

Macroscopic Fluctuation Theory for Stationary Non-Equilibrium States

L. Bertini,¹ A. De Sole,² D. Gabrielli,³ G. Jona-Lasinio,⁴ and C. Landim⁵

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We formulate a dynamical fluctuation theory for stationary non-equilibrium states (SNS) which is tested explicitly in stochastic models of interacting particles. In our theory a crucial role is played by the time reversed dynamics. Within this theory we derive the following results: the modification of the Onsager–Machlup theory in the SNS; a general Hamilton–Jacobi equation for the macroscopic entropy; a non-equilibrium, nonlinear fluctuation dissipation relation valid for a wide class of systems; an H theorem for the entropy. We discuss in detail two models of stochastic boundary driven lattice gases: the zero range and the simple exclusion processes. In the first model the invariant measure is explicitly known and we verify the predictions of the general theory. For the one dimensional simple exclusion process, as recently shown by Derrida, Lebowitz, and Speer, it is possible to express the macroscopic entropy in terms of the solution of a nonlinear ordinary differential equation; by using the Hamilton–Jacobi equation, we obtain a logically independent derivation of this result.

KEY WORDS: Stationary non-equilibrium states; large deviations; boundary driven lattice gases.

¹ Dipartimento di Matematica, Università di Roma La Sapienza, P.le A. Moro 2, 00185 Roma, Italy; e-mail: lorenzo@carpenter.mat.uniroma1.it

² Department of Mathematics, MIT, 77 Massachusetts Avenue, Cambridge, MA 02139-4307; e-mail: desole@math.mit.edu

³ Dipartimento di Matematica, Università dell’Aquila, 67100 Coppito, L’Aquila, Italy; e-mail: gabriell@univaq.it

⁴ Dipartimento di Fisica and INFN, Università di Roma La Sapienza, P.le A. Moro 2, 00185 Roma, Italy; e-mail: jona@roma1.infn.it

⁵ IMPA, Estrada Dona Castorina 110, J. Botânico, 22460 Rio de Janeiro, Brazil, CNRS UPRES-A 6085, Université de Rouen, 76128 Mont-Saint-Aignan Cedex, France; e-mail: landim@impa.br

1. INTRODUCTION

The Boltzmann–Einstein theory of equilibrium thermodynamic fluctuations, as described for example in Landau–Lifshitz,⁽¹⁾ states that the probability for a fluctuation from equilibrium in a macroscopic region of volume V is proportional to

$$\exp\{V\Delta S/k\}$$

where ΔS is the variation of entropy density calculated along a reversible transformation creating the fluctuation and k is the Boltzmann constant. This theory is well established and has received a rigorous mathematical formulation in classical equilibrium statistical mechanics via the so called large deviation theory.⁽²⁾ The rigorous study of large deviations has been extended to hydrodynamic evolutions of stochastic interacting particle systems.⁽³⁾ In a dynamical setting one may ask new questions, for example what is the most probable trajectory followed by the system in the spontaneous emergence of a fluctuation or in its relaxation to equilibrium. The Onsager–Machlup theory⁽⁴⁾ gives the following answer under the assumption of time reversibility. In the situation of a linear macroscopic equation, that is, close to equilibrium, the most probable emergence and relaxation trajectories are one the time reversal of the other. Developing the methods of ref. 3, this theory has been extended to nonlinear hydrodynamic regimes.⁽⁵⁾

In the present paper we formulate a general theory of large deviations for irreversible processes, i.e., when detailed balance does not hold. This question was previously addressed in ref. 6 for finite dimensional diffusions and in ref. 7 for lattice gases. Natural examples are boundary driven stationary non-equilibrium states (SNS), e.g., a thermodynamic system in contact with two reservoirs. In such a situation there is a flow of matter or other physical property like heat, charge,... through the system. As we shall see, the spontaneous fluctuations of the process are described by the time reversed dynamics, which is defined below.

Spontaneous fluctuations, including Onsager–Machlup symmetry, have been observed in stochastically perturbed reversible electronic devices.⁽⁸⁾ In their work, these authors study also nonreversible systems and observe violation of Onsager–Machlup symmetry; in the present work we shall connect such violations to the time reversed dynamics.

We are interested in many body systems in the limit of infinitely many degrees of freedom. The basic assumptions of our theory are the following.

(1) The microscopic evolution is given by a Markov process X_t which represents the configuration of the system at time t . This hypothesis probably is not so restrictive because also the Hamiltonian case discussed

in ref. 9 in the end is reduced to the analysis of a Markov process. The stationary non-equilibrium state (SNS) is described by a stationary, i.e., invariant with respect to time shifts, probability distribution P_{st} over the trajectories of X_t .

