instead, martingale theory provides second laws involving conditional expectations

$$\langle Z(X_{[r,u]}) \,|\, X_{[s,t]} \rangle \geq Z(X_{[s,t]}), \tag{9.2}$$

for all $0 \leq r \leq s \leq t \leq u$. Hence, with martingale theory we can address how knowledge about a system's trajectory affects the second law of thermodynamics.

Figure 9.1 illustrates the "tree"-like hierarchy of the different formulations of the Second Law of Thermodynamics that we derive from the martingales of Sections 6.2–6.3. The different formulations of the second law depend on the amount of knowledge we have available about a system's trajectory. The versions of the second law of thermodynamics that appear at the bottom of the tree assume that the observer has detailed knowledge available about the system's trajectory, while the observer's knowledge decreases when ascending the tree leading to weaker version of the second law of thermodynamics.

In this chapter, we assume for simplicity that X_t is a Markov process in discrete or continuous time, even though most of the results can also be formulated for generic stochastic processes.

9.1. *Conditional strong second laws (CSSL)*

The martingale properties for entropic functionals discussed in Chapter 6 can be interpreted as conditional strong second laws, which constrain the average of entropic functionals in a future time t conditioned on the fact that the system traces a specific trajectory $X_{[0,s]}$ up to a previous time $t \leq s$.

9.1.1. *Conditional strong second law for Λ-stochastic entropic functionals (CSSL-Λ)*

The submartingale condition (6.77) for Λ-stochastic entropic functionals states that

$$\left\langle \Lambda_t^{\mathcal{P},\mathcal{Q}} \middle| X_{[0,s]} \right\rangle \geq \Lambda_s^{\mathcal{P},\mathcal{Q}}, \tag{9.3}$$

for all $0 \leq s \leq t$. In other words, it is not possible to anticipate a decrease in $\Lambda_s^{\mathcal{P},\mathcal{Q}}$ based on knowledge of the past trajectory $X_{[0,s]}$. A physical example of a conditional strong second law is

$$\langle S_t^{\text{hk}} | X_{[0,s]} \rangle \geq S_s^{\text{hk}}, \tag{9.4}$$

where S_t^{hk} is the housekeeping entropy production, as defined in Equation (6.68).

9.1.2. *Conditional strong second law for Σ-stochastic entropic functionals when $\mathcal{Q} = \mathcal{Q}^{\text{st}}$ (CSSL-Σ_{st})*

As we have discussed in Chapter 6.2, Σ-stochastic entropic functionals are in general not submartingales, unless the reference path probability $\mathcal{Q}$ is time independent, stationary, and time homogeneous, i.e., $\mathcal{Q} = \mathcal{Q}^{\text{st}}$. In this case, the the submartingale condition (6.97) reads

$$\left\langle \Sigma_t^{\mathcal{P},\mathcal{Q}^{\text{st}}} \middle| X_{[0,s]} \right\rangle \geq \Sigma_s^{\mathcal{P},\mathcal{Q}^{\text{st}}}. \tag{9.5}$$

for all $0 \leq s \leq t$, which means that it is not possible to anticipate a decrease in $\Sigma_t^{\mathcal{P},\mathcal{Q}^{\text{st}}}$ based on the knowledge of the past trajectory $X_{[0,s]}$. If moreover $\mathcal{P}$ (or X_t) is a stationary Markov process, i.e., $\mathcal{P} = \mathcal{P}^{\text{st}}$, and it holds that $\Sigma_t^{\mathcal{P}^{\text{st}},\mathcal{P}^{\text{st}}} = S_t^{\text{tot}}$, with S_t^{tot} the total entropy production given in Equation (6.33), then the conditional strong second law equation (9.5) for S_t^{tot} reads

$$\left\langle S_t^{\text{tot}} \middle| X_{[0,s]} \right\rangle \geq S_s^{\text{tot}}. \tag{9.6}$$

Note that (9.6) is Equation (7.10) in Chapter 7.

On the other hand, if $\mathcal{P}$ (or X_t) is nonstationary, then the total entropic functional Σ_t^{tot} and the total stochastic entropy production S_t^{tot} do not satisfy conditional strong second laws. The same reasoning applies to the excess stochastic entropy production S_t^{ex} given in Equation (6.64).

9.1.3. *Conditional strong second law for the generalized Σ-stochastic entropic functional (CSSL-Σ_g)*

Generalized Σ-stochastic entropic functionals $\Sigma_{[r,s],t}^{\mathcal{P},\mathcal{Q}}$ with $[r,s] \subseteq [0,t]$ are forward submartingales with respect to s when r and t are fixed (see Equation (6.122)) and backward submartingales with respect to r when s and t are fixed (see Equation (6.130)). We unify these two statements by formulating a conditional strong second law.

The generalized Σ-stochastic entropic functional $\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t}$ with $[r,s] \subseteq [0,t]$, as defined in Equation (6.108), obeys the following **conditional strong second law (CSSL-Σ_g)**:

$$\left\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{[r',s'],t} \middle| X_{[r,s]} \right\rangle \geq \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t}, \tag{9.7}$$

for all $0 \leq r' \leq r \leq s \leq s' \leq t$. In words, $\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t}$ *conditionally increases* with respect to the final time s and *conditionally decreases* with respect to the initial time r.

The CSSL-Σ_g given in Equation (9.7) implies all the conditional strong second laws presented in Section 9.1.2 and is the root of many of the most well-known formulations of the second law of thermodynamics, see Figure 1.4; for example, it implies the second laws equations (8.20) and (8.41).

The conditional strong second law (9.7) together with the relation (6.139) proved in Chapter 6 gives for arbitrary Markovian process the following relation. For all $0 \leq r' \leq r \leq s \leq s' \leq t$, it holds that

$$\left\langle \left(\ln \left(\frac{\rho_{r'}(X_{r'})}{\rho^{\mathcal{Q}^{(t)}}_{t-s'}(X_{s'})} \right) + S^{env,\mathcal{P},\widehat{\mathcal{Q}}^{(t,s')}}_{s'} - S^{env,\mathcal{P},\widehat{\mathcal{Q}}^{(t,r')}}_{r'} \right) \middle| X_{[r,s]} \right\rangle$$
$$\geq \ln \left(\frac{\rho_{r}(X_{r})}{\rho^{\mathcal{Q}^{(t)}}_{t-s}(X_{s})} \right) + S^{env,\mathcal{P},\widehat{\mathcal{Q}}^{(t,s)}}_{s} - S^{env,\mathcal{P},\widehat{\mathcal{Q}}^{(t,r)}}_{r}, \tag{9.8}$$

in terms of the environmental $\widehat{\mathcal{Q}}$-stochastic entropy change (6.27). Here $\widehat{\mathcal{Q}}^{(t,.)}$ is the path probability of a Markovian process with generator given in (6.134). In the same way, with the relation (6.140) proved in Chapter 6, we obtain for arbitrarily Markovian process the **conditional strong second law** for all $0 \leq r' \leq r \leq s \leq s' \leq t$

$$\left\langle \left(\ln \left(\frac{\rho_{s'}(X_{s'})}{\rho^{\mathcal{Q}^{(t)}}_{t-s'}(X_{s'})} \right) + S^{\mathcal{P},\widehat{\mathcal{Q}}^{(t,s')}}_{s'} - S^{\mathcal{P},\widehat{\mathcal{Q}}^{(t,r')}}_{r'} \right) \middle| X_{[r,s]} \right\rangle \geq$$
$$\ln \left(\frac{\rho_{s}(X_{s})}{\rho^{\mathcal{Q}^{(t)}}_{t-s}(X_{s})} \right) + S^{\mathcal{P},\widehat{\mathcal{Q}}^{(t,s)}}_{s} - S^{\mathcal{P},\widehat{\mathcal{Q}}^{(t,r)}}_{r}, \tag{9.9}$$

in term of the $\widehat{\mathcal{Q}}$-stochastic entropy production.

As a special case of (9.8), the relation (6.141) of Chapter 6 allows to derive the following **conditional strong second law** for all $0 \leq r' \leq r \leq s \leq s' \leq t$:

$$\left\langle \underbrace{\ln \left(\frac{\rho_{r'}(X_{r'})}{\tilde{\rho}^{(t)}_{t-s'}(X_{s'})} \right)}_{\alpha^{(t)}_{r',s'}} + S^{\text{env}}_{s'} - S^{\text{env}}_{r'} \middle| X_{[r,s]} \right\rangle \geq \underbrace{\ln \left(\frac{\rho_{r}(X_{r})}{\tilde{\rho}^{(t)}_{t-s}(X_{s})} \right)}_{\alpha^{(t)}_{r,s}} + S^{\text{env}}_{s} - S^{\text{env}}_{r}, \tag{9.10}$$

which generalizes Equation (8.20) and where S^{env}_{s} is the environment entropy change defined in Equation (6.32). Furthermore, using the decomposition (6.33) of total entropy production, we obtain the following **conditional strong second law** for generic Markovian process and for all $0 \leq r' \leq r \leq s \leq s' \leq t$:

$$\left\langle \underbrace{\ln \frac{\rho_{s'}(X_{s'})}{\tilde{\rho}^{(t)}_{t-s'}(X_{s'})}}_{\delta^{(t)}_{s'}} + S^{\rm tot}_{s'} - S^{\rm tot}_{r'} \middle| X_{[r,s]} \right\rangle \geq \underbrace{\ln\left(\frac{\rho_s(X_s)}{\tilde{\rho}^{(t)}_{t-s}(X_s)}\right)}_{\delta^{(t)}_{s}} + S^{\rm tot}_{s} - S^{\rm tot}_{r}, \tag{9.11}$$

which generalizes Equation (8.41). This relation extends the conditional strong second law (9.6) to the nonstationary setup.

9.1.4. *Conditional version of the historical second law (CSSL-H) for Markovian processes*

From the CSSL-Σ_g given in Equation (9.7), it is possible to derive many well-known formulations of the second law of thermodynamics.

Let us consider the following Σ-stochastic entropic functional that only depends on the state X_r at the initial time r of the interval of interest $[r,s]$, viz.,

$$\Sigma^{\mathcal{P},\mathcal{P}^{\rm h,(t)}}_{[r,s],t} = \ln\left(\frac{\rho_r}{\rho'_r}(X_r)\right). \tag{9.12}$$

Here, ρ'_r represents the instantaneous density of a Markov process that has the same generator $\mathcal{L}$ as the process X_t, but with an initial density ρ'_0 that may be different from ρ_0, the probability density of X_0 under its native measure $\mathcal{P}$.

The path probability $\mathcal{Q} = \mathcal{P}^{\rm h,(t)}$ that determines the generalized Σ-stochastic entropic functional in Equation (9.12) has a similar structure to the excess path probability $\mathcal{P}^{{\rm ex},(t)}$, as defined in Section 6.1.6. In particular, $\mathcal{P}^{\rm h,(t)}$ is the path probability of a process with initial density $\rho_0^{\mathcal{P}^{\rm h,(t)}} = \rho'_t$ and with a Markovian generator that is given by the generalized Doob's h-transform

$$\mathcal{L}^{h,(t)}_s \equiv \left(\rho'_{t-s}\right)^{-1} \circ \mathcal{L}^\dagger_{t-s} \circ \rho'_{t-s} - \left(\rho'_{t-s}\right)^{-1}\left(\mathcal{L}^\dagger_{t-s}\rho'_{t-s}\right), \tag{9.13}$$

which holds for $s \leq t$, and $\circ$ denotes here the composition operator. See Ref. [82] for additional information about continuous-time Doob's h-transform. Note that, if we replace in Equation (9.13) the density ρ'_t by the accompanying density π_t, as defined in Equation (6.66), then we get the Markovian generator associated with the "excess" dynamics $\mathcal{P}^{\rm ex,(t)}$, see Equation (6.65). [14]

Specializing the backward submartingale relation (9.7) to the choice (9.12) yields the following **conditional version** of the **"historical" second law (CSSL-*H*)**, viz.,

$$\left\langle \ln\left(\frac{\rho_r(X_r)}{\rho'_r(X_r)}\right) \middle| X_{[s,t]} \right\rangle \geq \ln\left(\frac{\rho_s(X_s)}{\rho'_s(X_s)}\right) \tag{9.14}$$

for all $0 \leq r \leq s \leq t$. Because $r \leq s$, Equation (9.14) implies that $\ln \frac{\rho_r(X_r)}{\rho'_r(X_r)}$ is conditionally increasing in the reverse flow of time.

Now, we consider two examples for which the conditional version of the historical strong second law CSSL-H is particularly beautiful.

- *"Canonical" setup*: Let us consider X_t, a process which starts from an arbitrary initial distribution $\rho_0(X_0)$ and has a stationary density given by the Gibbs canonical distribution $\rho_{\rm st}(x) = \exp(-(H(x) - G^{\rm eq})/T)$, with the equilibrium free energy $G^{\rm eq} = \int_{\mathcal{X}} {\rm d}x \exp(-H(x)/T)$. Such dynamics, starting from a non-Gibbsian initial distribution, is sometimes called *a relaxation process*. This is the case for example of isothermal Langevin processes [Langevin equation (3.65) with Einstein relation (3.69)] with time-independent potential and no external forces. For such relaxation dynamics, we have

$$\ln\left(\frac{\rho_t(X_t)}{\rho_{\rm st}(X_t)}\right) = \ln(\rho_t(X_t)) + \frac{H(X_t) - G^{\rm eq}}{T}, \tag{9.15}$$

where in the right-hand side, we recognize the **nonequilibrium free energy** which is defined as

$$G_t^{\rm ne} = H(X_t) + T\ln(\rho_t(X_t)), \tag{9.16}$$

which is a fluctuating quantity whose ensemble average is given by [201–203]

$$\left\langle G_t^{\rm ne}\right\rangle = \langle H(X_t)\rangle + T\langle \ln\rho_t(X_t)\rangle = \langle H(X_t)\rangle - T\langle S_t^{\rm sys}\rangle. \tag{9.17}$$

For the choice $\rho_t' = \rho_{\rm st}$, the CSSL-H (9.14) with Equation (9.15) and using the definition (9.16), we derive a universal constraint for the expected value of the nonequilibrium free energy for such relaxation processes.

> Let X_t represent a process that relaxes under isothermal conditions to the stationary Gibbs canonical density $\rho_{\rm st}(x) = \exp(-(H(x) - G^{\rm eq})/T)$, starting from an arbitrary initial state $\rho_0(X_0)$. In this case, the CSSL-H, given in Equation (9.14), implies that
>
> $$\left\langle G_r^{\rm ne}\middle| X_{[s,t]}\right\rangle \geq G_s^{\rm ne}, \tag{9.18}$$
>
> for all $0 \leq r \leq s \leq t$. Hence, the **nonequilibrium free energy**, given in Equation (9.16), of a relaxation processes under isothermal conditions is a **backward submartingale**.

- *"Microcanonical" setup*: Let us consider X_t, a process which has a homogeneous stationary density $\rho_{\rm st}$ (i.e., a driven Langevin process on a ring with constant force considered in Section 1.6), the CSSL-H given in Equation (9.14) for the choice $\rho_t' = \rho_{\rm st}$ gives that for all $0 \leq r \leq s \leq t$, one has

$$\left\langle \ln(\rho_r(X_r))\middle| X_{[s,t]}\right\rangle \geq \ln(\rho_s(X_s)). \tag{9.19}$$

The above equation can be formulated in terms of a constraint for the nonequilibrium system entropy $S_t^{\rm sys} = -\ln\rho_t(X_t)$, see Equation (5.14), as follows.

For relaxation processes towards a homogeneous stationary state, the **system entropy** is a **backward supermartingale**, i.e.,

$$\left\langle S_r^{\rm sys} \middle| X_{[s,t]} \right\rangle \leq S_s^{\rm sys}, \tag{9.20}$$

for all $0 \leq r \leq s \leq t$. Hence, in a "microcanonical" setup, the system entropy conditionally decreases in the reverse flow of time.

Note that there exist two types of second laws, those that consider the expected value of an observable in the future given its past history, and those that consider the expected value of an observable in the past given its current history. For example, the stochastic entropy production in a stationary process is a submartingale in the forward dynamics, implying we cannot anticipate a decrease of entropy in the universe based on knowledge of the past's history of a system. On the other hand, the nonequilibrium free energy in a relaxation process is a submartingale in the backward dynamics, implying that we expect free energy to have decreased in the past, irrespective of our knowledge of the system's trajectory. Both laws imply that knowledge of a system's trajectory does not affect the second law, irrespective whether we look forwards or backwards in time.

9.2. *One-time conditional second laws (CSL)*

In Section 9.1, we have introduced second-law-like inequalities for ensembles of trajectories satisfying constraints that involve their values over a finite time window. Such conditional strong second laws can be simplified when considering ensembles of trajectories $X_{[0,t]}$ for which their value at a given time, i.e., X_s for $s \leq t$ is constrained. We call these relations one-time conditional second laws, which we abbreviate as CSL.

9.2.1. *One-time conditional second law for Σ-stochastic entropic functionals (CSL-Σ) and Λ-stochastic entropic functionals (CSL-Λ)*

From the definition of generalized Σ-stochastic entropic functional over the subset interval $[r,s] \subseteq [0,t]$, see Equation (6.108), we find

$$\Sigma_{[0,t],t}^{\mathcal{P},\mathcal{Q}} = \Sigma_t^{\mathcal{P},\mathcal{Q}}, \quad \Sigma_{[s,s],t}^{\mathcal{P},\mathcal{Q}} = \ln\left(\frac{\rho_s}{\rho_{t-s}^{\mathcal{Q}}}(X_s)\right). \tag{9.21}$$

Then, the Conditional Strong Second Law for generalized Σ-stochastic entropic functionals, i.e., the CSSL-Σ_g given in Equation (9.7), implies a one-time Conditional Second Law for the Σ-stochastic entropic functional (**CSL-Σ**), viz., for $0 \leq s \leq t$ and for an arbitrary auxiliary process $\mathcal{Q}$,

$$\langle \Sigma_t^{\mathcal{P},\mathcal{Q}} \,|\, X_s \rangle \geq \ln\left[\frac{\rho_s(X_s)}{\rho_{t-s}^{\mathcal{Q}}(X_s)}\right]. \tag{9.22}$$

Note that this result follows also from the choice $Z(X_{[0,t]}) = \delta(X_s - x)$ in the mother fluctuation relation (6.19) and applying Jensen's inequality. We also note that the right-hand side of Equation (9.22) can be negative. Similarly, one can also prove an analogous result, the one-time conditional second law for Λ-stochastic entropic functionals (**CSL**-Λ):

$$\langle \Lambda_t^{\mathcal{P},\mathcal{Q}} \,|\, X_s \rangle \geq \ln\left[\frac{\rho_s(X_s)}{\rho_s^{\mathcal{Q}}(X_s)}\right], \tag{9.23}$$

which holds for any $0 \leq s \leq t$, and an arbitrary $\mathcal{Q}$. Averaging Equations (9.22) and (9.25) over all possible values of X_s, we obtain for any $0 \leq s \leq t$ the *deterministic refinements* of the second laws

$$\langle \Sigma_t^{P,Q} \rangle \geq D\left[\rho_s(x)||\rho_{t-s}^{\mathcal{Q}}(x)\right] \tag{9.24}$$

and

$$\langle \Lambda_t^{P,Q} \rangle \geq D\left[\rho_s(x)||\rho_s^{\mathcal{Q}}(x)\right]. \tag{9.25}$$

Notably, Equation (9.24) extends the Kawai–Parrondo–Van Den Broeck relation derived in Ref. [204] to arbitrary nonequilibrium Markovian processes.

9.2.2. *One-time conditional second law for isothermal Markovian systems*

For X_t an overdamped Markovian nonequilibrium process in isothermal conditions, we showed in Section 6.1.5.2 that the total Σ-stochastic entropic functional can be written in terms of the fluctuating work and the equilibrium free energy change, as $\Sigma_t^{\rm tot} = [W_t - (G_t^{\rm eq} - G_0^{\rm eq})]/T$, see Equation (6.51). This result holds for driven isothermal systems initially in thermal equilibrium, i.e., $\rho_0(x) = \exp(-(H_0(x) - G_0^{\rm eq})/T)$. As we showed in Section 6.1.5.3, to obtain this simple relation between $\Sigma_t^{\rm tot}$ and W_t one needs to choose as auxiliary process that with initial density $\rho_0^{\mathcal{Q}}(x) = \exp(-(H_t(x) - G_t^{\rm eq})/T)$ with the "naive" time reversal of the Markov generator of the original process $\mathcal{L}_s^{\mathcal{Q}} = \mathcal{L}_{t-s}$ $(s \leq t)$. Applying the results from Section 9.2.1 to the functional $\Sigma_t^{\rm tot} = [W_t - (G_t^{\rm eq} - G_0^{\rm eq})]/T$ has important physical consequences that we explain below.

(1) First, specializing Equation (9.24) to the choice $\Sigma_t^{\rm tot} = [W_t - (G_t^{\rm eq} - G_0^{\rm eq})]/T$ and setting $s = t$, one gets a refined second law for the fluctuating work exerted on an isothermal system,

$$\langle W_t \rangle \geq G_t^{\rm eq} - G_0^{\rm eq} + TD_{\rm KL}\left[\rho_t(x) \,||\, \exp\left(-\frac{H_t(x) - G_t^{\rm eq}}{T}\right)\right] = \left\langle G_t^{\rm ne}\right\rangle - \left\langle G_0^{\rm ne}\right\rangle. \tag{9.26}$$

The second equality in (9.26) follows from the definition (9.17) for the average nonequilibrium free energy $\langle G_t^{\rm ne}\rangle = \langle H_t(X_t)\rangle + T\langle \ln \rho_t(X_t)\rangle$ and the fact that $\langle G_0^{\rm ne}\rangle = G_0^{\rm eq}$ since the system is initially in thermal equilibrium. This refinement of the second law was derived in [172], see also [201].

(2) Second, specializing Equation (9.22) to the choice $\Sigma_t^{\rm tot} = [W_t - (G_t^{\rm eq} - G_0^{\rm eq})]/T$, and setting $s = t$ equal to the final time, one retrieves the conditioned second law

$$\langle\, W_t |\, X_t \,\rangle + G_0^{\rm eq} \geq T \ln\left(\rho_t\left(X_t\right)\right) + H_t\left(X_t\right). \tag{9.27}$$

Then, using Bayes' theorem in (9.27) we obtain for any subset $\Omega \subseteq \mathcal{X}$ of the phase space $\mathcal{X}$,

$$\begin{aligned}\langle\, W_t |\, X_t \in \Omega\rangle + G_0^{\rm eq} &\geq T\frac{\int_\Omega {\rm d}x \rho_t\left(x\right) \ln\left(\rho_t(x)\right)}{\int_\Omega {\rm d}x\rho_t\left(x\right)} + \frac{\int_\Omega {\rm d}x\rho_t\left(x\right) H_t(x)}{\int_\Omega {\rm d}x\rho_t\left(x\right)} \\ &= T\frac{\int_\Omega {\rm d}x\rho_t\left(x\right) \ln\left(\frac{\rho_t(x)}{\exp\left(-H_t(x)/T\right)}\right)}{\int_\Omega {\rm d}x\rho_t\left(x\right)}.\end{aligned} \tag{9.28}$$

Equation (9.28) suggests introducing the *conformational free energy* [205]

$$G_t^{\Omega} = -T \ln\left(\int_{\Omega} \mathrm{d}x \exp\left(-\frac{H_t(x)}{T}\right)\right), \tag{9.29}$$

which is in general different to the equilibrium free energy G_t^{eq} in which the integral is done over $\mathcal{X}$, see Equation (6.48).

Equation (9.28) can be understood as a conditional second law for the fluctuating work exerted along an arbitrary nonequilibrium process in isothermal conditions:

$$\langle W_t | X_t \in \Omega\rangle \geq G_t^{\Omega} - G_0^{\mathrm{eq}} + T \ln\left(\int_{\Omega} \mathrm{d}x\, \rho_t(x)\right). \tag{9.30}$$

Analogously, plugging relation $\Sigma_t^{\mathrm{tot}} = [W_t - (G_t^{\mathrm{eq}} - G_0^{\mathrm{eq}})]/T$ in Equation (9.22) but this time for $s = 0$, we get after some analogue algebra the initial time Condition Second Law for the fluctuating work exerted on an isothermal system

$$\langle W_t \,|\, X_0 \in \Omega\rangle \geq (G_t^{\mathrm{eq}} - G_0^{\Omega}) - T \ln\left(\int_{\Omega} \mathrm{d}x\, \rho_t^{\Omega}(x)\right) \quad . \tag{9.31}$$

Note that, because $\int_{\Omega} \mathrm{d}x\rho_t(x) \leq \int_{\mathcal{X}} \mathrm{d}x\rho_t(x) = 1$, then the last term in Equation (9.30) is negative, which implies that the average work done over trajectories that belong to the subset $X_t \in \Omega$ can be below the conformational free energy change.

Proof of Equation (9.30): We have from the relation (9.28) that

$$\langle W_t | X_t \in \Omega\rangle + G_0^{\mathrm{eq}} - G_t^{\Omega} \geq T \int_{\Omega} \mathrm{d}x\rho_{t,\Omega}(x) \ln\left(\frac{\rho_{t,\Omega}(x) \int_{\Omega} \mathrm{d}y\rho_t(y)}{\exp\left(-\frac{H_t(x)-G_t^{\Omega}}{T}\right)}\right), \tag{9.32}$$

where

$$\rho_{t,\Omega}(x) = \frac{\rho_t(x)\, 1_{\Omega}(x)}{\displaystyle\int_{\Omega} \mathrm{d}x\rho_t(x)}, \tag{9.33}$$

is the normalized density over the subset Ω. Equation (9.32) can also be written as follows:

$$\begin{aligned}\langle W_t | X_t \in \Omega\rangle + G_0^{\mathrm{eq}} - G_t^{\Omega} &\geq T \int_{\Omega} \mathrm{d}x\rho_{t,\Omega}(x) \ln\left(\frac{\rho_{t,\Omega}(x)}{\exp\left(-\frac{H_t(x)-G_t^{\Omega}}{T}\right)}\right) + T \ln\left(\int_{\Omega} \mathrm{d}y\rho_t(y)\right)\\ &\geq T \ln\left(\int_{\Omega} \mathrm{d}x\rho_t(x)\right),\end{aligned} \tag{9.34}$$

where in the second line we have used the fact that the first term in the right-hand side of the first line is positive because it is a Kullback–Leibler divergence. This concludes the proof of conditional second law for the fluctuating work (9.30).

Note that Equations (9.30) and (9.31) were previously derived, respectively, in the context of the energetics of symmetry breaking and symmetry restoration in Ref. [206]. They provide the generalization of Landauer's principle and a rationale for the energetics of Szilard's engine. These relations, and related generalizations, have also been derived in Refs. [207–209], and fruitfully applied to uncover thermodynamic properties of biopolymers in single-molecule experiments.

9.3. *Strong second laws (SSL)*

The conditional strong second laws presented in Section 9.1 have as interesting colloraries the, so-called, strong second laws, which involve the rate of change of the average of Λ-stochastic, Σ-stochastic, and generalized Σ-stochastic entropic functionals. Moreover, it is also possible to recover a "historical" formulation of the second law, which we discuss below in Section 9.3.3.

9.3.1. *Strong second law for Λ-stochastic (SSL-Λ) and Σ-stochastic (SSL-Σ_{st}) entropic functionals of stationary auxiliary process $\mathcal{Q} = \mathcal{Q}^{\mathrm{st}}$*

The conditional strong second law for entropic functionals CSSL-Λ, given in Equation (9.3), implies that the average of a Λ-stochastic entropic functional increases with time, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \Lambda_t^{\mathcal{P},\mathcal{Q}} \right\rangle \geq 0, \tag{9.35}$$

for all $t \geq 0$. This motivates us to call $\Lambda_t^{\mathcal{P},\mathcal{Q}}$ a Lyapunov function [96], as it is, on average, an increasing function of time. An example of the strong second law (9.35) is when $\Lambda_t^{\mathcal{P},\mathcal{Q}}$ is the housekeeping entropy production, see Equation (6.86).

Similarly, the CSSL-Σ_{st} for Σ-stochastic entropic functionals with stationary auxiliary reference process implies a strong second law (SSL-Σ_{st}), i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \Sigma_t^{\mathcal{P},\mathcal{Q}_{st}} \right\rangle \geq 0, \tag{9.36}$$

for all $t \geq 0$. Equation (9.35) implies that functionals of the form $\Sigma_t^{\mathcal{P},\mathcal{Q}_{st}}$ increase on average in time. We note, however, that this result does not imply the concavity in time, sometimes postulated for entropy production in classical thermodynamics [167].

We provide some remarks concerning the SSL-Λ (9.35) and the SSL-Σ_{st} (9.36).

(1) Analogously as what we have discussed in Section 9.1.2 for the CSSL-Σ_{st}, if the process X_t is not stationary, then the total entropic functional Σ_t^{tot} and the stochastic entropy production S_t^{tot} do not necessarily obey strong second laws. Analogously, the excess stochastic entropy production S_t^{ex}, given in Equation (6.64), does not satisfy, in general, a strong second law.

(2) If the process X_t is stationary, i.e., $\mathcal{P} = \mathcal{P}_{st}$, then the total Σ-stochastic entropic functional Σ_t^{tot} defined in (6.31) fulfills a strong second law. This includes the case of the total stochastic entropy production S_t^{tot} (6.33). Lastly, for X_t an overdamped isothermal stationary process, the associated second law (9.35) is the second law for fluctuating work exerted on isothermal system, viz., $\mathrm{d}\langle W_t\rangle/\mathrm{d}t \geq 0$.

