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Large deviation approach to non equilibrium processes in stochastic lattice gases

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Abstract. We present a review of recent work on the statistical mechanics of non equilibrium processes based on the analysis of large deviations properties of microscopic systems. Stochastic lattice gases are non trivial models of such phenomena and can be studied rigorously providing a source of challenging mathematical problems. In this way, some principles of wide validity have been obtained leading to interesting physical consequences.

Keywords: interacting particle systems, large deviations, hydrodynamic limit.

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1 A Physicist motivation

In equilibrium statistical mechanics there is a well defined relationship, established by Boltzmann, between the probability of a state and its entropy. This fact was exploited by Einstein to study thermodynamic fluctuations. So far it does not exist a theory of irreversible processes of the same generality as equilibrium statistical mechanics and presumably it cannot exist. While in equilibrium the Gibbs distribution provides all the information and no equation of motion has to be solved, the dynamics plays the major role in non equilibrium.

When we are out of equilibrium, for example in a stationary state of a system in contact with two reservoirs, even if the system is in a local equilibrium state so that it is possible to define the local thermodynamic variables e.g. density or magnetization, it is not completely clear how to define the thermodynamic potentials like the entropy or the free energy. One possibility, adopting the Boltzmann-Einstein point of view, is to use fluctuation theory to define their non equilibrium

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analogs. In fact, in this way extensive functionals can be obtained although not necessarily simply additive due to the presence of long range correlations which seem to be a rather generic feature of non equilibrium systems.

Let us recall the Boltzmann-Einstein theory of equilibrium thermodynamic fluctuations. The main principle is that the probability of a fluctuation in a macroscopic region of fixed volume V is

$$P \propto \exp\{V \Delta S/k\} \tag{1.1}$$

where ΔS is the variation of the specific entropy calculated along a reversible transformation creating the fluctuation and k is the Boltzmann constant. Eq. (1.1) was derived by Einstein simply by inverting the Boltzmann relationship between entropy and probability. He considered (1.1) as a phenomenological definition of the probability of a state. Einstein theory refers to fluctuations for equilibrium states, that is for systems isolated or in contact with reservoirs characterized by the same chemical potentials. When in contact with reservoirs ΔS is the variation of the total entropy (system + reservoirs) which for fluctuations of constant volume and temperature is equal to $-\Delta \mathcal{F}/T$, that is minus the variation of the free energy of the system divided by the temperature.

We consider a stationary non-equilibrium state (SNS), namely, due to external fields and/or different chemical potentials at the boundaries, there is a flow of physical quantities, such as heat, electric charge, chemical substances, across the system. To start with, it is not always clear that a closed macroscopic dynamical description is possible. If the system can be described by a hydrodynamic equation, a fact which can be rigorously established in stochastic lattice gases, a reasonable goal is to find an explicit connection between the thermodynamic potentials and the dynamical macroscopic properties like transport coefficients. The study of large fluctuations provides such a connection.

Besides the definition of thermodynamic potentials, in a dynamical setting a typical question one may ask is the following: what is the most probable trajectory followed by the system in the spontaneous emergence of a fluctuation or in its relaxation to an equilibrium or a stationary state? To answer this question one first derives a generalization of the Boltzmann-Einstein formula from which the most probable trajectory can be calculated by solving a variational principle. For equilibrium states and small fluctuations an answer to this type of questions was given by Onsager and Machlup in 1953 [24]. The Onsager-Machlup theory gives the following result under the assumption of time reversibility of the microscopic dynamics: the most probable creation and relaxation trajectories of a fluctuation are one the time reversal of the other.

We discuss this issue in the context of stochastic lattice gases in a box of linear size N with birth and death process at the boundary modeling the reservoirs. We consider the case when there is only one thermodynamic variable, the local density denoted by ρ. Its macroscopic evolution is given by the continuity equation

$$\partial_t \rho \;=\; \nabla \cdot \Big[D(\rho)\nabla\rho - \chi(\rho)E \Big] \;=\; -\nabla \cdot J(\rho) \tag{1.2}$$

where $D(\rho)$ is the diffusion matrix, $\chi(\rho)$ the mobility and E the external field. Here $J(\rho)$ is the macroscopic instantaneous current associated to the density profile ρ. Finally the interaction with the reservoirs appears as boundary conditions to be imposed on solutions of (1.2). We shall denote by u the macroscopic space coordinate and by $\bar\rho = \bar\rho(u)$ the unique stationary solution of (1.2), i.e. $\bar\rho$ is the typical density profile for the SNS.

This equation derives from the underlying stochastic dynamics through an appropriate scaling limit in which the microscopic time and space coordinates are rescaled diffusively. The hydrodynamic equation (1.2) thus represents the law of large numbers for the empirical density of the stochastic lattice gas. The convergence has to be understood in probability with respect to the law of the stochastic lattice gas. Finally, the initial condition for (1.2) depends on the initial distribution of particles. Of course many microscopic configurations give rise to the same initial condition $\rho_0(u)$.

Let us denote by ν^N the invariant measure of the stochastic lattice gas. The free energy $\mathcal{F}(\rho)$, defined as a functional of the density profile $\rho = \rho(u)$, gives the asymptotic probability of fluctuations of the empirical measure π^N under the invariant measure ν^N. More precisely

$$\nu^N\big(\pi^N \approx \rho\big) \sim \exp\big\{ - N^d \mathcal{F}(\rho) \big\} \tag{1.3}$$

where d is the dimensionality of the system, $\pi^N \approx \rho$ means closeness in the weak topology and $\sim$ denotes logarithmic equivalence as $N \to \infty$. In the above formula we omitted the dependence on the temperature since it does not play any role in our analysis; we also normalized $\mathcal{F}$ so that $\mathcal{F}(\bar\rho) = 0$.

In the same way, the behavior of space time fluctuations can be described as follows. Let us denote by $\mathbb{P}_{\nu^N}$ the stationary process of the stochastic lattice gas, i.e. the initial distribution is given by the invariant measure ν^N. The probability that the evolution of the random variable π^N_t deviates from the solution of the hydrodynamic equation and is close to some trajectory $\hat\rho_t$ is exponentially small and of the form

$$\mathbb{P}_{\nu^N}\big(\pi^N_t \approx \hat\rho_t,\ t \in [t_1, t_2]\big) \sim \exp\big\{ - N^d \big[\mathcal{F}(\hat\rho_{t_1}) + I_{[t_1,t_2]}(\hat\rho) \big] \big\} \tag{1.4}$$

where $I(\hat{\rho})$ is a functional which vanishes if $\hat{\rho}_t$ is a solution of (1.2) and $\mathcal{F}(\hat{\rho}_{t_1})$ is the free energy cost to produce the initial density profile $\hat{\rho}_{t_1}$. Therefore $I(\hat{\rho})$ represents the extra cost necessary to follow the trajectory $\hat{\rho}_t$ in the time interval $[t_1, t_2]$.

To determine the most probable trajectory followed by the system in the spontaneous creation of a fluctuation, we consider the following physical situation. The system is macroscopically in the stationary state $\bar{\rho}$ at $t = -\infty$ but at $t = 0$ we find it in the state ρ. According to (1.4) the most probable trajectory is the one that minimizes I among all trajectories $\hat{\rho}_t$ connecting $\bar{\rho}$ to ρ in the time interval $[-\infty, 0]$, that is the optimal path for the variational problem

$$V(\rho) = \inf_{\hat{\rho}} I_{[-\infty,0]}(\hat{\rho}) \tag{1.5}$$

The functional $V(\rho)$, called the quasi-potential, measures the probability of the fluctuation ρ. Moreover, the optimal trajectory for (1.5) determines the path followed by the system in the creation of the fluctuation ρ. As shown in [1, 2, 10] this minimization problem gives the non equilibrium free energy, i.e. $V = \mathcal{F}$. As we discuss here, by analyzing this variational problem for SNS, the Onsager-Machlup relationship has to be modified in the following way: the spontaneous emergence of a macroscopic fluctuation takes place most likely following a trajectory which can be characterized in terms of the time reversed process.

Beside the density, a very important observable is the current flux. This quantity gives informations that cannot be recovered from the density because from a density trajectory we can determine the current trajectory only up to a divergence free vector field. We emphasize that this is due to the loss of information in the passage from the microscopic level to the macroscopic one.

To discuss the current fluctuations in the context of stochastic lattice gases, we introduce the empirical current w^N which measures the local net flow of particles. As for the empirical density, it is possible to prove a dynamical large deviations principle for the empirical current which is informally stated as follow. Given a vector field $j : [0, T] \times \Lambda \to \mathbb{R}^d$, we have

$$\mathbb{P}_{\eta^N}\big(w^N \approx j(t, u)\big) \sim \exp\big\{ - N^d \, \mathcal{I}_{[0,T]}(j)\big\} \tag{1.6}$$

where $\mathbb{P}_{\eta^N}$ is the law of the stochastic lattice gas with initial condition given by $\eta^N = \{\eta^N_x\}$, which represents the number of particles in each site, and the rate functional is

$$\mathcal{I}_{[0,T]}(j) \;=\; \frac{1}{2}\int_0^T dt \,\big\langle \,[j - J(\rho)]\,,\, \chi(\rho)^{-1}\,[j - J(\rho)]\,\big\rangle \tag{1.7}$$

in which we recall that

$$J(\rho) = -D(\rho)\nabla\rho + \chi(\rho)E \ .$$

Moreover, $\rho = \rho(t, u)$ is obtained by solving the continuity equation $\partial_t \rho + \nabla \cdot j = 0$ with the initial condition $\rho(0) = \rho_0$ associated to η^N. The rate functional vanishes if $j = J(\rho)$, so that ρ solves (1.2). This is the law of large numbers for the observable w^N. Note that equation (1.7) can be interpreted, in analogy to the classical Ohm's law, as the total energy dissipated in the time interval $[0, T]$ by the extra current $j - J(\rho)$.

Among the many problems we can discuss within this theory, we study the fluctuations of the time average of the empirical current over a large time interval. We show that the probability of observing a time-averaged fluctuation J can be described by a functional $\Phi(J)$ which we characterize in terms of a variational problem for the functional $\mathcal{I}_{[0,T]}$

$$\Phi(J) = \lim_{T\to\infty} \inf_{j} \frac{1}{T} \mathcal{I}_{[0,T]}(j) \ , \tag{1.8}$$

where the infimum is carried over all paths $j = j(t, u)$ having time average J. We finally analyze the variational problem (1.8) for some stochastic lattice gas models and show that different scenarios take place. In particular, for the symmetric exclusion process with periodic boundary condition the optimal trajectory is constant in time. On the other hand for the KMP model [22], also with periodic boundary conditions, this is not the case: we show that a current path in the form of a traveling wave leads to a higher probability.

