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Stochastic interacting particle systems out of equilibrium

L Bertini[1], A De Sole[1,2], D Gabrielli[3], G Jona-Lasinio[4] and C Landim[5,6]

[1] Dipartimento di Matematica, Università di Roma La Sapienza, Piazzale Aldo Moro 2, I-00185 Roma, Italy
[2] Mathematics Department, Harvard University, Cambridge, MA, USA
[3] Dipartimento di Matematica, Università dell'Aquila, I-67100 Coppito, L'Aquila, Italy
[4] Dipartimento di Fisica and INFN, Università di Roma La Sapienza, Piazzale Aldo Moro 2, I-00185 Roma, Italy
[5] IMPA, Estrada Dona Castorina 110, J. Botanico, 22460 Rio de Janeiro, Brazil
[6] CNRS UPRES-A 6085, Université de Rouen, F-76128 Mont-Saint-Aignan Cedex, France
E-mail: lorenzo@carpenter.mat.uniroma1.it, desole@math.harvard.edu, gabriell@univaq.it, gianni.jona@roma1.infn.it and landim@impa.br

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Abstract. This paper provides an introduction to some stochastic models of lattice gases out of equilibrium and a discussion of results of various kinds obtained in recent years. Although these models are different in their microscopic features, a unified picture is emerging at the macroscopic level, applicable, in our view, to real phenomena where diffusion is the dominating physical mechanism. We rely mainly on an approach developed by the authors based on the study of dynamical large fluctuations in stationary states of open systems. The outcome of this approach is a theory connecting the non-equilibrium thermodynamics to the transport coefficients via a variational principle. This leads ultimately to a functional derivative equation of Hamilton–Jacobi type for the non-equilibrium free energy in which local thermodynamic variables are the independent arguments. In the first part of the paper we give a detailed introduction to the microscopic dynamics considered, while the second part, devoted to the macroscopic properties, illustrates many consequences of the Hamilton–Jacobi equation. In both parts several novelties are included.

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Contents

1. Introduction

Models have played a fundamental role in equilibrium statistical mechanics. The Ising model provided the first proof that statistical mechanics can explain the existence of phase transitions and was a main guide in the study of critical behaviour. A reason for this effectiveness is the circumstance that the macroscopic behaviour is, to a considerable extent, independent of the microscopic details. Hence different systems exhibit qualitatively the same phenomenology at large scales.

Out of equilibrium the situation is more complex. First the variety of non-equilibrium phenomena one can conceive makes it more difficult to define general classes of phenomena for which a unified study is possible. Furthermore the details of the microscopic dynamics play a far greater role than in equilibrium. Since the first attempts to construct a non-equilibrium thermodynamics, a guiding idea has been that of local equilibrium. This means the following. Locally on the macroscopic scale it is possible to define thermodynamic variables like density, temperature, chemical potentials, etc, which vary smoothly on the same scale. Microscopically this implies that the system reaches local equilibrium in a time which is short compared to the times typical of macroscopic

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evolutions, as described, for example, by hydrodynamic equations. So what characterizes situations in which this description applies is a separation of scales both in space and time. There are important cases, however, where local equilibrium apparently fails like ageing phenomena in disordered systems due to insufficient ergodicity.

The simplest non-equilibrium states one can imagine are stationary states of systems in contact with different reservoirs and/or under the action of external fields. In such cases, to the contrary of equilibrium, there are currents (electrical, heat, matter of various chemical constitutions, etc) through the system whose macroscopic behaviour is encoded in transport coefficients like the diffusion coefficient, the conductivity or the mobility. The ideal would be to approach the study of these states starting from a microscopic model of atoms interacting with realistic forces and evolving with Newtonian dynamics. This is beyond the reach of present-day mathematical tools and much simpler models have to be adopted in the reasonable hope that some essential features are adequately captured.

In the last decades stochastic lattice gases have provided a very useful laboratory for studying properties of stationary non-equilibrium states (SNS). Besides many interesting results specific to the different models considered, the following features of general significance have emerged.

(1) Local equilibrium and hydrodynamic equations have been derived rigorously from the microscopic dynamics for a wide class of stochastic models.

(2) A definition of non-equilibrium thermodynamic functionals has emerged via a theory of dynamic large fluctuations; moreover, a general equation which they have to satisfy has been established. This is a time-independent Hamilton–Jacobi (H–J) equation whose independent arguments are the local thermodynamic variables and requires as input the transport coefficients. These coefficients can be either calculated explicitly for given models or obtained from measurements so that H–J can be used also as a phenomenological equation.

(3) Non-equilibrium long range correlations, which have been observed experimentally in various types of fluids [22], appear to be generic consequences of H–J. An important connection between the behaviour of the mobility and the sign of these correlations can be derived from the H–J equation.

(4) An analysis of the fluctuations of the currents averaged over long times has revealed the possibility of different dynamical regimes, which are interpreted as dynamical phase transitions. Such phase transitions have actually been proved to exist in some models. This theoretical prediction should be investigated experimentally.

As an overall comment we may say that the macroscopic theory obtained so far encompasses the theory developed long ago by Onsager [45] and then by Onsager–Machlup [46] for states close to equilibrium and we believe to be applicable in general to states where diffusion is the dominant dynamical mechanism.

The present paper intends to provide a unified introduction to models studied intensively in the last decade for which several results have been obtained. We shall concentrate on time-independent properties that are mainly on the topics (2) and (3) mentioned above. Our treatment is based on an approach developed by the authors in [2]–[5]. For item (1) we refer to [39, 49, 50] for the case of periodic boundary conditions

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and to [26, 27] for open systems. For item (4), which we do not discuss here, see [6]–[9], [13]–[15]. For recent overviews on non-equilibrium phenomena see also [34, 44].

There are two parts in this paper, due to the natural separation into microscopic and macroscopic properties. As a rule we do not include proofs except for statements which require a short argument. Most of the results discussed here are in published articles to which we shall refer for the details. We do outline, however, the following new results which will be the subject of forthcoming papers. In section 2.4 we consider the KMP process [38]. We give an explicit representation of the invariant measure of this process in the case of a single oscillator and we compute exactly the two-point correlations for the general case. In section 3.3 we show, for a particular class of one-dimensional models, that non-equilibrium long range correlations are positive if the mobility is convex and negative if it is concave. The general case is discussed in [10]. In section 3.4 we show that for *any* weakly asymmetric model with periodic boundary conditions the non-equilibrium free energy does not depend on the external field, so that it coincides with the equilibrium one and there are no long range correlations. In section 3.6 we consider the one-dimensional boundary-driven totally asymmetric exclusion process. For a particular choice of the parameters, starting from the results in [23] we obtained a new variational representation of the non-equilibrium free energy. In particular, while the representation in [21] requires the maximization of a trial functional, we show how it can be formulated as a minimization problem.

2. Nonreversible microscopic models

Stochastic lattice gases are—loosely speaking—a collection of random walks moving in the lattice and interacting with each other. These 'particles' are to be considered indistinguishable. Accordingly, the microscopic state is specified by giving the occupation number in each site of the lattice. The effect of the interaction is that the *jump rates* depend on the local configuration of the particles. For non-isolated systems we model the effect of the reservoirs by adding creation/annihilation of particles at the boundary. The effect of an external field is modelled by perturbing the rates and giving a net drift toward a specified direction.

In section 2.1 we give the precise definition of non-equilibrium stochastic lattice gases. Some special models, the *zero-range process* and the *exclusion process*, are discussed in sections 2.2 and 2.3. For the zero-range process the invariant measure is always product and can be computed explicitly. On the other hand, the boundary-driven exclusion process carries long range correlations, which can be computed explicitly in the one-dimensional case. In section 2.4 we recall the definition of the KMP process [38] and we compare it with the exclusion process. In section 2.5 we consider *gradient* lattice gases with periodic boundary conditions; the peculiarity of such models is that the invariant measure does not depend on the applied external field. In section 2.6 we consider the *Glauber + Kawasaki* model, in which a reaction term allowing creation/annihilation of particles in the bulk is added. We discuss under which conditions on the reaction rates it is reversible. Finally, in section 2.7 we consider the boundary-driven totally asymmetric exclusion process and we recall the representation of the invariant measure obtained in [23]. This representation suggests a new variational expression for the non-equilibrium free energy that will be discussed in section 3.6.

2.1. Stochastic lattice gases

As basic microscopic model we consider a stochastic lattice gas in a finite domain, with an external field, and either with periodic boundary conditions or with particle reservoirs at the boundary. The process can be informally described as follows. At each site, independently from the others, particles wait exponential times, at the end of which one of them jumps to a neighbouring site. In the case of particle reservoirs, in addition to this dynamics, we have creation and annihilation of particles, at exponential times, at the boundary. To define formally the microscopic dynamics, recall that a continuous time Markov chain ω_t on some state space Ω can be described in terms of its infinitesimal *generator* L defined as follows. Let $f : \Omega \to \mathbb{R}$ be an observable, then

$$\mathbb{E}(f(\omega_{t+h})|\omega_t) = (Lf)(\omega_t)h + \mathrm{o}(h) \tag{2.1}$$

where $\mathbb{E}(|)$ is the conditional expectation, so that the *expected* infinitesimal increment of $f(\omega_t)$ is $(Lf)(\omega_t)\,\mathrm{d}t$. The transition probability of the Markov process ω_t is then given by the kernel of the semigroup generated by L, i.e.

$$p_t(\omega, \omega') = \mathrm{e}^{tL}(\omega, \omega'). \tag{2.2}$$

Let Λ be the d-dimensional torus of side length one, i.e. $(\mathbb{R}/\mathbb{Z})^d$, respectively a smooth domain in $\mathbb{R}^d$, and, given an integer $N > 1$, set $\Lambda_N := (\mathbb{Z}/N\mathbb{Z})^d$, respectively $\Lambda_N := (N\Lambda) \cap \mathbb{Z}^d$. The configuration space is X^{Λ_N}, where X is a subset of $\mathbb{N}$, e.g. $X = \{0, 1\}$ when an exclusion principle is imposed and $X = \mathbb{N}$ when there is no limitation on the number of particles. The number of particles at the site $x \in \Lambda_N$ is denoted by $\eta_x \in X$ and the whole configuration by $\eta \in X^{\Lambda_N}$. The microscopic dynamics is then specified by a continuous time Markov chain on the state space X^{Λ_N} with infinitesimal generator given by $L_N = L_{0,N}$, resp. $L_N = [L_{0,N} + L_{b,N}]$, if Λ is the torus, resp. a smooth domain in $\mathbb{R}^d$, where, for functions $f : X^{\Lambda_N} \to \mathbb{R}$,

$$L_{0,N} f(\eta) = \tfrac{1}{2} \sum_{\substack{x,y\in\Lambda_N \\ |x-y|=1}} c_{x,y}(\eta)[f(\sigma^{x,y}\eta) - f(\eta)] \tag{2.3}$$

$$L_{b,N} f(\eta) = \tfrac{1}{2} \sum_{\substack{x\in\Lambda_N, y\notin\Lambda_N \\ |x-y|=1}} \{c_{x,y}(\eta)[f(\sigma^{x,y}\eta) - f(\eta)] + c_{y,x}(\eta)[f(\sigma^{y,x}\eta) - f(\eta)]\}. \tag{2.4}$$

Here $|x|$ stands for the usual Euclidean norm. For $x, y \in \Lambda_N$, $\sigma^{x,y}\eta$ is the configuration obtained from η by moving a particle from x to y, i.e.

$$(\sigma^{x,y}\eta)_z = \begin{cases} \eta_z & \text{if } z \neq x, y \\ \eta_y + 1 & \text{if } z = y \\ \eta_x - 1 & \text{if } z = x \end{cases}$$

and similarly, if $x \in \Lambda_N$, $y \notin \Lambda_N$, then $\sigma^{y,x}\eta$ is obtained from η by creating a particle at x, while $\sigma^{x,y}\eta$ is obtained by annihilating a particle at x. Therefore, for $x, y \in \Lambda_N$, $c_{x,y}$ is the rate at which a particle at x jumps to y. We assume that $c_{x,y}(\eta) = 0$ if $\sigma^{x,y}\eta \notin X^{\Lambda_N}$ so that $L_{0,N}$ and $L_{b,N}$ are well defined linear operators on the set of functions $f : X^{\Lambda_N} \to \mathbb{R}$. The generator $L_{0,N}$ describes the bulk dynamics which preserves the total number of particles whereas $L_{b,N}$ models the particle reservoirs at the boundary of Λ_N.

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We assume that the bulk rates $c_{x,y}$, $x,y \in \Lambda_N$, are obtained starting from reversible rates $c^0_{x,y}$ satisfying the *detailed balance* with respect to a Gibbs measure defined by a Hamiltonian $\mathcal{H}$, and perturbing them with an external field F. Likewise, in the case of particle reservoirs, we assume that the boundary rates $c_{x,y}$, $c_{y,x}$, $x \in \Lambda_N$, $y \notin \Lambda_N$, are obtained from rates $c^0_{x,y}$, $c^0_{y,x}$ satisfying the local detailed balance with respect to $\mathcal{H}$ and in presence of a chemical potential λ_0, and again perturbed by the external field F. Our analysis is restricted to the high temperature phase: in particular, we shall assume that the correlations in the Gibbs measure decay exponentially.

