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Non Equilibrium Current Fluctuations in Stochastic Lattice Gases

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We study current fluctuations in lattice gases in the macroscopic limit extending the dynamic approach for density fluctuations developed in previous articles. More precisely, we establish a large deviation principle for a space-time fluctuation j of the empirical current with a rate functional $\mathcal{I}(j)$. We then estimate the probability of a fluctuation of the average current over a large time interval; this probability can be obtained by solving a variational problem for the functional $\mathcal{I}$. We discuss several possible scenarios, interpreted as dynamical phase transitions, for this variational problem. They actually occur in specific models. We finally discuss the time reversal properties of $\mathcal{I}$ and derive a fluctuation relationship akin to the Gallavotti-Cohen theorem for the entropy production.

KEY WORDS: Stationary non equilibrium states, Stochastic lattice gases, Current fluctuations, Gallavotti-Cohen symmetry.

1. INTRODUCTION

1.1. Thermodynamic Functionals for Non Equilibrium Systems

In equilibrium statistical mechanics there is a well defined relationship, established by Boltzmann, between the probability of a state and its entropy. This

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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 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. This possibility has been pursued in recent years leading to a considerable number of interesting results. One can recognize two main lines. The first, as well exemplified by the work of Derrida, Lebowitz and Speer,[13–15] consists in exact calculations in specific models of stochastic lattice gases. The second is based on a macroscopic dynamical approach for Markovian microscopic evolutions, of which stochastic lattice gases are a main example, that leads to some general variational principles. We introduced this approach in Refs. (3, 4) and developed it in Refs. (5, 6). Both approaches have been very effective and of course give the same results when a comparison is possible.

Let us recall the Boltzmann–Einstein theory of equilibrium thermodynamic fluctuations, as described for example in Ref. (25). 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. Equation (1.1) was derived by Einstein[17] 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 $-\Delta F / T$, that is minus the variation of the free energy of the system divided by the temperature.

We consider a stationary nonequilibrium 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. As we discussed in Refs. (3–6), the study of large fluctuations provides such a connection. It leads in fact to a dynamical theory of the free energy which is shown to satisfy a Hamilton–Jacobi equation in infinitely many variables requiring as input the transport coefficients. In the case of homogeneous equilibrium states the solution of the Hamilton–Jacobi equation is easily found, and the equilibrium free energy is recovered together with the well known fluctuation-dissipation relationship, widely used in the physical and physical-chemical literature. On the other hand in SNS the Hamilton–Jacobi equation is hard to solve. There are few one-dimensional models where it reduces to a non linear ordinary differential equation which, even if it cannot be solved explicitly, leads to the important conclusion that the non equilibrium free energy is a non local functional of the thermodynamic variables. This implies that correlations over macroscopic scales are present. The existence of long range correlations is probably a generic feature of SNS and more generally of situations where the dynamics is not invariant under time reversal.[2] As a consequence if we divide a system into subsystems the free energy is not necessarily simply additive.

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. The free energy is then related to the logarithm of the probability of such a trajectory and satisfies the Hamilton–Jacobi equation associated to this variational principle. For equilibrium states and small fluctuations an answer to this type of questions was given by Onsager and Machlup in 1953.[30] 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. As we show in Refs. (3, 4), 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.

1.2. Macroscopic Dynamics and Large Fluctuations

We consider many-body systems in the limit of infinitely many degrees of freedom. Microscopically we assume that the evolution is described by a Markov

process X_τ which represents the state of the system at time τ. This hypothesis probably is not so restrictive because also the dynamics of Hamiltonian systems interacting with thermostats finally is reduced to the analysis of a Markov process, see e.g. Ref. (16). To be more precise X_τ represents the set of variables necessary to specify the state of the microscopic constituents interacting among themselves and with the reservoirs. The SNS is described by a stationary, i.e. invariant with respect to time shifts, probability distribution P_{st} over the trajectories of X_τ. We denote by μ the invariant measure of the process X_τ. The measure μ is a probability on the configuration space and for each fixed time τ we have $P_{st}(X_\tau = \omega) = \mu(\omega)$.

We assume that the system admits a macroscopic description in terms of density fields which are the local thermodynamic variables ρ_i. The usual macroscopic interpretation of Markovianity is that the time derivatives of the thermodynamic variables $\dot{\rho}_i$ at a given instant of time depend only on the ρ_i's and the affinities (thermodynamic forces) $\frac{\partial F}{\partial \rho_i}$ at the same instant, recall that F is the free energy. As we discussed in Ref. (6), for non equilibrium systems, the affinities, defined as the derivative of the non equilibrium free energy, do not determine the macroscopic evolution of the variables ρ_i. There is an additional non dissipative term which however does not modify the rate of approach to the stationary state.

For simplicity of notation we assume that there is only one thermodynamic variable ρ e.g. the local density. For conservative systems the evolution of the field $\rho = \rho(t, u)$, where t and u are the macroscopic time and space coordinates, is then given by the continuity equation

$$\partial_t \rho = \nabla \cdot \left[\frac{1}{2} D(\rho) \nabla \rho - \chi(\rho) E \right] = -\nabla \cdot J(\rho) \tag{1.2}$$

where $D(\rho)$ is the diffusion matrix, $\chi(\rho)$ the mobility and E the external field. Finally the interaction with the reservoirs appears as boundary conditions to be imposed on solutions of (1.2). We shall denote 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 microscopic dynamics through an appropriate scaling limit in which the microscopic time and space coordinates τ, x are rescaled diffusively: $t = \tau/N^2$, $u = x/N$ where N is the linear size of the system so that the number of degrees of freedom is proportional to N^d. The hydrodynamic Eq. (1.2) represents a law of large numbers with respect to the probability measure P_{st} conditioned on an initial state X_0. This conditional probability will be denoted by P_{X_0}. The initial conditions for (1.2) are determined by X_0. Of course many microscopic configurations give rise to the same value of $\rho(0, u)$. In general $\rho = \rho(t, u)$ is the limit of the local density $\pi_N(X_\tau)$.

The free energy $F(\rho)$, defined as a functional of the density profile $\rho = \rho(u)$, gives the asymptotic probability of density fluctuations for the invariant measure μ.

More precisely

$$\mu(\pi_N(X) \approx \rho) \sim \exp\{-N^d F(\rho)\} \tag{1.3}$$

where d is the dimensionality of the system, $\pi_N(X) \approx \rho$ means closeness in some metric 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 F so that $F(\bar{\rho}) = 0$.

In the same way, the behavior of space time fluctuations can be described as follows. The probability that the evolution of the random variable $\pi_N(X_\tau)$ deviates from the solution of the hydrodynamic equation and is close to some trajectory $\hat{\rho}(t)$ is exponentially small and of the form

$$P_{st}(\pi_N(X_{N^2 t}) \approx \hat{\rho}(t),\ t \in [t_1, t_2]) \sim \exp\{-N^d[F(\hat{\rho}(t_1)) + \mathcal{F}_{[t_1,t_2]}(\hat{\rho})]\} \tag{1.4}$$

where $\mathcal{F}(\hat{\rho})$ is a functional which vanishes if $\hat{\rho}(t)$ is a solution of (1.2) and $F(\hat{\rho}(t_1))$ is the free energy cost to produce the initial density profile $\hat{\rho}(t_1)$. Therefore $\mathcal{F}(\hat{\rho})$ represents the extra cost necessary to follow the trajectory $\hat{\rho}(t)$ in the time interval $[t_1, t_2]$. Equation (1.4) is a dynamical generalization of the Boltzmann–Einstein formula, we shall refer to it as the *dynamical large deviation principle* with dynamical *rate functional* $\mathcal{F}$. For stochastic lattice gases, as shown in Ref. (4), the functional $\mathcal{F}$ can be calculated explicitly.

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 $\mathcal{F}$ among all trajectories $\hat{\rho}(t)$ connecting $\bar{\rho}$ to ρ in the time interval $[-\infty, 0]$. As shown in Refs. (3, 4) this minimization problem gives the non equilibrium free energy, i.e.

$$F(\rho) = \inf_{\hat{\rho}} \mathcal{F}_{[-\infty,0]}(\hat{\rho}) \tag{1.5}$$

To this variational principle it is naturally associated a Hamilton–Jacobi equation which plays a crucial role in the analysis developed in Refs. (3–6). We emphasize that the functional $\mathcal{F}$, hence the corresponding Hamilton–Jacobi equation for F, is determined by the macroscopic transport coefficients $D(\rho)$ and $\chi(\rho)$, which are experimentally accessible, see e.g. Ref. (1). We can thus regard (1.5) as a far reaching generalization of the fluctuation-dissipation theorem since it allows to express a static quantity like the free energy in terms of the dynamical macroscopic features of the system.

1.3. Current Fluctuation and Related Thermodynamic Functionals

Beside the density, a very important observable is the current flux.[12,20,27,31,32] 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.

In the previous paper[7] we have introduced a Boltzmann–Einstein type formula for current fluctuations. This formula shows that the asymptotic probability, as the number of degrees of freedom increases, of observing a current fluctuation j on a space–time domain $[0, T] \times \Lambda$ can be described by a rate functional $\mathcal{I}_{[0,T]}(j)$. In the present paper we develop the approach introduced in Ref. (7) and illustrate some relevant applications.

To discuss the current fluctuations, we introduce a vector-valued observable $\mathcal{J}^N(\{X_\sigma, 0 \le \sigma \le \tau\})$ of the trajectory X which measures the local net flow of particles. As for the density, for stochastic lattice gases, we shall be able to derive a dynamical large deviations principle for the current. Recall that P_{X_0} stands for the probability P_{st} conditioned on the initial state X_0. Given a vector field $j : [0, T] \times \Lambda \to \mathbb{R}^d$, we have

$$P_{X_0}(\mathcal{J}^N(X) \approx j(t, u)) \sim \exp\left\{-N^d \mathcal{I}_{[0,T]}(j)\right\} \tag{1.6}$$

where the rate functional is

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

in which we recall that

$$J(\rho) = -\frac{1}{2} D(\rho) \nabla \rho + \chi(\rho) E.$$

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 X_0. The rate functional vanishes if $j = J(\rho)$, so that ρ solves (1.2). This is the law of large numbers for the observable $\mathcal{J}^N$. Note that Eq. (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 $j - J(\rho)$.

The functional $\mathcal{I}$ describes the fluctuation properties of the current, the density and all observables related to them, as proved in Sec. 3. Among the many problems we can discuss within this theory, we study the fluctuations of the time average of the current $\mathcal{J}^N$ over a large time interval. This is the question addressed in Ref. (9) in one space dimension by postulating an "additivity principle" which relates the fluctuation of the time averaged current in the whole system to the fluctuations in subsystems. We show that the probability of observing a given

divergence free time average fluctuation J can be described by a functional $\Phi(J)$ which we characterize, in any dimension, 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. The static additivity principle postulated in Ref. (9) gives the correct answer only under additional hypotheses which are not always satisfied. Let us denote by U the functional obtained by restricting the infimum in (1.8) to divergence free current paths j, i.e.

$$U(J) = \inf_\rho \frac{1}{2}\langle [J - J(\rho)],\, \chi(\rho)^{-1}[J - J(\rho)]\rangle \tag{1.9}$$

where the infimum is carried out over all the density profiles $\rho = \rho(u)$ satisfying the appropriate boundary conditions. From (1.8) and (1.9) it follows that $\Phi \le U$. In one space dimension the functional U is the one introduced in Ref. (9).

There are cases in which $\Phi = U$ and in Subsec. 6.1 below we give sufficient conditions on the transport coefficients D, χ for the coincidence of Φ and U. On the other hand, while Φ is always convex the functional U may be non convex. In such a case $U(J)$ underestimates the probability of the fluctuation J. In Ref. (7) we interpreted the lack of convexity of U, and more generally the strict inequality $\Phi < U$, as a dynamical phase transition. In the present paper we investigate in more detail the occurrence of this phenomenon. Let us denote by U^{**} the convex envelope of U; then $\Phi \le U^{**}$ and in Subsection 6.3 we give an example where $U^{**} < U$.

We shall also consider the fluctuation of the time averaged current with periodic boundary conditions. In Subsec. 6.2 we discuss the behavior of U and Φ under appropriate conditions on the transport coefficient and the external field. In particular we show that for the Kipnis–Marchioro–Presutti (KMP) model,[22] which is defined by a harmonic chain with random exchange of energy between neighboring oscillators, we have $U(J) = (1/2)J^2/\chi(m) = (1/2)J^2/m^2$, where m is the (conserved) total energy. In addition we show, for J large enough, $\Phi(J) < U(J)$. This inequality is obtained by constructing a suitable travelling wave current path whose cost is less than $U(J)$. We mention that, by using the space-time approach introduced in Ref. (7), the possibility of taking advantage of travelling waves has been first envisaged by Bodineau and Derrida[10,11] for the periodic simple exclusion process with external field. Referring to Subsec. 6.2 for a more detailed discussion, we here emphasize that for the KMP process this phenomenon is rather striking as it occurs even in equilibrium, i.e. without external field.

We study also the behavior of $\mathcal{I}$ and Φ under time reversal and derive a fluctuation relationship akin to the Gallavotti-Cohen theorem for the entropy

production;[18,24,26] this is also naturally discussed within a space-time Gibbsian formalism, see Ref. (28) and references therein. In this paper we show, in the present context of lattice gases, that the anti-symmetric part of Φ is equal to the power produced by the external field and the reservoirs independently of the details of the model. From this relationship we derive a macroscopic version the fluctuation theorem for the entropy production.