2 Boundary driven simple exclusion process

For an integer $N \geq 1$, let $\Lambda_N := \{1, \dots, N-1\}$. The sites of Λ_N are denoted by x, y, and z while the macroscopic space variable (points in the interval $[0, 1]$) by u. We introduce the microscopic state space as $\Sigma_N := \{0, 1\}^{\Lambda_N}$ which is endowed with the discrete topology; elements of Σ_N, called configurations, are denoted by η. In this way $\eta(x) \in \{0, 1\}$ stands for the number of particles at site x for the configuration η.

The one dimensional boundary driven simple exclusion process is the Markov process on the state space Σ_N with infinitesimal generator defined as follows.

Given $\alpha, \beta \in (0,1)$ we let

$$\begin{aligned}(L_N f)(\eta) \;&:=\; \frac{N^2}{2}\sum_{x=1}^{N-2}\big[f(\sigma^{x,x+1}\eta)-f(\eta)\big]\\ &+\; \frac{N^2}{2}\,[\alpha\{1-\eta(1)\}+(1-\alpha)\eta(1)]\big[f(\sigma^1\eta)-f(\eta)\big]\\ &+\; \frac{N^2}{2}\,[\beta\{1-\eta(N-1)\}+(1-\beta)\eta(N-1)]\big[f(\sigma^{N-1}\eta)-f(\eta)\big]\end{aligned}$$

for every function $f : \Sigma_N \to \mathbb{R}$. In this formula $\sigma^{x,y}\eta$ is the configuration obtained from η by exchanging the occupation variables $\eta(x)$ and $\eta(y)$:

$$(\sigma^{x,y}\eta)(z) \;:=\; \begin{cases}\eta(y) & \text{if } \; z=x\\ \eta(x) & \text{if } \; z=y\\ \eta(z) & \text{if } \; z\neq x,y\end{cases}$$

and $\sigma^x\eta$ is the configuration obtained from η by flipping the configuration at x:

$$(\sigma^x\eta)\,(z) \;:=\; \eta(z)[1-\delta_{x,z}] \;+\; \delta_{x,z}[1-\eta(z)]\;,$$

where $\delta_{x,y}$ is the Kronecker delta. The parameters α, β, which affect the birth and death rates at the two boundaries, represent the densities of the reservoirs. Without loss of generality, we assume $\alpha \le \beta$. Notice finally that L_N has been speeded up by N^2; this corresponds to the diffusive scaling.

The Markov process $\{\eta_t : t \ge 0\}$ associated to the generator L_N is irreducible. It has therefore a unique invariant measure, denoted by $\nu^N_{\alpha,\beta}$. The process is reversible if and only if $\alpha = \beta$, in which case $\nu^N_{\alpha,\alpha}$ is the Bernoulli product measure with density α

$$\nu^N_{\alpha,\alpha}\,\{\eta : \eta(x)=1\} \;=\; \alpha$$

for $1 \le x \le N-1$.

If $\alpha \neq \beta$ the process is not reversible and the measure $\nu^N_{\alpha,\beta}$ carries long range correlations. Since $E_{\nu^N_{\alpha,\beta}}[L_N\eta(x)] = 0$, it is not difficult to show that $\rho^N(x) = E_{\nu^N_{\alpha,\beta}}[\eta(x)]$ is the solution of the linear equation

$$\begin{cases}\Delta_N\rho^N(x) = 0\;, & 1\le x\le N-1\;,\\ \rho^N(0)=\alpha\;, & \rho^N(N)=\beta\;,\end{cases} \tag{2.1}$$

where Δ_N stands for the discrete Laplacian. Hence

$$\rho^N(x) = \alpha + \frac{x}{N}\,(\beta-\alpha) \tag{2.2}$$

Computing $L_N \eta(x)\eta(y)$, it is also possible to obtain a closed expression for the correlations

$$E_{\nu^N_{\alpha,\beta}}[\eta(x);\eta(y)] = E_{\nu^N_{\alpha,\beta}}[\eta(x)\eta(y)] - E_{\nu^N_{\alpha,\beta}}[\eta(x)]E_{\nu^N_{\alpha,\beta}}[\eta(y)]$$

As shown in [11, 25], for $1 \le x < y \le N-1$ we have

$$E_{\nu^N_{\alpha,\beta}}[\eta(x);\eta(y)] = -\frac{(\beta-\alpha)^2}{N-1}\,\frac{x}{N}\Big(1-\frac{y}{N}\Big) \tag{2.3}$$

Note that, if we take x, y at distance $O(N)$ from the boundary, then the covariance between $\eta(x)$ and $\eta(y)$ is of order $O(1/N)$. Moreover the random variables $\eta(x)$ and $\eta(y)$ are negatively correlated. This is the same qualitative behavior as the one in the canonical Gibbs measure given by the uniform measure on $\Sigma_{N,k} = \{\eta \in \Sigma_N : \sum_{x=1}^{N-1} \eta(x) = k\}$.

3 Stationary large deviations of the empirical density

Denote by $\mathcal{M}_+$ the space of positive measures on $[0,1]$ with total mass bounded by 1. We consider $\mathcal{M}_+$ endowed with the weak topology. For a configuration η in Σ_N, let π^N be the measure obtained by assigning mass N^{-1} to each particle and rescaling space by N^{-1}

$$\pi^N(\eta) \ := \ \frac{1}{N}\sum_{x=1}^{N-1} \eta(x)\,\delta_{x/N} \ ,$$

where δ_u stands for the Dirac measure concentrated on u. Denote by $\langle \pi^N, H\rangle$ the integral of a continuous function $H : [0,1] \to \mathbb{R}$ with respect to π^N

$$\langle \pi^N, H\rangle \ = \ \frac{1}{N}\sum_{x=1}^{N-1} H(x/N)\eta(x) \ .$$

We use the same notation for the inner product in $L_2([0,1], du)$. Analogously we denote the space integral of a function f by $\langle f\rangle = \int_0^1 du\ f(u)$.

The law of large numbers for the empirical density under the stationary state $\nu^N_{\alpha,\beta}$ is proven in [11, 16, 17].

Theorem 3.1. *For every continuous function $H : [0,1] \to \mathbb{R}$ and every $\delta > 0$,*

$$\lim_{N\to\infty} \nu^N_{\alpha,\beta}\Big\{ \Big|\langle \pi^N, H\rangle - \langle \bar\rho, H\rangle\Big| > \delta\Big\} \ = \ 0 \ ,$$

where

$$\bar{\rho}(u) = \alpha(1-u) + \beta u \,. \tag{3.1}$$

We remark that $\bar{\rho}$ is the solution of the elliptic linear equation

$$\begin{cases} \Delta\rho = 0 \,, \\ \rho(0) = \alpha \,, \quad \rho(1) = \beta \,, \end{cases}$$

which is the continuous analog of (2.1). Here and below Δ stands for the Laplacian.

Once a law of large numbers has been established, it is natural to consider the deviations around the typical value $\bar{\rho}$. From the explicit expression of the microscopic correlations (2.3) it is possible to prove a central limit theorem for the empirical density under the stationary measure $\nu^N_{\alpha,\beta}$. We refer to [25] for a more detailed discussion and to [19] for the mathematical details.

Fix a profile $\gamma : [0,1] \to [0,1]$ different from $\bar{\rho}$ and a neighborhood $V_\varepsilon(\gamma)$ of radius $\varepsilon > 0$ around the measure $\gamma(u)du$ in $\mathcal{M}_+$. The mathematical formulation of the Boltzmann-Einstein formula (1.1) consists in determining the exponential rate of decay, as $N \uparrow \infty$, of

$$\nu^N_{\alpha,\beta}\big\{\pi^N \in V_\varepsilon(\gamma)\big\} \,.$$

Derrida, Lebowitz and Speer [12, 13] derived, by explicit computations, the large deviations principle for the empirical density under the stationary state $\nu^N_{\alpha,\beta}$. This result has been obtained by a dynamical/variational approach in [2], a rigorous proof is given in [3]. The precise statement is the following.

Theorem 3.2. *For each profile $\gamma : [0,1] \to [0,1]$,*

$$\limsup_{\varepsilon\to 0} \limsup_{N\to\infty} \frac{1}{N} \log \nu^N_{\alpha,\beta}\big\{\pi^N \in V_\varepsilon(\gamma)\big\} \;\le\; -\mathcal{F}(\gamma) \,,$$

$$\liminf_{\varepsilon\to 0} \liminf_{N\to\infty} \frac{1}{N} \log \nu^N_{\alpha,\beta}\big\{\pi^N \in V_\varepsilon(\gamma)\big\} \;\ge\; -\mathcal{F}(\gamma) \,,$$

where

$$\begin{aligned} \mathcal{F}(\gamma) \;=\; \int_0^1 du \,\Big\{ & \gamma(u) \log \frac{\gamma(u)}{F(u)} \\ & + \; [1-\gamma(u)] \log \frac{1-\gamma(u)}{1-F(u)} + \log \frac{F'(u)}{\beta-\alpha} \Big\} \end{aligned} \tag{3.2}$$

and $F \in C^1([0,1])$ is the unique increasing solution of the non linear boundary value problem

$$\begin{cases} F'' = \big(\gamma - F\big) \dfrac{\big(F'\big)^2}{F(1-F)} \,, \\ F(0) = \alpha \,, \quad F(1) = \beta \,. \end{cases} \tag{3.3}$$

It is interesting to compare the large deviation properties of the stationary state $\nu^N_{\alpha,\beta}$ with the one of $\mu^N_{\alpha,\beta}$, the product measure on Σ_N which has the same marginals as $\nu^N_{\alpha,\beta}$, i.e.

$$\mu^N_{\alpha,\beta}\{\eta : \eta(x) = 1\} \; = \; \rho^N(x) \; ,$$

where ρ^N is given by (2.2). It is not difficult to show that in this case

$$\begin{aligned}
&\limsup_{\varepsilon\to 0}\limsup_{N\to\infty} \frac{1}{N} \log \mu^N_{\alpha,\beta}\big\{\pi^N \in V_\varepsilon(\gamma)\big\} \; \le \; -\mathcal{F}_0(\gamma) \; , \\
&\liminf_{\varepsilon\to 0}\liminf_{N\to\infty} \frac{1}{N} \log \mu^N_{\alpha,\beta}\big\{\pi^N \in V_\varepsilon(\gamma)\big\} \; \ge \; -\mathcal{F}_0(\gamma) \; ,
\end{aligned} \tag{3.4}$$

where

$$\mathcal{F}_0(\gamma) \; = \; \int_0^1 du \left\{\gamma(u) \log \frac{\gamma(u)}{\bar\rho(u)} \; + \; [1-\gamma(u)] \log \frac{1-\gamma(u)}{1-\bar\rho(u)}\right\} \tag{3.5}$$

and $\bar\rho$ is given in (3.1). Notice that the functional $\mathcal{F}_0$ is local while $\mathcal{F}$ is not. Moreover, it is not difficult to show [3, 13] that $\mathcal{F}_0 \le \mathcal{F}$. Therefore, fluctuations have less probability for the stationary state $\nu^N_{\alpha,\beta}$ than for the product measure $\mu^N_{\alpha,\beta}$. This bound reflects at the large deviations level the negative correlations observed in (2.3).