The above conditions are met by the following formal definitions. Consider jump rates $c^0_{x,y}$ satisfying the detailed balance with respect to the Gibbs measure associated to the Hamiltonian $\mathcal{H} : X^{\Lambda_N} \to \mathbb{R}$ with free boundary conditions. For the bulk rates this means

$$c^0_{x,y}(\eta) = \exp\{-[\mathcal{H}(\sigma^{x,y}\eta) - \mathcal{H}(\eta)]\} c^0_{y,x}(\sigma^{x,y}\eta), \qquad x, y \in \Lambda_N. \tag{2.5}$$

Note that we included the inverse temperature in $\mathcal{H}$. As before if $\sigma^{x,y}\eta \notin X^{\Lambda_N}$ we assume $c^0_{x,y}(\eta) = 0$. From a mathematical point of view, the detailed balance condition means that the generator is self-adjoint w.r.t. the Gibbs measure $\mu(\eta) \propto \mathrm{e}^{-\mathcal{H}(\eta)}$; namely if we let $L^0_{0,N}$ be the generator in (2.3) with c replaced by c^0, for each $f, g : X^{\Lambda_N} \to \mathbb{R}$ we have

$$\langle f, L^0_{0,N} g\rangle_\mu := \sum_\eta \mu(\eta) f(\eta) L^0_{0,N} g(\eta) = \langle L^0_{0,N} f, g\rangle_\mu. \tag{2.6}$$

Let $\overline{\Lambda}_N := \{x \in \mathbb{Z}^d \,|\, \exists\, y \in \Lambda_N \text{ with } |x-y| \le 1\}$ be the 1-neighbourhood of Λ_N. When Λ_N is the discrete torus we agree that $\overline{\Lambda}_N = \Lambda_N$. We also let $\partial\Lambda_N := \overline{\Lambda}_N \setminus \Lambda_N$. In the case when Λ is not the torus, the boundary dynamics with no external field is specified as follows. Denote by $\lambda_0 : \partial\Lambda_N \to \mathbb{R}$ the chemical potential of the reservoirs. If $x \in \Lambda_N$, $y \notin \Lambda_N$ the detailed balance condition (2.5) is modified by adding the chemical potential λ_0:

$$c^0_{x,y}(\eta) = \exp\{-[\mathcal{H}(\sigma^{x,y}\eta) - \mathcal{H}(\eta)] - \lambda_0(y)\} c^0_{y,x}(\sigma^{x,y}\eta), \qquad x \in \Lambda_N, y \notin \Lambda_N. \tag{2.7}$$

We denote by $\mathcal{B}(\Lambda_N) := \{(x,y) | x, y \in \overline{\Lambda}_N, \{x,y\} \cap \Lambda_N \ne \emptyset, |x-y| = 1\}$ the collections of ordered bonds intersecting Λ_N. A *discrete vector field* is then defined as a real function $F : \mathcal{B}(\Lambda_N) \to \mathbb{R}$ satisfying $F(x,y) = -F(y,x)$ for any $(x,y) \in \mathcal{B}(\Lambda_N)$. An *asymmetric lattice gas* is defined by the jump rates

$$c_{x,y}(\eta) := \mathrm{e}^{F(x,y)} c^0_{x,y}(\eta), \tag{2.8}$$

where c^0 are the unperturbed rates and F is a discrete vector field.

The case of *weakly asymmetric models* is obtained by choosing

$$F(x,y) \equiv F_N(x,y) = E\left(\frac{x+y}{2N}\right) \cdot \frac{y-x}{N}, \tag{2.9}$$

where $E : \Lambda \to \mathbb{R}^d$ is a smooth vector field and $\cdot$ denotes the inner product in $\mathbb{R}^d$. Namely, for N large, by expanding the exponential, particles at site x feel a drift $N^{-1}E(x/N)$.

We can rewrite the full generator L_N, using the notation introduced above, as follows:

$$L_N f(\eta) = \tfrac{1}{2} \sum_{(x,y)\in\mathcal{B}(\Lambda_N)} c_{x,y}(\eta)[f(\sigma^{x,y}\eta) - f(\eta)]. \tag{2.10}$$

Fix an initial condition $\eta \in X^{\Lambda_N}$. The trajectory of the Markov process $\eta(t)$, $t \geq 0$, is then an element on the path space $D(\mathbb{R}_+; X^{\Lambda_N})$, which consists of piecewise constant paths with values in X^{Λ_N}. We shall denote by $\mathbb{P}_\eta^N$ the probability measure on $D(\mathbb{R}_+; X^{\Lambda_N})$ corresponding to the distribution of the process $\eta(t)$, $t \geq 0$, with initial condition η. It is related to the generator L_N by $\mathbb{P}_\eta^N(\eta(t) = \eta') = \mathrm{e}^{tL_N}(\eta, \eta')$.

A probability measure μ_N on X^{Λ_N} is an *invariant* measure for the process $\eta(t)$ if

$$\sum_{\eta\in X^{\Lambda_N}} \mu_N(\eta)\mathrm{e}^{tL_N}(\eta, \eta') = \mu_N(\eta') \tag{2.11}$$

namely, if we distribute the initial condition η according to μ_N, then the distribution of $\eta(t)$ is μ_N for any $t \geq 0$. According to general results on Markov processes, if the process is *irreducible*, i.e. there is a strictly positive probability to go from any state to any other, then the invariant measure is unique and it encodes the long time behaviour of the system. More precisely, starting from any configuration η the distribution of $\eta(t)$ converges to μ_N as $t \to \infty$. In the case of a stochastic lattice gas with particle reservoirs, if $c_{x,y}(\eta) > 0$ for any $\eta \in X^{\Lambda_N}$ and any $(x, y) \in \mathcal{B}(\Lambda_N)$ such that $\sigma^{x,y}\eta \in X^{\Lambda_N}$, then the process is irreducible and there exists a unique invariant measure. On the other hand, if Λ_N is the discrete torus, the total number of particles $\sum_{x\in\Lambda_N} \eta_x$ is conserved and there exists a one-parameter family of invariant measures. Since in general the transition probability cannot be expressed in a closed form, condition (2.11) is not convenient. However, it is easy to obtain a necessary and sufficient infinitesimal condition for a measure to be invariant. The measure μ_N is invariant for the process generated by L_N if and only if, for any $f : X^{\Lambda_N} \to \mathbb{R}$, we have

$$\mu_N(L_N f) = 0, \tag{2.12}$$

where hereafter for a measure μ and an observable f we denote by $\mu(f)$ the expectation of f with respect to μ.

If the generator L_N satisfies the detailed balance condition with respect to some measure μ_N, namely

$$\mu_N(gL_N f) = \mu_N(fL_N g) \qquad \forall f, g : X^{\Lambda_N} \to \mathbb{R}, \tag{2.13}$$

then μ_N is necessarily an invariant measure. In such a case the process is said to be *reversible*. This terminology is due to the following fact. Let $\mathbb{P}_{\mu_N}^N$ the stationary process, i.e. the distribution on the path space induced by the Markov process with initial condition distributed according to the invariant measure μ_N. Since μ_N is invariant, the measure $\mathbb{P}_{\mu_N}^N$ is invariant with respect to time shifts. We can thus regard $\mathbb{P}_{\mu_N}^N$ as a measure on paths defined also for $t \leq 0$, i.e. as a probability on $D(\mathbb{R}; X^{\Lambda_N})$. This probability is invariant under time reversal if and only if the measure μ_N is reversible, i.e. (2.13) holds. More generally, if we denote by ϑ the time reversal, i.e. $(\vartheta\eta)(t) := \eta(-t)$, we have that $\mathbb{P}_{\mu_N}^N \circ \vartheta$ is the stationary process with generator L_N^*, the adjoint to L_N in $L_2(\mathrm{d}\mu_N)$. In particular, if (2.13) holds, we have $\mathbb{P}_{\mu_N}^N \circ \vartheta = \mathbb{P}_{\mu_N}^N$.

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When there is a unique invariant measure which is not reversible, we say the corresponding process is *non-reversible*. As we shall discuss, non-equilibrium models are necessarily non-reversible, while there exist non-reversible processes describing equilibrium phenomena, see, for example, [1], [30]–[32]. The main topic that we shall discuss is the asymptotic behaviour, as N diverges, of the invariant measure μ_N for specific classes of non-reversible models.

Conditions (2.5) and (2.7) are called *local* detailed balance for the following reason. If the chemical potential λ_0 is constant, it is easy to show that the Gibbs measure $\mu(\eta) \propto \mathrm{e}^{-\mathcal{H}(\eta)+\lambda_0 \sum_z \eta_z}$ is reversible with respect to the generator L_N^0, that is (2.10) with rates $c_{x,y}^0$. On the other hand, if λ_0 is not constant, the boundary dynamics forces a current in the system which becomes non-reversible.

We discuss next the effect of the external field. A very particular choice of F is that of a discrete *gradient* vector field, such that

$$F(x,y) = \tfrac{1}{2}[\lambda(y) - \lambda(x)] \tag{2.14}$$

for some function $\lambda : \overline{\Lambda}_N \to \mathbb{R}$. If we further assume that $\lambda(y) = \lambda_0(y)$ for $y \in \partial\Lambda_N$, recall that λ_0 is the chemical potential of the boundary reservoirs, then it is easily shown that the generator L_N in (2.10) is reversible w.r.t. the measure

$$\mu_N^\lambda(\eta) = \frac{1}{Z_N^\lambda} \exp\left\{-\mathcal{H}(\eta) + \sum_{x\in\Lambda_N} \lambda(x)\eta_x\right\}, \tag{2.15}$$

where Z_N^λ is the appropriate normalization constant. In this situation the reversibility of the process is due to the fact that the driving from the reservoirs and the external field compensate.

An equivalence principle. We can interpret the above result from two different perspectives, getting the answer to two opposite questions.

Consider a model with a given chemical potential λ_0 at the boundary. We ask if we can find an external field F which compensates the driving from the boundary, namely such that the corresponding stationary measure μ_N is reversible. The answer to this question is certainly yes. In fact, from the above consideration, we have a whole family of external fields that fulfil this condition: take a gradient vector field F as in (2.14) with λ such that $\lambda(y) = \lambda_0(y)$ for $y \in \partial\Lambda_N$. In this case the corresponding stationary measure happens to be the Gibbs measure (2.15).

Conversely, suppose that we have an asymmetric model with a given external field F. We ask if we can find a chemical potential $\lambda_0 : \partial\Lambda_N \to \mathbb{R}$ such that the model is reversible. We can immediately answer affirmatively this question if we know that the external field F is gradient, i.e. (2.14) holds for some $\lambda : \bar{\Lambda}_N \to \mathbb{R}$. In this case we can just fix, up to an overall additive constant, $\lambda_0(y) = \lambda(y), y \in \partial\Lambda_N$.

2.2. Zero-range process

The so-called *zero-range process* is a special case of the lattice gases introduced in section 2.1. In each site any number of particles is allowed so that $X = \mathbb{N}$ and the bulk symmetric jump rates are

$$c_{x,y}^0(\eta) = g(\eta_x), \qquad x, y \in \Lambda_N, |x-y| = 1, \tag{2.16}$$

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where $g : \mathbb{N} \to \mathbb{R}_+$ is a function satisfying $g(0) = 0$ with at most linear growth. In other words, the jump rate from x to y depends only on the occupation number at x; this explains the name of the model. Given $\lambda_0 : \partial\Lambda_N \to \mathbb{R}$, we choose the boundary rates as

$$c^0_{x,y}(\eta) = g(\eta_x), \qquad c^0_{y,x}(\eta) = \mathrm{e}^{\lambda_0(y)}, \qquad x \in \Lambda_N, y \in \partial\Lambda_N, |x - y| = 1. \tag{2.17}$$

It is not hard to check that the detailed balance conditions (2.5) and (2.7) are satisfied with the Hamiltonian

$$\mathcal{H}(\eta) = \sum_{x\in\Lambda_N} \log(g(\eta_x)!),$$

where, by definition, $g(0)! = 1$ and $g(k)! = g(1)\cdots g(k)$ for $k \geq 1$. The particular case in which g is the identity, i.e. $g(k) = k$, $k \in \mathbb{N}$, corresponds to independent random walks described in terms of the occupation variables $\eta \in \mathbb{N}^{\Lambda_N}$.

A peculiar feature of this model is that its invariant measure, both with particle reservoirs and external field, is always product. Consider this model with external field F. Denote by $\psi : \overline{\Lambda}_N \to \mathbb{R}_+$ the solution to

$$\begin{aligned} &\sum_{\substack{y\in\overline{\Lambda}_N\\ |x-y|=1}} [\mathrm{e}^{F(y,x)}\psi(y) - \mathrm{e}^{F(x,y)}\psi(x)] = 0, \qquad x \in \Lambda_N \\ &\psi(x) = \exp\{\lambda_0(x)\}, \qquad x \in \partial\Lambda_N. \end{aligned} \tag{2.18}$$

The invariant measure of the zero-range process with external field F and boundary chemical potential λ_0 is then the grand-canonical product measure $\mu_N = \prod_{x\in\Lambda_N} \mu_x$ with marginal distributions

$$\mu_x(\eta_x = k) = \frac{1}{Z(\psi(x))} \frac{\psi(x)^k}{g(k)!}, \tag{2.19}$$

where

$$Z(\varphi) = \sum_{k=0}^{\infty} \frac{\varphi^k}{g(k)!} \tag{2.20}$$

is the normalizing constant. This can be verified by showing that (2.12) holds. If Λ_N is the discrete torus and F vanishes, any constant ψ solves (2.18) and the corresponding invariant measures are thus the grand-canonical measures with arbitrary chemical potential. Since the invariant measure is always product, the zero-range process never exhibits long range correlations.

2.3. Exclusion process

The exclusion process is a much studied stochastic lattice gas. In this model an exclusion principle is imposed. In each site $x \in \Lambda_N$ at most one particle is allowed so that $X = \{0, 1\}$ and there is no other interaction. The symmetrical bulk rates are defined by

$$c^0_{x,y}(\eta) = \eta_x(1 - \eta_y), \qquad x, y \in \Lambda_N, |x - y| = 1 \tag{2.21}$$

namely a particle at x jumps to a nearest-neighbour site y with rate 1/2 if that site is empty. Then (2.5) holds with $\mathcal{H} = 0$. Note that the rates (2.21) satisfy the constraint

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$c^0_{x,y}(\eta) = 0$ if $\sigma^{x,y}\eta \notin \{0,1\}^{\Lambda_N}$. Given a chemical potential $\lambda_0 : \partial\Lambda_N \to \mathbb{R}$, the local detailed balance condition (2.7) is met by choosing the boundary rates as

$$\begin{aligned} &c^0_{x,y}(\eta) = \eta_x K(y), \qquad c^0_{y,x}(\eta) = (1-\eta_x)K(y)\mathrm{e}^{\lambda_0(y)}, \\ &x \in \Lambda_N, \quad y \in \partial\Lambda_N, \quad |x-y| = 1 \end{aligned} \tag{2.22}$$

for some $K : \partial\Lambda_N \to \mathbb{R}_+$.