(2) The system admits also a macroscopic description in terms of density fields which are the local thermodynamic variables. For simplicity of notation we assume there is only one thermodynamic variable ρ . The evolution of the field $\rho = \rho(t, u)$ where u is the macroscopic space coordinate, is given by a diffusion type hydrodynamical equation of the form

$$\partial_t \rho = \frac{1}{2} \nabla \cdot (D(\rho) \nabla \rho) = \frac{1}{2} \sum_{1 \leq i, j \leq d} \partial_{u_i} (D_{i,j}(\rho) \partial_{u_j} \rho) = \mathfrak{D}(\rho) \quad (1.1)$$

The interaction with the reservoirs appears as boundary conditions to be imposed on solutions of (1.1). We assume that there exists a unique stationary solution $\bar{\rho}$ of (1.1), i.e., a profile $\bar{\rho}(u)$, which satisfies the appropriate boundary conditions such that $\mathfrak{D}(\bar{\rho}) = 0$. This holds if the diffusion matrix $D_{i,j}(\rho)$ in (1.1) is strictly elliptic, namely there exists a constant $c > 0$ such that $D(\rho) \geq c \mathbb{1}$ (in matrix sense).

This equation derive from the underlying microscopic dynamics through an appropriate scaling limit. The hydrodynamic equation (1.1) represents a law of large numbers with respect to the probability measure P_{st} conditioned on an initial state X_0 . The initial conditions for (1.1) is 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 an appropriate limit of a $\rho_N(X_t)$ as the number N of degrees of freedom diverges.

(3) Let us denote by θ the time inversion operator defined by $\theta X_t = X_{-t}$. The probability measure P_{st}^* describing the evolution of the time reversed process X_t^* is given by the composition of P_{st} and θ^{-1} that is

$$P_{st}^*(X_t^* = \phi_t, t \in [t_1, t_2]) = P_{st}(X_t = \phi_{-t}, t \in [-t_2, -t_1]) \quad (1.2)$$

Let L be the generator of the microscopic dynamics. We remind that L induces the evolution of observables (functions on the configuration space) according to the equation $\partial_t E_{X_0}[f(X_t)] = E_{X_0}[(Lf)(X_t)]$, where E_{X_0} stands for the expectation with respect to P_{st} conditioned on the initial state X_0 , see, e.g., ref. 10, Chap. X. The time reversed dynamics is generated by the adjoint L^* of L with respect to the invariant measure μ , that is

$$E^\mu[fLg] = E^\mu[(L^*f)g] \quad (1.3)$$

The measure μ , which is the same for both processes, is a distribution over the configurations of the system and formally satisfies $\mu L = 0$. The expectation with respect to μ is denoted by E^μ and f, g are observables. We note that the probability P_{st} , and therefore P_{st}^* , depends on the invariant measure μ . The finite dimensional distributions of P_{st} are in fact given by

$$P_{st}(X_{t_1} = \phi_{t_1}, \dots, X_{t_n} = \phi_{t_n}) = \mu(\phi_{t_1}) p_{t_2-t_1}(\phi_{t_1} \rightarrow \phi_{t_2}) \cdots p_{t_n-t_{n-1}}(\phi_{t_{n-1}} \rightarrow \phi_{t_n}) \quad (1.4)$$

where $p_t(\phi_1 \rightarrow \phi_2)$ is the transition probability. According to (1.2) the finite dimensional distributions of P_{st}^* are

$$\begin{aligned} P_{st}^*(X_{t_1}^* = \phi_{t_1}, \dots, X_{t_n}^* = \phi_{t_n}) \\ &= \mu(\phi_{t_1}) p_{t_2-t_1}^*(\phi_{t_1} \rightarrow \phi_{t_2}) \cdots p_{t_n-t_{n-1}}^*(\phi_{t_{n-1}} \rightarrow \phi_{t_n}) \\ &= \mu(\phi_{t_n}) p_{t_n-t_{n-1}}(\phi_{t_n} \rightarrow \phi_{t_{n-1}}) \cdots p_{t_2-t_1}(\phi_{t_2} \rightarrow \phi_{t_1}) \end{aligned} \quad (1.5)$$

in particular the transition probabilities $p_t(\phi_1 \rightarrow \phi_2)$ and $p_t^*(\phi_1 \rightarrow \phi_2)$ are related by

$$\mu(\phi_1) p_t(\phi_1 \rightarrow \phi_2) = \mu(\phi_2) p_t^*(\phi_2 \rightarrow \phi_1) \quad (1.6)$$

which reduces to the well known detailed balance condition if $p_t(\phi_1 \rightarrow \phi_2) = p_t^*(\phi_1 \rightarrow \phi_2)$.