2. MICROSCOPIC MODEL

As the basic microscopic model we consider a stochastic lattice gas with a weak external field and particle reservoirs at the boundary. The process can be informally described as follows. We consider particles evolving on a finite domain. At each site, independently from the others, particles wait exponential times at the end of which one of them jumps to a neighboring site. Superimposed to this dynamics, at the boundary particles are created and annihilated at exponential times. More precisely, let $\Lambda \subset \mathbb{R}^d$ be a smooth domain and set $\Lambda_N = N\Lambda \cap \mathbb{Z}^d$. We consider a Markov process on the state space X^{Λ_N}, where X is a subset of $\mathbb{N}$, e.g. $X = \{0, 1\}$ when an exclusion principle is imposed. The number of particles at site $x \in \Lambda_N$ is denoted by $\eta_x \in X$ and the whole configuration by $\eta \in X^{\Lambda_N}$. The dynamics is specified by a continuous time Markov process on the state space X^{Λ_N} with infinitesimal generator $L_N = N^2[L_{0,N} + L_{b,N}]$ defined as follows: for functions $f : X^{\Lambda_N} \to \mathbb{R}$,

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

$$L_{b,N} f(\eta) = \frac{1}{2} \sum_{\substack{x \in \Lambda_N, y \notin \Lambda_N \\ |x-y|=1}} \{c_{x,y}(\eta)[f(\sigma^{x,y}\eta) - f(\eta)] + c_{y,x}(\eta)[f(\sigma^{y,x}\eta) - f(\eta)]\}. \tag{2.1}$$

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

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

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 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. Note that we already speeded up the microscopic time by N^2 in the definition of L_N, which corresponds to the diffusive scaling.

Assume that the bulk rates $c_{x,y}$, $x, y \in \Lambda_N$, satisfy the local detailed balance[26] with respect to a Gibbs measure defined by a Hamiltonian $\mathcal{H}$ and in presence of an external vector field $E = (E_1, \dots, E_d)$ smooth on the macroscopic scale. Likewise, assume that the boundary rates $c_{x,y}, c_{y,x}, x \in \Lambda_N, y \notin \Lambda_N$, satisfy the local detailed balance with respect to $\mathcal{H}$ and in presence of a chemical potential $\lambda_0(y/N)$ smooth on the macroscopic scale.

The above requirements are met by the following formal definitions. Fix a smooth function $\lambda_0 : \Lambda \to \mathbb{R}$ and a Hamiltonian $\mathcal{H}$. Consider jump rates $c^0_{x,y}$ satisfying the detailed balance with respect to the Gibbs measure associated to $\mathcal{H}$ with free boundary conditions if $x, y \in \Lambda_N$, while if $x \in \Lambda_N$, $y \notin \Lambda_N$ we add the chemical potential $\lambda_0(y/N)$:

$$c^0_{x,y}(\eta) = \exp -\{\mathcal{H}(\sigma^{x,y}\eta) - \mathcal{H}(\eta)\} c^0_{y,x}(\sigma^{x,y}\eta), \quad x, y \in \Lambda_N;$$
$$c^0_{x,y}(\eta) = \exp -\{\mathcal{H}(\sigma^{x,y}\eta) - \mathcal{H}(\eta) + \lambda_0(y/N)\} c^0_{y,x}(\sigma^{x,y}\eta), \quad x \in \Lambda_N, y \notin \Lambda_N.$$

Note that we included the inverse temperature in the Hamiltonian $\mathcal{H}$. Of course if $\eta_x = 0$ then $c^0_{x,y}(\eta) = 0$.

Fix a smooth vector field $E = (E_1, \dots, E_d) : \Lambda \to \mathbb{R}^d$ and let

$$c_{x,x+e_i}(\eta) := e^{N^{-1}E_i(x/N)} c^0_{x,x+e_i}(\eta), \quad c_{x+e_i,x}(\eta) := e^{-N^{-1}E_i(x/N)} c^0_{x+e_i,x}(\eta), \tag{2.2}$$

where $\{e_1, \dots, e_d\}$ stands for the canonical basis in $\mathbb{R}^d$. Namely, for N large, by expanding the exponential, particles at site x feel a drift $N^{-1}E(x/N)$.

Typically, for a non equilibrium model, we would consider Λ as the d-dimensional cube of side one, the system under a constant field E/N and a chemical potential λ_0 satisfying $\lambda_0(y/N) = \gamma_0$ if the first coordinate of y is 0, $\lambda_0(y/N) = \gamma_1$ if the first coordinate of y is N, imposing periodic boundary conditions in the other directions of Λ.

By setting $c_{x,y} = 0$ if both x and y do not belong to Λ_N, we can rewrite the full generator L_N as follows

$$L_N f(\eta) = \frac{N^2}{2} \sum_{\substack{x,y \in \mathbb{Z}^d \\ |x-y|=1}} c_{x,y}(\eta)[f(\sigma^{x,y}\eta) - f(\eta)] \tag{2.3}$$

We consider an initial condition $\eta \in X^{\Lambda_N}$. The trajectory of the Markov process $\eta(t)$, $t \geq 0$, is an element on the path space $D\big(\mathbb{R}_+; X^{\Lambda_N}\big)$, which consists of piecewise constant paths with values in X^{Λ_N}. We shall denote by $\mathbb{P}^N_\eta$ the probability measure on $D\big(\mathbb{R}_+; X^{\Lambda_N}\big)$ corresponding to the distribution of the process $\eta(t)$, $t \geq 0$ with initial condition η.

Examples of stochastic lattices gases are the simple exclusion processes in which $X = \{0, 1\}$, $\mathcal{H} = 0$ and $c^0_{x,y}(\eta) = \eta_x[1 - \eta_y]$ and zero range processes in

which $X = \mathbb{N}$, $\mathcal{H}(\eta) = \sum_x \sum_{1\le k\le\eta(x)} \log g(k)$, for some function $g : \mathbb{N} \to \mathbb{R}_+$ such that $g(0) = 0$, and $c^0_{x,y}(\eta) = g(\eta_x)$.

3. MACROSCOPIC DESCRIPTION OF LATTICE GASES

The empirical density π^N can be naturally defined as follows. To each microscopic configuration $\eta \in X^{\Lambda_N}$ we associate a macroscopic profile $\pi^N(u)$, $u \in \Lambda$, by requiring that for any smooth function $G : \Lambda \to \mathbb{R}$

$$\langle \pi^N, G\rangle = \int_\Lambda du\, \pi^N(u)\, G(u) = \frac{1}{N^d} \sum_{x\in\Lambda_N} G(x/N)\eta_x \tag{3.1}$$

so that $\pi^N(u)$ is the local density at the macroscopic point $u = x/N$ in Λ. Of course $\pi^N(u)$ is really a sum of point masses at the points x/N with weight η_x/N^d; in the limit $N \to \infty$ it will however weakly converge to a "true" function $\rho(u)$.

The definition of the empirical current is slightly more complicated. Indeed it is not a function of the configuration $\eta \in X^{\Lambda_N}$ but of the trajectory $\{\eta(t)\}_{t\ge0} \in D(\mathbb{R}_+; X^{\Lambda_N})$. Given an oriented bond (x, y), let $\mathcal{N}^{x,y}(t)$ be the number of particles that jumped from x to y in the time interval $[0, t]$. Here we adopt the convention that $\mathcal{N}^{x,y}(t)$ is the number of particles created at y due to the reservoir at x if $x \notin \Lambda_N$, $y \in \Lambda_N$ and that $\mathcal{N}^{x,y}(t)$ represents the number of particles that left the system at x by jumping to y if $x \in \Lambda_N$, $y \notin \Lambda_N$. The difference $Q^{x,y}(t) = \mathcal{N}^{x,y}(t) - \mathcal{N}^{y,x}(t)$ is the net number of particles flown across the bond $\{x, y\}$ in the time interval $[0, t]$. Given a trajectory $\eta(s)$, $0 \le s \le t$, the instantaneous current across $\{x, y\}$ is defined as $dQ^{x,y}_t/dt$. This is a sum of δ–functions localized at the jump times with weight $+1$, resp. -1, if a particle jumped from x to y, resp. from y to x.

For a given realization of the process $\eta(t)$ in $D\big(\mathbb{R}_+; X^{\Lambda_N}\big)$, we define the corresponding empirical current $\mathcal{J}^N$ as follows. Let $T > 0$ and pick a smooth vector field $G = (G_1, \dots, G_d)$ defined on $[0, T] \times \Lambda$. We then set

$$\begin{aligned}\langle\!\langle \mathcal{J}^N, G\rangle\!\rangle_T &= \int_0^T dt \int_\Lambda du\, G(t, u) \cdot \mathcal{J}^N(t, u)\\ &= \frac{1}{N^{d+1}} \sum_{i=1}^d \sum_x \int_0^T G_i(t, x/N)\, dQ^{x,x+e_i}(t),\end{aligned} \tag{3.2}$$

where $\cdot$ stands for the inner product in $\mathbb{R}^d$ and we sum over all x such that either $x \in \Lambda_N$ or $x + e_i \in \Lambda_N$. The empirical current $\mathcal{J}^N$ is therefore a signed measure on $\big([0, T] \times \Lambda\big)^d$, while we recall that the empirical density is a positive measure on Λ. The normalization $N^{-(d+1)}$ in (3.2) has been chosen so that the empirical current has a finite limit as $N \to \infty$.

The local conservation of the number of particles is expressed by

$$\eta_x(t) - \eta_x(0) + \sum_{y:|x-y|=1} Q^{x,y}(t) = 0.$$

It gives the following continuity equation for the empirical density and current. Let G be a smooth function on a neighborhood of the closure of Λ. Denote by $\nabla_N G$ the vector field whose coordinates are $(\nabla_N G)_i(u) = N[G(u + e_i/N) - G(u)]$. Then

$$\langle \pi^N(T), G\rangle - \langle \pi^N(0), G\rangle = \langle\!\langle \mathcal{J}^N, \nabla_N G\rangle\!\rangle_T - \int_0^T \frac{1}{N^d} \sum_{\substack{x\in\Lambda_N, y\notin\Lambda_N \\ |x-y|=1}} G(y/N) d\,Q^{x,y}(t)$$

The above equation can be formally stated as the continuity equation

$$\partial_t \pi^N + \nabla_N \cdot \mathcal{J}^N = 0 \tag{3.3}$$

In particular, given the initial condition, the trajectory of the process, described by the empirical density π^N can be completely recovered from the empirical current $\mathcal{J}^N$.

We briefly discuss at the heuristic level the law of large numbers, as $N \to \infty$, for the empirical density and the empirical current. Details are given in Appendix A. Fix a sequence of configurations η^N and assume that its associated empirical measure π^N converges to $\rho_0(u)du$ for some density profile $\rho_0 : \Lambda \to \mathbb{R}_+$. Let us denote by $\rho = \rho(t,u)$, $J = J(t,u)$, the limiting values of $\pi^N(t,u)$, $\mathcal{J}^N(t,u)$, respectively. Here $\pi^N(t,u)$ is the empirical density associated to the configuration $\eta(t)$ and $\mathcal{J}^N(t,u)$ has been defined in (3.2).

The microscopic relation (3.3) implies the continuity equation

$$\partial_t \rho + \nabla \cdot J = 0 \tag{3.4}$$

To derive a closed evolution for ρ and J, we need to express the current J in terms of the density ρ. To simplify the exposition, we assume the process to be gradient: there exist local functions $h_0^{(i)}(\eta)$, $i = 1, \dots, d$, depending on the configuration η around 0, so that for any $i = 1, \dots, d$

$$c^0_{x,x+e_i}(\eta) - c^0_{x+e_i,x}(\eta) = h_x^{(i)}(\eta) - h_{x+e_i}^{(i)}(\eta)$$

where $h_x^{(i)}$ is the function $h_0^{(i)}$ evaluated on the configuration η translated by x.

Denote by μ_λ the infinite volume grand canonical ensemble relative to the Hamiltonian $\mathcal{H}$ with chemical potential λ. Choose the chemical potential $\lambda = \lambda(\rho)$ so that $\mu_\lambda[\eta_0] = \rho$ and define

$$d^{(i)}(\rho) \;=\; \mu_{\lambda(\rho)}\big[h_0^{(i)}\big]\,, \quad \chi^{(i)}(\rho) \;:=\; (1/2)\mu_{\lambda(\rho)}\big[c^0_{0,e_i} + c^0_{e_i,0}\big] \tag{3.5}$$

We show in Appendix A. that the current J can be expressed in terms of the density ρ as

$$J = -\frac{1}{2}D(\rho)\nabla\rho + \chi(\rho)E =: J(\rho) \tag{3.6}$$

where D and χ are $d \times d$ diagonal matrices with entries $D_{ii}(\rho) = \frac{d}{d\rho}d^{(i)}(\rho)$ and $\chi_{ii}(\rho) = \chi^{(i)}(\rho)$.

For non gradient systems the diffusion matrix D and the mobility χ are not in general diagonal. In such a situation D is given by a Green–Kubo formula [see Ref. (33), II.2.2] and χ can be obtained by linear response theory [see Ref. (33), II.2.5]. These coefficients are related by 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 to the Hamiltonian $\mathcal{H}$,[33].