4 Diffusivity, Mobility and Einstein relation

The large deviation principle presented in the previous section holds for a general class of interacting particle systems. To state these results we introduce two thermodynamical quantities which describe the macroscopic time evolution of the system. To avoid an interminable sequence of definition, notation and assumptions, we will be vague in the description of the dynamics.

Consider a boundary driven interacting particle system evolving on E^{Λ_N}, where E is a subset of $\mathbb{Z}_+$, and having an hydrodynamic scaling limit with a diffusive rescaling. Assume that the total number of particles is the unique locally conserved quantity. For fixed parameters $0 \le \alpha \le \beta$, denote by $\nu^N_{\alpha,\beta}$ the unique stationary state whose density on the left (resp. right) boundary is α (resp. β).

For $0 \le x \le N-1$, denote by $Q_t^{x,x+1}$ the net flow of particles through the bond $\{x, x+1\}$ in the *microscopic* time interval $[0, t]$. This is the total number of particles which jumped from x to $x+1$ in the time interval $[0, t]$ minus the total number of particles which jumped from $x+1$ to x in the same time interval.

Microscopic means that time has not been rescaled. If $\alpha < \beta$, we expect $Q_t^{x,x+1}$ to be of order $tN^{-1}(\beta - \alpha)$, while for $\beta = \alpha$, we expect $(Q_t^{x,x+1})^2$ to be of order t.

Let $C(E)$ be the convex hull of E. The diffusivity $D : C(E) \to \mathbb{R}_+$ is defined by

$$D(\alpha) \;=\; \lim_{\beta \downarrow \alpha} \lim_{N\to\infty} \frac{N}{t(\alpha - \beta)} \, \mathbb{E}_{\nu^N_{\alpha,\beta}} \left[Q_t^{x,x+1} \right] ,$$

and the mobility $\chi : C(E) \to \mathbb{R}_+$ is defined by

$$\chi(\alpha) \;=\; \lim_{N\to\infty} \frac{1}{t} \, \mathbb{E}_{\nu^N_{\alpha,\alpha}} \left[(Q_t^{x,x+1})^2 \right] ,$$

The diffusivity and the mobility are related through the Einstein relation

$$D(\alpha) = \frac{1}{\sigma(\alpha)} \chi(\alpha) \;,$$

where $\sigma(\alpha)$ is the static compressibility given by

$$\sigma(\alpha) \;=\; \lim_{N\to\infty} \sum_{x\in\Lambda_N} E_{\nu^N_{\alpha,\alpha}} [\eta(x) ; \eta(N/2)] \;.$$

Below is a list of the diffusivity and the mobility of different models. Here $\Phi : \mathbb{R}_+ \to \mathbb{R}_+$ is a smooth strictly increasing function and $a : \mathbb{R}_+ \to \mathbb{R}_+$ is a smooth strictly positive function.

	$D(\alpha)$	$\chi(\alpha)$
Exclusion	1	$\alpha(1-\alpha)$
Zero-range	$\Phi'(\alpha)$	$\Phi(\alpha)$
Ginzburg-Landau	$a(\alpha)$	1
KMP	1	α^2

The law of large numbers for the empirical measure under the stationary state $\nu^N_{\alpha,\beta}$, presented in the previous section for the symmetric exclusion process, holds for a large class of models. It takes the following form. For every continuous function $H : [0,1] \to \mathbb{R}$, and every $\delta > 0$,

$$\lim_{N\to\infty} \nu^N_{\alpha,\beta} \left\{ \left| \langle \pi^N, H \rangle - \langle \bar\rho, H \rangle \right| > \delta \right\} \;=\; 0 \;,$$

where $\bar\rho$ is the unique weak solution of the elliptic equation

$$\begin{cases} \nabla [D(\rho)\nabla\rho] \;=\; 0 \;, \\ \rho(0) \;=\; \alpha \;, \quad \rho(1) \;=\; \beta \;. \end{cases} \tag{4.1}$$

A large deviations principle for the empirical measure under the equilibrium state $\nu^N_{\alpha,\alpha}$, similar to (3.4), also holds. The large deviations rate function $\mathcal{F}_0$ is given by

$$\mathcal{F}_0(\gamma) \;=\; \int_0^1 \big\{\gamma(u)R_\alpha(\gamma(u)) - \log Z_\alpha(R_\alpha(\gamma(u)))\big\}\,du\;,$$

where $R_\alpha : C(E) \to \mathbb{R}$ is given by

$$R_\alpha(\theta) \;=\; \int_\alpha^\theta \frac{1}{\sigma(u)}\,du \quad \text{and} \quad Z_\alpha(0) \;=\; 1\;, \quad \frac{Z'_\alpha(\theta)}{Z_\alpha(\theta)} \;=\; R_\alpha^{-1}(\theta)\;. \qquad (4.2)$$

In particular,

$$\frac{\delta\mathcal{F}_0(\gamma)}{\delta\gamma} \;=\; R_\alpha(\gamma(u))\;.$$

The stationary law of large numbers and the equilibrium large deviations can be proved in all dimensions, using, for example, the arguments of the following sections. In higher dimension, we consider particles evolving on $\Lambda_N \times \mathbb{T}_N^{d-1}$, where $\mathbb{T}_N^d$ is a discrete d-dimensional torus with N^d points and assume that the system is in contact at both extremities

$$\big\{x \in \Lambda_N \times \mathbb{T}_N^{d-1} : x_1 = 1\big\}\,,\;\big\{x \in \Lambda_N \times \mathbb{T}_N^{d-1} : x_1 = N-1\big\}$$

with infinite reservoirs at different densities.

The goal of the next sections is to prove a large deviations principle for the empirical measure under the stationary state $\nu^N_{\alpha,\beta}$ through a dynamical approach and to identify the rate function.

5 Hydrodynamics and dynamical large deviations of the density

We discuss the asymptotic behavior, as $N \to \infty$, of the evolution of the empirical density. Denote by $\{\eta^N_t : t \geq 0\}$ a Markov process introduced in the previous section, accelerated by a factor N^2, and let $\pi^N_t = \pi^N(\eta^N_t)$. Fix a profile $\gamma : [0,1] \to [0,1]$ and assume that π^N_0 converges to $\gamma(u)du$ as $N \uparrow \infty$. Observing the time evolution of the process, we expect π^N_t to relax to the stationary profile $\bar\rho(u)du$ according to some trajectory $\rho_t(u)du$. This result, stated in Theorem 5.1 below, is usually referred to as the hydrodynamic limit. It has been proved for the boundary driven simple exclusion process [16, 17], but the approach, based on the entropy method, can be adapted to the non-gradient models in any dimension.

Fix $T > 0$ and denote, respectively, by $D([0,T],\mathcal{M}_+)$, $D([0,T],\Sigma_N)$ the space of $\mathcal{M}_+$-valued, Σ_N-valued cadlag functions endowed with the Skorohod topology. For a configuration η^N in Σ_N, denote by $\mathbb{P}_{\eta^N}$ the probability on the path space $D([0,T],\Sigma_N)$ induced by the initial state η^N and the Markov dynamics.

Theorem 5.1. *Fix a profile $\gamma : [0,1] \to [0,1]$ and a sequence of configurations η^N such that $\pi^N(\eta^N)$ converges to $\gamma(u)du$, as $N \uparrow \infty$. Then, for each $t \geq 0$, π_t^N converges in $\mathbb{P}_{\eta^N}$-probability to $\rho_t(u)du$ as $N \uparrow \infty$. Here $\rho_t(u)$ is the solution of the parabolic equation*

$$\begin{cases} \partial_t \rho_t \;=\; (1/2)\nabla\left[D(\rho_t)\nabla\rho_t\right] \;, \\ \rho_0 \;=\; \gamma \;, \\ \rho_t(0) \;=\; \alpha \;, \quad \rho_t(1) = \beta \;. \end{cases} \tag{5.1}$$

In other words, for each $\delta, T > 0$ and each continuous function $H : [0,1] \to \mathbb{R}$ we have

$$\lim_{N\to\infty} \mathbb{P}_{\eta^N}\left(\sup_{t\in[0,T]} \left|\langle \pi_t^N, H\rangle - \langle \rho_t, H\rangle\right| > \delta \right) \;=\; 0 \;.$$

Equation (5.1) describes the relaxation path from γ to $\bar{\rho}$ since ρ_t converges to the stationary path $\bar{\rho}$ as $t \uparrow \infty$. To examine the fluctuations paths, we need first to describe the large deviations of the trajectories in a fixed time interval. This result requires some notation.

Fix a profile γ bounded away from 0 and 1: for some $\delta > 0$ we have $\delta \leq \gamma \leq 1-\delta$ du-a.e. Denote by C_γ the following subset of $D([0,T],\mathcal{M}_+)$. A trajectory π_t, $t \in [0,T]$ is in C_γ if it is continuous and, for any $t \in [0,T]$, we have $\pi_t(du) = \lambda_t(u)du$ for some density $\lambda_t(u) \in [0,1]$ which satisfies the boundary conditions $\lambda_0 = \gamma$, $\lambda_t(0) = \alpha$, $\lambda_t(1) = \beta$. The latter are to be understood in the sense that, for each $t \in [0,T]$,

$$\lim_{\delta\downarrow 0} \frac{1}{\delta} \int_0^\delta du\, \lambda_t(u) = \alpha \;, \qquad \lim_{\delta\downarrow 0} \frac{1}{\delta} \int_{1-\delta}^1 du\, \lambda_t(u) = \beta \;.$$

We define a functional $I_{[0,T]}(\cdot|\gamma)$ on $D([0,T],\mathcal{M}_+)$ by setting $I_{[0,T]}(\pi|\gamma) = +\infty$ if $\pi \notin C_\gamma$ and by a variational expression for $\pi \in C_\gamma$. Referring to [3, Eq. (2.4)–(2.5)] for the precise definition, here we note that if $\pi_t(du) = \lambda_t(u)du$ for some smooth density λ we have

$$I_{[0,T]}(\pi|\gamma) \;=\; \frac{1}{2}\int_0^T dt \int_0^1 du\, \chi(\lambda_t(u))\big[\nabla H_t(u)\big]^2 \;. \tag{5.2}$$

Here, χ is the mobility introduced in the previous section and H_t is the unique solution of

$$\partial_t \lambda_t = (1/2)\nabla[D(\lambda_t)\nabla\lambda_t] - \nabla\big[\chi(\lambda_t)\nabla H_t\big]\,, \tag{5.3}$$

with the boundary conditions $H_t(0) = H_t(1) = 0$ for any $t \in [0, T]$. As before, ∇ stands for $\frac{d}{du}$. Hence, to compute $I_{[0,T]}(\pi|\gamma)$, we first solve equation (5.3) in H and then plug it in (5.2).