We require that also the evolution generated by L^* admits a hydrodynamic description, that we call the adjoint hydrodynamics, which, however, is not necessarily of the same form as (1.1). In fact we shall discuss a model in which the adjoint hydrodynamics is nonlocal in space.

In order to avoid confusion we emphasize that what is usually called an equilibrium state, as distinguished from a SNS, corresponds to the special case $L^* = L$, i.e., the detailed balance principle holds. In such a case P_{st} is invariant under time reversal and the two hydrodynamics coincide.

(4) The stationary measure P_{st} admits a principle of large deviations describing the fluctuations of the thermodynamic variable appearing in the hydrodynamic equation. This means the following. The probability that in a macroscopic volume V containing N particles the evolution of the variable ρ_N deviates from the solution of the hydrodynamic equation and is close to some trajectory $\hat{\rho}(t)$, is exponentially small and of the form

$$P_{st}(\rho_N(X_t) \sim \hat{\rho}(t), t \in [t_1, t_2]) \approx e^{-N[S(\hat{\rho}(t_1)) + J_{[t_1, t_2]}(\hat{\rho})]} = e^{-N I_{[t_1, t_2]}(\hat{\rho})} \quad (1.7)$$

where $J(\hat{\rho})$ is a functional which vanishes if $\hat{\rho}(t)$ is a solution of (1.1) and $S(\hat{\rho}(t_1))$ is the entropy cost to produce the initial density profile $\hat{\rho}(t_1)$. We

adopt the convention for the entropy sign opposite to the usual one, so that it takes the minimum value in the equilibrium state. We also normalize it so that $S(\bar{\rho}) = 0$. The functional $J(\hat{\rho})$ represents the extra cost necessary to follow the trajectory $\hat{\rho}(t)$. Finally $\rho_N(X_t) \sim \hat{\rho}(t)$ means closeness in some metric and \approx denotes logarithmic equivalence as $N \rightarrow \infty$. This formula is a generalization of the Boltzmann–Einstein formula. We set the Boltzmann constant $k = 1$.

This paper is divided in two parts. In the first one we present a general fluctuation theory of SNS based on the hypotheses formulated above assuming the knowledge of the functional $J(\hat{\rho})$. The main results are outlined below.

1. The Onsager–Machlup relationship has to be modified in the following way: *“In a SNS the spontaneous emergence of a macroscopic fluctuation takes place most likely following a trajectory which is the time reversal of the relaxation path according to the adjoint hydrodynamics.”*

2. We show that the macroscopic entropy $S(\rho)$ solves Hamilton–Jacobi equation generalizing to a thermodynamic context known results for finite dimensional Langevin equations.^(6, 8, 11)

3. For a large class of systems we obtain a non-equilibrium nonlinear fluctuation dissipation relationship which links the hydrodynamics of the system and of its time reversal to the thermodynamic force, that is the derivative of $S(\rho)$. If $S(\rho)$ is known this relationship determines the adjoint hydrodynamics.

4. From the last two results we derive an H Theorem for $S(\rho)$: it is decreasing along the solutions of both the hydrodynamics and the adjoint hydrodynamics.

In the second part we test the theory outlined above in two boundary driven stochastic models of interacting particle systems: the zero range and the simple exclusion processes. The main results are outlined below.

1. For the boundary driven zero range process, as observed in ref. 12, the invariant measure is a product measure. It is therefore possible to write the functional $S(\rho)$, which in this case is a local functional of ρ , in a closed form and to construct the microscopic time reversed process explicitly. We derive both the hydrodynamics and the adjoint hydrodynamics. We compute the functionals $J(\hat{\rho})$ and $J^*(\hat{\rho})$ and verify the generalized Onsager–Machlup principle and the fluctuation dissipation relationship.

2. For the boundary driven simple exclusion process the invariant measure has long range correlations and is not explicitly known. The hydrodynamics has been obtained in ref. 13; we obtain the asymptotics of the probability of large deviations, that is we calculate $J(\hat{\rho})$. In one

space dimension, Derrida *et al.*⁽¹⁴⁾ have recently shown that the action functional S can be expressed in terms of the solution of a nonlinear ordinary differential equation. We show how this result can be recovered by our approach: the Hamilton–Jacobi equation for $S(\rho)$ (which is a functional derivative equation) can be reduced to the solution of the ordinary differential equation obtained in ref. 14. By using the fluctuation dissipation relationship we also find the adjoint hydrodynamics. Moreover, in any spatial dimension, we can deduce a lower bound for the macroscopic entropy in terms of the entropy of an equilibrium state. In the one dimensional case this bound has been independently obtained in ref. 14.