To conclude the description of the evolution, it remains to examine the evolution at the boundary of Λ. We claim that the density is fixed there because we speeded up diffusively the non-conservative Glauber dynamics at the boundary:

$$\lambda\big(\rho(t,u)\big) = \lambda_0(u) \qquad u \in \partial\Lambda \tag{3.7}$$

The macroscopic evolution of the density and the current is thus described by the equation

$$\begin{cases} \partial_t\rho + \nabla\cdot J = 0, & u \in \Lambda \\ J = -\frac{1}{2}D(\rho)\nabla\rho + \chi(\rho)E, & u \in \Lambda \\ \lambda\big(\rho(t,u)\big) = \lambda_0(u), & u \in \partial\Lambda \\ \rho(0,\cdot) = \rho_0(\cdot). \end{cases}$$

The stationary density profile $\bar\rho = \bar\rho(u)$, $u \in \Lambda$, is the stationary solution of the hydrodynamic equation, that is

$$\begin{cases} \nabla\cdot J(\bar\rho(u)) = 0\,, & u \in \Lambda \\ \lambda(\bar\rho(u)) = \lambda_0(u) & u \in \partial\Lambda, \end{cases}$$

If we let the macroscopic time diverge, $t \to \infty$, $\rho(t) \to \bar\rho$ and $J(\rho(t))$ converges to $J(\bar\rho)$, which is the current maintained by the stationary state.

We next discuss the large deviation properties of the empirical current. More details are given in Appendix A. As before we consider a sequence of initial configuration η^N such that the empirical density $\pi^N(\eta^N)$ converges to some density profile ρ_0. We fix a smooth vector field $j : [0,T] \times \Lambda \to \mathbb{R}^d$. The large deviation principle for the current states that

$$\mathbb{P}^N_{\eta^N}(\mathcal{J}^N(t,u) \approx j(t,u),\ (t,u) \in [0,T]\times\Lambda) \sim \exp\left\{-N^d\,\mathcal{I}_{[0,T]}(j)\right\} \tag{3.8}$$

where the rate functional $\mathcal{I}$ is

$$\mathcal{I}_{[0,T]}(j) \;=\; \frac{1}{2}\int_0^T dt\, \langle [j(t) - J(\rho(t))],\, \chi(\rho(t))^{-1}[j(t) - J(\rho(t))]\rangle \tag{3.9}$$

in which $\rho(t) = \rho(t,u)$ is obtained by solving the continuity equation

$$\begin{cases} \partial_t \rho(t,u) + \nabla \cdot j(t,u) = 0 \\ \rho(0,u) = \rho_0(u) \end{cases} \tag{3.10}$$

and $J(\rho)$ is given by (3.6).

Of course there are compatibility conditions to be satisfied, for instance if we have chosen a j such that $\rho(t,u)$ becomes negative for some $(t,u) \in [0,T]\times\Lambda$ then $\mathcal{I}_{[0,T]}(j) = +\infty$. Notice that, even if not indicated explicitly in the notation, the rate functional $\mathcal{I}$ depends on the initial density profile ρ_0, through equation (3.10).

We note that in the large deviation functional (3.9) the fluctuation of the density $\rho(t)$ is determined by the current $j(t)$. The large deviations properties of the density, which we described in Refs. (3–5) for non equilibrium stochastic lattice gases, can thus be deduced from the ones of the current, see Appendix A. for the details. This is due to the fact that the continuity equation, as already remarked, holds exactly at the microscopic level, see (3.3). On the other hand the constitutive Eq. (3.6) holds only in the limit $N \to \infty$ when fluctuations can be neglected.

4. LARGE DEVIATION OF THE TIME AVERAGED CURRENT

We want to study the fluctuations of the time average of the empirical current over a large time interval $[0, T]$; the corresponding probability can be obtained from the space time large deviation principle (3.8). Fix $T > 0$ and a divergence free vector field $J = J(u)$. We introduce the set of possible paths j of the current with time average J

$$\mathcal{A}_{T,J} = \left\{ j = j(t,u) \;:\; \frac{1}{T}\int_0^T dt\; j(t,u) = J(u) \right\}$$

The condition of vanishing divergence on J is required by the local conservation of the number of particles. By the large deviations principle (3.8), for T and N large we have

$$\mathbb{P}^N_{\eta^N}\left(\frac{1}{T}\int_0^T dt\; \mathcal{J}^N(t) \approx J \right) \sim \exp\{-N^d T\, \Phi(J)\} \tag{4.1}$$

where the logarithmic equivalence is understood by sending *first* $N \to \infty$ and *then* $T \to \infty$. In Subsec. 6.4 below we shall show that for the zero range process

the limits can be taken in the opposite order; we expect this to be true in general. The functional Φ is given by

$$\Phi(J) = \lim_{T\to\infty} \inf_{j\in\mathcal{A}_{T,J}} \frac{1}{T}\,\mathcal{I}_{[0,T]}(j) = \inf_{T>0} \inf_{j\in\mathcal{A}_{T,J}} \frac{1}{T}\,\mathcal{I}_{[0,T]}(j) \tag{4.2}$$

By a standard sub–additivity argument we show that the limit $T\to\infty$ exists and coincides with the infimum in T. Indeed, given $j_1\in\mathcal{A}_{T,J}$ and $j_2\in\mathcal{A}_{S,J}$, we have

$$\mathcal{I}_{[0,T+S]}(j) = \mathcal{I}_{[0,T]}(j_1) + \mathcal{I}_{[0,S]}(j_2) \tag{4.3}$$

where j is obtained by gluing j_1 and j_2. Here we used the invariance of $\mathcal{I}$ under time shift and that $j_1\in\mathcal{A}_{T,J}$ implies that the corresponding density ρ_1, obtained by solving the continuity Eq. (3.10), satisfies $\rho_1(0)=\rho_1(T)$ so that the densities match at $t=T$. From the previous equation we get the sub–additivity property:

$$\inf_{j\in\mathcal{A}_{T+S,J}} \mathcal{I}_{[0,T+S]}(j) \le \inf_{j\in\mathcal{A}_{T,J}} \mathcal{I}_{[0,T]}(j) + \inf_{j\in\mathcal{A}_{S,J}} \mathcal{I}_{[0,S]}(j)$$

Even if the rate functional $\mathcal{I}$ depends on the initial density profile ρ_0, by taking the limit in (4.2) it is easy to show Φ does not.

We now prove that Φ is a convex functional. Let $0<p<1$ and $J=pJ_1+(1-p)J_2$, we want to show that $\Phi(J)\le p\Phi(J_1)+(1-p)\Phi(J_2)$. By (4.2), given $\varepsilon>0$ we can find $T>0$, $j_1\in\mathcal{A}_{pT,J_1}$, and $j_2\in\mathcal{A}_{(1-p)T,J_2}$ so that

$$\Phi(J_1) \ge \frac{1}{pT}\,\mathcal{I}_{[0,pT]}(j_1) - \varepsilon$$
$$\Phi(J_2) \ge \frac{1}{(1-p)T}\,\mathcal{I}_{[0,(1-p)T]}(j_2) - \varepsilon$$

By the same arguments used in (4.3), the path obtained by gluing j_1 with j_2, denoted by j, is in the set $\mathcal{A}_{T,J}$. Therefore,

$$\Phi(J) \le \frac{1}{T}\,\mathcal{I}_{[0,T]}(j) \le p\,\Phi(J_1) + (1-p)\,\Phi(J_2) + \varepsilon$$

which proves the convexity of Φ. These arguments are standard in proving the existence and convexity of thermodynamic functions in statistical mechanics.

We next study the variational problem on the right hand side of (4.2). We begin by deriving an upper bound. Given $\rho=\rho(u)$ and $J=J(u)$, $\nabla\cdot J=0$, let us introduce the functionals

$$\mathcal{U}(\rho,J) = \frac{1}{2}\langle J-J(\rho),\,\chi(\rho)^{-1}[J-J(\rho)]\rangle \tag{4.4}$$

$$U(J) = \inf_{\rho}\,\mathcal{U}(\rho,J) \tag{4.5}$$

where the minimum in (4.5) is carried over all profiles ρ satisfying the boundary condition (3.7) and $J(\rho)$ is given by (3.6). When J is constant, that is, in the one-dimensional case, the functional U is the one introduced in Ref. (9).

We claim that

$$\Phi(J) \le U(J). \tag{4.6}$$

The strategy to prove this bound is quite simple, see also Ref. (9). Let $\hat\rho = \hat\rho(J)$ be the density profile which minimizes the variational problem (4.5). Given the initial density profile ρ_0, we choose some fixed time $\tau > 0$ and a current $\hat\jmath = \hat\jmath(u)$ which moves the density from ρ_0 to $\hat\rho$ in a time lag τ, namely such that $\tau\nabla\cdot\hat\jmath = \rho_0 - \hat\rho$. We now construct the path $j = j(t,u)$, $(t,u) \in [0,T]\times\Lambda$ as follows

$$j(t) = \begin{cases} \hat\jmath & \text{if } 0 \le t < \tau \\ \frac{T}{T-2\tau}\, J & \text{if } \tau \le t < T-\tau \\ -\hat\jmath & \text{if } T-\tau \le t \le T \end{cases}$$

The corresponding density $\rho(t)$ is obtained by solving the continuity equation (3.10), i.e.

$$\rho(t) = \begin{cases} \rho_0 + \frac{t}{\tau}(\hat\rho - \rho_0) & \text{if } 0 \le t < \tau \\ \hat\rho & \text{if } \tau \le t < T-\tau \\ \rho_0 + \frac{T-t}{\tau}(\hat\rho - \rho_0) & \text{if } T-\tau \le t \le T \end{cases}$$

It is straightforward to verify that $j \in \mathcal{A}_{T,J}$, as well as $\lim_{T\to\infty} \frac{1}{T}\,\mathcal{I}_{[0,T]}(j) = U(J)$.

By the convexity of $\Phi(J)$ we can improve the upper bound (4.6) for free. Let us denote by U^{**} the convex envelope of U, i.e. the largest convex functional below U. By taking the convex envelope in (4.6) we get

$$\Phi(J) \le U^{**}(J) \tag{4.7}$$

We next discuss a lower bound for the variational problem (4.2). We denote by $\widetilde{\mathcal{U}}$ and $\widetilde{U}$ the same functionals as in (4.4)–(4.5), but now defined on the space of all currents without the conditions of vanishing divergence. Let also $\widetilde{U}^{**}$ be the convex envelope of $\widetilde{U}$. Let $j \in \mathcal{A}_{T,J}$. By the convexity of $\widetilde{U}^{**}$ in the set of all currents, we get

$$\begin{aligned} \frac{1}{T}\mathcal{I}_{[0,T]}(j) &= \frac{1}{T}\int_0^T dt\, \widetilde{\mathcal{U}}(\rho(t), j(t)) \;\ge\; \frac{1}{T}\int_0^T dt\, \widetilde{U}(j(t)) \\ &\ge \frac{1}{T}\int_0^T dt\, \widetilde{U}^{**}(j(t)) \;\ge\; \widetilde{U}^{**}(J) \end{aligned}$$

which implies

$$\Phi(J) \;\ge\; \widetilde{U}^{**}(J) \tag{4.8}$$

The upper and lower bounds (4.7) and (4.8) are different in general. For a divergence free J we have $\widetilde{U}(J) = U(J)$ but since the convex envelopes are considered in different spaces, we only have $\widetilde{U}^{**}(J) \le U^{**}(J)$.

The derivation of the upper bound shows that our result differs from the one in Ref. (9) if U is not convex. Moreover, if $\Phi(J) < U(J)$, the optimal density path ρ in the variational problem (4.2) must be time dependent.

We now examine how different behaviors of the solution to the variational problem (4.2) reflect different dynamical regimes that we interpret as dynamical phase transitions. It is convenient to work in the time interval $[-T, T]$ instead of $[0, T]$. We consider the system in the ensemble defined by conditioning on the event $(2T)^{-1}\int_{-T}^{T} dt\ \mathcal{J}^N(t) = J$ with N and T large. The parameter J plays therefore the role of an intensive thermodynamic variable and the convexity of Φ expresses a stability property with respect to variations of J.

If $\Phi(J) = U(J)$ and the minimum for (4.5) is attained for $\rho = \hat{\rho}(J)$ we have a state analogous to a unique phase: by observing the system at any fixed time t we see, with probability converging to one as $N, T \to \infty$, the density $\pi^N(t) \sim \hat{\rho}(J)$ and the current $\mathcal{J}^N(t) \sim J$.

When $\Phi(J) = U^{**}(J) < U(J)$, we have a state analogous to a phase coexistence. Suppose for example $J = pJ_1 + (1-p)J_2$ and $U(J) > U^{**}(J) = pU(J_1) + (1-p)U(J_2)$ for some p, J_1, J_2. The values p, J_1, J_2 are determined by J and U. The density profile is then not determined, but rather we observe with probability p the profile $\hat{\rho}(J_1)$ and with probability $1-p$ the profile $\hat{\rho}(J_2)$. Actually there is a memory of initial condition: if we take $\rho(-T) = \rho(T) = \hat{\rho}(J_1)$ we will see a density close to $\hat{\rho}(J_1)$ in the time intervals $[-T, -(1-p+\delta)T]$ and $[(1-p+\delta)T, T]$, and a density close to $\hat{\rho}(J_2)$ in the time interval $[-(1-p-\delta)T, (1-p-\delta)T]$; here $\delta > 0$.

Consider now the case in which a minimizer for (4.2) is a function $\hat{\jmath}(t)$ not constant in t. This is possible (an example will be given in Subsection 6.2) only when $\Phi(J) < U^{**}(J)$. Suppose first that $\hat{\jmath}(t)$ is periodic with period τ and denote by $\hat{\rho}(t)$ the corresponding density. Of course we have $\tau^{-1}\int_0^\tau dt\ \hat{\jmath}(t) = J$. In such a case we have in fact a one parameter family of minimizers which are obtained by a time shift $\alpha \in [0, \tau]$. By choosing $2T$ an integral multiple of τ and $\rho(-T) = \hat{\rho}(\alpha)$ for some $\alpha \in [0, \tau]$ then the empirical density in the conditional ensemble will follow the path $\hat{\rho}(t + \alpha + T)$. This behavior is analogous to a non translation invariant state in equilibrium statistical mechanics, like a crystal. Finally if $\hat{\jmath}(t)$ is time dependent and not periodic the corresponding state is analogous to a quasi–crystal.