The rate function $I_{[0,T]}$ should be understood as follows. Fix a smooth function $H : [0, T] \times [0, 1] \to \mathbb{R}$ vanishing at the boundary $u = 0$, $u = 1$. If particles where performing random walks with jump rates $(1/2) + N^{-1}(\nabla H)(t, x/N)$ to the right and $(1/2) - N^{-1}(\nabla H)(t, x/N)$ to the left, the hydrodynamic equation would be

$$\partial_t \lambda_t = (1/2)\nabla\big[D(\lambda_t)\nabla\lambda_t\big] - \nabla\big[\chi(\lambda_t)\nabla H_t\big] \,.$$

Thus, for λ_t fixed, one finds an external field H which turns λ a typical trajectory. To prove the large deviations principle, it remains to compute the cost for observing the trajectory λ, which is given by the relative entropy of the dynamics in which particles jump with rates $(1/2) \pm N^{-1}(\nabla H)(t, x/N)$ with respect to the original dynamics in which particles jump with constant rate $1/2$. It has been shown [14, 23] that this entropy is asymptotically equal to $I_{[0,T]}(\lambda)$.

The following theorem states the dynamical large deviation principle for boundary driven interacting particle systems. It has been proven in [3] for boundary driven symmetric exclusion processes by developing the techniques introduced in [14, 23].

Theorem 5.2. *Fix $T > 0$ and a profile γ bounded away from 0 and 1. Consider a sequence η^N of configurations associated to γ in the sense that $\pi^N(\eta^N)$ converges to $\gamma(u)du$ as $N \uparrow \infty$. Fix π in $D([0, T], \mathcal{M}_+)$ and a neighborhood $V_\varepsilon(\pi)$ of π of radius ε. Then*

$$\limsup_{\varepsilon\to 0}\limsup_{N\to\infty} \frac{1}{N}\log \mathbb{P}_{\eta^N}\big\{\pi^N \in V_\varepsilon(\pi)\big\} \;\le\; -I_{[0,T]}(\pi|\gamma) \;,$$

$$\liminf_{\varepsilon\to 0}\liminf_{N\to\infty} \frac{1}{N}\log \mathbb{P}_{\eta^N}\big\{\pi^N \in V_\varepsilon(\pi)\big\} \;\ge\; -I_{[0,T]}(\pi|\gamma) \;.$$

We may now formulate the following exit problem. Fix a profile γ and a path π such that $\pi_0 = \bar\rho\, du$, $\pi_T = \gamma\, du$. The functional $I_{[0,T]}(\pi|\bar\rho)$ measures the cost of observing the path π. Therefore,

$$\inf_{\pi_T = \gamma du} I_{[0,T]}(\pi|\bar\rho)$$

measures the cost of joining $\bar\rho$ to γ in the time interval $[0, T]$ and

$$V(\gamma) \;:=\; \inf_{T>0}\inf_{\pi_T=\gamma du} I_{[0,T]}(\pi|\bar\rho) \tag{5.4}$$

measures the cost of observing γ starting from the stationary profile $\bar{\rho}$. The functional V is called the quasi-potential.

The quasi-potential is the rate functional of the large deviations principle for the empirical density under the stationary state $\nu^N_{\alpha,\beta}$. This fact, expected to be generally true, establishes a relation between a purely dynamical functional, the quasi-potential, and a purely static functional, the large deviation rate function under the stationary state.

This result has been proved by Bodineau and Giacomin [10], in the sequel of the work of Bertini et al. [1, 2], adapting to the infinite dimensional setting the method introduced by Freidlin and Wentzell [18] in the context of small perturbations of dynamical systems. Bodineau and Giacomin proved for d-dimensional boundary driven symmetric simple exclusion processes the following theorem.

Theorem 5.3. *Let $I_{[0,T]}$ be the rate function in Theorem 5.2 and define the quasi-potential as in* (5.4)*. Then the empirical density under the stationary state satisfies a large deviation principle with rate functional given by the quasi-potential.*

The method of the proof applies to other particle systems provided one is able to show that the dynamical rate function $I_{[0,T]}$ is convex, lower semi-continuous and has compact level sets.

Theorem 5.3 is not totally satisfactory, as the large deviations rate function is given by a variational formula. There are two classes of boundary driven examples (illustrated respectively in section 6.4 and 6.5), however, where one can exhibit the path φ_t which solves (5.4) and derive an explicit description of the quasi-potential, as the one given in Theorem 3.2 for the boundary driven simple exclusion process. Both class of examples are one-dimensional and include the (also weakly asymmetric) simple exclusion process, the zero range processes, the Ginzburg-Landau processes and the KMP model [1, 7, 15].

6 Dynamical approach to stationary large deviations

In this section we characterize the optimal path for the variational problem (5.4) and derive an explicit formula for the quasi-potential for two classses of one-dimensional boundary-driven interacting particle systems. Unless explicitly stated, the arguments presented in this section hold for interacting particle systems under general assumptions. To simplify the notation, given a density path $\pi \in D([0,T]; \mathcal{M}_+)$ such that π_t is absolutely continuous with respect to the Lebesgue measure for each $t \in [0,T]$, $\pi_t(du) = \lambda_t(u)du$, we shall write $I_{[0,T]}(\lambda|\gamma)$ instead of $I_{[0,T]}(\pi|\gamma)$.

6.1 The reversible case

Let $\varphi_t(u)$ be the optimal path for the variational problem (5.4) on the interval $(-\infty, 0]$ instead of $[0, \infty)$. In the reversible case, $\alpha = \beta$, from Onsager-Machlup we expect that it is equal to the time reversal of the relaxation trajectory $\rho_t(u)$ solution of (5.1), $\varphi_t(u) = \rho_{-t}(u)$. We show that this is indeed the case.

The cost of the path φ is not difficult to compute. By definition of φ and by (5.1), $\partial_t \varphi_t = -(1/2)\nabla[D(\varphi_t)\nabla\varphi_t]$. In particular, if $\sigma(\cdot)$ stands for the static compressibility, $\nabla H_t = \sigma(\varphi_t)^{-1}\nabla\varphi_t$ solves (5.3) so that

$$I_{(-\infty,0]}(\varphi|\bar\rho) \;=\; \frac{1}{2}\int_{-\infty}^{0} dt \int_0^1 du\, \frac{D(\varphi_t)^2}{\chi(\varphi_t)}(\nabla\varphi_t)^2 \;\cdot$$

Recall from (4.2) the definition of R_α. Since $R'_\alpha = D/\chi$, we may rewrite the integrand as $D(\varphi_t)\nabla\varphi_t \times \nabla R_\alpha(\varphi_t)$. Since $R_\alpha(\alpha) = 0$ and since $\varphi(t, 0) = \varphi(t, 1) = \alpha$, we may integrate by parts in space to obtain that

$$I_{(-\infty,0]}(\varphi|\bar\rho) \;=\; -\frac{1}{2}\int_{-\infty}^{0} dt \int_0^1 du\, \nabla\,[D(\varphi_t)\nabla\varphi_t]\, R_\alpha(\varphi_t) \;\cdot$$

Since $\partial_t\varphi = -(1/2)\nabla[D(\varphi_t)\nabla\varphi_t]$, and since $\delta\mathcal{F}_0(\varphi)/\delta\varphi = R_\alpha(\varphi)$, the previous expression is equal to

$$\begin{aligned}
\int_{-\infty}^{0} dt \int_0^1 du\, \dot\varphi_t \frac{\delta\mathcal{F}_0(\varphi_t)}{\delta\varphi_t} \;&=\; \int_{-\infty}^{0} dt\, \frac{d}{dt}\mathcal{F}_0(\varphi_t) \\
&=\; \mathcal{F}_0(\varphi_0) - \mathcal{F}_0(\varphi_{-\infty}) \\
&=\; \mathcal{F}_0(\gamma)
\end{aligned}$$

because $\mathcal{F}_0(\bar\rho) = 0$. This proves that $V \le \mathcal{F}_0$.

The proof of Lemma 6.1 below, with $\nabla R_\alpha(\lambda_t)$ instead of $\nabla\{\delta W(\lambda_t)/\delta\lambda_t\}$, shows that the cost of any trajectory λ_t joining $\bar\rho$ to a profile γ in the time interval $[0, T]$ is greater or equal to $\mathcal{F}_0(\gamma)$:

$$I_{[0,T]}(\lambda|\bar\rho) \;\ge\; \mathcal{F}_0(\gamma)\;.$$

In particular, the trajectory φ is optimal and $V(\gamma) = \mathcal{F}_0(\gamma)$.

6.2 The Hamilton-Jacobi equation

We have seen in Subsection 6.1 that the optimal path for reversible systems is the relaxation path reversed in time. In the non reversible case, the problem is much more difficult and, in general, we do not expect to find the solution in a closed form. We first derive a Hamilton-Jacobi equation for the quasi-potential by interpreting the large deviation rate functional $I_{[0,T]}(\cdot|\bar{\rho})$ as an action functional

$$
\begin{aligned}
I_{[0,T]}(\lambda|\bar{\rho}) &= \frac{1}{2}\int_0^T dt \int_0^1 du\, \frac{1}{\chi(\lambda_t)} \Big\{\nabla^{-1}\big[\partial_t \lambda_t - (1/2)\nabla\{D(\lambda_t)\nabla\lambda_t\}\big]\Big\}^2 \\
&=: \int_0^T dt\, \mathcal{L}(\dot{\lambda}_t, \lambda_t)\ .
\end{aligned}
$$

The quasi-potential V may therefore be written as

$$
V(\gamma) = \inf_{T>0} \inf_{\substack{\lambda_0=\bar{\rho} \\ \lambda_T=\gamma}} \int_0^T dt\, \mathcal{L}(\dot{\lambda}_t, \lambda_t)\ . \tag{6.1}
$$

From this variational formula, taking the Legendre transform of the Lagrangian, we derive the Hamilton-Jacobi equation for the quasi-potential:

$$
\Big\langle \nabla \frac{\delta V(\gamma)}{\delta\gamma}, \chi(\gamma)\nabla\frac{\delta V(\gamma)}{\delta\gamma}\Big\rangle + \Big\langle \frac{\delta V(\gamma)}{\delta\gamma}, \nabla\{D(\gamma)\nabla\gamma\}\Big\rangle = 0 \tag{6.2}
$$

and $\delta V(\gamma)/\delta\gamma$ vanishes at the boundary.

