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Statistical characterization of non-equilibrium states
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Chapter 1

Introduction on non-equilibrium systems

1.1 Several ways to be out of equilibrium

Systems composed of many particles involve a very large number of degrees of freedom, and it is most often uninteresting—not to say hopeless—to try to describe in a detailed way the microscopic state of the system. The aim of statistical physics is rather to restrict the description of the system to a few relevant macroscopic observables, and to predict the average values of these observables, or the relations between them. The standard equilibrium formalism of statistical physics has been developed for systems of physical particles having reached a statistical steady state in the absence of external driving (like heat flux or shearing forces for instance).

Interestingly, there are many possible ways to be out-of-equilibrium, since equilibrium actually corresponds to a rather singular situation. Among these many possibilities, one can single out a few types of idealized situations that are conceptually interesting:

- Relaxation to equilibrium, yielding a time-dependent behavior. This type of situation becomes particularly interesting if the relaxation is very slow, involving many different time scales, like in the physics of glasses where many intriguing non-equilibrium effects can be observed [1, 2].

- Driven steady-state; this corresponds to the case of a system maintained into a non-equilibrium stationary state by external sources (for instance a system in contact with two heat reservoirs at different temperatures, or a system sheared by external mechanical forces) [3, 4].

- Steady-state of a system composed of macroscopic interacting “entities”, like sand grains, animals or social agents. Here, the non-equilibrium character of the system not only comes from its macroscopic state, but also from the microscopic dynamics, which may significantly differ from the dynamics ruling physical particles (atoms, molecules,...). Though sometimes well-beyond the realm of physics, such systems have, in the last twenty years, raised a lot of interest in the statistical physics community [5, 6, 7].

Although more complicated situations can obviously occur (for instance, a driven system can also be in a non-stationary state), these three classes of problems may already yield interesting insights into non-equilibrium statistical physics. In the present manuscript, we shall mostly focus on steady-state properties, though time-dependent problems might occasionally be mentioned.
1.2 Motivation and outline of the manuscript

One of the main challenges of non-equilibrium statistical physics is to understand which principles rule the description of nonequilibrium steady states, if such principles exists. My research project over the last eight years has been mainly motivated by the following issues regarding the statistical description of non-equilibrium systems:

- What are the relevant macroscopic parameters to describe non-equilibrium systems? Can one generalize the notion of intensive thermodynamic parameters (temperature, pressure, chemical potential,...) which is at the heart of the equilibrium approach?

- Beyond average values, how can one describe the fluctuations of macroscopic (or global) observables, that are often observed to be non-Gaussian in non-equilibrium systems (for instance in the presence of dissipation)? How are these physical phenomenon linked to probability theory (breaking of the central limit theorem,...)?

- How far can standard statistical physics methods and concepts be applied to systems of interacting macroscopic entities? Is for instance the concept of phase transition relevant in these systems?

The present manuscript mostly follows the above questions. In Chapter 2 and 3, issues related to the definition of intensive thermodynamics parameters are investigated. Chapter 2 is specifically devoted to the study of non-equilibrium effective temperatures arising from generalized fluctuation-dissipation relations. Chapter 3 is dedicated to the study of other types of intensive thermodynamics parameters, those conjugated to conserved quantities when available (for instance, energy is often not a conserved quantity in non-equilibrium systems, so that tentative definitions of temperature need to rely on other approaches). Chapter 4 addresses the issue of non-Gaussian fluctuations in correlated (e.g., driven) systems, and briefly investigates some connections to more probabilistic aspects. Finally, different examples of systems composed of a large number of interacting agents, modeling in a very simplified way the behavior of social agents or animals, are presented in Chapter 5. Emphasis is put on the collective behavior and on possible emergent phenomena like phase transitions.

The spirit of the present manuscript is essentially to illustrate the above questions through the use of simple solvable models. Such models can of course not be claimed to be generic, but their main interest lies in their illustrative power, since explicit results can be provided at the cost of only moderately difficult calculations. Along this line of thought, we present in this introductory chapter two examples of such models, yielding a simple and interesting illustration of the way the probability of microscopic configurations is modified in non-equilibrium situations.

1.3 Explicit examples of nonequilibrium models

From a statistical viewpoint, the main characteristics of non-equilibrium systems is that the probability distribution of microscopic configurations does not follow any of the standard equilibrium forms, the most common one being the canonical distribution which describes the equilibrium statistics of a system in contact with a heat reservoir. It is thus of interest to characterize quantitatively the probability distribution of microscopic configurations, from which all (one-time) macroscopic
properties can in principle be derived. Determining this distribution is in general a very difficult task, but it can at least be derived in some very simplified models, as illustrated below.

1.3.1 Aging dynamics and trap model

Although many systems converge to a stationary state on times shorter than or comparable to the observation time, it turns out that some systems do not reach a steady state and keep evolving on time scales that can be very large compared to standard observation times. This is the case for instance of glasses, which keep aging for years or more [1, 8, 2]. The same type of mechanism is at play in laser cooling experiments [9, 10]. It is also likely that aging mechanisms, or slow relaxation effects, play a significant role in many different types of complex systems. Even though the aging mechanisms may differ from one situation to the other, it is certainly of interest to investigate one of the simplest known aging phenomena, illustrated by the trap model, which we describe here within a generic formalism that does not rely on a specific physical realization.

Let us consider a model system in which to each configuration \( C \) is associated a given lifetime \( \tau \). This lifetime \( \tau \) is the mean time spent in configuration \( C \) before moving to another configuration. As we consider only temporal aspects of the dynamics, and not other types of observables (energy, magnetization,...), we simply label the configurations by their lifetime \( \tau \). We then choose a simple form for the transition rate \( W(\tau' | \tau) \), namely:

\[
W(\tau' | \tau) = \frac{1}{\tau} \psi(\tau') .
\]  

The function \( \psi(\tau') \) is the a priori probability distribution of the configurations \( \tau' \), meaning that the selected new configuration is chosen completely at random. From the normalization condition \( \int_0^\infty d\tau' \psi(\tau') = 1 \), we have

\[
\int_0^\infty d\tau' W(\tau' | \tau) = \frac{1}{\tau},
\]  

so that the characteristic escape time from a configuration with lifetime \( \tau \) is precisely \( \tau \). For simplicity, we also assume that all lifetimes \( \tau \) are greater than a value \( \tau_0 \), that we set to \( \tau_0 = 1 \) in the following. The master equation then reads:

\[
\frac{\partial P}{\partial t}(\tau, t) = -P(\tau, t) \int_1^\infty d\tau' W(\tau' | \tau) + \int_1^\infty d\tau' W(\tau | \tau') P(\tau', t)
\]
\[= -\frac{1}{\tau} P(\tau, t) + \psi(\tau) \int_1^\infty \frac{d\tau'}{\tau'} P(\tau', t).
\]

(1.3)

At equilibrium, the probability to be in a configuration with lifetime \( \tau \) is proportional to \( \tau \) and to the a priori distribution \( \psi(\tau) \) of configurations:

\[
P_{eq}(\tau) = \frac{1}{\langle \tau \rangle} \tau \psi(\tau),
\]

(1.4)

where \( \langle \tau \rangle \) is defined as

\[
\langle \tau \rangle = \int_1^\infty d\tau \tau \psi(\tau).
\]

(1.5)

An interesting situation appears when the distribution \( \psi(\tau) \) takes a power-law form, namely

\[
\psi(\tau) = \frac{\alpha}{\tau^{1+\alpha}}, \quad \tau > 1, \quad \alpha > 0.
\]

(1.6)
This is realized for instance in the case of a particle trapped into potential wells of random depth \( \varepsilon \), with an exponential distribution

\[
\rho(\varepsilon) = \frac{1}{\varepsilon_0} e^{\varepsilon/\varepsilon_0}, \quad \varepsilon < 0.
\]  

(1.7)

The lifetime \( \tau \) is given by the standard Arrhenius law

\[
\tau = \tau_0 e^{\varepsilon_0/\varepsilon},
\]

where \( \tau_0 = 1 \) is a microscopic time scale. Using the relation \( \psi(\tau)|d\tau| = \rho(\varepsilon)|d\varepsilon| \), one precisely finds the form (1.6) for \( \psi(\tau) \), with \( \alpha = T/\varepsilon_0 \).

In the case \( \alpha > 1 \), \( \langle \tau \rangle \) is finite, but if \( \alpha \leq 1 \) then \( \langle \tau \rangle \) is infinite, so that the equilibrium distribution (1.4) does not exist, as it is not normalizable. As a result, no stationary state can be reached, and the system keeps drifting toward configurations with larger and larger lifetimes \( \tau \).

It is then of interest to determine the time-dependent probability distribution \( P(\tau, t) \) in the long-time regime. We postulate the following scaling form

\[
P(\tau, t) = \frac{1}{t} \phi \left( \frac{\tau}{t} \right).
\]  

(1.9)

Introducing this scaling form in the master equation (1.3), we get after some algebra the expression for \( \phi(u) \) [8, 10]:

\[
\phi(u) = \frac{\sin(\pi \alpha)}{\Gamma(\alpha)} \frac{1}{u} e^{-1/u} \int_0^{1/u} dv v^{\alpha-1} e^v,
\]  

(1.10)

where \( \Gamma(\alpha) = \int_0^\infty x^{\alpha-1}e^{-x}dx \) is the Euler Gamma function. It is rather easy to show that \( \phi(u) \sim u^{-\alpha} \) for \( u \to 0 \), and that \( \phi(u) \sim u^{-1-\alpha} \) for \( u \to \infty \), leading for \( P(\tau, t) \) to

\[
P(\tau, t) \propto \tau \psi(\tau), \quad \tau \ll t,
\]  

(1.11)

\[
P(\tau, t) \propto \psi(\tau), \quad \tau \gg t.
\]  

(1.12)

These asymptotic behaviors can be interpreted rather easily: configurations with lifetimes \( \tau \ll t \) have been visited a large number of times, so that they are quasi-equilibrated; in contrast, configurations with lifetimes \( \tau \gg t \) have been visited at most once, and the precise value of \( \tau \) is not yet felt by the dynamics (\( \tau \) appears as essentially infinite).

The trap model is a toy model implicitly involving a rather small number of particles, in the sense that the energies scales involved are assumed to remain of the same order as the temperature, and thus cannot become extensive with respect to the total number of particles in a macroscopic system. Hence, in the picture of the trap model, a macroscopic system should rather be viewed as a collection of a large number \( N \) of independent trap models with energy \( \varepsilon_i \), each of them describing the local dynamics within a coherent domain.

The probability distribution \( P(\{\varepsilon_i\}) \) of the macroscopic system is then given by

\[
P(\{\varepsilon_i\}) = \prod_{i=1}^N p(\varepsilon_i).
\]  

(1.13)

At equilibrium, for \( T > T_g \), the distribution \( p(\varepsilon_i) \) is equal to \( p(\varepsilon_i) = Z_1^{-1} e^{-\beta\varepsilon_i} \), and the distribution \( P(\{\varepsilon_i\}) \) takes the expected equilibrium canonical form

\[
P(\{\varepsilon_i\}) = \frac{1}{Z_N} e^{-\beta E}
\]  

(1.14)
with \( E = \sum \varepsilon_i \) the total energy of the system.

In contrast, in the aging regime \( T < T_g \), the distribution \( \mathcal{P}(\{\varepsilon_i\}, t) \) remains time-dependent, and takes the form

\[
\mathcal{P}(\{\varepsilon_i, t\}) = \frac{1}{t^N} \prod_{i=1}^{N} \phi \left( \frac{\tau_0}{t} e^{\varepsilon_i/T} \right),
\]

(1.15)

which cannot be recast onto the familiar equilibrium canonical form. Only in the limit where all domains have a small energy \( |\varepsilon_i| \ll T \ln(t/\tau_0) \) does one recover \( \mathcal{P}(\{\varepsilon_i, t\}) \propto e^{-\beta E} \). The discrepancy between this non-equilibrium form and the equilibrium canonical form leads to interesting phenomenon like, e.g., the violation of fluctuation-dissipation relations [11, 12].

### 1.3.2 A dissipative system on a tree

As a second illustration of non-equilibrium systems, we now consider the case of a dissipative system, where energy is injected at large scales, and dissipated at small scales. Examples include hydrodynamic turbulence [13], wave turbulence in fluids, plasma [14], and vibrating plates [15], fracture [16] and friction [17], granular materials and foams [18]. A natural question is to know whether in the limit of small, but nonzero dissipation, the steady state of the system becomes close to some equilibrium state to be determined. One may expect that adding a tiny amount of injection and dissipation to a conservative system breaks energy conservation, but leads to small fluctuations around a given energy level selected by the injection and dissipation mechanisms. The system would thus merely behave as if it was at equilibrium at this energy.

Whether this scenario holds in general is an open issue. Such approaches have been proposed in the context of two-dimensional turbulence [19], for which the flux of dissipated energy vanishes in the small viscosity limit. However, in other situations like three-dimensional turbulence [13] or granular gases [20], the dissipated flux remains finite for small viscosity, suggesting that the system does not converge to any equilibrium state.

In order to give further insights into these issues, we study a simple solvable stochastic transport model, namely an open Zero Range Process [21], that describes in a schematic way the transfer of energy between scales, in the presence of injection and dissipation. To account for the hierarchical organization of scale space, we define our model on a Cayley tree [22], each level being interpreted as a given scale. The advantage of this specific geometry with respect to more conventional ones (e.g., one-dimensional lattice) is twofold: the tree is self-similar, so that subsystems have the same structure as the global model, and scales are spaced logarithmically, which allows interactions to

![Figure 1.1: Sketch of the dissipative model, illustrating the tree geometry.](image-url)
be treated as local. We show that depending on the energy transfer dynamics, the dissipative stationary state of the model converges in the weak dissipation limit either to an equilibrium state, or to a well-defined far-from-equilibrium state with a finite dissipated flux. The simplicity of our model (non-linear interactions at play in real systems are replaced by an effective diffusion process) allows us to compute the exact stationary distribution and macroscopic observables of interest. Possible implications of our results for more realistic systems are then discussed.

The model is defined on a Cayley tree composed of $M$ successive levels (see Fig. 1.1): at any given level $j < M$, all sites have $m > 1$ forward branches that link them to level $j + 1$, so that the number of sites at level $j$ is $m^{j-1}$. Sites are thus labeled by the level index $j$, and the index $i = 1, \ldots, m^{j-1}$ within level $j$. The energy on each site $(j, i)$ of the tree is assumed to take only discrete values proportional to an elementary amount $\varepsilon_0$, namely $\varepsilon_{j,i} = n_{j,i}\varepsilon_0$. Energy transfer proceeds as follows: an energy amount $\varepsilon_0$ is moved, either forward or backward, along any branch between levels $j$ and $j + 1$ with a rate $\nu_j$. In the absence of driving and dissipation, the dynamics satisfies detailed balance. Energy injection is implemented by connecting the site $(1, 1)$ to a thermostat of temperature $T_{\text{ext}} = \beta_{\text{ext}}^{-1}$, with a coupling frequency $\nu_{\text{ext}}$. Dissipation proceeds through the random withdrawal of an amount of energy $\varepsilon_0$ at site $(j, i)$ with rate $\Delta_j$.

The steady-state probability distribution can be searched for under the form:

$$P_{\text{st}}(\{n_{j,i}\}) = \frac{1}{Z} \prod_{j=1}^{M} \prod_{i=1}^{m^{j-1}} e^{-\beta_j n_{j,i}\varepsilon_0}$$

where $\beta_j$ is an effective inverse temperature (to be determined) associated to level $j$, and $Z$ is a normalization factor. Inserting expression (1.16) of the stationary distribution into the master equation describing the stochastic dynamics [23], one finds a set of equations to be satisfied by the parameters $z_j = \exp(-\beta_j\varepsilon_0)$, for $j = 2, \ldots, M - 1$:

$$\nu_{j-1}(z_{j-1} - z_j) - m\nu_j(z_j - z_{j+1}) = \Delta_j z_j$$

with the boundary conditions

$$\nu_{\text{ext}}(e^{-\beta_{\text{ext}}\varepsilon_0} - z_1) - m\nu_1(z_1 - z_2) = \Delta_1 z_1$$

$$\nu_{M-1}(z_{M-1} - z_M) = \Delta_M z_M.$$  

Note that these equations correspond to the local balance of the diffusive fluxes $\nu_j(z_j - z_{j+1})$ and dissipative fluxes $\Delta_j z_j$. In the absence of dissipation, namely if $\Delta_j = 0$ for all $j$, the equilibrium solution $\beta_1 = \ldots = \beta_M = \beta_{\text{ext}}$ is recovered. To study the dissipative case, we need to choose a specific form of the frequency $\nu_j$ and the dissipation rate $\Delta_j$. A generic form is the following:

$$\nu_j = \nu_1 k_j^\alpha, \quad \Delta_j = D k_j^\gamma, \quad \gamma > 0,$$

where we have introduced a pseudo-wavenumber $k_j = m^{j-1}$, to map the tree structure onto physical space. Parameters $\nu_1$ and $D$ are respectively a frequency characterizing the large scale dynamics, and a dissipation coefficient. We impose the condition $\alpha < \gamma$, so that dissipation becomes the dominant effect at small scales (large $k_j$). The transfer rate $\nu_j$ and the dissipation rate $\Delta_j$ are balanced for a wavenumber $k_j = K$ given by

$$K = \left(\frac{\nu_1}{D}\right)^{1/(\gamma - \alpha)}.$$
Figure 1.2: Numerical solution of Eqs. (1.17), (1.18) and (1.19) for γ = 2 and D = 10^{-x}, with x given in (a); same symbols for all four figures. (a) Energy flux Φ as a function of α; the full line corresponds to the theoretical prediction \[23\]. (b) Temperature \(T_j = \beta_j^{-1}\) versus \(\ln k_j\) for \(\alpha = -2\); the full line is \(T_{ext}\). (c) \(\beta_j\) versus \(\ln k_j\) for \(\alpha = 1\); full line: \(\beta_j^{eq}\) defined in Eq. (1.23). (d) Same data as (c) plotted as \(T_j\), on the same window of \(\ln k_j\) as (b). Arrows in (b) and (c) indicate the value of \(K\) for each \(D\). Other parameters: \(M = 50, m = 2, \nu_1 = 1, \nu_{ext} = 0.1, \beta_{ext} = 1, \varepsilon_0 = 1\).

which goes to infinity in the limit of small dissipation coefficient \(D\), \((\nu_1 / D)\) is similar to the Reynolds number in hydrodynamics). For large \(K\), we shall call the ranges \(k_j \ll K\) and \(k_j \gg K\) the inertial and dissipative ranges respectively. The solution of Eqs. (1.17), (1.18) and (1.19) can be evaluated numerically. We are interested in the inertial range behavior, where energy transfer dominates over dissipative effects, so that we shall explore the solutions by varying \(\alpha\) while keeping \(\gamma\) fixed. We first compute the mean energy flux \(\Phi\) injected by the reservoir,

\[
\Phi = \nu_{ext} \left( e^{-\beta_{ext}\varepsilon_0} - e^{-\beta_1\varepsilon_0} \right).
\]

(1.22)

The flux \(\Phi\) is plotted as a function of \(\alpha\) in Fig. 1.2(a), for a broad range of values of the dissipation coefficient \(D\). We observe a transition around the value \(\alpha = -1\): for \(\alpha < -1\), \(\Phi \to 0\) when \(D \to 0\), while for \(\alpha > -1\), \(\Phi\) converges to a finite value in the small \(D\) limit. These two regimes are also clearly seen in Fig. 1.2 (b), (c), and (d) by plotting the temperature \(T_j = \beta_j^{-1} = -\varepsilon_0 / \ln z_j\) as a function of \(\ln k_j = (j - 1) \ln m\). A first trivial observation is that \(K\) increases more rapidly when decreasing \(D\) for larger values of \(\alpha\). More interestingly, we observe that for \(\alpha = -2\) [Fig. 1.2(b)], the temperature profile slowly converges to the equilibrium profile \(T_j^{eq} = \beta_j^{-1}\) when \(D \to 0\), while for \(\alpha = 1\) [Fig. 1.2(c) and (d)], it converges to a well-defined nonequilibrium profile, which is linear for \(k_j \lesssim K\) when plotting \(\beta_j\) as a function of \(\ln k_j\) [see Fig. 1.2(c)]. These results can be interpreted as follows. When the transfer mechanism is inefficient at small scales (\(\alpha < -1\)), dissipative scales are not ‘fedded’, so that energy accumulates at large scales, generating an effective equilibrium.
Figure 1.3: $\langle Y \rangle$ as a function of $\alpha$, for $D = 10^{-x}$; $Y$ is defined in Eq. (1.24). The full line is the asymptotic value of $\langle Y \rangle$ for $D \to 0$. Other parameters: same as in Fig. 1.2.

In the opposite case ($\alpha > -1$), the transfer mechanism is efficient at small scales, thus ‘pumping’ energy from large scales to dissipative ones.

The above behavior can be understood using a simpler form of the dissipation, which leads to analytically tractable calculations. Assuming that $\Delta_j = 0$ for all $j < M$, and leaving a nonzero dissipation rate $\Delta_M$ only on the last level $j = M$ of the tree, we get after some calculations [23] the nonequilibrium (inverse) temperature profile

$$\beta_{neq}^j = \frac{1}{\xi_0} (1 + \alpha) \ln k_j + \beta_{ext} + \frac{1}{\xi_0} \ln C,$$

where $C$ is a known constant. Although this profile has been obtained with a simplified version of the model, one sees on Fig. 1.2(c) that $\beta_j$ computed numerically in the original model also converges to $\beta_{neq}^j$. Let us mention that $\beta_{neq}^j$ does not depend on parameters related to dissipation, but only on parameters characterizing injection and transfer. In addition, the temperature profile is continuous with $\alpha$, namely $\beta_j \to \beta_{ext}$ when $\alpha \to -1^+$. To sum up, it turns out that an equilibrium approach to the stationary state of the present model in the weak dissipation limit is meaningful only if $\alpha < -1$. In this case, the probability distribution $P_{st}(\{n_{j,i}\})$ converges, in a weak sense, to the equilibrium distribution of temperature $\beta_{ext}$. In the opposite case $\alpha > -1$, the probability distribution $P_{st}(\{n_{j,i}\})$ converges when $D \to 0$ to a well-defined nonequilibrium probability distribution $P_{neq}(\{n_{j,i}\})$, given by Eqs. (1.16) and (1.23)

$^{1}$In order to discuss the implications of such different behaviors, we now compute the average value of a large scale observable, which is not sensitive to small scale details of the distribution. As an example, we consider the observable $Y$ defined as

$$Y = \sum_{j=1}^{M} \left( \frac{1}{k_j^2} \sum_{i=1}^{n_{j-1}} n_{j,i} \right),$$

Fig. 1.3 illustrates the convergence of $\langle Y \rangle$ as a function of $\alpha$. When $\alpha < -1$, $\langle Y \rangle$ converges to the equilibrium value $\langle Y \rangle_{eq}$. In contrast, for $\alpha > -1$, $\langle Y \rangle$ converges to the nonequilibrium value $\langle Y \rangle_{neq}$ (computed from the distribution $P_{neq}$), which depends on $\alpha$ and thus on the energy transfer.

$^{1}$The zero dissipation limit should however be taken after the infinite size limit; otherwise, equilibrium is recovered.
Chapter 2

Fluctuation-dissipation relations and effective temperatures

The definition of macroscopic quantities that can characterize nonequilibrium systems is a challenging and active field in statistical physics. Several approaches have been proposed in the literature, by generalizing thermodynamic [24] or statistical physics approaches [25, 26, 27, 28, 29]. One of these approaches is based on the possible generalization to nonequilibrium situations of intensive thermodynamic parameters (chemical potential, compactivity...) conjugated to conserved quantities [30, 31, 32, 33]. Such parameters are then defined as the logarithmic derivative of a generalized partition function with respect to the corresponding conserved quantity. Yet, energy is in general not conserved in nonequilibrium systems, and other approaches are necessary in order to define a nonequilibrium temperature. Along this line, the introduction of effective temperatures in nonequilibrium systems through generalized fluctuation-dissipation relations (FDR) has played a major role [34, 26].

In equilibrium the FDR turns out to be a powerful tool to describe the relaxation of slightly perturbed systems towards their equilibrium states. The fluctuation-dissipation theorem relies on the principle that the response of a system in thermodynamic equilibrium to a small perturbation is the same as its response to a spontaneous fluctuation. Accordingly, there is a direct relation between the fluctuation characteristics of the thermodynamic system for a given observable and its linear response. This is a very strong property, because it is valid for all systems in equilibrium, independent of the details of the microscopic dynamics and the observable considered. Hence the relation gives rise to a universal proportionality factor, precisely given by the equilibrium temperature.

However, in a nonequilibrium system this relation is a priori not valid. The theoretical investigation of the breaking of the fluctuation-dissipation theorem in spin-glass systems [35, 34] and in turbulence [36] has stimulated a wide range of experimental and numerical studies aiming to define an effective temperature in many different systems, ranging from granular materials [37, 38, 39, 40] to glasses [41, 42, 43, 44, 45, 46], spin-glasses [47, 48], gels and colloidal suspensions [49, 50, 51], liquid crystals [52], or turbulent flows [53]. Despite the large body of theoretical work devoted to nonequilibrium generalizations of the FDR [34, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72], the question of the observable-dependence of the effective temperature defined from the FDR has mainly been studied case by case in specific models [45, 46, 37, 11, 12, 73, 74, 75, 76], and no clear rationale has been proposed to interpret the observable-dependence.
In this chapter we study, following our recent papers [77, 78], how the characteristics of a nonequilibrium distribution of the microstates influence the possibility to define an observable-independent temperature in the system. We relate the observable-dependence of the FDR-temperature to the “lack of entropy”, defined as the entropy difference between the nonequilibrium distribution and the equilibrium distribution with the same energy. We also observe that the entropy production, which is a natural characterization of nonequilibrium systems [79, 54, 80], seems to bear no systematic relation to the dependence of the temperature on the choice of observable. Our study is however restricted to systems that remain close to an equilibrium state, and where correlation functions decay to zero on a single time scale. Most aging systems [2] are thus excluded from our analysis.

The chapter is organized as follows. In Sect. 2.1 we present the general framework, introducing a generalized fluctuation-dissipation relation and the notion of lack of entropy. We also relate quantitatively the observable-dependence of the effective temperature to the lack of entropy. In Sect. 2.2, this relation is quantitatively illustrated on three different stochastic models. First, an exactly solvable energy transport model on a ring in contact to a reservoir is studied (Sect. 2.2.1). In this model, the internal flux results from the bulk dynamics rather than from an external drive. In the second example, an external drive is introduced (Sect. 2.2.2). More specifically, we consider a fully connected model in contact with two heat baths at slightly different temperatures, resulting in a nonequilibrium steady state [77]. As a last example, we discuss a variant of the latter model, in which the system is connected to a single heat bath at zero temperature (Sect. 2.2.3). This dynamics leads to a slow relaxation towards the ground state, during which the non-stationary distribution can be computed. Finally, Sect. 2.3 summarizes and briefly discusses the obtained results.

2.1 General framework

2.1.1 Evaluation of the response function

We first introduce the form of the generalized fluctuation-dissipation relation, that we use to define the out-of-equilibrium effective temperatures. We shall consider a generic system that is described by a set of $N$ variables $x_i$, $i = 1, \ldots, N$. Since we are interested in the observable-dependence of the effective temperatures we introduce a family of observables $B_p$ indexed by an integer $p$. In analogy to the equilibrium response theory, we are interested in the dynamics of the observables due to the application of a perturbation to a system that is in a nonequilibrium steady state, or relaxing to equilibrium. This response will then be related to the fluctuations in the system in the absence of perturbation. In order to perturb the system, a small external field $h$, conjugated to an observable $M$, can be applied. The following protocol allows for the definition of the linear response of the observable $B_p$ to the external probe field. The field $h$ takes a constant and small non-zero value until time $t_s$, and it is then suddenly switched off. The subsequent evolution of the observable $B_p$ then provides the linear response to the probe field. More precisely, the two-time linear response $\chi_p(t, t_s)$ is defined, for $t > t_s$, as

$$\chi_p(t, t_s) = \frac{\partial}{\partial h} \bigg|_{h=0} \langle \langle B_p(t, t_s) \rangle \rangle,$$  \hspace{1cm} (2.1)

where $\langle \langle \cdots \rangle \rangle$ denotes an average over the dynamics corresponding to the field protocol described above.
The basic idea of the FDR is to relate the linear response function \( \chi_p(t, t_s) \) to the correlation function (computed in the absence of field)

\[
C_p(t, t_s) = \langle (B_p(t) - \langle B_p(t) \rangle) (M(t_s) - \langle M(t_s) \rangle) \rangle .
\] (2.2)

In general, such a relation is not necessarily linear. However, in cases when it is linear, a FDR is said to hold, namely

\[
\chi_p(t, t_s) = \frac{1}{T_p(t_s)} C_p(t, t_s) , \quad t > t_s .
\] (2.3)

The proportionality factor is the inverse of the effective temperature \( T_p \). In equilibrium, \( T_p \) depends neither on time nor on the observable, it is simply the bath temperature. In contrast, out of equilibrium, \( T_p \) can be time-dependent, and it can a priori depend on \( p \), that is, on the observable.

In the specific case of nonequilibrium steady state, the above FDR simplifies to, setting \( t_s = 0 \),

\[
\chi_p(t) = \frac{1}{T_p} C_p(t) ,
\] (2.4)

where \( T_p \) becomes time-independent.

In the following we will consider situations such that a fluctuation-dissipation relation as given in Eq. (2.3) or (2.4) exists, and we shall focus on the possible dependence of \( T_p \) on the choice of the observable \( B_p \). We shall mainly consider steady-state systems, but we will also briefly study a nonstationary model (Sect. 2.2.3), so that we keep a time-dependent formalism. The response of an observable to the perturbation can be formally rewritten using the distribution \( P(\{x_i\}, h, t_s) \) of the microstate \( \{x_i\} \equiv \{x_i, i = 1, \ldots, N\} \) in the presence of the field \( h \). To this aim we express \( \langle \langle B_p(t, t_s) \rangle \rangle \) as

\[
\langle \langle B_p(t, t_s) \rangle \rangle = \int \prod_{i=1}^{N} dx_i dx'_i B_p(\{x_i\}) \times G^0_{t, t_s}(\{x_i\}|\{x'_i\}) P(\{x'_i\}, h, t_s)
\] (2.5)

where \( G^0_{t, t_s}(\{x_i\}|\{x'_i\}) \) is the zero-field propagator, that is the conditional probability to be in a microstate \( \{x_i\} \) at time \( t \) given that the system was in a microstate \( \{x'_i\} \) at time \( t_s \), in the absence of the probe field. Taking the derivative of Eq. (2.5) with respect to \( h \) at \( h = 0 \), and using the relation \( \partial P / \partial h = P \partial \ln P / \partial h \), we get

\[
\chi_p(t, t_s) = \left\langle B_p(t) \frac{\partial \ln P}{\partial h}(\{x_i(t_s)\}, 0, t_s) \right\rangle ,
\] (2.6)

the average being computed at zero field. Similar forms of this expression of the response function can be found in the literature [81, 71, 70, 72]. In the case of a steady-state system, with a distribution \( P(\{x_i\}, h) \), the result does not depend on \( t_s \), so that we set \( t_s = 0 \), yielding

\[
\chi_p(t) = \left\langle B_p(t) \frac{\partial \ln P}{\partial h}(\{x_i(0)\}, 0) \right\rangle .
\] (2.7)
2.1.2 Properties of the phase-space distribution

Uniform distribution on energy shells

In order to go beyond the formal expression (2.6) of the response function, we need to choose a specific form of the distribution \( P(\{x_i\}, h, t_s) \). We first consider the case when the distribution only depends on the total energy \( E_h \), namely

\[
P(\{x_i\}, h, t_s) = Z(t_s)^{-1} \exp\left[-\theta(E_h, t_s)\right],
\]

with \( Z(t_s) \) being the normalization constant. The distribution \( P(\{x_i\}, h, t_s) \) is thus uniform over constant energy surfaces in phase-space for all times. A linear time-independent \( \theta(E_h, t_s) = \beta E + \theta_0 \) corresponds to the equilibrium canonical ensemble. However, we consider here the more general case of a regular function \( \theta(E_h, t_s) \) monotonically increasing with the total energy. It is easy to check that for \( h = 0 \),

\[
\frac{\partial \ln Z}{\partial h} = \langle M \theta' \rangle = 0,
\]

so that \( \frac{\partial \ln P}{\partial h} = M \theta' \), where \( \theta' \) is the derivative of \( \theta \) with respect to the total energy. For a macroscopic system, the average in Eq. (2.6) is dominated by the most probable energy level \( E^*(t_s) \). From a saddle-point evaluation, we obtain

\[
\chi_p(t, t_s) = \frac{\partial \theta}{\partial E}(E^*(t_s), t_s) C_p(t, t_s).
\]

Hence a fluctuation-dissipation temperature

\[
T_{FD}(t_s) = \left( \frac{\partial \theta}{\partial E}(E^*(t_s), t_s) \right)^{-1},
\]

independent of the observable, can be defined. As the value \( E^*(t_s) \) maximizes the energy distribution \( \rho(E, t_s) \propto \exp[\theta(E, t_s)] \), where \( \theta \) is the microcanonical entropy, it turns out that

\[
\frac{\partial \theta}{\partial E}(E^*(t_s), t_s) = S'(E^*(t_s)),
\]

so that the standard definition of temperature is recovered.

Beyond uniformity: the lack of entropy

In a more general situation, the distribution \( P(\{x_i\}, h, t_s) \) is not uniform over the shells of constant energy, and the above simplification does not occur, leading generically to an observable dependence of the fluctuation-dissipation temperature \(^1\). The above remarks suggest that this dependence on the observable could be related to a macroscopic quantity, namely the Shannon entropy difference between the stationary state and the equilibrium state with the same average energy. When the distribution is uniform over the most probable energy shell, the entropy is maximal, so that a non-uniform state necessarily corresponds to a lower entropy. The entropy difference may thus be interpreted as a measure of the deviation from equilibrium.

In the rest of this section, we focus on steady-state distributions in order to simplify the notations, but our argument can straightforwardly be extended to situations where the distribution \( P(\{x_i\}, h, t_s) \) depends on time. As a general framework, we consider in the following a class of stochastic markovian models, where an energy \( E = \sum_{i=1}^{N} \varepsilon_h(x_i) \) is exchanged in a random way between the internal degrees of freedom. Either the internal dynamics, or in more realistic scenarios additional external sinks and sources, drive the system into a nonequilibrium steady state. The resulting drive can be encompassed by a dimensionless parameter \( \gamma \), like a normalized temperature difference or external force. Note that in some cases the parameter \( \gamma \) may be the square of the physical driving force, as we define \( \gamma \) as the order of magnitude of the leading correction to the

\(^1\)If the FDR is non linear, the fluctuation-dissipation temperature is not even defined for a given observable.
equilibrium distribution (see below). In the absence of driving \((\gamma = 0)\), detailed balance is satisfied and the system is described by an equilibrium distribution

\[
P_{\text{eq}}(\{x_i\}, h) = Z_N^{-1} \exp \left(-\beta \sum_{i=1}^{N} \varepsilon_h(x_i)\right)
\]  

(2.10)

where \(\beta = 1/T\) is the inverse temperature of the thermal bath, and \(Z_N\) is the canonical partition function.