9.3.2. *Strong second laws for generalized Σ-stochastic entropic functionals (SSL-Σ_g)*

Strong second laws also hold for the generalized Σ-stochastic entropic functionals in the subset interval $[r,s] \subseteq [0,t]$, for which we have shown that they fulfill two conditional strong second laws, one forward and another backwards in time, see Equation (9.7). This allows us to derive two strong second laws, one with respect to a decreasing initial observation time r, and another one with respect to an increasing final observation timed s. Indeed, averaging the CSSL-Σ_g relation (9.7) implies the following strong second laws for the generalized Σ-stochastic entropic functional (SSL-Σ_g):

$$\frac{\partial}{\partial s}\left\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t} \right\rangle \geq 0 \tag{9.37}$$

and

$$\frac{\partial}{\partial r}\left\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t} \right\rangle \leq 0, \tag{9.38}$$

where $0 \leq r \leq s \leq t$. This result implies that $\Sigma^{\mathcal{P},\mathcal{Q}}_{[r,s],t}$ is *increasing* with time s and decreasing with time r. Note that the SSL-Σg does not imply that $\frac{\partial}{\partial t}\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{t} \rangle \geq 0$; in general, the average Σ-stochastic entropic functional, given by $\langle \Sigma^{\mathcal{P},\mathcal{Q}}_{t} \rangle = \langle \Sigma^{\mathcal{P},\mathcal{Q}}_{[0,t],t} \rangle$, does *not* increase monotonically a function of t,[15] as setting $s = t$ in the relation (9.38) after taking the derivative $\partial/\partial s$ is different from setting $s = t$ before taking the derivative with respect to s.

9.3.3. *Historical strong second law (SSL-H) for Markovian processes*

Below, we derive the "historical" formulation of the strong second law as a direct consequence from the CSSL-Σ_g. This is an important point, as it reinforces the physical interest in the conditional strong second law.

Averaging the Conditional version of the Historical Strong Second Law (9.14) over $X_{[s,t]}$ (recall that $X_{[s,t]}$ is random in (9.14)), one retrieves the "historical" formulation of the second law (**SSL-H**) which is formulated as follows. Let $\rho_t(x)$ be the instantaneous density at time t of a generic stochastic process, and $\rho'_t(x)$ the density at the same time of a process which has the same dynamics but an arbitrary initial density ρ'_0 that may be different from the actual initial density of the process ρ_0. For all $t \geq 0$, it follows that

$$\frac{\mathrm{d}}{\mathrm{d}t} D_{\mathrm{KL}}\left[\rho_t(x) \| \rho'_t(x)\right] \leq 0, \tag{9.39}$$

with equality for the special case $\rho'_0(x) = \rho_0(x)$ which implies that $\rho_t(x) = \rho'_t(x)$ for all t. Equation (9.39) is considered by many authors "the" historical second law associated to a Markovian process in many place in the literature, see the books and reviews [4,73,142,158] and also and the classic article [210].

We now provide some additional remarks about the SSL-H (9.39).

(1) Let us consider the "microcanonical" relaxation setup introduced in Section 9.1.4, i.e., a system with arbitrary initial distribution that relaxes towards a homogeneous stationary distribution ρ_{st}. Averaging the CSSL-H (9.20) over $X_{[s,t]}$, we obtain that the system entropy increases with time on average $d\langle S^{\mathrm{sys}}_t \rangle/\mathrm{d}t \geq 0$.

(2) Following an analogous procedure for the case of "canonical" relaxations (i.e., a system such that its stationary density ρ_{st} exist and is the Gibbs canonical density) introduced in Section 9.1.4, we obtain $d\langle G^{\mathrm{ne}}_t \rangle/\mathrm{d}t \leq 0$.

9.4. *Second laws for entropic functionals (SL)*

To finalize our journey through the tree of second laws, Figure 9.1, we quote here second laws that follow readily as corollaries from the *strong* second laws presented in Section 9.3.

9.4.1. *Second law for Σ-stochastic entropic functionals (SL-Σ) and for Λ-stochastic entropic functionals (SL-Λ)*

From the definitions of the Λ-stochastic and Σ-stochastic entropic functionals, we have shown in Equation (6.17) that

$$\langle \Lambda_t^{\mathcal{P},\mathcal{Q}} \rangle \geq 0, \quad \text{and} \quad \langle \Sigma_t^{\mathcal{P},\mathcal{Q}} \rangle \geq 0, \tag{9.40}$$

for all $t \geq 0$, which we refer to as the second law for Λ-stochastic entropic functionals (SL-Λ) and the second law for Σ-stochastic entropic functionals (SL-Σ), respectively.

Consequently, the SL-Σ holds for all the examples of Σ-stochastic entropic functionals introduced in Chapter 6, inter alia, Σ_t^{tot}, S_t^{tot}, and S_t^{ex}, and analogously, the SL-Λ holds for all examples of Λ-stochastic entropic functionals considered, such as S_t^{hk}.

9.4.2. *Second law for generalized Σ-stochastic entropic functionals (SL-Σ_g)*

We derive a second law for generalized Σ-stochastic entropic functionals from the strong second law equation (9.38).

The definition of $\Sigma_{[r,s]}^{\mathcal{P},\mathcal{Q}}$, given in Equation (6.108), specialized to $s = r$, yields

$$\Sigma_{[r,r],t}^{\mathcal{P},\mathcal{Q}} = \ln\left(\frac{\rho_r}{\rho_{t-r}^{\mathcal{Q}}}(X_s)\right), \tag{9.41}$$

for all $0 \leq r \leq t$. Using Equation (9.41) in the SSL-Σ_g (9.38), we find that

$$\left\langle \Sigma_{[r,s],t}^{\mathcal{P},\mathcal{Q}} \right\rangle \geq D_{\text{KL}}\left[\rho_r(x) \| \, \rho_{t-r}^{\mathcal{Q}}(x)\right], \tag{9.42}$$

for all $0 \leq r \leq s \leq t$. As the Kullback–Leibler divergence is nonnegative, the second law

$$\left\langle \Sigma_{[r,s],t}^{\mathcal{P},\mathcal{Q}} \right\rangle \geq 0, \tag{9.43}$$

for all $0 \leq r \leq s \leq t$, ensues. The second law equation (9.43) holds for generalized Σ-stochastic entropic functionals (SL-Σ), as given in Equation (6.116). The (8.42) is a specific example of the second law equation (9.43).

This concludes our almanac of second laws derived from the martingale properties of entropic functionals.

Chapter 10. Martingales in progressive quenching

We are from the very beginning illogical and thus unjust beings and can recognize this.
F. Nietzsche, from "Human, All Too Human".

In this chapter, we meet with the martingale in physics in a different route from the path-probability ratio, which has been discussed in the previous two chapters. We mostly use a discrete-"time" variable. We hope this chapter may provide with a new look at the martingale process in physics and inspire the readers to explore its consequence in their domain of research.

10.1. *Introduction*

The conservation laws in physics are in many cases related to some form of invariance under symmetry operations. When a system has such a symmetry, the consequent conservation law imposes an ever-lasting memory of the initial condition. The martingale property is a kind of *stochastic conservation* property. Unlike the sub- or super-martingale, the expectation of a random variable is kept constant once its value is observed at some point of time. Then the natural questions might be : (i) What form of memory is brought by the martingale property? and (ii) Is there any invariance behind its martingale property? Below we will give, through the study of the concrete model which we call Progressive Quenching (PQ), answers to these questions.

As a part of this review on the martingale in physics, this chapter brings two ingredients that might be of general interest for those who are entering this domain. First we take the route to the martingale through the so-called *tower rule* (or *tower property*) (see Equation 2.3), which is a route distinct from the path-probability ratio mainly discussed in the precedent chapters. Second we show the case in which the martingale is found in the mean drift of the stochastic evolution of the principal process of interest. In the language of stochastic differential equations, $\dot{X}_t = G_t(X_t) + \sqrt{2D}\dot{B}_t$, it is $G_t(X_t)$ that is martingale. For such case, we coin a word *hidden martingale* relative to the process X_t.

Below we will show that the martingale can be used for the inference of the past state and, moreover, for the prediction of the future probability distribution, beyond just some conditional expectations. In Section 10.2, we introduce the notion of PQ process. Then in Section 10.3, we introduce the model we focus on, which is of discrete states and discrete time. We show the presence of martingale process behind the main stochastic process. In Section 10.4, we describe the consequences of the hidden martingale process, concerning the inference and the prediction. We conclude this chapter in Section 10.5.

10.2. *Progressive quenching as a neutral operation*

We sometimes encounter the situations in which system's degrees of freedom become progressively fixed. When a molten material as a fluid system is pulled out as a string from a furnace and is quickly cooled down [211], the fluid degrees of freedom associated to fluid particles are progressively fixed (quenched), see Figure 10.1. The roughness exponents of the diffusion-type field, such as the surface undulation of the string, show the modified and anisotropic exponents as compared with the equilibrium one [212]. Although the analogy is not close, we might also consider the process of decision-making by a community, in which the members progressively make up her or his mind before the referendum. In both examples, the already fixed part can influence the behavior of the part whose degrees of freedom are not yet fixed. We shall call these types of processes the progressive quenching, PQ. It is largely unknown what generic aspects are in this type of problem. In the non-equilibrium statistical mechanics viewpoint, the PQ should be categorized in such class that (1) the system's dynamics breaks the local detailed balance (because the fixed part will never be unfixed afterwords) and that (2) the partition between the system and the external system is revised. While the progress has been made a lot in understanding the repartition between the system and the bath since the last decade [25], the similar question for the system and the external system has been much less explored.

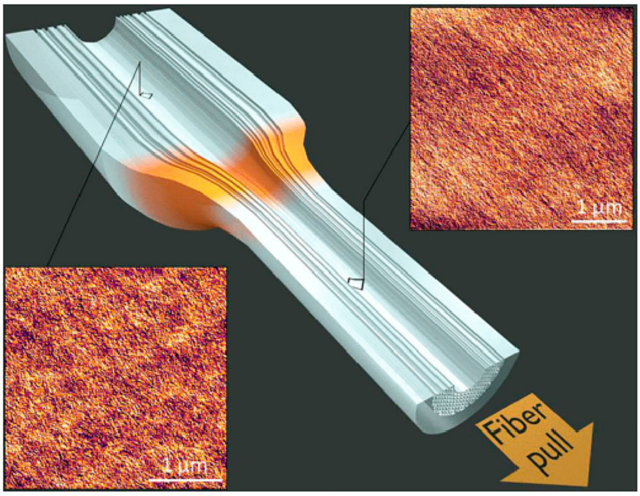

Figure 10.1. Sketch of the drawing of hollow fibers. See [211] for the details. Figure taken from Figure 1 of [211].

To have an intuition of PQ, we first describe this process for a one-dimensional ferromagnetic Ising chain up to the second-nearest neighbor interaction [213], whose energy H can be written as

$$-H = J_0 \sum_{i=1}^{N-1} s_i s_{i+1} + J_1 \sum_{i=1}^{N-2} s_i s_{i+2} + h \sum_{i=1}^{N} s_i. \quad (10.1)$$

The protocol of PQ is described in Figure 10.2. After an event of quenching (see below) is done, the unquenched part is re-equilibrated. Then the polarity of a specified number of spins (one spin in the case of Figure 10.2a) is fixed at their orientations that they took at the moment. This is the quenching event. The orientation of the newly fixed spins is, therefore, sampled from the equilibrium ensemble of the unquenched spins' configurations, but these spins are subject to the interactions with the *quenched spins* in addition to the interaction among the unquenched part. We should note that this process is *not* quasi-static although the unfixed spins are completely re-equilibrated. It is in the sense that the fixing of some spins implies to raise the barrier for the flipping of these spins so that the mean flipping interval exceeds the time-scale of observation/operation (see Chapter 7.1 of [25]).

If $J_1 = 0$, then the system has only the nearest neighbor interaction and we can directly use the technique of the transfer matrix. For $J_1 > 0$, we can still use this technique by introducing the composite variable, $\xi_p \equiv \{s_{2p-1}, s_{2p}\}$. Using this technique it was found that, for all the four models of PQ shown in Figure 10.2, the statistics of the finally quenched spins over the entire semi-infinite chain is identical to the equilibrium ensemble characterized by the temperature at which each spin has been quenched. This result is somehow counterintuitive because the protocol of PQ is very far from equilibrium, breaking the local detailed-balance (LDB) symmetry. A lesson that we might obtain from this solvable example is that PQ is a kind of *neutral* or non-invasive operation. For those unfixed spins which are just ahead of the quenching frontier, the fixation of the frontier spins is not "sensed" in the sense that the *statistics of* their equilibrium average is not biased nor modified by this operation. In general, the fixed part can cause the persistence in the process of unfixed part through the coupling between fixed part and unfixed one.

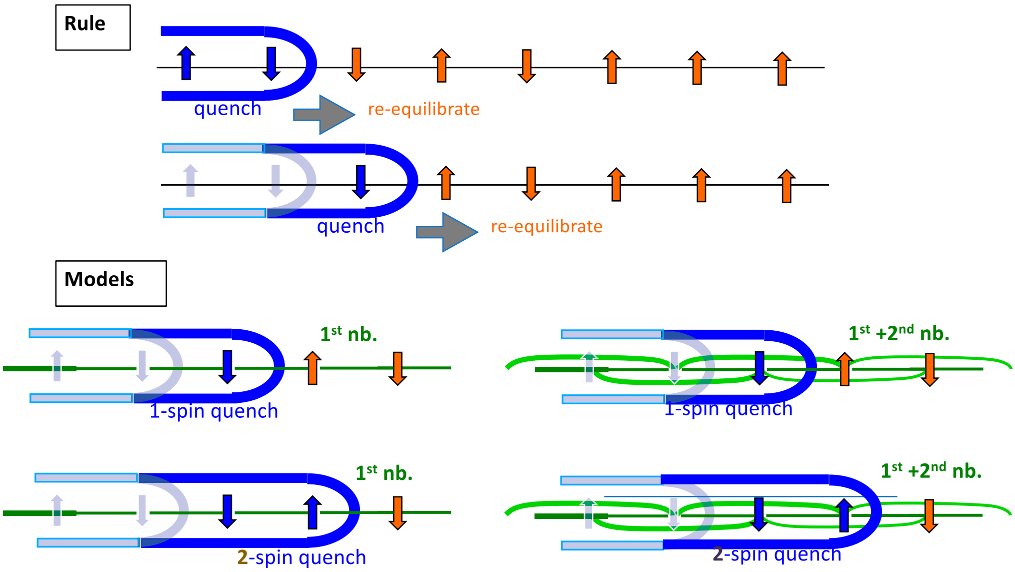

Figure 10.2. [Rule] shows elementary iterative step of progressive quenching applied to 1D Ising models. After the unquenched part is re-equilibrated, a specified number of spins are fixed at their orientation that they took at the moment. [Models] present different systems and different quenching units. In the first row in [Models] the spins interact with their first nearest neighbors, while in the lower row in [Models] the spins interact also with their second nearest neighbors. In the left column in [Models] a single spin is quenched at a time, while in the right column in [Models] a pair of spins are quenched at a time. (Figures are adopted from [213].)

10.3. *Globally coupled spin model and hidden martingale*

10.3.1. *Setup of model and protocol*

In [214], the authors took the ferromagnetic Ising model on a complete network, that is, the model in which any one of the spins interacts with all the other spins with equal coupling constant, j_0/N_0, where N_0 is the total number of spins. Each spin s_k takes the value ± 1. We mean by the stage-T, or simply T, the stage there are T *fixed* spins, see Figure 10.3(a) for illustration. The integer T acts as a fictive time of discrete stochastic processes. In this chapter, we avoid purposely the notation of usual time t because T should be better understood as the parameter characterizing the hybrid statistical ensemble consisting of the statistics of thermally fluctuating spins and that of fixed spins. At the stage-T, those $N = N_0 - \mathsf{T}$ unfixed spins are subject under the field consisting of two parts, $h = (-\frac{j_0}{N_0}M) + h_{\text{ext}}$. The part $-\frac{j_0}{N_0}M$ is the "molecular field" due to the quenched magnetization $M = \sum_{k=1}^{\mathsf{T}} s_k$, where we have relabeled the spins for our convenience. The other part, h_{ext}, is the genuine external field to perturb the process of PQ. The energy function then reads

$$\mathcal{H}_{\mathsf{T},M} = -\frac{j_0}{N_0} \sum_{\mathsf{T}+1 \le i < j \le N_0} s_i s_j + \left(-\frac{j_0}{N_0}M + h_{\text{ext}} \right) \sum_{i=\mathsf{T}+1}^{N_0} s_i. \tag{10.2}$$

The protocol of PQ is the cycle of re-equilibration of the unfixed spins and the fixation of a single spin at ± 1 just in the state it took at the moment of fixation. Because of the canonical equilibrium of unfixed spins, the probabilities for fixing in ± 1 are, respectively, $(1 \pm m^{(\text{eq})}_{\mathsf{T},M})/2$, see Figure 10.3(b), where $m^{(\text{eq})}_{\mathsf{T},M}$ is the canonical average of the unfixed spins with the probability weight

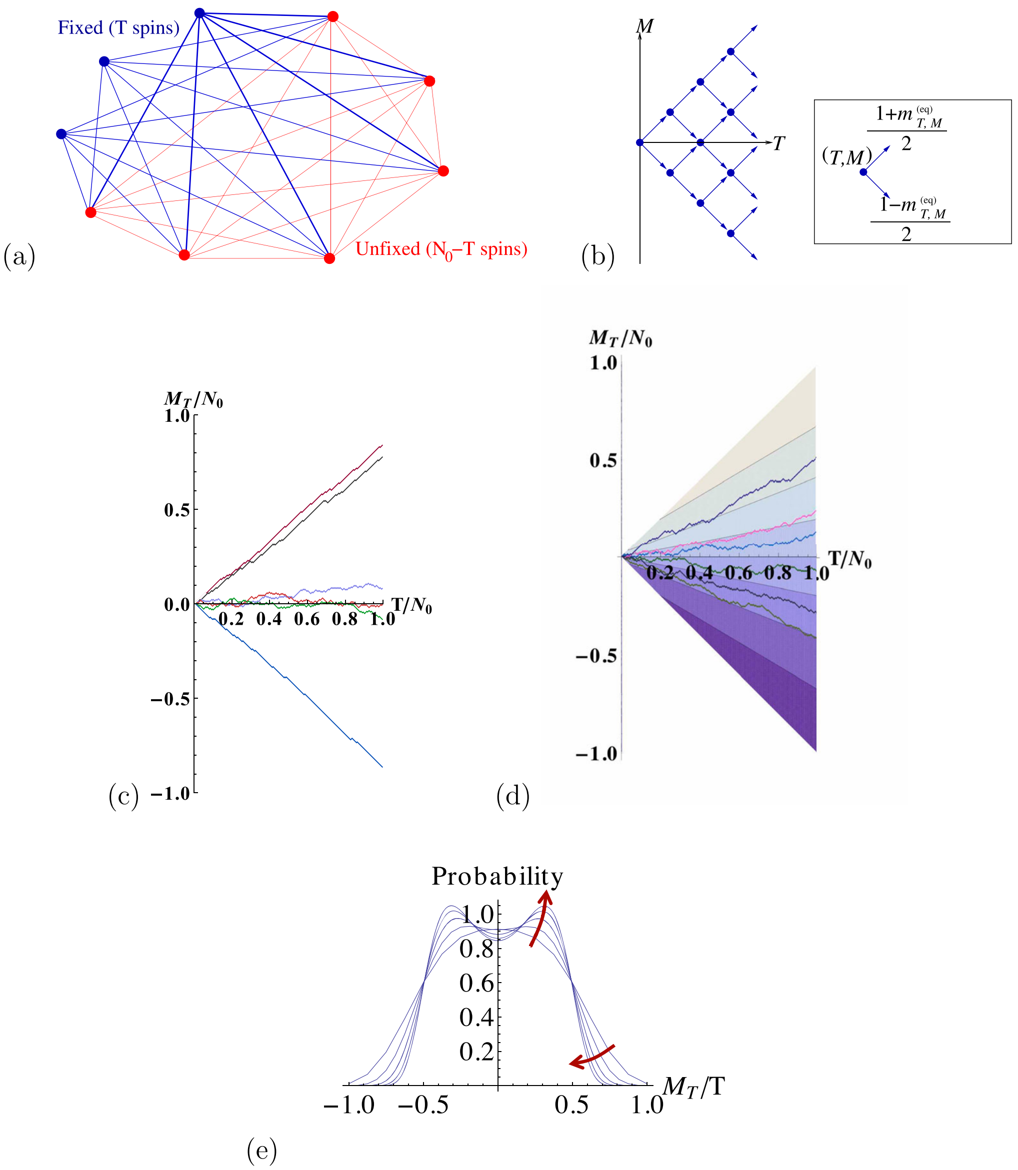

Figure 10.3. (a) In the complete network of $N_0(=9)$ spins, $\mathsf{T}(=3)$ spins have been fixed and there remain $N_0-\mathsf{T}$ unfixed spins. (b) PQ process of a complete spin network is a Markovian process on the 2D directed lattice coordinated by T and $M=\sum_{k=1}^{\mathsf{T}} s_k$. Those lattice points which are not visited are masked. (c) Three sample histories with $j_0 = 1.5$ (curves near the diagonals), and three others with $j_0 = 0$ (curves near the horizontal axis) are shown by different colors (brightness) for the system with the total size $N_0 = 256$. (d) The six sample histories (curves of different colors (brightness)) with $j_0 = j_{0,c}(\simeq 1.030)$, the "critical coupling" with the size $N_0 = 256$, are superposed on the contour plot of $m^{(\mathrm{eq})}_{\mathsf{T},M}$ for the same j_0 (almost straight lines inside the triangle with gradient of color (brightness)). The value of $m^{(\mathrm{eq})}_{\mathsf{T},M}$ is positive [negative], respectively, above [below] the horizontal axis. (e) Probability distributions of the mean *fixed* spin value, $M_{\mathsf{T}}/\mathsf{T}$, at different stages, $\mathsf{T}=2^k$ with integers $k = 4-8$. The system size is $N_0 = 2^8 = 256$. The initial conditions is $M_0 = 0$. The increment of T is indicated by the thick red arrows. Figures adapted from [214,215].

$\exp(-\beta\mathcal{H}_{\mathsf{T},M})$, where β is the inverse of the temperature times the Boltzmann constant. If we are quenching the spin $s_{\mathsf{T}+1}$ having already quenched $\{s_1,\ldots,s_{\mathsf{T}}\} \equiv s_{[1,\mathsf{T}]}$, its conditional expectation, $\langle s_{\mathsf{T}+1}|s_{[1,\mathsf{T}]}\rangle$, is $m^{(\text{eq})}_{\mathsf{T},M_{\mathsf{T}}}$ where $M_{\mathsf{T}} = \sum_{i=1}^{\mathsf{T}} s_i$. As we focus on the quenched magnetization, M_{T}, this relation may be rather written as

$$M_{\mathsf{T}+1} = M_{\mathsf{T}} + s_{\mathsf{T}+1}, \quad \langle s_{\mathsf{T}+1}|M_{[0,\mathsf{T}]}\rangle = m^{(\text{eq})}_{\mathsf{T},M_{\mathsf{T}}}. \tag{10.3}$$

Hereafter we shall use the energy unit so that $\beta = 1$. When we follow a process of PQ, the fixed magnetization, M, realizes an *observable stochastic process*, if we regard T as the discrete time. We will denote this process by M_{T}. Besides, though it may be *hidden* behind M_{T}, the equilibrium fixed spin, $m^{(\text{eq})}_{\mathsf{T},M_{\mathsf{T}}}$, also realizes a stochastic process, which we will denote by m_{T}. Both processes, M_{T} and m_{T}, will play crucial roles in our analysis. Figure 10.3(b) shows that the PQ is a Markovian stochastic process for M_{T}. When the coupling parameter j_0 is either too small (i.e., too high temperature) or the opposite (i.e., too low temperature) the process of PQ is trivial as shown in Figure 10.3(c), that is, M_{T} undergoes either almost unbiased random walk or almost polarized, $M_{\mathsf{T}} \simeq \pm\mathsf{T}$, the polarity of which is determined during the first few stages, respectively. To explore the most non-trivial case, j_0 will be chosen at the "critical" point. Because of the finite size $N_0 < \infty$, the true paramagnetic susceptibility χ is bounded as $\mathcal{O}(N_0)$. Therefore, the critical coupling, $j_{0,\text{crit}}$, is determined as the best fit of χ to the Curie's law; $\chi \sim (j_{0,\text{crit}} - j_0)^{-1}$. We found $j_{0,\text{crit}} \simeq 1.030$ for $N_0 = 2^8$.

The stochastic process M_{T} starting with this critical coupling gives rise to the trajectories that are far from the unbiased random walks and look to follow more or less contour lines of $m^{(\text{eq})}_{\mathsf{T},M}$ as shown in Figure 10.3(d). This quasi-ballistic trajectory is a sort of persistent random walk. At the ensemble level, Figure 10.3(e) shows that the probability density of the mean *fixed spin,* $M_{\mathsf{T}}/\mathsf{T}$, evolves from a single peaked form to the double peaked one [214]. Although one might suppose some spontaneous symmetry breaking mechanism behind the double peak, it is not the case because the effective coupling among the *unfixed* spins, $j_{\text{eff}} = j_{0,\text{crit}}(1 - \frac{\mathsf{T}}{N_0})$ is below critical for $\mathsf{T} \geq 1$.

10.3.2. *Hidden martingale process*

In [214], it was found that the process M_{T} that shows apparently the long-term memory in Figure 10.3(d) can be characterized by the *hidden* martingale of the stochastic process, $m_{\mathsf{T}}(\equiv m^{(\text{eq})}_{\mathsf{T},M_{\mathsf{T}}})$. In mathematical term, it can be shown that

$$\langle m_{\mathsf{T}+1}|M_{[0,\mathsf{T}]}\rangle = m_{\mathsf{T}}, \tag{10.4}$$

where $\langle X|M_{[0,\mathsf{T}]}\rangle$ means to take the conditional expectation of X under the given *sub-history*, $M_{[0,\mathsf{T}]}$, that is, under the specified data of M_{T} from $\mathsf{T} = 0$ up to T. In the present model of PQ, specifying the sub-history is equivalent to listing the values of the fixed spin up to the stage-T, i.e., $s_{[1,\mathsf{T}]}$, or $M_{[0,\mathsf{T}]}$ with $M_0 = 0$ is understood. The value of m_{T} on the right-hand side is, therefore, known for a given $M_{[0,\mathsf{T}]}$. In the present case, the process M_{T} is Markovian and we could replace $M_{[0,\mathsf{T}]}$ by the information of the last stage, M_{T}.

Equation (10.4) or, equivalently, $\langle (m_{\mathsf{T}+1} - m_{\mathsf{T}})|M_{[0,\mathsf{T}]}\rangle = 0$, guides the evolution of the total fixed spin, $M_{\mathsf{T}+1} - M_{\mathsf{T}}$, which takes only the binary values, ± 1.[16] By inductively applying (10.4), we can show (see also [216])

$$\langle m_{\mathsf{T}'}|M_{[0,\mathsf{T}]}\rangle = m_{\mathsf{T}}, \quad \mathsf{T} \leq \forall \mathsf{T}' \leq N_0. \tag{10.5}$$

The relationship (10.5) means that, as far as the average value is concerned, we need not integrate the discrete-time master equation from T to T' to evaluate $m_{\mathsf{T}'}$.

In [214], (10.4) has been derived up to a possible stochastic error of $\mathcal{O}({N_0}^{-2})$ using the large N_0-expansion of the formula of quasi-canonical expectation of $m^{(\mathrm{eq})}_{\mathsf{T}+1,M_{\mathsf{T}+1}}$. More recently [217], however, it was noted that (10.4) holds precisely and from general principle of tower rule (Equation 2.3). The following argument follows the line of Appendix B.2. Since those unquenched spins at the stage T, i.e., $\{s_{\mathsf{T}+1}, \ldots, s_{N_0}\}$, are all equivalent (*homogeneity*), we can replace $s_{\mathsf{T}+1}$ in the second part of (10.3) by s_{N_0}, the last spin to be fixed. *If* $(m_{\mathsf{T}} =)\langle s_{N_0}|M_{[0,\mathsf{T}]}\rangle$ *can be regarded as* $\langle Z|X_{[0,\mathsf{T}]}\rangle$ in Appendix B.2 with the mappings, $Z \mapsto s_{N_0}$ and $X_t \mapsto M_t$, then it follows the higher order tower rule (Equation 2.3); for $0 < \mathsf{T} \le \mathsf{T}' \le N_0$,

$$\langle\langle s_{N_0}|M_{[0,\mathsf{T}']}\rangle \,|\, M_{[0,\mathsf{T}]}\rangle = \langle s_{N_0}|\, M_{[0,\mathsf{T}]}\rangle. \tag{10.6}$$

This means (10.5), i.e., $\langle m_{\mathsf{T}'}|\, M_{[0,\mathsf{T}]}\rangle = m_{\mathsf{T}}$. We would stress that the hidden martingale property shown here holds irrespective of the initial coupling parameter j_0, either near critical or not.

10.4. *Consequences of hidden martingale process*

The next step is to find the consequence of this (hidden) martingale property in the (principal) stochastic process $\{M_{\mathsf{T}}\}$. Noting $M_{N_0} = M_{\mathsf{T}} + \sum_{j=\mathsf{T}+1}^{N_0} s_j$ and $\langle s_j|M_{[0,\mathsf{T}]}\rangle = \langle\langle s_j|M_{[0,j-1]}\rangle\,|M_{[0,\mathsf{T}]}\rangle = \langle m_{j-1}\,|M_{[0,\mathsf{T}]}\rangle = m_{\mathsf{T}}$ for $j > \mathsf{T}$, we have the *hidden martingale formula* (discrete version):

$$\langle M_{N_0}|M_{[0,\mathsf{T}]}\rangle = M_{\mathsf{T}} + (N_0 - \mathsf{T})m_{\mathsf{T}}. \tag{10.7}$$

At the end of this section, we will discuss the continuum version of (10.7).

10.4.1. *Inference*

Below are given the examples of the usage of the hidden martingale formula (10.7) to infer the past stage, which will also provide with an elementary demonstration of this theorem.