Part of the results presented here have been briefly reported in ref. 15. Rigorous mathematical treatment of the boundary driven simple exclusion process will be given in ref. 16.

We conclude with some remarks to clarify the differences between equilibrium and non-equilibrium states. The main problem in the SNS derives from the following situation. In equilibrium states the thermodynamic properties are determined by the Gibbs distribution which is specified by the Hamiltonian without solving a dynamical problem. On the contrary, in a SNS we cannot construct the appropriate ensemble without calculating first the invariant measure. At thermodynamic level, we do not need all the information carried by the invariant measure, but only the functional $S(\rho)$ appearing in the generalized Boltzmann–Einstein formula (1.7). In general $S(\rho)$, contrary to the equilibrium case, is a nonlocal functional of the profile ρ . It turns out that the entropy $S(\rho)$ can be obtained, both in equilibrium and non-equilibrium, from $J(\hat{\rho})$, which is therefore the basic object of the macroscopic theory. This step is simple for equilibrium, but highly nontrivial in non-equilibrium.

2. GENERAL THEORY

2.1. Generalized Onsager–Machlup Relationship

We now derive a first consequence of our assumptions, that is the relationship between the action functionals I and I^* associated to the dynamics L and L^* . From Eq. (1.2) and our assumptions it follows that P_{st}^* also admits a large deviation principle with functional I^* given by

$$I_{[t_1, t_2]}^*(\hat{\rho}) = I_{[-t_2, -t_1]}(\theta\hat{\rho}) \quad (2.1)$$

with obvious notation. More explicitly this equation reads

$$S(\hat{\rho}(t_1)) + J_{[t_1, t_2]}^*(\hat{\rho}) = S(\hat{\rho}(t_2)) + J_{[-t_2, -t_1]}(\theta\hat{\rho}) \quad (2.2)$$

where $\hat{\rho}(t_1)$, $\hat{\rho}(t_2)$ are the initial and final points of the trajectory and $S(\hat{\rho}(t_i))$ the entropies associated with the creation of the fluctuations $\hat{\rho}(t_i)$ starting from the SNS. The functional J^* vanishes on the solutions of the adjoint hydrodynamics. From (2.2) we can obtain the generalization of Onsager–Machlup relationship for SNS.

The physical situation we are considering is the following. The system is macroscopically in the stationary state $\bar{\rho}$ at $t = -\infty$ but at $t = 0$ we find it in the state ρ . We want to determine the most probable trajectory followed in the spontaneous creation of this fluctuation. According to (1.7) this trajectory is the one that minimizes J among all trajectories $\hat{\rho}(t)$ connecting $\bar{\rho}$ to ρ in the time interval $[-\infty, 0]$. From (2.2), recalling that $S(\bar{\rho}) = 0$, we have that

$$J_{[-\infty, 0]}(\hat{\rho}) = S(\rho) + J_{[0, \infty]}^*(\theta\hat{\rho}) \quad (2.3)$$

The right hand side is minimal if $J_{[0, \infty]}^*(\theta\hat{\rho}) = 0$ that is if $\theta\hat{\rho}$ is a solution of the adjoint hydrodynamics. The existence of such a relaxation solution is due to the fact that the stationary solution $\bar{\rho}$ is attractive also for the adjoint hydrodynamics. We have therefore the following generalization of Onsager–Machlup to SNS

“In a SNS the spontaneous emergence of a macroscopic fluctuation takes place most likely following a trajectory which is the time reversal of the relaxation path according to the adjoint hydrodynamics.”

We note that the reversibility of the microscopic process X_t , which we call microscopic reversibility, is not needed in order to deduce the classical Onsager–Machlup principle (i.e., that the trajectory which creates the fluctuation is the time reversal of the relaxation trajectory). In fact the classical Onsager–Machlup principle holds if and only if the hydrodynamics coincides with the adjoint hydrodynamics, which we call macroscopic reversibility. Indeed it is possible to construct microscopic non-reversible models in which the classical Onsager–Machlup principle holds, see refs. 17–19.

2.2. The Hamilton–Jacobi Equation for the Entropy

We assume that the functional J has a density (which plays the role of a Lagrangian), i.e.,

$$J_{[t_1, t_2]}(\hat{\rho}) = \int_{t_1}^{t_2} dt \mathcal{L}(\hat{\rho}(t), \partial_t \hat{\rho}(t)) \quad (2.4)$$

From (2.3) we have that the entropy is related to J by

$$S(\rho) = \inf_{\hat{\rho}} J_{[-\infty, 0]}(\hat{\rho}) \quad (2.5)$$

where the minimum is taken over all trajectories $\hat{\rho}(t)$ connecting $\bar{\rho}$ to ρ . Therefore S must satisfy the Hamilton–Jacobi equation associated to the action functional J . Let us introduce the Hamiltonian $\mathcal{H}(\rho, H)$ as the Legendre transform of $\mathcal{L}(\rho, \partial_t \rho)$, i.e.,

$$\mathcal{H}(\rho, H) = \sup_{\xi} \{ \langle \xi, H \rangle - \mathcal{L}(\rho, \xi) \} \quad (2.6)$$

where $\langle \cdot, \cdot \rangle$ denotes integration with respect to the macroscopic space coordinates u , that is the inner product in $L_2(du)$. This notation will be employed throughout the whole paper.