As a simplification, we assume that the \(N\)-body steady-state distribution \(P(\{x_i\}, h)\) can be factorized according to \(P(\{x_i\}, h) = \prod_{i=1}^{N} p(x_i, h)\), meaning that the degrees of freedom are statistically independent. The system can thus be fully described by means of the single-variable probability distribution \(p(x, h)\). We now consider the small driving limit \(|\gamma| \ll 1\), and expand \(p(x, h)\) around the equilibrium distribution \(p_{\text{eq}}(x, h) = Z_1^{-1} \exp\left[-\beta \varepsilon_h(x)\right]\) as

\[
p(x, h) = p_{\text{eq}}(x, h) \left[1 + \gamma F(\varepsilon_h(x)) + \mathcal{O}(\gamma^2)\right].
\]  

(2.11)

Such a perturbation is consistent with some recent generic results on nonequilibrium distributions [82]. The constraints of normalization of \(p(x, h)\) and \(p_{\text{eq}}(x, h)\) imply that \(\langle F(\varepsilon) \rangle_{\text{eq}} = 0\), where \(\varepsilon\) is a shorthand notation for \(\varepsilon_h(x)\) and \(\langle \cdots \rangle_{\text{eq}}\) denotes the equilibrium average. If \(p(x, h)\) follows Eq. (2.11), the factorized \(N\)-body distribution \(P(\{x_i\}, h)\) is generically not a function of the total energy \(E = \sum_{i=1}^{N} \varepsilon_h(x_i)\), so that \(P(\{x_i\}, h)\) is not uniform over the shells of constant energy. It follows that the nonequilibrium Shannon entropy is lower than the entropy of the reference equilibrium state having the same energy. Accordingly, the entropy difference between the equilibrium and nonequilibrium states with the same average energy provides a characterization of the deviation from equilibrium. To determine the entropy difference, we compute the average energy \(E(\beta, \gamma)\) of the out-of-equilibrium system, and we evaluate the temperature \(\beta^*\) for which \(E(\beta, \gamma) = E_{\text{eq}}(\beta^*)\), where \(E_{\text{eq}}(\beta^*)\) is the equilibrium energy at temperature \(\beta^*\). As the distribution \(P(\{x_i\}, h)\) is factorized, the Shannon entropy of the whole system is simply computed as the sum of the entropies associated to each variables \(x_i\). Hence only the Shannon entropy associated to a single degree of freedom,

\[
S = - \int dx \, p(x, h) \ln p(x, h),
\]  

(2.12)

needs to be computed. We denote by \(S_{\text{eq}}(\beta)\) the equilibrium entropy at temperature \(\beta\), and by \(S(\beta, \gamma)\) the entropy in the nonequilibrium steady-state characterized by \(\beta\) and \(\gamma\). We then define the entropy difference \(\Delta S\) per degree of freedom through the relation

\[
\Delta S = S_{\text{eq}}(\beta^*) - S(\beta, \gamma).
\]  

(2.13)

A rather straightforward calculation yields (see [78] for details):

\[
\Delta S = \frac{\gamma^2}{2} \left( \langle F(\varepsilon)^2 \rangle_{\text{eq}} - \langle \varepsilon \rangle_{\text{eq}}^2 \langle F(\varepsilon) \rangle_{\text{eq}}^2 \right).
\]  

(2.14)

We have checked [78] that \(\Delta S \geq 0\) as expected, even though this property does not appear explicitly in Eq. (2.14). In the case of a linear \(F(\varepsilon)\), one finds \(\Delta S = 0\), which can be understood from the fact that the distribution \(p(x, h)\) can be recast into an effective equilibrium form –see Eq. (2.11). Considering now a generic function \(F(\varepsilon)\), we parameterize it as

\[
F(\varepsilon) = a + b \varepsilon + \eta f(\varepsilon),
\]  

(2.15)
where \( \eta \) characterizes the amplitude of the nonlinearity. The normalization condition \( \langle F(\varepsilon) \rangle_{\text{eq}} = 0 \) fixes the value of the parameter \( a \). We then obtain the generic result

\[
\Delta S = \gamma^2 \eta^2 \omega ,
\]

where \( \omega \) is a constant which depends on the detailed expression of the functions \( f(\varepsilon) \) and \( \varepsilon_h(x) \). As an example, considering a nonlinearity of the form \( f(\varepsilon) = \varepsilon^2 \) and a zero-field local energy \( \varepsilon_0(x) = \frac{1}{2}x^2 \), one finds

\[
\Delta S = \frac{3\gamma^2 \eta^2}{4\beta^4} .
\]

### 2.1.3 Fluctuation-dissipation relation and effective temperatures

We now proceed to derive the FDR associated to the variable \( B_p \), and to analyze the dependence of the effective temperature on \( p \). To this aim, we further restrict the class of models considered by making an additional simplification. Namely, we assume that each time a variable \( x_i \) is modified by a dynamical event, its new value is decorrelated from the previous one. Examples of models satisfying this assumption are given below (see also [57]). Qualitatively, such an assumption can be interpreted as a coarse-graining of the dynamics on a time scale of the order of the correlation time of the system. Note that we focus here on systems with a single relaxation time scale, so that the present approach does not necessarily apply to systems with a more complex dynamics involving different time scales, like glassy systems. This assumption of local decorrelation implies that the correlation function \( C_p(t) \) is proportional to the persistence probability \( \Phi(t) \) [57], defined as

\[
\Phi(t) = \left\langle \frac{1}{N} \sum_{i=1}^{N} \phi_i(t) \right\rangle ,
\]

where the history-dependent local random variables \( \phi_i(t) \) are equal to 1 if no redistribution involving site \( i \) occurred between \( t = 0 \) and \( t \), and are equal to 0 otherwise. As a consequence we can express the different averages involved in expressions (2.2) and (2.7) in terms of \( \Phi(t) \).

We expand the local energy \( \varepsilon_h(x) \) for small field \( h \), namely \( \varepsilon_h(x) = \varepsilon_0(x) - h\psi(x) + \mathcal{O}(h^2) \), assuming \( \psi(x) \) to be an odd function. It follows that the observable \( M \), conjugated to the field \( h \), is defined as

\[
M = \sum_{i=1}^{N} \psi(x_i) .
\]

For the family of observables \( B_p \), we choose the following definition:

\[
B_p = \sum_{i=1}^{N} x_i^{2p+1}
\]

with \( p \geq 0 \) an integer number. In this way, \( B_p \) has a zero mean value in the absence of the field, which slightly simplifies the calculations.

Using the fact that the random variables \( x_i \) and \( x_j \) are independent for \( i \neq j \), and that \( \langle B_p \rangle = \langle M \rangle = 0 \), one can simplify the expression (2.2) for the correlation function, leading to

\[
C_p(t) = N \langle x(t)^{2p+1} \psi(x(0)) \rangle .
\]
Further using the assumption of decorrelation by the local dynamical events, we get

\[ C_p(t) = N \langle x^{2p+1} \psi(x) \rangle \Phi(t) \, . \] (2.22)

The average in the last expression is performed on the steady-state distribution. From Eq. (2.7), the response function can also be evaluated using the decorrelation assumption, yielding

\[ \chi_p(t) = N \left[ \beta \langle x^{2p+1} \psi(x) \rangle - \gamma \langle x^{2p+1} \psi(x) F'(\varepsilon_0) \rangle \right] \Phi(t) \] (2.23)

where \( \varepsilon_0 \) is a simplified notation for \( \varepsilon_0(x) \). The average in the second term can be replaced by the equilibrium average, neglecting higher order terms in \( \gamma \). One can then express \( \Phi(t) \) as a function of \( C_p(t) \) from Eq. (2.22), which leads to a FDR of the form (2.4). The corresponding temperature \( \beta_p = T_p^{-1} \) is given by

\[ \beta_p = \beta - \gamma \frac{\langle x^{2p+1} \psi(x) F'(\varepsilon_0) \rangle_{eq}}{\langle x^{2p+1} \psi(x) \rangle_{eq}} \, . \] (2.24)

As anticipated, the \( p \)-dependence in Eq. (2.24) does not cancel in general, so that the temperature \( T_p \) generically depends on the observable. A notable exception is the case of a linear \( F(\varepsilon) \), namely \( F(\varepsilon) = a + b\varepsilon \), where the effective temperature \( \beta_p = \beta - \gamma b \) is observable independent.

When \( F(\varepsilon) \) has a nonlinear contribution, parameterized as \( F(\varepsilon) = a + b\varepsilon + \eta f(\varepsilon) \), the temperature difference between two distinct observables is proportional to the amplitude \( \eta \) of the nonlinearity. More precisely, one finds from Eq. (2.24) that

\[ |\beta_p - \beta_0| = \kappa_p \sqrt{\Delta S} \, , \] (2.26)

where we have introduced a dimensionless and positive constant \( \kappa_p \). This constant a priori depends on \( p \), as well as on the functional forms of \( f(\varepsilon) \) and of the local energy \( \varepsilon_h(x) \). Note however that \( \kappa_p \) does not depend on \( \gamma \) and \( \eta \). In the following section, we give two examples of models for which \( \kappa_p \) can be determined exactly.

From the above analysis, it turns out that the dependence of the fluctuation-dissipation temperature on the choice of observable is a direct measure of the deviation from equilibrium. As already mentioned, the above argument can be generalized to time-dependent probability distributions. In this case, \( \beta_p \), \( \kappa_p \), and \( \sqrt{\Delta S} \) may all depend on time. Let us however emphasize again that the main assumptions made, namely that the distribution remains close to some equilibrium state, and that local decorrelation occurs in a single step, may not apply to glassy systems.
Figure 2.1: Left: Scheme of the energy transport model on a ring in contact with a bath at temperature $T$. Energy is injected from the bath to the ring with rate $J(\mu)$ and dissipated from the ring to the bath with rate $\varphi(\mu|\epsilon)$. Right: Internal dynamics of the ring. An fraction $\mu$ of the local energy $\epsilon_i = \frac{x^2_i}{2}$ is transported from site $i$ to site $i+1$ on the ring according to the transport rate $\varphi(\mu|\epsilon_i)$.

2.2 Illustration on simple models

2.2.1 A simple energy transfer model on a ring

Model and steady-state solution

To illustrate the above results let us consider as a first example an energy transfer model on a ring geometry that is connected to a bath with temperature $T$ (see Fig. 2.1). The model is defined on a one-dimensional lattice with periodic boundary conditions. To every site $i$, $i=1\ldots N$, is attached a real quantity $x_i$, associated to a local energy $\epsilon_i = \frac{x^2_i}{2}$. A fraction $\mu$ of the local energy $\epsilon_i$ is transferred from site $i$ to site $i+1$, according to the site independent rate

$$\varphi(\mu|\epsilon_i) = v(\mu) \frac{g(\epsilon_i - \mu)}{g(\epsilon_i)}, \quad g(\rho) = \rho^\delta - 1,$$

(2.27)

with $\delta > 0$, and $v(\mu)$ an arbitrary positive function. After the transport, the new variables denoted as $x'_i$ and $x'_{i+1}$ take the values

$$x'_i = \pm \sqrt{x_i^2 - 2\mu}, \quad x'_{i+1} = \pm \sqrt{x_{i+1}^2 + 2\mu},$$

(2.28)

with equiprobable and uncorrelated random signs. We consider a continuous time dynamics, where sites are updated in an asynchronous way. As can be easily checked, these transport rules locally conserve the energy. The choice of the function $g(\rho)$ entering the transport rates also ensures that the system remains homogeneous (no condensation occurs) [83].

In addition, each site $i$ of the system is also connected to an external heat bath at temperature $T$, according to the following dynamics. An amount of energy $\mu$ is injected from the bath with a probability rate $J(\mu)$ given by

$$J(\mu) = v(\mu)e^{-\mu/T}.$$  

(2.29)

Energy is transferred back to the bath with the same energy transport rate $\varphi(\mu,\epsilon_i)$ as for the internal transport.
Given this dynamics, the steady-state probability distribution for a microscopic state \( \{x_i\} \) takes the factorized form
\[
P_0(\{x_i\}) = \frac{1}{Z_N} \prod_{i=1}^{N} \left\{ |x_i| g \left( \frac{x_i^2}{2} \right) \right\} e^{-\frac{1}{T} \sum_i \frac{1}{2} x_i^2} ,
\]
(2.30)
with \( Z_N \) the normalization factor of the distribution, and where the index 0 indicates a zero-field dynamics.

In the following, we show that the temperature defined from the FDR does not necessarily coincide with the bath temperature, consistently with Sect. 2.1 and with the results obtained in a similar model [57]. The two temperature definitions become equivalent only for the special choice \( \delta = 1/2 \) in the transport rates (2.27), when the probability distribution has an equilibrium form.

Fluctuation-dissipation relations

To relate the spontaneous fluctuations present in this stochastic system to the response of an observable to a small perturbation, let us introduce an external field \( h(t) \) perturbing the system. A natural way to couple the field to the system is to add to the energy a linear term proportional to the external field:
\[
E_h = \sum_{i=1}^{N} \frac{1}{2} x_i^2 - h \sum_{i=1}^{N} x_i + \frac{N h^2}{2} = \sum_{i=1}^{N} \frac{1}{2} (x_i - h)^2 ,
\]
(2.31)
where we included for convenience an additional shift to the energy \( Nh^2/2 \) which is only changing the reference of the energy scale without loss of generality. Note that Eq. (2.31) implies \( \psi(x) = x \) and \( M = \sum_{i=1}^{N} x_i \). Introducing the new variables \( v_i = x_i - h \) we ask that they obey the same dynamics as the former variables \( x_i \), that are given in Eqs. (2.27) and (2.28). Further we assume the same protocol for the externally applied perturbation as described in the previous section: the field \( h(t) \) is non-zero at times \( t < 0 \), but small in comparison to the mean value \( \langle x \rangle \) of the variables. We assume that the nonequilibrium steady state is established for \( t < 0 \). At time \( t = 0 \) the field is switched off in order to analyze the response of an observable \( B_p(t) \) to this variation of the field.

Following Sect. 2.1, we consider the observables \( B_p \) defined as \( B_p = \sum_{i=1}^{N} x_i^{2p+1} \), with \( p \) a positive integer number. Given that the distribution (2.30) is factorized, the results of Sect. 2.1 can be applied, and the steady-state correlation function \( C_p(t) = \langle B_p(t) M(0) \rangle \) (we recall that \( \langle B_p \rangle = \langle M \rangle = 0 \)) is given by
\[
C_p(t) = N \langle x(t)^{2p+1} x(0) \rangle .
\]
(2.32)
To obtain the general formulation of the response function we use expression (2.7) with \( P(\{x_i(0)\}, h) \) being the distribution for the nonequilibrium steady state in the presence of the field \( h \). This distribution is given by (2.30) with respect to the new variables \( v_i = x_i - h \), namely \( P(\{x_i(0)\}, h) = P_0(\{v_i(0)\}) \), meaning that the dynamics of the variables \( \{x_i\} \) in the presence of the field \( h \) can be effectively described as a zero-field dynamics, once expressed in terms of the variables \( \{v_i\} \).

For arbitrary values of the integer \( p \geq 0 \), we obtain the following relation between the response and the correlation in the system for the observable \( B_p(t) \) (details are given in Appendix [78]):
\[
\chi_p(t) = \frac{2p+1}{2(p+\delta)} \frac{1}{T} C_p(t) .
\]
(2.33)
The temperature defined by the fluctuation-dissipation relation generically depends on $p$ and therefore on the observable chosen

$$T_p = \frac{2(p + \delta)}{(2p + 1)} T.$$  \hfill (2.34)

Only for $\delta = 1/2$, when the energy distribution (2.30) is uniform, the temperature takes independently of the observable the value $T_p = T$. But for non-uniform energy distributions, the temperature determined from the slope of the FDR depends on the observable and is therefore not well-defined.

To study the weakly nonequilibrium regime, we consider values of $\delta$ close to the equilibrium value $\delta = 1/2$, namely $\delta = 1/2 + \gamma$ with $|\gamma| \ll 1$. We find for the linear correction $F(\varepsilon)$ to the probability distribution $p(x, h)$, as defined in Eq.(2.11), the following expression:

$$F(\varepsilon) = \ln \varepsilon + C_\beta,$$  \hfill (2.35)

where $C_\beta = \ln \beta - \psi_0(1/2)$, and $\psi_0$ denotes the digamma function, defined as the logarithmic derivative of the Euler gamma function (numerically, $\psi_0(1/2) \approx -1.963$). Knowing $F(\varepsilon)$ then allows for the determination of all important quantities, necessary for the establishment of the crucial relation (2.26). Thus we end up with a quantitative expression of the observable-dependence of the FDR-temperature in terms of the lack of entropy. From Eq. (2.24), the observable dependence can be expressed through

$$\frac{|\beta_p - \beta_0|}{\beta} = |\gamma| \frac{4p}{2p + 1}.$$  \hfill (2.36)

Besides, the entropy difference can be evaluated from Eq. (2.14), yielding

$$\Delta S = \frac{\gamma^2}{2} \left[ \langle (\ln \varepsilon + C_\beta)^2 \rangle - 2\beta^2 \langle \varepsilon (\ln \varepsilon + C_\beta) \rangle^2 \right]$$

$$= \frac{\gamma^2}{2} \left[ \psi_0' \left( \frac{1}{2} \right) - 2 \right], \hfill (2.37)$$

where $\psi_0'$ is the derivative of $\psi_0$. Numerically, we find $\Delta S/\gamma^2 \approx 1.467$. From the relation (2.26), we then get

$$\kappa_p = \frac{4p}{2p + 1} \left[ \frac{2}{\psi_0' \left( \frac{1}{2} \right) - 2} \right]^{1/2}, \hfill (2.38)$$

which is, as expected, independent of the physical parameters of the system, like the driving $\gamma$ and the temperature $\beta$.

**Discussion of the transport model results**

We learn from the study of this exactly solvable transport model several interesting facts. First, this model illustrates explicitly how a probability distribution that is not uniform on energy shells (namely, $\delta \neq 1/2$) leads to a FDR-temperature which depends on the observable. The results for expression (2.26), that uniquely depend on the form of the probability distribution, do not depend on the energy flux in the system. Therefore the energy flux in the bulk of the system does not play a crucial role for the results. We chose the rules of the dynamics such that the transport of energy
is totally biased. But it is known that the symmetric case, where energy is transported with the same probability to the left or to the right, leads to exactly the same probability distribution for the microstates [83]. More precisely the distribution only depends on the transport rates, but the direction of the transport, that defines the total flux, is not of any influence.

Further, it is interesting to compare the characterization in terms of $\Delta S$ with that in terms of entropy production. On general grounds, the entropy production $\sigma_s$ can be defined from a balance equation involving rate of entropy change, and the entropy fluxes with the reservoirs to which the system is connected:

$$\frac{dS}{dt} = \sum_{i=1}^{n} \frac{J_i}{T_i} + \sigma_s,$$

where $J_i$ is the energy flux exchanged with the $i^{th}$ bath at temperature $T_i$. In the present model, the steady-state implies $dS/dt = 0$. The system is in contact with a single bath, and the energy flux $J$ is zero. Thus the entropy production is also equal to zero. This means that in the framework of this model the entropy production cannot give any information about the observable dependence of the effective temperature in the system.

In the next section we present a different situation, where the nonequilibrium character no longer results from an artificial bulk dynamics, but rather from an external drive.

### 2.2.2 Fully connected model driven by two heat baths

**Model and evolution equation**

In general we would expect that the non-uniformity of the probability distribution results from the fact that the system is externally driven into a nonequilibrium steady state, for example by two reservoirs at different temperatures [77]. In the following we consider a model with $N$ fully connected sites, associated to variables $x_i$, such that the local energy $\varepsilon_i = \frac{1}{2}(x_i - h)^2$ can be transferred between any pair of sites and with two different thermal baths. A sketch of the model is shown on Fig. 2.2. Energy transfers correspond to the dynamical rules (2.28) in terms of variables $x_i$. An amount of energy $\mu$ is transferred from an arbitrary site $i$, with energy $\varepsilon_i$, to any other site $j$ with a rate

$$\varphi(\mu|\varepsilon_i) = \frac{g(\varepsilon_i - \mu)}{g(\varepsilon_i)} , \quad g(\rho) = \rho^{-\frac{1}{2}} .$$

![Diagram of the fully connected model](image-url)
Such a rate is similar to the rate (2.27) for $\delta = 1/2$ and $\nu(\mu) = 1$. The value $\delta = 1/2$ is chosen such that equilibrium is recovered when the two baths have the same temperature. Energy is transferred to the baths with the same rate (2.40) as in the bulk, but weighted with a factor $\nu$ characterizing the coupling strength between the baths and the system. The injection from the bath is defined as the transfer, with a rate $\nu\varphi(\mu|\varepsilon)$, from an equilibrated site having a distribution $P_{\text{eq}}(\varepsilon, \beta_\alpha)$ at inverse temperature $\beta_\alpha$, leading to

$$J_\alpha(\mu) = \nu \int_\mu^\infty d\varepsilon \varphi(\mu|\varepsilon) P_{\text{eq}}(\varepsilon, \beta_\alpha).$$  

(2.41)

A straightforward calculation then yields

$$J_\alpha(\mu) = \nu e^{-\beta_\alpha \mu}.$$  

(2.42)

At this stage, it is convenient to describe the dynamics in terms of the local energy $\varepsilon_i$ rather than with the variables $x_i$. In the thermodynamic limit $N \to \infty$, the master equation governing the $N$-body distribution can be recast into a nonlinear evolution equation for the one-site probability distribution $P(\varepsilon)$, namely

$$\frac{\partial P(\varepsilon, t)}{\partial t} = \int_0^\varepsilon d\mu \left( J_1(\mu) + J_2(\mu) \right) P(\varepsilon - \mu, t) - \int_0^\infty d\mu \left( J_1(\mu) + J_2(\mu) \right) P(\varepsilon, t)$$

$$+ (2\nu + 1) \int_0^\infty d\mu \varphi(\mu|\varepsilon + \mu) P(\varepsilon + \mu, t) - (2\nu + 1) \int_0^\varepsilon d\mu \varphi(\mu|\varepsilon) P(\varepsilon, t)$$

$$+ \int_0^\varepsilon d\mu \varphi_{\text{in}}(\mu, t) P(\varepsilon - \mu, t) - \int_0^\infty d\mu \varphi_{\text{in}}(\mu, t) P(\varepsilon, t).$$  

(2.43)

The distribution $\varphi_{\text{in}}(\mu, t)$ accounts for the energy transfer coming from all the other sites, given by the averaged transport rate $\varphi(\mu|\varepsilon)$:

$$\varphi_{\text{in}}(\mu, t) = \int_\mu^\infty d\varepsilon \varphi(\mu|\varepsilon) P(\varepsilon, t).$$  

(2.44)

The local energy distribution $P(\varepsilon, t)$ is related to the distribution $p(x, h, t)$ through

$$p(x, h, t) = \frac{1}{2} P(\varepsilon, t) \left| \frac{d\varepsilon_h}{dx} \right|$$  

(2.45)

where $\varepsilon = \varepsilon_h(x) = \frac{1}{2}(x - h)^2$.

**Stationary distribution for a small bath temperature difference**

In order to determine the steady-state distribution of the model, we consider the case of a small temperature difference $|\beta_1 - \beta_2| \ll (\beta_1 + \beta_2)/2$, and parameterize the bath temperatures as $\beta_1 = \beta(1 - \lambda)$ and $\beta_2 = \beta(1 + \lambda)$, with $\lambda \ll 1$. We then assume that the stationary distribution $P(\varepsilon)$ has an analytical expansion as a function of $\lambda$. The linear term in $\lambda$ is excluded by a simple symmetry argument: exchanging the two bath temperatures changes $\lambda$ into $-\lambda$, but should not modify the distribution $P(\varepsilon)$ since the two heat baths play a symmetric role. The leading correction should thus behave as $\lambda^2$, so that $P(\varepsilon)$ can be written as

$$P(\varepsilon) = P_{\text{eq}}(\varepsilon) \left[ 1 + \lambda^2 F(\varepsilon) + \mathcal{O}(\lambda^4) \right],$$  

(2.46)
Figure 2.3: Test of the analyticity of $P(\varepsilon)$. Numerical simulations of the fully connected model show that the curves for $[P(\varepsilon) - P_{eq}(\varepsilon)]/\lambda^2$ match to a very good accuracy for small values of $\lambda$, justifying the assumption of analyticity of the $\lambda$-expansion made in Eq. (2.46). Parameter values: $\nu = 1$, $\beta = 1$, $T_{\text{max}} = 10^8$.

in analogy to expression (2.11) with $\gamma = \lambda^2$. The distribution

$$P_{eq}(\varepsilon) = \sqrt{\frac{\beta}{\pi}} e^{-\frac{1}{\beta} e^{-\beta \varepsilon}}$$  \hspace{1cm} (2.47)

is the known equilibrium distribution, namely the stationary solution of the equation (2.43) for $\beta_1 = \beta_2 = \beta$. The scaling form (2.46) is validated by numerical simulations, as shown on Fig. 2.3.

The function $F(\varepsilon)$ determined from numerical data is also shown in Fig. 2.4 for different values of the coupling strength $\nu$. The numerical results were obtained by directly simulating the stochastic dynamics, on a system of size $N = 102$. Such a relatively small size allows for long time averaging, over time $T_{\text{max}}$ of the order of $10^7$ or $10^8$, in order to reach a sufficient statistics. Note that the time unit is defined in such a way that all sites have typically experienced about one redistribution event in a unit of time.

It can be checked that Eq. (2.43) has no exact solution involving a finite polynomial function $F(\varepsilon)$. To find the best polynomial approximation $F^{(L)}(\varepsilon)$ at a given order $L$ we use a variational procedure, as detailed in [78]. We approximate the function $F(\varepsilon)$ by a polynomial of order $L$, $F^{(L)}(\varepsilon) = \sum_{n=0}^{L} a_n^{(L)} \beta^n \varepsilon^n$. The best approximation is then obtained analytically by minimizing the error, under the constraints of normalization and zero net flux with the baths, in the evolution equation (2.43) linearized with respect to the parameter $\gamma = \lambda^2$. The error is defined as the equilibrium average of the square of the r.h.s. in the linearized equation.

If we use for example $F^{(2)}(\varepsilon)$ to approximate $F(\varepsilon)$, the normalization constraint and the constraint of zero net flux in the system yields for the coefficients $a_0^{(2)}$ and $a_1^{(2)}$ [78]:

$$a_1^{(2)} = \frac{3}{2} - 4a_2^{(2)}, \hspace{0.5cm} a_0^{(2)} = -\frac{3}{4} + \frac{5}{4} a_2^{(2)}.$$

Hence the only remaining free parameter is $a_2^{(2)}$. Minimizing the error with respect to $a_2^{(2)}$ yields an analytic expression for the coefficient $a_2^{(2)}$ as a function of the coupling strength $\nu$ [78]

$$a_2^{(2)}(\nu) = \frac{3\nu(7 + 37\nu)}{13 + 136\nu + 358\nu^2}.$$

(2.49)
Note that in the limit of small $\nu$ this expression vanishes linearly in $\nu$, whereas the coefficients $a_0^{(2)}$ and $a_1^{(2)}$ take the finite values $-\frac{3}{4}$ and $\frac{3}{2}$ respectively.

Similarly, one can find analytically higher order approximations for $F(\varepsilon)$. Through this procedure we find that for approximations with $L > 2$ the coefficients $a_k^{(L)}$, $k > 2$, in the expansion are numerically small, as illustrated in Fig. 2.4 (right). A second order polynomial is thus already a good approximation of $F(\varepsilon)$ for $\nu \lesssim 1$ [see Fig. 2.4 (left)]. Taking into account higher order terms in $F(\varepsilon)$, we find that the relation (2.26) between the observable dependence and the entropy difference is satisfied to a good accuracy, as seen in Fig. 2.5. We have also checked for $L \leq 5$ that in the limit $\nu \to 0$, the coefficients $a_k^{(L)}$, $k > 1$ vanish while $a_0^{(L)} \to -\frac{3}{4}$ and $a_1^{(L)} \to \frac{3}{2}$.

**Observable-dependence and its relation to the lack of entropy**

In terms of the variable $x$, the stationary one-body distribution $p(x, h)$ reads, to second order in $\lambda$

$$p(x, h) = \sqrt{\frac{\beta}{2\pi}} e^{-\frac{1}{2} \beta (x-h)^2} \left[ 1 + \lambda^2 F \left( \frac{1}{2} (x-h)^2 \right) \right]. \quad (2.50)$$

Following our standard procedure, we introduce the response $\chi_p(t)$ of the observable $B_p$ to a small perturbing field $h$. From Sect. 2.1 we know how to obtain the FDR-temperature and the entropy difference using the correction $F(\varepsilon)$. As shown above $F(\varepsilon)$ can be well approximated by a quadratic function $F^{(2)}(\varepsilon) = a_0^{(2)} + a_1^{(2)} \beta \varepsilon + a_2^{(2)} \beta^2 \varepsilon^2$. Consequently we obtain for the observable-dependent inverse temperature, using Eq. (2.24) with $\psi(x) = x$

$$\beta_p = \beta - \lambda^2 \frac{\langle \varepsilon^{p+1} (a_1^{(2)} + 2a_2^{(2)} \beta \varepsilon) \rangle_{eq}}{\langle \varepsilon^{p+1} \rangle_{eq}} \quad (2.51)$$

leading to

$$\frac{|\beta_p - \beta_0|}{\beta} = 2p\lambda^2 |a_2^{(2)}|. \quad (2.52)$$
The calculation of $\Delta S$ using Eq. (2.14) with $F^{(2)}(\varepsilon)$ is also simple, involving averages of different powers of the energy, and the result takes the form

$$\Delta S = \frac{3}{4} \lambda^4 (\sigma_2(2))^2.$$  

Thus we obtain for the relation between the entropy difference $\Delta S$ and observable-dependence of the temperature

$$\frac{|\beta_p - \beta_0|}{\beta} = \frac{4p}{\sqrt{3}} \sqrt{\Delta S}$$

in agreement with the general results presented in Section 2.1 –see Eq. (2.26).

**Discussion of the fully-connected model**

The study of this model shows that observable dependence occurs as soon as the dynamics results in non-uniform probability distributions for the microstates. Further it is again possible to use the proposed general approach to characterize this non-uniformity by the entropy difference $\Delta S$. For small driving we find a direct relation between this entropy difference and the observable dependence (2.54). The proportionality factor turns out to be independent of the coupling strength and the driving parameter. However, in the zero coupling limit, where $F(\varepsilon)$ becomes linear, both $\Delta S$ and $|\beta_p - \beta_0|/\beta$ vanish, meaning that for small coupling we expect no observable dependence.

To compare these results with the information given by the entropy production $\sigma_s$ we calculate the total energy fluxes caused by the contact to the different baths. We denote as $J_{\text{out}}$ the total energy flux transferred from the systems to both heat baths, and by $J_{\text{in}}$ the total flux injected by the baths. In steady state, one has $|J_{\text{out}}| = |J_{\text{in}}|$. The flux $J_{\text{in}}$ is computed as

$$J_{\text{in}} = \int_0^\infty d\mu (J_1(\mu) + J_2(\mu)) \mu.$$  

Expanding the above integral to second order in $\lambda$, we obtain

$$J_{\text{in}} = \frac{\nu}{\beta^2} \left[ 2 + 6\lambda^2 + \mathcal{O}(\lambda^4) \right].$$  

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A similar calculation yields for the net energy fluxes $J_\alpha$ exchanged by the bath $\alpha$ with the system

$$J_1 = \int_0^\infty d\mu J_1(\mu) - \frac{1}{2} |J_{\text{out}}|$$

$$= 2\frac{\lambda \nu}{\beta^2} + O(\lambda^3)$$

(2.57)

$$J_2 = \int_0^\infty d\mu J_2(\mu) - \frac{1}{2} |J_{\text{out}}|$$

$$= -2\frac{\lambda \nu}{\beta^2} + O(\lambda^3) .$$

(2.58)

These results lead to an entropy production

$$\sigma_s = -(\beta_1 J_1 + \beta_2 J_2) = \frac{4\nu \lambda^2}{\beta} .$$

(2.59)

Hence we can relate $|\beta_p - \beta_0|$ to the entropy production as follows:

$$\frac{|\beta_p - \beta_0|}{\beta} = \zeta(\nu) \frac{p \beta}{2} \sigma_s$$

(2.60)

with $\zeta(\nu) = |a_2^{(2)}(\nu)|/\nu$, the coefficient $a_2^{(2)}(\nu)$ being given in Eq. (2.49). Consequently in the framework of this model it is possible to relate the dependence of the temperature on the observable to the entropy production.

The quantity $|\beta_p - \beta_0|/\beta$ results linear in $\sigma_s$ in contrast with the characterization through the entropy difference –see Eq. (2.54). Similarly to Eq. (2.54) the proportionality factor does not depend on the bath temperature difference $\lambda$. But contrary to the characterization via the lack of entropy, the coupling strength $\nu$ now enters into relation (2.60). Hence the entropy difference $\Delta S$ seems to be more directly related to $|\beta_p - \beta_0|$ than the entropy production $\sigma_s$. Note however that in the small coupling limit $\zeta(\nu)$ becomes a constant, so that the dependence upon the coupling constant disappears in this limit.

### 2.2.3 Slow relaxation model

**Model and time dependent probability distribution**

The former results seem to indicate that in the case of driven systems the observable dependence is a direct result of the non-uniformity of the phase space distribution. In Sect. 2.1, we argued that
such results also hold in the time-dependent case. In the following we will investigate a similar fully connected model as in the above example, but put into contact with a single heat bath at zero temperature (see Fig. 2.6). Interestingly this model can be solved exactly in the non-stationary regime. In this case the evolution equation for the probability distribution of the microstates in the thermodynamic limit reads

\[
\frac{\partial P(\varepsilon, t)}{\partial t} = (\nu + 1) \int_0^\infty d\mu \varphi(\mu | \varepsilon + \mu) P(\varepsilon + \mu, t) \\
- (\nu + 1) \int_0^\varepsilon d\mu \varphi(\mu | \varepsilon) P(\varepsilon, t) \\
+ \int_0^\varepsilon d\mu \varphi_{in}(\mu, t) P(\varepsilon - \mu, t) \\
- \int_0^\infty d\mu \varphi_{in}(\mu, t) P(\varepsilon, t),
\]

(2.61)

with \( \varphi_{in}(\mu, t) \) given in Eq. (2.44). Using as an ansatz the time-dependent Gibbs distribution \( P(\varepsilon, t) = \frac{1}{\sqrt{2\pi T(t)}} e^{-\beta(t)\varepsilon} \) in Eq. (2.61), we find the following differential equation, which should be valid for all \( \varepsilon > 0 \):

\[
\frac{1}{2} \dot{\beta} - \dot{\beta} \varepsilon = \frac{\nu}{\beta} - 2\nu \varepsilon,
\]

(2.62)

where \( \dot{\beta} \) denotes the time derivative of \( \beta(t) \). One can easily check that the above equation implies \( \dot{\beta} = 2\nu \). Hence, starting at \( t = 0 \) from an equilibrium distribution at temperature \( T(0) = \beta^{-1}_\text{init} \), the probability distribution is for \( t > 0 \) a Gibbs-like distribution at temperature \( T(t) = \beta(t)^{-1} \) given by

\[
T(t) = \frac{1}{\beta^{-1}_\text{init} + 2\nu t}.
\]

(2.63)

Once expressed in terms of the variable \( x \), the distribution reads

\[
p(x, h, t) = \frac{1}{\sqrt{2\pi T(t)}} \exp \left[ -\frac{(x - h)^2}{2T(t)} \right].
\]

(2.64)

The entropy difference \( \Delta S \) is thus equal to zero for all times.

**Fluctuation dissipation relation**

From Eq. (2.6), and taking into account the factorization property, the response \( \chi_p(t, t_s) \) of the observable \( B_p \) is given for \( t > t_s \) by

\[
\chi_p(t, t_s) = N \left\langle x(t)^{2p+1} \frac{\partial \ln p(x(t), 0, t_s)}{\partial h} (x(t_s), 0, t_s) \right\rangle,
\]

(2.65)

the average being computed at zero field. Therefore, we obtain the following result for the fluctuation-dissipation relation, using the probability density \( p(x, h, t_s) \) given by Eq. (2.64)

\[
\chi_p(t, t_s) = N \beta(t_s) \left\langle x(t)^{2p+1} x(t_s) \right\rangle = \beta(t_s) C(t, t_s),
\]

(2.66)
where \( C(t, t_\alpha) = N(x(t)^{2p+1} x(t_\alpha)) \) denotes the two time correlation function for the relaxation dynamics without field. Thus the FDR defines an effective temperature that is independent of the observable. This result is consistent with the generic relation (2.26) we obtained between the entropy difference and the observable dependence of the FDR (although \( \kappa_p \) does not have here a well-defined value).