We first discuss this symmetric case. In the case of periodic boundary conditions there is a one-parameter family of invariant measures which are the Bernoulli measures with an arbitrary parameter. Since the total number of particles is conserved, given $k > 0$, we can consider the process on the set $\Sigma_{N,k} = \{\eta \in \{0,1\}^{\Lambda_N} : \sum_{x\in\Lambda_N} \eta_x = k\}$. In this set the process is irreducible and the unique invariant measure is the uniform measure on $\Sigma_{N,k}$ which is the *canonical* ensemble associated to the Bernoulli measures. In the case with particles reservoirs, if the chemical potential λ_0 is constant then the unique invariant measure is the Bernoulli measure with parameter $\bar\rho = \mathrm{e}^{\lambda_0}/(1+\mathrm{e}^{\lambda_0})$, i.e. $\mu_N(\eta) = \mathrm{e}^{\lambda_0 \sum_{x\in\Lambda_N}\eta_x}/(1+\mathrm{e}^{\lambda_0})^{|\Lambda_N|}$. In both these situations the process is reversible.

One-dimensional boundary-driven exclusion process. Unlike the zero-range model, if λ_0 is not constant, so that this becomes a non-equilibrium model, the invariant measure is not a product measure and carries long range correlations. Let us discuss in more detail the one-dimensional case. Assume that $\Lambda = (0,1)$ so that $\Lambda_N = \{1,\ldots,N-1\}$; we also let $\lambda_0 := \lambda_0(0)$ and $\lambda_1 := \lambda_0(N)$ be the two chemical potentials of the reservoirs.

An old result by Kingman [37] computes the marginals of the unique invariant measure for a special choice of the injection rates. More precisely, in the case analysed by Kingman the bulk rates are as in (2.21) while the boundary rates are obtained by the following limiting procedure. In (2.22) choose $K(0) = (\mathrm{e}^A + \mathrm{e}^{-A})^{-1}\mathrm{e}^{-\lambda_0/2}$ and $K(N) = (\mathrm{e}^A + \mathrm{e}^{-A})^{-1}\mathrm{e}^{-\lambda_1/2}$ for some $A \in \mathbb{R}$. Consider then the asymmetric model with rates $c_{x,y}$ as in (2.8) by introducing the external field F given by $F(0,1) = F(N-1,N) = A$, $F(1,0) = F(N,N-1) = -A$, and $F(x,y) = 0$ in all the remaining bonds. Finally we take the limit $A \to \infty$ obtaining

$$c_{0,1}(\eta) = (1-\eta_1)\mathrm{e}^{\lambda_0/2}, \qquad c_{N-1,N}(\eta) = \eta_{N-1}\,\mathrm{e}^{-\lambda_1/2}, \qquad c_{1,0}(\eta) = c_{N,N-1}(\eta) = 0 \tag{2.23}$$

i.e. from the left endpoint particles enter with rate $(1/2)\mathrm{e}^{\lambda_0/2}$ but do not exit, while particles from the right endpoint exit with rate $(1/2)\mathrm{e}^{-\lambda_1/2}$ but do not enter.

By some smart duality computations, Kingman shows that, for this particular choice of the boundary rates, the marginals of the invariant measure μ_N are

$$\mu_N(\eta_{x_1} = 1, \ldots, \eta_{x_m} = 1) = \frac{(A-m-x_1)(A-m-x_2+1)\cdots(A-1-x_m)}{(B-m)(B-m+1)\cdots(B-1)}, \tag{2.24}$$

where $1 \le x_1 < x_2 < \cdots < x_m \le N-1$ are lattice sites and the parameters A and B are defined as

$$A = N + \mathrm{e}^{\lambda_1/2}; \qquad B = N - 1 + \mathrm{e}^{\lambda_1/2} + \mathrm{e}^{-\lambda_0/2}. \tag{2.25}$$

More recent work based on matrix methods allows us to get some representation of the invariant measure in the general one-dimensional case, see, for example, [42, 47] and references therein.

We consider now the one-dimensional boundary-driven symmetric exclusion model with boundary rates as in (2.22) with $K(0) = (1 + \mathrm{e}^{\lambda_0})^{-1}$ and $K(N) = (1 + \mathrm{e}^{\lambda_1})^{-1}$. As before λ_0 and λ_1 are the chemical potentials of the boundary reservoirs. Letting $\rho_i = \mathrm{e}^{\lambda_i}/(1 + \mathrm{e}^{\lambda_i})$, $i = 0, 1$, be the corresponding densities, we then get

$$c_{1,0}(\eta) = (1 - \rho_0)\eta_1, \qquad c_{0,1}(\eta) = \rho_0(1 - \eta_1),$$
$$c_{N-1,N}(\eta) = (1 - \rho_1)\eta_{N-1}, \qquad c_{N,N-1} = \rho_1(1 - \eta_{N-1}).$$

Let μ_N be the unique invariant measure, it is not difficult to show that the density profile $\mu_N(\eta_x)$ is linear so that

$$\mu_N(\eta_x) = \rho_0 + \frac{x}{N}(\rho_1 - \rho_0). \tag{2.26}$$

As first shown in [48], it is also possible to obtain a closed expression for the two-point correlations. For $1 \le x < y \le N - 1$ we have

$$\mu_N(\eta_x; \eta_y) := \mu_N(\eta_x \eta_y) - \mu_N(\eta_x)\mu_N(\eta_y) = -\frac{(\rho_1 - \rho_0)^2}{N - 1}\frac{x}{N}\left(1 - \frac{y}{N}\right). \tag{2.27}$$

To prove this result it is enough to compute $L_N(\eta_x \eta_y)$, i.e. the action of L_N on the function $\eta_x \eta_y$, and solve the equation

$$\mu_N(L_N(\eta_x \eta_y)) = 0. \tag{2.28}$$

Note that, if we take $x < y$ at distance $\mathrm{O}(N)$ from the boundary, then the covariance between η_x and η_y is of the order of $\mathrm{O}(1/N)$. Moreover the random variables η_x and η_y are negatively correlated. This is the same qualitative behaviour of the two-point correlation for the uniform measure on $\Sigma_{N,k}$. As we shall show below, quite the opposite behaviour is found in another model, the KMP process.

One-dimensional periodic asymmetric exclusion process. We finally discuss the case of the asymmetric exclusion process on the discrete torus. It is defined by the jump rates

$$c_{x,x+1}(\eta) = \mathrm{e}^{F}\eta_x(1 - \eta_{x+1}) \qquad c_{x+1,x}(\eta) = \mathrm{e}^{-F}\eta_{x+1}(1 - \eta_x) \tag{2.29}$$

for some $F \in \mathbb{R}$ so that (2.8) holds with constant external field F. A simple computation shows that the Bernoulli measure μ_ρ with arbitrary $\rho \in [0, 1]$ is an invariant measure. Note, however, that for $F \neq 0$ the process is not reversible; in fact the stationary process w.r.t. μ_ρ carries the mean current $\rho(1 - \rho)\sinh(F)$. Unlike the zero range, if the external field F is not constant the invariant measures are in general not anymore product. Note, however, that if F is a *gradient* vector field, as shown before, the process is reversible w.r.t. a product measure. We emphasize that a constant vector field on the torus is not gradient.

2.4. The boundary-driven KMP process

The Kipnis–Marchioro–Presutti (KMP) model [38] describes a chain of one-dimensional harmonic oscillators which are mechanically uncoupled but interact stochastically as follows. Each pair of nearest-neighbour oscillators waits an exponential time of rate one and then redistributes uniformly its total energy. The two oscillators at the end points are coupled to heat reservoirs. Since the single spin space state is not discrete and the elementary dynamics is associated to the bonds, this model does not really fit in the framework introduced in section 2. However, the precise definition of the model is straightforward. Let $\Lambda = (0,1)$ so that $\Lambda_N = N\Lambda \cap \mathbb{Z} \equiv \{1,\ldots,N-1\}$. We denote by ξ_x the energy of the oscillator at the site $x \in \Lambda_N$, so that the state space is $\mathbb{R}_+^{\Lambda_N}$. On it we introduce the Markov generator L_N as follows. Given $(x,y) \in \mathcal{B}(\Lambda_N)$ and $p \in [0,1]$ we let $\xi^{(x,y),p}$ be the configuration obtained from ξ by moving a fraction p of the total energy $\xi_x + \xi_y$ across the bond (x,y) to x and a fraction $1-p$ to y, i.e.

$$(\xi^{(x,y),p})_z := \begin{cases} \xi_z & \text{if } z \neq x, y \\ p(\xi_x + \xi_y) & \text{if } z = x \\ (1-p)(\xi_x + \xi_y) & \text{if } z = y. \end{cases}$$

We then set $L_N := \sum_{x=0}^{N-1} L_{x,x+1}$ where, for $f : \mathbb{R}_+^{\Lambda_N} \to \mathbb{R}$, the bulk dynamics is given by

$$L_{x,x+1} f(\xi) := \int_0^1 \mathrm{d}p\, [f(\xi^{(x,x+1),p}) - f(\xi)], \qquad x = 1,\ldots,N-2$$

while the boundary generators $L_{0,1}$ and $L_{N-1,N}$ are

$$\begin{aligned} L_{0,1} f(\xi) &:= \int_0^\infty \mathrm{d}\xi_0\, \frac{1}{T_0} \mathrm{e}^{-(\xi_0/T_0)} \int_0^1 \mathrm{d}p\, [f(\xi^{(0,1),p}) - f(\xi)] \\ L_{N-1,N} f(\xi) &:= \int_0^\infty \mathrm{d}\xi_N\, \frac{1}{T_1} \mathrm{e}^{-(\xi_N/T_1)} \int_0^1 \mathrm{d}p\, [f(\xi^{(N-1,N),p}) - f(\xi)]. \end{aligned} \tag{2.30}$$

Namely, we suppose that there is an energy exchange across the ghost bonds $(0,1)$ and $(N-1,N)$, and we put at the sites 0 and N oscillators whose energies are randomly chosen according to the Gibbs distributions with temperatures T_0 and T_1.

We emphasize that the above choice of the boundary dynamics differs slightly from the original one in [38]. Besides being more natural, this choice simplifies some microscopic computations. Note that in the case $T = T_0 = T_1$, namely of an equilibrium model, the above process is reversible with respect to the Gibbs measure

$$\mathrm{d}\mu_N(\xi) = \prod_{x=1}^{N-1} \frac{1}{T} \mathrm{e}^{-\xi_x/T}\, \mathrm{d}\xi_x \tag{2.31}$$

which is just the product of exponential distributions.

Later, in order to find a closed expression for the microscopic two-point correlation functions, we introduce a more general class of boundary dynamics which is obtained by replacing in (2.30) the two exponential distributions on boundary sites 0 and N by the other two probability measures on $\mathbb{R}_+$. Of course the macroscopic behaviour is the same for any reasonable choice of the boundary dynamics.

Invariant measure for a single oscillator. We consider the KMP model with a single oscillator, i.e. $N = 2$. Even in this case, as the system is in thermal contact with two reservoirs, its stationary state is not trivial. We next show that the invariant measure is a mixture of the Gibbs distributions with temperatures between T_0 and T_1. Furthermore we compute the weight of each distribution which turns out to be the arcsine law in the interval $[T_0, T_1]$; here we assume $T_0 \leq T_1$. We emphasize that this result depends on the specific choice of the boundary dynamics.

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We claim that the invariant measure (a probability measure on $\mathbb{R}_+$) is absolutely continuous w.r.t. the Lebesgue measure $\mathrm{d}\xi$ and its density can be expressed as

$$\frac{\mathrm{d}\mu}{\mathrm{d}\xi} = \int_{T_0}^{T_1} \mathrm{d}\varrho_{T_0,T_1}(T) \frac{1}{T} \mathrm{e}^{-\xi/T}, \tag{2.32}$$

where ϱ_{T_0,T_1} is the arcsine distribution in the interval $[T_0, T_1]$, namely for T in this interval we have

$$\mathrm{d}\varrho_{T_0,T_1}(T) = \frac{1}{\pi} \frac{1}{\sqrt{(T_1 - T)(T - T_0)}}\, \mathrm{d}T. \tag{2.33}$$

To show that μ in (2.32) is the invariant measure of the KMP process with a single oscillator, we need to check that, for each smooth real function, f on $\mathbb{R}_+$ (2.12) holds. By linearity and approximation by linear combinations of exponential functions, it is enough to show that (2.12) holds if $f(\xi) = \exp\{-\lambda\xi\}$, $\lambda > 0$. With this choice we have

$$\begin{aligned} Lf(\xi) &= \int_0^\infty \frac{\mathrm{d}\xi_0}{T_0} \mathrm{e}^{-\xi_0/T_0} \int_0^\infty \frac{\mathrm{d}\xi_2}{T_1} \mathrm{e}^{-\xi_2/T_1} \int_0^1 \mathrm{d}p\, [\mathrm{e}^{-\lambda p(\xi_0+\xi)} + \mathrm{e}^{-\lambda p(\xi+\xi_2)} - 2\mathrm{e}^{-\lambda\xi}] \\ &= \int_0^1 \mathrm{d}p \left[\frac{1}{1+\lambda p T_0} \mathrm{e}^{-\lambda p \xi} + \frac{1}{1+\lambda p T_1} \mathrm{e}^{-\lambda p \xi} - 2\mathrm{e}^{-\lambda\xi} \right]. \end{aligned}$$

If we now take the average of the above expression when ξ is an exponential random variable of parameter T we get

$$\int_0^\infty \frac{\mathrm{d}\xi}{T} \mathrm{e}^{-\xi/T} Lf(\xi) = \int_0^1 \mathrm{d}p \left[\frac{1}{(1+\lambda p T_0)(1+\lambda p T)} + \frac{1}{(1+\lambda p T)(1+\lambda p T_1)} - \frac{2}{1+\lambda T} \right]. \tag{2.34}$$

We next note that the arcsine distribution in the interval $[T_0, T_1]$ is characterized by the following property. For each $\gamma \geq 0$ we have

$$\int \mathrm{d}\varrho_{T_0,T_1}(T) \frac{1}{1+\gamma T} = \frac{1}{\sqrt{(1+\gamma T_0)(1+\gamma T_1)}}. \tag{2.35}$$

The integral on the lhs can be, in fact, computed by using the density in (2.33) and the residue theorem. Conversely, by expanding the above equation in power series of γ, we get that the moments of ϱ_{T_0,T_1} are determined.