The asymptotic (4.1) can be formulated in terms of the Laplace transform of the empirical current as follows. For each divergence free, time independent, vector field $\lambda = \lambda(u)$ we have

$$\lim_{T\to\infty}\lim_{N\to\infty}\frac{1}{T\,N^d}\log \mathbb{E}^N_{\eta^N}\left(e^{N^d\langle\!\langle \mathcal{J}^N,\lambda\rangle\!\rangle_T}\right) = \Phi^*(\lambda) \tag{4.9}$$

where $\Phi^*(\lambda)$ is the Legendre transform of $\Phi(J)$:

$$\Phi^*(\lambda) = \sup_J \{\langle \lambda, J\rangle - \Phi(J)\},$$

where the supremum is carried over all the divergence free vector fields J. It follows from (4.6) that $U^* \le \Phi^*$.

We conclude this section deriving a variational expression for U^*. Recall the definitions (4.4), (4.5) of U.

$$\begin{aligned} U^*(\lambda) &= \sup_{J,\rho} \left\{ \langle \lambda, J\rangle - \frac{1}{2}\langle [J - J(\rho)], \chi(\rho)^{-1}[J - J(\rho)]\rangle \right\} \\ &= \sup_{J,\rho} \left\{ -\frac{1}{2}\langle [J - J(\rho) - \chi(\rho)\lambda], \chi(\rho)^{-1}[J - J(\rho) - \chi(\rho)\lambda]\rangle \right. \\ &\qquad \left. + \frac{1}{2}\langle \lambda, \chi(\rho)\lambda\rangle + \langle \lambda, J(\rho)\rangle \right\} \end{aligned}$$

To compute the supremum over J we decompose the vector field $J(\rho) + \chi(\rho)\lambda$ as follows

$$J(\rho) + \chi(\rho)\lambda = \chi(\rho)\nabla\psi + [J(\rho) + \chi(\rho)\big(\lambda - \nabla\psi\big)] \tag{4.10}$$

where ψ solves

$$\begin{cases} \nabla \cdot \big(\chi(\rho)\nabla\psi\big) = \nabla \cdot (J(\rho) + \chi(\rho)\lambda\big) & u \in \Lambda \\ \psi(u) = 0 & u \in \partial\Lambda \end{cases}$$

Since the second term in the decomposition (4.10) is divergence free we get

$$U^*(\lambda) \;=\; \sup_\rho \left\{ -\frac{1}{2}\langle \nabla\psi, \chi(\rho)\nabla\psi\rangle + \frac{1}{2}\langle \lambda, \chi(\rho)\lambda\rangle + \langle \lambda, J(\rho)\rangle \right\} \tag{4.11}$$

where the supremum is over all density profiles ρ satisfying $F_0'(\rho(u)) = \lambda_0(u)$, $u \in \partial\Lambda$.

5. TIME–REVERSAL AND GALLAVOTTI–COHEN SYMMETRY

In this Section we discuss the properties of the rate functional for the current under time reversal. We also show that the functional Φ, which measures the probability of deviations of the time averaged current, satisfies a fluctuation theorem analogous to the Gallavotti–Cohen symmetry.

5.1. Time–Reversal Properties of the Rate Functional

In the previous Sections we discussed a large deviation principle given a fixed initial condition η^N associated to a density profile ρ_0, i.e. $\pi^N(\eta^N) \to \rho_0$. Now we

consider instead the stationary process, namely the initial condition is distributed according to the invariant measure μ^N which is defined by $\sum_\eta \mu^N(\eta) L_N f(\eta) = 0$ for any observable $f : X^{\Lambda_N} \to \mathbb{R}$; recall the generator L_N has been defined in (2.3). As discussed in the Introduction, the large deviations of the empirical density under the distribution μ^N are described by the non equilibrium free energy F, i.e.,

$$\mu^N(\pi^N \approx \rho) \sim \exp\{-N^d F(\rho)\} \tag{5.1}$$

In Refs. (3, 4) we show that the functional F, which for equilibrium states is trivially related to the free energy, can be characterized by a variational problem on the dynamical rate functional for the density $\mathcal{F}$ introduced in (1.4), see also (A.15). To this variational problem is associated a Hamilton–Jacobi equation which plays a crucial role.

In order to analyze the large deviations properties of the stationary process, since the initial condition is not fixed, it is natural to consider the joint fluctuations of the empirical density and current. We have

$$\mathbb{P}^N_{\mu^N}\left(\pi^N \approx \rho, \mathcal{J}^N \approx j \;\; t \in [-T, T]\right) \sim \exp\left\{ - N^d \mathcal{G}_{[-T,T]}(\rho, j)\right\} \tag{5.2}$$

Here $\mathbb{P}^N_{\mu^N}$, a probability measure on the space $D(\mathbb{R}; X^{\Lambda_N})$, is the stationary process. Of course, fluctuations of the density and of the current are not independent since the continuity equation $\partial_t \rho + \nabla \cdot j = 0$ must be satisfied. Therefore the large deviation functional is

$$\mathcal{G}_{[-T,T]}(\rho, j) = \begin{cases} F(\rho(-T)) + \mathcal{I}_{[-T,T]}(j) & \text{if } \partial_t \rho + \nabla \cdot j = 0 \\ +\infty & \text{otherwise} \end{cases} \tag{5.3}$$

where $\mathcal{I}$ has been introduced in (3.9). If we are interested only in the current fluctuations in the stationary process we get the appropriate rate functional by projecting (5.3),

$$\inf_{\rho_0} \{F(\rho_0) + \mathcal{I}_{[-T,T]}(j)\}.$$

Let us denote by L^a_N the adjoint of the generator L_N (2.3) with respect to the invariant measure μ^N. We call the process generated by L^a_N, which is still Markovian, the adjoint process. We remark that the invariant measure of the adjoint process is again μ^N. Given a path $\eta \in D(\mathbb{R}; X^{\Lambda_N})$ its time reversed is naturally defined as $[\vartheta \eta](t) = \eta(-t)$. The stationary adjoint process, that we denote by $\mathbb{P}^{N,a}_{\mu^N}$, is the time reversal of $\mathbb{P}^N_{\mu^N}$, i.e. we have $\mathbb{P}^{N,a}_{\mu^N} = \mathbb{P}^N_{\mu^N} \circ \vartheta^{-1}$. We extend the definition of the time reversal operator ϑ to the current as $[\vartheta j](t) = -j(-t)$. Note that the current j changes sign under time–reversal. Then

$$\mathbb{P}^N_{\mu^N}\left(\pi^N \approx \rho, \mathcal{J}^N \approx j \; t \in [-T, T]\right) = \mathbb{P}^{N,a}_{\mu^N}\left(\pi^N \approx \vartheta\rho, \mathcal{J}^N \approx \vartheta j \; t \in [-T, T]\right)$$

At the level of large deviations this implies

$$\mathcal{G}_{[-T,T]}(\rho, j) = \mathcal{G}^a_{[-T,T]}(\vartheta\rho, \vartheta j) \tag{5.4}$$

where $\mathcal{G}^a_{[-T,T]}$ is the large deviation functional for the adjoint process.

The relationship (5.4) has far reaching consequences. We next show that it implies a fluctuation dissipation relation for the current. We assume that the adjoint process has a dynamical large deviations principle of the same form as (5.3) with $\mathcal{I}$ replaced by $\mathcal{I}^a$ where

$$\mathcal{I}^a_{[-T,T]}(j) \;=\; \frac{1}{2}\int_{-T}^{T} dt\, \langle [j(t) - J^a(\rho(t))],\, \chi(\rho(t))^{-1}[j(t) - J^a(\rho(t))]\rangle,$$

in which $J^a(\rho)$ is the typical value of the current of the adjoint process. We divide both sides of (5.4) by $2T$ and take the limit $T \to 0$. By using (5.3) we get

$$\left\langle \frac{\delta F}{\delta \rho}, \partial_t \rho \right\rangle = \frac{1}{2}\langle j - J(\rho),\, \chi(\rho)^{-1}[j - J(\rho)]\rangle - \frac{1}{2}\langle j + J^a(\rho),\, \chi(\rho)^{-1}[j + J^a(\rho)]\rangle$$

recalling that $\partial_t \rho + \nabla \cdot j = 0$, this is equivalent to

$$-\left\langle \frac{\delta F}{\delta \rho}, \nabla \cdot j \right\rangle = -\langle J(\rho) + J^a(\rho),\, \chi(\rho)^{-1} j\rangle + \frac{1}{2}\langle J(\rho) + J^a(\rho),\, \chi(\rho)^{-1}[J(\rho) - J^a(\rho)]\rangle$$

which has to be satisfied for any ρ and j. By using that $\delta F/\delta\rho$ vanishes at the boundary of Λ, see Ref. (4), we can integrate by parts the left hand side above and get

$$J(\rho) + J^a(\rho) = -\chi(\rho)\nabla \frac{\delta F}{\delta \rho} \tag{5.5}$$

$$\langle J(\rho),\, \chi(\rho)^{-1} J(\rho)\rangle = \langle J^a(\rho),\, \chi(\rho)^{-1} J^a(\rho)\rangle. \tag{5.6}$$

Equation (5.5) is a fluctuation dissipation for the current analogous to the one for the density discussed in Ref. (4). It also extends the relationships between currents and thermodynamic forces, see e.g. Ref. (29), to a non equilibrium setting. By plugging (5.5) into (5.6) we also get another derivation of the Hamilton–Jacobi equation mentioned before, i.e.

$$\frac{1}{2}\left\langle \nabla \frac{\delta F}{\delta \rho}, \chi(\rho)\nabla \frac{\delta F}{\delta \rho} \right\rangle - \left\langle \frac{\delta F}{\delta \rho}, \nabla \cdot J(\rho) \right\rangle = 0$$

Let us now consider the variational problem (4.2) as well as the same problem for the functional $\mathcal{I}^a$, we denote by Φ^a the corresponding functional. From (5.4) we get

$$\Phi(J) = \Phi^a(-J) \tag{5.7}$$

For reversible process this symmetry states that the functional Φ is even.

Let us consider a path $j(t), t \in [-T, T]$ such that $(2T)^{-1} \int_{-T}^{T} dt\ j(t) = J$ for some divergence free vector field J. Recalling (3.6) and that $D(\rho)\chi(\rho)^{-1} = F_0''(\rho)$ we have

$$\chi(\rho)^{-1} J(\rho) = -\frac{1}{2} \nabla F_0'(\rho) + E$$

Since $F_0'(\rho(u)) = \lambda_0(u), u \in \partial\Lambda$, by developing the square in (3.9) and integrating by parts we get

$$\frac{1}{2T} \mathcal{G}_{[-T,T]}(\rho, j) = \frac{1}{2T} \mathcal{G}_{[-T,T]}(\vartheta\rho, \vartheta j) - 2\langle J, E\rangle + \int_{\partial\Lambda} d\Sigma\ \lambda_0\, J \cdot \hat{n} \qquad (5.8)$$

where $d\Sigma$ is the surface measure on $\partial\Lambda$ and $\hat{n}$ is the outward normal to Λ. In particular this relation implies that if $\hat{\rho}, \hat{j}$ is an optimal path for the variational problem defining $\Phi(J)$ then $\vartheta\hat{\rho}, \vartheta\hat{j}$ is an optimal path for the variational problem defining $\Phi(-J)$.

By taking the limit $T \to \infty$ in (5.8) we get

$$\Phi(J) - \Phi(-J) = \Phi(J) - \Phi^a(J) = -2\langle J, E\rangle + \int_{\partial\Lambda} d\Sigma\ \lambda_0\, J \cdot \hat{n} \qquad (5.9)$$

which is a Gallavotti–Cohen type symmetry in our space time dependent setup for macroscopic observables. Note that the right hand side of (5.9) is the power produced by the external field and the boundary reservoirs (recall E is the external field and λ_0 the chemical potential of the boundary reservoirs). We mention that the functional U, as defined in (4.5), also satisfies the relationship (5.9); in the one-dimensional case this has been observed in Ref. (9).

5.2. Entropy Production

Recall that we denote by $\mathbb{P}^N_{\mu^N}$ the stationary state and by $\mathbb{P}^{N,a}_{\mu^N}$ its time reversed, i.e. the stationary adjoint process. In the context of Markov processes the Gallavotti–Cohen observable is defined as

$$W_N(T) = -\frac{1}{2TN^d} \log \frac{d\mathbb{P}^{N,a}_{\mu}}{d\mathbb{P}^N_{\mu}}\bigg|_{[-T,T]} \qquad (5.10)$$

where the subscript means that we consider both distributions in the time interval $[-T, T]$. We introduced the factor $2T\,N^d$ in order to discuss the asymptotic $N, T \to \infty$. As discussed in Ref. (26), §2.4, $W_N(T)$ can be interpreted as the microscopic production of the Gibbs entropy. For N fixed and $T \to \infty$ the functional W_N satisfies a large deviation principle with rate function f_N namely,

$$\mathbb{P}^N_{\mu^N}(W_N(T) \approx q) \ \sim\ \exp\{-2TN^d\, f_N(q)\} \qquad (5.11)$$

In Refs. (18, 24, 26) it is shown that W_N satisfies the Gallavotti–Cohen symmetry, which states that the odd part of f_N is linear with a universal coefficient: $f_N(q) - f_N(-q) = -q$.