Noting that $\mathcal{H}(\bar{\rho}, 0) = 0$, the Hamilton–Jacobi equation associated to (2.5) is

$$\mathcal{H} \left(\rho, \frac{\delta S}{\delta \rho} \right) = 0 \quad (2.7)$$

This is an equation for the functional derivative $A(\rho) = \delta S / \delta \rho$ but not all the solutions of the equation $\mathcal{H}(\rho, A(\rho)) = 0$ are the derivative of some functional. Of course only those which are the derivative of some functional are relevant for us. Furthermore, as well known in mechanics, the Hamilton–Jacobi equation (2.7) has many solutions and we shall discuss later the criterion to select the correct one.

Let also introduce the pressure $G = G(h)$, where $h = h(u)$ can be interpreted as a chemical potential profile, as the Legendre transform of the entropy $S(\rho)$, namely

$$G(h) = \sup_{\rho} \{ \langle h, \rho \rangle - S(\rho) \} \quad (2.8)$$

Then, by Legendre duality, we have $\delta G / \delta h = \rho$ and $\delta S / \delta \rho = h$ so that $G(h)$ satisfies the dual Hamilton–Jacobi equation

$$\mathcal{H} \left(\frac{\delta G}{\delta h}, h \right) = 0 \quad (2.9)$$

We now specify the Hamilton–Jacobi equation (2.7) for boundary driven lattice gases. We assume that the large deviation functional J may be expressed as a quadratic functional of $\partial_i \hat{\rho}$

$$\begin{aligned} J_{[t_1, t_2]}(\hat{\rho}) &= \frac{1}{2} \int_{t_1}^{t_2} dt \langle \nabla^{-1}(\partial_i \hat{\rho} - \mathfrak{D}(\rho)), \chi(\hat{\rho})^{-1} \nabla^{-1}(\partial_i \hat{\rho} - \mathfrak{D}(\rho)) \rangle \\ &= \frac{1}{2} \int_{t_1}^{t_2} dt \langle \nabla^{-1}(\partial_i \hat{\rho} - \frac{1}{2} \nabla \cdot (D(\hat{\rho}) \nabla \hat{\rho})), \\ &\quad \chi(\hat{\rho})^{-1} \nabla^{-1}(\partial_i \hat{\rho} - \frac{1}{2} \nabla \cdot (D(\hat{\rho}) \nabla \hat{\rho})) \rangle \end{aligned} \quad (2.10)$$

where $D(\rho) = D_{i,j}(\rho)$ is the diffusion matrix in the hydrodynamic equation (1.1) and by $\nabla^{-1}f$ we mean a vector field whose divergence equals f . The form (2.10), which we derive in the models discussed below, is expected to be very general; the functional $J(\hat{\rho})$ measures how much $\hat{\rho}$ differs from a solution of the hydrodynamics (1.1) and the matrix $\chi(\rho) = \chi_{i,j}(\rho)$ reflects the intensity of the fluctuations. See ref. 20, II.3.7 for a heuristic derivation of (2.10) for reversible lattice gases. This form of J is also typical for diffusion processes described by finite dimensional Langevin equations.⁽¹¹⁾

In this case the Lagrangian \mathcal{L} is quadratic in $\partial_i \hat{\rho}(t)$ and the associated Hamiltonian is given by

$$\mathcal{H}(\rho, H) = \frac{1}{2} \langle \nabla H, \chi(\rho) \nabla H \rangle + \frac{1}{2} \langle H, \nabla \cdot (D(\rho) \nabla \rho) \rangle \quad (2.11)$$

so that the Hamilton–Jacobi equation (2.7) takes the form

$$\left\langle \nabla \frac{\delta S}{\delta \rho}, \chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right\rangle + \left\langle \frac{\delta S}{\delta \rho}, \nabla \cdot (D(\rho) \nabla \rho) \right\rangle = 0 \quad (2.12)$$

We remark that the macroscopic entropy S , given by the variational principle (2.5), depends only on the action functional J and is therefore stable with respect to microscopic perturbations which do not affect the dynamical large deviations.