Recalling (2.34), to complete the proof of (2.32) it remains to show that

$$\int \mathrm{d}\varrho_{T_0,T_1}(T) \int_0^1 \mathrm{d}p \left[\frac{1}{(1+\lambda p T_0)(1+\lambda p T)} + \frac{1}{(1+\lambda p T)(1+\lambda p T_1)} - \frac{2}{1+\lambda T} \right] = 0,$$

which, in view of (2.35), is equivalent to

$$\begin{aligned} &\int_0^1 \mathrm{d}p \left[\frac{1}{(1+\lambda p T_0)^{3/2}(1+\lambda p T_1)^{1/2}} + \frac{1}{(1+\lambda p T_0)^{1/2}(1+\lambda p T_1)^{3/2}} \right] \\ &\qquad = \frac{2}{(1+\lambda T_0)^{1/2}(1+\lambda T_1)^{1/2}}. \end{aligned}$$

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By a direct integration we get

$$\int_0^1 \mathrm{d}p \, \frac{1}{(1+\lambda p T_0)^{3/2}(1+\lambda p T_1)^{1/2}} = \frac{2}{\lambda(T_1-T_0)}\left[\frac{\sqrt{1+\lambda T_1}}{\sqrt{1+\lambda T_0}} - 1\right]$$

and simple algebraic computations yield the result.

It seems quite hard to obtain an analogous representation for $N \geq 3$. On the other hand, we compute explicitly below the one-and two-point correlation functions of μ_N for any $N \geq 2$.

Two-point correlations. We here consider the KMP process with boundary dynamics given by

$$L_{0,1} f(\xi) := \int_0^\infty \mathrm{d}\nu_0^N(\xi_0) \int_0^1 \mathrm{d}p \, [f(\xi^{(0,1),p}) - f(\xi)]$$

$$L_{N-1,N} f(\xi) := \int_0^\infty \mathrm{d}\nu_1^N(\xi_N) \int_0^1 \mathrm{d}p \, [f(\xi^{(N-1,N),p}) - f(\xi)],$$

where ν_i^N, $i = 0, 1$, are probability measures on $\mathbb{R}_+$ with mean T_i and variance

$$\nu_i^N([\xi - T_i]^2) = T_i^2 + \frac{(T_1 - T_0)^2}{N(N+1)} \qquad i = 0, 1 \tag{2.36}$$

and note that the exponential distributions chosen in (2.30) fail to satisfy the above condition only by a term $\mathrm{O}(N^{-2})$.

Given $T_0 \leq T_1$, let μ_N be the invariant measure of the KMP process with $N-1$ oscillators and set $E_N(x) := \mu_N(\xi_x)$, $x = 1, \ldots, N-1$, as well as $E_N(0) := T_0$, $E_N(N) := T_1$. By choosing linear functions f in (2.12) and computing $L_N \xi_x$, $x = 1, \ldots, N-1$, we get a closed equation for E_N which yields

$$E_N(x) = T_0 + (T_1 - T_0)\frac{x}{N}. \tag{2.37}$$

Let $C_N(x,y) := \mu_N(\xi_x;\xi_y) = \mu_N(\xi_x \xi_y) - E_N(x)E_N(y)$, $x, y \in \{1, \ldots, N-1\}$, be the two-point correlation function of μ_N. We also set $C_N(0,0) := \nu_0^N([\xi - T_0]^2)$, $C_N(N,N) := \nu_1^N([\xi - T_1]^2)$, $C_N(0,y) = C_N(x,N) := 0$ for $1 \leq y \leq N$, $0 \leq x \leq N-1$. By choosing quadratic functions in (2.12), by some elementary but tedious computations we get that $C_N(\cdot,\cdot)$ solves

$$(\Delta_x^N + \Delta_y^N) C_N(x,y) = 0 \qquad 1 \leq x \leq y \leq N-1, \quad y - x \geq 2$$

$$C_N(x,x+2) + C_N(x-1,x+1) - \tfrac{10}{3} C_N(x,x+1) + \tfrac{1}{3} C_N(x,x) + \frac{1}{3} C_N(x+1,x+1)$$
$$= \frac{2}{3}\left(\frac{T_1 - T_0}{N}\right)^2 + \frac{2}{3} E_N(x) E_N(x+1) \qquad 1 \leq x \leq N-2$$

$$C_N(x-1,x-1) + C_N(x+1,x+1) + 2C_N(x-1,x) + 2, C_N(x,x+1) - 4C_N(x,x)$$
$$= -2\left(\frac{T_1 - T_0}{N}\right)^2 - 2E_N(x)^2 \qquad 1 \leq x \leq N-1,$$

where $\Delta_x^N f(x,y) = f(x+1,y) + f(x-1,y) - 2f(x,y)$ is the discrete Laplacian w.r.t. x and Δ_y^N is the discrete Laplacian w.r.t. y.

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As can be easily checked, the solution is given by

$$C_N(x,y) = \begin{cases} \dfrac{(T_1-T_0)^2}{N+1}\dfrac{x}{N}\left(1-\dfrac{y}{N}\right) & 0 \le x < y \le N \\ E_N(x)^2 + 2\dfrac{(T_1-T_0)^2}{N+1}\dfrac{x}{N}\left(1-\dfrac{x}{N}\right) + \dfrac{(T_1-T_0)^2}{N(N+1)} & 0 \le x = y \le N. \end{cases} \tag{2.38}$$

Comparing (2.38) with (2.27) we observe that the off-diagonal terms are essentially the same in the macroscopic limit $N \to \infty$. We emphasize, however, that the sign is different: while for the boundary-driven symmetric exclusion the occupation variables η_x, $x \in \Lambda_N$, are negatively correlated, for the KMP process the local energies ξ_x, $x \in \Lambda_N$, are positively correlated. As we shall discuss in section 3.3, this qualitative difference is related to the different convexity properties of the mobilities of the two models. For the exclusion it is concave while it is convex for KMP.

We mention that an analogous computation has been recently performed for a somewhat similar model, see [33].

2.5. Gradient models with periodic boundary conditions

In this section we consider only the case of periodic boundary conditions, namely Λ_N is the discrete torus $(\mathbb{Z}/N\mathbb{Z})^d$. We also assume that the model is translationally covariant in the sense that, for any $(x,y) \in \mathcal{B}(\Lambda_N)$, $z \in \Lambda_N$, and $\eta \in X^{\Lambda_N}$, we have

$$c_{x,y}(\eta) = c_{x+z,y+z}(\tau_z \eta), \tag{2.39}$$

where τ_z is the space shift, i.e. $(\tau_z\eta)_x := \eta_{x-z}$.

Let the bulk rates $c^0_{x,y}$ satisfy (2.5). The *expected instantaneous current* across the bond $(x,y) \in \mathcal{B}(\Lambda_N)$ is, up to a factor 2,

$$j^0_{x,y}(\eta) := c^0_{x,y}(\eta) - c^0_{y,x}(\eta).$$

The corresponding lattice gas (with no external field) satisfies the *gradient condition* if the discrete vector field $j^0_{x,y}(\eta)$ is gradient for any $\eta \in X^{\Lambda_N}$, namely there exist functions $h_x : X^{\Lambda_N} \to \mathbb{R}$, $x \in \Lambda_N$, such that for any $(x,y) \in \mathcal{B}(\Lambda_N)$

$$j^0_{x,y}(\eta) = h_y(\eta) - h_x(\eta). \tag{2.40}$$

The zero-range process of section 2.2 is a gradient lattice gas for any choice of the function g. Indeed, for the rates (2.16) condition (2.40) holds with $h_x(\eta) = -g(\eta_x)$. Also the exclusion process is gradient, (2.40) holding with $h_x(\eta) = -\eta_x$.

In the stochastic gases literature, see [39, 49], the gradient condition is usually stated in a stronger form. More precisely, one considers a translationally invariant lattice gas on the whole lattice $\mathbb{Z}^d$ and says that the model is gradient if there exists a function $\tilde{h} : X^{\mathbb{Z}^d} \to \mathbb{R}$ which is *local*, i.e. it depends on η_x only for a finite number of $x \in \mathbb{Z}^d$, and such that for any $(x,y) \in \mathcal{B}(\mathbb{Z}^d)$ and $\eta \in X^{\mathbb{Z}^d}$

$$j^0_{x,y}(\eta) = \tilde{h}(\tau_y\eta) - \tilde{h}(\tau_x\eta). \tag{2.41}$$

Of course (2.41) implies (2.40) for N large enough. Conversely, it is possible to show that if (2.40) holds then there exists a function $\tilde{h} : X^{\Lambda_N} \to \mathbb{R}$ such that (2.41) holds for any $(x,y) \in \mathcal{B}(\Lambda_N)$.

Consider now a lattice gas with constant (non-zero) external field F. By this we mean that $F(x, x \pm e_i) = \pm F_i$, where e_i, $i = 1, \dots, d$ is the canonical basis in $\mathbb{R}^d$ and $(F_1, \dots, F_d)$ is a vector in $\mathbb{R}^d$. As discussed in [36], if the bulk rates c^0 satisfy the gradient condition (2.41) then the grand-canonical Gibbs measures $\exp\{-\mathcal{H}(\eta) + \lambda \sum_{x\in\Lambda_N} \eta_x\}$, $\lambda \in \mathbb{R}$, which are the invariant measures for the system with no external field, are invariant also for the process with external field F, i.e. with rates $c_{x,x\pm e_i} = c^0_{x,x\pm e_i} \mathrm{e}^{\pm F_i}$, $i = 1, \dots, d$. In particular this result shows that *gradient* lattice gases with constant external field and periodic boundary conditions do not exhibit long range correlations. In section 3.1 we show that, from a macroscopic point of view, *any* weakly asymmetric lattice gas with periodic boundary conditions does not have long range correlations.

We next discuss, from a microscopic point of view, gradient lattice gases in some more detail, obtaining the above mentioned result as a particular case. Let us consider an asymmetric lattice gas with external field $F : \mathcal{B}(\Lambda_N) \to \mathbb{R}$, rates $c_{x,y}$ as in (2.8) and generator given by (2.10). We look for an invariant measure of the form (2.15) for some $\lambda : \Lambda_N \to \mathbb{R}$. The condition for a stationary state is

$$\sum_{\eta\in X^{\Lambda_N}} \mu_N^\lambda(\eta) \sum_{(x,y)\in\mathcal{B}(\Lambda_N)} c_{x,y}(\eta)[f(\sigma^{x,y}\eta) - f(\eta)] = 0, \qquad \forall f : X^{\Lambda_N} \to \mathbb{R}. \tag{2.42}$$

Performing some change of variables and using the conditions (2.5) and (2.7) of local detailed balance, (2.42) becomes

$$\sum_{\eta\in X^{\Lambda_N}} f(\eta)\mu_N^\lambda(\eta) \sum_{(x,y)\in\mathcal{B}(\Lambda_N)} \mathrm{e}^{-\lambda(x)}\mathrm{e}^{F(x,y)} \left[\mathrm{e}^{\lambda(y)} c^0_{y,x}(\eta) - \mathrm{e}^{\lambda(x)} c^0_{x,y}(\eta)\right] = 0. \tag{2.43}$$

Let

$$\begin{aligned} G^\lambda(x,y) &:= \mathrm{e}^{-\lambda(x)}\mathrm{e}^{F(x,y)} - \mathrm{e}^{-\lambda(y)}\mathrm{e}^{F(y,x)} \\ j^\lambda_{y,x}(\eta) &:= \mathrm{e}^{\lambda(y)} c^0_{y,x}(\eta) - \mathrm{e}^{\lambda(x)} c^0_{x,y}(\eta). \end{aligned}$$

Note that, if F is a discrete vector field, i.e. it satisfies $F(x,y) = -F(y,x)$, then e^F is *not* a discrete vector field but G^λ and j^λ are indeed discrete vector fields. We then get that (2.43) is equivalent to

$$\sum_{(x,y)\in\mathcal{B}(\Lambda_N)} G^\lambda(x,y) j^\lambda_{y,x}(\eta) = 0, \qquad \forall \eta \in X^{\Lambda_N}. \tag{2.44}$$

Notice that (2.44) is an orthogonality condition. In general there is no solution to (2.44); note, in fact, that it is a system of $|X|^{|\Lambda_N|}$ equations (corresponding to different particle configurations) but we have only $|\Lambda_N|$ parameters (corresponding to the chemical potential profile $\lambda : \Lambda_N \to \mathbb{R}$). Non-existence of solutions to (2.44) means that the invariant measure is not of the form (2.15). There are, however, few remarkable cases in which (2.44) can be easily solved.

If the model is gradient, so that (2.40) holds, we claim that $\mu_N^\lambda(\eta)$ in (2.15) with $\lambda \in \mathbb{R}$ constant is an invariant measure for any asymmetric lattice gas provided the external field F satisfies

$$\sum_{y:|x-y|=1} [\mathrm{e}^{F(x,y)} - \mathrm{e}^{F(y,x)}] = 0 \qquad \forall x \in \Lambda_N \tag{2.45}$$

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that is, the discrete vector field G^λ, $\lambda \in \mathbb{R}$, has vanishing discrete divergence. Conversely, if we require that $\mu_N^\lambda(\eta)$, $\lambda \in \mathbb{R}$, is an invariant measure for any external field satisfying (2.45), we get that the rates $c^0_{x,y}$ have to satisfy (2.40) for some functions $h_x : X^{\Lambda_N} \to \mathbb{R}$, $x \in \Lambda_N$. The proof of both statements is accomplished by some computations which essentially amounts to proving the Hodge theorem in a discrete setting, see [43].