An elementary computation, analogous to the one in Ref. (26), shows that, for the stochastic lattice gases as introduced in Sec. 2, we can express the functional W_N in terms of the empirical current. More precisely, we have

$$W_N(T) = -\frac{1}{2TN^d}\Bigg\{ \log\frac{\mu^N(\eta(T))}{\mu^N(\eta(-T))} + \mathcal{H}(\eta(T)) - \mathcal{H}(\eta(-T)) \\ - \frac{2}{N}\sum_{j=1}^{d}\sum_{x} E_j(x/N)Q^{x,x+e_j}([-T,T]) + \sum_{\substack{x\in\Lambda_N \\ y\notin\Lambda_N}} \lambda_0(y/N)Q^{x,y}([-T,T])\Bigg\},$$

where the summation is carried over all x such that either $x \in \Lambda_N$ or $x + e_j \in \Lambda_N$. The previous equation can be understood as an entropy balance. Indeed, in the right hand side the first term is, for N large, the difference of the non equilibrium free energy at times T and $-T$, the second is the difference of the energy and the third is the work done by the external field E and the boundary reservoirs. Therefore, W_N can be interpreted as the total entropy produced by the system in the time interval $[-T, T]$.

Recalling the definition of the empirical current $\mathcal{J}^N$, we can rewrite the above equation as

$$W_N(T) = \frac{1}{2T}\Bigg\{ -\frac{1}{N^d}\left[\log\frac{\mu^N(\eta(T))}{\mu^N(\eta(-T))} + \mathcal{H}(\eta(T)) - \mathcal{H}(\eta(-T))\right] \\ + 2\langle\!\langle \mathcal{J}^N, E\rangle\!\rangle_{[-T,T]} - \frac{1}{N^d}\sum_{\substack{x\in\Lambda_N \\ y\notin\Lambda_N}} \lambda_0(y/N)Q^{x,y}([-T,T])\Bigg\} \tag{5.12}$$

We emphasize that, while the empirical current is a vector in $\mathbb{R}^d$, $W_N(t)$ is a scalar.

From the previous expression it follows that, for any $\delta > 0$

$$\lim_{T\to\infty}\lim_{N\to\infty} \mathbb{P}^N_{\eta^N}\left(\left| W_N(T) - 2\langle E, J(\bar\rho)\rangle + \int_{\partial\Lambda} d\Sigma\ \lambda_0 J(\bar\rho)\cdot\hat n\right| > \delta\right) = 0 \tag{5.13}$$

where we recall that $J(\bar\rho) = -(1/2)D(\bar\rho)\nabla\bar\rho + \chi(\bar\rho)E$ is the typical current.

We note that as $T \to \infty$ we can neglected the first line on the r.h.s. of (5.12) because it is a boundary term. We thus define

$$\widetilde{W}_N(T) = \frac{1}{2T}\left\{ 2\langle\!\langle \mathcal{J}^N, E\rangle\!\rangle_{[-T,T]} - \frac{1}{N^d}\sum_{\substack{x\in\Lambda_N \\ y\notin\Lambda_N}} \lambda_0(y/N)Q^{x,y}[-T,T]\right\} \tag{5.14}$$

which satisfies, as $T \to \infty$ with N fixed, the large deviation estimate (5.11) with the same rate function f_N.

On the other hand, since $\widetilde{W}_N(T)$ is a function of the empirical current, we can apply the large deviation principle (5.2). We then get, by taking *first* the limit $N \to \infty$ and *then* $T \to \infty$,

$$\mathbb{P}^N_{\mu^N}(\widetilde{W}_N(T) \approx q) \sim \exp\{-2TN^d\, f(q)\} \tag{5.15}$$

where the rate function f can be expressed in terms of the functional $\mathcal{I}$ namely

$$f(q) = \lim_{T\to\infty} \inf_{j\in\mathcal{B}_{T,q}} \frac{1}{2T}\mathcal{I}_{[-T,T]}(j)$$

in which we introduced the set of currents

$$\mathcal{B}_{T,q} := \left\{ j \,:\, \frac{1}{2T}\left[2\int_{-T}^{T} dt\, \langle j(t), E\rangle - \int_{-T}^{T} dt \int_{\partial\Lambda} d\Sigma\, \lambda_0 j(t)\cdot\hat{n}\right] = q \right\} \tag{5.16}$$

where we recall $d\Sigma$ is the surface measure on $\partial\Lambda$ and $\hat{n}$ is the outward normal to Λ.

Finally, since E and λ_0 are time independent we can take the time average of the empirical current in (5.16). Recalling (4.2), we get

$$f(q) = \inf_{J\in\mathcal{B}_q} \Phi(J) \tag{5.17}$$

where

$$\mathcal{B}_q := \left\{ J \,:\, 2\langle J, E\rangle - \int_{\partial\Lambda} d\Sigma\, \lambda_0 J\cdot\hat{n} = q\,,\ \nabla\cdot J = 0 \right\} \tag{5.18}$$

where we inserted the condition $\nabla\cdot J = 0$ because other things do not happen. The content of the variational problem (5.17) is to look for, among all possible currents, the best one to have a fixed entropy production. It is straightforward to verify that the symmetry (5.9) implies the classical Gallavotti–Cohen symmetry for the limiting functional f, i.e. $f(q) - f(-q) = -q$. On the other hand, if $d > 1$, Eq. (5.9) is more general than the classical Gallavotti–Cohen symmetry.

In the above argument we first took the limit $N \to \infty$ and next $T \to \infty$, but we expect that these limits could be taken in any order. In particular these would imply $\lim_{N\to\infty} f_N(q) = f(q)$. In Section 6.4 we prove that this is the case for the zero range process. We finally note that in the one–dimensional case, setting $\Lambda = [0, 1]$, we can easily solve (5.17). We get

$$f(q) = \Phi\left(\frac{q}{2\langle E\rangle - [\lambda_0(1) - \lambda_0(0)]}\right)$$

6. DYNAMICAL PHASE TRANSITIONS: EXAMPLES

As we have discussed in Sec. 4, we always have the following inequalities

$$\widetilde{U}^{**}(J) \le \Phi(J) \le U^{**}(J) \le U(J) \tag{6.1}$$

for any divergence free J. A natural question is when the above inequalities are strict and when are equalities, in particular when $\Phi = U$. As discussed in Section 4, the strict inequality $\Phi(J) < U(J)$ is a dynamical phase transition on the ensemble defined by conditioning on the event in which the time average current equals J. In this Section we discuss several examples which show that different scenarios actually do take place in concrete models. As we have shown in Section 3 the macroscopic behavior (including the probability of large fluctuations) of the system is determined by the transport coefficients $D(\rho)$ and $\chi(\rho)$. In this Section we consider these as given functions and discuss the properties of the variational problem defining Φ. Specific choices of D and χ correspond to well studied microscopic models, such as the simple exclusion processes, the zero range process, and the KMP model.[22]

In Subsec. 6.1 we find sufficient conditions on D and χ implying $\Phi = U$. In Subsec. 6.2 we discuss periodic boundary conditions: under appropriate conditions on the transport coefficient and the external field we show that the minimizer for the variational problem defining U is obtained when ρ is constant (in space). Moreover, by considering travelling waves, we find for J large a better (space-time dependent) strategy so that $\Phi < U$. These conditions hold in particular for the KMP model with no external field. Moreover, for the exclusion process with sufficiently large external field, we show that there exists a travelling wave path of current whose cost is strictly less than the constant (in time and space) one. This was first observed in Ref. (11). In Subsec. 6.3, we give an example where U is non convex which implies $\Phi < U$. Finally, in Subsec. 6.4 we compute the Legendre transform of U for the one dimensional zero range process in the presence of external field. As a byproduct, we show that the macroscopic limit $N \uparrow \infty$ and $T \uparrow \infty$ can be interchanged.

6.1. A Sufficient Condition for $\Phi = U$

We consider the case when the matrices $D(\rho)$ and $\chi(\rho)$ are multiple of the identity, i.e., there are strictly positive scalar functions still denoted by $D(\rho)$, $\chi(\rho)$, so that $D(\rho)_{i,j} = D(\rho)\delta_{i,j}$, $\chi(\rho)_{i,j} = \chi(\rho)\delta_{i,j}$, $i, j = 1, \dots, d$. We denote derivatives with a superscript. Let us first consider the case with no external field, i.e. $E = 0$, we shall prove that if

$$D(\rho)\chi''(\rho) \le D'(\rho)\chi'(\rho) \quad \text{for any } \rho \tag{6.2}$$

then $\Phi = U$. In this case U is necessarily convex.

Moreover we show that if

$$D(\rho)\chi''(\rho) = D'(\rho)\chi'(\rho) \quad \text{for any } \rho \tag{6.3}$$

then we have $\Phi = U$ for any external field E. We mention that under the condition (6.3), as shown in Ref. (8), §7, also the non equilibrium free energy F can be computed explicitly and it is a local functional.

Condition (6.2) is satisfied e.g. for the symmetric simple exclusion process, where $D = 1$ and $\chi(\rho) = \rho(1-\rho)$, $\rho \in [0,1]$. Condition (6.3) is satisfied either if D is proportional to χ' or χ is constant and D arbitrary. Examples are 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 the non interacting Ginzburg–Landau model, where $D(\rho)$, $\rho \in \mathbb{R}$, is an arbitrary strictly positive function and $\chi(\rho)$ is constant.

Let us consider first the case when $E = 0$ and condition (6.2) holds. In view of (3.9) and (4.4), to prove that $\Phi = U$ it is enough to show that for each $j = j(t,u) \in \mathcal{A}_{T,J}$, i.e., such that $T^{-1}\int_0^T dt\ j(t) = J$, and $\rho(t)$ such that $\partial_t \rho(t) + \nabla \cdot j(t) = 0$ we have

$$\frac{1}{T}\mathcal{I}_{[0,T]}(j) = \frac{1}{T}\int_0^T dt\ \mathcal{U}(\rho(t), j(t)) \geq U(J) \tag{6.4}$$

Instead of ρ we introduce a new variable α so that $\alpha = d(\rho) := \int^\rho d\rho' D(\rho')$. Condition (6.2) is then equivalent to the concavity of the function $X(\alpha) := \chi\big(d^{-1}(\alpha)\big)$ where d^{-1} is the inverse function of d. We introduce the functional

$$\mathcal{V}(\alpha, j) := \mathcal{U}(d^{-1}(\alpha), j) = \frac{1}{2}\left\langle j + \frac{1}{2}\nabla\alpha, \frac{1}{X(\alpha)}\left[j + \frac{1}{2}\nabla\alpha\right]\right\rangle$$

where we used (3.6). We claim that the functional $\mathcal{V}$ is jointly convex in (α, j). Let us first show that this implies the lower bound (6.4). We have

$$\begin{aligned}
\frac{1}{T}\int_0^T dt\ \mathcal{U}(\rho(t), j(t)) &= \frac{1}{T}\int_0^T dt\ \mathcal{V}(\alpha(t), j(t)) \\
&\geq \mathcal{V}\left(\frac{1}{T}\int_0^T dt\ \alpha(t), \frac{1}{T}\int_0^T dt\ j(t)\right) \\
&\geq \inf_\alpha \mathcal{V}(\alpha, J) = \inf_\rho \mathcal{U}(\rho, J) = U(J)
\end{aligned}$$

in which we used the convexity of $\mathcal{V}$ in the second step and $j \in \mathcal{A}_{T,J}$ in the third.

To prove that $\mathcal{V}$ is jointly convex we write

$$\mathcal{V}(\alpha, j) = \sup_a \mathcal{V}_a(\alpha, j)\,, \qquad \mathcal{V}_a(\alpha, j) := \left\langle j + \frac{1}{2}\nabla\alpha, a\right\rangle - \frac{1}{2}\langle a, X(\alpha)a\rangle$$

and the supremum is taken over all smooth vector fields $a = a(u)$ on Λ. Since $X(\alpha)$ is concave, for each fixed a the functional $\mathcal{V}_a$ is jointly convex. The claim follows.

In the case with non vanishing E, we can use the same argument, but the functional $\mathcal{V}$ is given by

$$\mathcal{V}(\alpha, j) := \mathcal{U}(d^{-1}(\alpha), j) = \frac{1}{2}\left\langle j + \frac{1}{2}\nabla\alpha - X(\alpha)E, \frac{1}{X(\alpha)}\left[j + \frac{1}{2}\nabla\alpha - X(\alpha)E\right]\right\rangle$$

Condition (6.3) is equivalent to $X''(\alpha) = 0$; in this case we can easily show, as before, that $\mathcal{V}$ is jointly convex.

6.2. Periodic Boundary Conditions

In this subsection we consider the case when $\Lambda = \mathbb{T}$, the one dimensional torus of side length one and constant external field E. If there is no external field, $E = 0$, then it is an equilibrium model; non equilibrium if $E \neq 0$.

Due to the periodic boundary conditions, we have the possibility of constructing a space time path $(\rho(t, u), j(t, u))$ of density and current in the form of a travelling wave for the variational problem (4.2) defining the functional Φ. In Ref. (11) Bodineau and Derrida perform the linear stability analysis of the constant (in space and time) profile showing, in particular, that for the weakly asymmetric simple exclusion process it becomes unstable for sufficiently large external field. However to prove the strict inequality $\Phi < U$ one should first show that the optimal density profile for the variational problem (4.5) defining U is indeed the constant one. By a numerical computation (with a finite N), in Ref. (11) is shown that the travelling wave path is the optimal one.