2.3. The Adjoint Hydrodynamics and a Non-Equilibrium Fluctuation Dissipation Relation

By assuming the quadratic form (2.10) also for J^* , we deduce a twofold generalization of the celebrated fluctuation dissipation relationship: it is valid in non-equilibrium states and in nonlinear regimes.

Such a relationship will hold provided the rate function J^* of the time reversed process is of the form (2.10) with a different hydrodynamic equation (the adjoint hydrodynamics) that we write in general as

$$\partial_t \rho^* = \mathfrak{D}^*(\rho^*) \quad (2.13)$$

with the same boundary conditions as (1.1).

We then assume J^* has the form

$$J_{[t_1, t_2]}^*(\hat{\rho}) = \frac{1}{2} \int_{t_1}^{t_2} dt \langle (\nabla^{-1}(\partial_t \hat{\rho} - \mathfrak{D}^*(\hat{\rho})), \chi(\hat{\rho})^{-1} \nabla^{-1}(\partial_t \hat{\rho} - \mathfrak{D}^*(\hat{\rho}))) \rangle \quad (2.14)$$

By taking the variation of the equation (2.2), we get

$$\mathfrak{D}(\rho) + \mathfrak{D}^*(\rho) = \nabla \cdot \left(\chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right) \quad (2.15)$$

This relation holds for the non-equilibrium zero range process which we discuss later. We also note that it holds for the equilibrium reversible models for which the large deviation principle has been rigorously proven such as the simple exclusion process,⁽³⁾ the Landau–Ginzburg model⁽²¹⁾ and its nongradient version.⁽²²⁾ It is also easy to check that the linearization of (2.15) around the stationary profile $\bar{\rho}$ yields a fluctuation dissipation relationship which reduces to the usual one in equilibrium. Accordingly, the matrix $\chi(\rho)$ coincides with the Onsager matrix as defined in refs. 18–20.

In order to verify the fluctuation dissipation relation (2.15), we need $\mathfrak{D}(\rho)$, $\mathfrak{D}^*(\rho)$ and $\delta S/\delta \rho$. On the other hand, it can be used to obtain the adjoint hydrodynamics from $\mathfrak{D}(\rho)$ and $\delta S/\delta \rho$; the first is typically known and the second can be calculated from the Hamilton–Jacobi equation (2.12).

Suppose we can decompose the hydrodynamics as the sum of a gradient of some functional V and a vector field \mathcal{A} orthogonal to it in the metric induced by the operator K^{-1} where $Kf = -\nabla \cdot (\chi(\rho) \nabla f)$, namely

$$\mathfrak{D}(\rho) = \frac{1}{2} \nabla \cdot \left(\chi(\rho) \nabla \frac{\delta V}{\delta \rho} \right) + \mathcal{A}(\rho)$$

with

$$\left\langle K \frac{\delta V}{\delta \rho}, K^{-1} \mathcal{A}(\rho) \right\rangle = \left\langle \frac{\delta V}{\delta \rho}, \mathcal{A}(\rho) \right\rangle = 0$$

If $\delta V/\delta\rho$, like the thermodynamic force $\delta S/\delta\rho$, vanishes at the boundary, it is easy to check that the functional V solves the Hamilton–Jacobi equation.

Conversely, given $S(\rho)$, by using the fluctuation dissipation relationship (2.15), we can introduce a vector field $\mathcal{A}(\rho)$ such that

$$\mathfrak{D}(\rho) = \frac{1}{2} \nabla \cdot \left(\chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right) + \mathcal{A}(\rho)$$

$$\mathfrak{D}^*(\rho) = \frac{1}{2} \nabla \cdot \left(\chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right) - \mathcal{A}(\rho)$$

and the Hamilton–Jacobi equation implies the orthogonality condition

$$\left\langle \frac{\delta S}{\delta \rho}, \mathcal{A}(\rho) \right\rangle = 0$$

Note the analogy with ref. 11, Thm. IV.3.1 for diffusion processes.

2.4. H Theorem

We show that the functional S is decreasing along the solutions of both the hydrodynamic equation (1.1) and the adjoint hydrodynamics

$$\partial_t \rho = \mathfrak{D}^*(\rho) = \nabla \cdot \left(\chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right) - \mathfrak{D}(\rho) \quad (2.16)$$

Let $\rho(t)$ be a solution of (1.1) or (2.16), by using the Hamilton–Jacobi equation (2.12), we get

$$\begin{aligned} \frac{d}{dt} S(\rho(t)) &= \left\langle \frac{\delta S}{\delta \rho}(\rho(t)), \partial_t \rho(t) \right\rangle \\ &= -\frac{1}{2} \left\langle \nabla \frac{\delta S}{\delta \rho}(\rho(t)), \chi(\rho(t)) \nabla \frac{\delta S}{\delta \rho}(\rho(t)) \right\rangle \leq 0 \end{aligned} \quad (2.17)$$

In particular we have that $\frac{d}{dt} S(\rho(t)) = 0$ if and only if $\frac{\delta S}{\delta \rho}(\rho(t)) = 0$. Since we assumed there exists a unique stationary profile $\bar{\rho}$, this implies that $\bar{\rho}$ is globally attractive also for the adjoint hydrodynamics (2.16).