**Discussion of the relaxation model**

We could show within this model that even for relaxation dynamics, the generic relation (2.26) that we derived for the observable-dependence of the fluctuation-relation temperature still holds. We find that the probability distribution has a Gibbs form for all times, which results in zero entropy difference and no observable-dependence of the fluctuation-dissipation temperature.

Can we have similar predictions using the entropy production, as was the case in the former model? The definition of the entropy production (2.39) is not valid for a zero temperature bath. Such a situation is however a theoretical idealization. The entropy production can be evaluated for an arbitrarily small bath temperature. In this limit the entropy production becomes arbitrarily large, in contrast to the entropy difference which is zero. Thus again, like in the example of the ring model, the entropy production cannot be considered as a relevant characterization of the observable-dependence of the fluctuation-dissipation temperature.

**2.3 Discussion and conclusion**

In this work we were aiming for some general statements regarding the issue of observable dependent temperatures defined from fluctuation-dissipation relations. We studied two stochastic models with non-uniform probability distributions and another stochastic model in a relaxation regime, that exhibits a time-dependent distribution of Gibbs form. These studies, complemented by the more general arguments developed in Sect. 2.1, support the view that the observable-dependence of fluctuation-dissipation temperatures in driven systems results from the non-uniformity of the phase space distribution.

In order to find a characterization of the observable dependence we related the non-uniformity of microstate distribution on a given energy shell to a quantity we call “lack of entropy” or “entropy difference” \( \Delta S \), namely the Shannon entropy difference of the non-equilibrium system with respect to the equilibrium state with the same average energy. We generically found that the difference between the temperatures associated to two different observables is proportional to the square-root of \( \Delta S \). This relation has been confirmed in the three explicit examples studied. In contrast, another quantity deeply rooted in nonequilibrium theory, namely the entropy production, does not seem to provide a systematic characterization of the dependence of the effective temperature upon the observable. A summary of the results is presented in Table 2.1.

It would be interesting to further test the present approach in experiments or numerical simulations of realistic models. One possibility would be to measure on the one hand the FDR-temperature for different observables and different driving intensities, and on the other hand the correction \( F(\varepsilon) \) to the equilibrium distribution, from which \( \Delta S \) could be evaluated. This independent determination of \( \beta_p \) and of \( \Delta S \) would then allow for a test of the relation (2.26) between these two quantities. Alternatively, assuming the validity of Eq. (2.26), one could estimate the order of magnitude of the observable-dependence of the FDR-temperature from the knowledge of \( \Delta S \) (assuming that \( \kappa_p \) is of
Table 2.1: Summary of the results obtained for the three different models used as illustration, recalling the values of the entropy difference $\Delta S$ and of the entropy production $\sigma_s$, together with the observable-dependence of the FDR-temperature.

| Model Description | $\Delta S^{1/2} \propto \frac{|\beta_p - \beta_0|}{\beta}$ | $\Delta S^{1/2} \propto \frac{|\beta_p - \beta_0|}{\beta}$ | $\Delta S = 0$, $\beta_p = \beta_0$ |
|-------------------|---------------------------------------------------|---------------------------------------------------|----------------------------------|
| One dimensional model on a ring | $\sigma_s = 0$ | $\sigma_s \propto \zeta(\nu) \frac{|\beta_p - \beta_0|}{\beta}$ | $\sigma_s \to \infty$ |
| Fully connected model, two reservoirs | | | |
| Fully connected model, one bath at $T = 0$ | | | |

We argued that in out-of-equilibrium systems, the effective temperature generically depends on the observable. Our derivation relies on some rather strong assumptions (statistical independence of the degrees of freedom, and local decorrelation by each dynamical event), but there is no reason to imagine that the observable-independence of the FDR-temperature would be restored when such assumptions are not fulfilled. We also believe that our arguments qualitatively extend beyond the perturbative regime obtained for weak driving forces, in the sense that we expect the non-uniformity of the phase-space distribution on energy shells to yield, in a generic way, an observable-dependence of the FDR-temperature (even though Eq. (2.26) may not be valid in a strong forcing regime). Hence the notion of effective temperature defined from fluctuation-dissipation relations in non-equilibrium systems seems to have a limited range of applicability. Recently, others types of generalization have been proposed, not relying on a notion of temperature, but rather relating the response function to a suitable, and often more complicated, correlation function [58, 71, 69, 70, 51]. Such an approach is certainly promising as it allows the deviations from the equilibrium FDR to be understood in more details [69]. These deviations often appear in the form of an additive term [58, 68], as can also be seen from Eqs. (2.22) and (2.23). In the framework of Langevin equations, such additive corrections have been interpreted in terms of dissipated energy flux [58]. In some case, for instance when a particle is trapped in a moving potential well, an equilibrium form of the FDR can be restored by moving from the standard eulerian frame to the lagrangian frame associated to the trap [51]. Finally, we note that it would be interesting to further clarify the link between the present work and the results of [54]. In the latter, an upper bound for the deviation from equilibrium FDR was reported in the context of Langevin equations. This upper bound is a function of the entropy production, and implies that there should be no deviation from the equilibrium FDR if the entropy

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production is zero. In the ring model presented in Sec. 2.2.1, we found a systematic deviation in the FDR, although the entropy production remains equal to zero. Although there is strictly speaking no contradiction with the results of [54] since the latter apply to Langevin systems, it would be interesting to understand through which mechanism the bound provided by [54] can be violated.
Chapter 3

Thermodynamic parameters conjugated to conserved quantities

The general concept of intensive thermodynamic parameters plays a crucial role in equilibrium statistical mechanics. For systems in contact, ITPs like temperature, pressure or chemical potential equalize their values once the equilibrium state is reached, provided that their associated quantities, energy, volume or number of particles, can be exchanged. Since this property holds even in the case of systems that exhibit different microscopic dynamics, this equalization became the key criterion in equilibrium statistical mechanics to study the influence of the environment on a given system, for example when a reservoir is connected to it. Moreover the theory of phase coexistence as well as the measurement of, for instance, temperature with a thermometer draw on this powerful concept.

Indeed this potency of the ITP formalism motivates the endeavor to generalize the notion of ITPs to nonequilibrium systems. There exist several different approaches mostly focusing on the generalization of temperature out of equilibrium. For stationary nonequilibrium systems that fulfill a local equilibrium condition, equilibrium properties are locally recovered, so that ITPs can be naturally defined on macroscopic scales that remain small in comparison with the system size [79]. Beyond local equilibrium, more phenomenological endeavors based on thermodynamic grounds [24] have been proposed, as well as statistical approaches illustrated on some specific models [40, 84, 28, 57, 85]. Finally, in the case of non-stationary slow dynamics, a notion of temperature may be derived from a generalized fluctuation-dissipation relation (FDR) [34, 56, 59, 29] in analogy to equilibrium statistical mechanics, as discussed in Chapter 2.

Besides, other notions of ITPs have appeared in the recent literature on nonequilibrium systems. For instance, in the context of stochastic models with a conserved mass $M$ (or number of particles), like the Zero Range Process or different kinds of mass transport models [21], a formal grand-canonical ensemble has been defined, in which systems with a total mass $M$ appear with a probability weight proportional to $\exp(-\mu M)$, $\mu$ being called a chemical potential. We call this ensemble a “formal” one, since no definition of the chemical potential is given prior to the grand-canonical construction, and no physical mechanism allowing for fluctuations of the total mass (like, e.g., a contact with a reservoir) is described. Hence, the grand-canonical distributions introduced so-far appear more as mathematical tools with interesting properties, as it may be considered as a Laplace transform with respect to $M$ of the canonical distribution for which $M$ is fixed [86, 21]. Even more importantly, if this formal grand-canonical ensemble was to be considered as defining the chemical potential, nothing could be said from it on the possible equalization of this parameter...
between two subsystems of a globally isolated system, since in the grand-canonical ensemble, the chemical potential is externally imposed.

The aim of the present chapter is to introduce a precise and general theoretical background allowing for the definition of ITPs conjugated to conserved quantities in nonequilibrium systems. Note that the systems considered here are out of equilibrium not due to the presence of gradients imposed, for instance, by boundary reservoirs, but because of the breaking of microreversibility (that is, time-reversal invariance) at the level of the microscopic dynamics in the bulk. Accordingly, the ITPs are in most cases not space dependent, as would be the case for systems that fulfill the local equilibrium assumption. We state the hypotheses underlying the present construction, and clarify the physical interpretation of the grand-canonical ensemble. We then discuss the relevance and usefulness of the concept of ITP, with particular emphasis on the description of phase coexistence. Although the proposed generalization of ITPs appears to be rather natural, it turns out that non-trivial problems arise as soon as systems with different dynamics are put into contact. This issue is essential if one wants to measure an ITP using a small auxiliary system—just like temperature is measured with a thermometer—and points at one of the main difficulties of nonequilibrium statistical mechanics.

This chapter, summarizing the results published in [31, 32, 33], is organized as follows. Sec. 3.1 introduces the concept of intensive thermodynamic parameters in the framework of nonequilibrium systems, and presents a few direct applications. Sec. 3.2 discusses the effect of the dynamics at the contact between two systems on the equalization or not of ITPs. Finally, Sec. 3.3 investigates the constraints imposed by the balance of fluxes in non-trivial geometries.

3.1 Nonequilibrium intensive thermodynamic parameters

3.1.1 Framework and definitions

Systems with conserved quantities

Let us start by considering a general macroscopic system that exhibits a steady state, and such that the dynamics conserves some additive quantities, referred to as $Q_k$, $k = 1, \ldots, \ell$, in the following. Such systems have been extensively studied for instance in the context of markovian stochastic models, and simple examples include the zero-range process (ZRP) [21], more general mass transport models [83, 88, 89], or the asymmetric exclusion process (ASEP) in a closed geometry [86]. On the microscopic level, the nonequilibrium character of the dynamics manifests itself (apart from the lack of detailed balance) in the presence of a non-trivial dynamical weight $f_\alpha$ associated with each microscopic configuration $\alpha$, in the steady-state probability $P_\alpha$. More precisely, the latter reads

$$P_\alpha = \frac{f_\alpha}{Z(Q_1, \ldots, Q_\ell)} \prod_{k=1}^\ell \delta(Q_k^\alpha - Q_k),$$

(3.1)

where the product of delta distributions ensures the conservation of the quantities $Q_k$. The function

$$Z(Q_1, \ldots, Q_\ell) = \sum_\alpha f_\alpha \prod_{k=1}^\ell \delta(Q_k^\alpha - Q_k)$$

(3.2)

serves as normalization factor, which will be referred to as “partition function” in analogy to equilibrium statistical mechanics. Let us emphasize that in equilibrium systems, the probability
steady state distribution (where sites are labelled by $i$). Some rather large classes of nonequilibrium systems will be illustrated in the following examples.

In the thermodynamic limit with $\beta$ being the inverse temperature. On the contrary, in a nonequilibrium system, the weights $f_\alpha$ also account for purely dynamical effects related to the absence of microreversibility (the latter being deeply rooted in the hamiltonian properties of equilibrium systems), so that these weights generically depart from a constant, even if no conserved quantity is exchanged with a reservoir.

To introduce a definition for ITPs in nonequilibrium situations, we first recall that their equilibrium definition is related to the exchanges of conserved quantities between subsystems, and ensures the equality of ITPs in different parts of the system. Following the same line of thought in a nonequilibrium context, let us divide our system, in an arbitrary way, into two subsystems $S_a$ and $S_b$. The sum $Q_{ka} + Q_{kb} = Q_k$ is kept constant due to the conservation law, whereas exchanges of these quantities between the two subsystems are allowed. The microstate $\alpha$ is now defined as the combination of the two microstates $\{\alpha_a, \alpha_b\}$ of the subsystems, so that the probability of a microstate is denoted as $P_{\alpha_a, \alpha_b}$. An important quantity in the following approach is the conditional probability $\Psi(Q_{1a}, \ldots, Q_{Na}, Q_{1b}, \ldots, Q_{Nb})$ that the conserved quantities have values $Q_{ka}$ in subsystem $S_a$, given their total values $Q_k$

$$\Psi(\{Q_{ka}\}|\{Q_k\}) = \sum_{\alpha_a, \alpha_b} P_{\alpha_a, \alpha_b} \prod_{k=1}^\ell \delta(Q_{ka}^\alpha - Q_k). \quad (3.3)$$

The key assumption in the following derivation is that the logarithm of $\Psi(\{Q_{ka}\}|\{Q_k\})$ satisfies an asymptotic additivity property, namely

$$\ln \Psi(\{Q_{ka}\}|\{Q_k\}) = \ln Z_a(\{Q_{ka}\}) + \ln Z_b(\{Q_k - Q_{ka}\}) - \ln Z(\{Q_k\}) + \epsilon_N(\{Q_{ka}\}, \{Q_k\}) \quad (3.4)$$

with

$$|\epsilon_N(\{Q_{ka}\}, \{Q_k\})| \ll |\ln \Psi(\{Q_{ka}\}|\{Q_k\})|, \quad (3.5)$$

in the thermodynamic limit $N \to \infty$. In Eq. (3.4), $Z_\nu(\{Q_{ka}\})$ refers to the isolated subsystem $S_\nu$, $\nu \in \{a, b\}$, and $N$ is the number of degrees of freedom. That this additivity condition is fulfilled for some rather large classes of nonequilibrium systems will be illustrated in the following examples.

Some of the simplest systems that fulfill Eqs. (3.4), (3.5) are lattice models with a factorized steady state distribution (where sites are labelled by $i = 1, \ldots, N$, and $\alpha = \{\alpha_i\}$)

$$P_\alpha = \frac{1}{Z(Q_1, \ldots, Q_l)} \prod_{i=1}^N f_i, \alpha_i \prod_{k=1}^l \delta \left( \sum_{i=1}^N Q_{ki}^\alpha_i - Q_k \right), \quad (3.6)$$

in which case the term $\epsilon_N$ vanishes. Well-known examples of models with factorized steady-states are for instance the ZRP [21] and other general mass transport models [83, 88]. Accordingly, the physical interpretation of the additivity condition given in Eqs. (3.4), (3.5) is that, on large scale, the system behaves essentially as if the probability weight was factorized, although the genuine probability weight may not be factorized.

As mentioned above, our aim is to define a parameter that takes equal values within the two (arbitrary) subsystems $S_a$ and $S_b$. Guided by the equilibrium procedure, we consider the most
probable value of $Q_{ka}$, denoted by $Q_{ka}^*$, which maximizes the probability $\Psi({Q_{ka}}|{Q_k})$. This most probable value satisfies
\[
\frac{\partial \ln \Psi({Q_{ka}}|{Q_k})}{\partial Q_{ka}} \bigg|_{Q_{ka}^*} = 0. \tag{3.7}
\]
Using the additivity condition (3.4), (3.5), we obtain the following relation
\[
\frac{\partial \ln Z_a}{\partial Q_{ka}} \bigg|_{Q_{ka}^*} = \frac{\partial \ln Z_b}{\partial Q_{kb}} \bigg|_{Q_{k} - Q_{ka}^*}. \tag{3.8}
\]
Hence, it is natural to define the ITP $\lambda_k$ conjugated to the conserved quantity $Q_k$ in a nonequilibrium system as
\[
\lambda_k = \frac{\partial \ln Z}{\partial Q_k}, \quad k = 1, \ldots, \ell. \tag{3.9}
\]
Once the steady state is reached, this quantity equalizes in the two subsystems $S_a$ and $S_b$ due to Eq. (3.8), and thus satisfies the basic requirement for the definition of an ITP.

Actually, for the approach to be fully consistent, one has to check that the value of $\lambda_k$ does not depend on the choice of the partition, as long as both subsystems remain macroscopic. We show in [32] that this is indeed the case, at least under the assumption (which is consistent with the additivity condition) that $\ln Z$ is extensive. To achieve this result one shows that the ITP $\lambda_k$ obtained from the subsystems is equal to the global ITP defined on the whole system from Eq. (3.9), independently of the partition chosen (see [32]). Thus from now on, we compute the ITP $\lambda_k$ using Eq. (3.9) for the whole system.

**Nonequilibrium “grand-canonical” ensemble**

Now that we have defined the notion of ITP, it is natural to try to introduce a grand-canonical ensemble describing a system in contact with a reservoir of conserved quantities, that imposes its values of $\{\lambda_k\}$ to the system. Let us consider a partition of a large isolated system into two subsystems $S_a$ and $S_b$, such that one of the macroscopic systems is much smaller than the other. The larger subsystem, say $S_b$, serves as a reservoir for the $\{Q_k\}$, leading to a natural definition of a “grand-canonical” distribution. This distribution is obtained by integrating the “canonical” distribution (3.1) over the degrees of freedom of the reservoir
\[
\hat{P}_{\alpha_a} = \frac{f_{\alpha_a}}{Z(Q_1, \ldots, Q_\ell)} \sum_{\alpha_b} f_{\alpha_b} \prod_{k=1}^\ell \delta(Q_{ka}^\alpha + Q_{kb}^\alpha - Q_k) = \frac{f_{\alpha_a}}{Z(Q_1, \ldots, Q_\ell)} Z_b(\{Q_k - Q_{ka}^\alpha\}). \tag{3.10}
\]
Note that in the above equation, we assume the factorization property $f_{\alpha_a,\alpha_b} = f_{\alpha_a} f_{\alpha_b}$, that is we neglect possible boundary contributions, similarly to the assumptions often made in the equilibrium context. Expanding the logarithm of the partition function $Z_b$ for $Q_{ka}^\alpha \ll Q_k$, one finds to leading order in $Q_{ka}^\alpha$
\[
\ln Z_b(\{Q_k - Q_{ka}^\alpha\}) \approx \ln Z_b(\{Q_k\}) - \sum_{k=1}^\ell \frac{\partial \ln Z_b}{\partial Q_{kb}} \bigg|_{Q_{ka}^\alpha} Q_{ka}^\alpha,
\approx \ln Z_b(\{Q_k\}) - \sum_{k=1}^\ell \lambda_k Q_{ka}^\alpha, \tag{3.11}
\]

where we approximated
\[
\frac{\partial \ln Z_b}{\partial Q_{kb}} |_{Q_k} \approx \frac{\partial \ln Z_b}{\partial Q_{kb}} |_{Q_k} = \lambda_k .
\] (3.12)

This is justified in the limit \( N_a/N \to 0 \). Therefore we obtain for the “grand-canonical” distribution the following expression
\[
\tilde{P}_{\alpha a} = \frac{f_{\alpha a}}{Z(\lambda_1, \ldots, \lambda_\ell)} \exp \left( - \sum_{k=1}^{l} \lambda_k Q_{ka}^{\alpha a} \right).
\] (3.13)

which defines the grand-canonical partition function
\[
\tilde{Z}(\lambda_1, \ldots, \lambda_\ell) = \sum_{\alpha a} f_{\alpha a} \exp \left( - \sum_{k=1}^{l} \lambda_k Q_{ka}^{\alpha a} \right).
\] (3.14)

Interestingly, the cumulants \( \langle Q_{k_1} Q_{k_2} \cdots Q_{k_n} \rangle_c \) may be expressed as a derivative of the logarithm of the grand-canonical partition function \( \tilde{Z}(\{\lambda_k\}) \), which thus appears as the associated generating function, as follows:
\[
\langle Q_{k_1} Q_{k_2} \cdots Q_{k_n} \rangle_c = (-1)^n \frac{\partial}{\partial \lambda_{k_1}} \frac{\partial}{\partial \lambda_{k_2}} \cdots \frac{\partial}{\partial \lambda_{k_n}} \ln \tilde{Z}(\{\lambda_k\})
\] (3.15)

Note that some of the indices among \( k_1, \ldots, k_n \) may be the same. This result generalizes the corresponding well-known equilibrium result \[90\]. Accordingly, checking the validity of such relations in a given system does not show that microstates compatible with the constraints are equiprobable, contrary to what is sometimes implicitly assumed (e.g., in the context of granular matter \[91\]).

### 3.1.2 Applicability to nonfactorized steady states

As stated above every nonequilibrium system that exhibits a product measure automatically fulfills the additivity property given in Eqs. (3.4), (3.5), since \( \epsilon_N \) vanishes in this case. The aim of this section is to discuss some typical cases for which the steady-state distribution does not factorize, but still satisfies the additivity condition. As a result, the ITP framework is relevant for such systems. There are two important classes of models with nonfactorized steady states: systems where the stationary state can be expressed by a matrix product ansatz, and models described by a transfer matrix.

**Matrix product ansatz**

Practically speaking, considering a matrix product ansatz means that, in a one-dimensional system with periodic boundary conditions, one expresses the probability weight \( f_\alpha \) in the form
\[
f_\alpha = \text{Tr} \prod_{i=1}^{N} M_{\alpha i}
\] (3.16)

where \( M_{\alpha i} \) is a (possibly infinite) matrix, \( \alpha_i \) is the state of site \( i \), and \( \text{Tr} \) is the trace operation over the matrices. For nonperiodic boundary conditions, a slightly different ansatz is used, namely
\[
f_\alpha = \langle W | \prod_{i=1}^{N} M_{\alpha i} | V \rangle
\] (3.17)
where the vectors \( \langle W \rangle \) and \( \langle V \rangle \) are determined by the boundary conditions (reflecting boundaries or injection of particles from a reservoir for instance). Matrix product ansatz have proved particularly useful in the context of the ASEP, where particles obeying an exclusion principle (that is, at most one particle per site is allowed) perform a biased stochastic motion on a one-dimensional lattice [3, 92, 86].

To test the additivity condition (3.4), (3.5) for such models, let us consider a generic lattice model with periodic boundary conditions. A variable \( q_i \) is defined on each site \( i = 1, \ldots, N \), and we assume that the quantity \( Q = \sum_{i=1}^{N} q_i \) is conserved by the dynamics. The steady-state distribution is assumed to be described by a matrix product ansatz:

\[
P(\{q_i\}) = \frac{1}{Z(Q)} \prod_{i=1}^{N} M(q_i) \delta \left( \sum_{i=1}^{N} q_i - Q \right),
\]

(3.18)

where \( M(q) \) is a square matrix. Let us also introduce the matrix \( R(Q) \) through

\[
R(Q) = \int \prod_{i=1}^{N} dq_i \ M(q_i) \delta \left( \sum_{i=1}^{N} q_i - Q \right),
\]

(3.19)

so that the normalizing factor \( Z(Q) = \text{Tr} \ R(Q) \). This leads for the conditional probability distribution \( \Psi(Q_a|Q) \) to:

\[
\Psi(Q_a|Q) = \frac{1}{Z(Q)} \text{Tr}[R_a(Q_a)R_b(Q - Q_a)]
\]

(3.20)

Loosely speaking, the additivity condition holds if the last factor \( \text{Tr}[R_a(Q_a)R_b(Q - Q_a)] \) behaves essentially as \( Z_a(Q_a)Z_b(Q - Q_a) \). It can be shown [32] that the additivity property (3.4), (3.5) is generically fulfilled for a system described by a matrix product ansatz with \textit{finite} matrices. Whether it also holds for some classes of infinite matrices \( M(q) \) remains an open issue.

**Models with transfer matrices**

Another matrix method that has become very popular, in equilibrium as well as in nonequilibrium statistical physics, is the transfer matrix one. The main idea of this method is to formulate the partition function in terms of a product of a matrix, the so-called transfer matrix.

To give an example of the application of this method for nonfactorized steady states let us consider, as previously, a one-dimensional transport model on a ring, with a local variable \( q_i \) on each site \( i \), and such that the sum \( Q = \sum_{i=1}^{N} q_i \) is conserved. The variables \( q_i \) may either be discrete or continuous. Let us now assume a steady-state distribution of the form

\[
P(\{q_i\}) = \frac{1}{Z(Q)} \prod_{i=1}^{N} g(q_i, q_{i+1}) \delta \left( \sum_{i=1}^{N} q_i - Q \right)
\]

(3.21)

with \( q_{N+1} \equiv q_1 \), and \( g(q_i, q_{i+1}) \) is a symmetric function. The partition function \( Z(Q) \) is given by

\[
Z(Q) = \int \prod_{i=1}^{N} dq_i \ g(q_i, q_{i+1}) \delta \left( \sum_{i=1}^{N} q_i - Q \right)
\]

(3.22)
Note that a model of this type has been studied in [89], showing interesting nonequilibrium condensation properties. Let us introduce the quantity $S_N(Q,q_1,q_{N+1})$ defined as

$$S_N(Q,q_1,q_{N+1}) \equiv \int dq_2 \ldots dq_N$$

$$\times \prod_{i=1}^{N} g(q_i,q_{i+1}) \delta \left( \sum_{i=1}^{N} q_i - Q \right)$$

where $q_1$ is no longer identified with $q_{N+1}$, contrary to Eq. (3.21). Then one has

$$Z(Q) = \int_0^{\infty} dq_1 S_N(Q,q_1,q_1),$$

and the distribution $\psi(Q_a|Q)$ can be written as

$$\Psi(Q_a|Q) = \frac{1}{Z(Q)} \int_0^{\infty} dq_1 \int_0^{\infty} dq_{N_a+1}$$

$$\times S_{N_a}(Q_a,q_1,q_{N_a+1}) S_{N_b}(Q - Q_a,q_{N_a+1},q_1)$$

From this expression, a calculation similar in spirit to the one presented in [32] for the case of matrix product ansatz, allows one to show that the additivity condition (3.4), (3.5) holds. The derivation makes use of the Laplace transform $\hat{S}_N(s,q_1,q_{N+1})$ of $S_N(Q,q_1,q_{N+1})$ with respect to $Q$, which can be written as a matrix product (hence the name transfer matrix method):

$$\hat{S}_N(s,q_1,q_{N+1}) = e^{-s(q_1-q_{N+1})/2} T_s^{N_a}(q_1,q_{N+1})$$

where the transfer matrix $T_s$ is defined by

$$T_s(q,q') = g(q,q') e^{-s(q+q')/2}$$

Let us mention, here again, that the derivation of the additivity condition relies on some properties of the transfer matrix that are well established for finite matrices, but that might not be fulfilled for infinite matrices.

### 3.1.3 ITPs at work on simple models

**Mass transport model with factorized steady-state**

As a first example we consider a simple one-dimensional mass transport model on a ring with only one globally conserved quantity, referred to as mass $M = \sum_{i=1}^{N} m_i$, as introduced in Ref. [83]. The masses $m_i$ are a priori positive and real variables. The continuous time stochastic dynamics is defined as follows. A mass $\mu$ is transferred from a randomly chosen site $i$, containing the mass $m_i$, to site $i+1$ according to the following rate

$$\varphi_i(\mu|m_i) = v(\mu) \frac{f_i(m_i - \mu)}{f_i(m_i)}.$$ 

Thus transport is totally biased, which generates a flux of mass along the ring. With the above rate, the steady-state distribution is of the form [83]

$$P(m_i) = \frac{1}{Z(M)} \prod_{i=1}^{N} f_i(m_i) \delta \left( \sum_{i=1}^{N} m_i - M \right),$$

$$39$$
where the single-site weight $f_i(m_i)$ may be site-dependent. Let us here consider for $f_i(m_i)$ the simple form $f_i(m_i) = m_i^{\eta_i - 1}$ with $\eta_i > 0$ for all $i$.

To calculate the ITP corresponding to the conserved mass in the system we need to find the dependence of the partition function $Z$ on $M$:

$$Z(M) = \int N \prod_{i=1}^{N} [dm_i m_i^{\eta_i - 1}] \delta \left( \sum_{i=1}^{N} m_i - M \right),$$

(3.30)

where the integrals are over the positive real axis. A simple rescaling $m_i = x_i M$ reveals the searched dependence:

$$Z(M) = M^{\sum_{i=1}^{N} \eta_i - 1} \int N \prod_{i=1}^{N} [dx_i x_i^{\eta_i - 1}] \delta \left( \sum_{i=1}^{N} x_i - 1 \right)$$

$$= M^{\sum_{i=1}^{N} \eta_i - 1} \prod_{i=1}^{N} [dx_i x_i^{\eta_i - 1}] \delta \left( \sum_{i=1}^{N} x_i - 1 \right) = K_N M^{N \eta - 1}$$

(3.31)

with $\eta = N^{-1} \sum_{i=1}^{N} \eta_i$, and where $K_N$ is a constant independent of $M$. The ITP is obtained from the derivative of $\ln Z$

$$\lambda = \frac{d \ln Z}{dM} = \frac{N \eta - 1}{M}$$

(3.32)

leading in the thermodynamic limit $N \to \infty$ to

$$\lambda = \frac{\eta}{\rho},$$

(3.33)

where $\rho = M/N$ denotes the average density.

**Model with pair-factorized steady-state**

Let us now consider a second example to illustrate that our approach works as well on systems that do not exhibit a factorized steady state. We therefore consider a model similar to that used in the preceding section, but with a transport rate that depends, besides the mass on the concerned site, also on the masses on the two neighboring sites:

$$\varphi(\mu|m_{i-1}, m_i, m_{i+1}) = v(\mu) \frac{g(m_{i-1}, m_i - \mu)}{g(m_{i-1}, m_i)} \times \frac{g(m_{i} - \mu, m_{i+1})}{g(m_{i}, m_{i+1})}.$$ 

(3.34)

Note that this is a generalization of the dynamics introduced in [89], defined for discrete masses. It can be shown [32] that these dynamics lead to a pair-factorized steady-state of the form

$$P(\{m_i\}) = \prod_{i=1}^{N} \frac{g(m_i, m_{i+1})}{Z(M)} \delta \left( \sum_{i=1}^{N} m_i - M \right),$$

(3.35)

Choosing, as a simple example, the function $g(m, n)$ as

$$g(m, n) = (m^\alpha n^\beta + m^\beta n^\alpha)^\gamma$$

(3.36)
with $\alpha, \beta, \gamma \geq 0$, we obtain the behavior of the partition function on $M$, using again a simple scaling argument:

$$Z(M) = \int \prod_{i=1}^{N} [dm_i \, g(m_i, m_{i+1})] \, \delta \left( \sum_{i=1}^{N} m_i - M \right)$$

$$= M^{N[\gamma(\alpha+\beta)+1]} \int \prod_{i=1}^{N} [dx_i \, g(x_i, x_{i+1})]$$

$$\times \delta \left( \sum_{i=1}^{N} x_i - 1 \right)$$

$$= \tilde{K}_N M^{N[\gamma(\alpha+\beta)+1]-1} \quad (3.37)$$

with a prefactor $\tilde{K}_N$ independent of $M$. Thus the ITP conjugated to the conserved mass reads

$$\lambda = \frac{d\ln Z}{dM} = \frac{N[\gamma(\alpha + \beta) + 1] - 1}{M} \quad (3.38)$$

yielding in the thermodynamic limit

$$\lambda = \frac{\gamma(\alpha + \beta) + 1}{\rho} \quad (3.39)$$

Note that here, we did not checked the additivity condition (3.4), (3.5), while the distribution (3.35) would lead to an infinite transfer matrix. Yet, we check in Sec. 3.2.4, on a specific example, that the above results are indeed consistent.

### 3.1.4 Relevance of ITP’s to describe phase coexistence

#### Principle of the approach

One of the main interest of the notion of ITP, which made its success in equilibrium, is that such parameters take equal values in different subsystems of a given system, regardless of their macroscopic state. Indeed, subsystems may for instance have different densities of a given conserved quantity, but they should have the same value of the associated ITP. A case of great interest where this situation arises is that of phase coexistence. At equilibrium, phase coexistence is described by the equality of the different ITPs (temperature, pressure, chemical potential). We shall now argue that the present ITP formalism allows for a similar description of nonequilibrium phase coexistence, at least when this phenomenon is related to a conservation law, and when the additivity condition (3.4), (3.5) holds.

As a simple illustration, we shall consider in this section a well-studied example of nonequilibrium phase coexistence, namely condensation transitions. Such transitions have been reported in ZRP [93, 94, 95, 21], and in more general mass transport models [88, 89]. These models have in common a critical density $\rho^{crit}$ above which a condensation transition occurs, that is, a finite fraction of the total mass condenses onto a given site (or on a small domain [89]).

The standard way to compute the critical density in ZRP for instance, is to use the grand-canonical partition function $\tilde{Z}$, considered as a function of the fugacity $z = e^{-\lambda}$ [21]:

$$\tilde{Z}(z) = \sum_{N=0}^{\infty} z^N Z_N(M) \quad (3.40)$$
where \( z \) is fixed by the density

\[
\rho = \frac{M}{N} = \frac{z \partial \ln \tilde{Z}}{N \partial z},
\]

and to look for the convergence radius of \( \tilde{Z}(z) \) in the complex plane of \( z \). To study the condensed phase in more details, it is necessary to use a canonical ensemble approach where the total mass is fixed [88]. Accordingly, the present ITP formalism turns out to be well-suited for such a study.

In Sect. 3.1.4 and 3.1.4, we illustrate in a pedagogical manner how ITPs may give a natural quantitative description of the condensation phenomenon, on the example of simple mass transport models. Qualitatively, the general procedure proposed is the following. Interpreting the condensation as the coexistence of a fluid phase and a condensed phase, one concludes that from the definition of ITPs, the value of the ITPs should equalize in the two phases. The ITP for the single-site condensate is often easily obtained, in which case the value of the ITP in the fluid phase is also known. Then the equation of state of the fluid phase, computed in the grand-canonical ensemble, can be used to determine the density of this phase (which turns out to be the critical density). Hence, the total mass of the fluid phase is known. From the knowledge of the total mass, one finally deduces the mass of the condensate.

Such a description of phase coexistence is a good illustration of the application of ITPs to a rather simple out-of-equilibrium situation. It is also a first step toward the description of the more complex situation of the contact between two different systems. As we shall see in Sect. 3.2, this case may reveal some difficulties, unexpected within a formal analogy with equilibrium (for instance by defining a formal grand-canonical distribution, or through the introduction of an effective hamiltonian), but well enlightened in the present framework.

**Mass transport model with one species**

*Homogeneous model.*— As a first example of the application of the ITP concept in phase coexistence let us return to the model described in chapter 3.1.3, defined by the transport rates given in Eq. (3.28). Assuming that \( f_i(m) = f(m) \) for all \( i \), and that \( f(m) \sim m^{-\gamma} \) for \( m \to \infty \), one finds for \( \gamma > 2 \) a condensation if the average density exceeds a critical value [21, 88]. In the following we revisit this condensation transition, and show how our approach of equalized ITPs can reveal the physics behind this phenomenon. If we assume that the condensate, which occurs on a randomly chosen site \( j \), carries the macroscopic mass \( M_c = O(N) \), its canonical partition function yields

\[
Z_c(M_c) = \int_0^\infty dm_j f(m_j) \delta(m_j - M_c) = f(M_c) \sim M_c^{-\gamma}.
\]

(3.42)

The ITP conjugated to \( M_c \) is the chemical potential \( \lambda_c \) of the condensate, which is given by

\[
\lambda_c = \frac{d \ln Z_c}{d M_c} \approx -\frac{\gamma}{M_c}.
\]

(3.43)

In the thermodynamic limit \( M_c \to \infty \), one thus obtains \( \lambda_c = 0 \). The equality of ITPs for the condensed and the fluid phase therefore leads to \( \lambda_f = \lambda_c = 0 \). The density \( \rho_f \) of the fluid phase, associated to \( \lambda_f \), can be determined from the equation of state computed in the grand-canonical ensemble

\[
\rho_f = \frac{\int_0^\infty dm f(m)e^{-\lambda_f m}}{\int_0^\infty dm f(m)e^{-\lambda_f m}} = \frac{\int_0^\infty dm f(m)}{\int_0^\infty dm f(m)}.
\]

(3.44)

42
and exactly gives the critical density $\rho^{\text{crit}}$ [88]. Note that for a value of $\gamma < 2$ the critical density becomes infinite, which means that no condensation occurs. Accordingly, the mass of the condensate is given by

$$M_c = M - N\rho^{\text{crit}},$$

(3.45)

if the overall density $\rho = M/N$ is larger than $\rho^{\text{crit}}$. This therefore leads to a thorough description of the condensation in this system.