In this subsection, by soft arguments (Jensen inequality and convexity properties of the transport coefficients), we find sufficient conditions on D, χ, E and J implying that the optimal profile for the variational problem (4.5) defining the functional U is the constant one. Under other appropriate conditions, we can show that a suitable travelling wave, for J large enough, is better, for the variational problem (4.2), than the constant profile. These arguments, applied to the weakly asymmetric simple exclusion process with large enough external field, imply that there exists a travelling wave path which is better than the constant profile. On the other hand, for the KMP process with no external field the above arguments allow to give a complete analytical proof of the strict inequality $\Phi < U$.

In the context of periodic boundary conditions, the proof that $\Phi = U$ presented in the previous subsection applies if D is constant. In other words, we have that $\Phi(J) = U(J)$ for all J provided D is constant, χ is concave and $E = 0$.
Let $\mathcal{M}_m(\mathbb{T})$ the convex set of positive functions ρ on the torus $\mathbb{T}$ such that $\int_0^1 du\, \rho(u) = m$; we call m the mass of ρ. In this context,

$$U(J) \;=\; \inf_{\rho} \frac{1}{2}\int_0^1 du\, \frac{\{J - J(\rho)\}^2}{\chi(\rho)},$$

where the infimum is carried over $\mathcal{M}_m(\mathbb{T})$ and $J(\rho)$ is defined in (3.6). For each $v \in \mathbb{R}$, let $\Psi_v : \mathbb{R} \to \mathbb{R}_+$ be defined by

$$\Psi_v(J) = \inf_\rho \frac{1}{2} \int_0^1 du \, \frac{\{J + v[\rho - m] - J(\rho)\}^2}{\chi(\rho)} \tag{6.5}$$

where the infimum is carried over $\mathcal{M}_m(\mathbb{T})$.

We claim that for each $v \in \mathbb{R}$

$$\Phi \le \Psi_v \tag{6.6}$$

Indeed, consider a profile ρ_0 in $\mathcal{M}_m(\mathbb{T})$. Let $T = v^{-1}$ and set $\rho(t,u) = \rho_0(u - vt)$, $j(t,u) = J + v[\rho_0(u - tv) - m]$ in the time interval $[0, T]$. An elementary computation shows that the continuity equation holds and that the time average over the time interval $[0, T]$ of $j(\cdot, u)$ is equal J. In particular,

$$\Phi(J) \le \frac{1}{T} \int_0^T dt \, \mathcal{U}(\rho(t), j(t))$$

On the other hand, it is easy to show by periodicity that the right hand side is equal to

$$\frac{1}{2} \int_0^1 du \, \frac{\{J + v[\rho_0 - m] - J(\rho_0)\}^2}{\chi(\rho_0)}$$

By optimizing over the profile ρ_0, we conclude the proof of 6.6.

Fix a mass m, an external field E and a current J. If $J^2/\chi + E^2\chi$ is a convex function then

$$U(J) = \frac{1}{2} \frac{\{J - E\chi(m)\}^2}{\chi(m)} \tag{6.7}$$

and the optimal profile for the variational problem defining $U(J)$ is the constant profile $\rho(u) = m$. In particular if $1/\chi$ and $E^2\chi$ are convex functions then (6.7) holds for any J so that U is trivially convex.

Indeed, fix a mass m, a current J and an external field E. For any profile ρ in $\mathcal{M}_m(\mathbb{T})$,

$$\int_0^1 du \, \frac{\{J - J(\rho)\}^2}{\chi(\rho)} = \int_0^1 du \, \frac{\{J - E\chi(\rho)\}^2}{\chi(\rho)} + \int_0^1 du \, \frac{[(1/2)\nabla d(\rho)]^2}{\chi(\rho)}$$

because the cross term vanishes upon integration; here $d(\rho)$ is such that $d'(\rho) = D(\rho)$. We thus have

$$\begin{aligned} \int_0^1 du \, \frac{\{J - E\chi(\rho)\}^2}{\chi(\rho)} &= \int_0^1 du \left[\frac{J^2}{\chi(\rho)} + E^2\chi(\rho) \right] - 2EJ \\ &\ge \frac{J^2}{\chi(m)} + E^2\chi(m) - 2EJ \end{aligned}$$

where we used Jensen inequality, the convexity of $J^2/\chi + E^2\chi$, and $\rho \in \mathcal{M}_m(\mathbb{T})$. Therefore, for all profiles ρ in $\mathcal{M}_m(\mathbb{T})$,

$$\int_0^1 du\, \frac{[J - J(\rho)]^2}{\chi(\rho)} \geq \frac{\{J - E\chi(m)\}^2}{\chi(m)}.$$

Since the cost of the constant profile $\rho(u) = m$ is $(1/2)\{J - E\chi(m)\}^2/\chi(m)$, (6.7) is proven.

Fix a mass m, $e \in \mathbb{R}$ and take the external field $E = eJ$. If

$$[1 - e^2\chi(m)^2]\chi''(m) > 0 \tag{6.8}$$

we claim that there exists w in $\mathbb{R}$ such that

$$\limsup_{|J|\to\infty} \frac{\Psi_{wJ}(J)}{J^2} < \frac{\{1 - e\chi(m)\}^2}{2\chi(m)} \tag{6.9}$$

where Ψ_v has been defined in (6.5).

Fix a mass m, a current J, an external field $E = eJ$ and take $v = wJ$. For ρ in $\mathcal{M}_m(\mathbb{T})$, by expanding the square we get that

$$\begin{aligned}\int_0^1 du\, \frac{\{J + wJ[\rho - m] + (1/2)\nabla d(\rho) - E\chi(\rho)\}^2}{\chi(\rho)} \\ = J^2 \int_0^1 du\, \frac{\{1 + w[\rho - m] - e\chi(\rho)\}^2}{\chi(\rho)} + \frac{1}{4}\int_0^1 du\, \frac{[\nabla d(\rho)]^2}{\chi(\rho)}.\end{aligned} \tag{6.10}$$

because the cross term vanishes. Expand the square on the first integral. Let $F(r) = F_{w,m}(r)$ be the smooth function defined by

$$F(r) = \frac{\{1 + w[r - m]\}^2}{\chi(r)} - 2e + e^2\chi(r).$$

An elementary computation shows that

$$\begin{aligned}F''(m) = \frac{1}{\chi(m)^3}\{2\chi(m)^2w^2 - 4\chi(m)\chi'(m)w + 2\chi'(m)^2 \\ - \chi(m)\chi''(m) + e^2\chi''(m)\chi(m)^3\}.\end{aligned}$$

Let $w = \chi'(m)/\chi(m)$. For this choice $F''(m) < 0$. In particular, we can choose a non constant profile $\rho(u)$ in $\mathcal{M}_m(\mathbb{T})$ close to m such that $F''(\rho(u)) < 0$ for every u. Hence, by Jensen inequality, the coefficient of J^2 in (6.10) is strictly less than

$$\frac{\{1 - e\chi(m)\}^2}{\chi(m)}.$$

The statement follows.

For the simple exclusion process we have $D(\rho) = 1$ and $\chi(\rho) = \rho(1-\rho)$. In the case of no external field, $E = 0$, since χ is concave and χ^{-1} is convex, it satisfies both the hypotheses for $\Phi = U$ and the ones for (6.7); hence $\Phi(J) = (1/2)J^2/m(1-m)$. If $E \neq 0$ the assumptions for (6.7) holds only if $|E/J| \leq 4$; in such a case we can conclude that the constant density profile is optimal for U but we do not know if it coincides with Φ. On the other hand for $|E/J| > [m(1-m)]^{-1}$ (6.8) holds so that we can conclude, by (6.9), that for J large there exists a travelling wave whose cost is strictly less than the one of the constant profile $\rho(u) = m$. As discussed above this is however not enough to prove the strict inequality $\Phi(J) < U(J)$.

For the KMP model[8,22] we have $D(\rho) = 1$ and $\chi(\rho) = \rho^2$. Since χ and $1/\chi$ are convex functions, the assumptions for (6.7) are satisfied for any external field E. Hence $U(J) = 1/2\,[J - Em^2]^2/m^2$ and the corresponding optimal density profile is always the constant one. Fix now e such that $|e| < 1/m^2$ (in particular $e = 0$), then (6.8) holds. Therefore for the KMP process with external field $E = eJ$, by (6.6), (6.7) and (6.9), we have $\Phi(J) < U(J)$ for all sufficiently large currents J.

We conclude by giving, for the KMP process with no external field, an interpretation of the strict inequality $\Phi < U$ in terms of the power necessary, according to (A.10), to sustain a time average current J. To get $U(J) = (1/2)J^2/m^2$ we switch on a constant external field equal to J/m^2 which provides exactly the power $U(J)$. On the other hand we can impose a time average current J by imposing a space time dependent external field of the type $F(u - vt)$; the corresponding density and current paths are then travelling waves. By exploiting the convexity of ρ^2 we have shown that, for J large, the second strategy requires less power.

6.3. An Example with Non Convex U

We discuss here a special choice of the macroscopic transport coefficients D and χ for which the functional U defined in (4.5) is not convex. In particular the upper bound (4.7) with the convex envelope differs from (4.6).

We take $d = 1$, $\Lambda = (0, 1)$, $E = 0$, $D(\rho) = 1$, and $\chi(\rho)$ a smooth function with $\chi(0) = \chi(1) = 0$ (accordingly the density satisfies $0 \leq \rho \leq 1$) such that there exist $0 < A < B < 1$, $\ell \in \mathbb{R}$ for which $\chi(\rho) = e^{-\ell\rho}$ if $A \leq \rho \leq B$. Furthermore we take the equilibrium boundary conditions $\rho(0) = \rho(1) = \bar{\rho} = (A + B)/2$. We show that, for a suitable choice of the parameters A, B, ℓ, there are $J_1 < J_2$ so that $U''(J) < 0$ for any $J \in (J_1, J_2)$.

Although we did not construct explicitly a microscopic lattice gas model in which the macroscopic transport coefficients meet the above requirements, we believe it would be possible to exhibit a model which has the same qualitative behavior.

For $d = 1$, $D = 1$, $E = 0$, and $J \in \mathbb{R}$, the Euler–Lagrange equation for the variational problem (4.5) defining the functional $U(J)$ is

$$\begin{cases} \frac{1}{2}\rho''(u) = -\frac{\chi'(\rho(u))}{\chi(\rho(u))}\left[J^2 - \frac{1}{4}\rho'(u)^2\right], \quad u \in (0,1) \\ \rho(0) = \rho_0, \quad \rho(1) = \rho_1 \end{cases} \tag{6.11}$$

For the above choice of χ and of the boundary conditions, provided $4|J| \leq B - A$, a solution of (6.11) is given by

$$\hat{\rho}_J(u) = \bar{\rho} + \frac{2}{\ell}\log\frac{\cosh[J\ell(u-1/2)]}{\cosh[J\ell/2]} \tag{6.12}$$

as can be easily verified. Note indeed that $A \leq \hat{\rho}_J \leq B$ since we assumed $4|J| \leq B - A$.

We shall prove below that, under the above conditions, (6.12) is the unique solution of the boundary value problem (6.11). A simple computation then gives

$$U(J) = \frac{2e^{\ell\bar{\rho}}}{\ell^2}\,\frac{J\ell}{2}\tanh\frac{J\ell}{2}$$

Let $F(z) := z\tanh z$ and z^* be the unique positive root of $z^{-1} = \tanh z$. Then $F''(z) = 2(1 - \tanh^2 z)\,(1 - z\tanh z) < 0$ for $z > z^*$. Hence $U''(J) < 0$ if $|J| \in \big(2z^*/\ell, (B-A)/4\big)$. This interval is not empty provided ℓ is chosen large enough.

To show that (6.12) is the unique solution of the boundary value problem (6.11), let us first prove that, given $J \neq 0$, any solution of (6.11) satisfies the *a priori bound* $|\rho'| \leq 2|J|$. Since $\rho(0) = \rho(1)$, we can exclude the possibility that $|\rho'(u)| \geq 2|J|$ for every $u \in [0,1]$. By the continuity of ρ', it is therefore enough to prove that $|\rho'(u)| \neq 2|J|$ for every $u \in [0,1]$. Suppose conversely that there exists $u^* \in [0,1]$ such that $\rho'(u^*) = 2J$. Then, by the uniqueness of the Cauchy problem $\frac{1}{2}\rho'' = \frac{\chi'(\rho)}{\chi(\rho)}[J^2 - \frac{1}{4}\rho'^2]$, $\rho(u^*) = \rho^*$, $\rho'(u^*) = 2J$, we would get that the solution of (6.11) is $\rho(u) = \rho(u^*) + 2J(u - u^*)$. Since this function does not satisfy the boundary conditions in (6.11) we find the desired contradiction.

Since $4|J| \leq B - A$, the *a priori bound* $|\rho'| \leq 2|J|$ implies that any solution ρ of (6.11) satisfies $A \leq \rho \leq B$. For such values we have that $\chi'(\rho)/\chi(\rho) = -\ell$. Uniqueness of the solution to (6.11) can then be easily proven by explicit computations.

6.4. Zero Range Processes

In this section we consider the so-called one-dimensional zero-range processes which models a non-linear diffusion of lattice gases[21] under constant external field E. The model is described by positive integer-valued variables η_x representing the number of particles at site x. The particles jump with rates

$(1/2)g(\eta_x))\exp\{E/N\}$ to right, $(1/2)g(\eta_x))\exp\{-E/N\}$ to the left, respectively. The function $g(k)$ is such that $g(k+1)-g(k)\geq a$ for some $a>0$ and $g(0)=0$. We assume that our system interacts with particle reservoirs at the sites 0 and N whose activity is given by φ_0, φ_1.