Generalized gradient models. Consider asymmetric lattice gases with constant external fields F. Some computations show that μ_N^λ as in (2.15) is an invariant measure for any constant $\lambda \in \mathbb{R}$ if and only if the rates $c^0_{x,y}$ satisfy

$$\sum_{x\in\Lambda_N} j^0_{x,x+e_i}(\eta) = 0, \qquad \forall \eta \in X^{\Lambda_N}, \forall i = 1, \ldots, d, \tag{2.46}$$

which is exactly the condition that identifies the orthogonal complement, w.r.t. the inner product defined in (2.44), of the constant vector fields. Moreover (2.46) is equivalent to the following *generalized gradient condition*. There is a function $h_{i,j} : X^{\Lambda_N} \to \mathbb{R}$, $i, j = 1, \ldots, d$, such that

$$j^0_{x,x+e_i}(\eta) = \sum_{j=1}^{d} [h_{i,j}(\tau_{x+e_j}\eta) - h_{i,j}(\tau_x\eta)], \qquad i = 1, \ldots, d. \tag{2.47}$$

We finally mention that (2.47) is a particular case of the condition stated in [39, Def. 2.5].

To summarize the previous discussion, gradient models in the sense of (2.40) have the property that any external field satisfying (2.45) will not change the invariant measure, while generalized gradient models in the sense of (2.47) have this property only for constant external fields.

2.6. Glauber + Kawasaki dynamics

Unlike the models discussed so far, the so-called *Glauber + Kawasaki* process is not a lattice gas in the sense that the number of particles is not locally conserved. A reaction term allowing creation/annihilation of particles is added in the bulk. We consider the case with exclusion rule so that $X = \{0, 1\}$ and discuss only the one-dimensional case with periodic boundary condition, Λ_N a ring with N sites. The generator is defined as

$$L_N f(\eta) = \frac{1}{2} \sum_{(x,y)\in\mathcal{B}(\Lambda_N)} \eta_x(1-\eta_y)[f(\sigma^{x,y}\eta) - f(\eta)] + \frac{1}{N^2} \sum_{x\in\Lambda_N} c_x(\eta)[f(\sigma^x\eta) - f(\eta)], \tag{2.48}$$

where σ^x denotes the particle flip at x, i.e. $(\sigma^x\eta)_x = 1 - \eta_x$ and $(\sigma^x\eta)_y = \eta_y$ for $y \neq x$. The first term of the generator corresponds to the symmetric exclusion process while the second one involves the reaction defined by the corresponding rates c_x, $x \in \Lambda_N$. The factor N^2 in (2.48) has been inserted to get, after diffusive rescaling, a meaningful macroscopic evolution.

The first question one can ask is when there exists a reversible measure for this process. As we shall see, this happens only if we impose some restrictions on the reaction rates c_x. The condition of reversibility w.r.t. the measure μ_N is (2.6), which in this case,

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after some algebra, is

$$\tfrac{1}{2}\sum_{\eta}\sum_{x\in\Lambda_N} g(\eta)f(\eta^{x,x+1})[\mu_N(\eta)-\mu_N(\eta^{x,x+1})] \\ +\frac{1}{N^2}\sum_{\eta}\sum_{x\in\Lambda_N} g(\eta)f(\sigma^x\eta)[c_x(\eta)\mu_N(\eta)-c_x(\sigma^x\eta)\mu_N(\sigma^x\eta)]=0, \tag{2.49}$$

where $\eta^{x,x+1}$ denotes the configuration obtained from η by exchanging the occupation numbers in x and $x+1$. Since this equality must hold for every g and f, this condition is equivalent to

$$\begin{aligned} &\mu_N(\eta)-\mu_N(\eta^{x,x+1})=0\\ &c_x(\eta)\mu_N(\eta)-c_x(\sigma^x\eta)\mu_N(\sigma^x\eta)=0 \end{aligned} \tag{2.50}$$

for any η and x. The first condition imposes that the measure μ_N has the form

$$\mu_N(\eta)=M_N\left(\sum_{x\in\Lambda_N}\eta_x\right) \tag{2.51}$$

namely μ_N must assign an equal weight to configurations with the same number of particles. The second condition, with a μ_N of this type, is a restriction on the reaction rates and on the function M_N. The most general form of $c_x(\eta)$ that satisfies this condition is

$$c_x(\eta)=A_1(1-\eta_x)h(\tau_x\eta)+A_2\eta_x h(\tau_x\eta), \tag{2.52}$$

where A_1, A_2 are arbitrary positive constants, and $h:\{0,1\}^{\Lambda_N}\to\mathbb{R}_+$ is an arbitrary positive function such that $h(\sigma^0\eta)=h(\eta)$, i.e. it does not depend on η_0. Recall that τ_x denotes the shift by x. Notice that the rates $c_x(\eta)$ in (2.52) are translation invariant, namely they satisfy $c_x(\eta)=c_0(\tau_x\eta)$. With this choice, the unique reversible measure μ_N is the Bernoulli measure with parameter $p=A_1/(A_1+A_2)$ [32].

We emphasize that periodic boundary conditions are crucial for the validity of (2.52) with a nontrivial h. In this special case there are no long range correlations. In section 3.5 we show that if the rates c_x are not of type (2.52) then—generically—there are long range correlations.

2.7. Totally asymmetric exclusion process

The one-dimensional totally asymmetric exclusion process is the particular case of the one-dimensional asymmetric exclusion process introduced in section 2.3 in which particles jump only to the right. As discussed there, in the case of periodic boundary conditions, the invariant measures are the Bernoulli measures with any density. We instead consider here the boundary-driven model. As usual we set $\Lambda_N=\{1,\ldots,N-1\}$ and we let λ_0 and λ_1 be the chemical potentials of the two reservoirs. The bulk jump rates are

$$c_{x,x+1}(\eta)=\eta_x(1-\eta_{x+1}),\qquad c_{x+1,x}(\eta)=0\qquad x=1,\ldots,N-2 \tag{2.53}$$

while the boundary rates are

$$c_{0,1}(\eta)=\eta_1\mathrm{e}^{\lambda_0/2},\qquad c_{N-1,N}(\eta)=\eta_N\mathrm{e}^{-(\lambda_1/2)},\qquad c_{1,0}(\eta)=c_{N,N-1}(\eta)=0. \tag{2.54}$$

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These rates can be obtained from our standard choice by a limiting procedure analogous to the one described to get (2.23).

The unique invariant measure for this model has an interesting representation due to Duchi and Schaeffer [23] that we briefly recall. We duplicate the variables by introducing new random variables $\xi \in \{0,1\}^{\Lambda_N}$. We then define a joint distribution ν_N for the variables (η, ξ) as follows. Let

$$E_x := \sum_{z=1}^{x} (\eta_z + \xi_z) - x, \qquad x = 1, \ldots, N-1$$

and $E_0 := 0$. The measure ν_N gives positive weight only to *complete configurations*, defined by the conditions

$$E_{N-1} = 0, \qquad E_x \geq 0, \qquad x = 1, \ldots, N-1. \tag{2.55}$$

Given a complete configuration we give some labels to the lattice sites according to the following rules:

$x \in \Lambda_N$ has label W if $\xi_x = 0$ and $E_{x-1} = E_x = 0$;

$x \in \Lambda_N$ has label B if $\xi_x = 1$, $E_{x-1} = 0$ and there are no sites on the left of x labelled W.

Let us denote by $N_W = N_W(\eta, \xi)$ the number of sites with label W for the complete configuration (η, ξ) and by $N_B = N_B(\eta, \xi)$ the number of sites with label B. The measure ν_N is then defined as

$$\nu_N(\eta, \xi) = \frac{1}{Z_N} \exp\{N_W \lambda_1/2 - N_B \lambda_0/2\}, \tag{2.56}$$

where $Z_N = Z_N(\lambda_1, \lambda_2)$ is the appropriate normalization constant.

The invariant measure of the boundary-driven totally asymmetric exclusion process is then the first marginal of the measure ν_N, i.e.

$$\mu_N(\eta) = \sum_{\xi \in \{0,1\}^{\Lambda_N}} \nu_N(\eta, \xi). \tag{2.57}$$

This result is proven by constructing a suitable Markov dynamics on the complete configurations (η, ξ) such that its projection to the η variables coincides with the dynamics of the totally asymmetric exclusion process. The invariant measure of the enlarged Markov dynamics can be easily computed and yields (2.56).

3. Macroscopic theory

As previously stated, an issue that we want to discuss is the asymptotic behaviour of the invariant measure μ_N. Let us first briefly recall the situation of reversible models. For definiteness consider a stochastic lattice gas with reservoirs at the boundary and assume that the chemical potential λ_0 of the boundary reservoirs is constant and that there is no external field. As discussed in section 2.1 the unique invariant measure is the grand-canonical Gibbs distribution

$$\mu_N^{\lambda_0}(\eta) = \frac{1}{Z_N(\lambda_0)} \exp\left\{-\mathcal{H}(\eta) + \lambda_0 \sum_{x \in \Lambda_N} \eta_x\right\}, \tag{3.1}$$

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where, letting $\Sigma_{N,k} := \{\eta \in X^{\Lambda_N} \mid \sum_{x\in\Lambda_N} \eta_x = k\}$, the grand-canonical partition function $Z_N(\lambda)$ is

$$Z_N(\lambda) = \sum_{k\geq 0} \mathrm{e}^{\lambda k} \sum_{\eta\in\Sigma_{N,k}} \mathrm{e}^{-\mathcal{H}(\eta)}. \tag{3.2}$$

We then define $p_0(\lambda)$ as

$$p_0(\lambda) := \lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log \mu_N^{\lambda_0}(\mathrm{e}^{\lambda \sum_{x\in\Lambda_N} \eta_x}), \tag{3.3}$$

where $|\Lambda_N|$ is the number of sites in Λ_N. Note that p_0 can be easily related to the pressure. Let in fact $\bar{p}_0(\lambda) := \lim_{N\to\infty} |\Lambda_N|^{-1} \log Z_N(\lambda)$ be the pressure, then $p_0(\lambda) = \bar{p}_0(\lambda_0 + \lambda) - \bar{p}_0(\lambda_0)$.

We then define the free energy f_0 as the Legendre transform of p_0, i.e.

$$f_0(\rho) := \sup_{\lambda\in\mathbb{R}} \{\lambda\rho - p_0(\lambda)\}. \tag{3.4}$$

According to the normalization chosen f_0 is a convex function which takes its minimum at the density associated to the chemical potential λ_0, i.e. at $\rho_0 = p_0'(0) = \bar{p}_0'(\lambda_0)$. Moreover $f_0(\rho_0) = 0$.

According to the Einstein fluctuation formula [24, 40], see also Lanford's lectures [41] for a complete mathematical treatment, the free energy f_0 gives the asymptotic probability of observing a fluctuation of the density, namely

$$\mu_N^{\lambda_0}\left(\frac{1}{|\Lambda_N|} \sum_{x\in\Lambda_N} \eta_x \approx \rho\right) \sim \exp\{-|\Lambda_N| f_0(\rho)\}. \tag{3.5}$$

Here $a \approx b$ means closeness in $\mathbb{R}$ and $\sim$ denotes logarithmic equivalence as $|\Lambda_N|$ diverges.

In discussing non-equilibrium models, which are not translationally invariant, it is important to establish a generalization of the above fluctuation formula. We want to compute the asymptotic probability of a fluctuation not of the average density but of the density profile. In fact, already Einstein [24] considered density profiles in small fluctuations from equilibrium. We introduce the empirical density as follows. To each microscopic configuration $\eta \in X^{\Lambda_N}$ we associate a macroscopic profile $\pi^N(u) = \pi^N(\eta; u)$, $u \in \Lambda$, by requiring that for each smooth function $G : \Lambda \to \mathbb{R}$

$$\langle \pi^N, G\rangle = \int_\Lambda \mathrm{d}u\, \pi^N(u) G(u) = \frac{1}{N^d} \sum_{x\in\Lambda_N} G(x/N)\eta_x \tag{3.6}$$

so that $\pi^N(u)$ is the local density at the macroscopic point $u = x/N$ in Λ. Let $\rho = \rho(u)$ be a given density profile. Then (3.5) can be recast as

$$\mu_N^{\lambda_0}(\pi^N \approx \rho) \sim \exp\{-N^d \mathcal{F}_0(\rho)\}. \tag{3.7}$$

Here $\rho \approx \rho'$ means that their averages over macroscopically small neighbourhoods are close and $\mathcal{F}_0(\rho)$ is the local and convex functional

$$\mathcal{F}_0(\rho) = \int_\Lambda \mathrm{d}u\, f_0(\rho(u)). \tag{3.8}$$

For non-reversible systems we shall look for a fluctuation formula like (3.7) which, in the same spirit as Einstein, we shall consider as the definition of the non-equilibrium free energy. While in the reversible setting discussed above the invariant measure μ_N is given by the Gibbs distribution (3.1), in a non-reversible system μ_N is not, in general, explicitly known. For special models, powerful combinatorial methods have been used [19]–[21], [25]. In the following we shall discuss instead the strategy introduced in [2, 3] which is based on the following idea. As N diverges the evolution of the thermodynamic variables is described by a closed macroscopic evolution called the hydrodynamic equation. The microscopic details are then encoded in the transport coefficients appearing in the hydrodynamic equation. In the cases discussed here, these transport coefficients are the diffusion coefficient and the mobility. For the Glauber + Kawasaki dynamics the reaction rates are also involved. We then compute the asymptotic probability of fluctuations from the typical hydrodynamical behaviour generalizing to a dynamical setting the Einstein fluctuation formula (3.7). The non-equilibrium free energy $\mathcal{F}$ is then characterized as the solution of a variational problem, from which we derive a Hamilton–Jacobi equation involving the transport coefficients. This is an infinite-dimensional strategy analogous to the Freidlin–Wentzell theory for diffusion processes [29].

Of course, in the case of reversible systems, the solution to the Hamilton–Jacobi equation coincides with the equilibrium free energy $\mathcal{F}_0$. This is essentially the characterization of $\mathcal{F}_0$ given by Onsager–Machlup [46], extended to a nonlinear context.