One is tempted to solve the Hamilton-Jacobi to find the quasi-potential and then to look for a trajectory whose cost is given by the quasi-potential. The problem is not that simple, however, because the theory of infinite dimensional Hamilton-Jacobi equations is not well established. Moreover, it is well known that, even in finite dimension the solution may develop caustics in correspondence to the Lagrangian singularities of the unstable manifold associated to the stationary solution $\bar{\rho}$, see e.g. [20]. Finally, the Hamilton-Jacobi equation has more than one solution. In particular, even if one is able to exhibit a solution, one still needs to show that the candidate solves the variational problem (6.1).

The next lemma shows that a solution W of the Hamilton-Jacobi equation is always smaller or equal than the quasi-potential:

Lemma 6.1. *Let W be a solution of the Hamilton-Jacobi equation* (6.2)*. Then, $W(\gamma) - W(\bar{\rho}) \le V(\gamma)$ for all profiles γ.*

Sketch of the proof. Fix $T > 0$, a profile γ, and consider a path λ in $C_{\bar{\rho}}$ such that $\lambda_T = \gamma$. We need to show that

$$
I_{[0,T]}(\lambda|\bar{\rho}) \ \ge\ W(\gamma) - W(\bar{\rho})\,.
$$

The functional $I_{[0,T]}(\lambda|\bar\rho)$ can be rewritten as

$$\begin{aligned} &\frac{1}{2}\int_0^T dt \Big\langle \chi(\lambda_t)\Big\{\nabla H_t - \nabla\frac{\delta W(\lambda_t)}{\delta\lambda_t}\Big\}^2\Big\rangle \\ &+ \int_0^T dt \Big\langle \chi(\lambda_t)\,(\nabla H_t)\Big(\nabla\frac{\delta W(\lambda_t)}{\delta\lambda_t}\Big)\Big\rangle - \frac{1}{2}\int_0^T dt \Big\langle \chi(\lambda_t)\Big\{\nabla\frac{\delta W(\lambda_t)}{\delta\lambda_t}\Big\}^2\Big\rangle . \end{aligned} \tag{6.3}$$

Since $\delta W(\lambda_t)/\delta\lambda_t$ vanishes at the boundary, an integration by parts gives that the second integral is equal to

$$-\int_0^T dt \Big\langle \frac{\delta W(\lambda_t)}{\delta\lambda_t}, \nabla\big(\chi(\lambda_t)\nabla H_t\big)\Big\rangle .$$

Since W is a solution of the Hamilton-Jacobi equation, the third integral is equal to

$$\int_0^T dt \Big\langle \frac{\delta W(\lambda_t)}{\delta\lambda_t}, (1/2)\nabla\left\{D(\lambda_t)\nabla\lambda_t\right\}\Big\rangle .$$

Summing this two expressions and keeping in mind that H_t solves (5.3), we obtain that $I_{[0,T]}(\lambda|\bar\rho)$ is greater than or equal to

$$\int_0^T dt \Big\langle \frac{\delta W(\lambda_t)}{\delta\lambda_t}, \dot\lambda_t\Big\rangle \;=\; W(\lambda_T) - W(\lambda_0) \;=\; W(\gamma) - W(\bar\rho) .$$

This proves the lemma. □

To get an identity in the previous lemma, we need the first term in (6.3) to vanish. This corresponds to have $\nabla H_t = \nabla\delta V(\lambda_t)/\delta\lambda_t$, i.e. to find a path λ which is the solution of

$$\partial_t\lambda_t = (1/2)\nabla\left\{D(\lambda_t)\nabla\lambda_t\right\} - \nabla\Big\{\chi(\lambda_t)\nabla\frac{\delta V(\lambda_t)}{\delta\lambda_t}\Big\} .$$

Its time reversal $\psi_t = \lambda_{-t}$, $t\in[-T,0]$ solves

$$\begin{cases} \partial_t\psi_t \;=\; -(1/2)\nabla\left\{D(\psi_t)\nabla\psi_t\right\} + \nabla\Big\{\chi(\psi_t)\nabla\dfrac{\delta V(\psi_t)}{\delta\psi_t}\Big\} , \\ \psi_{-T} \;=\; \gamma , \\ \psi_t(0) \;=\; \alpha , \quad \psi_t(1) = \beta . \end{cases} \tag{6.4}$$

As we argue in the next subsection, equation (6.4) corresponds to the hydrodynamic limit of the empirical density under the time reversed dynamics; this is the Markov process on Σ_N whose generator is the adjoint to L_N in $L_2(\Sigma_N, \nu^N_{\alpha,\beta})$.

The next lemma shows that a weakly lower semi-continuous solution W of the Hamilton-Jacobi equation is an upper bound for the quasi-potential V if one can prove that the solution of (6.4) relax to the stationary profile $\bar{\rho}$.

Lemma 6.2. *Let W be a solution of the Hamilton-Jacobi equation* (6.2), *lower semi-continuous for the weak topology. Fix a profile γ. Let ψ_t be the solution of* (6.4) *with V replaced by W. If ψ_0 converges $\bar{\rho}$ for $T \uparrow \infty$, then $V(\gamma) \leq W(\gamma) - W(\bar{\rho})$.*

Sketch of the proof. To prove the lemma, given $\varepsilon > 0$, it is enough to find $T_\varepsilon > 0$ and a path φ_t such that

$$\varphi_0 = \bar{\rho}, \quad \varphi_{T_\varepsilon} = \gamma, \quad I_{[0,T_\varepsilon]}(\varphi|\bar{\rho}) \leq W(\gamma) - W(\bar{\rho}) + \varepsilon.$$

Fix $T > 0$ and let ψ_t be the solution of equation (6.4) in the time interval $[-T, -1]$ with initial condition $\psi_{-T} = \gamma$. Consider then an appropriate interpolation between ψ_{-1} and $\bar{\rho}$ which we again denote ψ_t, $t \in [-1, 0]$. Let $\varphi_t = \psi_{-t}$, which is defined in the time interval $[0, T]$. By definition of $I_{[0,T]}$,

$$I_{[0,T]}(\varphi|\bar{\rho}) = I_{[0,1]}(\varphi|\bar{\rho}) + I_{[1,T]}(\varphi|\psi_{-1}) .$$

Since ψ_{-1} converges to $\bar{\rho}$ as $T \uparrow \infty$, the first term can be made as small as we want by taking T large. The second one, by definition of ψ_t and by the computations performed in the proof of Lemma 6.1, is equal to $W(\gamma) - W(\psi_{-1})$. Since ψ_{-1} converges to $\bar{\rho}$ and since W is lower semi-continuous we have $W(\bar{\rho}) \leq \liminf_{T\to\infty} W(\psi_{-1})$. Hence

$$\limsup_{T\to\infty} I_{[0,T]}(\varphi|\bar{\rho}) \leq W(\gamma) - W(\bar{\rho}).$$

This proves the lemma. □

Putting together the two previous lemmata, we get the following statement.

Theorem 6.3. *Let W be a solution of the Hamilton-Jacobi equation, lower semi-continuous for the weak topology. Suppose that the solution ψ_t of* (6.4), *with V replaced by W, is such that ψ_0 converges to $\bar{\rho}$ as $T \uparrow \infty$ for any initial profile γ. Then $V(\gamma) = W(\gamma) - W(\bar{\rho})$. Moreover, $\varphi_t = \psi_{-t}$ is the optimal path for the variational problem* (6.1) *defined in the interval* $(-\infty, 0]$ *instead of* $[0, \infty)$.

6.3 Adjoint hydrodynamic equation

We have just seen that equation (6.4) plays an important role in the derivation of the quasi-potential. We show in this subsection that (6.4) describes in fact the evolution of the density profile under the adjoint dynamics.

Consider a diffusive interacting particle system η_t^N satisfying the following assumptions.

(H1) The limiting evolution of the empirical density is described by a differential equation

$$\partial_t \rho = \mathcal{D}(\rho) \ ,$$

where $\mathcal{D}$ is a differential operator. In the symmetric simple exclusion process $\mathcal{D}(\rho) = (1/2)\Delta\rho$.

(H2) Denote by $\xi_t^N = \eta_{-t}^N$ the time-reversed process. The limiting evolution of its empirical density is also described by a differential equation

$$\partial_t \rho = \mathcal{D}^*(\rho) \tag{6.5}$$

for some integro-differential operator $\mathcal{D}^*$.

(H3) The empirical densities satisfy a dynamical large deviations principle with rate functions

$$\frac{1}{2}\int_0^T dt \left\langle \frac{1}{\chi(\lambda_t)} \Big[\nabla^{-1}\big(\partial_t \lambda_t - \mathcal{D}^i(\lambda_t)\big) \Big]^2 \right\rangle, \quad i = 1, 2$$

where $\mathcal{D}^1 = \mathcal{D}$ and $\mathcal{D}^2 = \mathcal{D}^*$ for the original and the time-reversed processes, respectively.

Under assumptions (H1)-(H3), in [1, 2] it is shown that

$$\mathcal{D}(\rho) \ + \ \mathcal{D}^*(\rho) \ = \ \nabla\Big(\chi(\rho)\nabla\frac{\delta V}{\delta\rho}\Big) \ . \tag{6.6}$$

In this general context, equation (6.4) takes the form

$$\partial_t \rho \ = \ -\mathcal{D}(\rho) + \nabla\Big(\chi(\rho)\nabla\frac{\delta V}{\delta\rho}\Big) \ = \ \mathcal{D}^*(\rho) \ .$$

Therefore, under the above assumptions on the dynamics, the solution of (6.4) represents the hydrodynamic limit of the empirical density under the adjoint dynamics. In particular, the following principle extends the Onsager-Machlup theory to irreversible systems.

Principle: For non reversible systems, the typical path which creates a fluctuation is the time-reversed relaxation path of the adjoint dynamics.