Suppose that the process starts by the stage-T ($\mathsf{T} > 0$) with a fixed magnetization M_{T}, and that we are given $\langle M_{N_0}|M_{[0,\mathsf{T}]}\rangle$ from a large ensemble of the final data $\{M_{N_0}\}$. Now in (10.7), the value of the left-hand side is known, while the right-hand side is a function of unknown M_{T} with a given T. Therefore, (10.7) is an (implicit) equation for M_{T}. In this manner, we can infer M_{T} with the cost of calculation of $\sim N_0$ (for a reliable expectation of M_{N_0}) instead of solving the master equation costing $\sim {N_0}^2$. It was numerically verified that this scenario indeed works very well.

10.4.2. *Prediction*

Another usage of the hidden martingale formula (10.7) is the prediction of the conditional expectation of the main stochastic process, $M_{\mathsf{T}'}$, for $\mathsf{T}' > \mathsf{T}$. In [215], the equivalent of (10.7) was shown:

$$\left\langle \frac{M_{\mathsf{T}'} - M_{\mathsf{T}}}{\mathsf{T}' - \mathsf{T}} \middle| M_{[0,\mathsf{T}]} \right\rangle = m_{\mathsf{T}}, \quad \mathsf{T}' > \mathsf{T}. \tag{10.8}$$

For example, in the case of $N_0 = \mathsf{T}' = 100$ and $\mathsf{T} = 5$, we can predict $\langle M_{100}|M_{[0,5]}\rangle$ to be $M_5 + 95 \times m_5$.

10.4.3. *Prediction of probability distribution function*

In the present model of PQ, the hidden martingale formula (10.7) allows to predict M_{N_0} from the data of Tth stage with $\mathsf{T} \ll N_0$:

$$M_{N_0} = M_{\mathsf{T}} + (N_0 - \mathsf{T})m_{\mathsf{T}} + \mathcal{O}((N_0 - \mathsf{T})^{\frac{1}{2}}), \tag{10.9}$$

where we recall $m_{\mathsf{T}} \equiv m^{(\text{eq})}_{\mathsf{T},M_{\mathsf{T}}}$ and the last term, $\mathcal{O}((N_0 - \mathsf{T})^{\frac{1}{2}})$, represents the sum, $\sum_{k=\mathsf{T}+1}^{N_0}(s_k - m_{\mathsf{T}})$, consisting of the terms deemed to vanish individually upon the conditional average, $\langle|M_{[0,\mathsf{T}]}\rangle$. The approximation (10.9), which ignores the diffusive aspect of the process after the Tth stage, may be called a *geometrical optics* approximation.[17] To know the probability distribution of M_{T} is a relatively easy task for $\mathsf{T} \ll N_0$ with the calculation cost of some power of T. The last formula (10.9) then allows to predict the final probability distribution of M_{N_0} (for the numerical procedure, see Section 10.4.4). Figure 10.4 demonstrates how it works well. In the left part of the figure, the PQ process is unbiased, where the distribution at $\mathsf{T} = 2^4$ is symmetric and unimodal (inset) while the final one is bimodal (dense dotted curve). The final distribution of M_{N_0} is predicted by the piecewise linear curve with $2^4 + 1$ nodes. In the right part of the figure, the PQ process is unbiased except at the stage-$(2^4 - 1)$, when the infinite external field, $h_{\text{ext}} = \infty$, is applied to force s_{2^4} is quenched to be $+1$. The distribution at the stage-2^4 (inset) is almost equal to the unbiased case but suffers the shift by $\Delta M = +1$. The subsequent unbiased PQ process leads then to the final bimodal but asymmetric distribution as shown by the dense dotted curve. Also in this case, the prescription described above (the piecewise linear curve with $2^4 + 1$ nodes) reproduces well the main feature of the full numerical result.

Amazingly this method of hidden martingale can predict the binodal distribution in the far future ($N_0 \gg \mathsf{T}$) given the data of unimodal distribution. Since $m^{(\text{eq})}_{\mathsf{T},M}$ is a monotonous function of M (not shown), the results are far from trivial. In case that N_0 and T constitute the double hierarchy $1 \ll \mathsf{T} \ll N_0$, our methodology may serve as a reasonable tool of numerical asymptotic analysis.

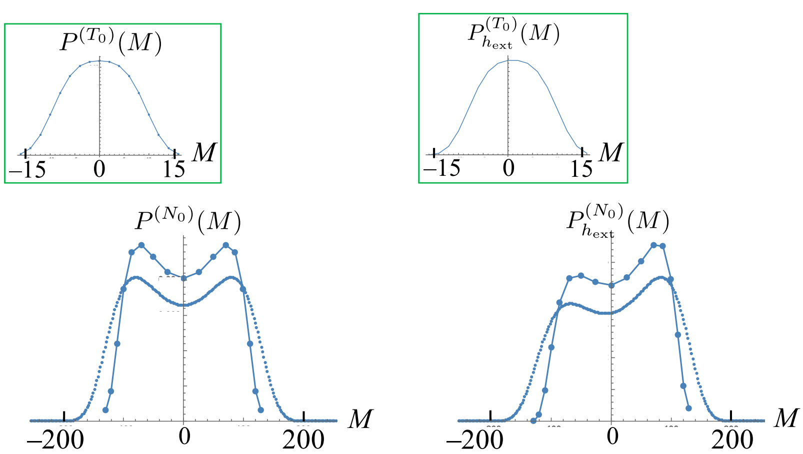

Figure 10.4. Comparison between the final distributions of M_{N_0} predicted by the hidden martingale property (joined $\mathsf{T} + 1$ dots) and those by full numerical solution (filled circles) with $\mathsf{T} = 2^4$ and $N_0 = 2^8$ [215]. See text for details.

10.4.4. *Numerical construction of the distribution from (10.9)*

We note that, in the absence of stochastic diffusion, i.e., the term $\mathcal{O}((N_0-\mathsf{T})^{\frac{1}{2}})$ in (10.9), the probability associated to any subset of the values of M_T at the stage T is directly conveyed to the corresponding subset of the values of M_{N_0} at the finale stage, somehow reminiscent of the Liouville's theorem that allows the probability to be carried along the Hamiltonian flow. Suppose that, at the stage T, we have an access to the probabilities, $P_i^{(\mathsf{T})}$, of having the fixed magnetization $M=-\mathsf{T}+2i\equiv\mu_i$ with $i=0,1,\ldots,\mathsf{T}$. Also we prepare the data of $m^{(\mathrm{eq})}_{\mathsf{T},M=\mu_i}$ with $i=0,1,\ldots,\mathsf{T}$. The object is to generate the normalized probability density, $p(M)$, with continuous variable $M\in[-N_0,N_0]$, of the final fixed magnetization through a piecewise linear approximation with $\mathsf{T}+1$ nodes. The assignment of the binning box may not be unique. Here we follow the Appendix C of [215] to use a simple trapezoidal rule to make Figure 10.4:

For the simplicity of notations, we introduce (see Equation 10.9)

$$x_i=\mu_i+(N_0-\mathsf{T})\,m^{(\mathrm{eq})}_{\mathsf{T},\mu_i}, \tag{10.10}$$

where $i=0,1,\ldots,\mathsf{T}$. We will make up the final probability *density* $p(x)$ so that its normalization is $\int_{x_0}^{x_\mathsf{T}}p(x)\,\mathrm{d}x=1$. We make a piecewise linear approximation of $p(x)$ whose joint points are $\{x_i,p(x_i)\}$. The normalization condition then reads

$$\begin{aligned}1&=\sum_{i=0}^{\mathsf{T}-1}\frac{p(x_i)+p(x_{i+1})}{2}(x_{i+1}-x_i)\\&=p(x_0)\frac{x_1-x_0}{2}+\sum_{i=1}^{\mathsf{T}-1}p(x_i)\frac{x_{i+1}-x_{i-1}}{2}+p(x_\mathsf{T})\frac{x_\mathsf{T}-x_{\mathsf{T}-1}}{2}.\end{aligned}\tag{10.11}$$

Then we define $p(x_i)$ through

$$\begin{aligned}p(x_0)\frac{x_1-x_0}{2}&=P_0^{(\mathsf{T})},\\p(x_i)\frac{x_{i+1}-x_{i-1}}{2}&=P_i^{(\mathsf{T})}\quad i=1,\ldots,\mathsf{T}-1\\p(x_\mathsf{T})\frac{x_\mathsf{T}-x_{\mathsf{T}-1}}{2}&=P_\mathsf{T}^{(\mathsf{T})}\end{aligned}\tag{10.12}$$

so that the "ray" of geometrical optics carries the probability from $\mathsf{T}=\mathsf{T}$ to $\mathsf{T}=N_0$. The uneven weight on both extremities is harmless because $P_0^{(\mathsf{T})}$ and $P_\mathsf{T}^{(\mathsf{T})}$ are very small. The martingale prediction of the probability densities in Figure 10.4 is thus made. Naturally, the prediction by hidden martingale gives narrower distributions than the full numerical results because the former method ignores the diffusion, whose contribution would fatten the distributions by $\sim(256-16)^{\frac{1}{2}}\simeq 15$.

Hidden martingale formula with continuous time ([215]*)* Before concluding the main results of this section, we give the continuum version of Equation (10.7). Suppose that the stochastic process X_t is generated by a hidden martingale system through the stochastic differential equation (SDE),

$$\dot{X}_t=G_t(X_t)+V_t(X_t)\dot{B}_t, \tag{10.13}$$

where B_t is a Wiener (or martingale) process and $G_t(X_t)$ is the *martingale drift* satisfying

$$\langle G_t(X_t)|M_{[0,s]}\rangle=G_s(X_s),\quad t\geq s. \tag{10.14}$$

Then

$$\left\langle \frac{X_t - X_s}{t-s} \middle| M_{[0,s]} \right\rangle = G_s(X_s), \quad t \geq s. \tag{10.15}$$

Proof Taking the conditional expectation of Equation (10.13) with the condition $M_{[0,s]}$ we have for all $\tau \geq s$,

$$\langle \dot{X}_\tau \mid M_{[0,s]} \rangle = \langle G_\tau(X_\tau) \mid M_{[0,s]} \rangle = G_s(X_s),$$

where (10.14) has been used in the second equality. By integrating the above equation with respect to τ from s up to t, we have $\langle X_t - X_s | M_{[0,s]} \rangle = G_s(X_s)\,(t-s)$. ∎

In the present model of our PQ, we may approach our process to an SDE by $dM_\tau := M_{\tau+1} - M_\tau$ and $\mathrm{d}\tau := 1$ for $\forall \tau \geq s$. Then a type of the Doob–Meyer decomposition, $\mathrm{d}M_\tau = m_\tau\,\mathrm{d}\tau + (s_{\tau+\mathrm{d}\tau} - m_\tau\,\mathrm{d}\tau)$, gives what corresponds to (10.13).

Remark 1 While the generalization from discrete version is straightforward, there can be functional constraints on $G_t(X_t)$ in order for $G_t(X_t)$ to be martingale with respect to $X_{[0,s]}$. The practical application of the continuous version has not been tested yet. Some analysis has been recently made for the case where $V_t(z) = 1$ and $G_t(z)$ is independent of time [218].

10.5. *Concluding discussion of this chapter*

When a martingale process is hidden behind the observed Markovian stochastic process, the former may bring long-lasting memory effects to the latter. If we regard (10.9) as a geometrical optics approximation of the full evolution, there may be a route to reach this form through the Freidlin–Wentzell approach [219] under the constraint of hidden martingale. Further theoretical studies are also needed.

The authors of [217] showed that the hidden martingale property (10.5) is equivalent to a *local invariance* of the path weights. This invariance may reflect an aspect of martingale as stochastic conservation although such invariance is not found with any martingale other than the present PQ model. In the latter case, the local invariance implies a constrained canonical structure of the statistics of M_T [217]. While the given quenched spins impose a permanent memory on the individual process, the neutral action of quenching allows to reflect the equilibrium statistics of the unquenched spins in the quenched ensemble. The constrained canonical structure makes compatible these two complementary aspects, see also [220] .

Chapter 11. Martingales in population genetics

It is remarkable, I think, that their behavior [of mutant frequencies] is calculable from the theory of stochastic processes, a theory which until recently has been regarded as too academic to have actual biological applications.

Motoo Kimura, from "The neutral theory of molecular evolution", 1983 [221].

Individuals belonging to natural populations are characterized by a certain degree of genetic diversity. Population genetics studies the distribution of these genetic variants as effect of mutations, natural selection, stochasticity, and other evolutionary forces. In particular, it is nowadays established that a large portion of mutations confer a negligible selective advantage (or disadvantage) to individuals carrying them. The fate of these mutations is therefore determined by pure chance without any deterministic selection. In population genetics, these mutations are called "neutral". The widespread occurrence and importance of neutral mutations was pointed out by Motoo Kimura [221]. Kimura's theory has encountered substantial resistance over the years – partially due to the fact that, historically, evolution was implicitly thought to be a deterministic process. In contrast, Kimura's neutral theory is inherently stochastic.

The distinction between neutral, advantageous, and deleterious mutations has become a cornerstone of modern population genetics. This concept provides us with a perfect example of the analogy between population genetics and non-equilibrium physical systems, and how martingales can be applied to population genetics.

11.1. *The Moran model*

To make our discussion more concrete, we introduce the Moran model of population genetics. The Moran model describes a population of N individuals reproducing asexually. The total number of individuals N is kept constant by resource availability, so that every time an individual dies another individual instantly reproduces. A number of individuals n in the population, with $0 \leq n \leq N$, carry a given mutation. We call these individuals the "mutants" and the remaining $(N - n)$ "wild-type individuals". For the time being, we assume the mutation to be neutral, i.e., mutants die and reproduce at the same rates as the wild type individuals. The number of mutants in the population evolves with rates

$$
\begin{aligned}
n &\to n+1 \quad \text{with rate } \frac{n(N-n)}{N} \\
n &\to n-1 \quad \text{with rate } \frac{n(N-n)}{N}
\end{aligned}
\tag{11.1}
$$

Equation (11.1) can be understood by thinking that the rate at which the number of mutants increase is proportional to the number $(n - N)$ of wild-type individuals, times the probability n/N that the dead individual is replaced by a copy of a mutant. Similar reasoning apply to the rate of decrease of n. The master equation defined by the rates (11.1) is characterized by two absorbing states, $n = 0$ and $n = N$. In the language of population genetics, if the absorbing state $n = N$ is reached we say that the mutation has "reached fixation". To understand the evolution of a population, it is important to compute the probability P_+ of this event. A short way of computing this probability is by noting that n_t is a martingale defined on a bounded interval, and therefore must satisfy Doob's optional stopping theorem. Calling τ the time at which one of the two absorbing states is reached, we obtain

$$
n_0 = \langle n_\tau \rangle = 0 \cdot P_- + N \cdot P_+ \to P_+ = \frac{n_0}{N}. \tag{11.2}
$$

Therefore, in the neutral Moran model, the probability of a mutation to reach fixation is equal to its current fraction in the population. This is a basic yet fundamental result of neutral population genetics.

We now generalize the Moran model to a case in which the mutation possibly confers a selective advantage to individuals carrying it. We define a selective advantage s as a relative increase in the reproduction rate. The transition rates of the model read

$$
\begin{aligned}
n &\to n+1 \quad \text{with rate } (1+s)\frac{n(N-n)}{N} \\
n &\to n-1 \quad \text{with rate } \frac{n(N-n)}{N}.
\end{aligned}
\tag{11.3}
$$

In the three cases $s > 0$, $s = 0$, and $s < 0$, the process is a submartingale, martingale, and surmartingale, respectively. In population genetics, if s is negligible, the mutation is considered to be neutral; if s is sufficiently large and positive the mutation is advantageous; and if s is negative and sufficiently large in absolute value, the mutation is deleterious. By analyzing the model, we will clarify what does it mean to be "negligible" and "sufficiently large". For simplicity, we study the model in the continuous approximation. Assuming N to be large, the fraction $X = n/N$ of mutants satisfies the Langevin equation

$$\dot{X}_t = sX_t(1 - X_t) + \sqrt{\frac{2X_t(1 - X_t)}{N}}\dot{B}_t. \tag{11.4}$$

The Langevin equation (11.4) is interpreted in the Itô sense and can be derived from the master equation by means of a Kramers–Moyal expansion [4]. We truncated this expansion at the first order in $1/N$ and assumed s to be order $1/N$, so that we neglected terms of order s/N.

Also Equation (11.4) is characterized by two absorbing states, in this case at $X = 0$ and $X = 1$. In this case, if $s \neq 0$ the process X_t is not a martingale. However, performing a change variable to $Y_t = \exp(-sNX_t)$ by means of the Itô formula we obtain

$$\dot{Y}_t = -sNY_t\sqrt{\frac{2X_t(1 - X_t)}{N}}\dot{B}_t \tag{11.5}$$

of Y_t is governed by an Itô stochastic differential equation without drift, the process Y_t is a martingale. It is interesting to note the analogy with stochastic thermodynamics, where entropy production is a submartingale whereas the exponential of minus the entropy production is a martingale. The range $X_t \in [0, 1]$ corresponds to a range $Y_t \in [\mathrm{e}^{-sN}, 1]$. We can therefore apply once more Doob's optional stopping theorem to the stopping time defined as the first time at which one of the two absorbing states is reached:

$$Y_0 = P_+ \exp(-sN) + P_-. \tag{11.6}$$

Using that $P_+ + P_- = 1$ and expressing the probabilities in terms of X_0, we find that the probability of fixation is

$$P_+ = \frac{1 - \exp(-sNX_0)}{1 - \exp(-sN)}. \tag{11.7}$$

Equation (11.7) is the celebrated Kimura's formula for the fixation probability of a mutation [222]. It is analogous to the expression (1.15) that we derived for the biased random walk. Equation (11.7) is singular for $s = 0$. However, it correctly predicts the neutral result $p_1 = X_0$ (see Equation (11.2)) in the limit $s \to 0$.

Importantly, Kimura's formula clarifies when a selective advantage is sufficiently large. Note that Kimura's formula depends on the parameters s and N only via the combination sN. It follows that mutations characterized by selective advantages $|s| \ll N^{-1}$ behaves essentially as neutral. This fact has deep consequences for the evolution of natural populations.

In population genetics, the model embodied in Equation (11.4) is used to describe the fate of mutations in real populations. However, the intensity of random fluctuations of mutation frequencies tends to be much larger than predicted by models such as Equation (11.4). An explanation is that many simplifying assumptions underlying the Moran process do not hold in reality. One of the most important is the assumption of constant population size: it can be shown that, in populations of variable size, evolution is strongly affected by "bottlenecks", i.e., epochs in which the population size happened to be small [223]. To compensate for these effects, when using the

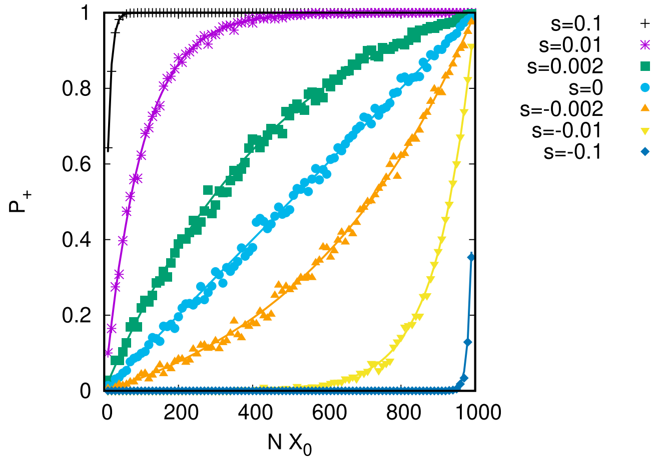

Figure 11.1. Kimura's fixation formula (11.7) (lines) compared to simulations of the Moran process (11.1) with $N = 1000$ (points). Each point is an average over 10^3 Gillespie simulations of a master equation with rates (11.3), where we set $\mu = 1$ and s as in the figure legend.

Moran model to describe real populations, the parameter N is taken as an effective parameter, called the "effective population size". For example, the effective population size estimated for humans from fluctuations of mutation frequencies is on the order of $N = 10^4$, whereas estimates for *Escherichia coli* range between 10^6 and 10^8. In general, Equation (11.7) reveals that mutations characterized by small selective advantages $s \ll 1/N$ do not significantly influence the fixation probability and therefore effectively behave as neutral. This fact implies that bacteria such as *E. coli*, characterized by a large effective population size, are much more sensitive to fitness differences than for example humans. For example, a mutation conferring a selective advantage $s = 10^{-5}$ would be seen as neutral by a human population, but as strongly advantageous by most bacteria (Figure 11.1).

An alternative approach to study Equation (11.5) is to perform a random time change

$$\mathcal{D}\tau = \mathcal{D}t X_t(1 - X_t) \tag{11.8}$$

so that Equation (11.5) becomes

$$\frac{\mathcal{D}}{\mathcal{D}\tau} X_\tau = s + \sqrt{\frac{2}{N}} \dot{B}'_\tau, \tag{11.9}$$

where $\dot{B}'_\tau$ is also a white Gaussian noise. In terms of the random time, the population dynamics is described by a simple Langevin process with constant drift and diffusion terms.

11.2. *Duality and martingales*

So far we analyzed the Moran process using a diffusion approximation, which paved the way to an analysis using martingales. In the following, we discuss another type of correspondence between discrete population models and Ito stochastic differential equations, based on the notion of duality, that does not rely on any approximation [224,225]. We consider a single population made up of a variable number n of individuals. Each individual reproduces at rate γ and dies at rate $\chi(n-1)$, proportional to the number of other individuals due to competition for resources:

$$\begin{aligned} n &\to n+1 \quad \text{with rate } \gamma n \\ n &\to n-1 \quad \text{with rate } \chi n(n-1) \end{aligned} \tag{11.10}$$

The corresponding master equation reads

$$\partial_t \rho_t(n) = \sum_m \omega(n,m)(\rho_t(m) - \rho_t(n)) \tag{11.11}$$

with the transition rates

$$\omega(n,m) = \gamma m \delta_{n,m+1} + \chi m(m-1)\delta_{n,m-1}. \tag{11.12}$$

We now associate to the Master equation (11.11) a Langevin dynamics

$$\dot{Z}_t = -\gamma Z_t(1-Z_t) + \sqrt{2\chi Z_t(1-Z_t)}\dot{B}_t. \tag{11.13}$$

We note that Equation (11.13) has the same form of Equation (11.4) if we perform the change of variable

$$X_t = 1 - Z_t. \tag{11.14}$$

With this mapping, Equation (11.13) can be seen as a (truncated) Kramers–Moyal expansion of the particle model defined in Equation (11.3), with selective advantage γ and constant population size χ^{-1}.

In this section, we shall instead relate Equation (11.13) with the Master equation (11.11), which does not conserve population size. This relation is very different in spirit to the one based on the Kramers–Moyal expansion and, in particular, does not rely on any approximation. The idea of this alternative approach is to combine the discrete process defined in Equation (11.10) with the continuous process described in Equation (11.13) to obtain a new process which is a martingale. To this aim, we consider the process Z_t^m, where m is an arbitrary integer number. Applying the Ito formula (2.88) yields

$$\dot{Z}_t^m = mZ_t^{m-1}\dot{Z}_t + \chi m(m-1)Z_t^{m-1}(1-Z_t). \tag{11.15}$$

Substituting Equations (11.13) and (11.12) into Equation (11.15) we obtain

$$\dot{Z}_t^m = \sum_{n=0}^{\infty} \omega(n,m)(Z_t^n - Z_t^m) + \sqrt{2\gamma} m Z_t^{m-1}\sqrt{Z_t(Z_t-1)}\dot{B}_t, \tag{11.16}$$

We now introduce the quantity

$$\mathcal{M}_t = \sum_{m=1}^{\infty} Z_t^m \rho_{T-t}(m), \tag{11.17}$$

where T is an arbitrary (reference) time. The process $\mathcal{M}_t$ combines a solution of the Langevin equation (11.13) with a backward solution $\rho_{T-t}(m)$ of the master equation (11.11). Independently of the choice of the time T and the initial conditions of the two processes, $\mathcal{M}_t$ is a martingale.

We can in fact prove from Equations (11.11) and (11.16) that $\mathcal{M}_t$ is governed by an Ito process without drift:

$$\dot{\mathcal{M}}_t = \sum_{m=1}^{\infty} \left(\dot{Z}_t^m \rho_{T-t}(m) + Z_t^m \partial_t \rho_{T-t}(m) \right)$$

$$= \sum_{m=1}^{\infty} \rho_{T-t}(m) \sqrt{2\gamma} m Z_t^{m-1} \sqrt{Z_t(Z_t - 1)} \dot{B}_t. \tag{11.18}$$

From its definition, the martingale $\mathcal{M}_t$ can be also expressed as

$$\mathcal{M}_t = \langle Z_t^{N_{T-t}} \rangle_N, \tag{11.19}$$

where with $\langle \dots \rangle_N$ we denote the expectation over trajectories N_{T-t} of the Master equation (11.11). We note that, while the continuous process Z_t progresses forward in time t, the discrete process N_{T-t} progresses backward in time. The martingality of $\mathcal{M}_t$ implies for example that

$$\langle Z_t^{N_0} \rangle_{Z,N} = \langle Z_0^{N_t} \rangle_{Z,N}, \tag{11.20}$$

where $\langle \dots \rangle_{Z,N}$ is the expectation over the forward continuous process and the backward discrete process. We remark that this equality is valid for any t, and any choices of the initial conditions of the two processes. By appropriate choices of initial conditions, this relation can be exploited to derive useful properties of the two processes [225].

Interestingly, these techniques can be also applied to spatially extended populations. A prototypical stochastic model describing the dynamics of spatial populations is the stochastic Fisher–Kolmogorov equation

$$\partial_t F_t(x) = sF_t(x)(1 - F_t(x)) + D\partial_x^2 F_t(x) + \sqrt{\frac{2F_t(x)(1 - F_t(x))}{N}} \xi_t(x). \tag{11.21}$$

Using duality it can be shown that the probability of a small, localized population described by the Fisher–Kolmogorov equation to grow up to a large size is still governed by the formula (11.7) for the fixation probability of a well-mixed population [225,226].

Chapter 12. Martingales in finance

> *October: This is one of the particularly dangerous months to invest in stocks. Other dangerous months are July, January, September, April, November, May, March, June, December, August and February.*
>
> Mark Twain, from "Pudd'nhead Wilson", 1894

We give here an overview of the use of martingales in finance. Since the theory of martingales had its early discussions in finance, it is no wonder that a huge amount of literature exists on this subject. In the treatment below, we do not aim to be exhaustive or rigorous in any way, and our primary (and perhaps only) motivation is to introduce the basic terminologies of quantitative finance and discuss how the theory of martingales arises naturally in this setting. In the process, we hope to get the readers excited about the field of quantitative finance. For further details, readers are directed to more specialized texts on the subject [227–230]. A concise and self-contained review on the topic, written from a physicist's point of view, is Ref. [231]. A reader aspiring to master all of stochastic calculus required for a rigorous formulation of quantitative finance may look up Refs. [232,233].

12.1. *Riskless and risky financial assets: bank deposits and stocks*

A riskless asset is one for which the return is fixed and guaranteed regardless of the market situation. A prominent example is a bank deposit $\mathcal{B}_t$, with t denoting time: an amount $\mathcal{B}_0$ deposited in a bank that offers a fixed interest rate r increases at a rate

$$\dot{\mathcal{B}}_t = r\mathcal{B}_t, \tag{12.1}$$

where the dot denotes derivative with respect to time. The above evolution implies an exponential growth in time and yields a fixed return with value $\mathcal{B}_t = \mathcal{B}_0 \exp(rt)$ at time t. Depending on r and $\mathcal{B}_0$, although that does sound like a fortune, it could be possible that the depositor earns more through investments whose worth is contingent on the evolution of the market. Such investments are in general risky, since unlike riskless assets no fixed return is guaranteed, but which when planned and managed well nevertheless offer the investor the unique opportunity to profit from market fluctuations.

An example of risky assets is what are called stocks or shares. A stock gives its holder the ownership of a small part of the company issuing the stock. A company that requires to raise its capital often does so by issuing stocks. By selling many such stocks, the company is able to raise its capital at typically lower costs than would have been possible if it were to borrow money from banks, which would ask for high interests on the money borrowed. It is evident that the stock price depends on the overall worth of the company in the market,[18] which in turn depends on how it has been performing in recent times, but also, interestingly, on how it is projected to perform in future. A small market fluctuation due to, i.e., a Government decision, which is anticipated to affect the future performance of the company, may lead to a change in the current price of its stocks. All the aforementioned factors lead to stock prices behaving erratically in time, an example of which is shown in Figure 12.1. In other words, the stock price S_t is a random function of time t; expressing its variation in time as

$$\dot{S}_t = R_t S_t, \tag{12.2}$$

where R_t is now the rate of return, which is itself a fluctuating quantity. In analogy with Equation (12.1), we may expect the “rate of return” R_t, a random function of time, to have a part representing the mean or expected rate of return and a part that varies randomly in time. The former part may be deducible on the basis of the average of the company’s past, present, and projected future performance, and is thus a deterministic or a predictable component, while all the uncertainty that got glossed over in computing the average is included in the random part. While there may be several ways to model the random part as a function of time, one of the most popular and simple ones in the field of quantitative finance is the so-called Geometric Brownian Motion (GBM) model. In this model, the rate of change in the stock price is

$$\dot{S}_t = \left(\mu + \sigma \dot{B}_t\right) S_t, \tag{12.3}$$

where the constants μ and σ represent respectively the expected rate of return and the standard deviation of returns, also called volatility, and where B_t is the standard Brownian motion or a Wiener process, as defined in Section 2.2.2. Volatility is a statistical measure of the dispersion of returns: the higher the volatility, the riskier is the stock.