The generator of this Markov process is given by (2.3) with $\Lambda_N=\{1,\dots,N\}$ and

$$c_{x,x+1}(\eta)=g(\eta_x)\,e^{E/N}\ ,\quad c_{x+1,x}(\eta)=g(\eta_{x+1})\,e^{-E/N}$$

for $1\leq x\leq N-1$. Moreover, at the boundary,

$$c_{0,1}(\eta)=\varphi_0\,e^{E/N},\quad c_{1,0}(\eta)=g(\eta_1)\,e^{-E/N},$$
$$c_{N,N+1}(\eta)=g(\eta_N)\,e^{E/N},\quad c_{N+1,N}(\eta)=\varphi_1\,e^{-E/N}.$$

Let $V(u)=Eu$ and let $\varphi_N(x)$ be the solution of

$$e^V\Delta_N\frac{\varphi_N}{e^V}=\frac{\varphi_N}{e^V}\Delta_N e^V$$

for $1\leq x\leq N$ and with boundary condition $\varphi_N(0)=\varphi_0$, $\varphi_N(N+1)=\varphi_1$. Here Δ_N stands for the discrete Laplacian.

The invariant measure μ_N is the grand–canonical measure $\mu_N=\prod_{x\in\Lambda_N}\mu_{x,N}$ obtained by taking the product of the marginal distributions

$$\mu_{x,N}(\eta_x=k)=\frac{1}{Z(\varphi_N(x))}\,\frac{\varphi_N(x)^k}{g(1)\cdots g(k)} \tag{6.12}$$

where $Z(\varphi)=\sum_{k\geq 0}\varphi^k/[g(1)\cdots g(k)]$ is the normalization constant. Let $R(\varphi)=\varphi Z'(\varphi)/Z(\varphi)$ and denote by Ψ its inverse function. For this process, the hydrodynamic Eq. (1.2) and the large deviations principle (1.4) can be obtained with $D(\rho)=\Psi'(\rho)$, $\chi(\rho)=\Psi(\rho)$, see Ref. (4). Moreover, $F_0'(\rho)=\log\Psi(\rho)$.

Let first show how, for this model, it is possible to solve explicitly the variational problem (4.11) for the Laplace transform of the total current. We note that the case $E=0$ has already been solved in Ref. (9); see Ref. (19) for more results on the current fluctuations in the zero range processes. Since we are in one space dimension, the condition $\nabla\cdot\lambda=0$ simply states that λ is a constant. Moreover we have $J(\rho)=-(1/2)\Psi'(\rho)\rho'+\Psi(\rho)E$, where hereafter the apices denotes differentiation w.r.t. the macroscopic variable u. Note that condition (6.3) holds so that $\Phi=U$. Changing variables in (4.11) by introducing $\varphi(u)=\Psi(\rho(u))$, $u\in[0,1]$; we get

$$U^*(\lambda)=\frac{1}{2}\sup_{\varphi}\int_0^1 du\,\{-\varphi(u)\psi'(u)^2+\lambda^2\varphi(u)-\lambda\varphi'(u)+2\lambda E\varphi(u)\}$$

where the supremum is over all positive φ such that $\varphi(0) = \varphi_0$, $\varphi(1) = \varphi_1$ and ψ solves

$$2(\varphi(u)\psi'(u))' = (-\varphi'(u) + 2[E + \lambda]\varphi(u))'$$

with boundary conditions $\psi(0) = \psi(1) = 0$. The solution is

$$\psi(u) = -\frac{1}{2}\log\frac{\varphi(u)}{\varphi_0} + (E + \lambda)u + A\int_0^u dv\ \frac{1}{\varphi(v)}$$

where

$$A = \left\{\frac{1}{2}\log\frac{\varphi_1}{\varphi_0} - (E + \lambda)\right\}\left\{\int_0^1 du\ \frac{1}{\varphi(u)}\right\}^{-1}$$

After elementary manipulations, the variational problem for $U^*(\lambda)$ becomes

$$U^*(\lambda) = \frac{1}{2}\sup_{\varphi}\left\{\left\{-\frac{1}{2}\log\frac{\varphi_1}{\varphi_0} + E + \lambda\right\}^2\left\{\int_0^1 du\ \frac{1}{\varphi(u)}\right\}^{-1} - \frac{1}{4}\int_0^1 du\frac{\varphi'(u)^2}{\varphi(u)} - E^2\int_0^1 du\ \varphi(u) + E(\varphi_1 - \varphi_0)\right\} \tag{6.13}$$

The associated extremality condition, which determines the optimal profile, is

$$\begin{aligned} &2\varphi''(u)\varphi(u) - (\varphi'(u))^2 - 4E^2\varphi(u)^2 \\ &= -4\left(-\frac{1}{2}\log\frac{\varphi_1}{\varphi_0} + E + \lambda\right)^2\left[\int_0^1 dv\ \frac{1}{\varphi(v)}\right]^{-2} \end{aligned} \tag{6.14}$$

with the boundary condition $\varphi(0) = \varphi_0$, $\varphi(1) = \varphi_1$.

In the case $E = 0$ it is not difficult to check that the solution of (6.14) is

$$\varphi(u) = C\left(u + \frac{e^{-\lambda}}{1 - e^{-\lambda}}\right)\left(u - \frac{\varphi_0 e^{\lambda}}{\varphi_0 e^{\lambda} - \varphi_1}\right)$$

where $C = -(1 - e^{-\lambda})(\varphi_0 e^{\lambda} - \varphi_1)$. We then get

$$U^*(\lambda) = -\frac{1}{4}[\varphi'(1) - \varphi'(0)] = \frac{1}{2}(1 - e^{-\lambda})(\varphi_0 e^{\lambda} - \varphi_1)$$

In the case $E \neq 0$, the solution of (6.14) is instead given by

$$\varphi(u) = C(e^{2Eu} - a)(e^{-2Eu} - b)$$

where

$$a = \frac{\varphi_0 e^{2E+\lambda} - \varphi_1}{\varphi_0 e^{\lambda} - \varphi_1} \qquad b = \frac{1 - e^{-\lambda-2E}}{1 - e^{-\lambda}}$$

and

$$C = \frac{(1-e^{-\lambda})(\varphi_0 e^{\lambda} - \varphi_1)}{(e^{2E}-1)(1-e^{-2E})}.$$

Notice that this solution converges, as $E \to 0$, to the solution with no external field. Plugging this solution into the variational formula for U^*, we get that

$$\begin{aligned} U^*(\lambda) &= -\frac{1}{4}[\varphi'(1) - \varphi'(0)] + \frac{1}{2}[\varphi_1 - \varphi_0] \\ &= E\Big\{\frac{\varphi_0}{1-e^{-2E}}(e^{\lambda}-1) + \frac{\varphi_1}{e^{2E}-1}(e^{-\lambda}-1)\Big\} \end{aligned} \tag{6.15}$$

We conclude this section showing that we may invert the order of limits in (4.9) for zero range models. For $0 \le x, y \le N+1$, $|x-y| = 1$, recall that we denote by $\mathcal{N}_t^{x,y}$ the total number of jumps from x to y in the time interval $[0,t]$. For $0 \le x \le N$, let $Q_t^{x,x+1} = \mathcal{N}_t^{x,x+1} - \mathcal{N}_t^{x+1,x}$ be the total current over the bond $(x, x+1)$. Note that we are including the boundary bonds.

Consider the limit as microscopic time t goes to infinity of the Laplace transform of the total current:

$$e_N(\lambda) = \frac{1}{N}\lim_{t\to\infty}\frac{1}{t}\log \mathbb{E}_{\eta^N}^N\left[\exp\left\{\lambda N^{-1}\sum_{x=0}^{N} Q_t^{x,x+1}\right\}\right]$$

and notice that f_N given by (5.11) is related to the Legendre transform of e_N by

$$f_N^*(\lambda) = e_N(\lambda\{2E - \log(\varphi_1/\varphi_0)\}).$$

Notice furthermore that this expression does not depend on the initial condition η^N by ergodicity.

Since two currents $Q_t^{x,x+1}$ $Q_t^{y,y+1}$ differ only by surface terms, in the asymptotic $t \uparrow \infty$, we may replace all currents by $Q_t^{0,1}$ and obtain that

$$e_N(\lambda) \;=\; \frac{1}{N}\lim_{t\to\infty}\frac{1}{t}\log \mathbb{E}_{\mu_N}\big[e^{\lambda Q_t^{0,1}}\big].$$

To compute the previous limit, we represent the zero range process in terms of interacting random walks. Let N_0 be the total number of particles at time 0: $N_0 = \sum_x \eta_x(0)$. We start labeling these particles. New particles entering the system at the boundary get new labels in an increasing order. Denote by $X^i(t)$ the position at time t of the i-th particle. X^1 performs a weakly asymmetric random walk on Λ_N with absorption at the boundary and mean $g(1)$ exponential waiting times. X^2 does the same but its clock rates are affected by X^1. If they occupy different sites, the X^2-exponential has rate $g(1)$, while if both occupy the same site, its exponential clock has rate $g(2) - g(1)$ and so on. We need for this construction the function g to be increasing. Moreover the condition $g(k+1) - g(k) \ge a > 0$ guarantees that these random walks will hit the boundary with probability one.

Let w_i (resp. u_i) the indicator function of the event that the i-th particle created at the left (resp. right) boundary is absorbed at $N+1$ (resp. 0). Denote by $N_\pm(t)$ a Poisson process of rate $\varphi_0/2$, $\varphi_1/2$ which represents the entrance of particles at either boundary. With this notation, up to negligible terms in the limit $t \uparrow \infty$,

$$Q_t^{0,1} \;=\; \sum_{i=1}^{N_-(t)} w_i - \sum_{i=1}^{N_+(t)} u_i .$$

In the above construction the interaction of the random walks affects only the jump rates but not the transition probabilities; the random variables w_i, u_j are therefore independent. An elementary computation now shows that

$$e_N(\lambda) = \frac{1}{N}\{(\varphi_0/2)p_N\{e^{\lambda}-1\} + (\varphi_1/2)q_N\{e^{-\lambda}-1\}\},$$

where $p_N = P[w_i = 1]$ (resp. $1-q_N$) is the probability that a random walk, absorbed in 0 and $N+1$, with transition probability $p(x,x+1) = e^{2E/N}/(e^{2E/N}+1) = 1-p(x,x-1)$ starting from 1 (resp. N) is absorbed in $N+1$ (resp. 0). These probabilities can be explicitly computed.

As $N \uparrow \infty$, we get that

$$\lim_{N\to\infty} e_N(\lambda) = E\Big\{\frac{\varphi_0}{1-e^{-2E}}(e^{\lambda}-1) + \frac{\varphi_1}{e^{2E}-1}(e^{-\lambda}-1)\Big\}$$

which agrees with (6.15).

APPENDIX A. SUPPLEMENT TO SECTION 3

We present here a derivation, at the heuristic level, of the law of large numbers and the large deviations, as $N \to \infty$, for the empirical density and the empirical current. Recall the notation introduced in Sec. 3. We have seen there that to prove the law of large numbers for the empirical measure and the current, we need to express the limit current J in terms of the density ρ.

In the context of stochastic lattice gases this is done by assuming a *local equilibrium state*. Roughly speaking, this means that in a large microscopic region Δ around u, still infinitesimal macroscopically, the system has relaxed to the Gibbs state (with Hamiltonian $\mathcal{H}$) conditioned to $\sum_{x\in\Delta}\eta_x = |\Delta|\pi^N(t,u)$. This assumption, which can be rigorously justified,[21] allows us to express the empirical current in terms of the empirical density. We next show how this can be done for the so–called *gradient* models.

By standard computations in the theory of Markov processes we have that, [see Ref. (33), Lemma II.2.3] for a bond $\{x, x+e_j\}$,

$$Q^{x,x+e_j}(t) \;=\; (1/2)N^2 \int_0^t ds\,[c_{x,x+e_j}(\eta_s) - c_{x+e_j,x}(\eta_s)] \;+\; M^{x,x+e_j}(t),$$

where $M^{x,x+e_j}(t)$ are martingales with bracket

$$\langle M^{x,x+e_i}, M^{y,y+e_j}\rangle(t) = (1/2)N^2\delta_{x,y}\delta_{i,j}\int_0^t ds\,[c_{x,x+e_i}(\eta(s)) + c_{x+e_i,x}(\eta(s))].$$

Let G be a smooth vector field as in (3.2) vanishing on $\partial\Lambda$. By definition of the martingales $M^{x,x+e_j}(t)$,

$$\langle\!\langle \mathcal{J}^N, G\rangle\!\rangle_T = \frac{1}{2}\frac{1}{N^d}\int_0^T dt \sum_{i=1}^d \sum_x G_i(t, x/N)N \times [c_{x,x+e_i}(\eta(t)) - c_{x+e_i,x}(\eta(t))] + \mathcal{M}_T^N(G), \tag{A.1}$$

where $\mathcal{M}_T^N(G)$ is a martingale term. An easy computation, based on the explicit formula for the quadratic variations of the martingales $M^{x,x+e_j}(t)$, shows that $\mathcal{M}_T^N(G)$ vanishes as $N \to \infty$. We next use definition (2.2) and Taylor expansion to write

$$\begin{aligned} &c_{x,x+e_i}(\eta) - c_{x+e_i,x}(\eta) \\ &\quad = c^0_{x,x+e_i}(\eta)\left[1 + \frac{1}{N}E_i(x/N)\right] - c^0_{x+e_i,x}(\eta)\left[1 - \frac{1}{N}E_i(x/N)\right] + O(1/N^2) \\ &\quad = \left[c^0_{x,x+e_i}(\eta) - c^0_{x+e_i,x}(\eta)\right] + \frac{1}{N}\left[c^0_{x,x+e_i}(\eta) + c^0_{x+e_i,x}(\eta)\right]E_i(x/N) + O(1/N^2) \end{aligned} \tag{A.2}$$