6.4 Explicit formula for the quasi-potential if $\chi'(\alpha) = CD(\alpha)$

We obtain in this section a solution of the Hamilton-Jacobi equation which satisfies the assumption of Theorem 6.3 in the case where $\chi'(\alpha) = CD(\alpha)$ for some non-negative constant C. This class includes zero-range and Ginzburg-Landau processes. In these two cases the stationary state $\nu^N_{\alpha,\beta}$ is a product measure and a stationary large deviations principle for the empirical measure can be proved directly.

Theorem 6.4. *Assume that $\chi'(\alpha) = CD(\alpha)$ for some non-negative constant C. Then,*

$$V(\gamma) \;=\; \int_0^1 \gamma\big\{R_\alpha(\gamma) - R_\alpha(\bar\rho)\big\} - \log\frac{Z_\alpha(R_\alpha(\gamma))}{Z_\alpha(R_\alpha(\bar\rho))}\,.$$

Notice that in this case the quasi-potential is an additive function and corresponds to the rate function (3.5) (for the exclusion process) one would obtain if the stationary states $\nu^N_{\alpha,\beta}$ were product measures.

Proof. Denote by $W(\gamma)$ the right hand side of the previous formula. To show that W is equal to the quasi-potential, we just need to check the three assumptions of Theorem 6.3. We first show that W solves the Hamilton-Jacobi equation.

Assume that $C \neq 0$. The proof for $C = 0$ is similar. An elementary computation shows that $\{\delta W/\delta\gamma\} = R_\alpha(\gamma) - R_\alpha(\bar\rho)$. Since $R'_\alpha(\gamma) = D(\gamma)/\chi(\gamma) = C^{-1}\chi'(\gamma)/\chi(\gamma)$ and since $R_\alpha(\gamma) - R_\alpha(\bar\rho)$ vanishes at the boundary, an integration by parts show that the left hand side of (6.2) with W in place of V is equal to

$$\frac{1}{C^2}\Big\{\Big\langle\chi(\gamma)\Big\{\frac{\nabla\chi(\gamma)}{\chi(\gamma)} - \frac{\nabla\chi(\bar\rho)}{\chi(\bar\rho)}\Big\}^2\Big\rangle \;-\; \Big\langle\Big\{\frac{\nabla\chi(\gamma)}{\chi(\gamma)} - \frac{\nabla\chi(\bar\rho)}{\chi(\bar\rho)}\Big\}\nabla\chi(\gamma)\Big\rangle\Big\}$$

$$=\; -\frac{1}{C^2}\Big\langle\frac{[\nabla\chi(\gamma) - \nabla\chi(\bar\rho)]\nabla\chi(\bar\rho)}{\chi(\bar\rho)} + \frac{[\nabla\chi(\bar\rho)]^2}{\chi(\bar\rho)} - \frac{\chi(\gamma)[\nabla\chi(\bar\rho)]^2}{\chi(\bar\rho)^2}\Big\rangle\,.$$

Since γ and $\bar\rho$ take the same value at the boundary, we may integrate by parts the first term to get that the previous expression is equal to

$$\frac{1}{C^2}\Big\langle\{\chi(\gamma) - \chi(\bar\rho)\}\,\frac{\Delta\chi(\bar\rho)}{\chi(\bar\rho)}\Big\rangle\,.$$

The previous expression vanishes because $\Delta\chi(\bar\rho) = C\nabla[D(\bar\rho)\nabla\bar\rho] = 0$.

Since it is easy to check that W is lower-semicontinuous, it remains to show that the solutions of the adjoint hydrodynamic equation relax to the stationary state $\bar\rho$. Since $\{\delta W/\delta\gamma\} = R_\alpha(\gamma) - R_\alpha(\bar\rho)$, the adjoint hydrodynamic equation (6.4) takes the form

$$\partial_t \psi_t \;=\; (1/2)\nabla\left[D(\psi_t)\nabla\psi_t\right] \;-\; \nabla\Big\{\chi(\psi_t)\frac{D(\bar\rho)}{\chi(\bar\rho)}\nabla\bar\rho\Big\}\;.$$

It is easy to check that the solution of this equation for any initial condition γ relaxes to equilibrium. This concludes the proof of the theorem. □

The adjoint hydrodynamic equation can be written as

$$\partial_t \psi_t \;=\; (1/2)\nabla\left[D(\psi_t)\nabla\psi_t\right] \;-\; \nabla\Big\{\chi(\psi_t)\nabla R_\alpha(\bar\rho)\Big\}\;.$$

Therefore, in order to obtain the adjoint hydrodynamic equation from the original hydrodynamic equation, one needs to add a weak external field $N^{-1}R_\alpha(\bar\rho)$ to the dynamics. Remark that the external field does not depend on the profile ψ_t. This property is rather peculiar and explains the simplicity of the quasi-potential.

6.5 Explicit formula for the quasi-potential if $\chi(\alpha) = a_0 + a_1\alpha + a_2\alpha^2$, $D(\alpha) = 1$

We obtain in this subsection a solution of the Hamilton-Jacobi equation which satisfies the assumptions of Theorem 6.3 in the case where the diffusivity is constant and the mobility is equal to a second order polynomial: $D(\alpha) = 1$, $\chi(\alpha) = a_0 + a_1\alpha + a_2\alpha^2$. We may assume without loss of generality that $a_2 \neq 0$, otherwise the system satisfy the conditions of the previous subsection. This class includes exclusion processes and the KMP model.

Theorem 6.5. *Assume that* $D(\alpha) = 1$, $\chi(\alpha) = a_0 + a_1\alpha + a_2\alpha^2$, $a_2 \neq 0$. *Then,*

$$V(\gamma) \;=\; \int_0^1 \gamma\big\{R_\alpha(\gamma) - R_\alpha(F)\big\} - \log\frac{Z_\alpha(R_\alpha(\gamma))}{Z_\alpha(R_\alpha(F))} - \frac{1}{a_2}\log\frac{F'}{\beta-\alpha}\;,$$

where F is the unique increasing solution of

$$\begin{cases} \dfrac{\Delta F}{[\nabla F]^2} \;=\; a_2\dfrac{F-\gamma}{\chi(F)}\;, \\[2ex] F(0) = \alpha,\;\; F(1) = \beta\;. \end{cases} \tag{6.7}$$

Proof. For a density profile γ and a smooth increasing function F, let

$$\mathcal{G}(\gamma, F) \;=\; \int_0^1 \gamma\big\{R_\alpha(\gamma) - R_\alpha(F)\big\} - \log\frac{Z_\alpha(R_\alpha(\gamma))}{Z_\alpha(R_\alpha(F))} - \frac{1}{a_2}\log\frac{F'}{\beta-\alpha}$$

and let $W(\gamma) = \mathcal{G}(\gamma, F(\gamma))$, where $F(\gamma)$ is the solution of (6.7). An elementary computation shows that $\delta\mathcal{G}(\gamma, F)/\delta F$ vanishes at $F = F(\gamma)$ for all γ because F solves (6.7). In particular, $\delta W/\delta\gamma = R_\alpha(\gamma) - R_\alpha(F)$.

We claim that $R_\alpha(\gamma) - R_\alpha(F)$ solves the Hamilton-Jacobi equation (6.2). Since $R'_\alpha = D/\chi$ and since γ and F assume the same value at the boundary, after an integration by parts, we get that the left hand side of (6.2) with W in place of V is given by

$$\left\langle \left\{ \frac{\nabla\gamma}{\chi(\gamma)} - \frac{\nabla F}{\chi(F)} \right\}^2 \chi(\gamma) \right\rangle - \left\langle \left\{ \frac{\nabla\gamma}{\chi(\gamma)} - \frac{\nabla F}{\chi(F)} \right\} \nabla\gamma \right\rangle =$$

$$- \left\langle \big\{ \nabla\gamma - \nabla F \big\} \frac{\nabla F}{\chi(F)} + \left(\frac{\nabla F}{\chi(F)} \right)^2 \big\{ \chi(F) - \chi(\gamma) \big\} \right\rangle .$$

Since $\gamma - F$ vanishes at the boundary, we may integrate by parts the first expression to get that the previous integral is equal to

$$\left\langle \{\gamma - F\} \left\{ \nabla \left(\frac{\nabla F}{\chi(F)} \right) + \left(\frac{\nabla F}{\chi(F)} \right)^2 \frac{\chi(F) - \chi(\gamma)}{F - \gamma} \right\} \right\rangle .$$

The expression inside braces vanishes because F is the solution of (6.7).

We now prove that the solutions of the adjoint hydrodynamic equation relax to the stationary profile $\bar\rho$.

Since $\delta W/\delta\gamma = R_\alpha(\gamma) - R_\alpha(F)$, the adjoint hydrodynamic equation (6.4) takes the form

$$\partial_t \psi_t \; = \; (1/2)\Delta\psi_t \; - \; \nabla\big\{ \chi(\psi_t) \nabla R_\alpha(F_t) \big\} \, , \tag{6.8}$$

where F_t is the solution of (6.7) with $\gamma = \psi_t$.

Observe that this equation gives an interpretation of the function F appearing in the equation (3.3): *For a fixed profile γ, $R_\alpha(F(\gamma))$ is the external field one needs to introduce to transform the hydrodynamic equation into the adjoint hydrodynamic equation.* In contrast with the examples discussed in Subsection 6.4, the external field now depends on the profile.

On the other hand, it seems hopeless to prove that the solution of the adjoint hydrodynamic equation relaxes to $\bar\rho$ since (ψ_t, F_t) solves a coupled of non-linear equation (6.7), (6.8). This means that for each fixed time t, we need to solve (6.7) with $\gamma = \psi_t$ and then plug the solution F_t in (6.8) to obtain the time evolution of ψ_t.

A miracle, however, takes place. Taking time derivative in (6.7), it is not difficult to show that F_t is solution of the heat equation! Thus, if for a fixed profile γ we define F_t, by

$$\begin{cases} \partial_t F_t \;=\; \dfrac{1}{2}\Delta F_t \\ F_t(0) \;=\; \alpha, \qquad F_t(1) \;=\; \beta, \\ F_0 \;=\; F(\gamma)\;, \end{cases}$$

where $F(\gamma)$ is the solution of (6.7), ψ_t defined by

$$\psi_t(u) = F_t(u) + \frac{1}{a_2}\chi(F_t)\frac{\Delta F_t(u)}{[\nabla F_t(u)]^2}$$

solves the adjoint hydrodynamic equation (6.8).