In section 3.1 we discuss the hydrodynamics and the associated dynamical large deviations principle of weakly asymmetric lattice gases. In section 3.2 we recall the derivation of the Hamilton–Jacobi equation and we discuss the form of the non-equilibrium free energy for the specific models introduced in section 2. We will also discuss a toy model for the invariant measure of the KMP process. In section 3.3 we obtain the macroscopic equation satisfied by the correlation functions and we discuss whether correlations are positive or negative. In section 3.4 we show that for weakly asymmetric lattice gases with periodic boundary conditions the non-equilibrium free energy coincides with the equilibrium one. In section 3.5 we discuss the macroscopic property of the Glauber + Kawasaki dynamics [1, 32]. Finally, in section 3.6, starting from the results in [23], we show how the representation for the non-equilibrium free energy of the totally asymmetric exclusion process obtained in [21] can be formulated as a minimization problem.

3.1. Hydrodynamics and dynamical large deviations

We consider an asymmetric model as defined by the rates (2.8). If the microscopic external field F is of order 1, the appropriate scaling is the Euler one, i.e. both space and time are rescaled by a factor N, and the hydrodynamic equation is given by a hyperbolic equation, see [39] and references therein. We here consider instead the case in which the external field is of the order $1/N$ as in (2.9). Then the hydrodynamic limit is obtained in the diffusive scaling and given by a parabolic equation. Let $\pi^N(t)$ be the empirical density, as defined in (3.6), corresponding to the particle's configuration at time N^2t; $\pi^N(t,u)$ is then a random space–time trajectory; as $N \to \infty$ it converges, however, to a deterministic function. Referring to [39, 49, 50] for periodic boundary conditions and to [3, 7, 26, 27] for open systems, we here state the law of large numbers, as $N \to \infty$, of the empirical density π^N for weakly asymmetric lattice gases. The macroscopic evolution of the density is described by a (in general nonlinear) diffusion equation with a transport term corresponding to the external field, namely

$$\partial_t \rho = \nabla \cdot [\tfrac{1}{2} D(\rho)\nabla\rho - \chi(\rho)E], \tag{3.9}$$

where D is the diffusion matrix, obtained from the microscopic dynamics by a Green-Kubo formula [49, II.2.2], and χ is the mobility matrix, obtained by linear response theory [49, II.2.5]. In (3.9) $\cdot$ denotes the standard inner product in $\mathbb{R}^d$. This equation has to be supplemented by the boundary conditions which are either periodic when Λ is the torus or the non-homogeneous Dirichlet condition

$$\lambda(\rho(t,u)) = \lambda_0(u), \qquad u \in \partial\Lambda \tag{3.10}$$

in the case of boundary-driven systems. Here $\partial\Lambda$ is the boundary of Λ, $\lambda(\rho) = f_0'(\rho)$ is the chemical potential associated with the microscopic Hamiltonian $\mathcal{H}$ and λ_0 is the chemical potential of the boundary reservoirs. Finally the initial condition for (3.9) is obtained as the limiting empirical density of the chosen microscopic initial configuration of particles.

We obtain an equilibrium model either if Λ is the torus and there is no external field or in the case of boundary-driven systems in which the external field in the bulk matches the driving from the boundary; in particular, if λ_0 is constant and E vanishes. In the other cases the stationary state supports a non-vanishing current and the systems is out of equilibrium.

The coefficients D and χ are related by the Einstein relation $D = R^{-1}\chi$, where R is the compressibility: $R^{-1} = f_0''$, in which f_0 is the equilibrium free energy associated with the Hamiltonian $\mathcal{H}$, see [49]. For gradient lattice gases, as defined in section 2.5, the diffusion matrix D and the mobility χ are multiples of the identity. For non-gradient models in general D and χ are not diagonal, however, as shown in [50, Lemma 8.3], if the Hamiltonian $\mathcal{H}$ is invariant w.r.t. rotation of $\pi/2$, then D and χ are diagonal.

We next discuss the large deviation properties of the empirical density; the derivation can be found in [3, 4, 39, 49]. Fix a smooth trajectory $\hat\rho \equiv \hat\rho(t,u)$, $(t,u) \in [0,T] \times \Lambda$. We want to compute the asymptotic probability that the empirical density π^N is in a small neighbourhood of $\hat\rho$. If $\hat\rho$ is not a solution to (3.9), this probability will be exponentially small and the corresponding rate is called the *large deviation dynamical rate functional*.

Consider an initial configuration η whose empirical measure approximates, as N diverges, $\hat\rho(0)$ and let $\mathbb{P}^N_\eta$ be the law of the microscopic process starting from such an initial condition. The dynamical large deviation principle for the empirical density states that

$$\mathbb{P}^N_\eta(\pi^N \approx \hat\rho) \sim \exp\{-N^d I_{[0,T]}(\hat\rho)\}, \tag{3.11}$$

where the rate functional $I_{[0,T]}$ is

$$I_{[0,T]}(\hat\rho) = \tfrac{1}{2}\int_0^T \mathrm{d}t \,\langle \nabla H, \chi(\hat\rho)\nabla H\rangle \tag{3.12}$$

in which $\langle , \rangle$ denotes integration in the space variables and $\nabla H \equiv \nabla H(t,u)$ is the extra gradient external field needed to produce the fluctuation $\hat\rho$, namely such that

$$\partial_t \hat\rho = \nabla \cdot [\tfrac{1}{2} D(\hat\rho)\nabla\hat\rho - \chi(\hat\rho)(E + \nabla H)]. \tag{3.13}$$

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The interpretation of (3.12) is straightforward; since χ is the mobility, $I_{[0,T]}(\hat{\rho})$ is the work done by the external field ∇H to produce the fluctuation $\hat{\rho}$ in the time interval $[0,T]$.

3.2. Thermodynamic functionals and Hamilton–Jacobi equation

Consider the following physical situation. The system is macroscopically in the stationary profile $\bar{\rho} \equiv \bar{\rho}(u)$, $u \in \Lambda$ (a stationary solution to (3.9)) at $t = -\infty$, but at $t = 0$ we find it in the state ρ. We want to determine the most probable trajectory followed in the spontaneous creation of this fluctuation. According to (3.11) this trajectory is the one that minimizes I among all trajectories $\hat{\rho}(t)$ connecting $\bar{\rho}$ to ρ in the time interval $[-\infty, 0]$. We thus define the so-called *quasi-potential* as

$$V(\rho) = \inf_{\substack{\hat{\rho}:\hat{\rho}(-\infty)=\bar{\rho} \\ \hat{\rho}(0)=\rho}} I_{[-\infty,0]}(\hat{\rho}). \tag{3.14}$$

As shown in [3, 5], the functional V solves the Hamilton–Jacobi equation

$$\frac{1}{2}\left\langle \nabla \frac{\delta V}{\delta \rho}, \chi(\rho) \nabla \frac{\delta V}{\delta \rho} \right\rangle + \left\langle \frac{\delta V}{\delta \rho}, \nabla \cdot \left[\frac{1}{2} D(\rho)\nabla\rho - \chi(\rho) E \right] \right\rangle = 0, \tag{3.15}$$

note that there is no uniqueness of solutions, e.g. $V = 0$ is always a solution. In [3] is discussed the appropriate selection criterion, that is V is the maximal solution to (3.15).

If the system is in equilibrium then the quasi-potential V coincides with the variation of the equilibrium free energy associated with the profile ρ. The latter can be characterized, by the Einstein fluctuation formula, as the rate of the asymptotic probability of observing a given density profile in the equilibrium measure. Namely, if μ_N is the invariant measure of the generator L_N, then

$$\mu_N(\pi^N \approx \rho) \sim \exp\{-N^d V(\rho)\}. \tag{3.16}$$

This relation holds also for non-equilibrium systems, see [3, 16], and, in this sense, the solution to the variational problem (3.14) is the appropriate generalization of the free energy for non-equilibrium systems. Finally, as discussed in [3], for *generic* non-equilibrium models the quasi-potential V is a *non-local* functional of ρ. Notable exceptions are the zero-range model and the case, discussed in section 3.4, of systems with weak external field and periodic boundary conditions. We next recall some results on the quasi-potential for specific lattice gases.

Zero-range process. We consider the zero-range process as introduced in section 2.2 either in the torus or in a bounded domain with a weak external field E. Recalling (2.19) and (2.20), we define the function $\Phi : \mathbb{R}_+ \to \mathbb{R}_+$ as the activity corresponding to the density α, i.e. such that

$$\alpha = \frac{1}{Z(\Phi(\alpha))} \sum_{k=0}^{\infty} k \frac{\Phi(\alpha)^k}{g(k)!}, \tag{3.17}$$

where $Z(\varphi)$ is defined in (2.20). In other words $\alpha \mapsto \Phi(\alpha)$ is the inverse of the function $\varphi \mapsto R(\varphi)$ defined by

$$R(\varphi) = \varphi \frac{Z'(\varphi)}{Z(\varphi)}. \tag{3.18}$$

As shown in [2, 3, 17, 39], the hydrodynamic equation for the zero-range process is then (3.9) with $D = \Phi'$ and $\chi = \Phi$. In the case of independent random walks, i.e. $g(k) = k$, Φ is the identity so that $D = 1$ and $\chi(\rho) = \rho$.

Since for the zero-range process, as discussed in section 2.2, the invariant measure is always a product measure, the quasi-potential V is a local functional. Its form can be computed directly from the invariant measure by requiring that (3.16) holds. On the other hand, it is also possible to solve explicitly the Hamilton–Jacobi equation (3.15). As shown in [2, 3] we get

$$V(\rho) = \int_\Lambda \mathrm{d}u \left[\rho(u) \log \frac{\Phi(\rho(u))}{\bar{\varphi}(u)} - \log \frac{Z(\Phi(\rho(u)))}{Z(\bar{\varphi}(u))}\right], \tag{3.19}$$

where $\bar{\varphi}(u) = \Phi(\bar{\rho}(u))$ is the stationary activity profile, $\bar{\rho}$ being the stationary solution to (3.9), i.e. the stationary density profile. Equivalently $\bar{\varphi}$ solves

$$\begin{cases} \frac{1}{2}\Delta\bar{\varphi} - \nabla \cdot (\bar{\varphi} E) = 0 & u \in \Lambda \\ \bar{\varphi}(u) = \exp\{\lambda_0(u)\} & u \in \partial\Lambda \end{cases} \tag{3.20}$$

which, recalling (2.9), is just the continuous limit of (2.18).

Boundary-driven symmetric exclusion process. We consider here the one-dimensional symmetric exclusion process as introduced in section 2.3 with $\Lambda = (0, 1)$. Let ρ_0 and ρ_1 be the boundary densities. As shown in [3, 26, 27], the hydrodynamic equation is (3.9) with $D = 1$ and $\chi(\rho) = \rho(1-\rho)$. For this model, if $\rho_0 \neq \rho_1$ the quasi-potential is non-local, which is the signature of macroscopic long range correlations. The quasi-potential cannot be written in a closed form, but can be obtained by solving a one-dimensional boundary value problem. This has been proven in [19, 20] by combinatorial methods and in [3, 4] by the dynamical/variational approach presented here. The result is the following:

$$V(\rho) = \sup_f \int_0^1 \mathrm{d}u \left[\rho \log \frac{\rho}{f} + (1-\rho) \log \frac{1-\rho}{1-f} + \log \frac{f'}{\rho_1 - \rho_0}\right], \tag{3.21}$$

where the supremum is carried out over all strictly monotone smooth functions f satisfying the boundary conditions $f(0) = \rho_0$, $f(1) = \rho_1$. It has also been shown that there exists a unique maximizer for the variational problem (3.21) which is the unique strictly monotone solution to the nonlinear boundary value problem

$$\begin{aligned} & f(1-f)\frac{f''}{(f')^2} + f = \rho \\ & f(0) = \rho_0, \qquad f(1) = \rho_1 \end{aligned} \tag{3.22}$$

in which $\rho = \rho(u)$ is the prescribed fluctuation. Knowing that (3.21) is the answer, the proof amounts to some lengthy but straightforward computations in showing that it solves the Hamilton–Jacobi equation (3.15), see [4] for the details. From (3.21), since V is expressed as the supremum of convex functionals we get 'for free' that V is a convex functional. However, as shown below, this convexity property does not hold in general.

Variational formulae like (3.21) are typical in statistical mechanics, but here the interpretation of it is rather unclear. Firstly it appears strange that we need to maximize and not to minimize, secondly the meaning of the test function f is not apparent.

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For the second issue we mention that a dynamical interpretation of f in terms of the hydrodynamics of the time-reversed process is discussed in [3]. For the first issue we shall show that it is connected with the convexity properties of the mobility χ.

We mention that an expression similar to (3.21) has also been obtained for the boundary-driven weakly asymmetric exclusion process in [25]. Also the Hamilton–Jacobi approach can be applied successfully, see [11].

Boundary-driven KMP process. We consider here the KMP process introduced in section 2.4. The hydrodynamic equation is (3.9) with $D = 1$ and $\chi(\rho) = \rho^2$. Note that here ρ is the energy density and not the particle density as for lattice gases. Similarly to the boundary-driven symmetric exclusion process, as shown in [12], the quasi-potential can be obtained by solving a one-dimensional boundary value problem. The result is the following:

$$V(\rho) = \inf_f \mathcal{G}(\rho, f), \tag{3.23}$$

where

$$\mathcal{G}(\rho, f) = \int_0^1 \mathrm{d}u \left[\frac{\rho}{f} - 1 - \log \frac{\rho}{f} - \log \frac{f'}{T_1 - T_0} \right], \tag{3.24}$$

and the infimum is carried out over all strictly monotone smooth functions f satisfying the boundary conditions $f(0) = T_0$, $f(1) = T_1$. It has also been shown that there exists a unique minimizer for the variational problem (3.23) which is the unique strictly monotone solution to the nonlinear boundary value problem

$$\begin{aligned} & f^2 \frac{f''}{(f')^2} - f = -\rho \\ & f(0) = T_0, \qquad f(1) = T_1 \end{aligned} \tag{3.25}$$

in which $\rho = \rho(u)$ is the prescribed fluctuation. As for the boundary-driven symmetric exclusion process, knowing that (3.23) is the answer, the proof amounts to some lengthy but straightforward computations in showing that it solves the Hamilton–Jacobi equation (3.15). Unlike the boundary-driven symmetric exclusion process, the quasi-potential for the KMP process is not convex.