Equation (12.3) is an example of an SDE, which may be solved subject to a given initial condition $S_{t_0} = s_0$. In terms a new random variable $Z_t \equiv \ln S_t$, on applying the Itô’s formula, see

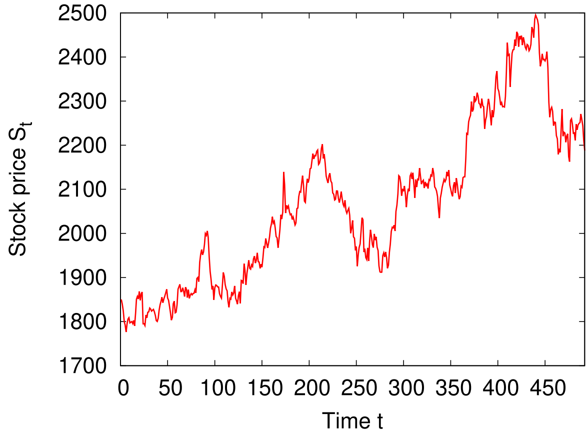

Figure 12.1. Representative stock price fluctuations as a function of time. The figure depicts data on the closing price of HDFC Bank on a daily basis from 19th September 2017 to 18th September 2019, i.e., over a period of 24 months. Source: National Stock Exchange, India.

Equation (B14) in Appendix B.3, and using Equation (12.3), we get

$$\dot{Z}_t = \mu - \frac{\sigma^2}{2} + \sigma \dot{B}_t, \tag{12.4}$$

which on integration with respect to time gives

$$Z_t = Z_{t_0} + \left(\mu - \sigma^2/2\right)(t - t_0) + \sigma\left(B_t - B_{t_0}\right), \tag{12.5}$$

with $Z_{t_0} = \ln s_0$; when expressed in terms of S_t, we get the following random function of time for the stock price S_t:

$$S_t = s_0 \exp\left(\left(\mu - \frac{\sigma^2}{2}\right)(t - t_0) + \sigma\left(B_t - B_{t_0}\right)\right). \tag{12.6}$$

Equation (12.4) implies that $Z_t - Z_{t_0}$ is normally distributed with mean $(\mu - \sigma^2/2)(t - t_0)$ and variance $\sigma^2(t - t_0)$, i.e., $Z_t - Z_{t_0} \sim \mathcal{N}((\mu - \sigma^2/2)(t - t_0), \sigma\sqrt{t - t_0})$. It then follows that the probability density of the stock price S_t at time t, subject to the initial condition $S_{t_0} = s_0$, is given by the log-normal distribution

$$\rho_{S_t}(s|S_{t_0} = s_0) = \frac{1}{s\sqrt{2\pi\sigma^2(t - t_0)}} \exp\left(-\frac{\left[\ln\left(\frac{s}{s_0}\right) - \left(\mu - \frac{\sigma^2}{2}\right)(t - t_0)\right]^2}{2\sigma^2(t - t_0)}\right). \tag{12.7}$$

12.2. *Options and the Black–Scholes equation for option pricing*

Stocks are sold and bought ("traded") in organized stock exchanges, such as the New York Stock Exchange, the NASDAQ Stock Market, and so on. Every stock exchange devises an index that is a representative of the daily average behavior of the corresponding market. Different from stocks whose intrinsic values are based directly on their market values and which therefore constitute primary financial assets for the holder, there are financial instruments called derivatives whose intrinsic values derive from the price of some underlying primary assets. Derivatives are also referred to as contingent claims as their values are contingent on that of the underlying asset. One such basic derivative is what are called options, which we will deal with now.

An option is a contract between two parties to buy or sell in future an underlying primary asset at an agreed price, regardless of the market situation prevailing at the time the asset is bought or sold. The two sides of the contract are called the buyer and the seller or the underwriter. European options can be exercised only on the future date (the maturity or expiration date) agreed in the contract, while American options can be exercised at any point of time until the expiration date. Here we will discuss only European options. The two common types of European options are calls and puts. An European call option gives the buyer the right, but not the obligation, to buy the underlying asset (stock S_t) at the strike price K specified in the contract on the expiration date $\mathcal{T}$, regardless of the current price (the spot price) $S_{\mathcal{T}}$ of the asset. If the call buyer exercises his option, the seller is accordingly obliged to sell the asset at price K. An European put option is quite similar to the call option, excepting that it gives the buyer the right, but not the obligation, to sell the underlying asset at price K on date $\mathcal{T}$ regardless of the spot price $S_{\mathcal{T}}$, and if exercised, the seller is then obliged to buy the asset at price K. Either way, due to the obligation to sell or buy at a predetermined price on date $\mathcal{T}$ regardless of the spot price $S_{\mathcal{T}}$, the seller may incur a loss, so that the buyer when entering into the option contract must compensate somewhat by paying on-spot a certain amount called the option premium to the seller. From the above, it is evident that investors buy calls or sell puts (respectively, sell calls or buy puts) when they anticipate that the price of the underlying asset will increase (respectively, decrease) in time.

Here, we discuss the concept of **price** of an option, from the point of view of a potential buyer of a call option, which would help us fix our ideas about option premium. If the spot price S_t at any time t exceeds the strike price K, it would make sense, in case it were possible, to exercise the call option, buy the asset from the seller at price K and sell it in the market at price S_t (buy low and sell high), thereby making a profit; we would then say that the option has a positive intrinsic value given by the difference $S_t - K$. If on the other hand one has $S_t < K$, it is cheaper to buy in the market itself, and it would be meaningless to exercise the call option; we would then say that the option has zero intrinsic value. This leads us to define the intrinsic value of a call option at time t to be the function $\max(S_t - K, 0)$. Besides the intrinsic value, the option would also have a time value that may be understood thus. At any time $t < \mathcal{T}$, suppose that we have $S_t > K$. Now, since there is still time left until expiration, there is a possibility that in course of time until $\mathcal{T}$, S_t will increase even further beyond K, which is to say that the option has a certain positive time value. It is clear that the further S_t is beyond K, higher is the probability that in the time until $\mathcal{T}$, S_t will increase even further beyond K, and so higher will be the time value. How about the case $S_t < K$? Again, since there is still time until expiration, there is still a chance that S_t will exceed K: the lower S_t is below K, of course, the smaller is this chance. All these lead us to conclude that the time value of the option is a monotonically increasing function of S_t. Moreover, the further one is from expiration, the higher is the time value. This is because longer is the time until expiration, higher is the investor's expectation and consequently, higher is the probability that market fluctuations may cause S_t to exceed K. The sum of the time value and the intrinsic value gives the option price $C \equiv C(S_t, t; K, \mathcal{T})$, where we have shown explicitly the factors on which the option price depends: the time at which we value the option and the spot price of the underlying asset, as well as the strike price K and the expiration date $\mathcal{T}$. Since the time value gets smaller as the expiration date gets closer, the call option price as t hits $\mathcal{T}$ is just the intrinsic value. These points are shown schematically in Figure 12.2(a).

We now discuss the price of a put option, from the point of view of a potential buyer. If the spot price S_t at any time t is below the strike price K, it would make sense, in case it were possible, to exercise the put option, sell the asset to the buyer at a higher price K, thereby making

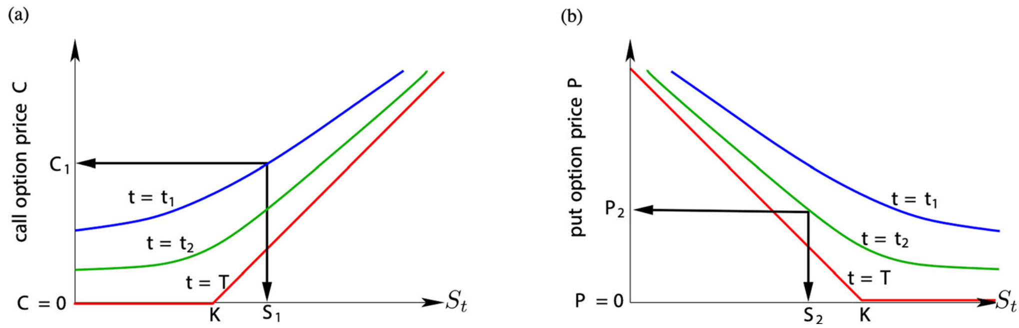

Figure 12.2. Price of a European call and put option; here, we have $t_1 < t_2 < \mathcal{T}$. The red line, which is the limit $t \to \mathcal{T}$ of the $t < \mathcal{T}$-curves, is also the intrinsic value of the option. Note that the origin of the S_t-axis is certainly not zero: you cannot have a stock priced at zero!

a profit; we would then say that the option has a positive intrinsic value given by the difference $K - S_t$. If on the other hand one has $S_t > K$, it is better to sell in the market itself, and it would be meaningless to exercise the put option; we would then say that the option has zero intrinsic value. The intrinsic value of a put option at time t is then the function $\max(K - S_t, 0)$. Coming to the time value, suppose at any time $t < \mathcal{T}$, we have $S_t < K$. Now, since there is still time left until expiration, there is a possibility that in course of time until $\mathcal{T}$, S_t will decrease even further below K, which is tantamount to saying that the option has a certain positive time value. The further S_t is below K, higher is the probability that in the time until $\mathcal{T}$, S_t will decrease even further below K, and so higher will be the time value. Summarizing, the time value of a put option is a monotonically decreasing function of S_t, and the further one is from expiration, the higher is the time value. The sum of the time value and the intrinsic value gives the put option price $P \equiv P(S_t, t; K, \mathcal{T})$. Since the time value gets smaller as the expiration date is approached, the put option price as t hits $\mathcal{T}$ is made up entirely of the intrinsic value. The discussed scenario is shown in Figure 12.2(b).

Now that we have discussed the scenario of a potential buyer of either a call or a put option, let us now proceed to discuss the situation of one who has already purchased the option. A buyer of a call option who has purchased the option at time $t_1 < \mathcal{T}$ when the spot price was $S_1 \equiv S_{t_1}$ and the corresponding cost was $C_1 \equiv C(S_1, t_1; K, \mathcal{T})$ had to pay as option premium the amount C_1 to the seller. A payoff diagram summarizes the net worth of the option from the point of view of the buyer and is shown in Figure 12.3(a). On the expiration date, the payoff is $-C_1$ if $S_{\mathcal{T}} < K$ and is $S_{\mathcal{T}} - K - C_1$ if $S_{\mathcal{T}} > K$. The payoff of a call option (buy) on maturity is thus given by

$$\text{payoff}_{\text{call}}^{\text{buy}} = \max(S_{\mathcal{T}} - K, 0) - C_1. \tag{12.8}$$

From the point of view of the seller, the call option payoff diagram is evidently just the mirror image of that for the buyer Figure 12.3(b): the maximum profit of the call option buyer is the maximum loss of the call option seller and vice versa. Moreover, the buyer has unlimited potential for profit, and correspondingly, the seller has unlimited loss potential.

Arguing as above, one may obtain the payoff diagram of a put option (buy) on maturity. Thus a buyer of a put option who has purchased the option at time $t_2 < \mathcal{T}$ when the spot price was $S_2 \equiv S_{t_2}$ and the corresponding cost was $P_2 \equiv P(S_2, t_2; K, \mathcal{T})$ has his payoff given by

$$\text{payoff}_{\text{call}}^{\text{buy}} = \max(K - S_{\mathcal{T}}, 0) - P_2, \tag{12.9}$$

while that from the point of view of the seller is the mirror image of that for the buyer (Figure 12.3 c,d). Comparing Figures 12.2 and 12.3, we see that the payoff curve at time $t < \mathcal{T}$ may be

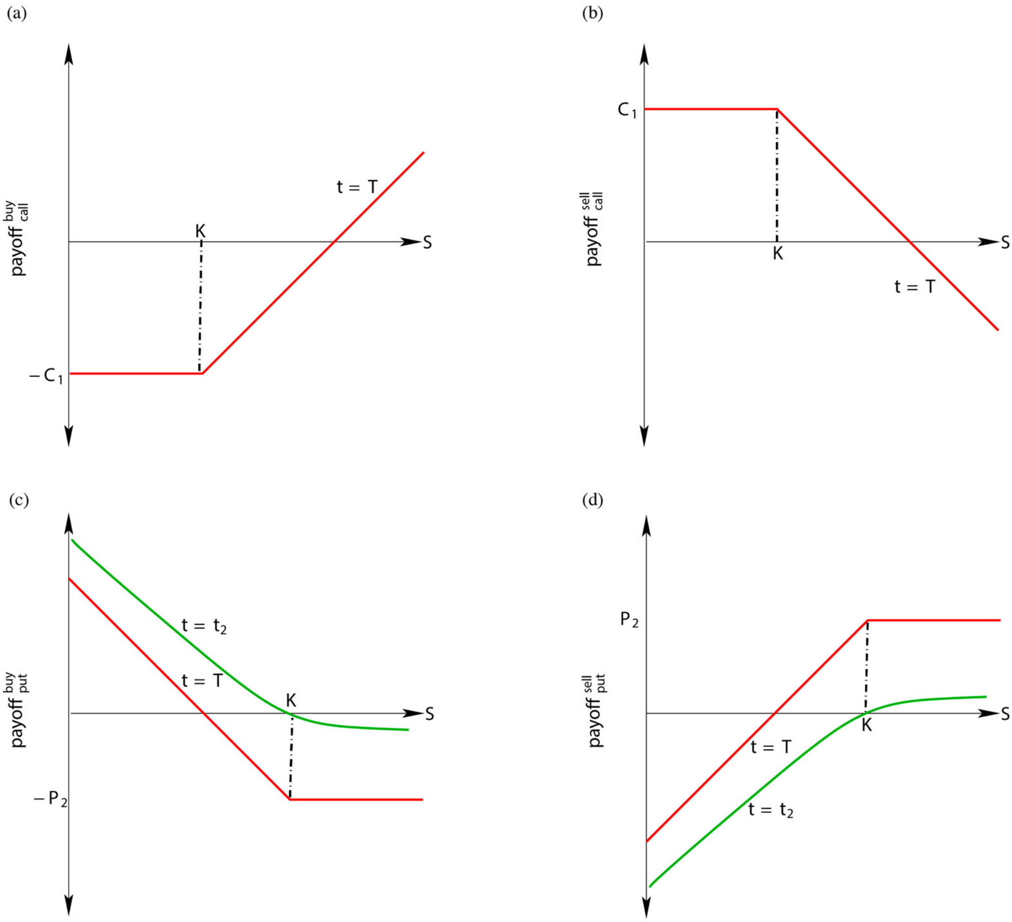

Figure 12.3. Payoff diagrams for call and put options. The quantities C_1 and P_2 are defined in Figure 12.2.

obtained from the corresponding cost curve in the former by shifting it (vertically down for the buyer and vertically up for the seller) by an amount given by the cost at the corresponding value of the stock (see Figure 12.3 c,d for an illustration).

From the above discussion, it is evident that the buyer and the seller of an option have different expectations from the market, so that a central question as regards entering into an option contract is: What should be the "right" option price $\mathcal{V}$ ($= C$ for call and $= P$ for put) that would ensure that none of the two sides of an option contract have an a-priori advantage to make profit, for it is the magnitude of $\mathcal{V}$ that enters into the payoff diagram for the buyer and the seller, see Figure 12.3: the buyer would not like a high $\mathcal{V}$ while the seller would very much like a high $\mathcal{V}$. The value of $\mathcal{V}$ depends on the dynamics of the underlying stock S_t. The question of finding the right $\mathcal{V}$, equivalent to finding a closed form expression for $\mathcal{V}$ as a function of $K, \mathcal{T}, S_t$, and time, has paramount importance in option pricing. It was answered in the most remarkable way by economists Black and Scholes [234] and Merton [235], a work that earned Scholes and Merton (Black had died by then) the Nobel prize in Economics in 1997. A crucial assumption behind deriving the model is that of a market with "no-arbitrage" opportunity, so we now digress to discuss briefly what an arbitrage opportunity means.

An investor who does not wish to make any initial commitment of money may still make money in the market in the following way. He may borrow a stock from someone who has it and sell it in the market. This process of selling an asset that one does not own is called short selling or shorting or taking a short position on the asset (buying the actual asset is what is termed "taking a long position on the asset"). The borrower has to eventually pay back the lender (i.e., he has to "close" his short position on the borrowed asset), so what he may do is to buy the same stock from the market on a later date, and return it to the lender, and in the process, if the stock price decreases, he makes a profit by this short selling; otherwise, he incurs a loss. Thus there is a risk involved in short selling, which may be compensated thus: he chooses a company that is listed in two different stock exchanges, say, exchange A and exchange B. Suppose he finds that at some point in time, the last traded price $S^{(\mathrm{A})}$ for selling a stock of the company in A is higher than the last traded price $S^{(\mathrm{B})}$ for buying a stock of the same company in B. He may then with no initial commitment short sell N stocks in A and use the proceeds to close his short position by buying N stocks in B, making in the process a riskless profit of $N(S^{(\mathrm{A})} - S^{(\mathrm{B})})$. This process of making a riskless profit, with no initial money at all, by entering simultaneously into transactions in two or more markets is called an arbitrage opportunity or an arbitrage, and those who exploit such opportunities are called arbitrageurs. A minute's thought would reveal that such arbitrage opportunities cannot last in the market for long, for selling the stock in A will decrease the price for selling a stock in A, while buying the stock in B will increase the price to buy a stock in B. As a result of these two competing tendencies, an equilibrium price for the stock in both the exchanges will be reached in time and then the arbitrage opportunity will no longer exist. The action of an arbitrageur is said to be self-destroying in that it is destroying the action itself, but the latter takes time, and in the process, the arbitrageur makes profit. An efficient market is then one that satisfies the no-arbitrage condition, that is, it does not allow anyone to make profit out of thin air (even if some short-term profit may be possible, it would not allow for any long-term profit). In common parlance, one says that there is no free lunch possible in an efficient market.

Besides arbitrageurs, there are hedgers in the market.[19] A hedge is defined to be an investment that protects one's finances from risks. Hedgers may use derivatives to reduce the risk in their portfolio in the following manner. Consider an investor with a long position on a stock, for whom the risk is associated with the possibility of the stock price going down in time. In this case, a hedging strategy could be to buy a put option on the stock, so that one would sell the stock only if the price goes below a certain level and can keep it with him if the price goes up. In the former case, the proceeds from selling the stock at a higher price (the strike price) than the spot price may minimize or offset somewhat the risk associated with the long position, and this comes at the price of the option premium that he paid in buying the put option. We may think of the option as like an insurance in the present scenario.

With the above background, we now move on to describe the Black–Scholes equation for option pricing. Here, we will discuss the Black–Scholes equation in a simple setting, while generalizations and a more detailed consideration may be found in [228]. To derive the equation, assume within our simple setting that there are two assets in the market: a bank deposit $\mathcal{B}_t$ and a stock S_t, whose dynamics are given respectively by Equations (12.1) and (12.3). The quantity r in Equation (12.1) is the interest rate offered by the bank to a depositor, but is also the interest rate the bank charges on money borrowed from the bank. Moreover, the market is assumed to be free of arbitrage opportunities. For a more extensive list of assumptions behind the Black–Scholes equation, the reader is directed to Ref. [228].

Let us define a financial portfolio as a combination of financial assets held by, i.e., individual investors and/or managed by financial professionals. To derive the Black–Scholes equation, consider a portfolio consisting of a long position on a European call option and a short position on Δ stocks. The option has strike price K and expiration date $\mathcal{T}$ on the underlying stock S_t. The question is what should be the value $C(S_t, t; K, \mathcal{T})$ of the option at time t subject to the boundary condition $C(S_\mathcal{T}, \mathcal{T}; K, \mathcal{T}) = \max(S_\mathcal{T} - K, 0)$. We take the portfolio to be self-financing, that is, in course of time no money is taken out of the portfolio and no additional money is put into it, so that any change the portfolio value may undergo is due to change in asset prices only. The value V_t of the portfolio at time t is given by

$$V_t = C(S_t, t) - \Delta\, S_t, \tag{12.10}$$

where we have suppressed the dependence of C on K and $\mathcal{T}$, for ease of notation. The minus sign on the right-hand side of Equation (12.10) is a reminder of the fact that we need to eventually close the short position on the stocks, and so we "owe" the market an amount $\Delta\, S_t$. As it will turn out, Δ will be a function of time: $\Delta = \Delta_t$. The portfolio is self-financing, which implies the following. Let us specialize to discrete times. The value of the portfolio at time $t = 0$ is

$$V_0 = C(S_0, 0) - \Delta_0 S_0, \tag{12.11}$$

which on its own will yield the value at the next time instant $t = 1$ as $C(S_1, 1) - \Delta_0 S_1$, while our strategy being self-financing, the new portfolio at time $t = 1$ should be able to be bought with the asset one has from the previous period, i.e.,

$$V_1 = C(S_1, 1) - \Delta_1 S_1 = C(S_1, 1) - \Delta_0 S_1, \tag{12.12}$$

yielding

$$S_1(\Delta_1 - \Delta_0) = 0. \tag{12.13}$$

In continuous times, we thus have

$$S_t \mathrm{d}\Delta_t = 0. \tag{12.14}$$

Using the above equation, we obtain from Equation (12.10) the rate of change in its value as given by

$$\dot{V}_t = \dot{C} - \Delta\, \dot{S}_t. \tag{12.15}$$

Equation (12.10) represents what is known as a **delta-hedging** portfolio. Delta hedging involves holding an option and shorting a quantity Δ of the underlying. Its practical importance and hedging implications will be discussed below.

Now, using Equation (12.3) and Itô's formula, see Appendix B.3.1, we have

$$\dot{C} = \frac{\partial C}{\partial t} + \mu S_t \frac{\partial C}{\partial S_t} + \frac{\sigma^2 S_t^2}{2} \frac{\partial^2 C}{\partial S_t^2} + \sigma S_t \frac{\partial C}{\partial S_t} \dot{B}_t, \tag{12.16}$$

which when used in Equation (12.15) yields

$$\dot{V}_t = \frac{\partial C}{\partial t} + \mu S_t \frac{\partial C}{\partial S_t} + \frac{\sigma^2 S_t^2}{2} \frac{\partial^2 C}{\partial S_t^2} - \mu \Delta\, S_t + \sigma S_t \left(\frac{\partial C}{\partial S_t} - \Delta \right) \dot{B}_t. \tag{12.17}$$

What the above equation gives is the value V_t of the portfolio in the future on knowing its value at the current instant t at which one knows with certainty the current stock price S_t. Note that when one says that the stock price S_t is a random function of time (see Equation 12.7), what one means is that although one knows the price at the current instant (one has to just visit a stock exchange), one cannot predict with certainty the price in the future. We will now show how, knowing S_t and V_t at the current instant t, the above equation allows to know with certainty the value of $\dot{V}_t$ and hence of V_t in future. To this end, let us choose Δ in such a way that one gets rid of the term involving $\dot{B}_t$ on the right hand side, namely, we choose Δ such that

$$\Delta = \frac{\partial C}{\partial S_t}. \tag{12.18}$$

With the above choice, Equation (12.17) gives

$$\dot{V}_t = \frac{\partial C}{\partial t} + \frac{\sigma^2 S_t^2}{2}\frac{\partial^2 C}{\partial S_t^2}. \tag{12.19}$$

It is now evident that knowing S_t allows one to compute the right-hand side and obtain with certainty the value of $\dot{V}_t$ (one has to evaluate the derivatives at S_t) and consequently, the value of $V_{t+\mathrm{d}t}$ (provided Equation (12.18) remains valid during the interval $[t, t+\mathrm{d}t]$), and hence, there is no more randomness or stochasticity in the evolution of V_t. In other words, V_t has a deterministic evolution in time, and so the portfolio becomes **risk free** for the choice given by Equation (12.18), i.e., for $\Delta = \partial C/\partial S_t$.

Now that we have a risk-free portfolio and the market is by assumption free of arbitrage opportunities, the portfolio would yield the same rate of return as we would get if we had deposited an equivalent amount of cash in a bank account, see Equation (12.1). This may be explained as follows: Suppose the rate of return $r_{\text{risk-free}}$ from the risk-free portfolio is different from r, and let us say that one has $r_{\text{risk-free}} > r$. Then, someone would borrow money from the bank (which would according to our assumptions ask for an interest rate r on the lent amount), and would invest it in the risk-free portfolio. He would then use the return from the portfolio to give back the money he owes to the bank, and in the process, pocket the difference of the return from the invested amount and the money given back to the bank, without making any initial investment. The market being arbitrage-free would not allow for such a possibility, and hence, we conclude that $r_{\text{risk-free}}$ should equal r. Then, we may write

$$\dot{V}_t = rV_t = r\left(C - \frac{\partial C}{\partial S_t}S_t\right), \tag{12.20}$$

where in obtaining the second equality we have used Equations (12.10) and (12.18).

Comparing Equations (12.19) and (12.20) yields the celebrated **Black–Scholes equation**

$$\frac{\partial C}{\partial t} + \frac{\sigma^2 S_t^2}{2}\frac{\partial^2 C}{\partial S_t^2} + rS_t\frac{\partial C}{\partial S_t} - rC = 0, \tag{12.21}$$

with the boundary condition

$$C(S_{\mathcal{T}}, \mathcal{T}) = \max(S_{\mathcal{T}} - K, 0). \tag{12.22}$$

As we have discussed earlier, hedging relates to reduction of risks in one's financial portfolio. We saw above that choosing $\Delta = \partial C/\partial S_t$, which corresponds to exploiting correlation between the option and the stock making up the portfolio (clearly, evolution of C depends on the dynamics of S_t), led to perfect elimination of risks in that the resulting portfolio has completely deterministic evolution (12.19). Such a strategy goes by the name of delta hedging. Note that the quantity $\partial C/\partial S_t$ continually changes in time. This implies that the amount Δ of stocks that one needs to short to offset the risk associated with the long position must change continually in time. Delta hedging is thus an example of a dynamic hedging strategy.

In obtaining the Black–Scholes equation (12.21), the only place where the nature of the derivative enters into the derivation is through the boundary condition (12.22). Thus it should be possible to generalize the derivation for the price of an arbitrary European option $F(S_t,t)$ with payoff $F(S_{\mathcal{T}},\mathcal{T}) = \Phi(S_{\mathcal{T}})$, where $\Phi(S)$ is a known function. The price $F(S_t,t)$ should then follow the equation:

$$\frac{\partial F}{\partial t} + \frac{\sigma^2 S_t^2}{2}\frac{\partial^2 F}{\partial S_t^2} + rS_t\frac{\partial F}{\partial S_t} - rC = 0, \tag{12.23}$$

with the boundary condition

$$F(S_{\mathcal{T}},\mathcal{T}) = \Phi(S_{\mathcal{T}}). \tag{12.24}$$

12.2.1. *Solution of the Black–Scholes equation (12.21)*

The treatment here follows the one given in Refs. [228,231]. The Black–Scholes equation (12.21) may be solved by performing the following transformation to a set of dimensionless variables that turns it into the heat equation or the Fokker–Planck equation for a free Brownian particle, both well known in physics:

$$\tau \equiv \frac{\mathcal{T}-t}{2/\sigma^2}, \quad x \equiv \ln(S_t/K), \quad u(x,\tau) \equiv \exp(\alpha x + \beta^2\tau)\frac{C(S_t,t)}{K},$$
$$\alpha \equiv \frac{1}{2}\left(\frac{2r}{\sigma^2} - 1\right), \quad \beta = \frac{1}{2}\left(\frac{2r}{\sigma^2} + 1\right). \tag{12.25}$$

In terms of transformed variables u, x, τ, Equation (12.21) reads [231] (for details, see Appendix G.1):

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2}, \tag{12.26}$$

while the condition (12.22) becomes an initial condition thus: Equation (12.22) gives the result $u(x,0)K/\exp(\alpha x) = \max(S_t - K, 0)$, that is,

$$u(x,0) = \max(S_t\exp(\alpha x)/K - \exp(\alpha x), 0) = \max(\exp((\alpha+1)x) - \exp(\alpha x), 0), \tag{12.27}$$

where we have used the fact that $S_t/K = \exp(x)$. Next, using $\alpha + 1 = \beta$, we finally have the desired initial condition:

$$u(x,0) = \max(\exp(\beta x) - \exp(\alpha x), 0). \tag{12.28}$$

Now, the heat Equation (12.26) is solved as

$$u(x,\tau) = \int_{-\infty}^{\infty} \mathrm{d}x'\, u(x',0)G(x,x'), \tag{12.29}$$

in terms of the Green's function for the heat equation: $G(x,x') = 1/\sqrt{4\pi\tau}\exp(-(x-x')^2/(4\tau))$. Using the initial condition (12.28) in the last equation allows to write $u(x,\tau)$ as

$$u(x,\tau) = I(\beta) - I(\alpha);\ I(a) \equiv \frac{1}{\sqrt{4\pi\tau}}\int_0^\infty \mathrm{d}x'\ \exp(ax' - (x-x')^2/(4\tau))$$
$$= \exp(ax + a^2\tau)N(d_a), \tag{12.30}$$

with

$$d_a \equiv \frac{x + 2a\tau}{\sqrt{2\tau}}, \tag{12.31}$$

and $N(x)$ being the cumulative distribution for a Gaussian random variable distributed as $\mathcal{N}(0,1)$:

$$N(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{x} \mathrm{d}y \exp(-y^2/2). \tag{12.32}$$

Using Equation (12.30) and reverting to the original variables of C, S_t, K, etc. by using Equation (12.25) lead to the following result:

The Black–Scholes formula for the price of a European call option:

$$C(S_t,t) = S_tN(d_1) - K\exp(-r(\mathcal{T}-t))N(d_2);$$
$$d_1 = \frac{\ln(S_t/K) + \left(r + \sigma^2/2\right)(\mathcal{T}-t)}{\sigma\sqrt{\mathcal{T}-t}},\quad d_2 = \frac{\ln(S_t/K) + \left(r - \sigma^2/2\right)(\mathcal{T}-t)}{\sigma\sqrt{\mathcal{T}-t}}. \tag{12.33}$$

Equation (12.33) is known as the Black–Scholes formula for option pricing: a closed expression to price an option in a market where there are two assets, namely, a bank deposit $\mathcal{B}_t$ subject to interest rate r and a stock S_t with expiration $\mathcal{T}$ and strike price K, and with the dynamics of $\mathcal{B}_t$ and S_t given respectively by Equations (12.1) and (12.3).