2.5. A Lower Bound for the Entropy S

Let us consider any functional $V(\rho)$, normalized so that $V(\bar{\rho}) = 0$, whose derivative satisfies the Hamilton–Jacobi equation (2.12) and the condition $\delta V(\rho)/\delta\rho = 0$ at the boundary. We shall prove the bound

$$S(\rho) = \inf_{\hat{\rho}} J_{[-\infty, 0]}(\hat{\rho}) \geq V(\rho) \quad (2.18)$$

where the trajectory $\hat{\rho}(t)$ connects $\bar{\rho}$ to ρ .

Fix $t_1 < t_2$, two profiles ρ_1, ρ_2 and a path $\hat{\rho}(t)$ in the time interval $[t_1, t_2]$ that joins ρ_1 to ρ_2 : $\hat{\rho}(t_1) = \rho_1, \hat{\rho}(t_2) = \rho_2$. Let H , vanishing at the boundary, be given by the equation

$$\partial_t \hat{\rho} = \frac{1}{2} \nabla \cdot (D(\hat{\rho}) \nabla \hat{\rho}) - \nabla \cdot (\chi(\hat{\rho}) \nabla H) \quad (2.19)$$

We then claim that

$$\begin{aligned} J_{[t_1, t_2]}(\hat{\rho}) &= V(\rho_2) - V(\rho_1) \\ &+ \frac{1}{2} \int_{t_1}^{t_2} dt \left\langle \nabla \left\{ H - \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}} \right\}, \chi(\hat{\rho}) \nabla \left\{ H - \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}} \right\} \right\rangle \end{aligned} \quad (2.20)$$

Since the last term above is positive the bound (2.18) follows from the above identity.

To prove (2.20) we note, recalling (2.10), that, since H is the solution of (2.19),

$$J_{[t_1, t_2]}(\hat{\rho}) = \frac{1}{2} \int_{t_1}^{t_2} dt \langle \nabla H, \chi(\hat{\rho}) \nabla H \rangle$$

We add and subtract in this expression $\nabla \{ \delta V(\hat{\rho}) / \delta \hat{\rho} \}$ to obtain

$$\begin{aligned} J_{[t_1, t_2]}(\hat{\rho}) &= \frac{1}{2} \int_{t_1}^{t_2} dt \left\langle \nabla \left\{ H - \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}} \right\}, \chi(\hat{\rho}) \nabla \left\{ H - \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}} \right\} \right\rangle \\ &+ \int_{t_1}^{t_2} dt \left\langle \nabla \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}}, \chi(\hat{\rho}) \nabla H \right\rangle \\ &- \frac{1}{2} \int_{t_1}^{t_2} dt \left\langle \nabla \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}}, \chi(\hat{\rho}) \nabla \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}} \right\rangle \end{aligned} \quad (2.21)$$

We leave the first term unchanged and we show that the sum of the second and third gives $V(\rho_2) - V(\rho_1)$. Since $\delta V(\hat{\rho})/\delta \hat{\rho}$ vanishes at the boundary, we may integrate by parts the second term; we get

$$-\int_{t_1}^{t_2} dt \left\langle \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}}, \nabla \cdot (\chi(\hat{\rho}) \nabla H) \right\rangle$$

By the Hamilton–Jacobi equation (2.12), the third term is equal to

$$\frac{1}{2} \int_{t_1}^{t_2} dt \left\langle \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}}, \nabla \cdot (D(\hat{\rho}) \nabla \hat{\rho}) \right\rangle$$

Adding together the previous two expressions, we obtain that the sum of the last two terms in (2.21) is equal to

$$\int_{t_1}^{t_2} dt \left\langle \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}}, \left\{ \frac{1}{2} \nabla \cdot (D(\hat{\rho}) \nabla \hat{\rho}) - \nabla \cdot (\chi(\hat{\rho}) \nabla H) \right\} \right\rangle$$

Since $\hat{\rho}$ is the solution of (2.19), this expression is equal to

$$\int_{t_1}^{t_2} dt \left\langle \frac{\delta V(\hat{\rho})}{\delta \hat{\rho}}, \partial_t \hat{\rho} \right\rangle = V(\hat{\rho}(t_2)) - V(\hat{\rho}(t_1)) = V(\rho_2) - V(\rho_1)$$

which proves the claim.