We have thus shown how a solution of the (non local, non linear) equation (6.8) can be obtained from the linear heat equation by performing the non local transformation (6.7) on the initial datum. In particular, since the solution $F_t(u)$ of the heat equation converges as $t \to \infty$ to $\bar{\rho}$, we see that the solution of the adjoint hydrodynamic relaxes to the stationary density profile $\bar{\rho}$.

To complete the proof, it remains to check that W is lower semi-continuous. This follows from the fact that W can be defined through a supremum or infimum in F of $\mathcal{G}(\gamma, F)$ (cf. [2, 3, 7]). □

7 Asymptotic behavior of the empirical current

We examine in this section the current fluctuations over a fixed macroscopic time interval. In particular we discuss the law of large numbers and the dynamical large deviations principle for the empirical current. We state these results in the context of the boundary driven symmetric exclusion process but similar results hold for more general dynamics and for periodic boundary conditions.

Consider the boundary driven symmetric simple exclusion process defined in Section 2. For $0 \le x \le N-1$, denote by $j_{x,x+1}$ the rate at which a particle jumps from x to $x+1$ minus the rate at which a particle jumps from $x+1$ to x. For $x = 0$, this is the rate at which a particle is created minus the rate at which a particle leaves the system. A similar interpretation holds at the right boundary. An elementary computation shows that

$$j_{x,x+1} \;=\; N^2 \begin{cases} \alpha - \eta(1) & \text{for} \quad x = 0, \\ \eta(x) - \eta(x+1) & \text{for} \quad 1 \le x \le N-2\;, \\ \eta(N-1) - \beta & \text{for} \quad x = N-1. \end{cases}$$

In view of (2.2), under the invariant measure $\nu^N_{\alpha,\beta}$, the average of $j_{x,x+1}$ is

$$E_{\nu^N_{\alpha,\beta}}[j_{x,x+1}] = N(\alpha - \beta)$$

Given a bond $\{x, x+1\}$, $0 \le x \le N-1$, let $J_t^{x,x+1}$ (resp. $J_t^{x+1,x}$) be the number of particles that have jumped from x to $x+1$ (resp. $x+1$ to x) in the time interval $[0,t]$. Here we adopt the convention that $J_t^{0,1}$ is the number of particles created at 1 and that $J_t^{0,1}$ represents the number of particles that left the system from 1. A similar convention is adopted at the right boundary. The difference $W_t^{x,x+1} = J_t^{x,x+1} - J_t^{x+1,x}$ is the net number of particles flown across the bond $\{x, x+1\}$ in the time interval $[0,t]$. Let us consider the stationary process $\mathbb{P}_{\nu^N_{\alpha,\beta}}$, i.e. the boundary driven symmetric simple exclusion process in which the initial condition is distributed according to the invariant measure $\nu^N_{\alpha,\beta}$. A simple martingale computation shows that $W_t^{x,x+1}/(Nt)$ converges, as $t \to \infty$, to $(\alpha-\beta)$ in probability. Namely, for each $N \ge 1$, $x = 0, \dots, N-1$, and $\delta > 0$, we have

$$\lim_{t\to\infty} \mathbb{P}_{\nu^N_{\alpha,\beta}}\Big[\Big| \frac{W_t^{x,x+1}}{Nt} - (\alpha - \beta) \Big| \; > \; \delta \Big] \; = \; 0 \; .$$

Let $\mathcal{M}$ be the space of bounded signed measures on $[0,1]$ endowed with the weak topology. For $t \ge 0$, define the *empirical integrated current* $W_t^N \in \mathcal{M}$ as the finite signed measure on $[0,1]$ induced by the net flow of particles in the time interval $[0,t]$:

$$W_t^N \;=\; N^{-2} \sum_{x=0}^{N-1} W_t^{x,x+1} \delta_{x/N} \; .$$

Notice the extra factor N^{-1} in the normalizing constant which corresponds to the diffusive rescaling of time. In particular, for a function F in $C([0,1])$, the integral of F with respect to W_t^N, also denoted by $\langle W_t^N, F\rangle$, is given by

$$\langle W_t^N, F\rangle \;=\; N^{-2} \sum_{x=0}^{N-1} F(x/N)\, W_t^{x,x+1} \; . \tag{7.1}$$

It is not difficult to prove the law of large numbers for the empirical current starting from an initial configuration associated to a density profile.

Proposition 7.1. *Fix a profile γ and consider a sequence of configurations η^N such that $\pi^N(\eta^N)$ converges to $\gamma(u)du$, as $N \uparrow \infty$. Let ρ be the solution of the heat equation* (5.1)*. Then, for each $T > 0$, $\delta > 0$ and F in $C([0,1])$,*

$$\lim_{N\to\infty} \mathbb{P}_{\eta^N}\Big[\Big| \langle W_T^N, F\rangle \;+\; (1/2) \int_0^T dt \int_0^1 F(u) \nabla \rho_t(u)\, du \Big| > \delta \Big] \;=\; 0 \; .$$

This result states that the empirical current W_t^N converges to the time integral of $-(1/2)\nabla\rho_t(u)$, which is the instantaneous current associated to the profile ρ_t. Thus, if we denote by $w(\gamma) = -(1/2)\nabla\gamma$ the instantaneous current of a profile γ, we have that

$$\lim_{N\to\infty} W_t^N \;=\; \int_0^t ds\, w(\rho_s)$$

in probability. Proposition 7.1 is easy to understand. The local conservation of the number of particles is expressed by

$$\eta_t(x) - \eta_0(x) = W_t^{x-1,x} - W_t^{x,x+1} \;.$$

It gives the following continuity equation for the empirical density and current. Let $G : [0,1] \to \mathbb{R}$ be a smooth function vanishing at the boundary and let $(\nabla_N G)(x/N) = N\{G(x+1/N) - G(x/N)\}$. Then,

$$\langle \pi_t^N, G\rangle - \langle \pi_0^N, G\rangle = \langle W_t^N, \nabla_N G\rangle \;.$$

The previous identity shows that the empirical density at time t can be recovered from the initial state and the empirical current at time t. In contrast, the empirical density at time t and at time 0 determines the empirical current at time t only up to a constant. Letting $N \uparrow \infty$ in the previous identity, since π^N converges to the solution of the heat equation (5.1), an integration by parts gives that

$$\langle W_t, \nabla G\rangle \;=\; \langle \rho_t, G\rangle - \langle \rho_0, G\rangle \;=\; \frac{1}{2}\int_0^t ds\, \langle \Delta\rho_s, G\rangle \;=\; -\frac{1}{2}\int_0^t ds\, \langle \nabla\rho_s, \nabla G\rangle \;.$$

where W_t is the limit of W_t^N.

After proving this law of large numbers for the current, we examine its large deviations properties. To state a large deviations principle for the current we need to introduce some notation. Fix $T > 0$ and recall that we denote by $w(\gamma) = -(1/2)\nabla\gamma$ the instantaneous current associated γ. For a density profile γ and a path W in $D([0,T], \mathcal{M})$, denote by $w_t = \dot{W}_t$ and let $\rho_t^{\gamma,W}$ the weak solution of

$$\begin{cases} \partial_t\rho_t \;+\; \nabla w_t \;=\; 0 \;, \\ \rho_0(u) \;=\; \gamma(u) \;, \\ \rho_t(0) \;=\; \alpha \;, \quad \rho_t(1) \;=\; \beta \;. \end{cases} \tag{7.2}$$

We note that the trajectory $\rho_t^{\gamma,W}$ is the one followed by the density profile if the initial condition is γ and the instantaneous current is w. As for the empirical density, the rate functional for the empirical current is given by a variational expression. Referring to [6] for the precise definition, we here note that for trajectories W in $D([0,T],\mathcal{M})$ the rate functional is finite only if the associated density path $\rho_t^{\gamma,W}du$ belongs to $C([0,T],\mathcal{M}_+)$; moreover when W is a smooth path we have

$$\mathcal{I}_{[0,T]}(W|\gamma) \;=\; \frac{1}{2}\int_0^T dt\left\langle \frac{1}{\chi(\rho_t^{\gamma,W})}\,\Big\{\dot{W}_t - w(\rho_t^{\gamma,W})\Big\}^2\right\rangle. \tag{7.3}$$

The following theorem is proven in [6] in the case of periodic boundary condition. The proof can easily be modified to cover the present setting of the boundary driven simple exclusion process.

Theorem 7.2. *Fix $T>0$ and a smooth profile γ bounded away from 0 and 1. Consider a sequence η^N of configurations associated to γ in the sense that $\pi^N(\eta^N)$ converges to $\gamma(u)du$ as $N\uparrow\infty$. Fix W in $D([0,T],\mathcal{M})$ and an associated neighborhood $V_\varepsilon(W)$ of radius ε. Then,*

$$\limsup_{\varepsilon\to 0}\limsup_{N\to\infty}\frac{1}{N}\log\mathbb{P}_{\eta^N}\Big\{W^N\in V_\varepsilon(W)\Big\} \;\le\; -\mathcal{I}_{[0,T]}(W|\gamma)\;,$$

$$\liminf_{\varepsilon\to 0}\liminf_{N\to\infty}\frac{1}{N}\log\mathbb{P}_{\eta^N}\Big\{W^N\in V_\varepsilon(W)\Big\} \;\ge\; -\mathcal{I}_{[0,T]}(W|\gamma)\;.$$

Since the trajectory of the empirical density can be recovered from the evolution of the current and the initial condition, the large deviations principle for the empirical density stated in Theorem 5.2 can be obtained from the large deviations principle for the current by the contraction principle, see [6] for the proof.

8 Large deviations of the time averaged empirical current

In this section we investigate the large deviations properties of the mean empirical current W_T^N/T as we let *first* $N\to\infty$ and *then* $T\to\infty$. As before, unless stated explicitly, the analysis carried out in this section does not depend on the details of the symmetric simple exclusion process so that it holds in a general setting.

Since the density is bounded, for T large the time averaged empirical current must be constant with respect to the space variable u. This holds in the present one-dimensional setting; in higher dimensions the condition required would be the vanishing of the divergence. Indeed, if this condition were not satisfied we would have an unbounded (either positive or negative) accumulation of particles. We next discuss the asymptotic probability that the time averaged empirical current equals some fixed constant.