From the foregoing, it is easy to write down the solution to Equation (12.23) for an arbitrary European option. Defining $u(x,\tau) \equiv \exp(\alpha x + \beta^2\tau)F(S_t,t)/K$, and following the same line of argument as the one followed in Equations (12.25)–(12.29), one obtains in analogy with Equation (12.29) that

$$u(x,\tau) = \int_{-\infty}^{\infty} \mathrm{d}x'\ \Phi(x')G(x,x'), \tag{12.34}$$

which when expressed in terms of variables F, S_t, K, etc. yields

$$F(S_t,t) = \frac{\exp(-r(\mathcal{T}-t))}{\sqrt{2\pi\sigma^2(\mathcal{T}-t)}}\int_0^\infty \mathrm{d}S'\ \frac{\Phi(S')}{S'}\exp\left[-\frac{\{\ln(S'/S_t) - (r-\sigma^2/2)(\mathcal{T}-t)\}^2}{2\sigma^2(\mathcal{T}-t)}\right]. \tag{12.35}$$

Equation (12.35) is the Black–Scholes formula for an arbitrary European option with payoff $F(S_{\mathcal{T}},\mathcal{T}) = \Phi(S_{\mathcal{T}})$, where $\Phi(S)$ is a known function. For a European call option, $F(S_t,t) = C(S_t,t)$ and $\Phi(S) = \max(S-K,0)$, while for a European put option, $F(S_t,t) = P(S_t,t)$ and $\Phi(S) = \max(K-S,0)$, where K is the strike price and $\mathcal{T}$ is the expiration time.

12.3. *Efficient market and the martingale approach*

The so-called martingale approach to an efficient market offers an alternative elegant way to arrive at the Black–Scholes equation. With the preliminaries on elements of probability theory that may be found in Appendix B.1, let us now describe the martingale approach to an efficient market.

12.3.1. *Equivalent martingale measure and the Girsanov theorem*

We have already seen that the standard Brownian motion is a martingale. We know that the probability density of the standard Brownian motion is a Gaussian:

$$\rho_{B_t}^{\mathcal{P}}(b) = \frac{1}{\sqrt{2\pi t}} \exp\left(-b^2/(2t)\right). \tag{12.36}$$

Using the defining property of a martingale, we may conclude that the motion with a drift, given by

$$\widetilde{B}_t = at + B_t; \quad 0 \le t \le \mathcal{T}, \tag{12.37}$$

is not a martingale precisely because of the presence of the drift a. The **Girsanov theorem** [66] states, however, that $\widetilde{B}_t$ becomes a standard Brownian motion with respect to the probability measure $\mathcal{Q}$ given by

$$\rho_{\widetilde{B}_t}^{\mathcal{Q}}(b) = M_{\widetilde{B}_t}(b)\rho_{\widetilde{B}_t}^{\mathcal{P}}(b), \tag{12.38}$$

where $M_{\widetilde{B}_t}(b)$ is the function

$$M_{\widetilde{B}_t}(b) = \exp\left(-ab + \frac{a^2 t}{2}\right). \tag{12.39}$$

Indeed, using

$$\rho_{\widetilde{B}_t}^{\mathcal{P}}(b) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\left(b - at\right)^2/(2t)\right), \tag{12.40}$$

we see that

$$\rho_{\widetilde{B}_t}^{\mathcal{Q}}(b) = \frac{1}{\sqrt{2\pi t}} \exp\left(-b^2/(2t)\right), \tag{12.41}$$

which indeed corresponds to the probability density of the standard Brownian motion. Thus, with respect to measure $\mathcal{Q}$, the process with drift, $\widetilde{B}_t$, becomes a standard Brownian motion and is thus a martingale. The measure $\mathcal{Q}$ is called the equivalent martingale measure.

Consider now the Geometric Brownian motion (12.3), which we rewrite below as

$$\mathrm{d}S_t = \sigma S_t \left(\frac{\mu}{\sigma}\,\mathrm{d}t + \mathrm{d}B_t\right) = \sigma S_t\,\mathrm{d}\widetilde{B}_t; \quad 0 \le t \le \mathcal{T}, \tag{12.42}$$

with

$$\widetilde{B}_t = \frac{\mu}{\sigma}t + B_t. \tag{12.43}$$

The Girsanov theorem would make $\widetilde{B}_t$ a standard Brownian motion with respect to the measure (12.38) with $a = \mu/\sigma$, and then the SDE (12.42) will have no drift so that the stochastic process S_t will be a martingale with respect to the measure $\mathcal{Q}$.

12.3.2. *The martingale approach to an efficient market*

With the above background, we now come to discuss about the main object of this section: the martingale approach to an arbitrage-free market. Consider a market comprising two assets $(\mathcal{B}_t, S_t)$, with $\mathcal{B}_t$ a risk-free asset (a bank deposit) and S_t a risky asset such as a stock that is modelled as a stochastic process. As implied by Equation (12.1), we have the growth law $\mathcal{B}_t = \mathcal{B}_0 \exp(rt)$, where $\mathcal{B}_0 \equiv \mathcal{B}_{t=0}$ is the initial amount deposited in the bank. Based on the information available up to time t_0, the expected price of S_t at a later time $t > t_0$ is $\langle S_t | S_{[0,t_0]} \rangle$ with $S_{[0,t_0]} = \{S_s\}_{s\in[0,t_0]}$, so that if the market is arbitrage-free, we now argue that the price at time t_0 should be $\langle S_t | S_{[0,t_0]} \rangle / \exp(r(t-t_0))$. For, if the stock is priced at time t_0 at a value $y < \langle S_t | S_{[0,t_0]} \rangle / \exp(r(t-t_0))$, then a buyer would take advantage of the situation by borrowing an amount of money y at time t_0 to buy the asset and then selling at time t to repay his debt of $y \exp(r(t-t_0))$, thereby pocketing at time t a positive profit of $\langle S_t | S_{[0,t_0]} \rangle - y \exp(r(t-t_0))$. On the other hand, if the stock is priced at $y > \langle S_t | S_{[0,t_0]} \rangle / \exp(r(t-t_0))$, then a seller would take advantage of the situation by selling the stock at time t_0 and lending an amount of money y so that at time t, he would receive an amount $y \exp(r(t-t_0))$ and would buy back the asset to make a positive profit of $y \exp(r(t-t_0)) - \langle S_t | S_{[0,t_0]} \rangle$. The market being arbitrage-free, it would not allow for both these opportunities of making profit out of thin air, and hence, the stock at time t_0 should be priced at $\langle S_t | S_{[0,t_0]} \rangle / \exp(r(t-t_0))$, which by definition is the actual price S_{t_0} at time t_0. Rewriting in terms of $\mathcal{B}(t)$, and recalling that a bank deposit is risk-free, i.e., non-stochastic, we get

$$\left\langle \frac{S_t}{\mathcal{B}_t} \middle| S_{[0,t_0]} \right\rangle_{\mathcal{Q}} = \frac{S_{t_0}}{\mathcal{B}_{t_0}}; \quad t \geq t_0. \tag{12.44}$$

From the definition of a martingale, it then follows that the stochastic process given by $\{S_t/\mathcal{B}_t\}_{t\geq 0}$ is a martingale. The ratio $S_t/\mathcal{B}_t$ is known as the discounted price of the stock S_t. Note that Equation (12.44) holds with the expectation calculated with respect to a suitable probability measure $\mathcal{Q}$.

In the light of the foregoing, we now state the two fundamental theorems of asset pricing.

First Fundamental Theorem of asset pricing. If in the market there exists at least one probability measure $\mathcal{Q}$ such that the discounted price $S_t/\mathcal{B}_t$ is a martingale with respect to the measure $\mathcal{Q}$, that is,

$$\left\langle \frac{S_t}{\mathcal{B}_t} \middle| S_{[0,t_0]} \right\rangle_{\mathcal{Q}} = \frac{S_{t_0}}{\mathcal{B}_{t_0}}; \quad t \geq t_0, \tag{12.45}$$

then the market does not admit arbitrage, or, in other words, the market is efficient. In words, an efficient market is one for which it should not be possible to make definite predictions about future price on the basis of the information available today, so that the best prediction that one can make for the expected future price discounted to the present time is today's price itself. One may ask when does the measure $\mathcal{Q}$ exist? If the market is arbitrage-free, the measure $\mathcal{Q}$ has to exist. For a mathematically-rigorous discussion of conditions for the existence of $\mathcal{Q}$, beyond the scope of this review, the reader is referred to, i.e., Refs. [236,237].

In the above backdrop, we now turn to the Black–Scholes model of option pricing. To this end, assume, as in Section 12.2, that there are two assets in the market: a bank deposit $\mathcal{B}_t$ and a stock

S_t, whose dynamics are given respectively by Equations (12.1) and (12.3). Moreover, the market is assumed to be free of arbitrage opportunities, which according to our discussions above is to be regarded as an efficient market. Using the fact that in an efficient market, all financial assets are martingales with respect to the measure $\mathcal{Q}$, we may now write for an arbitrary European option $F(S_t, t)$ with maturity $\mathcal{T}$ and payoff function $\Phi(S)$ that

$$\begin{aligned}\frac{F(S_t,t)}{\mathcal{B}_t} &= \left\langle \frac{F(S_{\mathcal{T}},\mathcal{T})}{\mathcal{B}_{\mathcal{T}}} \middle| S_{[0,t]} \right\rangle_{\mathcal{Q}} \\ &= \left\langle \frac{\Phi(S_{\mathcal{T}})}{\mathcal{B}_{\mathcal{T}}} \right\rangle_{\mathcal{Q};t,S_t},\end{aligned} \tag{12.46}$$

where in obtaining the second line, we have used the fact that $F(S_{\mathcal{T}},\mathcal{T}) = \Phi(S_{\mathcal{T}})$. In the second line, using $\mathcal{B}_t = \mathcal{B}_0 \exp(rt)$, and denoting by $\rho^{\mathcal{Q}}_{S_t}(s|S_{t_0} = s_0)$ the probability density under the measure $\mathcal{Q}$ of S_t with initial value $S_{t_0} = S_0$, the quantity $\langle\cdot\rangle_{\mathcal{Q};t,S}$ means the following:

$$F(S_t,t) = \exp\left[-r(\mathcal{T}-t)\right] \int_0^\infty \mathrm{d}s'\, \Phi(s') \rho^{\mathcal{Q}}_{S_{\mathcal{T}}}(s'|S_t = S_t). \tag{12.47}$$

To obtain $\mathcal{Q}$, consider the stochastic process

$$Z_t = \frac{S_t}{\mathcal{B}_t} = \exp(-rt) S_t, \tag{12.48}$$

so that

$$\mathrm{d}Z_t = r\exp(-rt)S_t\,\mathrm{d}t + \exp(-rt)\,\mathrm{d}S_t = \sigma Z_t\,\mathrm{d}\widetilde{B}_t; \quad \widetilde{B}_t = \frac{\mu - r}{\sigma} t + B_t, \tag{12.49}$$

where we have used Equation (12.3) to arrive at the second equality. The latter when rewritten in terms of the process $\widetilde{B}_t$ reads

$$\mathrm{d}S_t = rS_t\,\mathrm{d}t + \sigma S_t\,\mathrm{d}\widetilde{B}_t. \tag{12.50}$$

From our previous discussion on the Girsanov theorem, we know that one can construct a measure $\mathcal{Q}$ with respect to which the process $\widetilde{B}_t$ is a standard Brownian motion. Note that the measure $\mathcal{Q}$ will be different for different S_t's that would have in general different μ and different σ that gets reflected in having correspondingly different $\widetilde{B}_t$'s, see Equation (12.49). Then, Equation (12.50) has the same form as the Geometric Brownian motion (12.3), with mean rate of return given by $\mu = r$. The latter fact, which implies that risky stocks guarantee the same mean rate of return as the risk-free bank account, makes the pricing method based on the measure $\mathcal{Q}$ sometimes referred to as risk-neutral valuation. The measure $\mathcal{Q}$ with respect to which the discounted stock price $S_t/\mathcal{B}_t$ is a martingale is therefore said to be a risk-neutral measure.

Using Equation (12.7) and with the substitution $\mu = r, S_0 = S_t$, we thus have

$$\rho^{\mathcal{Q}}_{S_{\mathcal{T}}}(s'|S_t = s) = \frac{1}{s'\sqrt{2\sigma^2(\mathcal{T}-t)}} \exp\left[-\frac{\left\{\ln\left(s'/s\right) - \left(r - \sigma^2/2\right)(\mathcal{T}-t)\right\}^2}{2\sigma^2(\mathcal{T}-t)}\right], \tag{12.51}$$

which when used in Equation (12.47) yields

$$F(S_t,t) = \frac{\mathrm{e}^{-r(\mathcal{T}-t)}}{\sqrt{2\pi\sigma^2(\mathcal{T}-t)}} \int_0^\infty \mathrm{d}s'\, \frac{\Phi(s')}{s'} \exp\left[-\frac{\left\{\ln\left(s'/S_t\right) - \left(r - \sigma^2/2\right)(\mathcal{T}-t)\right\}^2}{2\sigma^2(\mathcal{T}-t)}\right], \tag{12.52}$$

the same as Equation (12.35).

In an efficient market, we know that at least one risk-neutral measure $\mathcal{Q}$ will exist. If a unique $\mathcal{Q}$ exists, there is a unique arbitrage-free price for every derivative, and the market is said to be complete. This brings us to the second fundamental theorem of asset of pricing:

> **Second Fundamental Theorem of asset pricing.** An arbitrage-free $(\mathcal{B}_t, S_t)$-market is complete if and only if the measure $\mathcal{Q}$ is unique.

For rigorous mathematical proof and implications of the two fundamental theorems of asset pricing, the reader is referred to Ref. [233].

To conclude, we see in this brief overview on use of martingales in the field of finance how an approach based on martingales allows to obtain rather straightforwardly the solution of the Black–Scholes equation without actually solving it using the rather nontrivial variable transformation discussed in Section 12.2. The martingality encodes the expectation that in an efficient market, all relevant information is already reflected in the prices, so that the best possible prediction for the expected future price would be today's price. The Nobel-winning Black–Scholes model for pricing an option contract with an underlying martingale structure provided one of the earliest and remarkable mathematical foundations to option-market activities around the world. The success of the model led to an eventual boom in options trading with people gaining confidence in engaging in such activities. The assumptions behind the model have over the years been relaxed and generalized in many directions, leading to a spectrum of models that are currently in wide use in derivative pricing and risk management all over the world.

Chapter 13. Final remarks and discussion

In the old days, you could type into our main computer "Edit explain life" and you got the answer "Life is a supermartingale"

Obituary: Joseph Leonard Doob, J. L. Snell, J. Appl. Prob. **42**, 247–256 (2005).

13.1. *Other revelations of martingales*

There exist other fields in science where martingales have found valuable applications. Here is a swift list of some of the miscellaneous topics that we have not covered in this treatise.

The main aim of **decision theory** is to develop algorithms that take fast and reliable decisions from the observations of a noisy process. Wald's sequential probability ratio test (SPRT) [47,238,239] is optimal amongst sequential hypothesis tests with a prescribed error probability when the observation process consists of a sequence of iid random variables, in the sense that it provides the minimum average time to decide between two competing hypothesis. In addition, for a broad class of observations processes Wald's SPRT is optimal in the asymptotic limit of small prescribed error probabilities when neglecting subleading order terms [47]. The recent work [240] shows that Wald's SPRT is optimal in an information theoretically sense for continuous observation processes, providing an information theoretical interpretation for the SPRT.

The SPRT takes sequential observations from a stream of data coming from a stochastic process X_t, and measures the weight of evidence through the log-likelihood ratio

$$\Lambda_t = \log \frac{\mathcal{P}(X_{[0,t]}|H_1)}{\mathcal{P}(X_{[0,t]}|H_2)}, \tag{13.1}$$

where $\mathcal{P}(X_{[0,t]}|H_1)$ and $\mathcal{P}(X_{[0,t]}|H_2)$ are the path probabilities for the sequence $X_{[0,t]}$ when the statistical hypothesis H_1 and H_2 are, respectively, true. Wald's SPRT takes a decision when the log-likelihood ratio leaves the interval $(-L_2, L_1)$ for the first time with $L_1 > 0$ and $L_2 > 0$ the decision thresholds, i.e.,

$$\mathcal{T} = \min\{t \geq 0 : \Lambda_t \leq -L_2 \text{ or } \Lambda_t \geq L_1\}\,. \tag{13.2}$$

When $\Lambda_{\mathcal{T}} \geq L_1$, then the SPRT test decides for H_1, whereas if $\Lambda_{\mathcal{T}} \leq -L_2$, then the SPRT decides for H_2. The decision thresholds are set by the prescribed error probabilities [47,238,239].

Reference [34] uses Wald's SPRT to decide on the direction of time's arrow from the observation of a trajectory drawn from a time-homogeneous stationary process. Interestingly, [34] shows that the mean decision is related to the entropy production rate of the process. Moreover, as the log-likelihood ratio (13.1) has the form of a Λ-stochastic entropic functional (see Chapter 6), it is possible to exploit the mathematical machinery of martingales to derive fluctuation relations for decision times [11] and to develop quantitative criteria on how far from Wald's optimality is a decision maker [241].

A field in physics where martingales have found profound applications and we did not discuss in this treatise are **quantum measurements**. Briefly, in models of iterated discrete (continuous) time measurements, the collapse of the system at large times can be rationalized in terms of the convergence theorem of submartingales (as Theorem 8 in Chapter 4 or more precisely version with almost sure convergence). More precisely, under a discrete iterated (resp. continuous) time measurement, the diagonal elements of the density matrix is a martingale, in a special basis called pointer basis and given by a non-demolition hypothesis [242]. For a pure state, such martingale is given by the modulus square of the projection of the ket in the pointer basis. This result has been shown for both continuous time [243] and discrete time [244].

Let us now we give a smell of this formulation in a physical example. In continuous-time quantum measurements, the equation for the evolution of the density matrix is called *quantum trajectory* [242]; it is given by a matricial stochastic differential equation with Gaussian and/or Poissonian white noise. If the Hilbert space of the system is two-dimensional with orthonormal basis $\{|+\rangle, |-\rangle\}$,[20] then the density matrix in this basis is parametrized by $\rho_t = \begin{pmatrix} X_t & Z_t \\ \bar{Z}_t & 1-X_t \end{pmatrix}$ where $X_t \in [0,1]$ and Z_t is the coherence of the density matrix. Then the quantum trajectory with Gaussian noise which results from the continuous measurements of the operator[21] $\frac{1}{4}\sigma_z = \frac{1}{4}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, is given by the Ito stochastic differential equation for X_t

$$\dot{X}_t = rX_t\,(1 - X_t)\,\dot{B}_t, \tag{13.3}$$

where r is a parameter quantifying the rate of measurement. Figure 13.1 shows representative trajectories for X_t obtained from numerical simulations.

Then, from the absence of drift in this stochastic differential equation, X_t is a bounded (local) Martingale and converges to $X_\infty \in \{0,1\}$ by virtue of continuous-time version of Theorem 8 in Chapter 4. Moreover, the martingale property implies that $X_0 = \langle X_\infty\rangle = 1 \times P(X_\infty = 1) + 0 \times P(X_\infty = 0)$. We then find the Born law as an emergent property:

$$\begin{cases} P\,(X_\infty = 1) = X_0 = \mathrm{Tr}\,(P_1\rho_0) \\ P\,(X_\infty = 0) = 1 - X_0 = \mathrm{Tr}\,(P_{-1}\rho_0) \end{cases} \quad \text{with} \quad \begin{cases} P_1 = |1\rangle\,\langle 1| \\ P_{-1} = |-1\rangle\,\langle -1| \end{cases}.$$

Lastly, let us mention two more interesting applications of martingales in statistical physics. In the context of **spin glass theory** [245,246], a full replica symmetry breaking theory for a spin

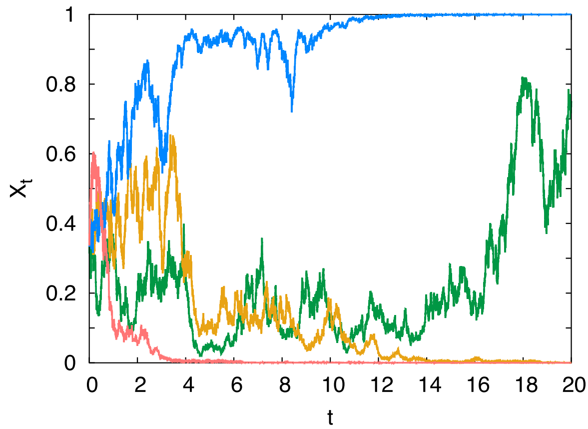

Figure 13.1. Representative time series of the process (13.3). Parameters: $r = 1$, $X_0 = 1/3$, $\mathrm{d}t = 10^{-3}$.

glass on a Bethe lattice, which is one of the main open challenges in this research area, has been formulated with the help of martingales [247,248]. In the **theory of critical phenomena**, Cardy's formula for the crossing probability of a stochastic Loewner evolution, which in the case of percolation gives the probability that there exist a percolating cluster, has been rederived and extended with martingales [249]. Martingales also play a key role in the study of **nonequilibrium properties of interacting particles**, see i.e., Spohn's treatise [250]. In particular, martingale theory was applied to prove directly weak convergence of path probabilities, which go beyond the convergence of moments as done in expansion techniques. Fruits of this approach, explicit proofs for the Green-Kubo formula, current statistics and various hydrodynamic limits can be retrieved through elegant calculations, see also Refs. [251–253].

Discussion

This treatise highlights the use of martingale theory in statistical physics, population dynamics, and quantitative finance. Although martingales have been used extensively in the latter two research areas, its relevance and usefulness for statistical physics, notably stochastic thermodynamics, is a recent endeavor. Taken together, the results and techniques reviewed here address *why a statistical physicist should learn martingale theory.* As we have shown, martingales are ubiquitous and their properties are fundamental in probability theory. Therefore, we think that martingale theory can be considered as relevant for statistical physics as, i.e., the theory of Markov processes or large deviation theory. Particularly interesting is the fact that once a martingale, submartingale, or supermartingale has been identified, we can use theorems from martingale theory to unveil universal physical principles. For random walks, the "martingale" approach is particularly useful when dealing with first-passage properties and extreme-value statistics. As we have shown with several examples, non-trivial extreme-value and first-passage-time calculations can be greatly simplified upon using Doob's theorems for stopping times. This leads to another key concept for physics unveiled by this treatise, viz., the *stopping time*. We have thoroughly reviewed the concept of stopping times in the context of stochastic processes as generalized first-passage times. Furthermore, upon applying several well-known martingale theorems to physically-relevant stopping times, we have presented several "shortcuts" to calculations of, i.e., absorption probabilities, first passage time statistics (mean, second moment, distributions), and finite-time statistics of extrema.

When dealing with the stochastic thermodynamics of small systems, the martingale approach provides novel insights with respect to conventional fluctuation theorems developed in the 1990s and 2000s. On one hand, the martingale structure of thermodynamically-relevant probability ratios leads to a tree-like hierarchy of second laws of thermodynamics, among which only some of them were known previously in the literature. Furthermore, applying mathematical properties of martingales to thermodynamics quantities unveils universal fluctuation relations for, i.e., stopping times, extrema, and absorption probabilities of entropy production in stationary states. Interestingly, for stationary processes one can overcome classical limits for, i.e., the efficiency of thermal machines, by stopping the dynamics of a system upon a cleverly-chosen time. On the other hand, we have shown that extra care is required when applying martingale concepts to non-stationary processes, as the second laws at stopping times are in this context nontrivial generalizations of the traditional second laws at fixed times. This leads to the so-called gambling opportunities, which allow an observer to extract more work from a system than given by the free energy difference between the initial and final state through several executions of a protocol stopped at a cleverly chosen strategy. For future work, it will be interesting to relate the martingale bounds on work extraction to the performance of Szilard demons or engines [179,254].

We expect that martingales will find use in statistical physics beyond the study of fundamental principles in stochastic thermodynamics. In biophysics, recent work proposed that small living systems (i.e., cells) can take accurate rapid decisions in noisy environments through applying threshold criteria (i.e., Wald's SPRT) to accumulated chemical species [255,256]. Similarly, in cognitive neuroscience it has been hypothesized that binary perceptual decisions taken by i.e., rhesus monkeys [257,258] result from the accumulation of neural evidence in the brain and the implementation of log-likelihood-ratio threshold tests. The plethora of second laws for path-probability ratios discussed in this work and the trade-off relations between speed and accuracy may thus shed further light in understanding decision making of living systems from the sub-cellular to the whole organism level [259,260]. Furthermore, stopping times form a versatile toolbox with applications in various research areas. A notable example is computer science [261], where the first thermodynamics insights brought by, i.e., Landauer and Bennett [262,263] were rationalized by the field of information thermodynamics [201]. The development of a comprehensive stochastic-thermodynamic framework of computation is, however, still in its infancy [264]. Stopping-time statistics could be pushed forward in unveiling novel generic thermodynamic laws that govern computational tasks executed by, i.e., finite automata, Turing machines, and quantum computers, and beyond.

Notes

1. "I went [to Venice's casino], taking all the gold I could get, and by means of what in gambling is called the martingale I won three or four times a day during the rest of the carnival".
2. For the example of a Markov chain, which we introduce below in Chapter 3, explicit time dependence occurs if the transition matrix in Equation (3.2) has a supplementary dependence on n, i.e., the path-probability equation (3.4) reads

$$\mathcal{Q}^{(n)}(x_{[0,n]}) = \rho_0(x_0) \prod_{j=1}^{n} w^{(n)}(x_{j-1}, x_j). \tag{2.20}$$

Note that this latter property is different than the time-inhomogeneity of a Markov chain for which the transition matrix has a supplementary dependency on the present time j and the path-probability equation (3.4) reads

$$\mathcal{Q}(x_{[0,n]}) = \rho_0(x_0)\prod_{j=1}^{n} w^{(j)}(x_{j-1},x_j). \tag{2.21}$$

This time inhomogeneity is not a problem for the last step of the derivation in Equation (2.19), which remains valid.

3. See [265] for generalizations where $\alpha \in \mathbb{R}$ and even space dependent.
4. The expression of the spurious drift depends on the convention chosen in Equation (3.65). In some references, it is claimed that the spurious term disappears in the anti-Itô convention ($\alpha = 1$ in Equation (2.85)) of the isothermal overdamped version of (3.65), and therefore the convention $\alpha = 1$ is often called the isothermal convention. Note, however, that the spurious drift disappears in the anti-Itô convention *only for the case* $\mathbf{D}_t(x) = g_t(x)\mathbf{D}_t$, with g a scalar function and $\mathbf{D}_t$ a space homogeneous matrix, i.e., if all the x dependence is in the scalar part. The latter condition holds in one dimension, but is not generally true for $d \geq 2$. See also [266,267]. An alternative perspective is to consider the Langevin equation (3.65) as the zero correlation time limit of Equation (3.65) but with a colored, Orsntein–Uhlenbeck noise, see [268,269]. Note that the limiting equation has also in general a non-vanishing spurious drift, except for the one-dimensional case if we choose to write Equation (3.65) in the Stratonovich convention. Such spurious drift is in general different to the spurious drift in Equation (3.65). For the expression and the proof of such spurious drift in the general case, we refer to Theorem 7.2 on page 497 of the book [270].
5. Indeed, if we apply Itô's formula to $\exp(Z)$, see Appendix B.3, with $Z = Y_t - Y_0 - [Y,Y]_t/2$, and use that $[Y,[Y,Y]] = 0$ and $[[Y,Y],[Y,Y]] = 0$, we obtain Equation (4.92). Note that the correction term inside the exponential can be understood from the passage of Equation (4.92) from the Itô convention to the Stratonovich convention (see Appendix B.3 on stochastic integrals).
6. The $\dot{X}_s$ in these relations must be interpreted in Stratonovich convention.
7. The Dynkin martingale approach does not provide a rigorous proof of martingality neither as $\exp(-s)$ is not a bounded function, which is required to show martingality, see Theorem 4.
8. See also the footnote in Section 2.1.3 for an example in the discrete-time setup.
9. Here, $\Lambda_{[s,t]}$ should depend on $X_{[s,t]}$ only.
10. An example of Markov process where we have condition (3) without condition (2) is a general Isothermal Langevin equation: (3.65) with Einstein relation (3.69), without external force $f_t = 0$, generic time-homogeneous potential $V_t = V$, and with the mobility matrix $\boldsymbol{\mu}_t$ having an explicit time dependence. For this example, the stationary density is the Gibbs density $\rho_{\rm st} \sim \exp(-H(x)/T)$, and if moreover $\rho_0 = \rho_{st}$, we have (3) without (2).
11. For all $0 \leq r \leq s \leq t$, we have the decomposition of the Markovian path probabilities

$$\mathcal{P}_{[0,s]}\left(X_{[0,t]}\right) = \frac{\mathcal{P}_{[0,r]}\left(X_{[0,t]}\right)\mathcal{P}_{[r,s]}\left(X_{[0,t]}\right)}{\rho_r\left(X_r\right)}, \tag{6.136}$$

and

$$\mathcal{Q}^{(t)}_{[t-s,t]}\left(\Theta_t X_{[0,t]}\right) = \frac{\mathcal{Q}^{(t)}_{[t-s,t-r]}\left(\Theta_t X_{[0,t]}\right)\mathcal{Q}^{(t)}_{[t-r,t]}\left(\Theta_t X_{[0,t]}\right)}{\rho^{\mathcal{Q}^{(t)}}_{t-r}\left(X_r\right)}. \tag{6.137}$$

12. This follows from stationarity which gives $\langle \Delta S^{\rm sys}_t\rangle = 0$, and the fact that the second law (6.29) holds for all normalized $\mathcal{Q}$.
13. The nonequilibrium free energy is formally defined as $G^{\rm ne}_t = V_t - TS^{\rm sys}_t$, see Equation (9.16) in Chapter 9, with E_t and $S^{\rm sys}_t$ the (stochastic) energy and nonequilibrium entropy of the system at time t. We will provide a proof of the second law (8.47) in Chapter 9, see Equation (9.26).
14. See p. 174–175 in [98] for a detailed proof of Equation (9.12)
15. Except for the case $\mathcal{Q} = \mathcal{Q}_{st}$ where we have (9.35).
16. Note that if we replaced $m_{\mathsf{T}+1}$ on the left-hand side by $s_{\mathsf{T}+1} = M_{\mathsf{T}+1} - M_{\mathsf{T}}$, the equation is nothing but the definition of our quenching protocol.
17. While the analogy is not close, let us regard the ensemble of the graphs $\{(t, M_t)\}_{T\leq t\leq N_0}$ representing the histories of the total magnetization on the (t, M)-plane as a light wave emitted from (T, M_T) in

the direction parallel to $(1, m_T)$. In the *wave* optics, when the wavelength of the light is non-negligible against the aperture of the light source, the flux of light is broadened as it propagates while the location of the maximum intensity goes along the "ray", $M_t = M_T + (t - T)m_T$ for $T \le t \le N_0$, according to the *geometrical* optics. Likewise, in the Progressive Quenching, the stochasticity causes diffusion of the trajectories around the mean history, $M_t = M_T + (t - T)m_T$ for $T \le t \le N_0$. While the broadening of the light flux grows linearly with distance from the source, the trajectories of Progressive Quenching will diffuses like $\sim (t - T)^{1/2}$ for $T \le t \le N_0$.