*Model with an impurity.*— Another well-known situation where condensation occurs is when a single impurity site exhibits a dynamics which differs from those of the other sites [21]. In this case the condensation no longer occurs on a randomly chosen site, but on the impurity itself. One of the simplest choice for the weights in such a model corresponds to

$$f_1(m) = f_{\text{imp}}(m) = e^{\xi m} \quad \text{with} \quad \xi > 0$$

(3.46)

for the impurity site and

$$f_i(m) = f_{\text{hom}}(m) = m^{n-1} \quad \text{with} \quad \eta > 0$$

(3.47)

for the remaining sites $i > 1$ (‘hom’ stands for ‘homogeneous’). In this case the canonical partition function for the condensate reads

$$Z_c(M_c) = e^{\xi M_c},$$

(3.48)

which amounts to an ITP for the condensate

$$\lambda_c = \frac{d \ln Z_c}{d M_c} = \xi.$$  

(3.49)

This yields for the fluid phase $\lambda_f = \xi$, again by equalizing the ITPs of the two phases. The equation of state $\rho_f(\lambda_f)$ for the fluid phase, computed in the grand-canonical ensemble, reads

$$\rho_f(\lambda_f) = \frac{\int_0^\infty dm m^\eta e^{-\lambda_f m}}{\int_0^\infty dm m^{\eta-1} e^{-\lambda_f m}} = \frac{\Gamma(\eta + 1)}{\lambda_f \Gamma(\eta)} = \frac{\eta}{\lambda_f}.$$  

(3.50)

Thus the equality of the chemical potentials forces the fluid to have a fixed density $\rho_0 = \eta/\xi$, as long as the condensate is present, that is for $\rho = M/N > \rho_0$. Interestingly, $\rho_0$ is not in itself the maximum density of the homogeneous fluid phase, but is simply a density imposed by the impurity.

Finally, let us also briefly mention the interesting case where the impurity is defined by

$$f_{\text{imp}}(m) = e^{\zeta m^2}$$

(3.51)

while the homogeneous phase is still defined by Eq. (3.47). Assuming again that there is a condensate on the impurity, one finds $\lambda_c = 2\zeta M_c \to \infty$. Thus one expects $\lambda_f \to \infty$, yielding $\rho_f = 0$ using Eq. (3.50). This case is of particular interest, since on the one hand there is a full localization of mass on the impurity in the thermodynamic limit, and on the other hand it cannot be studied within the framework of the grand-canonical ensemble, due to the faster-than-exponential divergence of $f_1(m)$.

Accordingly, the above calculations provide a simple description of the condensation in terms of the (out-of-equilibrium) “equilibration” of two coexisting phases. In particular, that the condensate may absorb all the excess mass is understood due to the fact that $\lambda_c$ is independent of $M_c$. 

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Mass transport model with two species

The approach explained above for a model with one conserved quantity can easily be extended to more complicated dynamics where more than one species are involved. In the case of two species, the general strategy is the following. Let us consider a lattice model with two conserved masses \( M_1 = \sum_{i=1}^{N} m_{1i} \) and \( M_2 = \sum_{i=1}^{N} m_{2i} \). We assume that a condensate takes place on a given site \( i_0 \). The key point of the approach is that the ITPs conjugated to \( M_1 \) and \( M_2 \) take equal values in both phases. We shall denote these common values as \( \lambda_k, k = 1, 2 \), regardless of the phase we are dealing with. Assuming a factorized steady-state, one can easily compute the values of \( \lambda_k \) in the condensate as a function of the condensed masses \( M_{1c} \) and \( M_{2c} \), leading to two equations of the form:

\[
\lambda_k = \lambda_{kc}(M_{1c}, M_{2c}) , \quad k = 1, 2 .
\] (3.52)

By analogy with the single-species case, it is expected that at least one of the ITPs vanishes in the condensate in the thermodynamic limit, as long as we consider a system without impurities; we thus assume that \( \lambda_1 = 0 \). Then, one needs to compute the densities in the fluid phase using the grand-canonical equation of state \( \rho_kf(\lambda_1 = 0, \lambda_2) \). Finally, the conservation of the total mass generically yields two coupled non-linear equations for the unknown variables \( M_{1c} \) and \( M_{2c} \):

\[
M_{kc} + N\rho_kf(0, \lambda_{2c}(M_{1c}, M_{2c})) = M_k , \quad k = 1, 2 .
\] (3.53)

These equations may be hard to solve analytically in general, but they could be solved numerically. In addition, simplifications may appear in some cases, as we now illustrate on a specific model.

Let us consider a model with two conserved masses as above, which are being transported on a lattice of arbitrary dimension \( d \), with periodic boundary conditions. The transfer rates for an amount of mass \( \mu_1 \) or \( \mu_2 \) from a random site to a neighboring one are given by \( \varphi_1(\mu_1|m_{1i}, m_{2i}) \) or \( \varphi_2(\mu_2|m_{1i}, m_{2i}) \) respectively, in accordance with

\[
\varphi_1(\mu_1|m_{1i}, m_{2i}) = v_1(\mu_1) \frac{h(m_{1i} - \mu_1, m_{2i})}{h(m_{1i}, m_{2i})}
\] (3.54)

\[
\varphi_2(\mu_2|m_{1i}, m_{2i}) = v_2(\mu_2) \frac{h(m_{1i}, m_{2i} - \mu_2)}{h(m_{1i}, m_{2i})}
\] (3.55)

For lattices of dimensions \( d > 1 \), one allows a symmetric mass transfer in any direction transverse to the flux with the same rates \( \varphi_1(\mu_1|m_{1i}, m_{2i}) \) and \( \varphi_2(\mu_2|m_{1i}, m_{2i}) \) as in the direction of the flux. The steady-state distribution in arbitrary dimension \( d \) is then given by

\[
P(\{m_{ki}\}) = \frac{\prod_{i=1}^{N} g(m_{1i}, m_{2i})}{Z(M_1, M_2)} \prod_{k=1}^{2} \delta \left( \sum_{i=1}^{N} m_{ki} - M_k \right) .
\] (3.57)

Guided by the studies of the two-species ZRP [95], we choose an exponential form for the weights

\[
h(m_1, m_2) = \exp(-\kappa m_1 m_2^\sigma)
\] (3.58)

with \( \kappa, \sigma > 0 \). To obtain the conditions under which a condensation occurs, we calculate the canonical partition function of the single-site condensate \( Z_c(M_{1c}, M_{2c}) = h(M_{1c}, M_{2c}) \). Hence one
obtains for the chemical potentials of the two species, computed in the condensate

\[ \lambda_1 = \frac{\partial \ln Z_c}{\partial M_{1c}} = -\frac{\kappa}{M_{2c}^{\sigma}}, \]

\[ \lambda_2 = \frac{\partial \ln Z_c}{\partial M_{2c}} = \kappa \sigma \frac{M_{1c}}{M_{2c}^{\sigma+1}} \].

(3.59) (3.60)

Therefore in the thermodynamic limit, one finds for the chemical potential of the first species \( \lambda_1 = 0 \). The densities in the fluid phase are then computed in the grand-canonical ensemble approach, which yields for \( \rho_{1f} \):

\[ \rho_{1f}(0, \lambda_2) = \frac{\int_0^\infty dm_2 e^{-\lambda_2 m_2} \int_0^\infty dm_1 m_1 e^{-\kappa m_1 m_2^\sigma}}{\int_0^\infty dm_2 e^{-\lambda_2 m_2} \int_0^\infty dm_1 e^{-\kappa m_1 m_2^\sigma}} \]

\[ = \frac{1}{\kappa \lambda_2^\sigma} \frac{\Gamma(1 + 2\sigma)}{\Gamma(1 + \sigma)} \].

(3.61)

For \( \rho_{2f} \), one obtains in the same way

\[ \rho_{2f}(0, \lambda_2) = \frac{\int_0^\infty dm_2 m_2 e^{-\lambda_2 m_2} \int_0^\infty dm_1 e^{-\kappa m_1 m_2^\sigma}}{\int_0^\infty dm_2 e^{-\lambda_2 m_2} \int_0^\infty dm_1 e^{-\kappa m_1 m_2^\sigma}} \]

The integration over \( m_1 \) is straightforward and leads to

\[ \rho_{2f} = \frac{1}{\lambda_2} \frac{\Gamma(2 + \sigma)}{\Gamma(1 + \sigma)} = \frac{\sigma + 1}{\lambda_2} \].

(3.62)

Hence if a condensate exists, one has \( \lambda_2 > 0 \) to ensure a finite positive density \( \rho_{2f} \) in Eq. (3.62). Then, from Eq. (3.60) one finds that \( M_{2c} \sim M_{1c}^{1/(\sigma+1)} \), which means that the condensed mass \( M_{2c} \) behaves subextensively, and the density of the fluid phase for the second species is thus equal to the overall density, \( \rho_{2f} = \rho_2 \). Due to Eq. (3.62) it follows that \( \lambda_2 \) is determined only by the value of \( \rho_2 \). Therefore, the value of \( \rho_{1f} \) is also fixed by the overall density \( \rho_2 \) of the second species, since it is only dependent on \( \lambda_2 \), as seen in Eq. (3.61). As a result, a condensate forms only under the condition that \( \rho_1 > \rho_{1c}^{\text{crit}}(\rho_2) \) given by

\[ \rho_{1c}^{\text{crit}}(\rho_2) = \rho_{1f}(0, \lambda_2(\rho_2)) = \frac{\Gamma(1 + 2\sigma)}{\kappa \Gamma(1 + \sigma)} \left( \frac{\sigma + 1}{\rho_2} \right)^\sigma \]

(3.63)

Using Eqs. (3.60) and (3.62), as well as the relation \( M_{1c} = N(\rho_1 - \rho_{1c}^{\text{crit}}) \), one finds the following expression for the condensed mass of the second species

\[ M_{2c} = \left[ \frac{\kappa \rho_2}{\sigma + 1} N(\rho_1 - \rho_{1c}^{\text{crit}}) \right]^{\frac{1}{\sigma+1}} \].

(3.64)

To sum up, we have shown in this section that in the framework of ITPs, a simple procedure can be developed to describe the coexistence of different nonequilibrium phases in mass transport models, based on the idea that ITPs equalize their values in these phases. We now turn to the more complex situation, where systems with a different microscopic dynamics are put into contact.
3.2 Contact of systems with different dynamics and ITP measure

3.2.1 General approach

Within the equilibrium context, the temperature, pressure and chemical potential of two different systems put into contact equalize, as long as the contact allows the conjugated conserved quantity (energy, volume or particles) to be exchanged. This is actually a strong statement, as it is true even if the two systems considered have very different microscopic dynamics, provided that both systems can be described by an Hamiltonian. Whether such property also holds in the present more general context of nonequilibrium ITP formalism is thus an essential issue. Potentially interesting applications are the description of the effect of the environment on a system, or the possibility to measure the value of an ITP using a small auxiliary system, in the same way as temperature is measured with a thermometer.

As we shall see in this section, the equalization of the values of the ITPs in two systems in contact is actually not automatically fulfilled in a nonequilibrium context due to the necessity to satisfy the additivity condition (3.4), (3.5), and the way the two systems are connected has to be considered carefully. To highlight this point, let us examine two different systems (that is, with different microscopic dynamics) $S_1$ and $S_2$ that separately conserve the same physical quantities $Q_i$, with values $Q_1$ and $Q_2$ respectively. When put into contact, the dynamics at the interface generates the distribution $\Phi(Q_1|Q)$ for the random partition of $Q = \sum_i q_i$ into $Q_1$ (in system $S_1$) and $Q_2 = Q - Q_1$ (in system $S_2$) respectively. Assuming, in the spirit of equilibrium calculations, that the two systems are weakly coupled, i.e. the only coupling is the exchange of $Q$, the global probability distribution reads

$$P(q_1) = \int_0^Q dQ_1 \Phi(Q_1|Q) P_1(q_1) P_2(q_2)$$

$$= \frac{\Phi(\sum_{i \in S_1} q_i|Q)}{Z_1(\sum_{i \in S_1} q_i) Z_2(Q - \sum_{i \in S_1} q_i)} \times F_1(q_1) F_2(q_2) \delta(Q - \sum_i q_i)$$

(3.65)

where $F_1(q_1)$ and $F_2(q_2)$ are the probability weights of systems $S_1$ and $S_2$ respectively, taken as isolated. For the ITP to equalize, the additivity condition (3.4), (3.5) has to be satisfied, when applied to $S_1$ and $S_2$ considered as the two subsystems of the global system. Intuitively, this additivity condition means that the probability weight essentially factorizes, as already mentioned when describing the grand-canonical ensemble. Due to the appearance of the quantity $\sum_{i \in S_1} q_i$ in Eq. (3.65), nonlocal contributions arise in the probability weights appearing in $P(q_1)$. For these weights to factorize (and thus for the additivity condition to be fulfilled), the prefactor $\Phi/Z_1 Z_2$ has to be equal to a constant (since it would otherwise depend on the nonlocal quantity $\sum_{i \in S_1} q_i$), which is nothing but $1/Z(Q)$, up to corrections vanishing in the thermodynamic limit. Thus $\Phi(Q_1|Q)$ should necessarily be of the form

$$\Phi(Q_1|Q) \approx \frac{Z_1(Q_1) Z_2(Q - Q_1)}{Z(Q)}$$

(3.66)

again up to possible small corrections. This result may alternatively be interpreted in the following way. The distribution $\Phi(Q_1|Q)$ is actually nothing but the conditional distribution $\Psi(Q_1|Q)$ introduced in Eq. (3.4), for the specific partition of the global system into $(S_1, S_2)$—whereas $\Psi(Q_1)$ is
a priori defined for an arbitrary partition. Eq. (3.66) is then simply the additivity condition (3.4), (3.5) applied to the partition \((S_1, S_2)\).

When putting into contact two nonequilibrium systems, \(\Phi(Q_1|Q)\) does not obey Eq. (3.66) in general, so that ITPs do not necessarily equalize. Yet for special cases, this equalization may be recovered, as we shall see in Sec. 3.2.2. In any case, it is an important challenge to be able to understand which microscopic properties the dynamics of the contact has to satisfy so that equalization of ITPs hold. This is the topic of Sec. 3.2.3.

To clarify the relation with the equilibrium case, let us consider for instance the equilibrium canonical ensemble, where the conserved quantity would be the number of particles. The system is described by a Boltzmann-Gibbs distribution, and assuming that the hamiltonian does not include long-range interactions, the additivity condition (3.4), (3.5) is satisfied. From this, one deduces that Eq. (3.66) is necessarily satisfied, since otherwise the additivity condition would not hold.

### 3.2.2 Connecting two different mass transport models

To illustrate an implementation of the above idea, we consider two single-species mass transport models in contact, as represented schematically in Fig. 3.1. The dynamical rules are site-independent within each system, but are different in \(S_1\) and \(S_2\). To be more specific, the transport rate within system \(S_\nu\) reads

\[
\varphi_\nu(\mu|m) = v(\mu) \frac{f_\nu(m - \mu)}{f_\nu(m)}, \quad \nu = 1, 2.
\]

Let us emphasize that the function \(v(\mu)\) is the same for both systems. A particular case where this condition holds is the ZRP one, where \(\mu = 1\) is the only allowed value, and \(v(1)\) is set to 1.

In order to define the dynamics at the contact, we extend the dynamical rules in such a way that a mass located at site \(i_1 \in S_1\) at the interface (see Fig. 3.1), is transferred with rate \(\varphi_1(\mu|m)\) either to the neighboring site \(i_1 + 1\) or with the same rate to site \(i_2 \in S_2\). A similar rule is applied for a mass located on site \(i_2\), regarding the transfer to \(i_1\). Hence the two homogeneous systems simply...
Figure 3.2: Time dependence of the masses of the condensates (a), the ITPs (b) and the densities of the fluid phases (c) in two mass transport models in contact, \( S_1 \) (full line) and \( S_2 \) (dashed line) – see Fig. 3.1. Both of them contain an impurity site. Parameter values are \( \xi_1 = 1.5 \) and \( \xi_2 = 1 \) for the impurities, \( \eta_1 = 2 \) and \( \eta_2 = 1 \) for the homogeneous parts – see text. The systems are separately in steady state (with overall initial densities \( \rho_1 = \rho_2 = 2 \)) before the contact is established at time \( t=0 \) (dotted line). Note that the ITPs eventually equalize, and that the difference between the fluid densities increases after the contact is established.

combine to an inhomogeneous one, for which one can find a factorized steady-state, as \( v(\mu) \) is site-independent, and as the graph on which the system is defined satisfies the required geometrical constraint [96]. It follows that in this case the additivity condition (3.4), (3.5) holds, and the ITPs of the two systems equalize.

Let us now give some examples illustrating the consequences of the equalization of ITPs for two systems in contact, within the framework of the above model. It should first be noticed that the equalization of ITPs enforces constraints on the densities of the two systems, which may thus differ one from the other if the two systems have different equations of state. An interesting situation arises in the presence of a condensate. To be more specific, let us consider two different mass transport models, without impurities. The two systems are initially both isolated, and we assume that the first one contains a condensate, while the second one does not. This means that, in this initial stage, \( \lambda_1 = 0 \) whereas \( \lambda_2 > 0 \). When put into contact, the dynamics will be such as to equalize the ITPs \( \lambda_1 \) and \( \lambda_2 \), through a transfer of mass between the two systems. As \( \lambda \) generically decreases when the density increases, mass has to be transferred from \( S_1 \) to \( S_2 \). Withdrawing mass from \( S_1 \) actually does not affect the fluid phase of \( S_1 \) (at least in a quasi-static limit) as long as the average density \( \rho_1 \) remains above the critical density \( \rho_1^{\text{crit}} \), and mass is taken from the condensate only, in this first stage. Assuming that the critical density of \( S_2 \), \( \rho_2^{\text{crit}} \), is infinite, the condensate in \( S_1 \) eventually disappears, and both ITPs converge to a strictly positive value that lies between the initial values of \( \lambda_1 \) and \( \lambda_2 \). Yet, the final densities of the two systems are different in general.

One may also think of more complex situations. Let us consider the case where each of the two systems contains an impurity (as defined in Sect. 3.1.4), with respective parameters \( \xi_1 \) and
\( \xi_2 (\xi_2 < \xi_1) \). In addition, we consider different functions \( f_{\text{hom}}(m) \) for the homogeneous part of each system, namely \( f_{\text{hom},\nu}(m) = m^{\nu - 1} \) in system \( S_\nu, \nu = 1, 2 \). Before the contact is switched on, both systems are in steady state and contain a condensate, so that \( \lambda_1 = \xi_1 \) and \( \lambda_2 = \xi_2 \). When the contact is established at \( t = 0 \), the ITPs tend to equalize, and as \( \lambda_2 < \lambda_1 \), mass is transferred from \( S_2 \) to \( S_1 \) (as \( \rho \) decreases with \( \lambda \)), independently of the values of \( \eta_1 \) and \( \eta_2 \). But as \( S_1 \) already contains a condensate, the density of the fluid phase is fixed, and all the mass brought to \( S_1 \) is actually transferred to the condensate. Hence, the final state corresponds to \( \lambda_1 = \lambda_2 = \xi_1 \), with \( S_1 \) containing a larger condensate than initially, and \( S_2 \) being at a density \( \rho_2(\lambda_2 = \xi_1) < \rho_2^{\text{crit}} = \rho_2(\lambda_2 = \xi_2) \), so that there is no more condensate in \( S_2 \). Fig. 3.2 presents the results of numerical simulations of the above situation, showing in particular that the condensate of \( S_2 \) disappears once the contact is established. In addition, this simulation confirms that the ITPs of the two systems are controlling the direction of the flux of mass. Indeed, mass is transferred from \( S_2 \) to \( S_1 \) even though the density of the fluid is larger in \( S_1 \) than in \( S_2 \), which might seem rather counterintuitive given that the two systems are in contact through their fluid phases only.

Note also that strictly speaking, the determination of \( \lambda \) using the equation of state is valid only in a steady state, so that one should wait until the density \( \rho \) is stationary before determining \( \lambda \) from \( \rho \). Still, for the purpose of illustration, we present here \( \lambda(t) \) deduced from the fluid density \( \rho_f(t) \) even in the nonstationary regime. This is meaningful if the exchanges between the two systems are slow enough so that each system may be considered in a quasi-steady state.

From the above result, one sees that the impurity in system \( S_1 \) (that is, the one with the larger value of \( \xi \)) plays the role of a reservoir of mass that fixes the value of the ITP of \( S_2 \) to \( \lambda_2 = \xi_2 \). Interestingly, \( S_1 \) only needs to contain a mass of the same order as that of \( S_2 \) to act as a reservoir, as the ITP \( \lambda_{1c} \) of the condensate is independent of its mass \( M_{1c} \) as long as \( M_{1c} \) is macroscopic. On the contrary, usual reservoirs require a mass much larger than that of the systems they are in contact with.

As we have seen on these simple examples, the notion of ITP allows one to make, essentially without calculations, non-trivial predictions about the behavior of mass transport models put into contact (for instance, the final densities of both systems); only the knowledge of the equation of state for each system taken separately is required. However, such predictions can be made only if the ITPs equalize. In the present case of mass transport models, this equalization holds as long as the transition rates obey the relation (3.67). What are the conditions for such an equalization to hold in more general situations will be the topic of the next section.

### 3.2.3 Characterization of the dynamics at the contact

In this section, we consider the more general case of two systems in contact as schematically illustrated in Fig. 3.3. The dimension \( d \) of the two systems is arbitrary, and the contact consists in a set of links between the two systems. Generically, the contact relates some parts of the borders of each system, as shown in Fig. 3.3, but one may also think of more complex types of contact.

As mentioned in Sect. 3.2.1, the dynamics at the contact plays an essential role in the possibility to equalize the ITPs of two connected systems. This equalization occurs if the condition (3.66), or equivalently, the additivity condition (3.4), (3.5), is fulfilled. Yet, testing this condition is a priori very difficult, and its interpretation in terms of the microscopic dynamics at the contact is not obvious. On the other hand, if two systems \( S_1 \) and \( S_2 \) are connected and globally isolated, the flux \( \phi_{1 \rightarrow 2} \) transferred from \( S_1 \) to \( S_2 \) through the contact has to be equal, in steady state, to the reverse flux \( \phi_{2 \rightarrow 1} \) going from \( S_2 \) to \( S_1 \).
Figure 3.3: Schematic drawing of two generic systems in contact. Arrows illustrate the possibility to transfer a conserved quantity between the two systems. Contrary to Fig. 3.1, the contact generally extends over many sites.

For the sake of simplicity, we now introduce some assumptions that allow one to analyze, at least in a simple case, this generic problem of the contact between two systems. For definiteness, let us consider lattice systems $S_1$ and $S_2$ that may exchange a globally conserved quantity. The set of sites belonging to the contact in system $S_\nu$, $\nu = 1, 2$, is denoted as $C_\nu$. As already mentioned, the situations considered correspond to the weak coupling limit. In the present context, this means that the flux per site crossing the contact is typically much smaller than the local flux between two sites of a given system, so that the contact does not perturb the dynamics of each system, apart from the (slow) exchange of $Q$. In addition, the specific assumptions used in the following arguments are that:

(i) the flux $\phi_{1 \rightarrow 2}$ depends only on $\lambda_1$, and not on the properties of $S_2$ such as $\lambda_2$; respectively, $\phi_{2 \rightarrow 1}$ depends only on $\lambda_2$ (yet, the total flux $\phi_{1 \rightarrow 2} - \phi_{2 \rightarrow 1}$ depends on both $\lambda_1$ and $\lambda_2$);

(ii) the probability weights of $S_1$ and $S_2$, each one considered as isolated, are factorized as products of one-site weights.

In the spirit of hypothesis (i), the dynamics at the contact is defined by the probability rate $\varphi_{i_1}^c(\mu|q_{i_1})$ to transfer $\mu$ from site $i_1 \in C_1$ in $S_1$ to $S_2$; a similar rate $\varphi_{i_2}^c(\mu|q_{i_2})$ defines the transfer from $i_2 \in C_2$ in $S_2$ to $S_1$. Under these assumptions, one can compute the fluxes $\phi_{1 \rightarrow 2}(\lambda_1)$ and $\phi_{2 \rightarrow 1}(\lambda_2)$; in particular, $\phi_{1 \rightarrow 2}(\lambda_1)$ reads

$$\phi_{1 \rightarrow 2}(\lambda_1) = \sum_{i \in C_1} \int_0^\infty dq_i \, P_1(q_i) \int_{0}^{q_i} d\mu \, \mu \varphi_{i_1}^c(\mu|q_i).$$

(3.68)

where $P_1(q_i)$ is the single site probability distribution in $S_1$. Given that $P_1(q) = c_1 f_1(q) \exp(-\lambda_1 q)$, $c_1$ being a normalization constant, it follows that

$$\phi_{1 \rightarrow 2}(\lambda_1) = c_1 \int_0^\infty dq \int_0^q d\mu \, \mu \varphi_{1}^{\text{tot}}(\mu|q)f_1(q) \, e^{-\lambda_1 q},$$

(3.69)

where we have introduced the “total” rate

$$\varphi_{1}^{\text{tot}}(\mu|q) = \sum_{i \in C_1} \varphi_{i}^c(\mu|q).$$

(3.70)

By exchanging the indexes of the systems, a similar relation holds for $\phi_{2 \rightarrow 1}(\lambda_2)$.

For the two systems to equalize their ITPs, it is necessary that the equality $\phi_{1 \rightarrow 2}(\lambda_1) = \phi_{2 \rightarrow 1}(\lambda_2)$ leads to $\lambda_1 = \lambda_2$, for arbitrary values of (say) $\lambda_1$. In other words, the two functions $\phi_{1 \rightarrow 2}(\lambda)$
and \( \phi_{2 \rightarrow 1}(\lambda) \) must be identical. Let us then compute the difference \( \phi_{1 \rightarrow 2}(\lambda) - \phi_{2 \rightarrow 1}(\lambda) \). After a straightforward calculation, this difference can be expressed as

\[
\phi_{1 \rightarrow 2}(\lambda) - \phi_{2 \rightarrow 1}(\lambda) = c_1 c_2 \int_0^\infty dq_1 \int_0^\infty dq_2 \int_0^{\mu_1} d\mu \mu e^{-\lambda(q_1 + q_2)} \times \\
\times [\phi_{1 \text{tot}}^\mu(q_1)f_1(q_1)f_2(q_2) - \phi_{2 \text{tot}}^\mu(q_2 + \mu)f_1(q_1 - \mu)f_2(q_2 + \mu)]
\]

In order that \( \phi_{1 \rightarrow 2}(\lambda) - \phi_{2 \rightarrow 1}(\lambda) \) vanishes for any value of \( \lambda \), it is necessary and sufficient that the expression between brackets vanishes, that is

\[
\phi_{1 \text{tot}}^\mu(q_1)f_1(q_1)f_2(q_2) = \phi_{2 \text{tot}}^\mu(q_2 + \mu)f_1(q_1 - \mu)f_2(q_2 + \mu)
\]

One can check that Eq. (3.72) is precisely a detailed balance relation between configurations \((q_1, q_2)\) and \((q'_1 = q_1 - \mu, q'_2 = q_2 + \mu)\). Yet, let us emphasize that this detailed balance relation does not concern the true microscopic dynamics at the contact, but rather an effective, coarse-grained dynamics, defined by \( \phi_{\nu\text{tot}}^\mu(q) \) that reduces the contact to a single effective link. To illustrate this point, one can imagine a contact made of two fully biased links between \( S_1 \) and \( S_2 \). The first link can only transfer the conserved quantity \( Q \) from \( S_1 \) to \( S_2 \), whereas the second one only allows \( Q \) to be transferred from \( S_2 \) to \( S_1 \). Then, the microscopic dynamics at the contact does not satisfy detailed balance, but the coarse-grained dynamics may fulfill this condition.

Note that if the true contact already consists in a single link as illustrated on Fig. 3.1, the effective dynamics is the true one, so that the dynamics at the contact really satisfies detailed balance. This is basically the interpretation of the condition used in Eq. (3.67), according to which \( v(\mu) \) has to be the same in the two systems: this condition ensures detailed balance at the contact, even though detailed balance breaks down in each system due to the presence of fluxes.

In summary, we have seen the importance of the dynamics of the contact, which must fulfill condition (3.66) to ensure the equalization of the ITPs among the connected systems. On the other hand, the effective detailed balance Eq. (3.72) is a priori a less general statement, due to the simplifying assumptions used to derive it. However it provides us with a physical interpretation of the conditions required for the dynamics at the contact. One may hope that the resulting physical picture might be relevant beyond the strict validity of Eq. (3.72).

### 3.2.4 Measure of an ITP

#### Notion of ITP-meter

An essential issue about ITPs would be the ability to measure them. In analogy to the measurement of temperature in equilibrium statistical mechanics, one could imagine to realize such a measurement by connecting an auxiliary system to the system under consideration. In this general framework, we shall call this (perhaps conceptual) instrument “ITP-meter”, in reference to the nomenclature “thermometer”. There are three essential requirements which have to be fulfilled to perform such an implementation. First, the values of \( \lambda \) in the gauged system and in the ITP-meter need to equalize. Second, the measured system must not be disturbed by the measurement, so that the ITP-meter should be small with respect to the system upon which the measure is performed. Third, the equation of state of the ITP-meter has to be known, since one needs to deduce the value of its ITP from the measure of a directly accessible physical quantity. Accordingly, these different conditions turn the realization of an ITP-meter into a highly nontrivial problem.
Figure 3.4: Measurement process on a system $S_1$ using an ITP-meter $S_2$. The values of the ITPs $\lambda_1$ (dashed line) and $\lambda_2$ (full line) are plotted versus time. The systems are characterized by parameters $\eta_1 = 3$, $\eta_2 = 5$ (see text). The contact is switched on at time $t = 0$. Initially, $\rho_1 = \rho_2 = 10$, so that $\lambda_1 = 0.3$ and $\lambda_2 = 0.5$. Note that $\lambda_1$ almost stays constant whereas after a sufficient time $\lambda_2$ converges to $\lambda_1$.

Nevertheless it is possible for certain simple cases to realize a measurement with an ITP-meter, using for instance two connected mass transport models as described in Sec. 3.2.2. The systems are similar to the ones shown in Fig. 3.1, but now $S_2$, used as an ITP-meter, is much smaller than $S_1$. We present in Fig. 3.4 numerical simulations in which each system $S_\nu$ ($\nu = 1, 2$) is homogeneous, and obeys the transport rate defined in Eq. (3.67) with $f_\nu(m) = m^{\eta_\nu - 1}$, where $\eta_1 \neq \eta_2$. By measuring the density $\rho_\nu$ of each system, one can determine the value of $\lambda_\nu$ using the equations of state, namely $\lambda_\nu = \eta_\nu / \rho_\nu$. In practice, one would of course only measure the density of the ITP-meter, but here we determine both $\lambda_1$ and $\lambda_2$ to check the validity of the approach.

Numerical simulations are run using systems of size $N_1 = 64510$ and $N_2 = 1024$, with equal initial densities, $\rho_1 = \rho_2 = \rho$, and with $\eta_1 < \eta_2$. Hence the initial values of the ITPs are different, namely $\lambda_1 = \eta_1 / \rho$ and $\lambda_2 = \eta_2 / \rho$. At time zero the contact between the two systems is switched on, and mass flows from $S_1$ to the ITP-meter $S_2$, since $\lambda_1 < \lambda_2$. As predicted theoretically and confirmed by the numerical simulations, the ITPs of the two systems equalize once the steady-state is reached. In addition, the value of $\lambda_1$ does not change significantly along this process, which is the basic requirement for a non-perturbative measurement. Accordingly, the ITP-meter indeed measures the value of $\lambda_1$. Quite importantly, this measure is done without knowing the value of the parameter $\eta_1$ defining the dynamics of $S_1$. This value was only used to determine $\lambda_1$ from $\rho_1$ in order to check the measurement.

The above example illustrates on a simple model that it is in principle possible to measure an ITP using an ITP-meter in nonequilibrium systems. Still, in more realistic situations, finding a suitable definition for the dynamics at the contact that allows for the equalization of ITPs turns out to be a major challenge. As seen in the preceding section, Eq. (3.72) gives a condition for the equalization of ITPs between the two systems, and it provides useful information to design the contact. Yet, it is important to notice that Eq. (3.72) is a detailed balance relation with respect to the stationary distributions of $S_1$ and $S_2$. Hence, to satisfy this relation, one requires some important information on the gauged system, namely its steady state weight $f_1(q)$. Such an information is usually unavailable in nonequilibrium systems, contrary to what happens in equilibrium, where
the weights are either uniform (microcanonical ensemble) or given by the Boltzmann-Gibbs factor (canonical ensemble).

**Measure within subsystems**

An alternative route, that has been exploited recently in the context of granular matter [97, 91], consists in trying to determine the ITP through an interpretation of direct measurements on the system, instead of using an auxiliary system (the ITP-meter) \(^1\). More precisely, let us consider a system with a globally conserved quantity \(Q\). Then, from Eq. (3.15), the variance of the quantity \(Q_N\), measured over a “mesoscopic” subsystem of size \(N\), obeys the following relation, derived from the grand-canonical ensemble:

\[
\langle Q_N^2 \rangle - \langle Q_N \rangle^2 = -\frac{d\langle Q_N \rangle}{d\lambda}.
\]

(3.73)

Let us assume, consistently with the additivity condition (3.4), (3.5), that the variance of \(Q_N\) is linear in the subsystem size \(N\), at least for \(1 \ll N \ll N_{\text{tot}}\), where \(N_{\text{tot}}\) is the size of the global system. Hence the variance may be written as

\[
\langle Q_N^2 \rangle - \langle Q_N \rangle^2 = Ng(\rho)
\]

(3.74)

with \(\rho = \langle Q_N \rangle/N\). Then Eq. (3.73) leads to

\[
g(\rho) = -\frac{d\rho}{d\lambda}.
\]

(3.75)

Given a reference point \((\rho_0, \lambda_0)\), one can then determine the equation of state of the system, simply by integrating Eq. (3.75) numerically:

\[
\lambda = \int_\rho^{\rho_0} \frac{d\rho}{g(\rho)} + \lambda_0.
\]

(3.76)

As a first example, we now apply this procedure to a mass transport model on a ring with dynamics defined by \(f(m) = (1 + m)^2\) and \(v(\mu) = 1\) (see Eq. (3.28)), for which the equation of state \(\lambda(\rho)\) cannot be determined easily by scaling arguments as in Sect. 3.1.3. By measuring in a numerical simulation the variance of the mass \(M_N\) over subsystems of different size \(N\), we find as expected a linear behavior in \(N\) already for small sizes (see inset of Fig. 3.5(a)), since the grand-canonical distribution is fully factorized. The result of the numerical integration for the equation of state is in very good agreement with the theoretical curve obtained using the grand-canonical ensemble (see Fig. 3.5(a)), for which \(\rho\) can be determined as a function of \(\lambda\), as done for instance in Eq. (3.44).

The fact that this procedure works as well for cases in which the steady state does not fully factorize, can be seen in another numerical experiment exhibiting a pair-factorized steady state. Let the dynamics be defined as in Eq. (3.34), with \(v(\mu) = 1\) and \(g(m, n) = m + n\), that is, we assume \(\alpha = 1\), \(\beta = 0\) and \(\gamma = 1\) in Eq. (3.36). Measuring again the variance of the mass \(M_N\) over subsystems of size \(N\), shows that the measurement of the ITP \(\lambda\) should be performed for higher values of \(N\) than in the fully factorized case to have access to the linear regime (see inset of Fig. 3.5(b)). Note that the results of the measurement (see Fig. 3.5(b)) agree equally well with

\(^1\)Note that, however, the procedure presented here is slightly different from that used in [97, 91].
Figure 3.5: Equation of state $\lambda$ as a function of $\rho$ in two mass transport models, obtained by numerical simulations using the measurement procedure described in the text ($\times$), compared with the theoretical prediction $\rho(\lambda)$ derived in the grand-canonical ensemble (full line); (a) fully factorized steady state with $f(m) = (1 + m)^2$, (b) pair-factorized case with $g(m,n) = m + n$. Insets: dependence of the variance on the subsystem size $N$ ($\ast$) for densities $\rho = 1.2$ (a) and $\rho = 0.5$ (b); full lines are linear fits.

the theoretical curve, which can be obtained in this case by the simple scaling argument presented in Sect. 3.1.3.