For a smooth profile γ bounded away from 0 and 1, let $\widetilde{\Phi} : \mathcal{M} \to [0, +\infty]$ be the functional defined by

$$\widetilde{\Phi}(J) = \begin{cases} \inf\limits_{T>0} \dfrac{1}{T} \inf\limits_{W \in \mathcal{A}_{T,q}} \mathcal{I}_{[0,T]}(W|\gamma) & \text{if } J(du) = q\,du \ \text{ for some } \ q \in \mathbb{R} \\ +\infty & \text{otherwise} \end{cases} \tag{8.1}$$

where $\mathcal{A}_{T,q}$ stands for the set of currents with time average equal to q

$$\mathcal{A}_{T,q} := \left\{ W \in D\big([0, T]; \mathcal{M}\big) \, : \, \frac{1}{T} \int_0^T dt\, \dot{W}_t(du) = q\, du \right\} .$$

It is not difficult to show that $\widetilde{\Phi}$ is convex. In the present context of the boundary driven simple exclusion process, it is also easy to verify that the functional $\widetilde{\Phi}$ does not depend on on the initial condition γ. We emphasize however that, in the case of periodic boundary condition $\widetilde{\Phi}$ depends on γ only through its total mass $\int du\, \gamma(u)$. Indeed, we may start by driving the empirical density from a profile γ to a profile γ' in the time interval $[0, 1]$ paying a finite price, note that in the periodic case γ and γ' must have the same mass. As $T \uparrow \infty$, this initial cost vanishes and the problem is reduced to the original one starting from the profile γ'. Let us finally introduce Φ as the lower semi-continuous envelope of $\widetilde{\Phi}$, i.e. the largest lower semi-continuous function below $\widetilde{\Phi}$. The next theorem states that, as we let first $N \uparrow \infty$ and then $T \uparrow \infty$ the time averaged empirical current W_T^N / T satisfies a large deviation principle with rate function Φ. We refer to [6] for the proof which is carried out by analyzing the variational problem $\inf_{W \in \mathcal{A}_{T,q}} T^{-1} \mathcal{I}_{[0,T]}(W|\gamma)$ as $T \uparrow \infty$ and showing that it converges, in a suitable sense, to the variational problem defining Φ.

Theorem 8.1. *Fix $T > 0$ and a smooth profile γ bounded away from 0 and 1. Consider a sequence η^N of configurations associated to γ in the sense that $\pi^N(\eta^N)$ converges to $\gamma(u)du$ as $N \uparrow \infty$. Fix $J \in \mathcal{M}$ and a neighborhood $V_\varepsilon(J)$ of radius ε. Then,*

$$\limsup_{\varepsilon \to 0} \limsup_{T \to \infty} \limsup_{N \to \infty} \frac{1}{TN} \log \mathbb{P}_{\eta^N}\Big[\frac{1}{T} W_T^N \in V_\varepsilon(J) \Big] \ \le \ -\Phi(J) \ ,$$

$$\liminf_{\varepsilon \to 0} \liminf_{T \to \infty} \liminf_{N \to \infty} \frac{1}{TN} \log \mathbb{P}_{\eta^N}\Big[\frac{1}{T} W_T^N \in V_\varepsilon(J) \Big] \ \ge \ -\Phi(J) \ .$$

A result analogous to Theorem 8.1 can be proven for other diffusive interacting particle systems. Consider a system with a weak external field $E = E(u)$, whose hydrodynamic equation, describing the evolution of the empirical density on the macroscopic scale, has the form

$$\partial_t \rho_t = \nabla\big(D(\rho_t)\nabla\rho_t\big) - \nabla\big(\chi(\rho_t)E\big)\ . \tag{8.2}$$

where $D(\rho)$ is the diffusion coefficient and $\chi(\rho)$ is the mobility. For the symmetric simple exclusion process $D = 1/2$ and $\chi(\rho) = \rho(1-\rho)$. In the general case, the large deviations functional $\mathcal{I}_{[0,T]}(\cdot|\gamma)$ has the same form (7.3) with $w(\gamma) = -D(\gamma)\nabla\gamma + \chi(\gamma)E$ and $\rho^{\gamma,W}$ the solution of (7.2). For systems with periodic boundary conditions, the boundary conditions in (7.2) is modified accordingly. In the remaining part of this section we analyze the variational problem (8.1) for different systems and show that different scenarios are possible.

A possible strategy for minimizing $\mathcal{I}_{[0,T]}(w|\gamma)$ with the constraint that $w \in \mathcal{A}_{T,q}$, i.e. that the time average of w is fixed, consists in driving the empirical density to a density profile γ^*, remaining there most the time and forcing the associated current to be equal to q. This is the strategy originally proposed by Bodineau and Derrida [8]. In view of (7.3) the asymptotic cost, as $T \uparrow \infty$, of this strategy is

$$\frac{1}{2}\Big\langle\big[q + D(\gamma^*)\nabla\gamma^*\big], \frac{1}{\chi(\gamma^*)}\big[q + D(\gamma^*)\nabla\gamma^*\big]\Big\rangle\ .$$

If we minimize this quantity over all profiles γ^* we obtain a functional U which gives the cost of keeping a current q at a fixed density profile:

$$U(q) := \inf_{\rho} \frac{1}{2}\Big\langle\big[q + D(\rho)\nabla\rho\big], \frac{1}{\chi(\rho)}\big[q + D(\rho)\nabla\rho\big]\Big\rangle\ . \tag{8.3}$$

where the infimum is carried out over all smooth density profiles $\rho = \rho(u)$ bounded away from 0 and 1 which satisfy the boundary conditions $\rho(0) = \alpha$, $\rho(1) = \beta$. As observed above, for boundary driven systems all density profiles are allowed while for periodic boundary condition only profiles with the same total mass $m = \int_0^1 du\, \rho(u)$ are allowed. In the latter case, the functional U depends on the total mass m and is denoted by U_m.

As proven in [4, 5, 6], for the symmetric simple exclusion process the strategy above is the optimal one, i.e. $\Phi = U$. It is in fact not difficult to show that in this case U is lower semi-continuous, so that $\widetilde{\Phi} = \Phi$. More generally we have the following result.

Lemma 8.2. *Let $E = 0$. If $D(\rho)\chi''(\rho) \le D'(\rho)\chi'(\rho)$ for any ρ, then $\Phi = U$.*

Besides the symmetric simple exclusion process, the hypothesis of the lemma is also satisfied for the zero range model, where $D(\rho) = \Psi'(\rho)$ and $\chi(\rho) = \Psi(\rho)$

for some strictly increasing function $\Psi : \mathbb{R}_+ \to \mathbb{R}_+$, and for the non interacting Ginzburg–Landau model, where $\rho \in \mathbb{R}$, $D(\rho)$ is an arbitrary strictly positive function and $\chi(\rho)$ is constant.

For systems with periodic boundary condition we have shown [5, 6] that the profile which minimizes U_m is the constant profile if $1/\chi(\rho)$ is convex.

Lemma 8.3. *Let $E = 0$. If the function $\rho \mapsto 1/\chi(\rho)$ is convex, then*

$$U_m(q) = \frac{1}{2}\frac{q^2}{\chi(m)}$$

and the constant profile $\rho(u) = m$ is optimal for the variational problem (8.3).

The assumption of this lemma is satisfied by the symmetric simple exclusion process as well as by the KMP model [7, 22], where $D(\rho) = 1$ and $\chi(\rho) = \rho^2$.

As first discussed in [4], the above strategy is not always the optimal one, i.e. there are systems for which $\Phi < U$. In [4, 5] we interpreted this strict inequality as a dynamical phase transition. In such a case the minimizers for (8.1) become in fact time dependent and the invariance under time shifts is broken. We now illustrate how different behaviors of the variational problem (8.1) leads to different dynamical regimes. We consider the system in the ensemble defined by conditioning on the event $(T)^{-1}W_T^N(du) = q\,du$, $q \in \mathbb{R}$, with N and T large. The parameter q plays therefore the role of an intensive thermodynamic variable and the convexity of Φ expresses a stability property with respect to variations of q.

If $\Phi(q) = U(q)$ and the minimum for (8.3) is attained for $\rho = \hat{\rho}(q)$ we have a state analogous to a unique phase: by observing the system at any fixed time $t = O(T)$ we see, with probability converging to one as $N, T \to \infty$, the density $\pi_T^N \sim \hat{\rho}(q)$ and the instantaneous current $\dot{W}_t^N \sim q$.

While the functional Φ is always convex, U may be not convex; an example of a system with this property is given in [5]. If Φ is equal to the convex envelope of U, we have a state analogous to a phase coexistence. Suppose for example

$$q = pq_1 + (1-p)q_2 \quad \text{and} \quad U(q) > U^{**}(q) = pU(q_1) + (1-p)U(q_2)$$

for some p, q_1, q_2; here U^{**} denotes the convex envelope of U. The values p, q_1, q_2 are determined by q and U. The density profile is then not determined, but rather we observe with probability p the profile $\hat{\rho}(q_1)$ and with probability $1-p$ the profile $\hat{\rho}(q_2)$.

Consider now the case in which a minimizer for (8.1) is a current path w_t not constant in t and suppose that it is periodic with period τ. We denote by $\hat{\rho}_t$ the corresponding density. Of course we have $\tau^{-1}\int_0^\tau dt\, w_t = q$. In this situation we have in fact a one parameter family of minimizers which are obtained by a time shift $\alpha \in [0, \tau]$. This behavior is analogous to a non translation invariant state in equilibrium statistical mechanics, like a crystal. Finally, if the optimal path for (8.1) is time dependent and not periodic the corresponding state is analogous to a quasi-crystal.

The explicit formula for U_m derived in Lemma 8.3 permits to show that under additional conditions on the transport coefficient D and χ, a dynamical phase transition occurs. We discuss only the case of periodic boundary conditions. In this situation a time-averaged current q may be produced using a traveling wave density profile, $\rho_t(u) = \rho_0(u - vt)$, with velocity $v \sim q$. Assume now that $E = 0$ and the function $\rho \mapsto \chi(\rho)$ is strictly convex for $\rho = m$. Then, for sufficiently large q, the traveling wave strategy is more convenient than the one using the constant profile m [4, 5]. In particular, if $\rho \mapsto 1/\chi(\rho)$ is convex so that Lemma 8.3 can be applied, we have

$$\Phi_m(q) \;<\; U_m(q) \tag{8.4}$$

for sufficiently large q. In the KMP model the above hypotheses are satisfied for any $m > 0$; we can thus conclude that a dynamical phase transition takes place for sufficiently large time-averaged currents.

The above analysis can also be applied to the weakly asymmetric simple exclusion process [5]. It yields that if $|E/q| > [m(1-m)]^{-1}$ for q large there exists a traveling wave whose cost is strictly less than the one of the constant profile $\rho(u) = m$. The analysis in [9] suggest however that the strict inequality (8.4) holds also in this case. Moreover, the numerical simulations in [9] indicate the existence, for the weakly asymmetric simple exclusion process, of a critical current q^* below which the optimal profile is constant and above which the optimal profile is a traveling wave.

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