A possible interpretation of (3.23) is the following. The local functional $\mathcal{G}(\rho, f)$ can be thought of as a joint rate functional for both the energy density ρ and the function f, which we can interpreted as a temperature profile. Then the minimization procedure of (3.23) corresponds to the application of a contraction principle. We therefore search for the best hidden temperature profile f associated to the energy density profile ρ. This is the inspiring idea behind the following toy model for the invariant measure.

We will show that the functional V in (3.23) is the large deviations rate functional of a measure on $\mathbb{R}_+^{\Lambda_N}$ which is 'simple' enough to be described explicitly and 'rich' enough to produce such a non-local rate functional. Recall that in section 2.4 we have obtained an explicit representation of the invariant measure of the KMP process with a single oscillator as a convex combination of exponential distributions.

We assume $T_0 \le T_1$ and let $t_1, \dots, t_{N-1}$ be independent uniform random variables on the interval $[T_0, T_1]$. Denote $t_{[1]} \le t_{[2]} \le \cdots \le t_{[N-1]}$ be order statistics of $t_1, \dots, t_{N-1}$,

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i.e. $t_{[1]}$ is the smallest among the t_i, $t_{[2]}$ the second smallest and so on. Denote by ϱ_N, the distribution of the random vector $t_{[1]}, \ldots, t_{[N-1]}$; note that ϱ_N is a probability on $[T_0, T_1]^{N-1}$. We then define ν_N as the probability measure on $\mathbb{R}_+^{\Lambda_N}$ whose density w.r.t. the Lebesgue measure $\mathrm{d}\xi = \prod_{x\in\Lambda_N} \mathrm{d}\xi_x$ is given by

$$\frac{\mathrm{d}\nu_N}{\mathrm{d}\xi} = \int \varrho_N(\mathrm{d}t_1, \ldots, \mathrm{d}t_{N-1}) \prod_{x\in\Lambda_N} \frac{1}{t_x} \exp\{-\xi_x/t_x\}. \tag{3.26}$$

That is, ν_N is a mixture of the exponential Gibbs distribution with temperature profile $T(x/N) = t_x$. The measure ν_N is not the invariant measure of the KMP process; if we compare (3.26) for a single oscillator, $N = 2$, with the exact expression in (2.32) we see that we replaced the arcsine distribution in $[T_0, T_1]$ with the uniform one. As N diverges, the measure ν_N is, however, a good approximation of the true invariant measure in the sense that it leads the rate function in (3.23). In particular it has the correct asymptotic form of the two-point correlations.

To prove the above statement, let us consider the probability measure $\tilde{\nu}_N$ on the space $\mathbb{R}_+^{\Lambda_N} \times [T_0, T_1]^{\Lambda_N}$ given by

$$\tilde{\nu}_N(\mathrm{d}\xi, \mathrm{d}t) = \varrho_N(\mathrm{d}t) \prod_{x\in\Lambda_N} \frac{1}{t_x} \exp\{-\xi_x/t_x\}\, \mathrm{d}\xi_x \tag{3.27}$$

so that ν_N in (3.26) is obtained as the first marginal of $\tilde{\nu}_N$, i.e. integrating on the second variable t. Recalling the definition (3.6) of the empirical density π^N, we likewise define the empirical temperature profile τ^N by requiring that for each smooth function G on $\Lambda\langle\tau^N, G\rangle = (1/N)\sum_{x\in\Lambda_N} G(x/N) t_x$. Given a smooth function $\rho : \Lambda \to \mathbb{R}_+$ and a smooth strictly increasing function $f : \Lambda \to [T_0, T_1]$ such that $f(0) = T_0$ and $f(1) = T_1$, we claim that

$$\tilde{\nu}_N(\pi^N \approx \rho, \tau^N \approx f) \sim \exp\{-N\mathcal{G}(\rho, f)\}, \tag{3.28}$$

where $\mathcal{G}$ was defined in (3.24). To obtain this result, we first observe that if $e_1, \ldots, e_N$ are N independent exponential random variables with parameter T, then

$$\mathbb{P}\left(\frac{1}{N}\sum_{i=1}^N e_i \approx \alpha\right) \sim \exp\{-N[\alpha/T - 1 - \log(\alpha/T)]\}.$$

We also recall, see, for example, [28, I.6], that the random variables $\Delta_1 := t_{[1]} - T_0, \Delta_2 := t_{[2]} - t_{[1]}, \ldots, \Delta_N := T_1 - t_{[N-1]}$ are distributed according to the product of N exponentials *conditioned* on $\Delta_1 + \cdots + \Delta_N = T_1 - T_0$. We then get

$$\varrho_N(\tau^N \approx f) \sim \exp\left\{-N\int_0^1 \mathrm{d}u\left[-\log\frac{f'(u)}{T_1 - T_0}\right]\right\}.$$

Since, conditionally on the random variables $t_{[x]}$, $x \in \Lambda_N$, the distribution of ξ is the product of exponentials, (3.28) follows. Finally, from (3.28), by maximizing over the possible values of f, we easily get that

$$\nu_N(\pi^N \approx \rho) \sim \exp\left\{-N \inf_f \mathcal{G}(\rho, f)\right\}. \tag{3.29}$$

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3.3. Macroscopic correlation functions

In sections 2.3 and 2.4 we found exact formulae for the two-point correlation functions $C_N(x,y) = \mu_N(\eta_x;\eta_y)$ of the invariant measure μ_N, both for the one-dimensional boundary-driven symmetric exclusion process, see (2.27), and for the boundary-driven KMP process, see (2.38). For both models we found that, out of equilibrium, they admit long range correlations of order $1/N$. More precisely we have

$$C_N(x,y) = \frac{1}{N} C\left(\frac{x}{N}, \frac{y}{N}\right) + \mathrm{O}\left(\frac{1}{N^2}\right),$$

with

$$C(u,v) = C(v,u) = -(\rho_1 - \rho_0)^2 u(1-v), \qquad 0 \le u < v \le 1 \tag{3.30}$$

for the boundary-driven symmetric exclusion process and

$$C(u,v) = C(v,u) = +(T_1 - T_0)^2 u(1-v), \qquad 0 \le u < v \le 1 \tag{3.31}$$

for the boundary-driven KMP process. Notice that the above functions (3.30) and (3.31) only differ by a sign. Moreover the off-diagonal part of the above covariance is proportional to the Green function of the Laplacian on the interval $[0,1]$ with Dirichlet boundary conditions

$$\Delta^{-1}(u,v) = \Delta^{-1}(v,u) = -u(1-v), \qquad 0 \le u \le v \le 1, \tag{3.32}$$

namely the solution to the problem $\partial_u^2 \Delta^{-1}(u,v) = \delta(u-v)$, $0 \le u, v \le 1$, with boundary condition $\Delta^{-1}(u,v) = 0$ if either u or v is 0 or 1.

In this section we will derive the above results from a purely macroscopic point of view. More precisely, we consider a one-dimensional boundary-driven system with $\Lambda = (0,1)$ and no external field and we assume that the transport coefficients in (3.9) are of the following form. The diffusion coefficient is constant, we set $D(\rho) = 1$ and $\chi(\rho)$ is quadratic so that χ'' is constant. We show that such models have positive, resp. negative, correlations if $\chi'' \ge 0$, resp. $\chi'' \le 0$.

Recall that the quasi-potential $V(\rho)$ solves the Hamilton–Jacobi equation (3.15), which in this context is

$$\left\langle \nabla \frac{\delta V}{\delta \rho}, \chi(\rho) \nabla \frac{\delta V}{\delta \rho} - \nabla \rho \right\rangle = 0. \tag{3.33}$$

The functional V assumes its minimum at $\bar\rho$, the stationary solution to (3.9), which in this case is a linear function. The correlation function $C(u,v)$, which measures the covariance of the density fluctuations with respect to the invariant measure, is then obtained in the quadratic approximation of V, i.e.

$$V(\rho) = \tfrac{1}{2}\langle(\rho - \bar\rho), C^{-1}(\rho - \bar\rho)\rangle + \mathrm{O}((\rho - \bar\rho)^3), \tag{3.34}$$

where C^{-1} denotes the inverse operator of C. We can therefore get an equation for $C(u,v)$ by expanding the Hamilton–Jacobi equation (3.33) up to second order in $(\rho - \bar\rho)$.

It is convenient to introduce the 'pressure' $G(h)$, see [3], defined as the Legendre transform of the quasi-potential $V(\rho)$,

$$G(h) = \sup_\rho \{\langle h, \rho\rangle - V(\rho)\}.$$

Here $h = h(u)$ can be interpreted as a chemical potential profile. By Legendre duality, equation (3.33) can be rewritten as the following Hamilton–Jacobi equation for the pressure,

$$\left\langle \nabla h, \chi\left(\frac{\delta G}{\delta h}\right)\nabla h - \nabla\frac{\delta G}{\delta h}\right\rangle = 0 \tag{3.35}$$

for any h which satisfies the boundary conditions $h(0) = h(1) = 0$. Moreover the expansion (3.34) gets translated into the following expansion for G,

$$G(h) = \langle h, \bar\rho\rangle + \tfrac{1}{2}\langle h, Ch\rangle + \mathrm{O}(h^3). \tag{3.36}$$

Hence the macroscopic correlation function C can be obtained by expanding equation (3.35) up to second order in h.

From equation (3.36) we have

$$\frac{\delta G}{\delta h(u)} = \bar\rho(u) + (Ch)(u) + \mathrm{O}(h^2). \tag{3.37}$$

If we thus plug (3.37) into (3.35) and neglect the terms of order h^3 we get

$$\langle \nabla h, \chi(\bar\rho)\nabla h - \nabla Ch\rangle = 0 \tag{3.38}$$

for all chemical potential profiles h such that $h(0) = h(1) = 0$. To derive the above equation we used the fact that $\bar\rho$ is linear. The macroscopic correlation function C can then be determined as the solution to equation (3.38) satisfying the boundary condition $C(u, v) = 0$ if $u \neq v$ and either u or v is 0 or 1. This condition is due to the fact that the values of the density at the boundary is fixed by the reservoirs.

We next define the non-equilibrium contribution to the covariance as the function B such that

$$C(u, v) = \chi(\bar\rho(u))\delta(u - v) + B(u, v), \qquad u, v \in \Lambda. \tag{3.39}$$

Note that, since $D = 1$, $\chi(\bar\rho(u))$ is the local equilibrium variance. By plugging (3.39) into (3.38), we get that B solves

$$(\partial_u^2 + \partial_v^2)B(u, v) = -(\nabla\bar\rho)^2\chi''\delta(u - v) \tag{3.40}$$

together with the boundary condition $B(u, v) = 0$ if either u or v is 0 or 1. The above equation can also be derived within the fluctuating hydrodynamic theory, see [48]. Hence

$$B(u, v) = -\tfrac{1}{2}(\nabla\bar\rho)^2\chi''\Delta^{-1}(u, v)$$

which, by (3.32) and recalling that $\chi(\rho) = \rho(1-\rho)$ for the exclusion process and $\chi(\rho) = \rho^2$ for the KMP process, agrees with (3.30) and (3.31).

In [10] we derive the equation satisfied by the off-diagonal covariance B for arbitrary dimension, D, χ, and external field E. This equation allows us to establish, for a class of models, whether the correlations are positive or negative.

3.4. Weakly asymmetric models with periodic boundary conditions

We consider here a lattice gas with periodic boundary conditions, namely Λ is the d-dimensional torus, and constant weak external field E. As discussed in section 2.5, from a microscopic point of view, if the model is *gradient* then the invariant measure does not depend on the external field E. As we show here, from a macroscopic point of view, *any* system behaves as gradient models.

The precise statement is the following. Consider the variational problem (3.14) defining the quasi-potential V in the present setting of periodic boundary conditions and constant external field E. Then V does not depend on E and therefore coincides with the solution to (3.14) with $E = 0$, namely with the free energy associated with the microscopic Hamiltonian $\mathcal{H}$.

We suppose given the transport coefficients D and χ in (3.12)–(3.13) so that the Einstein relationship $D(\rho) = R(\rho)^{-1}\chi(\rho)$ holds; recall that, while D and χ are matrices, the compressibility R is a scalar. In the case of periodic boundary conditions and constant field E there is a one-parameter family of stationary solutions to (3.9) which are simply the constant functions $\bar\rho(u) = m$, $m \in \mathbb{R}_+$. Given $m \in \mathbb{R}_+$ we define

$$f_m(\rho) = \int_m^\rho \mathrm{d}r \int_m^r \mathrm{d}r' \, \frac{1}{R(r')}$$

which is a strictly convex function with minimum at $\rho = m$. We claim that the solution of the variational problem (3.14) with $\bar\rho = m$ is the functional

$$\mathcal{F}_m(\rho) = \int_\Lambda \mathrm{d}u \, f_m(\rho(u)) \tag{3.41}$$

for any value of the external field E.

If $E = 0$, by using the Einstein relation $D(\rho) = f_m''(\rho)\chi(\rho)$, it is easy to check that $\mathcal{F}_m$ solves the Hamilton–Jacobi (3.15). If E is a constant, since the boundary conditions are periodic, we have that

$$\left\langle \frac{\delta \mathcal{F}_m}{\delta\rho}, \nabla\cdot\chi(\rho)E \right\rangle = 0,$$

hence $\mathcal{F}_m$ solves the Hamilton–Jacobi (3.15) for any (constant) external field E. It is also not difficult to check that $\mathcal{F}_m$ is the maximal solution to the Hamilton–Jacobi equation (3.15) so that the claim is proven.