In these examples, we obtained for simplicity a reference point $(\rho_0, \lambda_0)$ using the theoretical equation of state. In a more realistic situation where the equation of state is unknown, one can estimate as well a reference point only through the information obtained from the measured variances. Measuring numerically the function $g(\rho)$ for large values of $\rho$, one can fit its asymptotic (large $\rho$) expression with a power law, $g(\rho) \approx A \rho^\delta$; in the two models above, one has $\delta = 2$. Then, assuming that $\lambda$ vanishes when $\rho \to \infty$, and that $\delta > 1$, the reference value $\lambda_0$ corresponding to a given large density $\rho_0$ is obtained as

$$\lambda_0 = \int_{\rho_0}^{\infty} \frac{d\rho}{g(\rho)} \approx \int_{\rho_0}^{\infty} \frac{d\rho}{\rho^\delta} = \frac{1}{A(\delta - 1)\rho_0^{\delta-1}}. \quad (3.77)$$

Note that alternatively, one may also determine a reference point from the distribution of $Q_N$, as proposed in [98].

Accordingly, the present approach provides a rather simple way to measure experimentally or numerically ITPs in realistic systems for which no information on the microscopic probability distribution (like the weight factors $f(m)$ for instance) is available. As mentioned above, this method has already been used in the context of granular material [97, 91]. However, it was thought to rely on Edwards’ thermodynamic construction which explicitly assumes the equiprobability of states compatible with the constraints (conserved quantities), whereas this assumption is not necessary,
3.3 Influence of the balance of fluxes

We have seen that the contact dynamics may be a significant limitation to the practical use of ITPs. We now investigate the effect on ITP definition and measurement of another generic constraint arising in non-equilibrium systems, namely the balance of fluxes throughout the system. The influence of this dynamical constraint is particularly important when the system has a non-trivial geometry, with for instance several branches. To investigate this issue, we consider in this section a mass transport model defined on a three-branch geometry, summarizing the results presented in [33].

3.3.1 Mass transport model with three branches

Definition of the model

Using the methods presented in Sec. 3.2.4, we study here the issue of the local measurement of the chemical potential in a model where the local dynamics is essentially homogeneous, but where the heterogeneity results from the non-linearity of the geometry. We consider a mass transport model with three branches, corresponding to the geometry displayed in Fig. 3.6. The three branches are assumed to be oriented. The transfer rate from site $i$ to the neighboring site is $p \varphi(\mu|m_i)$ along the positive direction (according to the orientation of each branch) and $q \varphi(\mu|m_i)$ along the negative direction. The rate $\varphi(\mu|m)$ is defined according to Eq. (3.28), with a site-independent weight function $f(m)$. At the branching points ($A \rightarrow B \rightarrow C$), probability rates for the transfer to branches $B$ and $C$ are reweighted by factors $\gamma_B$ and $\gamma_C$, as shown on Fig. 3.6. For instance, at the lower branching point on Fig. 3.6, the transfer from branch $A$ occurs with rate $\gamma_B p \varphi(\mu|m_i)$ to branch $B$, and with rate $\gamma_C p \varphi(\mu|m_i)$ to branch $C$. Due to this specific geometry, the probability distribution does not necessarily factorize, even with the choice of transport rates $\varphi(\mu|m)$ given in Eq. (3.28).

For mass transport models defined on an arbitrary graph, a sufficient condition for the factorization of the probability distribution has been given in Ref. [96]. In the most general case, such models are defined by transport rates $\varphi_{ij}(\mu|m_i)$ from site $i$ to site $j$ of the form

$$\varphi_{ij}(\mu|m_i) = v_{ij}(\mu) \frac{f_i(m_i - \mu)}{f_i(m_i)} \tag{3.78}$$

where the function $v_{ij}(\mu)$ is identically zero if there is no directed link from $i$ to $j$. If the condition

$$\sum_{j \neq i} v_{ij}(\mu) = \sum_{j \neq i} v_{ji}(\mu) \tag{3.79}$$

holds for every site $i$, the probability distribution factorizes, with the local probability weight given by $f_i(m_i)$ [96]:

$$P(\{m_i\}) = \frac{1}{Z(M)} \prod_{i=1}^{N} f_i(m_i) \delta \left( \sum_{i=1}^{N} m_i - M \right). \tag{3.80}$$

In the case of the model with three branches, the branching sites violate the sufficient condition for factorization given Eq. (3.79), which is a strong indication that strict factorization does not hold.
Figure 3.6: Sketch of the model with three branches. Left panel: Mass is transported along each oriented branch according to the rate $p \varphi(\mu, m)$ in the positive direction, and to the rate $q \varphi(\mu, m)$ in the negative direction. Right panel: Zoom on the branching points, where specific rules are taken into account, some of the transfer rates being reweighted by factors $\gamma_B$ and $\gamma_C$.

Hence the exact solution of this model is not known, and it is not clear a priori whether the present model satisfies or not the “asymptotic factorization condition” given in Eq. (3.4) [31], which is a key criterion for the existence of a globally defined chemical potential. Indeed, although the strict factorization property is likely to be violated, one might ask whether this violation is ’localized’ around the branching points and if the local chemical potential in the bulk of the branches remains uniform. It is thus interesting in this situation to perform numerical measurements of the local chemical potential.

**Local measurement of the chemical potential**

To test this issue, we measure the chemical potential with a probe system attached to a bulk site of the branch considered, in analogy to the procedure explained in Sect. 3.2.4. The transport rates are the same in all branches as well as in the probe system, $\varphi(\mu|m) \equiv 1$. All three branches have the same number of sites $N_b$, so that the system size is $N = 3N_b$ (to be specific, the two branching points are included in branch A). Simulations are done with $p = 1$ and $\gamma_B = \gamma_C = \frac{1}{2}$. The results of the numerical implementation of the measurement are shown in Fig. 3.7. The locally measured chemical potential is denoted as $\tilde{\lambda}_\nu$ in branch $\nu = A$, $B$, or $C$. It turns out that we obtain equal values for the locally measured chemical potential in branches $B$ and $C$, but a very different value for branch $A$. In the rest of this section, we shall try to understand the origin of this discrepancy between the values measured in the different branches.

We first check whether this result, obtained by probing the system, depends on the measurement method. To this aim, we apply the alternative measurement technique involving local fluctuations, presented in Sec. 3.2.4, a technique which does not require any external device. Let us first define the quantity $g_\nu (\nu = A, B, \text{or} C)$ as the variance of the total mass $M_\nu$ in branch $\nu$ divided by the number of sites $N_\nu$ in this branch:

$$g_\nu = \frac{\langle M_\nu^2 \rangle - \langle M_\nu \rangle^2}{N_\nu}. \quad (3.81)$$
We have checked numerically that $g_\nu$ does not depend on the size of the subsystem chosen within a given branch. Consequently $g_\nu$ is an intensive quantity depending only on the local density, $g_\nu = g_\nu(\rho_\nu)$.

We choose the same parameters for the dynamics as above. Each branch is of the same size $N_b$ and the transport rates are given by $\varphi(\mu|m_i) \equiv 1$ everywhere. The result of a numerical implementation of the measurement of the function $g_\nu(\rho_\nu)$ in the three-branch model is shown in the left panel of Fig. 3.8. The functional behavior of $g_\nu(\rho_\nu)$ is seen to be the same for the three branches, and we denote this function simply as $g(\rho_\nu)$. We further observe on Fig. 3.8 that the numerically measured $g(\rho_\nu)$ is very close to the theoretical value $g(\rho_\nu) = \rho_\nu^2$ corresponding to a homogeneous system with the same local dynamics $\varphi(\mu|m) = 1$, so that we shall use this theoretical expression in the following.

Following the same procedure as in Sec. 3.2.4, we get

$$\bar{\lambda}_\nu = \Lambda(\rho_\nu) \equiv \int_{\rho_\nu}^{\infty} \frac{dp}{g(p)}$$

(3.82)

This means that the functional behavior of the local chemical potential $\Lambda$ with density $\rho_\nu$, that is the local equation of state, is the same in the three branches, namely $\Lambda(\rho_\nu) = \rho_\nu^{-1}$ for the specific dynamics chosen here. This result is not surprising since the local dynamics is the same everywhere and although the probability distribution does not factorize, only weak correlations are expected in the bulk of each branch. Taking into account the fact that the local densities $\rho_\nu$ in the three branches are not equal, it follows that the values $\bar{\lambda}_\nu = \Lambda(\rho_\nu)$ of the local chemical potential of the three branches differ as well: $\bar{\lambda}_A \neq \bar{\lambda}_B = \bar{\lambda}_C$. 

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Interpretation in terms of flux balance

This discrepancy can be understood by taking into account the balance of fluxes. To this aim, let us compute the flux of mass $\Phi$ crossing a site $i$ in the bulk of a given branch. Considering the rest of the system as a reservoir of mass, one finds for the probability distribution on site $i$

$$p_i(m_i) = \frac{1}{Q_i} f_i(m) e^{-\tilde{\lambda} m_i},$$

(3.83)

where $Q_i$ is a normalization constant, and $\tilde{\lambda}$ is the local chemical potential. The mass flux $\Phi$ crossing site $i$ can be expressed as

$$\Phi = (p-q) \int_0^\infty dm p_i(m) \int_0^m d\mu \varphi_i(\mu|m).$$

(3.84)

which can be rewritten, using Eqs. (3.83) and (3.28), as

$$\Phi = (p-q) \int_0^\infty d\mu \mu v(\mu) e^{-\tilde{\lambda} \mu}.$$  

(3.85)

From the expression (3.85) of the flux $\Phi$, we first note that if the function $v(\mu)$ in the transport rates is identically 1, $v(\mu) \equiv 1$, then the flux is given by $\Phi = 1/\tilde{\lambda}^2$ (note that the expression of the flux is independent of the form of $f(m)$). We use here the local chemical potential $\tilde{\lambda}$, as the flux is governed by the local dynamics –see Eq. (3.85). We shall come back to this point in Sec. 3.3.2. In the bulk of the branches, where the correlations are expected to be small, the different fluxes are given by $\Phi_A = 1/\tilde{\lambda}_A^2$ and $\Phi_B = 1/\tilde{\lambda}_B^2$ (fluxes in branches $B$ and $C$ are equal since $\gamma_B = \gamma_C$). Moreover we know that the flux in branch $A$ is twice the flux in branch $B$, which leads to the following relation between the chemical potentials of the different branches:

$$\tilde{\lambda}_A = \frac{\tilde{\lambda}_B}{\sqrt{2}} = \frac{\tilde{\lambda}_C}{\sqrt{2}}.$$  

(3.86)
This relation has been verified numerically for \( \varphi(\mu|m) \equiv 1 \), where we expect analytically \( \tilde{\lambda}_{\nu} = \rho_{\nu}^{-1} \), \( \nu = A, B, C \) – see the right panel of Fig. 3.8 and left panel of Fig. 3.9 for the numerical results. We can generalize this flux balance argument to situations where branches \( B \) and \( C \) do not have the same flux, in which case the relation reads:

\[
\tilde{\lambda}_A = \sqrt{\frac{\Phi_B}{\Phi_A}} \tilde{\lambda}_B = \sqrt{\frac{\Phi_C}{\Phi_A}} \tilde{\lambda}_C.
\] (3.87)

Note that at equilibrium, when the fluxes vanish, this correction is not present and all chemical potentials equalize. But as soon as a little bias is introduced in the dynamics, the value of the chemical potential in branch \( A \) differs from that of the two other branches. Let us emphasize that this difference is not perturbative with respect to the bias: \( \tilde{\lambda}_A - \tilde{\lambda}_B \) does not go to zero when \( p - q \to 0 \), but rather remains constant as long as \( p > q \).

From a more theoretical perspective, the discrepancy between \( \tilde{\lambda}_A, \tilde{\lambda}_B \) and \( \tilde{\lambda}_C \) questions the validity of the asymptotic factorization condition (3.4) required to define a global chemical potential from Eq. (3.9). It would thus be interesting to verify explicitly whether this asymptotic factorization property holds or not. This is a difficult task because (to our knowledge) the exact joint probability distribution is not known for generic rates in the present geometry, as it does not fulfill Eq. (3.79). Yet, the specific case of the Zero Range Process (ZRP), where masses are discrete, turns out to be solvable and thus deserves to be investigated in more details.

### 3.3.2 A solvable three-branch model

#### Zero-Range Process and factorized steady-state

The ZRP case, which has been intensively studied in the literature [21], corresponds to the choice \( v(\mu) = \delta(\mu - 1) \), so that masses \( m_i \) take integer values, denoted as \( n_i \) in the following. We study here the ZRP in the three branch geometry illustrated on Fig. 3.6. The dynamics is defined as...
in Sec. 3.3.1, except that $\mu$ can only take the value $\mu = 1$. To simplify the calculations, we set $\gamma_B = \gamma_C = 1$ and choose $p > q$.

The relation (3.85) between flux and local chemical potential reads in this case $\Phi_\nu = e^{-\tilde{\lambda}_\nu}$. Given that fluxes are different in the three branches, it is clear that the chemical potentials are not equal. More quantitatively, the balance of fluxes $\Phi_A = \Phi_B + \Phi_C$ implies $\tilde{\lambda}_A = -\ln(\Phi_A/\Phi_B) + \tilde{\lambda}_B$. From this expression we see that there is now a shift, given by the logarithm of the ratio of the fluxes, in the value of the chemical potential.

To better understand the origin of this shift, we compute the steady-state distribution of the ZRP with three branches. Interestingly, it has been shown that the steady-state distribution of the ZRP on an arbitrary graph remains factorized [96]. Slightly rephrasing the results of Ref. [96], one finds that the distribution $P(n_i)$ is given by

$$ P(n_i) = \frac{1}{Z(M)} \left( \prod_{i=1}^{N} f(n_i) z_i^{n_i} \right) \delta_{\sum n_i, M} \tag{3.88} $$

where $\delta$ is the Kronecker delta symbol, and where the local “fugacities” $z_i$ satisfy for all $i$ the equation

$$ \sum_{j \neq i} v_{ij} z_i = \sum_{j \neq i} v_{ji} z_j \tag{3.89} $$

with $v_{ij} \equiv v_{ij}(1)$ defined in Eq. (3.78). In the present three-branch model, $v_{ij}$ is equal to $p$ if there is a positively oriented link from $i$ to $j$, and to $q$ if the link is negatively oriented; $v_{ij} = 0$ in the absence of link. Note that the fugacities $z_j$ are defined only up to an overall arbitrary factor. Condition (3.89) then reads, for all site $i$ different from a branching point:

$$ pz_{i-1} - z_i + qz_{i+1} = 0. \tag{3.90} $$

The general solution of this linear equation (valid separately on each branch) is a linear combination of solutions of the form $z_j = r^j$, with a parameter $r$ obeying the relation

$$ qr^2 - r + p = 0. \tag{3.91} $$

Eq. (3.91) has two solutions, $r_1 = 1$ and $r_2 = p/q > 1$. As a result, $z_j$ can be expressed on each branch as a linear combination of the two independent solutions $r_1^j$ and $r_2^j$,

$$ z_j = \zeta_\nu \left[ 1 + K_\nu \left( \frac{q}{p} \right)^{N_\nu - j} \right] \tag{3.92} $$

where $\zeta_\nu$ and $K_\nu$ are constants ($\nu = A, B, \text{ or } C$) and $N_\nu$ denotes the number of sites in branch $\nu$. The total number of sites in the system is given by $N = N_A + N_B + N_C + 2$ (the last term accounts for the two nodes). Taking into account Eq. (3.89), formulated for the two branching points, one can match the expressions (3.92) corresponding to different branches and determine the constants $K_\nu$ as well as the ratios $\zeta_A/\zeta_B$ and $\zeta_A/\zeta_C$. In the limit where the sizes $N_A, N_B$ and $N_C$ of the three branches go to infinity, one finds $\zeta_A/\zeta_B = \zeta_A/\zeta_C = 2$. As $z_j$ is defined up to an overall prefactor, one can choose for instance $\zeta_B = \zeta_C = 1$ and $\zeta_A = 2$. Given that the terms proportional to $K_\nu$ are exponentially decaying corrections, it turns out that $z_j$ is almost constant, and equal to $\zeta_\nu$, on each branch $\nu$.

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Local versus global chemical potential

As the probability distribution of the ZRP is factorized, the definition of the chemical potential proposed in Sec. 3.1 [31, 32] can indeed be applied. Splitting the system into two parts, branch $A$ on one side, and branches $B$ and $C$ on the other side, one obtains

$$\lambda_A = \frac{\partial \ln Z_A}{\partial M_A}, \quad \lambda_{BC} = \frac{\partial \ln Z_{BC}}{\partial M_{BC}}. \quad (3.93)$$

with $M_A = \sum_{i \in A} n_i$ and $M_{BC} = \sum_{i \in B,C} n_i$ the respective masses of the two subsystems. Since $\xi_A = 2$, we get, neglecting the exponential corrections appearing in Eq. (3.92)

$$Z_A = 2^{M_A} Z_A^{(0)}, \quad Z_{BC} = Z_{BC}^{(0)}, \quad (3.94)$$

where $Z_A^{(0)}$ and $Z_{BC}^{(0)}$ are the standard partition functions of these two subsystems, that would be obtained by taking $z_i = 1$ for all $i$. In the large size limit, one then finds for the chemical potential, using the definition (3.9):

$$\lambda_A = \ln 2 + \tilde{\lambda}_A, \quad \lambda_{BC} = \tilde{\lambda}_{BC}. \quad (3.95)$$

We thus recover in this way the result directly obtained from the balance of fluxes, showing that this result is actually consistent with the asymptotic factorization condition on which the definition of the chemical potential is built (let us recall that the probability distribution of the present ZRP model is factorized). Note that the shift $\ln 2$ is independent of the precise value of the bias $p - q$, as long as this bias is non-zero. If $p = q$, equilibrium is recovered, and the bias vanishes. The presence of this bias is thus a genuine non-equilibrium effect, which appears non-perturbatively, in a discontinuous way.

It is also interesting to note that the shift $\ln 2$ cancels out from the one-site mass distribution. Indeed, one has for a site $i$ in the bulk of branch $A$, using Eq. (3.95)

$$p_i(n) = \frac{1}{Q_A} f(n) 2^n e^{-\lambda_A n} = \frac{1}{Q_A} f(n) e^{-\tilde{\lambda}_A n} \quad (3.96)$$

and for a site in branch $B$ or $C$

$$p_i(n) = \frac{1}{Q_{BC}} f(n) e^{-\tilde{\lambda}_{BC} n}. \quad (3.97)$$

Hence both distributions have exactly the same form as a function of the local chemical potential, making the shift undetectable from a local measurement.

3.3.3 Discussion: a tentative scenario

We now try to assess more generally, beyond the specific ZRP case, the consistency between flux balance and equality of the local chemical potentials. We have seen in the ZRP case that the discrepancy between the local chemical potentials $\tilde{\lambda}_\nu$ can be explained by the presence of exponential factors that differ from one subsystem to the other. It is tempting to try to generalize this scenario to the case of the mass transport model with continuous masses, although no analytical solution is available in this case. At a heuristic level, a more general form of Eq. (3.94) can be proposed, namely

$$Z_A = e^{\alpha(p) M_A} Z_A^{(0)}, \quad Z_{BC} = Z_{BC}^{(0)}, \quad (3.98)$$
since the global average density $\bar{\rho}$ is fixed, and can thus a priori enter as a parameter in the exponential factor. Eq. (3.95) is then replaced by

$$\lambda_A = \alpha(\bar{\rho}) + \bar{\lambda}_A, \quad \lambda_{BC} = \bar{\lambda}_{BC}. \tag{3.99}$$

Assuming that the asymptotic factorization condition holds, one has $\lambda_A = \lambda_{BC}$, so that

$$\alpha(\bar{\rho}) + \bar{\lambda}_A = \bar{\lambda}_{BC}. \tag{3.100}$$

The constant $\alpha(\bar{\rho})$ is determined as follows. Given a value of $\bar{\rho}$, one looks for the densities $\rho_A(\bar{\rho})$ and $\rho_{BC}(\bar{\rho})$ satisfying the constraints

$$\tilde{\Phi}(\rho_A) = 2\tilde{\Phi}(\rho_{BC}), \tag{3.101}$$

$$\bar{\rho} = \kappa\rho_A + (1 - \kappa)\rho_{BC} \tag{3.102}$$

with $\kappa = N_A/(N_A + N_{BC})$, and where $\tilde{\Phi}(\rho)$ is the value of the local flux for a local density $\rho$. The parameter $\alpha(\bar{\rho})$ is then obtained, consistently with Eq. (3.100), as

$$\alpha(\bar{\rho}) = \Lambda\left(\rho_{BC}(\bar{\rho})\right) - \Lambda\left(\rho_A(\bar{\rho})\right). \tag{3.103}$$

In the ZRP case, one recovers $\alpha = \ln 2$, independently of the density $\bar{\rho}$, while with continuous masses, assuming $v(\mu) = 1$ and $f(m) = m^{\eta-1}$, one finds

$$\alpha(\bar{\rho}) = \frac{\eta}{\bar{\rho}} \left(1 - 2\kappa + \frac{3\kappa - 1}{\sqrt{2}}\right). \tag{3.104}$$

This result is in agreement with the numerical findings of Sect. 3.3.1 where $\eta = 1$ and $\kappa = \frac{1}{3}$, yielding $\alpha = 1/(3\bar{\rho})$ (see right panel of Fig. 3.9). Hence, despite the absence of an exact solution of the mass transport model (beyond the specific ZRP case), this tentative scenario provides a consistent explanation of the numerical results obtained for the local chemical potential, showing that the asymptotic factorization condition may still hold while local measurements fail to find an equilibrated chemical potential throughout the system.

### 3.4 Conclusions

In this chapter, we highlighted that the notion of generalized ITPs for steady-state nonequilibrium systems serves as a new tool in the study of nonequilibrium phenomena. Within the range of validity of the additivity condition (3.4), (3.5), there is a vast variety of models for which our approach can be useful, like models with a factorized steady-state distribution, or one-dimensional systems described by a matrix product ansatz or the transfer matrix method (at least with finite matrices). The method should also be of interest for models which are well approximated by a mean field approach.

Introduced by generalizing the equilibrium concept, for which physical intuition is well developed, ITPs benefit from a rather clear physical interpretation. They provide a convenient way to describe the coexistence of two phases, as may be easily illustrated on the case of the condensation transition. An essential issue, which made the success of the ITP concept in equilibrium, is the possibility to equalize ITPs in different systems put into contact. Contrary to equilibrium situations,
such an equalization is not automatically fulfilled in the nonequilibrium case, and the dynamics at the contact turns out to play a major role. We have derived, under simplifying assumptions, a coarse-grained detailed balance relation that needs to be satisfied by the contact dynamics in order that ITPs equalize. Deriving a more general criterion by relaxing some of the assumptions made would be interesting to gain further insights on this important issue.

A related difficulty with the approach is that the additivity property (3.4), (3.5) may be hard to test directly. Still, measuring the variance of the globally conserved quantity over subsystems of a homogeneous system may lead to an indirect test of this property: indeed, one expects that the variance introduced in Eq. (3.73), becomes linear in $N$ for $N \gg 1$ if the additivity property is satisfied.

From the point of view of measurements, it turns out that realizing an ITP-meter remains a major challenge, mostly due to the difficulties with the choice of the dynamics at the contact. Indeed, one would need to find a dynamics for the contact that satisfies the condition for equalization of ITPs (that is, the coarse-grained detailed balance relation (3.72) or a generalization of it), without having information on the probability weights of the system on which the measure should be done. Alternatively, measurements of ITPs using the variance of the globally conserved quantity in subsystems of “mesoscopic” size seem to be a promising route.

In addition, we also attempted to clarify the influence of the flux balance condition on the generalized chemical potential in non-equilibrium mass transport models. We have seen in particular that even when the asymptotic factorization condition holds, locally measured values of the chemical potential may not equalize, while the theoretically-defined ones remain equal. This surprising property has been traced back to the presence of exponential factors appearing in the probability weights of different subsystems. These exponential factors cancel out at the level of the local statistics (for instance the single-site distribution) and are thus locally undetectable. But on the other hand these factors play an essential role in the global statistics to ensure the balance of flux. An important consequence of these results is that for branching geometries, it is not possible to define along the present lines a locally measurable chemical potential that would equalize throughout the system.
Chapter 4

Fluctuations of global observables

The ubiquitous appearance of asymmetric distributions in the study of fluctuations of global quantities in correlated systems has raised a lot of interest in recent years. Such non-Gaussian distributions, characterized by an exponential tail on one side and a rapid fall-off on the other side, have been observed in many models or experimental systems, in the context of turbulence [105, 106, 107, 108, 99], equilibrium critical systems [105, 109, 110, 111, 112], nonequilibrium models exhibiting self-organized criticality [109, 113], interface models [114], 1/f noise [115], Langevin equations [116], granular gas models [107, 104], or even the statistics of the level of the Danube river [117]. Quite strikingly, this analogy is not only qualitative, but many of the distributions observed in these very different systems actually fall [105, 109, 112, 104, 117], once suitably rescaled, close to the so-called Bramwell-Holdsworth-Pinton (BHP) distribution describing the magnetization of the XY model in the low temperature limit, as well as the roughness of the two-dimensional Edwards-Wilkinson surface model [110, 118]. Yet, as not all data collapse onto the BHP curve [111, 108], a more general distribution has been proposed to describe the data, namely the generalized Gumbel distribution $G_a(x)$, which includes a continuous shape parameter $a$ [109, 110, 111, 119, 117, 108, 104, 120]—see below for definition. Interestingly, this distribution, with $a = 1$, turns out to be the exact one for periodic Gaussian 1/f-noise [115]; it is also very close to the BHP one for $a \approx \pi/2$ [109, 104].

The distribution $G_a(x)$ originates, for integer values of $a$, from the study of extreme value statistics [101, 121], and describes the fluctuations of the $a$th largest value in a large set of identically distributed (independent) random variables $z_i$. Accordingly, there is no obvious theoretical motivation for the use of the distribution $G_a(x)$ in the study of fluctuations of global quantities. Rather, it is usually considered as a convenient fitting function, and a theoretical understanding of its relevance is still lacking.

These introductory comments lead us to the following questions:

• How generic and precise is the description through a generalized Gumbel distribution? Can one find simple physical models (for instance dissipative models) for which the fluctuations of a global quantity would be exactly described by a generalized Gumbel distribution?

• Is there a precise relationship between global fluctuations in correlated systems and extreme value statistics?

---

1This requires that $z$ has no upper bound, and that $P(z)$ decays faster than any power law at large $z$. 64
In this chapter, we investigate these issues, starting from the physical modeling point of view, and then going to more formal probabilistic issues.

### 4.1 Energy distribution in dissipative cascade models

#### 4.1.1 Energy cascade in Fourier space

As mentioned above, the standard Gumbel distribution has been reported to describe the fluctuations of the total energy (integrated spectrum) for the periodic $1/f$-noise model. In the framework of non-equilibrium systems, decaying energy spectrum are qualitatively obtained in systems where energy is injected at large scale and dissipated at small scales, the transfer between scales (described for instance by Fourier modes) occurring due to non-linear interactions.

As a first illustration, we present some preliminary results obtained from a dissipative energy transfer model rather similar to the one considered in Chapter 1, but with two significant differences. First, energies are positive real variables instead of being discrete. Second, the geometry is no longer a Cayley tree, but a one-dimensional lattice representing the Fourier space. Each site of the lattice carries an energy that can be interpreted as the sum of the energies of modes having a given wavenumber. Once a steady-state is reached, the distribution of the total energy is measured numerically. Results are shown on Fig. 4.1. Interestingly, the energy distribution is well fitted by a generalized Gumbel distribution $G_{\alpha}(x)$ with parameter $\alpha = 1.57 \approx \pi/2$ (which is also an excellent approximation of the BHP distribution mentioned above). Let us emphasize that these results are only preliminary, and that a more detailed study, varying the parameters of the model, remains to be done. However, this first result provides one further motivation to investigate the possible appearance of generalized Gumbel distributions in driven dissipative systems. This is the goal of the following section, which introduces a solvable nonequilibrium stochastic model.
4.1.2 An exactly solvable model

Let us consider the driven dissipative model defined by the following stochastic rules \[135\]. On each site \( n = 1, \ldots, N \) of a one-dimensional lattice, a positive continuous energy \( \rho_n \) is introduced. The (asynchronous) dynamics is defined through three different physical mechanisms involving energy, namely injection on –say– the left boundary, transport from one site to its right neighbor, and local dissipation. More precisely, an amount of energy between \( \mu \) and \( \mu + d\mu \) can be either injected on the leftmost site \( n = 1 \) with a rate (probability per unit time) \( J(\mu) \, d\mu \), transferred from site \( n \) to site \( n + 1 \) with rate \( \phi(\mu) \, d\mu \), or removed (i.e., dissipated) from site \( n \) with rate \( \Delta(\mu) \, d\mu \) –see Fig. 4.2.

On the rightmost site \( n = N \), the transferred energy is actually dissipated. Note that the above rates do not depend on the values of the local energies \( \rho_n \), apart from the obvious constraint that one cannot withdraw from site \( n \) (either for transport or dissipation) an energy \( \mu \) greater than \( \rho_n \).

The master equation governing the evolution of the probability distribution \( P(\{\rho_n\},t) \) reads:

\[
\frac{\partial P}{\partial t} = J(\mu) \int_0^{\rho_1} d\mu J(\mu)P(\{\rho_1 - \mu, \rho_j\},t) - J(\mu) \int_0^{\rho_N} d\mu J(\mu)P(\{\rho_j\},t) - \sum_{n=1}^{N-1} \int_0^{\rho_{n+1}} d\mu \phi(\mu)P(\{\rho_n + \mu, \rho_{n+1} - \mu, \rho_j\},t) - \sum_{n=1}^{N} \int_0^{\rho_n} d\mu \Delta(\mu) + \phi(\mu) \delta_{n,N} P(\{\rho_n + \mu, \rho_j\},t) - \sum_{n=1}^{N} \int_0^{\rho_n} d\mu [\phi(\mu) + \Delta(\mu)]P(\{\rho_j\},t)
\]  

(4.1)

where \( \rho_j \) generically stands for all the variables that are not affected by \( \mu \). In the following, we focus on the specific case where \( J(\mu) = e^{-\beta \mu} \phi(\mu) \) and \( \Delta(\mu) = (e^{\lambda \mu} - 1) \phi(\mu) \), introducing two positive parameters \( \beta \) and \( \lambda \). With these assumptions, the steady-state distribution \( P(\{\rho_n\}) \) proves
Figure 4.3: Distribution $P_E(x)$ of the rescaled (global) energy of the model, $x = (E - \langle E \rangle)/\sigma_E$. The analytical result $G_a(x)$ (full lines) is compared with numerical simulations with $\phi(\mu) = 1$, for $a \equiv 1 + \beta/\lambda = 1.7$ ($\circ$), 3.3 ($\triangledown$), and 6 ($\diamond$), showing an excellent agreement. Inset: zoom on the top of the curves, on a linear scale.

factorized and can be computed exactly [135]:

$$P(\{\rho_n\}) = \prod_{n=1}^{N} (\lambda n + \beta) e^{-(\lambda n + \beta)\rho_n}. \quad (4.2)$$

Anticipating the results of Sec. 4.2.2 below, we find that the fluctuations of the total energy $E = \sum_{n=1}^{N} \rho_n$ are described in the infinite $N$ limit —after rescaling $E$ to ensure zero mean and unit variance— by the generalized Gumbel [101, 102, 103] distribution $G_a(x)$, with $a = 1 + \beta/\lambda$ (see Fig. 4.3) [135]. Interestingly, we observe that in the limit of low dissipation $\lambda \to 0$, one recovers a Gaussian distribution, since $G_a(x)$ converges to a Gaussian for $a \to \infty$. Qualitatively, the parameter $a$ may be thought of as the number of sites having roughly the same energy, of the order of $1/\beta$.

Finally, we note that the ‘cascade’ mechanism illustrated by the above stochastic model should be considered as one possible mechanism, but perhaps not as the unique one. Indeed, in some systems like freely evolving granular gases [104], Gumbel distributions are indeed observed even though the global quantity of interest cannot be written in an obvious way as a sum of independent collective variables. Yet, it must be noticed that such a granular system does not reach a steady state since no energy is injected; fluctuations are then measured in a scaling regime where the average kinetic energy continuously decreases. Accordingly, one might expect another physical mechanism to be at play in this case.

4.2 Relation to extreme value statistics

4.2.1 Mapping between extremes and sums

In this section, we try to clarify how the statistics of global quantities, expressed as sums of non-identically distributed random variables, is related to extreme value problems, and how the generalized Gumbel distribution $G_a(x)$, with a real index $a$, emerges in the study of global fluctuations. Our starting point is the observation [115] that the integrated power spectrum $w$ of periodic...
Gaussian $1/f$ noise is distributed, after a suitable rescaling $x = (w - \langle w \rangle) / \sigma_w$ (where $\sigma_w^2$ is the variance of $w$) according to the Gumbel distribution $G_1(x)$. The model for $1/f$ noise used in [115] consists in a large number $N$ of statistically independent Gaussian Fourier modes with complex amplitudes $c_n = c^*_n$. Introducing $y_n \equiv |c_n|^2 + |c_{-n}|^2$, one has by definition $w = \sum_{n=1}^{N} y_n$. The distribution of $y_n$ reads

$$p_n(y_n) = n\kappa e^{-n\kappa y_n},$$

so that $w$ is simply the sum of $N$ independent random variables $y_n$, with non-identical exponential distributions. Note that the appearance of a non-Gaussian distribution is not surprising in itself, since the sum of the variances of the $y_n$’s converges when $N \to \infty$ [as $\text{var}(y_n) = 1/(n^2 \kappa^2)$], so that the central limit theorem is not expected to hold [for a detailed discussion on this point, see [125]]. Still, the fact that a Gumbel distribution precisely emerges might suggest the existence of some “hidden” extremal processes dominating the fluctuations of $w$, though no clear evidence for such processes has been found [119, 112].

Actually, a different perspective may be necessary to understand the relationship between the two problems. Indeed, instead of looking for extremal processes hidden in sums of random variables, one may look for sums of random variables with decreasing amplitudes when studying the statistics of extreme values. To this aim, we introduce the following procedure, illustrated in Fig. 4.4. Considering a set of $N$ random variables $z_n > 0$ ($1 \leq n \leq N$), all drawn from the same distribution $P(z)$, we introduce the variables $z'_n$ defined by ordering the original variables $z_n$: $z'_1 = z_{\sigma(n)}$, where $\sigma(n)$ is a permutation over the interval $[1, N]$ such that $z'_1 \geq z'_2 \geq \ldots \geq z'_N$. Thus $z'_1$ is simply the maximum value of the set $\{z_n\}$. We also define the interval $y_n$ between $z'_{n+1}$ and $z'_n$:

$$y_n = z'_n - z'_{n+1} \quad (1 \leq n \leq N - 1); \quad y_N = z'_N. \quad (4.4)$$

With these notations, one can write:

$$\max_{1 \leq n \leq N} (z_n) \equiv z'_1 = \sum_{n=1}^{N} y_n. \quad (4.5)$$

As a result, a problem of extreme value can be mapped onto a problem of sum of random variables. Still, it should be noticed that although the original variables $z_n$ are independent, the $y_n$’s are a priori correlated.