18. There are two types of markets – primary and secondary. When a company issues its shares, the process is called Initial Public Offering (IPO). Investors interested in buying the shares have to apply to procure the shares. In case there are more applications than the number of shares issued, applicants are chosen randomly. Selected applicants buy shares directly from the company. Stock exchanges have no part to play here. This is referred as the primary market. After the above process is complete, the company gets listed in the stock exchanges. Only after this can an investor trade (buy or sell) the stock of the company in the exchanges from another share holder. This is called the secondary market.
19. In the market, there are also speculators who unlike the hedgers like to take risks, by anticipating trends in the market and exploiting them to make profit [228].
20. Which will be here also the pointer basis.
21. This matrix is diagonal in the orthonormal basis $|\pm 1\rangle$; this is the meaning of the quantum non-demolition hypothesis here.
22. In mathematics, a set A is considered a subset of a set B, or, equivalently, B is a superset of A, if all elements of A are also elements of B.
23. We might appreciate this meaning from different facets: (1) When a pair of histories, ω and ω', realizes the identical set of data $X_{[0,n]}$, therefore also identical $\langle z|X_{[0,n]}\rangle$, it can occur that $z(\omega) \neq z(\omega')$. (2) When a history ω is given, $\langle z|X_{[0,n]}\rangle$ takes the average of z over all the histories $\{\omega'\}$ which share the same tata $X_{[0,n]}$. (3) z *can* be any function of n variables, $X_{[0,n]}$. Nevertheless, each of $X_{[0,n]}$ are *prefixed functions* of the history, being independent of z. While z is an object of observation, $X_{[0,n]}$ are the measureing apparatus for that. (4) Yet, z is not restricted to a linear combination of $X_{[0,n]}$ and, therefore, the functional subspace spanned by $\langle z|X_{[0,n]}\rangle$ is not n-dimensional.

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Appendix A. Appendix to Chapter 1

A.1. *Random walk between two absorbing boundaries*

Consider a random walker moving in discrete time steps on a one-dimensional lattice, with $X_t \in \{-L, -L+1, \ldots, L\}$ the sites of the lattice. At every discrete time step, the walker hops to its right-neighbor site with probability $0 \leq q \leq 1$ and to its left-neighbor site with a complementary probability $1-q$. The process terminates at the random time $\mathcal{T}$ when either $X_t = L$ or $X_t = -L$. This is the classical gambler's ruin problem, as formulated, for example, in Feller's treatise on probability theory [44]. Following Ref. [44], we determine here the splitting probabilities and mean-first passage time of the gambler's ruin problem, see also [8].

A.2. *Splitting probabilities*

We determine the probabilities $P_+(i)$ and $P_-(i)$ that the walker ends its excursion at $X_{\mathcal{T}} = L$ or $X_{\mathcal{T}} = -L$, respectively, given that the walker started its excursion from site $X_0 = i$.

The splitting probabilities satisfy the following recurrence equation:

$$P_-(i) = qP_-(i+1) + (1-q)P_-(i-1), \quad \text{for } i \in \{-L+1, -L+2, \ldots, L-1\}, \tag{A1}$$

with boundary conditions $P_-(-L) = 1$ and $P_-(L) = 0$. For $q \neq 1/2$, Equation (A1) admits solutions of the form $P_-(i) = \alpha^i$. Substitution in Equation (A1) gives $\alpha = q\alpha^2 + (1-q)$, which admits two solutions, $\alpha = 1$ and $\alpha = (1-q)/q$. Consequently,

$$P_-(i) = \alpha_0 + \beta_0 \left(\frac{1-q}{q}\right)^i \tag{A2}$$

where α_0 and β_0 are determined by the boundary conditions. Consequently,

$$P_-(i) = \frac{\left(\frac{1-q}{q}\right)^{2L} - \left(\frac{1-q}{q}\right)^{i+L}}{\left(\frac{1-q}{q}\right)^{2L} - 1} \tag{A3}$$

and analogously,

$$P_+(i) = \frac{\left(\frac{1-q}{q}\right)^{i+L} - 1}{\left(\frac{1-q}{q}\right)^{2L} - 1}. \tag{A4}$$

Note that since the solution to Equation (A1) with boundary conditions $P_-(-L) = 1$ and $P_-(L) = 0$ is unique, these are the expressions for the splitting probabilities.

For $q = 1/2$, we suggest a linear solution of the form

$$P_-(i) = \alpha_0 + \beta_0 i \tag{A5}$$

leading to

$$P_-(i) = 1 - \frac{i+L}{2L}. \tag{A6}$$

Equations (1.15) and (1.16) in the main text are obtained by setting $i = 0$ in Equations (A3)–(A6).

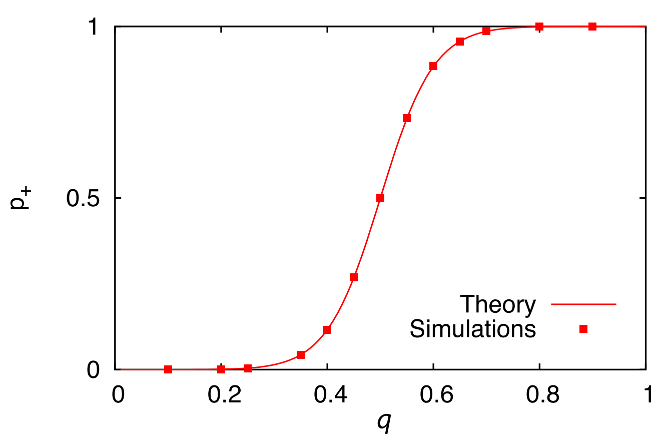

Figure A1. Comparing Equation (1.15) with results from simulations for $L = 5$. The data involve sampling 10^6 independent dynamical realizations.

A.3. *Mean first-passage time*

We determine the mean duration of the process, $\tau_i = \langle \mathcal{T} | X_0 = i \rangle$, which obey the recurrence relations

$$\tau_i = q\tau_{i+1} + (1-q)\tau_{i-1} + 1 \tag{A7}$$

with boundary conditions

$$\tau_{-L} = \tau_L = 0. \tag{A8}$$

For $q \neq 1/2$, the solution takes the form

$$\tau_i = \frac{i+L}{1-2q} + \alpha_0 + \beta_0 \left(\frac{1-q}{q}\right)^i \tag{A9}$$

Using the boundary conditions, we find

$$\tau_i = \frac{L+i}{1-2q} - \frac{2L}{1-2q} \frac{1-\left(\frac{1-q}{q}\right)^{i+L}}{1-\left(\frac{1-q}{q}\right)^{2L}} \tag{A10}$$

On the other hand, for $q = 1/2$ the solution takes a quadratic form

$$\tau_i = -i^2 + \alpha_0 + \beta_0 i, \tag{A11}$$

such that with boundary conditions

$$\tau_i = (i+L)(L-i). \tag{A12}$$

Equations (1.18) and (1.19) in the main text are obtained by setting $i = 0$ in Equations (A10) and (A12).

Appendix B. Appendix to Chapter 2

B.1. *A primer on probability theory*

Here, we provide a primer on probability theory, emphasizing in particular the elements that may prove to be both essential and useful in reading this review. For a more extensive treatise on probability theory within the ambit of quantitative finance, the reader is referred to Ref. [232]. While a physicist's notion of probability and measure may suffice to understand martingales, the rigorous mathematical foundation of probability theory, a glimpse of which is provided below, is absolutely necessary to comprehend scientific papers (regular postings may be found on the arXiv: https://arxiv.org/list/q-fin/new) and standard mathematical treatise on quantitative finance, i.e., Ref. [232]

B.1.1. *Probability space and σ-algebra*

In discussing probability, one talks about a random experiment or a random trial, namely, an experiment whose outcome is random, i.e., one gets in general a different outcome every time the experiment is repeated under identical conditions. Let Ω denote the sample space, i.e., the set of all possible elementary outcomes ω of the random trial. An event A is a subset[22] of Ω. The set of observable events is the collection $\mathcal{F}$ of subsets of Ω (conventionally called the family of subsets of Ω) with the following properties:

(1) $\emptyset \in \mathcal{F}$ and $\Omega \in \mathcal{F}$. Here, $\emptyset$ is the empty set, denoting the event "nothing happens", while Ω denotes the event "something happens".
(2) $A \in \mathcal{F} \implies A^c \in \mathcal{F}$, where A^c is the complement of A (if A is an event, "A does not happen" is also an event).
(3) $A_1, A_2, A_3, \ldots \in \mathcal{F} \implies \cup_i A_i \in \mathcal{F}$ (if a sequence of events can occur, then "at least one of them occurs" is also an event).

When the above properties are satisfied, $\mathcal{F}$ is said to form a σ-algebra on Ω. From the three properties, it follows that $A_1, A_2, A_3, \ldots \in \mathcal{F} \implies \cap_i A_i \in \mathcal{F}$. An element $A \in \mathcal{F}$ is called a measurable set or an observable event. The pair $(\Omega, \mathcal{F})$ forms the measure space.

Given a sample space Ω and a σ-algebra $\mathcal{F}$ on Ω, a probability measure is a function that assigns to each event $A \in \mathcal{F}$ a nonnegative real number ≤ 1. Specifically, a probability measure P is a function $P : \mathcal{F} \to [0, 1]$, such that

(1) $P(A) \geq 0 \; \forall A \in \mathcal{F}$,
(2) $P(\emptyset) = 0$ and $P(\Omega) = 1$, and
(3) For $A_1, A_2, \ldots \in \mathcal{F}$, if $A_i \cap A_j = \emptyset \forall i \neq j$, then $P(\cup_i A_i) = \sum_i P(A_i)$.

Altogether, the triple $(\Omega, \mathcal{F}, P)$ forms a probability space.

Let us consider an example:

- Random trial: Tossing a coin two times in a row.
- Sample space $\Omega = \{HH, TT, HT, TH\} = \{\omega_1, \omega_2, \omega_3, \omega_4\}$.
- Event: could be "getting identical result in the two throws": $A = \{\omega_1, \omega_2\}$.
- For $\mathcal{F}$, there are several possibilities:
  (1) The smallest σ-algebra: $\mathcal{F}_{\min} = \{\emptyset, \Omega\}$ (the events are "getting nothing" and "getting something"). $\mathcal{F}_{\min}$ contains what is known before the random trial is performed.
  (2) Another possibility: $\mathcal{F}_1 = \{\emptyset, \{\omega_1, \omega_2\}, \{\omega_3, \omega_4\}, \Omega\}$. $\mathcal{F}_1$ contains what can be observed after the first trial: whether the random trial gives identical or non-identical results for the two throws.
  (3) Another one: $\mathcal{F}_2 = \{\emptyset, \{\omega_3\}, \{\omega_4\}, \{\omega_1, \omega_2\}, \{\omega_3, \omega_4\}, \{\omega_1, \omega_2, \omega_4\}, \{\omega_1, \omega_2, \omega_3\}, \Omega\}$. $\mathcal{F}_2$ contains information on what can be observed after the second trial. Note that here, i.e., the element $\{\omega_3\}$ refers to the event "Observing *HT*", the element $\{\omega_1, \omega_2, \omega_4\}$ refers to observing the corresponding complement event, i.e., the event "Not observing *HT*". Here, we have assumed that $\mathcal{F}_s \subset \mathcal{F}_t$ for $s \leq t$, since a natural expectation is that with subsequent throws, we gain new information and do not discard the old ones.
  (4) The largest σ-algebra:

$$\mathcal{F}_{\max} = \{\emptyset, \{\omega_1\}, \{\omega_2\}, \{\omega_3\}, \{\omega_4\}, \{\omega_1, \omega_2\}, \{\omega_1, \omega_3\}, \{\omega_1, \omega_4\}, \{\omega_2, \omega_3\}, \{\omega_2, \omega_4\}, \{\omega_3, \omega_4\}, \{\omega_1, \omega_2, \omega_3\}, \{\omega_1, \omega_2, \omega_4\}, \{\omega_1, \omega_3, \omega_4\}, \{\omega_2, \omega_3, \omega_4\}, \Omega\}. \tag{B1}$$

  $\mathcal{F}_{\max}$ is the largest possible collection of events that can be observed on tossing a coin two times in a row.

Summarizing, we may think of a σ-algebra $\mathcal{F}$ as the amount of information contained in Ω that can be observed: The smaller the $\mathcal{F}$, the lesser is the amount of information we have of Ω.

From the above example, we see an illustration of the general result that the smallest σ-algebra $\mathcal{F}_{\min}$ consists of the empty set $\emptyset$ and the sample space Ω, while the largest σ-algebra $\mathcal{F}_{\max}$ consists of all subsets of Ω including the empty set and the set Ω itself ($\mathcal{F}_{\max}$ would conventionally be called the power set of Ω); note that the number of elements in $\mathcal{F}_{\max}$ is 2 raised to the power "number of elements in Ω", hence, one writes $\mathcal{F}_{\max} = 2^{\Omega}$. A σ-algebra $\mathcal{G}$ is a sub-σ-algebra of another σ-algebra $\mathcal{F}$ if $\mathcal{G} \subset \mathcal{F}$. In the above example of tossing a coin two times in a row, we have $\mathcal{F}_1 \subset \mathcal{F}_{\max}$.

B.1.2. *$\mathcal{F}$-measurability, random variables and stochastic processes*

We now discuss the concept of $\mathcal{F}$-measurability. Let $(\Omega, \mathcal{F}, P)$ be a probability space. A function $f : \Omega \to \mathbf{R}$ is said to be $\mathcal{F}$-measurable if to any given interval $(a, b) \in \mathbf{R}$ one can associate an event $A \in \mathcal{F}$. Consider throwing a die. Here, we have $\Omega = \{1, 2, 3, 4, 5, 6\}$. Next, consider the function $X \equiv X(\omega)$ that equals $+1$ if ω is either 1 or 3 or 5 and equals -1 if ω is either 2 or 4 or 6. Then, X is measurable with respect to the σ-algebra $\mathcal{F}_1 = \{\emptyset, \Omega, \{1, 3, 5\}, \{2, 4, 6\}\}$ but is not measurable with respect to the σ-algebra $\mathcal{F}_2 = \{\emptyset, \Omega, \{1, 2, 3\}, \{4, 5, 6\}\}$ or with respect to the σ-algebra $\mathcal{F}_3 = \{\emptyset, \Omega, \{1, 2\}, \{3, 4\}, \{5, 6\}\}$. A random variable X on a probability space $(\Omega, \mathcal{F}, P)$ is an $\mathcal{F}$-measurable function. A collection of random variables $\{X_t\}$ defined on the probability space $(\Omega, \mathcal{F}, P)$ and parametrized by the variable t is called a stochastic process. Taking t to be time, the stochastic process may be denoted as $\{X_t\}_{t \geq 0}$, or, when no confusion may arise, by simply X_t as in the Main Text.

B.1.3. *Filtration and adaptation*

Given a probability space $(\Omega, \mathcal{F}, P)$, a filtration is a collection $\{\mathcal{F}_t\}_{t \geq 0}$ of nested sub-σ-algebras of $\mathcal{F}$ such that $\mathcal{F}_s \subset \mathcal{F}_t$ for $0 \leq s \leq t$. The probability space with filtration $\{\mathcal{F}_t\}_{t \geq 0}$ is called the filtered probability space $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}, P)$. A stochastic process $\{X_t\}_{t \geq 0}$ defined on $(\Omega, \mathcal{F}, P)$ whose values can be completely determined from $\{\mathcal{F}_t\}_{t\geq 0}$ is said to be adapted to the filtration $\{\mathcal{F}_t\}_{t\geq 0}$. In other words, the process $\{X_t\}_{t\geq 0}$ is adapted to the filtration $\{\mathcal{F}_t\}_{t\geq 0}$ if X_t is $\mathcal{F}_t$-measurable for every $t \geq 0$. The natural filtration $\{\mathcal{F}_t^X\}_{t\geq 0}$ associated to a stochastic process $\{X_t\}_{t\geq 0}$ is a filtration that records the past behavior of the stochastic process at each time, i.e., the information contained in the trajectories $\{X_t\}$ up to time t. Thus, all information related to the process, and only that information, is available in the natural filtration. Note that $\{X_t\}_{t\geq 0}$ is obviously adapted to its natural filtration. The reader is referred to Ref. [271] in which several illustrative examples of filtration and adaptation are discussed.

B.1.4. *Conditional expectation*

Given a random variable X on a probability space $(\Omega, \mathcal{F}, P)$ and a sub-σ-algebra $\mathcal{F}' \subset \mathcal{F}$, one may define a new random variable as the conditional expectation of X:

$$Z \equiv \langle X|\mathcal{F}' \rangle, \tag{B2}$$

namely, the expected value of X, given the information contained in $\mathcal{F}'$, i.e., the conditional expectation. The conditional expectation satisfies $\langle X|\mathcal{F}\rangle = X$ if X is $\mathcal{F}$-measurable, and the property of iterated conditioning [232] given by $\langle\langle X|\mathcal{F}\rangle\rangle = \langle X\rangle$.

In more practical terms, for two discrete random variables X and Y, the conditional probability distribution of X given Y is the probability distribution of X when Y is known to have a particular value. Thus the conditional probability distribution of X given $Y = y$ is given by the Bayes' theorem from probability theory:

$$P(X = x|Y = y) = \frac{P_{X,Y}(x, y)}{P_Y(y)}. \tag{B3}$$

Here, $P_{X,Y}(x, y)$ is the joint distribution of the random variables X and Y, while $P_Y(y)$ is the probability distribution of the random variable Y alone. The definition in Equation (B3) holds also for continuous random variables. Considering the case of continuous random variables, we then have the conditional expectation

$$\langle X|Y\rangle = \int \mathrm{d}x\, xP(X = x|Y = y), \tag{B4}$$

so that

$$\begin{aligned}\langle\langle X|Y\rangle\rangle &= \int \mathrm{d}y\, P_Y(y) \int \mathrm{d}x\, xP(X = x|Y = y)\\ &= \int \mathrm{d}x\, x \int \mathrm{d}y\, P_{X,Y}(x, y)\\ &= \int \mathrm{d}x\, xP_X(x)\\ &= \langle X\rangle.\end{aligned} \tag{B5}$$

Here, in obtaining the second step, we have used Equation (B3).

B.2. *Tower rule*

In Section 2.1.3 we introduced the *conditional-expectation process* as a key example of martingale. For this route to the martingale the core is the *tower property*,

$$\langle\langle Z|X_{[0,n]}\rangle|X_{[0,m]}\rangle = \langle Z|X_{[0,m]}\rangle \quad 0 \leq m \leq n.$$

In the main text $Z = X_q$ $(q \geq n)$ has been taken, but Z can be any random variable whose statistical character is given once $X_{[0,m]}$ is known. See, for example, Chapter 10.

B.2.1. *Elementary tower rule*

We first recall Equation (B5) in Section B.1.4, that we write

$$\langle\, \langle Z|X \rangle\, \rangle = \langle Z \rangle. \tag{B6}$$

The fact that the conditional expectation $\langle Z|X\rangle$ is found at the inside of another expectation implies that X is also a random variable. In other words, the value of the condition $X = x$ occurs according to the probability of X, that is $\rho_X(x)$. The outer expectation is taken according to such probability distribution.

B.2.2. *Higher order tower rule*

We can immediately extend the above rule to a higher order Tower Rule,

$$\langle\, \langle Z|\, X_{[0,n]}\rangle | X_{[0,m]}\rangle = \langle Z|X_{[0,m]}\rangle, \quad 0 \le m \le n, \tag{B7}$$

where we have used the abbreviation $X_{[0,m]} = X_0, X_1, \dots, X_m$, etc., for the sequence of random variables with consecutive discrete time. Below we shall also abuse this notation for $x_{[0,m]} = x_0, x_1, \dots, x_m$, etc. The demonstration is done in the same line as (B6):

$$\begin{aligned}
\langle\, \langle Z|X_{[0,n]}\rangle \big|\, X_{[0,m]}\rangle &= \sum_{x_{[m+1,n]}} \langle Z|X_{[0,m]}, x_{[m+1,n]}\rangle \mathcal{P}_{X_{[m+1,n]}|X_{[0,m]}}(x_{[m+1,n]}|X_{[0,m]}) \\
&= \sum_{x_{[m+1,n]}} \left(\sum_z z \mathcal{P}_{Z|X_{[0,n]}}(z|X_{[0,m]}, x_{[m+1,n]}) \right) \mathcal{P}_{X_{[m+1,n]}|X_{[0,m]}}(x_{[m+1,n]}|X_{[0,m]}) \\
&= \sum_{x_{[m+1,n]}} \sum_z z \mathcal{P}_{X_{[m+1,n]},Z|X_{[0,m]}}(x_{[m+1,n]}, z|X_{[0,m]}) \\
&= \sum_z z \mathcal{P}_{Z|X_{[0,m]}}(z|X_{[0,m]}) = \langle Z|X_{[0,m]}\rangle,
\end{aligned} \tag{B8}$$

where we have used

$$\begin{aligned}
&\mathcal{P}_{Z|X_{[0,n]}}(z|X_{[0,m]}, x_{[m+1,n]}) \mathcal{P}_{X_{[m+1,n]}|X_{[0,m]}}(x_{[m+1,n]}|X_{[0,m]}) \\
&\quad = \frac{\mathcal{P}_{X_{[0,n]},Z}(X_{[0,m]}, x_{[m+1,n]}, z)}{\mathcal{P}_{X_{[0,n]}}(X_{[0,m]}, x_{[m+1,n]})} \frac{\mathcal{P}_{X_{[0,n]}}(X_{[0,m]}, x_{[m+1,n]})}{\mathcal{P}_{X_{[0,m]}}(X_{[0,m]})} \\
&\quad = \mathcal{P}_{X_{[m+1,n]},Z|X_{[0,m]}}(x_{[m+1,n]}, z|X_{[0,m]})
\end{aligned} \tag{B9}$$

and $\sum_{x_{[m+1,n]}} \mathcal{P}_{X_{[0,n]},Z}(X_{[0,m]}, x_{[m+1,n]}, z) = \mathcal{P}_{X_{[0,m]},Z}(X_{[0,m]}, z)$. It is worth noting the similarity of this derivation to the one for the martingality of the ratio of path probability densities, see (2.19). In fact both have the common origin in the inclusively ordered series of conditional probabilities, or, the ordered structure of the filtration, see Section B.1.3. In other words, behind these generic ways to make martingale processes, i.e., by the path probability ratios and by the higher order tower rule, there lies the tower rule for the conditional probability *function*.

We illustrate intuitively the tower property or tower-rule of the conditional expectation (B7). We hope this illustration helps a little for demystifying the martingale. Let z be a random variable (RV), that is, a function of the elementary event which we regard to be a sample history. In Figure B1, we schematize by the 3D space the functional space on the elementary events. For example, the RV, z, is a vector. When X_k's represents the value of an observable X at time k, it is also a function of the history, therefore, of the elementary event. Then the expectation $\langle z|X_{[0,n]}\rangle$ is also the function of the elementary event but through $X_1, \dots, X_n$. However, being different from z this expectation spans only a subspace of the whole functional space, which we symbolize by the 2D bottom plane in Figure B1. Then $\langle z|X_{[0,n]}\rangle$ is said to be the orthogonal projection of z onto the sub-space associated with $X_{[0,n]}$. Then it is understandable that $\langle z|X_{[0,m]}\rangle$ with $m < n$ as function of elementary event finds itself in the (further) sub-space associated with $(X_{[0,m]})$, which we schematize by an 1D edge in Figure B1.

Physically speaking we interpret $\langle z|X_{[0,n]}\rangle$ as a coarse-grained version of z as function of sample history such that its value is determined only through n data, $X_{[0,n]}$.[23] It is understandable that $\langle z|X_{[0,m]}\rangle$ with

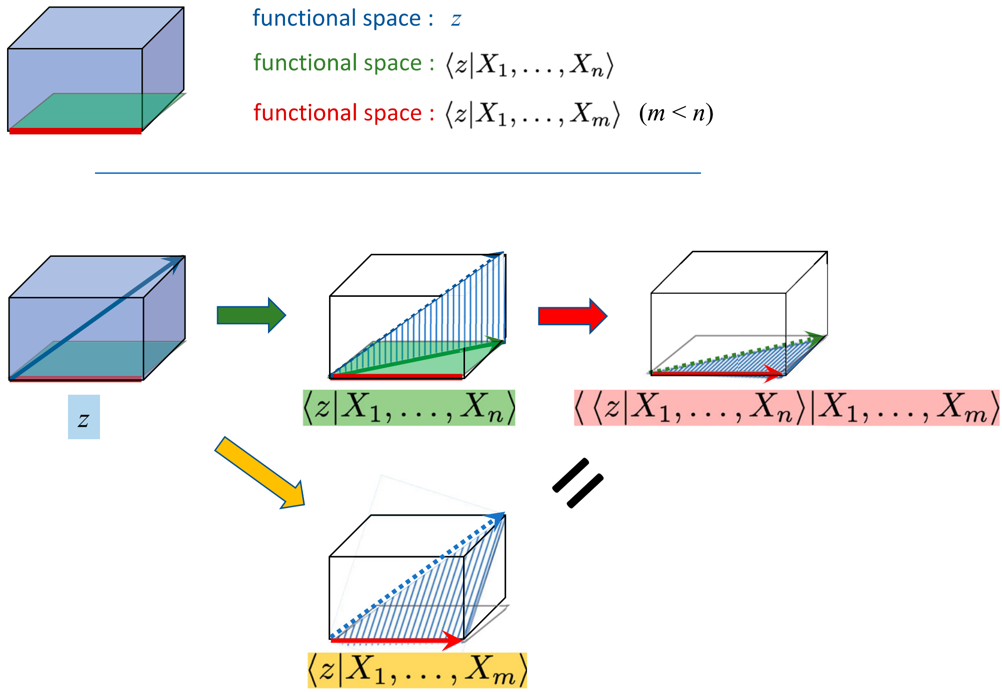

Figure B1. Schematic illustration of the tower property of the conditional expectation.

$m<n$ is even more coarse-grained than $\langle z|X_{[0,n]}\rangle$. Now the tower property or tower rule is nothing but an elementary extension of the *theorem of three perpendiculars* in Euclidean geometry, which claims that the orthogonal projection through an intermediate orthogonal projection is identical to the one obtained by the direct projection. In the present context, the coarse-grained observation of z through the data set, $X_{[0,m]}$, can be either obtained directly, $\langle z|X_{[0,m]}\rangle$, or passing through an intermediate version, $\langle z|X_{[0,n]}\rangle$ with $t>s$. In equation,

$$\langle z|X_{[0,m]}\rangle = \langle\,\langle z|X_{[0,n]}\rangle\,|\,X_{[0,m]}\rangle,$$

the martingale $M_m = \langle M_n\,|\,X_{[0,m]}\rangle$ emerges if we regard $M_n = \langle z|X_{[0,n]}\rangle$ as a process associated to the process $X_{[0,n]}$.

B.3. *Basics of stochastic calculus*

Let X_t be a stochastic process that obeys a stochastic differential equation. What is the stochastic differential equation of the process $Y_t = g(X_t)$, where g is a twice continuously, differentiable function? The rules of stochastic calculus, which we review here, provide a solution to this problem.

We first review the rules of stochastic calculus for the simplest case of a one-dimensional Itô process in Section B.3.1, and subsequently we consider the case of multi-dimensional Itô processes and semimartingales, which is loosely defined as any stochastic process that is a good integrator for the Itô integral, in Sections B.3.2 and B.3.3. Lastly, in Section B.3.4, we review how to express an Itô integral in terms of a Stratonovich integral. We follow the references [64,70].