3.5. Glauber + Kawasaki

We consider here the macroscopic behaviour of the Glauber + Kawasaki process introduced in section 2.6. The empirical density is defined as in (3.6). We emphasize that in this model the empirical density is not locally conserved due to the reaction terms in the microscopic dynamic (2.48). Accordingly, the hydrodynamic equation is given by the reaction–diffusion equation

$$\partial_t\rho = \tfrac{1}{2}\Delta\rho + b(\rho) - d(\rho), \tag{3.42}$$

where the reaction terms b and d, which are polynomials in ρ, are determined by the rates $c_x(\eta)$ in (2.48) as follows [18, 35]:

$$b(\rho) = \nu_\rho(c_0(\eta)(1-\eta_0)), \qquad d(\rho) = \nu_\rho(c_0(\eta)\eta_0), \tag{3.43}$$

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where ν_ρ is the Bernoulli measure with density ρ. In particular, in the reversible case where the rates $c_x(\eta)$ are as in (2.52), $b(\rho)$ and $d(\rho)$ have the form

$$b(\rho) = A_1(1-\rho)\varphi(\rho), \qquad d(\rho) = A_2\rho\varphi(\rho), \tag{3.44}$$

where $\varphi(\rho)$ is the expected value of $h(\eta)$ in (2.52) with respect to ν_ρ and A_1, $A_2 \geq 0$. We consider this system only with periodic boundary conditions. The equilibrium profile thus corresponds to a constant density $\bar{\rho}$ which solves $b(\rho) = d(\rho)$ and gives an absolute minimum of the potential U, defined by $U'(\rho) = -[b(\rho) - d(\rho)]$.

The associated large deviation asymptotics is in the same form as in (3.11), but here the rate functional $I_{[0,T]}$ is not simply quadratic in the external field. Indeed, in [35] it is proven that it is given by

$$\begin{aligned} I_{[0,T]}(\hat{\rho}) = \int_0^T \mathrm{d}t\,\{ &\tfrac{1}{2}\langle \nabla H, \hat{\rho}(1-\hat{\rho})\nabla H\rangle \\ &+ \langle b(\hat{\rho}), (1 - \mathrm{e}^H + H\mathrm{e}^H)\rangle + \langle d(\hat{\rho}), (1 - \mathrm{e}^{-H} - H\mathrm{e}^{-H})\rangle\}, \end{aligned} \tag{3.45}$$

where the external potential H is connected to the fluctuation $\hat{\rho}$ by

$$\partial_t\hat{\rho} = \tfrac{1}{2}\Delta\hat{\rho} - \nabla\cdot(\hat{\rho}(1-\hat{\rho})\nabla H) + b(\hat{\rho})\mathrm{e}^H - d(\hat{\rho})\mathrm{e}^{-H}. \tag{3.46}$$

As in section 3.2 we analyse the variational problem (3.14). The associated Hamilton–Jacobi equation [1] is

$$\mathfrak{H}\left(\rho, \frac{\delta V}{\delta\rho}\right) = 0, \tag{3.47}$$

where the 'Hamiltonian' $\mathfrak{H}$ is not anymore quadratic in the momenta and it is given by

$$\mathfrak{H}(\rho, H) = \tfrac{1}{2}\langle H, \Delta\rho\rangle + \tfrac{1}{2}\langle \nabla H, \rho(1-\rho)\nabla H\rangle - \langle b(\rho), 1 - \mathrm{e}^H\rangle - \langle d(\rho), 1 - \mathrm{e}^{-H}\rangle. \tag{3.48}$$

If b and d are as in (3.44) it is easy to find the solution V of (3.47) [32]. Let $\bar{\rho} = A_1/(A_1 + A_2)$, the unique root of $b(\rho) - d(\rho) = 0$, then

$$V(\rho) = \int_0^1 \mathrm{d}u \left[\rho \log\frac{\rho}{\bar{\rho}} + (1-\rho)\log\frac{1-\rho}{1-\bar{\rho}}\right]. \tag{3.49}$$

If the reaction rates $c_x(\eta)$ are of the form (2.52), then the invariant measure is Bernoulli and (3.49) follows. On the other hand, as shown in [32], there are choices of the reaction rates such that (2.52) fails but (3.44) holds. In this case (3.49) still holds and we may say that reversibility is restored at the macroscopic level or that time-reversal invariance is violated 'weakly' by the microscopic dynamics.

Correlation functions. In section 3.3 we studied long range correlations for some boundary-driven (hence non-equilibrium) conservative models. Here we consider equilibrium states for the Glauber + Kawasaki dynamics, which is non-conservative, and we study their macroscopic correlation functions. In particular we show that, if the microscopic dynamics violates time-reversal invariance 'strongly', that is (3.44) does not hold, long range correlations do appear [1].

Recall that, in order for the system to be reversible, the rates $c_x(\eta)$ of the Glauber dynamics should be of the form (2.52). Their relationship with the coefficients $b(\rho)$ and $d(\rho)$ in (3.42) is given in (3.43).

Equation (3.47) is a very complicated functional derivative equation which, as in section 3.3, can be solved by successive approximations by formal power series expansion in $\rho - \bar{\rho}$. Here $\bar{\rho}$ is a constant stationary solution of (3.42), i.e. a root of $b(\rho) - d(\rho) = 0$.

Let C be the correlation function. It gives the second-order approximation of the quasi-potential as in (3.34). Proceeding as in section 3.3, see [1] for further details, we get that C solves

$$\tfrac{1}{2}\partial_u^2 C(u,v) - (d_1 - b_1)C(u,v) - \tfrac{1}{2}\bar{\rho}(1-\bar{\rho})\partial_u^2\delta(u-v) + b_0\delta(u-v) = 0, \tag{3.50}$$

where

$$b_1 = b'(\bar{\rho}), \qquad d_1 = d'(\bar{\rho}), \qquad b_0 = b(\bar{\rho}) = d(\bar{\rho}) = d_0.$$

Notice that, if (3.44) holds, we get

$$\gamma := b_0 - \bar{\rho}(1-\bar{\rho})(d_1 - b_1) = 0 \tag{3.51}$$

and in this case, recalling (3.49), we of course have $C(u,v) = \bar{\rho}(1-\bar{\rho})\,\delta(u-v)$. Conversely, a solution of the form $C(u,v) = \alpha\delta(u-v)$, for some $\alpha \geq 0$, exists only if (3.51) holds and therefore $\alpha = \bar{\rho}(1-\bar{\rho})$.

The above considerations imply that long range correlations do appear whenever (3.51) fails. In this case we say that irreversibility persists at the macroscopic level. As in section 3.3, we introduce the off-diagonal covariance B such that

$$C(u,v) = \bar{\rho}(1-\bar{\rho})\delta(u-v) + B(u,v)$$

and we get that B solves

$$-\tfrac{1}{2}\partial_u^2 B(u,v) + (d_1 - b_1)B(u,v) = \gamma\delta(u-v), \tag{3.52}$$

where γ is defined in (3.51). Note that $d_1 - b_1$, being the second derivative of the potential calculated in a minimum, is positive. Let $R = (d_1 - b_1 - (1/2)\,\Delta)^{-1}$ be the resolvent of the Laplacian on the torus. Then the solution of (3.52) is

$$B(u,v) = \gamma R(u,v). \tag{3.53}$$

Since $R(u,v) \geq 0$, we conclude that the correlation $B(u,v)$ has the same sign as γ.

While $\gamma = 0$ corresponds to the macroscopically reversible situation, in general γ may have either sign. For instance, given $\alpha \in (-1,1)$, take the flip rates given by

$$c_0(\eta) = \eta_0\left(1 - \alpha\frac{\eta_{-1}+\eta_1}{2}\right) + (1-\eta_0)\left(1 + \alpha\frac{\eta_{-1}+\eta_1}{2}\right)$$

for $\alpha > 0$ the presence of surrounding particles enhances the birth rate and suppresses the death rate. We thus expect that the two-point correlation to be positive for $\alpha > 0$ and negative for $\alpha < 0$. We have $\gamma = \alpha(1-\alpha)(2-\alpha)^{-2}$ which shows that this is indeed the case.

In [18] it is shown that fluctuations from the hydrodynamical equation with standard Gaussian normalization converge, as $N \to \infty$, to an Ornstein–Uhlenbeck process. The stationary correlations of this process agree, as they should, with (3.53).

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3.6. Boundary-driven asymmetric exclusion process

We start from the representation of the invariant measure for the boundary-driven totally asymmetric exclusion process obtained in [23] and illustrated in section 2.7. We call π^N the empirical measure associated with the configuration η, γ^N the empirical measure associated with ξ and $\mathcal{G}(\rho, f)$ the joint rate functional

$$\nu_N\left(\pi^N \approx \rho, \gamma^N \approx f\right) \sim \mathrm{e}^{-N\mathcal{G}(\rho,f)}, \tag{3.54}$$

where ν_N is the measure (2.56). From formula (2.57), using the contraction principle of large deviations, we obtain directly

$$\mu_N(\pi^N \approx \rho) \sim \mathrm{e}^{-NV(\rho)}, \tag{3.55}$$

where

$$V(\rho) = \inf_f \mathcal{G}(\rho, f). \tag{3.56}$$

This argument suggests a different representation, from the one obtained in [21], for the non-local rate functional $V(\rho)$. In particular, while in [21] $V(\rho)$ is obtained either as an infimum or a supremum, depending on the values of the chemical potentials λ_0 and λ_1, here we write $V(\rho)$ always as an infimum.

We construct explicitly this new representation in the special case $\lambda_0 = \lambda_1 = 0$. In this case the measure ν^N is uniform on the set of complete configurations, defined by (2.55), and the joint rate functional $\mathcal{G}$ is easily obtained as a restriction of the one associated to the uniform measure over all configurations $(\eta, \xi) \in X^{\Lambda_N} \times X^{\Lambda_N}$. We define the set of *complete profiles*

$$\mathcal{C} := \left\{(\rho, f) : \int_0^u \mathrm{d}v\, [\rho(v) + f(v)] \geq u, u \in [0,1]; \int_0^1 \mathrm{d}v\, [\rho(v) + f(v)] = 1\right\}.$$

Remember that ρ and f are density profiles for configurations of particles satisfying an exclusion rule so that they take values in $[0, 1]$. Then in the special case $\lambda_0 = \lambda_1 = 0$ we have

$$\mathcal{G}(\rho, f) = \begin{cases} \displaystyle\int_0^1 \mathrm{d}u[h(\rho) + h(f)] & \text{if } (\rho, f) \in \mathcal{C} \\ +\infty & \text{otherwise,} \end{cases} \tag{3.57}$$

where $h(x) = x \log(2x) + (1 - x) \log[2(1 - x)]$. Note that we do not need to add a normalization constant due to the fact that the constant profiles $\left(\frac{1}{2}, \frac{1}{2}\right)$ belong to $\mathcal{C}$ and $\mathcal{G}\left(\frac{1}{2}, \frac{1}{2}\right) = 0$. Using (3.56) we obtain the following variational representation for the quasi-potential V,

$$V(\rho) = \inf_{\{f:(\rho,f)\in\mathcal{C}\}} \int_0^1 \mathrm{d}u[h(\rho) + h(f)], \tag{3.58}$$

that has to be compared with the one in [21]

$$V(\rho) = \sup_{\{f:f(0)=1,f(1)=0\}} \int_0^1 \mathrm{d}u\, \{\rho \log[\rho(1 - f)] + (1 - \rho) \log[(1 - \rho)f] + \log 4\}, \tag{3.59}$$

where the supremum is over monotone functions.

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In [21] it is shown that the supremum in (3.59) is obtained when $f = F'_\rho$ and

$$F_\rho(u) = \mathrm{CE}\left(\int_0^u \mathrm{d}v\,[1-\rho(v)]\right),$$

where CE means *concave envelope*. We will show next that F'_ρ is also the minimizer of the problem (3.58). This is equivalent to proving that

$$\inf_{\{F:(\rho,F')\in\mathcal{C}\}} \int_0^1 \mathrm{d}u\, h(F'(u)) = \int_0^1 \mathrm{d}u\, h(F'_\rho(u)). \tag{3.60}$$

Note that F' has to be a density profile so that F is increasing. Moreover F is defined up to an additive constant so we can choose $F(0) = 0$. The condition $(\rho, F') \in \mathcal{C}$ is easily seen as

$$F(0) = 0, \qquad F(u) \geq \int_0^u \mathrm{d}v[1-\rho(v)]\,\forall u \in [0,1], \qquad F(1) = \int_0^1 \mathrm{d}v\,[1-\rho(v)]. \tag{3.61}$$

It is clear that, if F satisfies condition (3.61), then also $\mathrm{CE}(F)$ satisfies (3.61); or, equivalently, if $(\rho, F') \in \mathcal{C}$ then also $(\rho, \mathrm{CE}(F)') \in \mathcal{C}$. Moreover the following elementary inequality holds due to the convexity of h:

$$\int_a^b \mathrm{d}u\, h(F'(u)) \geq (b-a)h\left(\frac{F(b)-F(a)}{b-a}\right) \tag{3.62}$$

which immediately implies

$$\int_0^1 \mathrm{d}u\, h(F'(u)) \geq \int_0^1 \mathrm{d}u\, h([\mathrm{CE}(F)]'(u)).$$

We thus conclude that we can restrict the infimum (3.60) over the set of concave functions F satisfying conditions (3.61). Still a direct application of (3.62) imposes that the minimizer has to be the smallest among them, that is F_ρ.

Using the above result we can finally prove the equivalence between the two different representations (3.58) and (3.59) of $V(\rho)$. In order to prove it we just have to show that, for any density profile ρ,

$$\int_0^1 \mathrm{d}u\{\rho \log(1-F'_\rho) + (1-\rho)\log F'_\rho\} = \int_0^1 \mathrm{d}u\,\{(1-F'_\rho)\log(1-F'_\rho) + F'_\rho \log F'_\rho\}. \tag{3.63}$$

The contributions on both sides in (3.63) from the domain of integration where $F'_\rho = 1-\rho$ are clearly equal. Consider now a maximal interval $[a,b]$ where $F'_\rho \neq 1-\rho$. Then on this interval we have

$$F'_\rho(u) = \frac{1}{b-a}\int_a^b \mathrm{d}v\,[1-\rho(v)], \qquad u \in [a,b].$$

From this fact, an easy computation shows that also the contributions on both sides of (3.63) from the integrations over $[a,b]$ are equal.

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