In the following, we show that in the specific case where $P(z)$ is an exponential distribution $P(z) = \kappa e^{-\kappa z}$, the $y_n$’s prove independent and distributed according to Eq. (4.3). The distribution
\[ P_N(\{y_n\}) \text{ reads:} \]
\[
P_N(\{y_n\}) = \kappa^N N! \int_0^\infty dz_N e^{-\kappa z_N} \ldots \int_0^\infty dz_1 e^{-\kappa z_1} \]
\[
\times \delta(y_N - z_N) \prod_{n=1}^{N-1} \delta[y_n - (z_n - z_{n+1})] \quad (4.6)
\]

where the integral over \(z_n\) is from \(z_{n+1}\) to \(\infty\), for \(1 \leq n \leq N - 1\). This expression can be understood as follows: either the variables \(\{z_n\}\) are already ordered, which straightforwardly gives the above integrals, or they are not, and then can be ordered through a permutation, which leads to the \(N!\) factor in front. Making the change of variables \(v_n = z_n - z_{n+1}\) (1 \(\leq n \leq N - 1\)) and \(v_N = z_N\) in Eq. (4.6), the different integrals factorize and one finds:
\[
P_N(\{y_n\}) = \prod_{n=1}^N n \kappa e^{-n \kappa y_n} \quad (4.7)
\]

Thus it turns out that in the specific case \(P(z) = \kappa e^{-\kappa z}\) the \(y_n\)'s are independent variables, distributed as the squared Fourier amplitudes in the 1/f noise model, i.e., according to Eq. (4.3). But as the sum of the \(y_n\)'s is precisely the maximum value of a set of exponentially distributed variables \(\{z_n\}\), we know that this sum has to be distributed (after a suitable rescaling) according to \(G_1(x)\), so that one recovers immediately the results of [115]. Accordingly, a clear relationship appears between the statistics of extreme values and that of sums of variables with decreasing amplitudes. This relationship can actually be understood at two different levels. On the one hand, starting from a set of (possibly correlated) variables \(\{z_n\}\), one can always define the interval \(y_n\) between two successive variables \(z'_n\) obtained by ordering the set \(\{z_n\}\) –see Eq. (4.5). Thus, on general grounds, the maximum value of correlated variables \(z_n\) can be formally written as a sum of correlated variables \(y_n\), but the corresponding extreme value distribution is usually unknown. On the other hand, it seems that the maximum value of a set \(\{z_n\}\) of independent variables is related to a sum of independent variables \(\{y_n\}\) only in the case where the \(z_n\)'s are drawn from an exponential distribution, leading to the Gumbel distribution \(G_1(x)\). Indeed, the factorization property of the exponential is essential to derive Eq. (4.7) from Eq. (4.6).

### 4.2.2 Generalized Gumbel distribution

The above result leads to some rather unexpected consequences. From the very definition of the variables \(\{z'_n\}\), \(z'_k\) is precisely the \(k\)th largest value of the original set \(\{z_n\}\). So we know that \(z'_k\) follows, once rescaled as \(x = (z'_k - \langle z'_k \rangle)/\sigma_k\) with \(\sigma_k^2 = \text{var}(z'_k)\), the generalized Gumbel distribution \(G_k(x)\) [101]. The distribution \(G_a(x)\) is defined for any positive real value \(a\) by:
\[
G_a(x) = \frac{\theta_a a^a}{\Gamma(a)} \exp \left\{ -a \left[ \theta_a (x + \nu_a) + e^{-\theta_a (x+\nu_a)} \right] \right\} \quad (4.8)
\]

with
\[
\theta_a^2 = \frac{d^2 \ln \Gamma}{da^2}, \quad \nu_a = \frac{1}{\theta_a} \left( \ln a - \frac{d \ln \Gamma}{da} \right) \quad (4.9)
\]
where $\Gamma(a)$ is the Euler Gamma function. Besides, $z'_k$ may also be expressed as a sum:

$$z'_k = \sum_{n=k}^{N} y_n = \sum_{n=1}^{N-k+1} \tilde{y}_n$$

(4.10)

with $\tilde{y}_n \equiv y_{n+k-1}$ distributed according to

$$p_{n,k}(\tilde{y}_n) = (n + k - 1) \kappa e^{-(n+k-1)\kappa \tilde{y}_n}.$$  

(4.11)

Thus the sum of independent random variables drawn from (4.11) is distributed, after a suitable rescaling, according to $G_k(x)$ in the limit $N \to \infty$. But then, one can forget the original extreme value problem, and consider only the statistics of the sum, so that there is no more reason to restrict $k$ to be integer. Since the generalized Gumbel distribution is obtained for integer $k$, it seems plausible that it also holds for real values $k = a > 0$. To be more specific, considering independent variables $u_n$ with distribution

$$p_{n,a}(u_n) = (n + a - 1) \kappa e^{-(n+a-1)\kappa u_n}, \quad 1 \leq n \leq N$$

(4.12)

the sum $X = \sum_{n=1}^{N} u_n$ is precisely distributed, in the limit $N \to \infty$, according to the generalized Gumbel distribution $G_a(x)$, where $x = (X - \langle X \rangle)/\sigma_X$. This result, suggested by the above heuristic argument, can be derived exactly, without reference to the extreme value problem [100].

Actually, a more general formulation of this result can also be given [100]. Instead of starting from the specific distribution (4.12) for the variables $\{u_n\}$, one can start from an arbitrary joint distribution belonging to a specific class, which turns out to be included in the basin of attraction of the generalized Gumbel distribution. Along the same line, classes of joint distributions belonging to basins of attraction of generalized Fréchet and Weibull distribution can also be proposed. The reader is referred to Ref. [100] for more details about these classes of distributions. Here, rather than presenting the detailed formalism, we rather turn to an application of this formalism to a (simplified) physical situation, the one-dimensional classical gas of independent particles in a gravity field [136].

### 4.3 Application: one-dimensional gas in a gravity field

One-dimensional gas models have a long history and have proved very useful for the illustration of statistical concepts [126, 127, 128, 129, 130, 131]. However, at variance with most previous studies on such a model, we consider here a gas confined both by a piston and by an external potential. We find that although the system is composed of independent and identical particles, the distributions of volume fluctuations are non-Gaussian, and described in the limit of a large number of particles by generalized extreme value distributions, indicating that correlations appear in the system. The nature of the correlations is however rather subtle: the local volume between particles is correlated, but their positions are not.

Note that connections between the one-dimensional classical gas of particles (or Jepsen gas) and extreme value statistics have already been reported when the gas can freely expand, in the absence of piston and potential [131]. However, these results concern the velocity of the rightmost particle rather than the volume of the gas, and are thus of a different nature.

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2Another reason for non-Gaussian fluctuations would be that the variance diverges, leading to Lévy-stable laws [132], but this is not the case here.
4.3.1 A simple model of a one-dimensional confined gas

We consider an ideal system composed of $N$ point-particles placed in a cylindrical container with long axis $z$ and with a small diameter with respect to its length (quasi one-dimensional geometry). The model is illustrated in a schematic way in Fig. 4.5. The position of the particles along the $z$-axis is denoted as $z_i$, $i = 1, \ldots, N$. A hard wall, acting as a reflecting boundary is placed at $z = 0$, so that particles are constrained to remain on the half-space $z > 0$. The container is closed by a piston that can freely move along the $z$-axis. The position of the bottom of the piston is denoted $z_p$, so that the volume of the system is given by $V = S z_p$, where $S$ is the cross-section of the cylinder. In addition, particles are subjected to an external potential $U(z)$, $z > 0$, that tends to confine them in the small $z$ region, that is $U(z)$ is assumed to be an increasing function of $z$. The piston is also subjected to an external potential $U_p(z_p)$, that may differ from the potential acting on the particle. The potential $U_p$ may for instance be the gravitational potential acting on the piston. It may also be the potential caused by an operator exerting a constant force $f_p$ on the piston, corresponding to a linear potential $U_p(z_p) = -f_p z_p$, or by a spring fixed on the piston, corresponding to a quadratic potential $U_p(z_p) = \frac{1}{2}K(z_p - z_0)^2$. $U_p(z_p)$ may also result from the superposition of the different types of potentials mentioned above.

The container plays the role of a heat bath that thermalizes the particles at a given temperature $T$. Collisions between the particles and the piston are elastic, so that the piston in turn thermalizes at temperature $T$ (the piston does not have any internal structure, only its translation degree of freedom thermalizes). Note that the present model differs from the so-called Jepsen gas [126, 127, 128, 129, 130], due to the presence of a heat reservoir and of an external potential.

4.3.2 Distribution of volume fluctuations

We now characterize quantitatively the volume fluctuations of the system through the position, $z_p$, of the piston. When all the particles and the piston are equilibrated at temperature $T$, the
equilibrium distribution reads, with \( z_i, z_p > 0 \),

\[
P_N(z_1, \ldots, z_N, z_p) = \frac{1}{Z} e^{-\beta U_p(z_p)} \prod_{i=1}^{N} e^{-\beta U(z_i)} \Theta(z_p - z_i),
\]

(4.13)

where \( \beta = 1/k_B T \) is the inverse temperature, \( Z \) is the partition function and \( \Theta(x) \) is the Heaviside function. The volume distribution \( Q_N(z_p) \) is obtained by integrating over the variables \( z_1, \ldots, z_N \), leading to

\[
Q_N(z_p) = \frac{1}{Z} e^{-\beta U_p(z_p)} \left( \int_{0}^{z_p} dz e^{-\beta U(z)} \right)^N.
\]

(4.14)

Before going into more detailed calculations, we briefly discuss two simple limiting cases of interest, namely \( U(z) = 0 \) and \( U(z) = U_p(z) \). The case \( U(z) = 0 \) is the most standard equilibrium case, for which

\[
Q_N(z_p) = \frac{1}{Z} z_p^N e^{-\beta U_p(z_p)},
\]

(4.15)

and Gaussian fluctuations are recovered in the large \( N \) limit [133].

In contrast, if the potential acting on the piston is the same as that acting on the particles, one can express \( P(z_p) \) in the following form:

\[
Q_N(z_p) = \frac{d}{dz_p} G(z_p)^{N+1},
\]

(4.16)

with

\[
G(z_p) = \frac{\int_{0}^{z_p} dz e^{-\beta U(z)}}{\int_{0}^{\infty} dz e^{-\beta U(z)}}.
\]

(4.17)

Volume fluctuations then exactly map onto an auxiliary problem of extreme values, namely, the fluctuations of the maximal height of \( N + 1 \) independent particles (with no piston) with positions \( z'_i \) in a potential \( U(z) \). The function \( G(z_p) \) is simply the probability that the position of a particle subjected to the potential \( U(z) \) is smaller than \( z_p \). Hence, \( G(z_p)^{N+1} \) is the probability that the positions of \( N + 1 \) particles are less than \( z_p \), which is nothing but the cumulative distribution of the maximum of the \( N + 1 \) positions \( z'_i \). From Eq. (4.16), it follows that \( P(z_p) \) is the distribution of \( \max(z'_1, \ldots, z'_{N+1}) \), so that in the large \( N \) limit, fluctuations of \( z_p \) are described by standard extreme value distributions.

Here, we are mostly concerned with the intermediate situation where particles are submitted to a force derived from a potential, but where this force is smaller than that acting on the piston. A typical situation of this type is that of a system placed in a gravitational field, as the piston generically has a mass larger than that of the particles.

Let us now compute the asymptotic volume distribution for general potentials \( U(z) \) and \( U_p(z) \). One way to tackle this issue could be to start directly from Eq. (4.14). Rather, as a short-cut, we take an alternative approach using the results derived in [100]. To this aim, we introduce the intervals between the ordered positions of the particles in the following way. For a given set of values \( z_1, \ldots, z_N \) satisfying \( 0 < z_i < z_p \) for all \( i \), we introduce a permutation \( \sigma \) of the integers \( 1, \ldots, N \) such that \( z_{\sigma(1)} \leq z_{\sigma(2)} \leq \cdots \leq z_{\sigma(N)} \), and we define the space interval \( h_i \) between particles through

\[
h_i = z_{\sigma(i)} - z_{\sigma(i-1)}, \quad i = 2, \ldots, N.
\]

(4.18)
For convenience, we also introduce the variables \( h_1 \) and \( h_{N+1} \),

\[
h_1 = z_{\sigma(1)}, \quad h_{N+1} = z_p - z_{\sigma(N)}.
\] (4.19)

It is then straightforward to express \( z_i \) as a function of the variables \( h_j \), namely

\[
z_i = \sum_{j=1}^{\sigma^{-1}(i)} h_j, \quad (i = 1, \ldots, N), \quad z_p = \sum_{j=1}^{N+1} h_j.
\] (4.20)

where \( \sigma^{-1} \) is the inverse permutation of \( \sigma \). The system can then be described by the set \((h_1, \ldots, h_{N+1})\), with \( h_i \geq 0 \) for all \( i \), up to an arbitrary permutation of the \( N \)istinguishable particles. A given set \((h_1, \ldots, h_{N+1})\) then corresponds to \( N! \) configurations of the particles (the position of the piston is fixed when the \( h_i \)'s are given). Summing over the corresponding \( N! \) configurations \((z_1, \ldots, z_N)\) in Eq. (4.13), one obtains the equilibrium probability distribution

\[
\tilde{P}_N(h_1, \ldots, h_{N+1}) = \frac{N!}{Z} e^{-\beta U_p \left(\sum_{j=1}^{N+1} h_j\right)} \prod_{k=1}^{N} e^{-\beta U \left(\sum_{j=1}^{k} h_j\right)},
\] (4.21)

where we relabelled the factors in the product using \( k = \sigma^{-1}(i) \). Note that this last equation is also obtained in the case when particles cannot cross each other. In this case, the ‘no-crossing’ constraint needs to be taken into account from the outset in Eq. (4.13), and Eq. (4.21) is rather straightforwardly obtained, since there is no need for reordering the positions of the particles. Note also that the case of indistinguishable particles leads to a result similar to that of distinguishable particles that cannot cross each other, since in both cases it is not possible to generate a different configuration through a permutation of the particles.

The distribution \( \tilde{P}_N(h_1, \ldots, h_{N+1}) \) given in Eq. (4.21) turns out to be quite similar to the joint distribution describing the class of correlated random variables introduced in [100]. Up to slight notation changes \(^3\), the latter reads:

\[
J_N(h_1, \ldots, h_{N+1}) = K_N \left[ F \left( \sum_{i=1}^{N+1} h_i \right) \right]^{N+1} \prod_{i=1}^{N} P \left( \sum_{j=1}^{i} h_i \right),
\] (4.22)

\( \Omega(F) \) is an arbitrary function of \( F \), with \( 0 < F < 1 \), and the function \( F(z) \) is defined as

\[
F(z) = \int_{z}^{\infty} P(z')dz'.
\] (4.23)

The function \( P(z) \) has the properties of a one-variable probability distribution, namely it is a positive function such that \( \int_{0}^{\infty} P(z')dz' = 1 \). In order to map the gas model onto Eq. (4.22), we make the following identification:

\[
P(z) = \lambda e^{-\beta U(z)},
\] (4.24)

\[
\Omega[F(z_p)]P(z_p) = e^{-\beta U_p(z_p)}.
\] (4.25)

\(^3\)Starting from the distribution \( J_N(u_1, \ldots, u_N) \) defined in [100], we change \( N \) into \( N + 1 \), and reverse the order of index, that is, we define the variables \( h_i = u_{N+2-i} \).
for all \( z, z_p > 0 \), and where \( \lambda \) is a normalization factor. With this identification, Eq. (4.21) can be rewritten as

\[
\tilde{P}_N(h_1, \ldots, h_{N+1}) = \frac{N!}{Z\lambda^N} \Omega \left[ F \left( \sum_{j=1}^{N+1} h_j \right) \right]^{N+1} P \left( \sum_{j=1}^k h_j \right),
\]

which is precisely the same form as in Eq. (4.22). As \( P(z) > 0 \) for all \( z > 0 \), it results from Eq. (4.23) that \( F(z) \) is a strictly decreasing function of \( z > 0 \), so that \( y = F(z) \) can be inverted into \( z = F^{-1}(y) \). Accordingly, Eq. (4.25) can be reformulated as

\[
\Omega(y) = \exp\left[\beta U_p(F^{-1}(y))\right],
\]

\[
= \frac{1}{\lambda} \exp \left[ \beta U(F^{-1}(y)) - \beta U_p(F^{-1}(y)) \right],
\]

for all \( y, 0 < y < 1 \). Eq. (4.27) actually gives a definition of the function \( \Omega(y) \). The key result of [100] is that if

\[
\Omega(y) \sim \Omega_0 y^{a-1}, \quad y \to 0, \quad (a > 0),
\]

the distribution of the sum \( z_p = \sum_{i=1}^{N+1} h_i \) converges, up to a suitable rescaling, to one of the generalized extreme value distributions with parameter \( a \). These distributions, illustrated in Fig. 4.6, belong to three different classes, depending on the large \( z \) behavior of \( P(z) \). If \( P(z) \) decays faster than any power law (typically, a power-law potential \( U(z) \)), the generalized Gumbel distribution \( G_a(x) \) is obtained, namely

\[
G_a(x) = C_g \exp (-\gamma y - ae^{-y}), \quad y = \theta(x + \nu),
\]

where \( \theta \) and \( \nu \) are rescaling factors introduced to have zero mean and unit variance, and \( C_g \) is a normalization factor –see Eq. (4.8). In the limit \( a \to \infty \), the generalized Gumbel distribution converges to the Gaussian distribution. If \( P(z) \) has a power law tail \( P(z) \sim z^{-1-\mu} \) when \( z \to \infty \), with \( \mu > 0 \) (corresponding, in the present mapping, to a logarithmic potential \( U(z) \)), one finds the generalized Fréchet distribution,

\[
F_{a,\mu}(x) = \frac{C_f}{x^{1+a\mu}} \exp \left(-bf x^{-\mu}\right), \quad x > 0.
\]

Finally, if \( P(z) \) vanishes above a certain value \( z_{\text{max}} \) (say, there is a hard wall at \( z_{\text{max}} \)), and behaves as a power-law \( P(z) \sim (z_{\text{max}} - z)^{\mu-1} \), for \( z \to z_{\text{max}} \), with \( \mu > 0 \), then the resulting distribution is of the generalized Weibull type,

\[
W_{a,\mu}(x) = C_w x^{a\mu-1} \exp (-b_w x^\mu), \quad x > 0.
\]

The parameters \( b_f \) and \( b_w \) are scale parameters, that can be tuned to obtain any of the distributions with unit mean or with unit variance (for the Fréchet distribution, this is only possible if \( \mu \) is large enough so that the mean or the variance are finite).

As a rather generic illustration, let us consider the case when the potentials \( U(z) \) and \( U_p(z_p) \) are given by

\[
U(z) = U_0 z^\alpha, \quad U_p(z_p) = U'_0 z_p^\gamma,
\]
with $\alpha, \gamma > 0$. If $\alpha = \gamma = 1$, the particles and the piston are in a constant external force field, like the (local) gravity field, in which case $U_0 = mg$ and $U'_0 = Mg$. If $\gamma = 2$, the piston is for instance linked to the hard wall situated at $z = 0$ with a spring of stiffness $k = 2U'_0$.

In order to determine the limit distribution of the volume fluctuations in the large $N$ limit, the parameter $a$ characterizing the small $y$ behavior of $\Omega(y)$ should be evaluated. Considering Eq. (4.27), one needs to compute first the function $F^{-1}(y)$ in the small $y$ limit, which is deduced from the large $z$ limit of $F(z)$. Given that

$$P(z) = \lambda e^{-\beta U_0 z^\alpha}, \quad \lambda = \frac{\alpha (\beta U_0)^{1/\alpha}}{\Gamma \left( \frac{1}{\alpha} \right)}, \quad (4.33)$$

with $\Gamma(t) = \int_0^\infty du u^{t-1}e^{-u}$ the Euler Gamma function, one has in the large $z$ limit

$$F(z) = \int_z^{\infty} \lambda e^{-\beta U_0 z^\alpha} dx \approx \frac{(\beta U_0)^{\frac{1}{\alpha} - 1}}{\Gamma \left( \frac{1}{\alpha} \right)} z^{\alpha - 1} e^{-z^\alpha} \quad (z \to \infty). \quad (4.34)$$

Inverting the relation $y = F(z)$ to get $z = F^{-1}(y)$, one finds to leading order in the limit $y \to 0$

$$F^{-1}(y) \approx \frac{1}{(\beta U_0)^{1/\alpha}} \left( \ln \frac{1}{y} - \left( 1 - \frac{1}{\alpha} \right) \ln \ln \frac{1}{y} - \ln \Gamma \left( \frac{1}{\alpha} \right) \right)^{1/\alpha}. \quad (4.35)$$

We now wish to compute $\Omega(y)$. Putting Eq. (4.35) into Eq. (4.27), one needs to distinguish between the cases $\alpha = \gamma$ and $\alpha \neq \gamma$.

If $\alpha = \gamma$, one gets

$$\Omega(y) \approx \frac{\Gamma \left( \frac{1}{\alpha} \right)^a y^{(a-1)(1-\frac{1}{\alpha})}}{\alpha (\beta U_0)^{1/\alpha}} \left( \ln \frac{1}{y} \right)^{a-1} \quad (y \to 0), \quad (4.36)$$

with $a = U'_0/U_0$. Therefore, $\Omega(y)$ behaves as a power law in the small $y$ limit, up to logarithmic corrections which do not modify the asymptotic distribution [136]. It follows that volume fluctuations are described by a Gumbel distribution with parameter $a$ [100], which compares the relative
intensity of the compression force acting on the piston and of the forces directly acting on the particles. In the limit of a strong compression force \( a \to \infty \), volume fluctuations asymptotically become Gaussian, as the generalized Gumbel distribution converges to the normal distribution in this limit. In the opposite limit \( a \ll 1 \) where the external compression force is small with respect to the forces acting on the particles, the generalized Gumbel distribution converges to an exponential distribution \([136]\).

In the case where the confining potential for the gas and that for the piston are of different functional form, \( \alpha \neq \gamma \), one finds for \( \Omega(y) \), dropping logarithmic corrections as well as constants of order unity,

\[
\Omega(y) \sim \frac{1}{y} \exp \left[ -\beta U_0' \left( \frac{1}{\beta U_0} \ln \frac{1}{y} \right)^{\gamma/\alpha} \right] \quad (y \to 0).
\]

Hence \( \Omega(y) \) does not behave as a power law when \( y \to 0 \), so that the results of \([100]\) do not apply. It can be shown that when \( \gamma > \alpha \), the limit distribution is a Gaussian law, while for \( \gamma < \alpha \) the limit distribution is exponential \([136]\). This result is consistent with the following intuitive argument. When \( \gamma > \alpha \), \( y \Omega(y) \) decays faster than any power law, and one expects this situation to be similar to the large \( a \) limit, for which a Gaussian distribution is recovered. In contrast, when \( \gamma < \alpha \), \( y \Omega(y) \) decays slower than any power law, which is expected to be similar to the limit \( a \to 0 \), in which case one obtains an exponential distribution. The physical interpretation is that for \( \gamma > \alpha \) the piston confines the gas more strongly that the bulk confining potential, so that the latter becomes irrelevant at large size, leading to a regular confined gas with standard thermodynamic properties. For \( \gamma < \alpha \) the reverse is true; the gas is confined by the bulk potential; the piston becomes irrelevant and its fluctuations become those of a piece of flotsam driven by the fluctuations of the confined gas below.

Note that we focused here on power law potentials, which correspond to a quite natural class of potentials. However, one could also consider logarithmic potentials \( U(z) \) and \( U_p(z_p) \), which would lead to Fréchet distributions given in Eq. (4.30) for the volume fluctuations. Alternatively, if the potential diverges for a finite value \( z_{\text{max}} \), (for instance by adding a rigid wall on top of the piston), the asymptotic distribution of fluctuations would be of the Weibull type, as described in Eq. (4.31).

### 4.3.3 Discussion: relation with thermodynamics

We have shown that the volume fluctuations of an ideal gas of classical and independent particles confined by an algebraic potential acting on both particles and piston along one dimension and by hard walls in the perpendicular directions, are described by generalized extreme value statistics. In the simple case when the piston is identical to the particles, the appearance of standard extreme value distributions is easily understood from a direct mapping of volume fluctuations onto an extreme value problem of independent and identically distributed (i.i.d.) random variables.

In a more general situation the piston can differ from the particles in two ways; either the confining potential is of the same form but of different amplitude, meaning that the restoring forces on the particle and piston are different. Or, the functional form is different. In the first situation non-Gaussian height fluctuations still occur in the limit of large \( N \) in the form of generalized extreme value distributions parameterized by a real variable, \( a = U'_0/U_0 \). If the restoring force on the piston becomes much larger than that on the particles, the distribution crosses over to Gaussian. Yet for fixed values of the forces, that is for fixed \( a \), the distributions are non-Gaussian for all system sizes and no crossover occurs as a function of \( N \). For different functional forms, a crossover does
occur as a function of system size, either to Gaussian fluctuations if the piston is strongly confined, or to one-body non-Gaussian statistics, with exponential height fluctuations if the piston is less strongly confined. Our results are, in principle valid for a system of arbitrary scale perpendicular to the \( z \) axis. However, non-Gaussian fluctuations should be observable for \( a \) of order unity only, which implies a piston of microscopic extent perpendicular to \( z \), ensuring that any experimental realization would be in the form of a quasi-one dimensional sample (another possibility could be to exert two different forces on the piston, that could be fine-tuned to compensate almost exactly).

Non-Gaussian volume fluctuations have strong consequences for the thermodynamics. In a different context, non-Gaussian order parameter fluctuations have been related to critical phenomena or to the fact that an ordered phase is unstable in low dimensions [134, 137]. Analogous physics occurs for the models considered here: non-Gaussian volume fluctuations lead to singular thermodynamics. To illustrate this we consider first the simplest case where piston and particles are identical, of mass \( m \) and confined by a gravitational force, \( mg \), so that \( \alpha = \gamma = 1 \). In this case the height difference variables \( h_j \) defined in (4.20), are independent and exponentially distributed:

\[
P(h_j) = (N - j + 1) \beta mg \exp[-(N - j + 1) \beta mgh_j],
\]

as seen from Eq. (4.21). One then has a 1/f-noise-like spectrum [115], \( \langle h_j \rangle = k_B T / (N - j + 1) mg \), giving directly

\[
\langle h_j \rangle = k_B T / mg, \quad \langle z_p \rangle \approx z_0 \ln(N + 1), \quad z_0 = \frac{k_B T}{mg},
\]

where \( z_0 \) is the characteristic length scale for the particles set by the gravitational field. Defining volume \( V = Sz_p \) and external pressure, \( P = mg/S \), leads to an equation of state for the confined ideal gas \( P(V) = k_B T \ln(N) \) in the large \( N \) limit. This singular non-extensive behavior signifies the crossover between a system confined by a bulk potential (the gravitational field on the particles) and an external constraint (the pressure imposed by the piston).

Let us now consider the case where the piston mass \( M \) is different from the mass \( m \) of the particles. In this case, the variables \( h_j \) are still exponentially distributed, but now with

\[
\langle h_j \rangle = \frac{k_B T}{mg(N - j + a)}, \quad a = \frac{U_0'}{U_0} = \frac{M}{m},
\]

similarly to the “truncated 1/f-noise” considered in [135, 100]. The average piston position \( \langle z_p \rangle \) is then given by

\[
\langle z_p \rangle = \sum_{j=1}^{N+1} \langle h_j \rangle = z_0 \sum_{j=1}^{N+1} \frac{1}{(N - j + a)}.
\]

For large \( N \), one can approximate the sum by an integral, yielding

\[
\langle z_p \rangle \approx z_0 \ln \left( \frac{N}{a} + 1 \right).
\]

Introducing again the (external) pressure \( P = Mg/S \), one finds the equation of state

\[
P(V) = ak_B T \ln \left( \frac{N}{a} + 1 \right),
\]

where now \( a \) is a function of pressure. Hence, again we find that non-Gaussian fluctuations are associated with non-extensive thermodynamics. The ratio \( N/a = Nm/M \) compares the total
mass \( Nm \) of the particles to the mass \( M \) of the piston (the mass \( M \) could also be an effective mass accounting for the constant force \( f_p \), positive or negative, exerted by an operator: \( M = M_0 - f_p/g \)). If the piston becomes macroscopic with total mass, \( M \), exceeding that of the gas, then we move into the regime where \( N/a \ll 1 \). In this regime, we recover the ideal gas equation of state, \( P \langle V \rangle = Nk_BT \), as well as Gaussian volume fluctuations. In the opposite case where \( N/a \gg 1 \) (typically if \( a \) is finite and \( N \) is large), one has non-Gaussian fluctuations as described in Sect. 4.3.3, and the non-extensive equation of state \( P \langle V \rangle \approx ak_BT \ln(N/a) \). Assuming that \( a \) is large but finite, and scaling the number of particles, \( N \), with all other parameters held fixed, one therefore begins in the extensive regime for small (but macroscopic) \( N \) and \( V \). In this regime \( \langle z_p \rangle \) is less than \( z_0 \) and the effect of the confining field on the particles is negligible. On increasing \( N \), one crosses over into the non-extensive regime when this length scale in exceeded. However, no crossover is observed in the statistics of fluctuations since \( a \) is large, and fluctuations are practically Gaussian even in the non-extensive regime. Taking \( \alpha = \gamma \neq 1 \) requires more calculation but leads to essentially equivalent results.

A consequence of these results is that in the non-extensive regime the volume fluctuations are abnormally small on the scale set by the mean volume or the number of particles. Through the fluctuation dissipation relation, this scale is given by

\[
-\frac{\partial \langle V \rangle}{\partial P} = \frac{1}{k_BT} \left( \langle V^2 \rangle - \langle V \rangle^2 \right),
\]

which, in the limit \( N/a \gg 1 \) is independent of \( \langle V \rangle \). Hence the isothermal compressibility, \( \kappa = -\langle 1/V \rangle \partial \langle V \rangle / \partial P \), a normally intensive measure of the fluctuations, varies as \( 1/\ln(N) \) and scales to zero in the limit \( N \rightarrow \infty \). Physically this result occurs because the potential confining the particles within the bulk of the sample suppresses the collective fluctuations present in the standard thermodynamic regime. The logarithmic dependence is characteristic of a marginal situation between the two regimes and is analogue to the marginal stability of an ordered phase at the lower critical dimension, such as the 2D-XY model [134], or one dimensional interface with long range interactions [115].

The case where the piston is more confined than the particles is best illustrated by removing the confining potential for the particles in the above example while keeping that for the piston. One now trivially finds the ideal gas equation of state, \( P \langle V \rangle = Nk_BT \) and regular thermodynamic fluctuations from Eq. (4.3.2).

### 4.4 Renormalization group approach

#### 4.4.1 Need for a more general framework to describe fluctuations

Through these simple examples, we have seen interesting connections between the study of fluctuations of global quantities in driven or correlated systems on one side, and statistics of sums and extreme values of random variables on the other side. The toy models presented have an illustrative value, but a more general approach to the study of large scale fluctuations in non-equilibrium correlated system would be desirable, and remains to be built. The renormalization group approach, that has proved very successful in the context of correlated equilibrium systems (in particular critical phenomena), is certainly a good candidate in this respect.

Such an ambitious goal is clearly far beyond the scope of the present manuscript. Yet, as a first modest step in this direction, it is of interest to reformulate the standard extreme value statistics
problem in a renormalization group language, given the connection emphasized above between extreme value statistics and global fluctuations. This is the goal of the present section.

4.4.2 Renormalization transformation for extreme values

In extreme value statistics (EVS) [101, 102], the integrated distribution $\mu(x)$ is a useful quantity, defined for a random variable $x$ as

$$\mu(x) = \int_{-\infty}^{x} \rho(x')dx',$$  \hspace{1cm} (4.45)

where $\rho(x)$ is the probability density function. It has the meaning of the probability of finding the variable at any value below $x$. In the simplest version of EVS, let us consider a set of $N$ i.i.d. random variables $x_i$, $i = 1, \ldots, N$. The probability that the maximum value in the set, $\max(x_1, \ldots, x_N)$, is smaller than a given value $x$ is equal to the probability that all the variables $x_i$ are less than $x$. As the variables are statistically independent, this yields

$$\text{Prob}(\max(x_1, \ldots, x_N) < x) = \mu(x)^N.$$  \hspace{1cm} (4.46)

Often $\mu$ is called the parent distribution, whence the extreme value distributions descend.

In what follows we give a flavor of the decimation method leading to the RG formalism presented afterwards. Let us split the set of sufficiently large $N$ random variables $x_i$ into $N' = N/p$ blocks of $p$ random variables each. Denoting by $y_j$ the maximum value in the $j^{th}$ block, one has

$$\max(x_1, \ldots, x_N) = \max(y_1, \ldots, y_{N'}).$$  \hspace{1cm} (4.47)

The variables $y_j$ are also i.i.d. random variables, with a distribution $\mu_p(y)$ given by

$$\mu_p(y) = \mu(y)^p.$$  \hspace{1cm} (4.48)

The above procedure, which can be further iterated, may thus be thought of as a RG transformation, since a problem involving a large number of random variables is transformed into a similar problem, involving a reduced number of variables obeying a renormalized distribution. Note however that this is a quite simple example of RG, as the variables are independent, while the RG was originally designed, in the context of critical phenomena, to deal with strongly correlated variables. Yet in EVS nonlinearities are important even in the i.i.d. case, and singularities may appear for large $N$, which can be dealt with easily by the RG approach. In particular, one can simply derive universal shape corrections associated to finite size effects that need a thorough mathematical study in a direct approach. Finally we note that the parameter $p$ is here a priori an integer number $p \geq 2$. In the following, we shall however consider the case of a continuous variable.

4.4.3 Renormalization flow

The RG operation

The discrete renormalization group (RG) transformation for the extreme value statistics of independent and identically distributed (i.i.d.) variables has been introduced and studied in Ref. [138, 139], considering a discrete iteration parameter $p$. An alternative approach, which as we shall see is well
adapted to analytical studies, is to consider the RG flow by means of a partial differential equation (PDE), obtained from the discrete RG by continuation in $p$. [140]. The RG transformation introduced in [138, 139] had the form

$$[\hat{R}_p \mu](x) = \mu(a(p)x + b(p))^p.$$  (4.49)

Here the scale and shift parameters $a(p), b(p)$, to be specified later, are included in contrast to the original formula (4.48). They aim at eliminating the degeneracy of the distribution developing in the large $p$ limit and allow the emergence of a limit distribution.

As iterating $n$ times the RG transform with a scale factor $p$ corresponds to an effective RG with a scale factor $p^n$, it is natural to introduce the variable

$$s = \ln p$$

in order to parameterize the RG flow. Indeed, iterations of the RG flow then correspond to a linear increase in $s$. The integrated distribution after $p = e^s$ iterations will thus be denoted as $\mu(x, s)$. For later convenience, we also write the integrated distribution into a double exponential form, namely

$$\mu(x, s) = e^{-e^{-g(x, s)}},$$

(4.51)

which defines the real function $g(x, s)$. In this way, $\mu(x, s)$ is necessarily bounded between 0 and 1 for all real values of $g(x, s)$. The parent distribution can be suitably taken as the function at $s = 0$

$$\begin{align*}
\mu(x, 0) &= \mu(x), \\
g(x, 0) &= g(x),
\end{align*}$$

(4.52a, 4.52b)

but we will also study trajectories in function space without reference to a specific parent, when the origin of “s” will be set by some other convention.

One of the major interests of the RG approach stems from the fact that it facilitates the study of the convergence to asymptotic distributions, including the finite size corrections to this limit distributions. However, from the practical viewpoint limit distributions are equivalent up to a linear rescaling $x \to ax + b$ of the random variable, with arbitrary finite parameters $a$ and $b$. In order to lift this ambiguity, we impose the following standardization conditions on the integrated distributions (two conditions are needed since there are two free parameters $a$ and $b$ in the above rescaling):

$$\begin{align*}
\mu(0, s) &= e^{-1}, \\
\partial_x \mu(0, s) &= e^{-1}.
\end{align*}$$

(4.53a, 4.53b)

In terms of the function $g(x, s)$, these conditions translate into

$$\begin{align*}
g(0, s) &= 0, \\
\partial_x g(0, s) &= 1.
\end{align*}$$

(4.54a, 4.54b)
Partial differential equation of the flow

We now turn to the derivation of the PDE for the RG flow. With the reparameterization (4.50), we first convert the subscript and argument from \( p \) to \( s \) in the RG transform (4.49), yielding the renormalized integrated distribution as

\[
\mu(x, s) \equiv \hat{R}_s \mu(x) = \mu(a(s)x + b(s))^s,
\]

where the functions \( a(s) \) and \( b(s) \) enforce the standardization conditions (4.53). In terms of the function \( g(x, s) \), the RG transform (4.55) can be rewritten, by taking the double logarithm, as

\[
g(x, s) = g(a(s)x + b(s)) - s.
\]

This is a very simple operation, a linear change of variable in the argument of the parent (4.52b) and a global shift, where \( a(s) \) and \( b(s) \) are determined so as to satisfy the nonlinear standardization conditions (4.54).