B.3.1. *Itô's formula*

Let $X_t \in \mathbb{R}$ be a stochastic process that solves a stochastic differential equation of the form

$$\dot{X}_t = b_t(X_{[0,t]}) + \sigma_t(X_{[0,t]})\dot{B}_t, \tag{B10}$$

where B_t is the one-dimensional Brownian motion, as defined in Section 2.2.2, and where

$$\mathcal{P}\left(\int_0^t \mathrm{d}s\sigma_s^2(X_{[0,s]}) < \infty, \quad \forall t \geq 0\right) = 1 \tag{B11}$$

and

$$\mathcal{P}\left(\int_0^t \mathrm{d}s|b_s(X_{[0,s]})| < \infty, \quad \forall t \geq 0\right) = 1. \tag{B12}$$

Let $g(t,x)$ be a twice continuously differentiable function in $t \in \mathbb{R}^+$ and $x \in \mathbb{R}$, then the process

$$Y_t = g(t, X_t) \tag{B13}$$

solves the stochastic differential equation [64]

$$\dot{Y}_t = \frac{\partial g}{\partial t}(t, X_t) + \frac{\partial g}{\partial x}\dot{X}_t + D_t(X_{[0,t]})\frac{\partial^2 g}{(\partial x)^2}(t, X_t), \tag{B14}$$

where

$$D_t = \frac{\sigma_t^2}{2}. \tag{B15}$$

Itô's formula can be understood from a Taylor expansion of $g(t + \mathrm{d}t, X_{t+\mathrm{d}t})$, viz.,

$$g(t + \mathrm{d}t, X_{t+\mathrm{d}t}) - g(t, X_t) = \frac{\partial g}{\partial t}\mathrm{d}t + \frac{\partial g}{\partial x}\mathrm{d}X_t + \frac{1}{2}\frac{\partial^2 g}{\partial t^2}(\mathrm{d}t)^2 + \frac{1}{2}\frac{\partial^2 g}{(\partial x)^2}(\mathrm{d}X_t)^2 + \frac{1}{2}\frac{\partial^2 g}{\partial t\partial x}\mathrm{d}t\mathrm{d}X_t + \cdots, \tag{B16}$$

Neglecting contributions of the order $O((\mathrm{d}t)^2)$, and using $\mathrm{d}X_t = \dot{X}_t\mathrm{d}t$ with X_t solving Equation (B10), we obtain

$$g(t + \mathrm{d}t, X_{t+\mathrm{d}t}) - g(t, X_t) = \frac{\partial g}{\partial t}\mathrm{d}t + \frac{\partial g}{\partial x}\mathrm{d}X_t + \frac{\partial^2 g}{(\partial x)^2}b_t\sigma_t\mathrm{d}t\mathrm{d}B_t + \frac{1}{2}\frac{\partial^2 g}{(\partial x)^2}\sigma_t^2(\mathrm{d}B_t)^2 + O((\mathrm{d}t)^2). \tag{B17}$$

Using in Equation (B17) that $\mathrm{d}t\mathrm{d}B_t \in o(\mathrm{d}t)$ and $(\mathrm{d}B_t)^2 = \mathrm{d}t$, we readily obtain the Itô formula (B14) after neglecting $o(\mathrm{d}t)$ terms.

To show that $(\mathrm{d}B_t)^2 = \mathrm{d}t$, we determine the probability distribution of $(\mathrm{d}B_t)^2$, see also Ref. [272]. The distribution of $\mathrm{d}B_t$ is a normal distribution with zero mean and variance $\mathrm{d}t$, i.e.,

$$\rho_{\mathrm{d}B_t}(x) = \frac{1}{\sqrt{2\pi\,\mathrm{d}t}}\exp\left(-\frac{x^2}{2\mathrm{d}t}\right). \tag{B18}$$

Consequently, we obtain for the distribution of $(\mathrm{d}B_t)^2$,

$$\rho_{(\mathrm{d}B_t)^2}(y) = \frac{1}{\sqrt{2\pi\,\mathrm{d}t}}\int_{-\infty}^{\infty}\mathrm{d}x\exp\left(-\frac{x^2}{2\mathrm{d}t}\right)\delta(y - x^2) = \frac{1}{\sqrt{2\pi\,\mathrm{d}t}}\frac{1}{\sqrt{y}}\exp\left(-\frac{y}{2\mathrm{d}t}\right). \tag{B19}$$

In the limit of $\mathrm{d}t \to 0$ it holds that $(\mathrm{d}B_t)^2 = \mathrm{d}t$. Indeed, the average $\langle(\mathrm{d}B_t)^2\rangle = \mathrm{d}t$ and $\langle(\mathrm{d}B_t)^4\rangle = 3(\mathrm{d}t)^2$, so that its variance is negligible.

B.3.2. *Multidimensional Itô formula*

We review the generalization of the Itô formula Equation (B14) to the multidimensional case.

Consider now

$$\dot{X}_t = b_t(X_{[0,t]}) + \sigma_t(X_{[0,t]})\dot{B}_t \tag{B20}$$

where $b_t = (b_t^1, b_t^2, \ldots, b_t^d)^\dagger \in \mathbb{R}^d$, where $\sigma_t \in \mathbb{R}^d \times \mathbb{R}^m$ is a matrix with entries σ_t^{ij} where $i = 1, 2, \ldots, d$ and $j = 1, 2, \ldots, m$; and where $B_t = (B_t^1, B_t^2, \ldots, B_t^m)$ is a vector of m independent Brownian motions.

We require that each of the individual b_t^i satisfy Equation (B12) and each of the individual σ_t^{ij} satisfy Equation (B11).

Let

$$Y_t = g(t, X_t), \tag{B21}$$

where $Y_t \in \mathbb{R}$ and where g is twice, continuously differentiable. It then holds that

$$\dot{Y}_t = \frac{\partial g}{\partial t}(t, X_t) + \sum_{i=1}^{d} \frac{\partial g}{\partial x_i}\dot{X}_t^i + \frac{1}{2}\sum_{i,j}\frac{\partial^2 g}{\partial x_i \partial x_j}\dot{X}_t^i \dot{X}_t^j, \tag{B22}$$

where $\dot{X}_t^i \dot{X}_t^j$ follows from applying the rules

$$\dot{B}_i \dot{B}_j = \delta_{i,j}\mathrm{d}t, \quad \dot{B}_i \mathrm{d}t = 0, \quad (\mathrm{d}t)^2 = 0 \tag{B23}$$

to Equation (B20).

B.3.3. *Meyer–Itô formula for semimartingales*

We review the Itô formula for so-called semimartingales X, which are stochastic processes that form good integrators of the Itô integral [70]. According to the Bichteler–Dellacherie theorem, a semimartingale can be decomposed into a local martingale (L) and a finite variation process (A) [70], viz.,

$$X_t = A_t + L_t. \tag{B24}$$

A process A_t is a finite variation process if with probability 1 the paths of A have a finite total variation $\sup_P \sum_{i=0}^{n-1} |A_{t_i} - A_{t_{i-1}}|$ on each compact interval $[0, t]$, where P is a finite partition of $[0, t]$, as defined in Section 2.2.2. Note that differently from Itô processes, semi-martingales may contain jumps; examples of semi-martingales are Itô processes, (inhomogeneous) Poisson processes, Lévy processes [273], and cádlág (right-continuous in t and with existing left limits) martingales and submartingales. The fractional Brownian motion is an example of a stochastic process that is not a semi-martingale, and hence the Itó integral does not exist for the latter [274].

Let us assume for simplicity that $X \in \mathbb{R}$, and let g be again a twice, continuously differentiable function, and consider

$$Y_t = g(t, X_t). \tag{B25}$$

It then holds that

$$\begin{aligned} Y_t - Y_0 = {} & \int_0^t (\partial_t g)(X_s)\mathrm{d}s + \int_{0^+}^t \frac{\mathrm{d}g}{\mathrm{d}x}(X_{s^-})\mathrm{d}X_s + \frac{1}{2}\int_0^t \frac{\mathrm{d}^2 g}{(\mathrm{d}x)^2}(X_{s^-})\mathrm{d}[X, X]_s^{\mathrm{c}} \\ & + \sum_{j=1}^{N_t}\left(g(X_{\mathcal{T}_j^+}) - g(X_{\mathcal{T}_j^-}) - \frac{\mathrm{d}g}{\mathrm{d}x}\left(X_{\mathcal{T}_j^-}\right)\left(X_{\mathcal{T}_j^+} - X_{\mathcal{T}_j^-}\right)\right), \end{aligned} \tag{B26}$$

where $[X, X]_s^{\mathrm{c}}$ is the continuous part of the quadratic variation $[X, X]$, defined in Equation (2.71), N_t denotes the number of jumps in the interval $[0, t]$, and $\mathcal{T}_j$ are the jump times (this is the same notation as used for Markov jump processes in Section 3.2.2).

In the particular case of an Itô process of the form (B10), $N_t = 0$ and

$$[X, X]_t^c = \int_0^t D_s \mathrm{d}s, \tag{B27}$$

and we recover Itô's formula (B14).

On the other hand, for a pure jump process,

$$[X,X]^c_t = 0, \tag{B28}$$

and

$$\int_{0^+}^t \frac{\mathrm{d}g}{\mathrm{d}x}(X_{s^-})\mathrm{d}X_s = \sum_{j=1}^{N_t} \frac{\mathrm{d}g}{\mathrm{d}x}\left(X_{\mathcal{T}_j^-}\right)\left(X_{\mathcal{T}_j^+} - X_{\mathcal{T}_j^-}\right) \tag{B29}$$

so that

$$Y_t - Y_0 = \int_0^t (\partial_t g)(X_s)\mathrm{d}s + \sum_{j=1}^{N_t}\left(g(X_{\mathcal{T}_j^+}) - g(X_{\mathcal{T}_j^-})\right). \tag{B30}$$

B.3.4. *Stratonovich integrals*

We revise here a generalization of Theorem 1 to semimartingales. Let $Y_t \in \mathbb{R}$ and $Z_t \in \mathbb{R}$ represent two semimartingales. Then, the following conversion formula holds [70]:

$$\int_0^t Z_{s^-} \circ \mathrm{d}Y_s = \int_0^t Z_{s^-}\mathrm{d}Y_s + \frac{1}{2}[Z,Y]^{\mathrm{c}}_t, \tag{B31}$$

where the left-hand side contains a Stratonovich integral and the right-hand side an Itô integral, see Equations (2.83) and (2.69) for definitions, and where $[X,Y]^{\mathrm{c}}_t$ is the continuous part of the covariation

$$[Z_t, Y_t] \equiv \lim_{\|P\|\to 0} \sum_{i=0}^{n-1}\left(Z_{t_i} - Z_{t_{i-1}}\right)\left(Y_{t_i} - Y_{t_{i-1}}\right). \tag{B32}$$

Let us consider the example for which Y and Z are Itô processes of the form

$$\dot{Y} = b^{(Y)}_t(X_{[0,t]}) + \sigma^{(Y)}(X_{[0,t]})\dot{B}_t \tag{B33}$$

and

$$\dot{Z} = b^{(Z)}_t(X_{[0,t]}) + \sigma^{(Z)}(X_{[0,t]})\dot{B}_t, \tag{B34}$$

where X solves Equation (B10). In this case, we obtain the quadratic covariation process by using the rules $(\mathrm{d}B_t)^2 = \mathrm{d}t$, $\mathrm{d}t\mathrm{d}B_t = 0$, and $(dt)^2 = 0$, yielding

$$[Y_t, Z_t]^{\mathrm{c}} = [Y_t, Z_t] = \int_0^t \sigma^{(Y)}(X_{[0,s]})\sigma^{(Z)}(X_{[0,s]})\mathrm{d}s. \tag{B35}$$

On the other hand, if Y and Z are pure jump processes, then

$$[Y_t, Z_t]^{\mathrm{c}} = 0 \tag{B36}$$

and the Stratonovich integral equals the Itô integral.

B.4. *Stochastic exponential for a simple random walk*

We show that the process equations (2.23) and (2.59) are martingales.

B.4.1. *Discrete time*

To show that the process $\mathcal{E}_n(z)$ given by Equation (2.23) is a martingale, we use that $\mathcal{E}_n(z)$ is a ratio of two probability densities R_n of the form (2.18).

The probability density of a trajectory $X_{[0,n]}$ is given by

$$\mathcal{P}(X_{[0,n]}) = \prod_{i=1}^{n} \left((1-q)\delta_{X_i - X_{i-1},-1} + q\delta_{X_i - X_{i-1},1}\right). \tag{B37}$$

Analogously, we can define the density

$$\mathcal{Q}(X_{[0,n]}) = \prod_{i=1}^{n} \left((1-\tilde{q})\delta_{X_i - X_{i-1},-1} + \tilde{q}\delta_{X_i - X_{i-1},1}\right). \tag{B38}$$

Hence, the ratio of $\mathcal{P}(X_{[0,n]})$ and $\mathcal{Q}(X_{[0,n]})$ is given by

$$R_n = \frac{\mathcal{Q}(X_{[0,n]})}{\mathcal{P}(X_{[0,n]})} = \exp(y(q,\tilde{q})X_n + z(q,\tilde{q})n), \tag{B39}$$

with

$$y(q,\tilde{q}) \equiv \frac{1}{2}\ln\left(\frac{(1-q)\tilde{q}}{q(1-\tilde{q})}\right), \quad z(q,\tilde{q}) \equiv \frac{1}{2}\ln\left(\frac{\tilde{q}(1-\tilde{q})}{q(1-q)}\right). \tag{B40}$$

Solving the first equation towards $\tilde{q}$, we obtain

$$\tilde{q} = \frac{q\exp(2y)}{1-q+q\exp(2y)}, \tag{B41}$$

and thus

$$z(q,\tilde{q}(y)) = \frac{1}{2}\ln\left(\frac{\exp(2y)}{[(1-q)+q\exp(2y)]^2}\right) = y - \ln[(1-q)+\exp(2y)q]. \tag{B42}$$

Substituting z in (B39) and writing everything as a function of y we obtain (2.23).

B.4.2. *Continuous time*

Using that

$$\langle \exp(z(B_t - B_s)) | B_{[0,s]} \rangle = \langle \exp(z(B_t - B_s)) \rangle = \exp\left(\frac{z^2}{2}(t-s)\right), \tag{B43}$$

we obtain

$$\left\langle \exp\left(zB_t - \frac{z^2 t}{2}\right) \middle| B_{[0,s]} \right\rangle = \exp\left(zB_s - \frac{z^2 s}{2}\right). \tag{B44}$$

Appendix C. Appendix to Chapter 5

C.1. *Derivation of Equation (5.26)*

The stochastic differential equation for $\dot{S}_t^{\mathrm{tot}}$, given by Equation (5.20), contains the Stratonovich integral S_t that solves

$$\dot{S}_t = \frac{J_{t,\rho}(X_t)}{\mu T \rho_t(X_t)} \circ \dot{X}_t, \tag{C1}$$

where $\dot{X}_t$ solves Equation (5.3), and thus

$$\dot{S}_t = \frac{F_t(X_t) J_{t,\rho}(X_t)}{T\rho_t(X_t)} + \left(\sqrt{\frac{2}{\mu T}} \frac{J_{t,\rho}(X_t)}{\rho_t(X_t)}\right) \circ \dot{B}_t, \tag{C2}$$

where F_t is the total force, as defined in Equation (5.9).

Using equations (B31), (C2) can be expressed as an Itô stochastic differential equation,

$$\dot{S}_t = \frac{F_t(X_t)J_{t,\rho}(X_t)}{T\rho_t(X_t)} + \left(\sqrt{\frac{2}{\mu T}}\frac{J_{t,\rho}(X_t)}{\rho_t(X_t)}\right)\dot{B}_t + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}[Z,B]_t, \tag{C3}$$

where

$$Z_t = \sqrt{\frac{2}{\mu T}}\frac{J_{t,\rho}(X_t)}{\rho_t(X_t)}, \tag{C4}$$

and we have used that for a continuous process $[Z,B]^{\mathrm{c}}_t = [Z,B]_t$. The quadratic covariation is given in Equation (B35), where $\sigma_t^{(B)} = 1$ and $\sigma_t^{(Z)}$ is the coefficient in front of the noise term of $\dot{Z}_t$. We obtain $\dot{Z}_t$ by applying Itô's formula (B14) to Z, yielding

$$\dot{Z}_t = \sqrt{\frac{2}{\mu T}}\frac{\left(\partial_x J_{t,\rho}\right)(X_t)}{\rho_t(X_t)}\dot{X} - \sqrt{\frac{2}{\mu T}}\frac{(\partial_x\rho_t)(X_t)J_{t,\rho}(X_t)}{\rho_t^2(X_t)}\dot{X} + \cdots, \tag{C5}$$

where we omitted the $\partial_t g$ and $D\partial_x^2 g$ terms in Itô's formula as they do not contain a noise term and hence do not contribute to $\sigma_t^{(Z)}$. Using Equation (5.3) in Equation (C5), we find

$$\dot{Z}_t = 2\left(\frac{\left(\partial_x J_{t,\rho}\right)(X_t)}{\rho_t(X_t)} - \frac{(\partial_x\rho_t)(X_t)J_{t,\rho}(X_t)}{\rho_t^2(X_t)}\right)\dot{B}_t + \cdots, \tag{C6}$$

where we identify

$$\sigma_t^{(Z)} = 2\left(\frac{\left(\partial_x J_{t,\rho}\right)(X_t)}{\rho_t(X_t)} - \frac{(\partial_x\rho_t)(X_t)J_{t,\rho}(X_t)}{\rho_t^2(X_t)}\right). \tag{C7}$$

Further using Equations (5.12) and (5.13), this yields

$$\sigma_t^{(Z)} = 2\left(-\frac{(\partial_t\rho_t)(X_t)}{\rho_t(X_t)} + \frac{J^2_{t,\rho}(X_t)}{\mu T\rho_t^2(X_t)} - \frac{F_t(X_t)J_{t,\rho}(X_t)}{T\rho_t(X_t)}\right). \tag{C8}$$

Hence,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}[Z,B]_t = -\frac{(\partial_t\rho_t)(X_t)}{\rho_t(X_t)} + \frac{J^2_{t,\rho}(X_t)}{\mu T\rho_t^2(X_t)} - \frac{F_t(X_t)J_{t,\rho}(X_t)}{T\rho_t(X_t)} \tag{C9}$$

and substituting in Equation (C3) gives

$$\dot{S}_t = \frac{J_{t,\rho}(X_t)}{\mu T\rho_t(X_t)}\circ\dot{X}_t = -\frac{(\partial_t\rho_t)(X_t)}{\rho_t(X_t)} + \frac{J^2_{t,\rho}(X_t)}{\mu T\rho_t^2(X_t)} + \left(\sqrt{\frac{2}{\mu T}}\frac{J_{t,\rho}(X_t)}{\rho_t(X_t)}\right)\dot{B}_t. \tag{C10}$$

Using Equation (C10) in Equation (5.20), we readily obtain Equation (5.26).

C.2. *Derivation of the inequality in Equation (5.90)*

We derive the inequality in Equation (5.90), namely, we show that

$$\sum_{(x,y)\in\mathcal{X}^2}\rho_t(x)\omega_t(x,y)\ln\left(\frac{\rho_t(x)\omega_t(x,y)}{\rho_t(y)\omega_t(y,x)}\right) \geq 0. \tag{C11}$$

The inequality follows from the nonnegativity of the Kullback–Leibler divergence

$$D(p||q) = \sum_{x\in\mathcal{S}}p(x)\ln\frac{p(x)}{q(x)} \geq 0, \tag{C12}$$

where $q(x), p(x) \geq 0$,

$$\sum_{x\in\mathcal{X}}p(x) = \sum_{x\in\mathcal{X}}q(x) = 1, \tag{C13}$$

and $\mathcal{X}$ is a finite set, see, for example Ref. [142].

Defining

$$\mathcal{N} = \sum_{(x',y')\in\mathcal{X}^2} \rho_t(x')\omega_t(x',y') > 0, \tag{C14}$$

the left-hand side of Equation (C15) can be written as

$$\sum_{(x,y)\in\mathcal{X}^2} \rho_t(x)\omega_t(x,y)\ln\left(\frac{\rho_t(x)\omega_t(x,y)}{\rho_t(y)\omega_t(y,x)}\right) = \mathcal{N}\sum_{(x,y)\in\mathcal{X}^2} \frac{\rho_t(x)\omega(x,y)}{\mathcal{N}}\ln\left(\frac{\rho_t(x)\omega_t(x,y)/\mathcal{N}}{\rho_t(y)\omega_t(y,x)/\mathcal{N}}\right). \tag{C15}$$

Identifying the two functions

$$p(x,y) = \frac{\rho_t(x)\omega_t(x,y)}{\mathcal{N}} \quad \text{and} \quad q(x,y) = \frac{\rho_t(y)\omega_t(y,x)}{\mathcal{N}}, \tag{C16}$$

equation (C15) reads

$$\sum_{(x,y)\in\mathcal{X}^2} \rho_t(x)\omega_t(x,y)\ln\left(\frac{\rho_t(x)\omega_t(x,y)}{\rho_t(y)\omega_t(y,x)}\right) = \mathcal{N}D(p||q) \geq 0. \tag{C17}$$

C.3. *Time independence of the time-reversed Lagrangian in the case of Markov jump processes*

We complete the derivation of the martingale property of $\exp(-S_t^{\text{tot}})$ in Section 5.4.1.2 by showing that $\mathcal{P}[\Theta_t(X_{[0,t]})]$ is not explicitly dependent on time, and hence we can write $\mathcal{P}[\Theta_t(X_{[0,t]})] = \mathcal{Q}[X_{[0,t]}]$ for a certain measure $\mathcal{Q}$. To this purpose, we show that the Lagrangian of $\mathcal{P}[\Theta_t(X_{[0,t]})]$ contains no explicit time dependency on t – see Equation (3.97) for the definition of a Lagrangian.

Indeed, Equation (5.98) can be written as

$$\begin{aligned}
\mathcal{P}\left(\Theta_t\left(X_{[0,t]}\right)\right) &= \frac{1}{\mathcal{N}}\rho_{st}\left(X_t\right)\exp\left(\sum_{i=1}^{N_t}\ln\left(w\left(X_{\mathcal{T}_i^+},X_{\mathcal{T}_i^-}\right)\right) - \int_0^t \lambda(X_s)\mathrm{d}s\right) \\
&= \frac{1}{\mathcal{N}}\rho_{st}\left(X_0\right)\exp\left(\sum_{i=1}^{N_t}\ln\left(\frac{\rho_{st}\left(X_{\mathcal{T}_i^+}\right)w\left(X_{\mathcal{T}_i^+},X_{\mathcal{T}_i^-}\right)}{\rho_{st}\left(X_{\mathcal{T}_i^-}\right)}\right) - \int_0^t \lambda(X_s)\mathrm{d}s\right) \\
&= \frac{1}{\mathcal{N}}\rho_{st}\left(X_0\right)\exp\left(-\int_0^t\left\{-\sum_{x,y}\ln\left(\frac{\rho_{st}\left(y\right)w\left(y,x\right)}{\rho_{st}\left(x\right)}\right)\dot{N}_s(x,y) + \lambda(X_s)\right\}\mathrm{d}s\right),
\end{aligned}$$

where in the last line we have used $\dot{N}_s(x,y)$ to denote the rate of change of the jump process, as defined in Equation (3.50).

Then, the Lagrangian transforms under time reversal as

$$(\Theta_t\mathcal{L})\left[X_s,\dot{N}_s\right] = -\sum_{x,y}\ln\left(\frac{\rho_{st}\left(y\right)w\left(y,x\right)}{\rho_{st}\left(x\right)}\right)\dot{N}_s(x,y) + \lambda(X_s).$$

The absence of an explicit t-dependence in the right-hand side of the last relation implies that the measure $\mathcal{P}\circ\theta_t$ has no explicit t-dependency.

C.4. *Exponentiated negative entropy production as an Itô integral for stationary Markov jump processes*

We derive the stochastic differential Equation (5.100) presented in Section 5.4.1.3 that describes the evolution in time of $\exp(-S_t^{\text{tot}})$, with M_t given by Equation (5.101).

Since X is a jump process, the rules for stochastic calculus as discussed in Appendix B.3 apply, in particular Equation (B30) implies in a differential form that

$$\frac{\mathrm{d}\exp(-S_t^{\mathrm{tot}})}{\mathrm{d}t} = \sum_{x\in\mathcal{X}\setminus\{X_{t^-}\}} \left(\exp(-S_t^{\mathrm{tot}}) - \exp(-S_{t-}^{\mathrm{tot}})\right) \dot{N}_t(X_{t^-},x)$$
$$= \exp(-S_{t-}^{\mathrm{tot}}) \sum_{x\in\mathcal{X}\setminus\{X_{t^-}\}} \left(\frac{\rho_{\mathrm{st}}(x)\omega(x,X_{t^-})}{\rho_{\mathrm{st}}(X_{t^-})\omega(X_{t^-},x)} - 1\right) \dot{N}_t(X_{t^-},x). \tag{C18}$$

Subsequently, we write the stationarity condition (5.93) as

$$\sum_{x\in\mathcal{X};x\neq y} (\rho_{\mathrm{st}}(x)\omega(x,y) - \rho_{\mathrm{st}}(y)\omega(y,x)) = \rho_{\mathrm{st}}(y) \sum_{x\in\mathcal{X};x\neq y} \left(\frac{\rho_{\mathrm{st}}(x)\omega(x,y)}{\rho_{\mathrm{st}}(y)\omega(y,x)} - 1\right) \omega(y,x) = 0. \tag{C19}$$

Using the latter equation for $y = X_{t^-}$, and subtracting it from Equation (C18), we get

$$\frac{\mathrm{d}\exp(-S_t^{\mathrm{tot}})}{\mathrm{d}t} = \exp(-S_{t-}^{\mathrm{tot}}) \sum_{x\in\mathcal{X}\setminus\{X_{t^-}\}} \left(\frac{\rho_{\mathrm{st}}(x)\omega(x,X_{t^-})}{\rho_{\mathrm{st}}(X_{t^-})\omega(X_{t^-},x)} - 1\right) \left(\dot{N}_t(X_{t^-},x) - \omega(X_{t^-},x)\right), \tag{C20}$$

which can also be written as

$$\frac{\mathrm{d}\exp(-S_t^{\mathrm{tot}})}{\mathrm{d}t}$$
$$= \exp(-S_{t-}^{\mathrm{tot}}) \sum_{x\in\mathcal{X}\setminus\{X_{t^-}\}} \left(\frac{\rho_{\mathrm{st}}(x)\omega(x,X_{t^-})}{\rho_{\mathrm{st}}(X_{t^-})\omega(X_{t^-},x)} - 1\right) \left(\dot{N}_t(X_{t^-},x) - \dot{\tau}(X_{t^-})\omega(X_{t^-},x)\right). \tag{C21}$$

Integrating over t, we obtain Equations (5.100) and (5.101) in Section 5.4.1.3, which we were meant to show.

C.5. *Novikov's condition for Markov jump processes*

We derive Novikov's condition (5.102) in Section 5.4.1.4 for the exponentiated negative entropy production of a Markov jump process.

We use Novikov's condition for Markov jump processes [135], viz.,

$$\left\langle \exp\left(\frac{1}{2}\langle M^c, M^c\rangle_t + \langle M^d, M^d\rangle_t\right)\right\rangle < \infty, \quad \forall t \geq 0, \tag{C22}$$

and where for our purpose here M is the martingale of Equation (5.101), i.e.,

$$M_t = \sum_{x,y\in\mathcal{X}^2} \left(\frac{\rho_{\mathrm{st}}(y)\omega(y,x)}{\rho_{\mathrm{st}}(x)\omega(x,y)} - 1\right) (N_t(x,y) - \tau_t(x)\omega(x,y)). \tag{C23}$$

The predictable quadratic variation $\langle M^c, M^c\rangle_t$ of the continuous part M^c of M equals zero, as also $[M^c, M^c] = 0$. Let us therefore determine the predictable quadratic variation $\langle M^d, M^d\rangle_t$ of the discontinuous component

$$M^d = \sum_{x,y\in\mathcal{X}^2} \left(\frac{\rho_{\mathrm{st}}(y)\omega(y,x)}{\rho_{\mathrm{st}}(x)\omega(x,y)} - 1\right) N_t(x,y). \tag{C24}$$

The quadratic variation of M^d is the process

$$[M^d, M^d] = \sum_{x,y\in\mathcal{X}^2} \left(\frac{\rho_{\mathrm{st}}(y)\omega(y,x)}{\rho_{\mathrm{st}}(x)\omega(x,y)} - 1\right)^2 N_t(x,y) \tag{C25}$$

and its compensator

$$\langle M^d, M^d\rangle = \sum_{x,y\in\mathcal{X}^2} \left(\frac{\rho_{\mathrm{st}}(y)\omega(y,x)}{\rho_{\mathrm{st}}(x)\omega(x,y)} - 1\right)^2 \omega(x,y)\tau_t(x). \tag{C26}$$

Substituting Equation (C26) in Equation (C22), we get Equation (5.102) that we were meant to show.

Appendix D. Appendix to Chapter 6

We give here explicit expressions to the excess stochastic entropy production (6.64) and explicit expressions for the housekeeping stochastic entropy production (6.68), by restricting ourselves the class of Markov process.