The *gradient condition*, see Ref. (33), II.2.4, holds if there exist local functions $h_0^{(i)}(\eta)$, $i = 1, \ldots, d$, depending on the configuration η around 0, so that for any $i = 1, \ldots, d$

$$c^0_{x,x+e_i}(\eta) - c^0_{x+e_i,x}(\eta) = h_x^{(i)}(\eta) - h^{(i)}_{x+e_i}(\eta) \tag{A.3}$$

where $h_x^{(i)}$ is the function $h_0^{(i)}$ evaluated on the configuration η translated by x. Let us plug the right hand side of (A.2) into (A.1). By the gradient condition (A.3) we can perform a summation by parts on the first term. Note that there are no boundary terms since we assumed G to vanish on the boundary. We get, with a negligible error as $N \to \infty$,

$$\langle\!\langle \mathcal{J}^N, G\rangle\!\rangle_T \approx \frac{1}{2}\frac{1}{N^d}\int_0^T dt \sum_{i=1}^d \sum_x \big\{\partial_i G_i(t, x/N)h_x^{(i)}(\eta) + G_i(t, x/N)\big[c^0_{x,x+e_i}(\eta(t)) + c^0_{x+e_i,x}(\eta(t))\big]E_i(x/N)\big\} \tag{A.4}$$

Recall the definition of the functions $d^{(i)}$, $\chi^{(i)}$ introduced in (3.5). By the local equilibrium assumption mentioned above and the equivalence of ensembles

from (A.4) we get

$$\langle\langle \mathcal{J}^N, G\rangle\rangle_T \approx \sum_{i=1}^{d} \int_0^T dt \int_\Lambda du \left\{ \frac{1}{2} \partial_i G_i(t,u) d^{(i)}(\pi^N(t,u)) + G_i(t,u) \chi^{(i)}(\pi^N(t,u)) E_i(u) \right\} \tag{A.5}$$

Taking the limit $N \to \infty$, the empirical density $\pi^N(t,u)$ converges to $\rho(t,u)$, whereas the empirical current $\mathcal{J}^N(t,u)$ converges to a vector field $J(t,u)$. Equation (A.5) then implies

$$J(\rho) = -\frac{1}{2} D(\rho) \nabla \rho + \chi(\rho) E \tag{A.6}$$

where D and χ are $d \times d$ diagonal matrices with entries $D_{ii}(\rho) = \frac{d}{d\rho} d^{(i)}(\rho)$ and $\chi_{ii}(\rho) = \chi^{(i)}(\rho)$.

We now turn to a heuristic derivation of the large deviations principle (3.8)–(3.9) for the current. Recall the statement and the notation introduced in Sec. 3.

In order to make the trajectory j typical, we introduce an extra weak time dependent external field $F = (F_1, \ldots, F_d)$ by perturbing the rates as in Sec. 2, namely

$$c^F_{x,x+e_i}(\eta) = c_{x,x+e_i}(\eta)\, e^{N^{-1} F_i(t,x/N)}, \quad c^F_{x+e_i,x}(\eta) = c_{x+e_i,x}(\eta)\, e^{-N^{-1} F_i(t,x/N)} \tag{A.7}$$

We denote by $\mathbb{P}^{N,F}_{\eta^N}$ the probability distribution of the perturbed process. Since these rates c^F are the same as the rates of the original process with E replaced by $E + F$ (cf. (2.2)), we have the following law of large numbers:

$$\lim_{N\to\infty} \mathbb{P}^{N,F}_{\eta^N}(\mathcal{J}^N \approx j) = 1$$

where

$$j = J(\rho) + \chi(\rho) F = -\frac{1}{2} D(\rho) \nabla \rho + \chi(\rho)(E + F) \tag{A.8}$$

and ρ satisfies the continuity Eq. (3.10).

We now read this equation in the opposite direction: given the trajectory j we first solve (3.10) to get ρ, then we determine the external field F which makes j the typical behavior, namely

$$F = \chi(\rho)^{-1} \left(j + \frac{1}{2} D(\rho) \nabla \rho \right) - E \tag{A.9}$$

By writing the original process in terms of the perturbed one we have

$$\mathbb{P}^N_{\eta^N}\left(\mathcal{J}^N(t,u)\approx j(t,u),\ (t,u)\in[0,T]\times\Lambda\right)=\mathbb{P}^{N,F}_{\eta^N}\left(\frac{d\mathbb{P}^N_{\eta^N}}{d\mathbb{P}^{N,F}_{\eta^N}}\,\mathbb{1}_{\{\mathcal{J}^N\approx j\}}\right)$$

The large deviation principle (3.8)–(3.9) will follow, recalling (A.9), once we compute the Radon–Nikodym derivative and show that on the event $\{\mathcal{J}^N\approx j\}$ we have, with a negligible error if $N\to\infty$,

$$\log\frac{d\mathbb{P}^N_{\eta^N}}{d\mathbb{P}^{N,F}_{\eta^N}}=-\log\frac{d\mathbb{P}^{N,F}_{\eta^N}}{d\mathbb{P}^N_{\eta^N}}\approx -N^d\frac{1}{2}\int_0^T dt\ \langle F,\chi(\rho)F\rangle \tag{A.10}$$

This equation can be interpreted, in analogy to the classical Ohm's law, as the total work done in the time interval $[0,T]$ by the external field F.

We shall need some basic tool from the general theory of jump Markov processes that we briefly recall, see e.g. Ref. (21), Appendix A1 or Ref. (4), Appendix A. Let Ω be a countable set and consider a continuous time jump Markov process X_t on the state space Ω with generator given by

$$Lf(\eta)=\sum_{\eta'\in\Omega}\lambda(\eta)p(\eta,\eta')\big[f(\eta')-f(\eta)\big] \tag{A.11}$$

where the rate λ is a positive function on Ω and $p(\eta,\eta')$ is a transition probability. We consider also another process X^F_t of the same type with time dependent rate $\lambda^F(\eta,t)$ and transition probability $p^F(\eta,\eta';t)$. Then, denoting by $\mathbb{P}_{\eta_0}$ and $\mathbb{P}^F_{\eta_0}$ the distribution of the two processes with initial condition η_0 we have

$$\begin{aligned}\frac{d\mathbb{P}^F_{\eta_0}}{d\mathbb{P}_{\eta_0}}(X_t,\ t\in[0,T]) \ &=\exp\left\{\sum_{i=1}^n\log\frac{\lambda^F(X_{\tau_{i-1}},\tau_i)p^F(X_{\tau_{i-1}},X_{\tau_i};\tau_i)}{\lambda(X_{\tau_{i-1}})p(X_{\tau_{i-1}},X_{\tau_i})}\right.\\ &\left.-\int_0^T dt\,[\lambda^F(X_t,t)-\lambda(X_t)]\right\}\end{aligned} \tag{A.12}$$

where $\tau_0=0$, $X_0=\eta_0$, τ_i, $i=1,\dots,n$ is the time in which the process jumped from $X_{\tau_{i-1}}$ to X_{τ_i}, and n is total number of jumps in the time interval $[0,T]$.

For the process $\eta(t)$ with generator (2.3) we have for x, y in $\mathbb{Z}^d$,

$$\lambda(\eta)\,p(\eta,\sigma^{x,y}\eta)=(1/2)N^2c_{x,y}(\eta)\qquad \lambda(\eta)=(1/2)N^2\sum_{x,y}c_{x,y}(\eta)$$

For the process $\eta(t)$ with rates (A.7) we have

$$\lambda^F(\eta,t)\,p^F(\eta,\sigma^{x,x+e_i}\eta,t)=(1/2)N^2c_{x,x+e_i}(\eta)e^{N^{-1}F_i(t,x/N)}$$

and a similar formula for $\lambda^F(\eta, t)\, p^F(\eta, \sigma^{x+e_i,x}\eta, t)$ so that

$$\lambda^F(\eta) = (1/2)N^2 \sum_{i=1}^{d} \sum_{x} \left\{ c_{x,x+e_i}(\eta) e^{N^{-1}F_i(t,x/N)} + c_{x+e_i,x}(\eta) e^{-N^{-1}F_i(t,x/N)} \right\}.$$

From (A.12) and the explicit expressions for the rates, we get that

$$\begin{aligned} \log \frac{d\mathbb{P}^{N,F}_{\eta^N}}{d\mathbb{P}^{N}_{\eta^N}} &= \frac{1}{N} \sum_{j=1}^{d} \sum_{x} \left\{ \sum_{\tau_{x,x+e_j}} F_j(\tau_{x,x+e_j}, x/N) - \sum_{\tau_{x+e_j,x}} F_j(\tau_{x+e_j,x}, x/N) \right\} \\ &\quad - \frac{N^2}{2} \int_0^T dt \left\{ c_{x,x+e_j}(\eta(t)) \left(e^{N^{-1}F(t,x/N)} - 1 \right) \right. \\ &\quad \left. + c_{x+e_j,x}(\eta(t)) \left(e^{-N^{-1}F(t,x/N)} - 1 \right) \right\}, \end{aligned}$$

where $\tau_{x,y}$ are the jump times from x to y. Expanding the exponentials and recalling the definition of the empirical current, we may rewrite the previous expression as

$$\begin{aligned} N^d \langle\!\langle \mathcal{J}^N, F \rangle\!\rangle_T &- \frac{N}{2} \int_0^T dt \sum_{x} \sum_{i=1}^{d} F_i(x/N, t) \left\{ c_{x,x+e_i}(\eta(t)) - c_{x+e_i,x}(\eta(t)) \right\} \\ &- \frac{1}{2} \int_0^T dt \sum_{x} \sum_{i=1}^{d} \left\{ c_{x,x+e_i}(\eta(t)) + c_{x+e_i,x}(\eta(t)) \right\} F_i(x/N, t)^2 + O(1/N), \end{aligned} \tag{A.13}$$

where we let $c_{x,y} = 0$ if $x, y \notin \Lambda_N$.

For gradient models condition (A.3) holds so that we can perform a summation by parts in the second term. Recalling the definition of the diffusion matrix D, the mobility χ and the local equilibrium assumption, we can express the second term of the right hand side of (A.13) in terms of the empirical density. Since we are assuming $\mathcal{J}^N \approx j$, we get that

$$\begin{aligned} \log \frac{d\mathbb{P}^{N,F}_{\eta^N}}{d\mathbb{P}^{N}_{\eta^N}} \approx N^d \left\{ \langle\!\langle j, F \rangle\!\rangle_T + \int_0^T dt \langle F, (1/2) D(\rho) \nabla \rho - \chi(\rho) E \rangle \right. \\ \left. - \frac{1}{2} \int_0^T dt \langle F, \chi(\rho) F \rangle \right\}. \end{aligned} \tag{A.14}$$

which, by the choice of F in (A.9), concludes the derivation of (A.10).

The rigorous derivation of action functional $\mathcal{I}$ requires some difficult estimates. In fact, while in the proof of the hydrodynamic limit it is enough to show that the local equilibrium assumption holds with a negligible error as $N \to \infty$, in the proof of the large deviations we need such an error to be $o(e^{-CN^d})$. This can be proven by the so called super exponential estimate, see Refs. (21, 23), which is the key point in the rigorous approach.

Recall the dynamical large deviations principle for the density stated in (1.4). The rate functional $\mathcal{F}$ is given by

$$\mathcal{F}_{[0,T]}(\rho) \;=\; \frac{1}{2}\int_0^T dt\, \langle \nabla H(t),\, \chi(\rho(t))\nabla H(t)\rangle \tag{A.15}$$

where, given the fluctuation ρ, the external potential $H = H(t,u)$ is chosen so that it vanishes at the boundary and

$$\partial_t \rho = \nabla\cdot\left(\frac{1}{2}D(\rho)\nabla\rho - \chi(\rho)[E+\nabla H]\right) \tag{A.16}$$

which is a Poisson equation for H.

We conclude this Appendix showing how the above result follows directly from the large deviation principle for the current. We fix a path $\rho = \rho(t,u)$, $(t,u)\in[0,T]\times\Lambda$. There are many possible trajectories $j = j(t,u)$, differing by divergence free vector fields, such that the continuity Eq. (3.10) is satisfied. The functional $\mathcal{F}_{[0,T]}(\rho)$ can be obtained by minimizing $\mathcal{I}_{[0,T]}(j)$ among all such paths j

$$\mathcal{F}_{[0,T]}(\rho) = \inf_{\substack{j:\\ \nabla\cdot j = -\partial_t\rho}} \mathcal{I}_{[0,T]}(j) \tag{A.17}$$

To derive the functional (A.15) we show that the infimum above is obtained when the external perturbation F introduced in (A.9) is a gradient vector field whose potential H solves (A.16). Let H be the solution of (A.16) and F as in (A.9), we write

$$F = \nabla H + \widetilde{F} \tag{A.18}$$

By the definition of H we get

$$\langle \nabla H,\, \chi(\rho)\widetilde{F}\rangle = -\left\langle H,\, \nabla\cdot j + \nabla\cdot\left(\frac{1}{2}D(\rho)\nabla\rho - \chi(\rho)E - \chi(\rho)\nabla H\right)\right\rangle = 0$$

Hence

$$\mathcal{I}_{[0,T]}(j) = \frac{1}{2}\int_0^T dt\, \{\langle \nabla H,\, \chi(\rho)\nabla H\rangle + \langle \widetilde{F},\, \chi(\rho)\widetilde{F}\rangle\}$$

Therefore the infimum in (A.17) is obtained when $\widetilde{F} = 0$, so that the functional defined in (A.17) coincides with (A.15).

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