In order to make the RG transformation more explicit we now compute the parameters \( a(s) \) and \( b(s) \). Setting \( x = 0 \) in (4.56), we get from (4.54a) that \( g(b(s)) = s \), so that

\[
b(s) = g^{-1}(s).
\]

Note that \( g(x) \) is a monotonously increasing function, invertible over the support of the parent distribution. To determine \( a(s) \), we first differentiate (4.56) with respect to \( x \), yielding

\[
\partial_x g(x, s) = a(s)g'(a(s)x + b(s)).
\]

Setting again \( x = 0 \) and using Eq. (4.54b), we get

\[
a(s) = 1/g'(b(s)).
\]

Since we aim at describing the continuous evolution of \( g(x, s) \) as a function of \( s \), we differentiate (4.56) with respect to \( s \) and obtain

\[
\partial_s g(x, s) = (\dot{a}(s)x + \dot{b}(s))g'(a(s)x + b(s)) - 1,
\]

where the dot denotes the derivative with respect to \( s \). Combining equations (4.57) and (4.59), we get

\[
\dot{b}(s) = a(s),
\]

which we substitute into Eq. (4.60). Then we use (4.58) in order to eliminate \( g' \) from Eq. (4.60), and if we introduce as well the notation

\[
\gamma(s) = \frac{\dot{a}(s)}{a(s)} = -\frac{g''(b(s))}{g'^2(b(s))},
\]

we eventually obtain the PDE

\[
\partial_s g(x, s) = (1 + \gamma(s)x)\partial_x g(x, s) - 1.
\]

This equation should be taken with initial condition defined by the parent distribution through (4.52), and the parent also determines \( \gamma(s) \) by (4.62). We emphasize that the original form (4.55)
of the RG transformation produces valid (monotonically increasing in $x$) distribution functions from a like initial function, thus the PDE, derived from (4.55), also must preserve monotonicity. This is a property maintained even if it is not obvious directly from the PDE. We note furthermore, that if the standardization condition (4.54a) is met then, as it is easy to see, the solution of the PDE automatically satisfies (4.54b).

In (4.63) the coefficient function $\gamma(s)$ can be considered as an “external” forcing, which, beside the initial condition, carries information on the parent. In this sense, (4.63) is a linear, parametrically driven PDE.

Interestingly, the same PDE (4.63) can be alternatively interpreted as an autonomous but nonlinear flow equation. For this purpose we start out from an arbitrary point on the flow $g(x,s)$ and apply an infinitesimal renormalization transformation to it as

$$g(x, s + ds) = [\dot{R}_{ds}]g(x, s).$$

(4.64)

Consistently with (4.56), this involves a linear change of variable and an overall shift, both infinitesimal as

$$g(x, s + ds) = g \left( (1 + \tilde{a}(s)ds)x + \tilde{b}(s)ds, s \right) − ds,$$

(4.65)

where the functions $\tilde{a}(s)$ and $\tilde{b}(s)$ are to be specified. Linearizing (4.65) with respect to $ds$, we get

$$\partial_s g(x, s) = (\tilde{a}(s)x + \tilde{b}(s))\partial_x g(x, s) − 1.$$  

(4.66)

Using the standardization conditions (4.54) we can hence determine the unknown functions $\tilde{a}(s)$ and $\tilde{b}(s)$. Setting $x = 0$ yields a constant $\tilde{b}(s) \equiv 1$, from which we recover the previously derived PDE (4.63), where in place of $\tilde{a}(s)$ the $\gamma(s)$ appears. As a final step in this reasoning, by once differentiating (4.63) in terms of $x$, setting $x = 0$, and using (4.54b) we find that

$$\gamma(s) = −\partial_x^2 g(0, s)$$

(4.67)

must hold. So in this picture the PDE is the same as (4.63), but the coefficient function $\gamma(s)$ is now interpreted as the initial curvature (4.67) of the field $g(x, s)$. Then one can try to find families of solutions of the PDE, where $\gamma(s)$ is calculated from the self-consistency condition (4.67). Note that the presence of $\gamma(s)$ defined by (4.67) makes the PDE nonlinear, and actually nonlocal because the curvature at $x = 0$ affects the evolution at all $x$’s, but without external driving.

In conclusion, the RG flow is described by (4.63), where the coefficient function $\gamma(s)$ is either an external forcing given by the parent $g(x)$ or defined by the initial curvature of the field $g(x, s)$ itself. The two definitions (4.62) and (4.67) are, however, identical, as can be shown by using the standardization (4.54) and the form (4.56) for the RG transformation.

**Fixed point**

Let us look for fixed point solutions $g(x, s) \equiv f(x)$ of the PDE (4.63), namely solutions that are independent of $s$. Then $f(x)$ must satisfy the stationary version of (4.63)

$$0 = (1 + \gamma x)f'(x) − 1,$$

(4.68)

where by (4.67) we must have a constant $\gamma$ arising in

$$\gamma = −f''(0).$$

(4.69)
Hence, using the standardization condition $f(0) = 0$, we get

$$f(x; \gamma) = \int_0^x (1 + \gamma y)^{-1} dy = \frac{1}{\gamma} \ln(1 + \gamma x),$$

from which the fixed point distribution reads

$$M(x; \gamma) = e^{-e^{f(x; \gamma)}} = e^{-(1+\gamma x)^{-1/\gamma}}.$$ \hspace{1cm} (4.71)

This is the well known generalized extreme value distribution, obtained here as a fixed line of the RG transformation [141, 101]. The above derivation of the universal limit distribution family is quite brief, and was made possible by the PDE-representation of the RG flow.

4.4.4 Concluding remarks

We have seen that the renormalization group language provides an efficient formalism in order to derive the asymptotic extreme value distributions. Actually, the renormalization approach also yields in a rather straightforward way the first finite size correction to the asymptotic distribution [138, 139, 140]. We have also reported interesting formal connections between extreme values and sums (different from that presented above) in this RG framework [140].

One might hope that the present RG application to extreme value statistics could trigger more involved studies, dealing with correlated problems. This could be a further step toward the understanding of the intriguing statistics of global observables in correlated systems, and more specifically in driven dissipative systems.
Chapter 5

Collective behavior of interacting agents

Standard statistical physics is mainly concerned with physical systems in which elementary entities are implicitly atoms or molecules. In this case, the laws of motion of the individual particles are known, and the main difficulty consists in being able to change the scale of description, going from the scale of particles to the system size.

However, our everyday life experience tells us that there exist many familiar systems that are composed of interacting macroscopic ‘entities’, that thus behave very differently from atoms or molecules: examples range from sand piles, foams, bacteria colonies, animal flocks, or road traffic, to quote only a few examples. In such cases, it is clear that the interacting objects, or individuals, cannot be described in the same way as molecules, and precise dynamical laws at the individual scale are most often not known.

The difficulties encountered when trying to apply a statistical physics approach to such assemblies of macroscopic ‘entities’ are then two-fold. On the one hand, a model should be given for the dynamics of individual, and it is often not clear how relevant or reliable such modeling are to describe realistic systems. On the other hand, reasonable models of individual dynamics usually do not have similar conservation laws and time-reversal symmetry as the Hamiltonian dynamics of molecular systems. Hence it is hard, even in specific cases, to build a statistical physics approach from a postulate similar to the hypothesis of equiprobability of configurations having the same energy. Interesting attempts in this direction, notably in the context of granular matter, have however been proposed [25].

In this last part, we illustrate on several examples how different statistical physics techniques can be devised, in specific cases, to describe assemblies of interacting agents. In the first example (the dynamics of residential moves in a city, Sec. 5.1), a mapping can be performed to an effective equilibrium system, yielding interesting insights. The second example (collective motion, Sec. 5.2) is studied through the so-called Boltzmann equation, a generic approach that can be used when interactions are limited to binary ‘collisions’, that are extremely localized in space and time. Finally, the last section (Sec. 5.3) deals with the example of a population of (human) agents that need to choose between two different shops when they wish to buy fresh food products, leading to an interesting symmetry breaking phenomenon.
5.1 Dynamics of residential moves

The intricate relations between the individual and collective levels are at the heart of many natural and social sciences. Different disciplines wonder how atoms combine to form solids [142, 143], neurons give rise to consciousness [144, 145] or individuals shape societies [146, 147]. However, scientific fields assume distinct points of view for defining the “normal”, or “equilibrium” aggregated state. Physics looks at the collective level, selecting the configurations that minimize the global free energy [143]. In contrast, economic agents behave in a selfish way, and equilibrium is attained when no agent can increase its own satisfaction [148]. Although similar at first sight, the two approaches lead to radically different outcomes.

In this section, we illustrate the differences between collective and individual dynamics on an exactly solvable model, similar to Schelling’s segregation model [149]. The model considers individual agents which prefer a mixed environment, with dynamics that lead to segregated or mixed patterns at the global level. A “tax” parameter monitors continuously the agents’ degree of altruism or cooperativity, i.e., their consideration of the global welfare. At high degrees of cooperativity, the system is in a mixed phase of maximal utility. As the altruism parameter is decreased, a phase transition occurs, leading to segregation. In this phase, the agents’ utilities remain low, in spite of continuous efforts to maximize their satisfaction. This paradoxical result of Schelling’s segregation model [149] has generated an abundant literature. Many papers have simulated how the global state depends on specific individual utility functions, as reviewed by [150]. There have been attempts at solving Schelling’s model analytically, in order to provide more general results concerning the consequences of individual preferences on segregation levels [151, 152, 153]. However, these are limited to specific utility functions. More recently, physicists have tried to use a statistical physics approach to understand the segregation transition [154, 155, 156]. The idea seems promising, since statistical physics has successfully bridged the gap between microscopic and macroscopic descriptions, for physical systems governed by collective dynamics. In this section, we introduce a rigorous generalization of the physicist’s notion of free energy, taking into account individual dynamics. By introducing a state function which is maximized in the stationary state, this approach provides us with a quantitative solution for very general utility functions.

5.1.1 Model and dynamics

Our model represents in a schematic way the dynamics of residential moves in a city. For simplicity, we include a single type of agents, but our results can readily be generalized to deal with agents of two “colors”, as in the original Schelling model [149]. The city is divided into $Q$ blocks ($Q \gg 1$), each block containing $H$ cells or flats. We assume that each cell can contain at most one agent, so that the number $n_q$ of agents in a given block $q$ ($q = 1, \ldots, Q$) satisfies $n_q \leq H$, and we introduce the density of agents $\rho_q = n_q / H$. Each agent has the same utility function $u(\rho_q)$, which describes the degree of satisfaction concerning the density of the block he is living in. The collective utility is defined as the total utility of all the agents in the city: $U(x) = H \sum_q \rho_q u(\rho_q)$, where $x \equiv \{\rho_q\}$ corresponds to the coarse-grained configuration of the city, i.e. the knowledge of the density of each block. For a given $x$, there is a large number of ways to arrange the agents in the different cells. This number of arrangements is quantified by its logarithm $S(x)$, called the entropy of the configuration $x$.

The dynamical rule allowing the agents to move from one block to another is the following. At each time step, one picks up at random an agent and a vacant cell, within two different blocks.
Then the agent moves in that empty cell with probability:

\[ P_{xy} = \frac{1}{1 + e^{-C/T}}, \]

where \( x \) and \( y \) are respectively the configurations before and after the move, and \( C \) is the cost associated to the proposed move. The positive parameter \( T \) is a “temperature” which introduces in a standard way [157] some noise on the decision process. It can be interpreted as the effect of features that are not explicitly included in the utility function but still affect the moving decision (urban facilities, friends...). We write the cost \( C \) as:

\[ C = \Delta u + \alpha(\Delta U - \Delta u) \]

(5.2)

where \( \Delta u \) is the variation of the agent’s own utility upon moving and \( \Delta U \) is the variation of the total utility of all agents. The parameter \( 0 \leq \alpha \leq 1 \) weights the contribution of the other agents’ utility variation in the calculation of the cost \( C \), and it can thus be interpreted as a degree of cooperativity (or altruism). For \( \alpha = 0 \), the probability to move only depends on the selfish interest of the chosen agent, which corresponds to the spirit of economic models such as Schelling’s. When \( \alpha = 1 \), the decision to move only depends on the collective utility change, as in physics models. Varying \( \alpha \) in a continuous way, one can interpolate between the two limiting behaviors of individual and collective dynamics.

5.1.2 Effective free energy

We wish to find the stationary probability distribution \( \Pi(x) \) of the microscopic configurations \( x \). If the cost \( C \) can be written as \( C = \Delta V \equiv V(y) - V(x) \), where \( V(x) \) is a function of the configuration \( x \), then the dynamics satisfies detailed balance [21] and the distribution \( \Pi(x) \) is given by

\[ \Pi(x) = \frac{1}{Z} e^{F(x)/T}, \]

(5.3)

with \( F(x) = V(x) + TS(x) \) and \( Z \) a normalization constant. The entropy has for large \( H \) the standard expression \( S(x) = H \sum_q s(\rho_q) \), with

\[ s(\rho) = -\rho \ln \rho - (1 - \rho) \ln(1 - \rho). \]

(5.4)

We now need to find the function \( V(x) \), if it exists. Given the form (5.2) of \( C \), finding such a function \( V(x) \) amounts to finding a function \( L(x) \), connecting the individual and collective levels, such that \( \Delta u = \Delta L \). The function \( V \) would thus be given by \( V(x) = (1 - \alpha)L(x) + \alpha U(x) \). By analogy to the entropy, we assume that \( L(x) \) can be written as a sum over the blocks, namely \( L(x) = H \sum_q \ell(\rho_q) \). Considering a move from a block at density \( \rho_1 \) to a block at density \( \rho_2 \), \( \Delta L \) reduces in the large \( H \) limit to \( \ell'(\rho_2) - \ell'(\rho_1) \), where \( \ell' \) is the derivative of \( \ell \). The condition \( \Delta u = \Delta L \) then leads to the identification \( \ell'(\rho) = u(\rho) \), from which the expression of \( \ell(\rho) \) follows:

\[ \ell(\rho) = \int_0^\rho u(\rho')d\rho'. \]

(5.5)

As a result, the function \( F(x) \) can be expressed in the large \( H \) limit as \( F(x) = H \sum_q f(\rho_q) \), with a block potential \( f(\rho) \) given by:

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\[ f(\rho) = -T \rho \ln \rho - T(1-\rho) \ln(1-\rho) + \alpha \rho u(\rho) + (1-\alpha) \int_0^\rho u(\rho') d\rho'. \] (5.6)

The probability \( \Pi(x) \) is dominated by the configurations \( x = \{\rho_q\} \) that maximize the sum \( \sum_q f(\rho_q) \) under the constraint of a fixed \( \rho_0 = Q^{-1} \sum_{q=1}^Q \rho_q \). To perform this maximization procedure, we follow standard physical methods used in the study of phase transitions (like liquid-vapor coexistence [158]), which can be summarized as follows. If \( f(\rho) \) coincides with its concave hull at a given density \( \rho_0 \), then the state of the city is homogeneous, and all blocks have a density \( \rho_0 \). Otherwise, a phase separation occurs: some blocks have a density \( \rho_1^s < \rho_0 \), while the others have a density \( \rho_2^s > \rho_0 \).

Interestingly, the potential \( F = (1-\alpha)L + \alpha U + TS \) appears as a generalization of the notion of free energy introduced in physical systems. Mapping the global utility onto the opposite of the energy of a physical system, it turns out that for \( \alpha = 1 \), the maximization of the function \( U + TS \) is equivalent to the minimization of the free energy \( E - TS \). For \( \alpha < 1 \), the potential \( F \) takes into account individual moves through the state function \( L \). Furthermore, the potential \( F \) can be calculated for arbitrary utility functions, allowing to predict analytically the global town state.

To obtain explicitly the equilibrium configurations, one needs to know the specific form of the utility function. To illustrate the dramatic influence of the cooperativity parameter \( \alpha \), we use the asymmetrically peaked utility function shown on Fig. 5.1 [159], which indicates that agents prefer mixed blocks. The overall town density is fixed at \( \rho_0 = 1/2 \) to avoid the trivial utility frustration resulting from the impossibility to attain the optimal equilibrium (\( \rho_q = 1/2 \) for all blocks). We also consider for simplicity the limit \( T \to 0 \), to avoid entropy effects. It can be shown that the qualitative behavior of the system is unchanged for \( \rho_0 \neq 1/2 \) or for low values of the temperature.

In the collective case (\( \alpha = 1 \)), the optimal state corresponds to the configuration that maximizes the global utility, which can be immediately guessed from Figure 5.1, namely \( \rho_q = 1/2 \) for all \( q \). On the contrary, in the selfish case (\( \alpha = 0 \)), maximization of the potential \( F(x) \) shows that the town settles in a segregated configuration where a fraction of the blocks are empty and the others have a density \( \rho_q > 1/2 \). Surprisingly, the city settles in this state of low utility in spite of agents’ continuous efforts to maximize their own satisfaction. To understand this frustrated configuration, note that the collective equilibrium (\( \rho_q = 1/2 \) for all \( q \)) is now an unstable Nash equilibrium at \( T > 0 \). The instability can be understood by noting that at \( T > 0 \) there is a positive probability that an agent accepts a slight decrease of its utility, and leaves a block with density \( \rho_q = 1/2 \). The agents remaining in its former block now have a lower utility and are more likely to leave to another \( \rho_q = 1/2 \) block. This creates an avalanche which empties the block, as each move away further decreases the utility of the remaining agents. This avalanche stops when the stable (Nash) equilibrium, given by the maximum of the potential \( F \), is reached. This state corresponds to a spatially inhomogeneous repartition of agents in the city. To understand the transition between mixed and segregated configurations, it is instructive to calculate the values of both the overall utility and the potential, for different values of \( m \) (at \( \alpha = 0 \)). In case of a homogeneous town (an unstable Nash equilibrium for which \( \rho_q = 1/2 \) for all \( q \)), the normalized collective utility is given by \( U^* = U/(\rho_0HQ) = u(\rho_0 = 1/2) = 1 \). The normalized link function equals, for all \( m, L^* = L/(\rho_0HQ) = \ell(\rho_0)/\rho_0 = 1/2 \), where \( \ell \) is given in Eq. 5.5. The values of \( L^* \) and \( U^* \) displayed in Table 2.1 show that the utility of the segregated equilibrium is lower but that its

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Figure 5.1: Asymmetrically peaked individual utility as a function of block density. The utility is defined as $u(\rho) = 2\rho$ if $\rho \leq 1/2$ and $u(\rho) = m + 2(1 - m)(1 - \rho)$ if $\rho > 1/2$, where $0 < m < 1$ is the asymmetry parameter. Agents strictly prefer half-filled neighborhoods ($\rho = 1/2$). They also prefer overcrowded ($\rho = 1$) neighborhoods to empty ones ($\rho = 0$).

Potential is higher, explaining its stability. Note that the gap between the link function values of the homogeneous and segregated configurations increases with $m$.

This helps understanding why the greater the $m$, the greater the value of $\alpha$ necessary to reach the homogeneous configuration. Indeed, the segregated states are separated from mixed ones by a phase transition at the critical value $\alpha_c = 1/(3 - 2m)$ - which increases with $m$ (Figure 5.2). This transition differs from standard equilibrium phase transitions known in physics, which are most often driven by the competition between energy and entropy. Here, the transition is driven by a competition between the collective and individual components of the agents dynamics. Another interesting effect is observed for $m > 2/3$ (Fig. 5.2). Considering a small value of $\alpha$ has no effect on the overall satisfaction, the utility remaining constant until a threshold level is attained at $\alpha_t = (3m - 2)/(6 - 5m)$.

5.1.3 Discussion

The present model can be thought of as a ”local mean-field” version of the original Schelling model [149], with the further difference that only one type of agent is present. It can however be generalized to take into account the existence of two types of agents [195], yielding qualitatively a similar behavior.

Besides, the present simple model raises a number of interesting questions about collective or individual points of view. In the purely collective case ($\alpha = 1$), the stationary state corresponds to the maximization of the average utility, in analogy to the minimization of energy in physics. In the opposite case ($\alpha = 0$), the stationary state strongly differs from the simple collection of individual optima [160]: the optimization strategy based on purely individual dynamics fails, illustrating the unexpected links between micromotives and macrobehavior [161]. However, the emergent collective state can be efficiently captured by the maximization of the link function $\ell(\rho)$ given in Eq. (5.5), up to constraints in the overall town density. This function intimately connects the individual and global points of view. First, it depends only on the global town configuration (given by the $\rho_q$), allowing a relatively simple calculation of the equilibrium. At the same time, it can be interpreted
Figure 5.2: Phase diagram of the global utility as a function of the cooperativity $\alpha$ and the asymmetry $m$, at $T \to 0$ and $\rho_0 = 1/2$. The average utility per agent $U^* = U/(H\rho_0)$ is calculated by maximizing the potential $F(x)$ for the peaked utility shown in Fig. 5.1. The plateau at high values of $\alpha$ corresponds to the mixed phase of optimal utility, which is separated from the segregated state by a phase transition arising at $\alpha_c = 1/(3 - 2m)$. The overall picture is qualitatively unchanged for low but finite values of the temperature.

as the sum of the individual marginal utilities gained by agents as they progressively fill the city after leaving a reservoir of zero utility. In the stationary state, a maximal value of the potential $L$ is reached. This means that no agent can increase its utility by moving (since $\Delta u = \Delta L$), consistently with the economists’ definition of a Nash equilibrium.

5.1.4 Application: socio-economic utility and chemical potential

As a by product of the above study, one can derive an interesting relationship between the socio-economic notion of utility and the physical notion of chemical potential [163]. To be more specific, the question we investigate here is whether the above physical description of socio-economic models can be extended to other basic concepts of statistical physics, such as the equalization of thermodynamic parameters like temperature or chemical potential. The equalization of these quantities throughout the system precisely results from the conservation of the conjugated extensive quantities, namely the energy or the number of particles. Although there is no notion of energy in socio-economic models, the dynamics indeed conserves the number of agents. A natural question is thus to know whether a chemical potential can be defined in such models, and what would be its relation to standard socio-economic concepts. This question is further motivated by the following remark. In spatial socio-economic models, the individual dynamics leads to a Nash equilibrium, where no agent has an incentive to move. If all agents are of the same type, the Nash equilibrium results in a spatially uniform utility, even if the environment is spatially inhomogeneous like in cities, where the center plays a specific role. This uniformity property is also expected from the chemical potential (if such a quantity can be defined), suggesting a possible relation between these two notions.

We consider here a model where agents belong to $m$ different groups, according for instance to their income, or to their cultural preferences. We further assume that the system can be described
by a state function as above, so that the steady-state probability distribution can be computed, and takes the form:

\[ P(\{\rho_{qi}\}) = \frac{1}{Z} \prod_q e^{H_f(\rho_{q1}, \ldots, \rho_{qm})/T} \prod_i \delta\left( \sum_q \rho_{qi} - Q\rho_i \right) \]  

(5.7)

where the effective free-energy \( f_q \) is given by

\[ f_q(\rho_{q1}, \ldots, \rho_{qm}) = l_q(\rho_{q1}, \ldots, \rho_{qm}) + Ts(\rho_{q1}, \ldots, \rho_{qm}), \]  

(5.8)

with an additive entropic contribution:

\[ s(\rho_{q1}, \ldots, \rho_{qm}) = -\sum_i \rho_{qi} \ln \rho_{qi}. \]  

(5.9)

In the following, we do not need to specify further the functional form of the function \( l_q(\rho_{q1}, \ldots, \rho_{qm}) \).

The configurations \( \{\rho_{qi}^*\} \) which maximize \( F = \sum_q f_q \) under the constraints of fixed global density \( \sum_q \rho_{qi} = Q\rho_i \) are the most probable (or equilibrium) configurations. Finding the equilibrium densities \( \{\rho_{qi}^*\} \) is then a constrained maximization problem. Let us introduce a Lagrangian

\[ \mathcal{L}(\{\rho_{qi}\}, \{\lambda_i\}) = \sum_q f_q(\rho_{q1}, \ldots, \rho_{qm}) - \sum_i \lambda_i \left( \sum_q \rho_{qi} - Q\rho_i \right), \]  

(5.10)

where the parameters \( \lambda_i \) are Lagrange multipliers associated to the conservation of the number of agents in each group. In physical terms, \( \lambda_i \) corresponds to the chemical potential of the agents of group \( i \). The equilibrium densities \( \{\rho_{qi}^*\} \) are then determined from the conditions \( \partial \mathcal{L} / \partial \rho_{qi} = 0 \) for all \( (q, i) \), yielding

\[ u_{qi}(\rho_{q1}^*, \ldots, \rho_{qm}^*) + T \frac{\partial s}{\partial \rho_{qi}}(\rho_{q1}^*, \ldots, \rho_{qm}^*) = \lambda_i. \]  

(5.11)

Equation (5.11) thus provides an answer to the question raised at the beginning of this section: there is indeed a direct relationship between the socio-economic utility and the chemical potential defined, in analogy to equilibrium physical systems, from the conservation of the number of particles. At zero temperature, both quantities can be identified. This result might come as a surprise: utility is often thought to be the socio-economic concept most similar to the physical concept of energy (or more precisely, the opposite of the energy), because agents seek to maximize their utility in social systems and physical particles minimize the energy in the zero temperature limit. Hence one might have intuitively expected the homogeneity of utility to be linked to a notion of temperature (the thermodynamic variable conjugated to energy), rather than to a chemical potential.

Interestingly, Eq. (5.11) not only provides a link between two apparently unrelated concepts, but also yields a non-trivial prediction on the variations of utility across the system at non-zero temperature. As the chemical potential remains uniform at any temperature, one sees from Eq. (5.11) that the utility \( u_{qi} = \lambda_i - T \partial s / \partial \rho_{qi} \) becomes non-uniform if \( T > 0 \), and that the corrections to uniformity are given by the derivative of the local entropy.

### 5.2 Collective motion of active particles

Another interesting example of collective behavior is the motion of large groups of self-propelled interacting agents. This subject has become in recent years an important topic of interest for
statistical physicists. Applications range from animal flocks (e.g. fish schools or bird flocks) [164], to bacteria colonies [165], human crowds [166], molecular motors [167], or even interacting robots [168]. Despite its ubiquity, it is only recently that physicists realized that this phenomenon was exhibiting universal emerging properties, depending only on a few general properties of interacting agents [169, 6]. From a physicist viewpoint, it is thus of primary importance to analyze generic minimal models that could capture the emergence of collective motion, without entering the details of the dynamics of each particular system. In this spirit, Vicsek et al. proposed a simple model [170], defined on a continuous plane, where “animals” are represented schematically as point particles with a velocity vector of constant magnitude. Noisy interaction rules tend to align the velocity of any given particle with its neighbors. A continuous transition from a disordered state at high enough noise to a state where a collective motion arises was found numerically [170]. Recent numerical simulations confirmed the existence of the transition, and suggested that the transition may be discontinuous, with strong finite size effects [171, 172]. In other approaches, velocity vectors have been associated with classical spins [173, 174]. Lattice Boltzmann models have also been proposed [175], with the drawback that the rotational symmetry of the velocities does not hold at the microscopic level.

However, apart from this large amount of numerical data, little analytical results are available. Some coarse-grained descriptions of the dynamics in terms of phenomenological hydrodynamic equations have been proposed [176, 177, 6, 178], on the basis of symmetry and conservation laws arguments. Accordingly, the coefficients entering these equations have no microscopic content, and their dependence upon external parameters is unknown. Renormalization group analysis [176] and numerical studies [178] confirm the presence of a nonequilibrium phase transition in such systems. Still, a first-principle analytical approach based on the dynamics of individuals would be desirable in order to gain a better understanding of the spontaneous symmetry breaking occurring in such two-dimensional non-equilibrium systems with continuous rotational symmetry (a phenomenon that cannot occur in equilibrium systems, as shown by Mermin and Wagner [137]).

In this section, we introduce a microscopic bidimensional model of self-propelled particles with noisy and local interaction rules tending to align the velocities of the particles. We derive analytically hydrodynamic equations for the density and velocity fields, within a Boltzmann approach. The obtained equations are consistent with previous phenomenological proposals [176, 177, 6, 178]. Most importantly, we obtain explicit expressions for the coefficients of these equations as a function of the microscopic parameters. This allows us to analyze the phase diagram of the model in the noise-density plane.

### 5.2.1 Definition of the model

We consider self-propelled point-like particles moving on a continuous plane, with a velocity vector $\mathbf{v}$ of fixed magnitude $v_0$ (to be chosen as the velocity unit) in a reference frame –hence, Galilean

![Figure 5.3: Schematic view of the dynamics of the model: (a) self-diffusion events, (b) binary collisions with alignment interactions –see text for notations.](image)
invariance no longer holds. The velocity of the particles is simply defined by the angle $\theta$ between $\mathbf{v}$ and an arbitrary reference direction. Particles evolve ballistically until they experience either a self-diffusion event (a random “kick”), or a binary collision that tends to align the velocities of the two particles. To be more specific, the velocity angle $\theta$ of any particle is changed with a probability $\lambda$ per unit time to a value $\theta' = \theta + \eta$ [Fig. 5.3(a)], where $\eta$ is a Gaussian noise with distribution $p_0(\eta)$ and variance $\sigma_0^2$. In addition, binary collisions occur when the distance between two particles becomes less than $d_0$ (in the following, we set $d_0 = \frac{1}{2}$). The velocity angles $\theta_1$ and $\theta_2$ of the two particles are then changed into $\theta'_1 = \overline{\theta} + \eta_1$ and $\theta'_2 = \overline{\theta} + \eta_2$ [Fig. 5.3(b)], where $\overline{\theta} = \text{Arg}(e^{i\theta_1} + e^{i\theta_2})$ is the average angle, and $\eta_1$ and $\eta_2$ are independent Gaussian noises with the same distribution $p(\eta)$ and variance $\sigma^2$, that may differ from $\sigma_0^2$.

### 5.2.2 Boltzmann equation

The Boltzmann equation describing the evolution of the one-particle phase-space distribution $f(r, \theta, t)$ reads

$$\frac{\partial f}{\partial t}(r, \theta, t) + e(\theta) \cdot \nabla f(r, \theta, t) = I_{\text{dif}}[f] + I_{\text{col}}[f]$$

where $I_{\text{dif}}[f]$ accounts for the self-diffusion phenomenon, and $I_{\text{col}}[f]$ describes the effect of collisions; $e(\theta)$ is the unit vector in the direction $\theta$. $I_{\text{dif}}[f]$ is given by

$$I_{\text{dif}}[f] = -\lambda f(r, \theta, t) + \lambda \int_{-\pi}^{\pi} d\theta' \int_{-\infty}^{\infty} d\eta p_0(\eta)$$

$$\times \sum_{m=-\infty}^{\infty} \delta(\theta' + \eta - \theta + 2m\pi) f(r, \theta', t)$$

(5.13)

The collision term $I_{\text{col}}[f]$ is evaluated as follows. By definition, two particles collide if their relative distance becomes less than $d_0$. In the referential of particle 1, particle 2 has a velocity $v'_2 = e(\theta_2) - e(\theta_1)$. Thus, particles that collide with particle 1 between $t$ and $t + dt$ are those that lie, at time $t$, in a rectangle of length $|v'_2|$ and of width $2d_0$. This leads to

$$I_{\text{col}}[f] = -f(r, \theta, t) \int_{-\pi}^{\pi} d\theta' |e(\theta') - e(\theta)| f(r, \theta', t)$$

$$+ \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_2 \int_{-\infty}^{\infty} d\eta p(\eta) |e(\theta_2) - e(\theta_1)|$$

$$\times f(r, \theta_1, t) f(r, \theta_2, t) \sum_{m=-\infty}^{\infty} \delta(\theta + \eta - \theta + 2m\pi)$$

(5.14)

with $\overline{\theta} = \text{Arg}(e^{i\theta_1} + e^{i\theta_2})$. It can be checked easily that the uniform distribution $f(r, \theta, t) = \rho/2\pi$, is a solution of Eq. (5.12) for any density, and whatever the form of the noise distributions $p_0(\eta)$ and $p(\eta)$.
5.2.3 Hydrodynamic equations

Let us now define the hydrodynamic density and velocity fields \( \rho(r, t) \) and \( u(r, t) \)
\[
\rho(r, t) = \int_{-\pi}^{\pi} d\theta f(r, \theta, t) \tag{5.15}
\]
\[
\rho(r, t) u(r, t) = \int_{-\pi}^{\pi} d\theta f(r, \theta, t) e(\theta) \tag{5.16}
\]

Integrating the Boltzmann equation (5.12) over \( \theta \) yields the continuity equation for \( \rho(r, t) \)
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{5.17}
\]

The derivation of a hydrodynamic equation for the velocity field is less straightforward, and involves an approximation scheme. Let us introduce the Fourier series expansion of \( f(r, \theta, t) \) with respect to \( \theta \)
\[
\hat{f}_k(r, t) = \int_{-\pi}^{\pi} d\theta f(r, \theta, t) e^{ik\theta} \tag{5.18}
\]

Multiplying Eq. (5.12) by \( e^{ik\theta} \) and integrating over \( \theta \) leads to an infinite set of coupled equations for the (space-dependent) Fourier coefficients \( \hat{f}_k(r, t) \). We note that, identifying complex numbers with two-dimensional vectors so that \( e^{i\theta} \) corresponds to \( e(\theta) \), the Fourier coefficient \( \hat{f}_1(r, t) \) is nothing but the “momentum” field \( w(r, t) = \rho(r, t) u(r, t) \). Thus the evolution equation for \( \hat{f}_1(r, t) \) should yield the hydrodynamic equation for \( u(r, t) \). Yet, as \( \hat{f}_k(r, t) \) is coupled to all others \( \hat{f}_l(r, t) \), a closure relation has to be found. In the following, we assume that \( u(r, t) \) is small compared to the individual velocity of particles, and that the hydrodynamic fields vary on length scales that are much larger than the microscopic length \( d_0 \). As a result, the velocity equation is obtained from the equation for \( \hat{f}_1 \) through an expansion to leading orders in \( \hat{f}_k(r, t) \) and in space and time derivatives. Noting that \( f_0(r, t) = \rho(r, t) = O(1) \), we set \( \hat{f}_1(r, t) = O(\epsilon) \), \( \epsilon \ll 1 \). A consistent scaling ansatz, confirmed by a numerical integration of Eq. (5.12) in the steady state, is \( \hat{f}_k(r, t) = O(\epsilon^{|k|}) \). Expanding to order \( \epsilon^3 \), one only keeps the terms in \( \hat{f}_1 \) and \( \hat{f}_2 \) in the evolution equation for \( \hat{f}_1 \). A similar expansion of the equation for \( \hat{f}_2 \) leads to a closure relation for the equation on \( \hat{f}_1 \), finally leading to the following hydrodynamic equation [179, 180]
\[
\frac{\partial w}{\partial t} + \gamma(w \cdot \nabla)w = -\frac{1}{2} \nabla(\rho - \kappa w^2) \tag{5.19}
\]
\[
+ (\mu - \xi w^2)w + \nu \nabla^2 w - \kappa(\nabla \cdot w)w
\]

where the different coefficients are given by
\[
\nu = \frac{1}{4} \left[ \lambda \left(1 - e^{-\sigma^2/2}\right) + \frac{4}{\pi} \rho \left(\frac{14}{15} + \frac{2}{3} e^{-2\sigma^2}\right) \right]^{-1} \tag{5.20}
\]
\[
\gamma = \frac{8\nu}{\pi} \left(\frac{16}{15} + 2 e^{-2\sigma^2} - e^{-\sigma^2/2}\right) \tag{5.21}
\]
\[
\kappa = \frac{8\nu}{\pi} \left(\frac{4}{15} + 2 e^{-2\sigma^2} + e^{-\sigma^2/2}\right) \tag{5.22}
\]
\[
\mu = \frac{4}{\pi} \rho \left(e^{-\sigma^2/2} - \frac{2}{3}\right) - \lambda \left(1 - e^{-\sigma^2/2}\right) \tag{5.23}
\]
\[
\xi = \frac{64
\nu}{\pi^2} \left(e^{-\sigma^2/2} - \frac{2}{5}\right) \left(\frac{1}{3} + e^{-2\sigma^2}\right) \tag{5.24}
\]
5.2.4 Phase diagram

We can now study the spontaneous onset of collective motion in the present model. As a first step, it is interesting to consider possible instabilities of the spatially homogeneous system, that is the appearance of a uniform nonzero field \( w \). Equating all space derivatives to zero leads to the simple equation

\[
\frac{\partial w}{\partial t} = (\mu - \xi w^2)w
\]

Clearly, \( w = 0 \) is solution for all values of the coefficients, but it becomes unstable for \( \mu > 0 \), when a nonzero solution \( w_0 = \sqrt{\mu/\xi} e \) appears, where \( e \) is an arbitrary unit vector. From Eq. (5.23), the value \( \mu = 0 \) corresponds to a threshold value \( \rho_t \)

\[
\rho_t = \frac{\pi \lambda (1 - e^{-\sigma_0^2/2})}{4(e^{-\sigma_0^2/2} - 2/3)}
\]

The transition line defined by \( \rho_t \) in the plane \( (\rho/\lambda, \sigma) \) is plotted in Fig. 5.4, for \( \sigma_0 = \sigma \) and for a fixed value \( \sigma_0 = 1 \). If \( \sigma_0 = \sigma \), the instability occurs at any density, provided the noise is low enough. On the contrary, at fixed \( \sigma_0 \), the instability disappears below a finite density \( \rho_t^0 = 3\pi \lambda (1 - e^{-\sigma_0^2/2})/4 \). Both transition lines saturate at a value \( \sigma_t = (2 \ln 3)^{1/2} \approx 0.90 \).