(1) For a pure jump process given by transition rates $\omega_t(x,y)$, we obtain from the generic formulae (6.64) the alternative expression for the excess stochastic entropy production [164,275] :

$$S_t^{ex} = -\ln(\rho_t(X_t)) + \ln(\rho_0(X_0)) + \sum_{j=1}^{N_t} \ln\left[\frac{\pi_{\mathcal{T}_j}(X_{\mathcal{T}_j^+})}{\pi_{\mathcal{T}_j}(X_{\mathcal{T}_j^-})}\right]. \tag{D1}$$

Moreover, the process with path probability $\mathcal{P}^{\text{ex}}$ in the relation (6.64), or equivalently with Markovian generator given by the dual generator $\mathcal{L}^{\text{ex}}$ (6.65), is the pure jump process given by the transition rates

$$\omega_s^{\text{ex}}(x,y) \equiv \frac{\omega_{t-s}(y,x)\pi_{t-s}(y)}{\pi_{t-s}(x)}.$$

On the other hand, we have the following explicit expression for the housekeeping stochastic entropy production [164,275]:

$$S_t^{\text{hk}} = \sum_{j=1}^{N_t} \ln\left[\frac{\pi_{\mathcal{T}_j}(X_{\mathcal{T}_j^-})\omega_{\mathcal{T}_j}(X_{\mathcal{T}_j^-}, X_{\mathcal{T}_j^+})}{\pi_{\mathcal{T}_j}(X_{\mathcal{T}_j^+})\omega_{\mathcal{T}_j}(X_{s^+}, X_{s^-})}\right].$$

These last expressions can be obtained from the generic formula (6.68) or, more simply, directly from the explicit expressions given before (6.36), (D1) and the Oono–Paniconi decomposition (6.63). Similarly of the total Σ-entropic functional, S_t^{hk} is finite only if for all x, y, $\omega_t(x,y) > 0$ implies $\omega_t(y,x) > 0$, condition which is sometimes call microreversibilty. Moreover, the process with path probability $\mathcal{P}^{\text{hk}}$ in the relation (6.68), or equivalently with Markovian generator given by the dual generator $\mathcal{L}^{\text{hk}}$ (6.69), is the pure jump process given by the transition rates

$$\omega_s^{\text{hk}}(x,y) \equiv \frac{\omega_s(y,x)\pi_s(y)}{\pi_s(x)}.$$

(2) For multidimensional Langevin equation (3.65) (even without Einstein relation (3.69)), we obtain from (6.64) the explicit expression for the excess stochastic entropy production [138,151,165] :

$$S_t^{\text{ex}} = -\ln(\rho_t(X_t)) + \ln(\rho_0(X_0)) + \int_0^t [\nabla \ln(\pi_s)](X_s) \circ \dot{X}_s \mathrm{d}s. \tag{D2}$$

Moreover, the process with path probability $\mathcal{P}^{\text{ex}}$ in the relation (6.64), or equivalently with Markovian generator given by the dual generator $\mathcal{L}^{\text{ex}}$ (6.65), is the Langevin equation in the Itô convention

$$\frac{\mathrm{d}X_s^{\text{ex}}}{\mathrm{d}s} = (-\boldsymbol{\mu}_{t-s}F_{t-s} + 2D_{t-s}\nabla(\ln \pi_{t-s}))(X_s^{ex}) + (\nabla\, \mathbf{D}_{t-s})\,(X_s^{ex}) + \sqrt{2\mathbf{D}_{t-s}(X_s^{ex})}\dot{B}_s. \tag{D3}$$

on the other hand side, S_t^{hk} exists only if the diffusion matrix D_t is invertible and is given by the explicit expression [138,151]:

$$S_t^{\text{hk}} = \int_0^t \left(\left(\boldsymbol{\mu}_s F_s\right)\mathbf{D}_s^{-1} - \nabla \ln \pi_s\right)(X_s) \circ \dot{X}_s \mathrm{d}s.$$

Again, these expressions can be obtained from the generic formula (6.68) or, more simply, directly from the explicit expressions given before, (D2) and the Oono–Paniconi decomposition (6.63). Moreover, the process with path probability $\mathcal{P}^{\text{hk}}$ in the relation (6.68), or equivalently with Markovian generator given by the dual generator $\mathcal{L}^{\text{hk}}$ (6.69), is the Langevin equation in the Itô convention

$$\frac{\mathrm{d}X_s^{\text{hk}}}{\mathrm{d}s} = (-\boldsymbol{\mu}_s F_s + 2D_s\nabla(\ln \pi_s))(X_s^{hk}) + (\nabla\, \mathbf{D}_s)\,(X_s^{hk}) + \sqrt{2\mathbf{D}_s(X_s^{hk})}\dot{B}_s. \tag{D4}$$

Appendix E. Appendix to Chapter 7

E.1. *Modified fluctuation relation and second law when* $\exp(-S_t^{\rm tot})$ *is a strict local martingale*

As mentioned in Section 5.2.2, we cannot exclude the possibility that there exist processes $X_{[0,t]}$ for which $\exp(-S_t^{\rm tot})$ is a strict local martingale, i.e., a local martingale that is not a martingales.

Therefore, we analyze here the implication of local martingality on the properties of $S_t^{\rm tot}$.

Since $\exp(-S_t^{\rm tot})$ is bounded from below, it is a supermartingale (see in Ref. [70]), yielding the following *modified martingale fluctuation relation:*

$$\langle \exp(-S_t^{\rm tot})|X_{[0,s]}\rangle \leq \exp(-S_s^{\rm tot}) \tag{E1}$$

for all $t > s > 0$.

Note that for a supermartingale with $S_0^{\rm tot} = 0$,

$$\langle \exp(-S_t^{\rm tot})\rangle \leq 1 \tag{E2}$$

and the equality is attained when $\exp(-S_t^{\rm tot})$ is a martingale.

Using Jensen's inequality $\exp(-\langle x\rangle) \leq \langle \exp(-x)\rangle$ together with $S_0^{\rm tot} = 0$, we obtain

$$\langle S_t^{\rm tot}|X_{[0,s]}\rangle \geq 0 \tag{E3}$$

which is the martingale version of the second law of thermodynamics. Hence, strict local martingales $\exp(-S_t^{\rm tot})$ are compatible with the second law of thermodynamics, which is one more indication that strict local martingales $\exp(-S_t^{\rm tot})$ are physical admissible.

Since the random time transformation of Section 5.2.3 applies to strict local martingales, also the universal properties of entropy production, such as the infimum law equation (5.79) and the universal splitting probabilities equations (7.19)–(7.20), hold for processes $\exp(-S_t^{\rm tot})$ that are strict local martingales and continuous.

Although the above arguments show that local martingales are compatible with physical laws, it will be interesting to find concrete examples of processes X for which $\exp(-S_t^{\rm tot})$ is a local martingale. A possible example are absolutely irreversible processes [276], as such processes obey a modified integral fluctuation relation of the form Equation (E2), although this possible connection between absolute irreversibility and local martingales requires a more careful study, see e.g. [277].

E.2. *Evaluation of the estimators* $\hat{s}_{\rm FPR}$ *and* $\hat{s}_{\rm TUR}$ *for a random walk on a two-dimensional lattice*

We derive Equations (7.69) and (7.71) for the estimators $\hat{s}_{\rm FPR}$ and $\hat{s}_{\rm TUR}$, respectively, of the random walk process on the two-dimensional lattice, as illustrated in Figure 7.11. To this purpose, we derive an explicit expression for the quantities P_-, $\langle \mathcal{T}\rangle$, and $\langle \mathcal{T}^2\rangle$ appearing in the definitions of $\hat{s}_{\rm FPR}$ and $\hat{s}_{\rm TUR}$ in (7.60). The expressions we require are first-passage quantities associated with the first-passage time $\mathcal{T}$ of the current J_t, as defined in Equations (7.55) and (7.66), respectively.

As will become soon evident, we can use the martingale theory of Section 4.1.5 to derive expressions for first-passage quantities associated with $\mathcal{T}$. In this appendix, we sketch this approach, and we refer for details to Appendices D and E of Ref. [35].

E.2.1. *A martingale in the 2D random walk process*

The key insight of the present derivations for $\langle \mathcal{T}\rangle$, $\langle \mathcal{T}^2\rangle$ and P_- is that the process

$$Z_t = \exp\left(zJ_t + tf(z)\right), \tag{E4}$$

where

$$\begin{aligned} f(z) \equiv\ & [1-\exp(z(1-\Delta))]\,\omega_1^+ + [1-\exp(-z(1-\Delta))]\,\omega_1^- \\ &+ [1-\exp(z(1+\Delta))]\,\omega_2^+ + [1-\exp(-z(1+\Delta))]\,\omega_2^-, \end{aligned} \tag{E5}$$

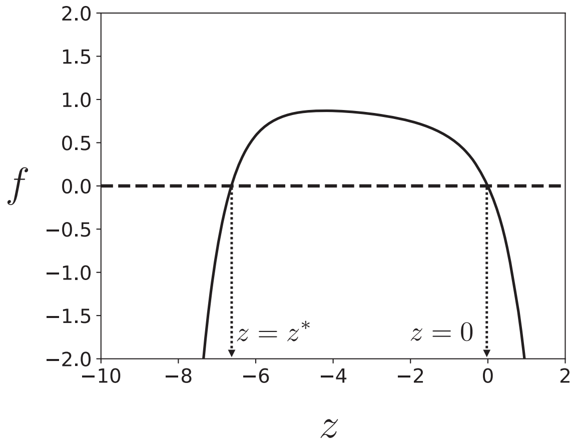

Figure E1. Plot of the function of f, as defined in Equation (E5), for $\Delta = 0.6$, and parameters $\omega_1^+ = \exp(\nu/2)/(4\cosh(\nu/2))$, $\omega_1^- = \exp(-\nu/2)/(4\cosh(\nu/2))$, $\omega_2^+ = \exp(\nu\rho/2)/(4\cosh(\nu/2))$, and $\omega_2^- = \exp(-\nu\rho/2)/(4\cosh(\nu/2))$ with $\rho = 2$ and $\nu = 5$, as in Panel (c) of Figure 7.11.

is a martingale for all values of $z \in \mathbb{R}$.

We plot the function f in Figure E1 for the same parameters as in Panel (c) of Figure 7.11. Observe that f has two roots, the trivial root $z = 0$ and a nontrivial root z^* that solves

$$f(z^*) = 0. \tag{E6}$$

The nontrivial root is negative when $\langle J_t \rangle > 0$ and is positive when $\langle J_t \rangle < 0$. In what follows, we assume that $\langle J_t \rangle > 0$ and hence $z^* < 0$.

Using Equation (4.51) from Doob's optional stopping theorem, we obtain that for all values $z \in \mathbb{R}$ for which $f(z) < 0$ (see Ref. [35]),

$$1 = \langle \mathbf{1}_{J_{\mathcal{T}} \geq \ell_+} \exp\left(z\ell_+[1 + o_{\ell_{\min}}(1)] + \mathcal{T} f(z)\right) + \mathbf{1}_{J(\mathcal{T}) \leq -\ell_-} \exp\left(-z\ell_-[1 + o_{\ell_{\min}}(1)] + \mathcal{T} f(z)\right)\rangle, \tag{E7}$$

where the factors $(1 + o_{\ell_{\min}}(1))$ take care of the overshoot $J_{\mathcal{T}} - \ell_\pm$.

Equation (E7) is central in the following derivations. Indeed, we obtain from this equation the splitting probabilities P_- and P_+, and the moments $\langle \mathcal{T} \rangle$ and $\langle \mathcal{T}^2 \rangle$.

E.2.2. *Splitting probabilities*

Using Equation (E7) for the nonzero value of z^* that solves Equation (E6), together with

$$P_- + P_+ = 1, \tag{E8}$$

we obtain, see also Appendix E of Ref. [35],

$$P_+ = \frac{1 - \exp\left(-\ell_-|z^*|\,[1 + o_{\ell_{\min}}(1)]\right)}{1 - \exp\left(-(\ell_- + \ell_+)|z^*|\,[1 + o_{\ell_{\min}}(1)]\right)} \tag{E9}$$

and

$$P_- = \exp\left(-\ell_-|z^*|\,[1 + o_{\ell_{\min}}(1)]\right) \frac{1 - \exp\left(-\ell_+|z^*|\,[1 + o_{\ell_{\min}}(1)]\right)}{1 - \exp\left(-(\ell_- + \ell_+)|z^*|\,[1 + o_{\ell_{\min}}(1)]\right)}. \tag{E10}$$

Again, we used the factors $[1 + o_{\ell_{\min}}(1)]$ in the exponentials, as in general $J_{\mathcal{T}}$ is not equal to either ℓ_+ or ℓ_- when J_t crosses one of the two threshold.

Hence, in the limit of $\ell_{\min} \to \infty$, we get

$$P_- = \exp\left(-\ell_-|z^*|\,[1 + o_{\ell_{\min}}(1)]\right). \tag{E11}$$

E.2.3. *Generating function of $\mathcal{T}$*

The generating function is defined as

$$g(y) \equiv \langle \exp(-y\mathcal{T}) \rangle = P_+ g_+(y) + P_- g_-(y), \tag{E12}$$

where

$$g_+(y) \equiv \langle \exp(-y\mathcal{T}) \,|\mathcal{T} \geq \ell_+ \rangle \quad \text{and} \quad g_-(y) \equiv \langle \exp(-y\mathcal{T}) \,|\mathcal{T} \leq -\ell_- \rangle. \tag{E13}$$

To obtain an expression for $g_+(y)$ and $g_-(y)$, we use the central equation (E7). In the range $z \notin [z^*, 0]$, for which $f(z) < 0$, we set

$$y = -f(z). \tag{E14}$$

Taking the functional inverse of f, we obtain two solution branches,

$$z_+(y) \in (-\infty, z^*] \quad \text{and} \quad z_-(y) \in [0, \infty), \tag{E15}$$

so that

$$f(z_\pm(y)) = y. \tag{E16}$$

Selecting these two solution in Equation (E7), we obtain the equations

$$1 = P_+ \exp\left(z_+(y)\ell_+ \left[1 + o_{\ell_{\min}}(1)\right]\right) g_+(y) + P_- \exp\left(-z_+(y)\ell_- \left[1 + o_{\ell_{\min}}(1)\right]\right) g_-(y) \tag{E17}$$

and

$$1 = P_+ \exp\left(z_-(y)\ell_+ \left[1 + o_{\ell_{\min}}(1)\right]\right) g_+(y) + P_- \exp\left(-z_-(y)\ell_- \left[1 + o_{\ell_{\min}}(1)\right]\right) g_-(y), \tag{E18}$$

respectively. Solving the above two equations towards $g_+(y)$ and $g_-(y)$, we obtain

$$g_+(y) = \frac{1}{P_+} \frac{1 - \exp\left(-[z_+(y) - z_-(y)]\ell_- \left[1 + o_{\ell_{\min}}(1)\right]\right)}{\exp\left(z_+(y)\ell_+ \left[1 + o_{\ell_{\min}}(1)\right]\right) - \exp\left(-[z_+(y)\ell_- - z_-(y)(\ell_- + \ell_+)] \left[1 + o_{\ell_{\min}}(1)\right]\right)} \tag{E19}$$

and

$$g_-(y) = \frac{1}{P_-} \frac{1 - \exp\left(-[z_-(y) - z_+(y)]\ell_+ [1 + o_{\ell_{\min}}(1)]\right)}{\exp\left(-z_+(y)\ell_- [1 + o_{\ell_{\min}}(1)]\right) - \exp\left(-[z_-(y)(\ell_- + \ell_+) - z_+(y)\ell_+] \left[1 + o_{\ell_{\min}}(1)\right]\right)}. \tag{E20}$$

Taking the limit $\ell_{\min} \to \infty$, it follows from Equations (E9), (E10), (E12), (E19) and (E20) that the generating function of $\mathcal{T}$ is given by

$$g(y) = g_+(y)(1 + O(\exp\left(\ell_- z^*\right))) \tag{E21}$$

with

$$g_+(y) = \exp\left(-z_-(y)\ell_+ \left[1 + o_{\ell_{\min}}(1)\right]\right), \tag{E22}$$

and where we have used that $z_+ < 0$ and $z_- > 0$.

E.2.4. *First moment and second moment of $\mathcal{T}$*

Equations (E21) and (E22) determine the generating function g of $\mathcal{T}$ in terms of the function $z_-(y)$ that solves Equation (E16) for $z_-(y) \in [0, \infty)$. Solving Equation (E16) is not an easy task, but since we only need the first two moments of $\mathcal{T}$, we can simplify the problem further. Indeed, expanding g in small values of y we obtain up to second order in y,

$$g(y) = 1 - y\langle\mathcal{T}\rangle + \frac{y^2}{2}\langle\mathcal{T}^2\rangle + O(y^3), \tag{E23}$$

and hence it is sufficient to solve Equation (E16) up to second order in y. In addition, using that $z_-(y) \approx 0$ for $y \approx 0$ and expanding Equation (E16) up to second order yields the equation

$$\begin{aligned}&\left[z(1-\Delta) + \frac{z^2(1-\Delta)^2}{2}\right]\omega_1^+ - \left[z(1-\Delta) - \frac{z^2(1-\Delta)^2}{2}\right]\omega_1^- \\ &+ \left[z(1+\Delta) + \frac{z^2(1+\Delta)^2}{2}\right]\omega_2^+ - \left[z(1+\Delta) - \frac{z^2(1+\Delta)^2}{2}\right]\omega_2^- + O(z^3) = y,\end{aligned} \tag{E24}$$

whose positive solution determines z_-.

Mean first-passage time $\langle\mathcal{T}\rangle$. The solution of Equation (E24) up to linear order in y is

$$z_- = \frac{y}{(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)} + O(y^2). \tag{E25}$$

Substituting Equation (E25) in Equations (E21) and (E22) gives

$$g(y) = \exp\left(-\frac{\ell_+\left(y + O(y^2)\right)}{(1-\Delta)(k_1^+ - k_1^-) + (1+\Delta)(k_2^+ - k_2^-)}(1 + o_{\ell_{\min}}(1))\right). \tag{E26}$$

Expanding the latter equation up to linear order in y and comparing with Equation (E23) gives

$$\langle\mathcal{T}\rangle = \frac{\ell_+}{(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)}(1 + o_{\ell_{\min}}(1)). \tag{E27}$$

Second moment $\langle\mathcal{T}^2\rangle$. Solving Equation (E24) up to quadratic order yields the solution

$$\begin{aligned} z_- =& \frac{y}{(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)} \\ &- \frac{y^2}{2}\left[\frac{(1-\Delta)^2\left(\omega_1^+ + \omega_1^-\right) + (1+\Delta)^2\left(\omega_2^+ + \omega_2^-\right)}{\left((1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)\right)^3}\right] + O(y^3).\end{aligned} \tag{E28}$$

Substituting Equation (E28) in Equations (E21) and (E22) and expanding up to second order in y gives

$$\begin{aligned} g_+(y) =& \exp\left(-\frac{\ell_+ y}{(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)}(1 + o_{\ell_{\min}}(1))\right) \\ &\times \exp\left(\frac{y^2\ell_+ + O(y^3)}{2}\left[\frac{(1-\Delta)^2\left(\omega_1^+ + \omega_1^-\right) + (1+\Delta)^2\left(\omega_2^+ + \omega_2^-\right)}{\left((1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)\right)^3}\right](1 + o_{\ell_{\min}}(1))\right).\end{aligned} \tag{E29}$$

Expanding the latter equation up to second order in y, and comparing with Equation (E23), we obtain

$$\begin{aligned}\langle\mathcal{T}^2\rangle =& \frac{\ell_+^2}{\left[(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)\right]^2} \\ &+ \ell_+\frac{(1-\Delta)^2\left(\omega_1^+ + \omega_1^-\right) + (1+\Delta)^2\left(\omega_2^+ + \omega_2^-\right)}{\left[(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)\right]^3},\end{aligned} \tag{E30}$$

and thus

$$\langle\mathcal{T}^2\rangle - \langle\mathcal{T}\rangle^2 = \frac{(1-\Delta)^2\left(\omega_1^+ + \omega_1^-\right) + (1+\Delta)^2\left(\omega_2^+ + \omega_2^-\right)}{\left[(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)\right]^3}. \tag{E31}$$

E.2.5. *Estimators* $\hat{s}_{\rm FPR}$ *and* $\hat{s}_{\rm TUR}$

Using the expressions (E11) and (E27) for P_- and $\langle\mathcal{T}\rangle$, respectively, in the definition of $\hat{s}_{\rm FPR}$, Equation (7.60), we obtain

$$\hat{s}_{\rm FPR} = |z^*| \left((1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)\right)(1 + o_{\ell_{\min}}(1)), \tag{E32}$$

which is Equation (7.69) we were meant to derive.

Analogously, using the expressions (E27) and (E31) for $\langle\mathcal{T}\rangle$ and $\langle\mathcal{T}^2\rangle - \langle\mathcal{T}\rangle^2$, respectively, in the definition of $\hat{s}_{\rm TUR}$, Equation (7.60), we obtain

$$\hat{s}_{\rm TUR} = \frac{2\langle T\rangle}{\langle\mathcal{T}^2\rangle - \langle\mathcal{T}\rangle^2} = \frac{2\left[(1-\Delta)(\omega_1^+ - \omega_1^-) + (1+\Delta)(\omega_2^+ - \omega_2^-)\right]^2}{(1-\Delta)^2\left(\omega_1^+ + \omega_1^-\right) + (1+\Delta)^2\left(\omega_2^+ + \omega_2^-\right)}(1 + o_{\ell_{\min}}(1)), \tag{E33}$$

which is Equation (7.71) that we were meant to derive.

Appendix F. Appendix to Chapter 8

F.1. *Derivation of Equation (8.16) demonstrating the exponential martingale for nonstationary processes*

The derivation of Equation (8.16) is similar to the derivation of Equation (5.42) in Chapter 5.

First, we use the definition of $\tilde{\rho}$ as the solution to the Fokker–Planck equation given by Equations (8.11)–(8.12) to write,

$$\frac{\mathrm{d}\left(-\ln\left(\tilde{\rho}_{\tau-s}\left(X_s\right)\right)\right)}{\mathrm{d}s} \tag{F1}$$

$$= -\frac{\left(\partial_s\tilde{\rho}_{\tau-s}\right)\left(X_s\right)}{\tilde{\rho}_{\tau-s}\left(X_s\right)} - \frac{\left(\partial_x\tilde{\rho}_{\tau-s}\right)\left(X_s\right)}{\tilde{\rho}_{\tau-s}\left(X_s\right)} \circ \dot{X}_s \tag{F2}$$

$$= \underbrace{-\frac{\left(\partial_s\tilde{\rho}_{\tau-s}\right)\left(X_s\right)}{\tilde{\rho}_{\tau-s}\left(X_s\right)} + \frac{\tilde{J}_{\tau-s,\tilde{\rho}}(X_s)}{\mu T\tilde{\rho}_{\tau-s}\left(X_s\right)} \circ \dot{X}_s}_{\frac{\mathrm{d}\hat{\Sigma}_s}{\mathrm{d}s}} \underbrace{- \frac{\partial_x V(X_s;\tilde{\lambda}_{\tau-s})}{T} \circ \dot{X}_s}_{\dot{Q}_s/T}, \tag{F3}$$

where we have used that $\tilde{\lambda}_{\tau-s} = \lambda_s$.

Hence, in Stratonovich convention

$$\frac{\mathrm{d}\hat{\Sigma}_s}{\mathrm{d}s} = -\frac{\left(\partial_s\tilde{\rho}_{\tau-s}\right)\left(X_s\right)}{\tilde{\rho}_{\tau-s}\left(X_s\right)} + \frac{1}{\mu T}\frac{\tilde{J}_{\tau-s,\tilde{\rho}}(X_s)}{\tilde{\rho}_{\tau-s}\left(X_s\right)} \circ \dot{X}_s. \tag{F4}$$

Substituting $\dot{X}_s$, given in Equation (8.4), in Equation (F4), and using

$$\partial_x V(x,\lambda_s) = \partial_x V(x,\tilde{\lambda}_{\tau-s}) = -\frac{\tilde{J}_{\tau-s,\tilde{\rho}}}{\mu\tilde{\rho}_{\tau-s}} - T\frac{\partial_x\tilde{\rho}_{\tau-s}}{\tilde{\rho}_{\tau-s}}, \tag{F5}$$

we get

$$\frac{\mathrm{d}\hat{\Sigma}_s}{\mathrm{d}s} = -\frac{\left(\partial_s\tilde{\rho}_{\tau-s}\right)\left(X_s\right)}{\tilde{\rho}_{\tau-s}\left(X_s\right)} + \frac{\tilde{J}_{\tau-s,\tilde{\rho}}\left(X_s\right)\left(\partial_x\tilde{\rho}_{\tau-s}\right)\left(X_s\right)}{\left(\tilde{\rho}_{\tau-s}\left(X_s\right)\right)^2} + v_s^S + \sqrt{2v_s^S} \circ \dot{B}_s, \tag{F6}$$

where we have used Equation (8.17) to identify v_s^S. Next, we use Theorem 1 to write the last term in the latter equation in the Itô convention, obtaining

$$\sqrt{v_s^S} \circ \dot{B}_s = \sqrt{v_s^S}\dot{B}_t + \frac{\left(\partial_x\tilde{J}_{\tau-s,\tilde{\rho}}\right)\left(X_s\right)}{\tilde{\rho}_{\tau-s}(X_s)} - \frac{\tilde{J}_{\tau-s,\tilde{\rho}}\left(X_s\right)\left(\partial_x\tilde{\rho}_{\tau-s}\right)\left(X_s\right)}{\left(\tilde{\rho}_{\tau-s}\left(X_s\right)\right)^2}. \tag{F7}$$

Lastly, using Equation (F7) into Equation (F6) together with

$$\partial_s \tilde{\rho}_{\tau-s} = -\partial_x \tilde{J}_{\tau-s,\tilde{\rho}}, \tag{F8}$$

we obtain

$$\frac{\mathrm{d}\hat{\Sigma}_s}{\mathrm{d}s} = v_s^S + \sqrt{2v_s^S}\dot{B}_s, \tag{F9}$$

which is Equation (8.16) that we were meant to derive.

F.2. *Origin of time reversal in the definition of* $\hat{\Sigma}_s$

In the definition Equation (8.9) of $\hat{\Sigma}_s$ we have set *t*/2, the origin of time reversal, equal to $\tau/2$. Here, we show that the process $\hat{\Sigma}_s$ is independent of the choice *t*/2 for the origin of time-reversal.

Let us therefore define the stochastic process

$$\hat{\Sigma}_s^{(t)} \equiv -\frac{Q_s}{T} + \ln \rho_{\mathrm{eq}}(X_0; \lambda_{\mathrm{i}}) - \ln \tilde{\rho}_{t-s}^{(t)}(X_s), \tag{F10}$$

where $\dot{Q}_s$ is the heat equation (8.10) as before, and where $\tilde{\rho}_{t-s}^{(t)}$ is the solution to the Fokker–Planck equation

$$\partial_s \tilde{\rho}_s^{(t)} + \partial_x \tilde{J}_{s,\tilde{\rho}}^{(t)} = 0, \tag{F11}$$

with

$$\tilde{J}_{s,\tilde{\rho}}^{(t)} = -\mu \partial_x V(x; \tilde{\lambda}_s^{(t)}) \tilde{\rho}_s^{(t)}(x) - \mu T \partial_x \tilde{\rho}_s^{(t)}(x), \tag{F12}$$

and with

$$\tilde{\lambda}_s^{(t)} \equiv \begin{cases} \lambda_{\mathrm{f}} & \text{if } s \leq t-\tau, \\ \lambda_{t-s} & \text{if } s \in [t-\tau, t], \\ \lambda_{\mathrm{i}} & \text{if } s \geq t, \end{cases} \tag{F13}$$

the time-reversed protocol. Note that in the time-reversed protocol $\tilde{\lambda}_s^{(t)}$ the time-reversal reflection point is *t*/2, and not $\tau/2$ as in Equation (8.13). To complete the definition of $\tilde{\rho}_s^{(t)}$ we specify the initial state of the time-reversal dynamics, which for $t \geq \tau$ given by

$$\tilde{\rho}_0^{(t)}(x) = \rho_{\mathrm{eq}}(x; \lambda_{\mathrm{f}}), \tag{F14}$$

and for $t \in [0, \tau]$ by

$$\tilde{\rho}_0^{(t)} = \tilde{\rho}_{\tau-t}^{(\tau)}. \tag{F15}$$

Note that in the case $t = \tau$, it holds that $\hat{\Sigma}_s^{(t)}$, as defined in Equation (8.9), equals $\hat{\Sigma}_s$, as defined in Equation (F10).

It follows from the definition equations (F11)–(F12) for the Fokker–Planck equation with initial condition equations (F14) or (F15) that

$$\tilde{\rho}_{t-s}^{(t)} = \tilde{\rho}_{\tau-s}^{(\tau)}, \tag{F16}$$

and hence

$$\hat{\Sigma}_s^{(t)} = \hat{\Sigma}_s^{(\tau)}. \tag{F17}$$

In other words, the origin *t*/2 of time reversal is not relevant in the definition of $\hat{\Sigma}_s^{(t)}$, as all processes are the same. For this reason, we have set $t = \tau$ as in Ref. [14], and we removed the index (τ) from the definition $\hat{\Sigma}_s^{(\tau)}$ in Equation (8.9).

Appendix G. Appendix to Chapter 12

G.1. *Derivation of Equation (12.26) from Equation (12.21)*

We start with considering the transformation (12.25) that implies the following identities:

$$\alpha+\beta=\frac{2r}{\sigma^2},\quad \alpha+1=\beta. \tag{G1}$$

Using $C(S_t,t)=Ku(x,\tau)\exp(-\alpha x-\beta^2\tau)$ and $\partial\tau/\partial t=-\sigma^2/2$, we get

$$\frac{\partial C}{\partial t}=-\frac{\sigma^2}{2}K\exp(-\alpha x-\beta^2\tau)\left(\frac{\partial u}{\partial \tau}-\beta^2 u\right). \tag{G2}$$

Next, using $\partial x/\partial S_t=1/S_t$, we get

$$\frac{\partial C}{\partial S_t}=\frac{K}{S_t}\exp(-\alpha x-\beta^2\tau)\left(\frac{\partial u}{\partial x}-u\alpha\right), \tag{G3}$$

so that $r=(\alpha+\beta)\sigma^2/2$ yields

$$rS_t\frac{\partial C}{\partial S_t}=\frac{(\alpha+\beta)\sigma^2}{2}K\exp(-\alpha x-\beta^2\tau)\left(\frac{\partial u}{\partial x}-u\alpha\right). \tag{G4}$$

Using Equation (G3) and $K/S_t=\exp(-x)$, we get

$$\frac{\partial^2 C}{\partial S_t^2}=\frac{1}{S_t}\exp(-(\alpha+1)x-\beta^2\tau)\left[-(2\alpha+1)\frac{\partial u}{\partial x}+\frac{\partial^2 u}{\partial x^2}+\alpha(\alpha+1)u\right]. \tag{G5}$$

It then follows that

$$\frac{\sigma^2 S_t^2}{2}\frac{\partial^2 C}{\partial S_t^2}=\frac{\sigma^2 K}{2}\exp(-\alpha x-\beta^2\tau)\left[-(2\alpha+1)\frac{\partial u}{\partial x}+\frac{\partial^2 u}{\partial x^2}+\alpha(\alpha+1)u\right]. \tag{G6}$$

Finally, we have

$$rC=\frac{(\alpha+\beta)\sigma^2 Ku}{2}\exp(-\alpha x-\beta^2\tau). \tag{G7}$$

We now substitute Equations (G2), (G4), (G6), and (G7) in Equation (12.21), and use

$$\beta^2+\alpha\beta-(\alpha+\beta)\alpha-(\alpha+\beta)=\beta(\alpha+1)+\alpha\beta-(\alpha+\beta)(\alpha+1)=0, \tag{G8}$$

where we have used the result $\alpha+1=\beta$; we finally get our desired result, namely, Equation (12.26):

$$\frac{\partial u}{\partial \tau}=\frac{\partial^2 u}{\partial x^2}. \tag{G9}$$