Note that, strictly speaking, the homogeneous field \( w_0 \) can only develop in some ideal geometrical conditions, namely in an infinite space or in presence of periodic boundary conditions. In finite geometries, the spontaneous field \( w(r) \) is locally equal to \( w_0 \) (with a space-dependent direction) plus some corrections which can be computed analytically [180].
Let us now test the stability against perturbations of the above spatially homogeneous flow \( w(r,t) = w_0 \), with finite density \( \rho_0 \), in an infinite space. From Eq. (5.25), it is clear that \( w_0 \) is stable against spatially homogeneous perturbations. Yet, this solution may be unstable against finite wavelength perturbations (note that for \( \rho < \rho_t \), the solution \( w = 0 \) is stable against finite wavelength perturbations [180]).

To check this issue, we introduce a perturbation around the homogeneous steady-state solution

\[
\rho(r,t) = \rho_0 + \delta\rho(r,t), \quad w(r,t) = w_0 + \delta w(r,t)
\]

and linearize Eq. (5.19) in \( \delta\rho(r,t) \) and \( \delta w(r,t) \). Linear stability is then tested with the ansatz

\[
\delta\rho(r,t) = \delta\rho_0 e^{st+i|q| \cdot r}, \quad \delta w(r,t) = \delta w_0 e^{st+i|q| \cdot r},
\]

where \( q \) is a given wavevector, by looking for the dispersion relation \( s(q) \). By choosing \( \delta w_0 \) and \( q \) along the same direction as \( w_0 \), one finds for the real part of \( s \)

\[
\Re(s) = \frac{\mu_0^2}{8\xi^3 w_0^3} |q|^2 - \frac{5\mu_0^4}{128\xi^7 w_0^6} |q|^4 + O(|q|^6)
\]

for small \( |q| \), with \( \mu_0 = 4(e^{-\sigma^2/2} - \frac{1}{2})/\pi \) and \( w_0 = |w_0| \), indicating the onset of a long wavelength instability since \( \Re(s) \) becomes positive at small enough \( |q| \). The spatially homogeneous states \( w = 0 \) and \( w = w_0 \) are thus both unstable, so that more complicated structures should eventually appear in the system. The “stripes” of higher density moving over a low density background, reported in [172], may be examples of such patterns.

### 5.2.5 Discussion

The hydrodynamic equations (5.17,5.19) have been derived in the framework of the Boltzmann approach and their validity is in principle restricted to a low density regime obtained if \( \lambda \) is chosen to be small. However, as verified for many systems, the validity of the Boltzmann equation often goes well-beyond the a priori expected limit. One also expects that in this low density regime, the hydrodynamic equations should not depend strongly on the details of the interactions—for instance, the precise shape of the distribution \( p(\eta) \). Another limitation comes from the assumption that \( w \) is small. However, other coarse-grained approaches derived through analogous expansions close to a transition, turn out to be valid quite far from the threshold [181].

Our analytical approach has several advantages when compared with pure numerical simulations of similar microscopic models. First, these equations may be used to get analytical solutions in reference cases with simple geometries, and to analyze their stability against perturbations. Second, in more complicated situations, these equations may be integrated numerically, allowing one to study much larger systems than with direct simulations of the particles. Moreover, the greatest advantage of our approach is to provide an explicit form, in terms of microscopic parameters, of the coefficients entering the hydrodynamic equations. This allows us first to draw the phase diagram in the density-noise variables, and second to perform a stability analysis of the homogeneous state with nonzero velocity, showing that this state is itself unstable against long wavelength perturbations. It is interesting to note that these perturbations that destabilize the long-range order correspond to longitudinal waves, at odds with what happens in the two-dimensional XY-model [182] which might be thought of as an equilibrium counterpart of the present model [176].

\footnote{An analogous instability has been reported in [177].}
5.3 Dynamical decision model

We now turn to a different type of symmetry breaking phase transition involving a large group of agents, in the context of a decision model. Phase transitions and are standard phenomena occurring in physical systems due to the presence of interactions [183], a prominent example being the ferromagnetic Ising model [184]. Outside physics, phase transitions are also often found in complex systems composed of many interacting “agents” (virtual entities representing in a schematic way human beings, animals or bacteria for instance) [161, 6, 185]. In these cases, interaction rules do not derive from an energy function as in physical systems, but still correspond to direct interactions between agents.

There however exist situations in which agents have no direct interactions between them, but rather interact with an external system, having its own dynamics, and producing a feedback on the agents. A simple example of such a situation is the case of an assembly of customers who go for shopping on a regular time basis—say, every week—and need to choose between several equivalent stores. In the absence of bias between shops, that is if customers choose any of the shops with equal probability, all stores should maintain the same activity level. If however, a fluctuation of activity occurs, one shop may become slightly less attractive because, for instance, the sold products get older (which may have significant consequences when selling, e.g., fresh food). One can intuitively expect that this feedback loop may, in some cases, result in an amplification mechanism leading to a symmetry breaking between shops.

Modelling the competition between stores is a difficult issue, which raised interest in the economic literature from different perspectives [186, 187, 188, 189, 190] as well as, marginally, in the physics literature [191]. Such models are often grounded in discrete choice theory [157, 192]. Despite the essential role played by prices in economic modelling, empirical studies show that pricing mechanisms for fresh products like fruits and vegetables are complex, and that other criteria related to the quality of the products also play an important role in customers decisions [193]. The freshness of products thus turns out to be an important ingredient to take into account when modelling shops selling perishable goods [187, 188, 194].

In the present section, we investigate a simple model in which the aging of products, and the corresponding decrease of utility, are the central ingredients. At variance with economic models, we neglect all financial aspects (like the price of products and the fixed costs that the shopkeeper has to pay), in order to single out a unique dynamical feedback mechanism (the freshness of products) between shops and customers, thus leading to a minimal dynamical model of shop competition. Focusing on the symmetry breaking phenomenon, we find both through numerical simulations and analytical mean-field approaches that a phase transition takes place between a symmetric state in which the two stores maintain the same level of activity, and a symmetry broken state where a majority of customers choose a given store, in which they can find fresher products.

5.3.1 Model of competing stores

Definition

The model is defined as follows. A set of $N_a$ agents randomly visit, on a regularly time basis, one of two competing stores selling the same products. Each store has the same number $N_p$ of products, which are all identical except for their age. The age $\tau$ defines the freshness $h(\tau)$ of the corresponding product, where $h(\tau)$ is a decreasing function, taking values between 0 and 1, of the
variable $\tau \geq 0$. A typical functional forms for $h(\tau)$ is

$$h(\tau) = e^{-\tau/\tau_1}$$

(5.30)

where $\tau_1$ is the characteristic aging time scale of products.

At discrete time steps $t_k = k\delta t$, with $\delta t = \tau_0/N$, an agent is chosen at random with uniform probability. This agent $i$ then randomly selects one of the two stores with a probability related to its satisfaction $S_{ij}$ with respect to each store $j = 1, 2$. To be more specific, the probability $p_i$ that agent $i$ chooses the first store is given by

$$p_i = \frac{1}{1 + e^{-\Delta S_i/T}}$$

(5.31)

where $\Delta S_i = S_{i1} - S_{i2}$ is the satisfaction difference of agent $i$ with respect to the two shops, and $T$ is a parameter playing the role of a temperature, taking into account the influence of other factors that are not described explicitly. The second store is chosen with probability $1 - p_i$. It is easy to check that this dynamical rule preserves the symmetry between the two shops, in the sense that $1 - p_i$ takes the same form as $p_i$ up to the replacement of $\Delta S_i$ by $-\Delta S_i$ in Eq. (5.31).

Note that Eq. (5.31) is known as the logit rule in the socio-economic literature [157], and that it is also formally similar to the Glauber transition probability used in physics, provided $-\Delta S_i$ can be interpreted as an energy (which is not necessarily the case in social models, see e.g. [195]).

Once agent $i$ has chosen a store $j = 1, 2$, it visits this store and buys one product chosen at random (we recall that only one type of product is sold, only the age $\tau$ differs from one to the other). The sold product is immediately replaced by a fresh one, with age $\tau' = 0$. The agent a posteriori assesses the freshness $h(\tau)$ of the bought product, and updates its satisfaction with respect to the store $j$ according to

$$S'_{ij} = \alpha S_{ij} + (1 - \alpha)h(\tau),$$

(5.32)

where $0 \leq \alpha < 1$ is a parameter characterizing the agents’ memory (all agents have the same value for $\alpha$). Then the process is iterated and a new agent is chosen randomly.

**Qualitative behavior of the model**

Simulating numerically the above model, we observe for low enough temperature a symmetry breaking between the two stores (see Fig. 5.5): one of the stores reaches a high level of commercial activity, resulting in a high freshness of the sold products, while the second one only maintains a low activity and a low freshness level. Interestingly, symmetry can be restored by varying the parameter $\tau_1$, which controls the aging rate of products, as seen on Fig. 5.5; both shops then keep the same level of freshness. Less surprisingly, symmetry is also restored at high temperature (not shown).

In the following sections, we quantitatively study this symmetry breaking phase transition, through both analytical and numerical methods. Section 5.3.2 is devoted to a mean-field approach that allows us to obtain the phase diagram of the model. We find in particular a transition line in the plane defined by the temperature $T$ and a control parameter $R$ related to the characteristic aging time $\tau_1$. Section 5.3.3 is then devoted to the comparison between mean-field results and numerical simulations.
5.3.2 Mean-field approach

Framework and basic dynamical equations

We now present an analytical approach of the above model, in order to characterize quantitatively the phase transition between symmetric and non-symmetric states of the two stores. Our analytical framework relies on the simplifying assumption that the fluctuations of the agents’ satisfaction can be neglected, so that all agents are considered to have a satisfaction equal to the average satisfaction $\Delta S$. In socio-economic terms, one would say that the set of agents is replaced by a “representative agent” [157]. To lighten the notations, we introduce $\sigma \equiv \Delta S$. From Eq. (5.32), we get

$$\sigma(t + \tau_0) = \alpha \sigma(t) + (1 - \alpha) (\bar{h}_1(t) - \bar{h}_2(t)) ,$$

where $\bar{h}_j(t)$ is the average freshness of products in the store $j$ at time $t$. This equation can be reformulated as

$$\frac{1}{\tau_0} (\sigma(t + \tau_0) - \sigma(t)) = \frac{1 - \alpha}{\tau_0} (-\sigma(t) + \bar{h}_1(t) - \bar{h}_2(t)) .$$

Hence $\sigma(t)$ varies significantly over a time scale of the order of $\tau_0/(1 - \alpha)$. In the limit of strong memory, $0 < 1 - \alpha \ll 1$, $\tau_0/(1 - \alpha) \gg \tau_0$ so that the variations of $\sigma$ are very small over a time $\tau_0$. Hence $\sigma(t)$ can be considered as a continuous function of the variable $t$, and the l.h.s. of Eq. (5.34) can be replaced by a time derivative. We thus end up with

$$\frac{d\sigma}{dt} = \gamma (-\sigma(t) + \bar{h}_1(t) - \bar{h}_2(t)) ,$$

with $\gamma = (1 - \alpha)/\tau_0$. It is convenient to rather express the dynamics in terms of the fraction $p$ of customers choosing the first store, instead of keeping the variable $\sigma$. Using Eq. (5.31) and replacing

Figure 5.5: Illustration of the dynamical behavior of the model, in cases when symmetry breaking occurs (left) or do not occur (right); the mean freshness $\langle h_j \rangle$ of products in each shop $j = 1, 2$ is plotted as a function of time. The inset on the left plot shows a short time-window corresponding to the transient state of the simulation starting from a non equilibrated initial conditions. Left panel: $\tau_1 = 16.7$; right panel: $\tau_1 = 40$. The other parameters are the same on both panels: $N_a = N_p = 500$, $T = 0.1$, $\tau_0 = 1$. 

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\[ \sigma = -T \ln \left( \frac{1-p}{p} \right), \]  
\text{(5.36)}

which can be plugged into Eq. (5.35), leading to
\[ \frac{dp}{dt} = \gamma p(1-p) \left[ T \ln \left( \frac{1-p}{p} \right) + \bar{\eta}_1(t) - \bar{\eta}_2(t) \right]. \]  
\text{(5.37)}

We now need to compute the average freshness \( \bar{\eta}_j \) as a function of \( p \). To this aim, we first determine the age distribution of products.

**Age distribution of products**

Let us denote as \( \lambda_j(t) \) the average fraction of products sold in store \( j \) per unit time, and \( \phi_j(\tau, t) \) the probability distribution of the age \( \tau \) of products in store \( j \) at time \( t \). This distribution evolves in time according to the following relation:
\[ \phi_j(\tau + dt, t + dt) = \phi_j(\tau, t) - \lambda_j(t) dt \phi_j(\tau, t), \]  
\text{(5.38)}

yielding
\[ \frac{\partial \phi_j}{\partial \tau}(\tau, t) + \frac{\partial \phi_j}{\partial t}(\tau, t) = -\lambda_j(t)\phi_j(\tau, t). \]  
\text{(5.39)}

Integrating this equation over \( \tau \) on the positive real axis yields \( \phi_j(0, t) = \lambda_j(t) \), which encodes the fact that sold products are immediately replaced by new ones, with age \( \tau = 0 \). The stationary solution of Eq. (5.39) is exponential, namely
\[ \phi_j^{st}(\tau) = \lambda_j e^{-\lambda_j \tau}. \]  
\text{(5.40)}

Using the exponential aging function given in Eq. (5.30), the corresponding average freshness is thus
\[ \bar{\eta}_j = \int_0^{\infty} d\tau \phi_j^{st}(\tau) e^{-\tau/\tau_1} = \left( 1 + \frac{1}{\lambda_j \tau_1} \right)^{-1}. \]  
\text{(5.41)}

In addition, the parameter \( \lambda_j \) can be identified with the flux per product of customers visiting store \( j \) since every time a customer comes to a shop, he will buy a product no matter his satisfaction for the shop, yielding
\[ \lambda_j = \frac{N_ap_j}{N_p \tau_0} \]  
\text{(5.42)}

with \( p_1 = p \) and \( p_2 = 1 - p \). We thus end up, as far as the average freshness is concerned, with
\[ \bar{\eta}_j = \left( 1 + \frac{R}{2p_j} \right)^{-1} \]  
\text{(5.43)}

where we have defined the control parameter
\[ R = \frac{2N_p \tau_0}{N_a \tau_1}, \]  
\text{(5.44)}

which combines the ratio of the numbers of customers and products, to the ratio of the aging time of products and the characteristic time of the agents’ dynamics. In the following, we use as an approximation the above steady-state distribution of the age of products, assuming that the satisfaction of agents evolves on time scales much longer than the turn-over of products. This assumption has, however, no consequence on the determination of the fixed points of the dynamics.
Figure 5.6: Illustration of the behavior of the free energy $f_{T,R}(m)$, for four different temperatures (from top to bottom: $T = 0.2$, 0.185, 0.16, and 0.12) and the same value $R = 0.2$, showing the onset of the two symmetric secondary minima.

**Determination of the phase transition**

Gathering results, we find for the time evolution of $p$ the following equation

$$\frac{dp}{dt} = \frac{\gamma}{T} p(1-p) \left[ T \ln \left( \frac{1-p}{p} \right) + \left( 1 + \frac{R}{2p} \right)^{-1} - \left( 1 + \frac{R}{2(1-p)} \right)^{-1} \right]. \quad (5.45)$$

Introducing $p = (1 + m)/2$, we can formally rewrite Eq. (5.45) as

$$\frac{dm}{dt} = \frac{\gamma}{T} (1 - m^2) g_{T,R}(m), \quad (5.46)$$

with $g_{T,R}(m)$ given by

$$g_{T,R}(m) = \frac{1}{2} \left[ T \ln \left( \frac{1 - m}{1 + m} \right) + \left( 1 + \frac{R}{1+m} \right)^{-1} - \left( 1 + \frac{R}{1-m} \right)^{-1} \right]. \quad (5.47)$$

The reason for excluding the factor $\gamma(1 - m^2)/T$ from the definition of $g_{T,R}(m)$ will be discussed in Sec. 5.3.4. In order to study possible phase transitions, it is convenient to define an effective free energy (or potential function) $f_{T,R}(m)$ through

$$f_{T,R}(m) = -\int_0^m g_{T,R}(m') \, dm', \quad (5.48)$$

so that

$$\frac{dm}{dt} = -\frac{df_{T,R}}{dm}(m). \quad (5.49)$$

It is easily seen that $m = 0$ is a steady-state solution of Eq. (5.46). To test the local stability of this solution, we expand the free energy $f_{T,R}(m)$ for small $m$, to order $m^2$, leading to

$$f_{T,R}(m) = \frac{1}{2} \left[ T - \frac{R}{(1+R)^2} \right] m^2 + \mathcal{O}(m^4). \quad (5.50)$$
Figure 5.7: Mean-field phase diagram, with four different regions. A: \( m = 0 \) is the only minimum of \( f_{T,R}(m) \). B: \( m = 0 \) is the global minimum, but secondary minima have appeared. C: \( m = 0 \) is only a local minimum, the two symmetric minima are the most stable. D: \( m = 0 \) is a local maximum, the two symmetric minima are the only stable states. The transition lines between those regions are respectively defined by \( T(R) = T_s \) between A and B, \( T_d \) between B and C, and \( T_c \) between C and D. \( T_c \) also separates A and D for \( R > R^* \approx 0.732 \), when the transition is continuous. The lower panels show the typical shape of \( f_{T,R}(m) \) for \( m > 0 \) (\( f_{T,R}(m) \) is a symmetric function) in each region.

The solution \( m = 0 \) is linearly stable if the bracket on the r.h.s. is positive. The critical temperature \( T_c \) is reached when the bracket vanishes, yielding

\[
T_c = \frac{R}{1 + R^2}.
\]

When this transition coincides with the onset of two symmetric minima for \( T < T_c \), the transition is continuous. For low values of \( R \), however, two symmetric secondary minima appear already for a value \( T_s > T_c \), when \( m = 0 \) is still the global minimum as illustrated on Fig. 5.6. This case corresponds to a discontinuous transition, which should be reached (in analogy to the equilibrium theory of phase transitions) at a temperature \( T_d \) such that all three minima have equal values \( f_{T,R}(m) = 0 \).

The resulting mean-field phase diagram is presented on Fig. 5.7. In region A, a single solution \( (m = 0) \) exists, while in region D, only the two symmetric solutions remain. In region B, between the lines \( T_s \) and \( T_d \), the symmetric solution \( m = 0 \) is the most stable, while in region C, between \( T_d \) and \( T_c \), the most stable solutions are the non-zero ones. The lines \( T_s, T_d \) and \( T_c \) meet at a value \( R^* = \sqrt{3} - 1 \).

The nature of the discontinuous transition however calls for a short comment. First of all, we note that the evolution equation (5.46) is deterministic, so that the system should remain trapped forever once it has reached a locally stable stationary solution. However, in a more realistic description, the finite size of the system should result in a small effective noise, making the system
Figure 5.8: Order parameter $m$, plotted either as a function of $R$ or as a function of temperature $T$. Lines correspond to the mean-field predictions, while dots with error bars are the results from numerical simulations. On all four figures, a phase transition, either continuous or discontinuous, is observed between a symmetric phase (both stores have the same activity) and a phase with broken symmetry (one of the stores has a higher activity level).

explore the vicinity of the stationary state. In this case, the most stable stationary states correspond to the absolute minima of $g_{T,R}(m)$ (either $m = 0$, or two symmetric values $m_0$ and $-m_0$).

5.3.3 Comparison between mean-field and numerical results

Measure of the order parameter

We now turn to the results of numerical simulations of the agent-based model, and compare them with the mean-field results. The numerical value for $m$ is obtained as a time average (over 10000 $\tau_0$) for a simulation usually involving $N_a = 500$ agents and as many products as agents ($N_p = N_a$). The memory parameter was set to $\alpha = 0.8$, a value sufficiently large for the continuous description to be approximately valid. We have however checked that setting this parameter in the range $0.5 \leq \alpha \leq 0.95$ only changes the numerical value of $m$ by less than a few percent for most values of $R$ and $T$.

We first plot on Fig. 5.8 the steady-state value of the order parameter $m$ as a function of temperature $T$ and parameter $R$. An overall good agreement is observed with the mean-field predictions, that are obtained as follows. The fixed points of Eq. (5.46) are solutions of $g_{T,R}(m) = 0$. Besides the trivial solution $m = 0$, a solution $m^* > 0$ exists below the transition line. An analytical expression for $m^*(T, R)$ is hard to obtain, but one can instead easily express $T$ as a function of $m$ and $R$:

$$T(m, R) = \frac{\left(1 + \frac{R}{1+m}\right)^{-1} - \left(1 + \frac{R}{1-m}\right)^{-1}}{\ln(1+m) - \ln(1-m)}$$ (5.52)
Figure 5.9: Left: behavior of the Binder cumulant $B$ as a function of temperature $T$ for different sizes $N_a = 16, 32, 64, 128, 256, 512$ ($R = 2$, simulation time size: $5 \times 10^5 \tau_0$). The critical point is obtained as the large $N$ limit of the intersections of successive curves. Right: crossing point of two successive curves $N_a = N/2$ and $N_a = N$, as a function of $N$.

Fixing $R$, it is then straightforward to plot $T$ as a function of $m$. One can also invert $T(R, m)$ to get $R(T, m)$, as shown on Fig. 5.8.

Determination of the transition line

We also compare on Fig. 5.10 numerical results for the phase diagram with the mean-field predictions. To determine the transition line, we have distinguished two methods for the cases of continuous and discontinuous phase transitions. For the discontinuous phase transition, the transition can be determined from the jump of the order parameter $m$ (shown as '+' on Fig. 5.10). In the continuous case, the transition is more difficult to determine from the average value of the order parameter, due to finite size effects close to the transition. We thus have used the standard technique of the Binder cumulant, which characterizes the deviation from Gaussianity of the probability distribution of the order parameter [196]. For a centered variable $m$, the Binder cumulant is defined as

$$B = 1 - \frac{\langle m^4 \rangle}{3 \langle m^2 \rangle^2}. \quad (5.53)$$

The main interest of the Binder cumulant is that when plotted as a function of the control parameter, curves corresponding to different system sizes intersect at the critical point, with only small finite size effects. This method allows for a rather precise estimate of the transition point. An illustration of the behavior of the Binder cumulant is given on Fig. 5.9.

Altogether, a rather good agreement is obtained between mean-field and numerical results, though some systematic deviations appear, as seen on Fig. 5.10. These deviations might be due to underevaluated finite size effects (the number of agents used in the simulation is $N_a \sim 500$), but it is more likely to result from the simplifying assumptions made in the derivation the mean-field equations. Note however that the ranges in which continuous and discontinuous transitions are observed numerically are well reproduced by the mean-field argument.
5.3.4 Discussion

In this section, we briefly discuss the relation between the present model and one of the most standard models exhibiting a symmetry breaking phase transition, namely the Ising model, before drawing some conclusions and perspectives.

Relation to the Ising model

In the present model, each agent has to choose between two options, namely going to the first or the second store. Such a binary choice can be encoded into a 'spin' variable \( s_i \), equal to 1 if agent \( i \) chooses the first shop, and to \(-1\) in the opposite case. Though somehow artificial, this definition has the advantage that the order parameter \( m \) introduced in Sec. 5.3.2 can be reexpressed as \( m = N_a^{-1} \sum_i s_i \). This naturally suggests that the present model may exhibit, to some extend, an analogy to the Ising model. This analogy can be made more precise, at the mean-field level, in the following way. Let us modify the model in such a way that the freshness of products (which drives the evolutions of the satisfaction of agents) is replaced by the opposite of the energy of the mean-field Ising model, \( E_{\text{Ising}} = -\frac{1}{2} N_a J m^2 \). Then the mean satisfaction \( \sigma \) introduced in Sec. 5.3.2 evolves according to

\[
\sigma(t + \tau_0) = \alpha \sigma(t) - (1 - \alpha) \Delta E,
\]

(5.54)

\( ^2 \)Strictly speaking, the magnetization \( m \) should be computed from the last choice of the \( N_a - 1 \) other agents.
with
\[ \Delta E = -\frac{1}{2}N_aJ \left[ (m + \frac{1}{N_a})^2 - (m - \frac{1}{N_a})^2 \right] = -2Jm. \] (5.55)

Note that the last equality has been obtained in the large \( N_a \) limit. We then get the evolution equation, in the large memory limit \( 1 - \alpha \ll 1 \),
\[ \frac{d\sigma}{dt} = \gamma[\sigma - 2Jm], \] (5.56)
which is the analog of Eq. (5.35). It is easy to check, using relation (5.36) to eliminate the variable \( \sigma \), that the time evolution equation for \( m \) is given by
\[ \frac{dm}{dt} = \frac{\gamma}{T}(1 - m^2) \left[ \frac{T}{2} \ln \left( \frac{1 - m}{1 + m} \right) + Jm \right]. \] (5.57)

Similarly to Eq. (5.46), the term between brackets can be written as the opposite of the derivative of a free energy \( f(m) \),
\[ f(m) = \frac{T}{2} (1 + m) \ln(1 + m) + \frac{T}{2} (1 - m) \ln(1 - m) - \frac{1}{2} Jm^2 \] (5.58)
which is, up to an additive constant \( T \ln 2 \), nothing but the standard mean-field free energy of the Ising model.

However, beyond mean-field, it is clear that the relation to the Ising model is at most an analogy. Indeed, the present model differs from standard equilibrium models in several respects: on the one hand, the interaction between agents is here mediated by the aging of products in each store rather than by an internal energy function, and on the other hand the dynamics is not Markovian since agents have a memory of their past visits to the shops.

**Conclusion and perspectives**

We have studied a simple model of competing shops selling fresh products, retaining as main ingredients the aging of products and the satisfaction of customers with respect to the freshness of products –considered to be the main factor influencing choices made by customers. Under these very simplifying assumptions, we found a surprisingly rich dynamics, with both continuous and discontinuous transitions between symmetric and symmetry-broken states. The overall agreement between numerical simulations and mean-field predictions was found to be satisfactory.

Several extensions could be interesting to study. For instance, other functional forms could be considered for the aging function \( h(t) \) introduced in Eq. (5.30), like
\[ h(\tau) = \left( 1 - \frac{\tau}{\tau_1} \right) \theta \left( 1 - \frac{\tau}{\tau_1} \right) \] (5.59)
where \( \theta(x) \) is the Heaviside function. Such a form would be rather natural for products that can be sold only up to expiration date. We have checked that the form (5.59) preserves the qualitative behavior of the model. Another natural extension of this work would be to include more than two shops. Although we did not study this case in detail, a simple argument can already be given here. With a fixed overall number of agents \( N_a \), adding shops reduces the nominal number of customers
for a given shop. As a first approximation, a model with more than two shops can be described by an effective number of agents \(N^* \approx N_a\), resulting in an effective parameter \(R^* > R\). Starting from a low value of \(R\) corresponding to the symmetric region, increasing the number of shops would then eventually lead to a value \(R^*\) in the symmetry broken phase. It is thus likely that, for a given total number of agents, there is a maximal number of shops that can maintain a good level of activity, which seems to be consistent with conventional wisdom.

Further possible extensions may include taking into account explicitly the prices of products, as well as the costs associated to the shops (e.g., rent or salaries). In this context, one can imagine to include, in a simplified way, a dynamics of the shopkeeper who could modify the prices, or diversify the products, as a function of the dynamical state of the store. One might guess that such a dynamics could contribute to stabilize the symmetric states.
Chapter 6

General conclusion

All along this manuscript, we have tried to answer, or at least illustrate on simple models, different questions related to the statistical description of non-equilibrium systems, mostly focusing on steady-state situations. These questions were related to:

- the possibility to define generalized notions of intensive thermodynamic parameters (temperature, chemical potential, etc.),
- the shape of the distribution of global observables in correlated physical systems, with a specific interest in driven dissipative systems,
- the statistical description of assemblies of interacting agents, focusing on similarities and differences with equilibrium systems, and with emphasis on possible phase transitions related to the non-equilibrium character of the model.

Let us now briefly summarize the results obtained. As for the first point, we have seen that the dependence of the fluctuation-dissipation temperature upon the observable considered seems to be generic for non-equilibrium steady-state systems, and that this dependence is related to the (Shannon) entropy difference between the considered non-equilibrium state and the equilibrium state having the same average energy. A consistent, observable-independent, definition of temperature thus does not seem possible along this way. Another track was the definition of thermodynamic parameters conjugated to conserved quantities, generalizing standard equilibrium approaches. We have basically seen that such a definition is possible as long as long-range correlations are absent. However, some difficulties appear here also when two systems are put into contact, and when the flux balance imposes some non-trivial additional constraints. Hence, the question to know whether these definitions of intensive parameters are the relevant ones to describe non-equilibrium systems remains open to some extent.

Turning to the second point, we have illustrated on simple models how generalized extreme distributions can appear in correlated systems, and we provided a rather straightforward link between the statistics of extreme values and that of specific types of random sums that are relevant in the context of correlated systems. In order to gain generality, renormalization group approaches would certainly be useful in order to understand the behavior of driven dissipative systems, and more general types of correlated systems. The reformulation of extreme value statistics in a renormalization language we have presented could be of interest in this respect.
Finally, we have tentatively addressed the third point by providing a few simple examples of applications of statistical physics methods and concepts to the description of assemblies of interacting agents. Let us emphasize that the three examples presented were dealt with using different methods. For the first model (a variant of Schelling’s model), we obtained a mapping onto an effective equilibrium model allowing us to predict a phase transition through standard methods, namely the non-convexity of an effective free-energy function. In the second model (collective motion), we used the generic approach of the Boltzmann equation, which is valid for many different types of systems, provided that interactions between particles (or agents) are binary, and essentially instantaneous. One of the advantages of the Boltzmann approach is to provide a coarse-grained, time- and space-dependent hydrodynamic description of the system. When such methods are not available (in particular if the conditions required are not fulfilled), it is still often possible to use an uncontrolled mean-field approximation, which yields in many cases a reasonable description, as illustrated on the decision model.

Note that all my research work published in the period 2004-2011 (that is, after obtaining my Ph.D) has not been presented in this manuscript. The interested reader is referred to the full publication list presented in Chapter 7 below.

In the near future, I would in particular like to go on working on the statistical physics modeling of systems composed of macroscopic “entities” (ranging from granular material to systems of self-propelled particles and to social systems), in the spirit of the work presented in Chapter 5. I would specifically like to investigate whether there exist generic concepts in this class of systems, or if each problem needs to be dealt with using a specific method.

Future perspectives also include several collaborations that already started over the last years. Some relationships between methods and concepts used in statistical physics and signal processing are currently investigated by F. Angeletti, in the framework of his Ph.D thesis I am supervising in collaboration with P. Abry at the ENS Lyon. Other more experimentally oriented collaborations will be carried on in the next years, like the one with J.-C. Géminard about problems related to soft matter and granular materials. In the same spirit, the collaboration with S. Ciliberto is presently becoming more active, with the Ph.D thesis of M. Mathieu (starting in October 2011), which we are supervising together. The topic of this thesis is the experimental and theoretical study of assemblies of interacting self-propelled particles. On this topic, interactions with several colleagues in Paris (O. Dauchot, G. Grégoire, H. Chaté), with whom I participated in an ANR project, will also be continued. Finally, and although this list is obviously not exhaustive, I would also like to mention the collaboration with P. Jensen from the Complex System Institute in Lyon (IXXI), with whom I had interesting interactions over the last few years in relation with the modeling of social systems.
Chapter 7

Publication list

Research articles

- *Influence of flux balance on the generalized chemical potential in mass transport models*

- *Symmetry-breaking phase transition in a dynamical decision model*

- *Linearization effect in multifractal analysis: Insights from the Random Energy Model*

- *Socio-economic utility and chemical potential*

- *Random barrier double-well model for resistive switching in tunnel barriers*

- *Aging of the frictional properties induced by temperature variations*

- *Renormalization flow in extreme value statistics*

- *Entropic aging and extreme value statistics*

- *Entropy-based characterization of the observable-dependence of the fluctuation-dissipation temperature*

- *Hydrodynamic equations for self-propelled particles: microscopic derivation and stability analysis*
• Competition between collective and individual dynamics

• Dependence of the fluctuation-dissipation temperature on the choice of observable

• Far-from-equilibrium state in a weakly dissipative model

• Intermittent outgassing through a non-newtonian fluid

• Extreme statistics and volume fluctuations in a confined one-dimensional gas

• Intensive thermodynamic parameters in nonequilibrium systems

• Generalised extreme value statistics and sum of correlated variables

• Boltzmann and hydrodynamic description for self-propelled particles

• Free volume distributions and compactivity measurement in a bidimensional granular packing

• Definition and relevance of nonequilibrium intensive thermodynamic parameters

• An exactly solvable dissipative transport model

• Global fluctuations and Gumbel statistics
  E. Bertin, Phys. Rev. Lett. 95, 170601 (2005) [cond-mat/0506166].

• Subdiffusion and dynamical heterogeneities in a lattice glass model

• Nonequilibrium temperatures in steady-state systems with conserved energy

• Reply to Comment on “Temperature in nonequilibrium systems with conserved energy”

• Real space analysis of inherent structures
• Dynamic phase diagram of the Number Partitioning Problem

• Temperature in nonequilibrium systems with conserved energy

• The Kovacs effect in model glasses

• Jamming transition of a granular pile below the angle of repose

• Cross-over from entropic to thermal dynamics in glassy models

• Linear and nonlinear response in the aging regime of the one dimensional trap model

• Subdiffusion and localization in the one dimensional trap model

• Dynamical ultrametricity in the critical trap model

• Effective nuclear temperature in a fluctuating spin system

Review article

• Global fluctuations in physical systems: a subtle interplay between sum and extreme value statistics

Pedagogical paper

• From laser cooling to aging: a unified Lvy flight description

Book

• A concise introduction to the statistical physics of complex systems
**Proceedings**

- *Effective free energy for individual dynamics*

- *Free volume distributions inside a bidimensional granular medium*

- *Transition and spin dynamics at very low temperature in the pyrochlores Yb2Ti2O7 and Gd2Sn2O7*

**Publications in national journals**

- *Une pragmatique des complexités*

- *Science et Danse, les mouvements collectifs*
Bibliography