2.6. Identification of the Entropy

In order to have a selection criterion for the solution $V(\rho)$ of the Hamilton–Jacobi equation, we consider the partial differential equation

$$\partial_t \rho = -\frac{1}{2} \nabla \cdot (D(\rho) \nabla \rho) + \nabla \cdot \left(\chi(\rho) \nabla \frac{\delta V}{\delta \rho} \right) \quad (2.22)$$

As in the previous Subsection we assume $V(\rho)$ is normalized so that $V(\bar{\rho}) = 0$ and satisfies $\delta V(\rho)/\delta \rho = 0$ at the boundary. Note that this is the adjoint hydrodynamics (2.16) if V coincides with S .

If $V = S$ we then have, by using the H Theorem (2.17), that the solution of the Cauchy problem (2.22) with initial condition ρ relaxes to the stationary profile $\bar{\rho}$ so that

$$\lim_{t \rightarrow \infty} V(\rho(t)) = V(\bar{\rho}) = 0 \quad (2.23)$$

Conversely if the above property holds, we can choose in (2.20) the trajectory $\hat{\rho}(t) = \rho(-t)$, where $\rho(t)$ solves (2.22). We then have $H = \delta V(\hat{\rho})/\delta \hat{\rho}$ in (2.20). The last term in (2.20) becomes thus zero and $V(\rho_1)$ can be made arbitrary small; therefore (2.18) holds as an equality.

The above argument shows that $V = S$ if and only if (2.23) holds.

2.7. Hamiltonian Interlude

As in Section 2.2, let us interpret the large deviation functional J as the action for the Lagrangian $\mathcal{L}(\rho, \partial_t \rho)$, see (2.4), and J^* as the action for the Lagrangian $\mathcal{L}^*(\rho, \partial_t \rho)$, see (2.14). Let also $\mathcal{H}(\rho, H)$ and $\mathcal{H}^*(\rho, H)$ be the corresponding Hamiltonians obtained as Legendre transforms, see (2.6).

The time reversal relationship (2.2) implies the following relation between Lagrangians:

$$\mathcal{L}(\rho, \partial_t \rho) = \mathcal{L}^*(\rho, -\partial_t \rho) + \left\langle \frac{\delta S}{\delta \rho}, \partial_t \rho \right\rangle \quad (2.24)$$

As a consequence we obtain

$$\mathcal{H}(\rho, H) = \mathcal{H}^*\left(\rho, \frac{\delta S}{\delta \rho} - H\right) \quad (2.25)$$

Since $\mathcal{L}(\rho, \partial_t \rho)$ and $\mathcal{L}^*(\rho, -\partial_t \rho)$ differ by a total time derivative, see (2.24), we have the following. Given any $\hat{\rho}$ solution of either $\partial_t \hat{\rho} = \mathfrak{D}(\hat{\rho})$ or $\partial_t \hat{\rho} = -\mathfrak{D}^*(\hat{\rho})$ then $\hat{\rho}$ is a solution of the Euler–Lagrange equation for the Lagrangian \mathcal{L} . Likewise given any $\hat{\rho}$ solution of either $\partial_t \hat{\rho} = \mathfrak{D}^*(\hat{\rho})$ or $\partial_t \hat{\rho} = -\mathfrak{D}(\hat{\rho})$ then $\hat{\rho}$ is a solution of the Euler–Lagrange equation for the Lagrangian \mathcal{L}^* .

In the case of the quadratic functional (2.10), we have

$$\mathcal{L}(\rho, \partial_t \rho) = \frac{1}{2} \langle \nabla^{-1}(\partial_t \hat{\rho} - \mathfrak{D}(\rho)), \chi(\hat{\rho})^{-1} \nabla^{-1}(\partial_t \hat{\rho} - \mathfrak{D}(\rho)) \rangle \quad (2.26)$$

The momentum conjugate to $\partial_t \rho$ is

$$H = \frac{\delta \mathcal{L}}{\delta(\partial_t \rho)} = -\nabla^{-1}(\chi(\rho)^{-1} \nabla^{-1}(\partial_t \rho - \mathfrak{D}(\rho))) \quad (2.27)$$

where we recall that $\mathfrak{D}(\rho) = \frac{1}{2} \nabla \cdot (D(\rho) \nabla \rho)$. Note that the above equation is the relationship (2.19); as we shall see later, H is the external field we have to add to the microscopic dynamics to produce the fluctuation $\hat{\rho}$.

The Hamiltonian is given by (2.11), so that the Hamilton equations are

$$\begin{cases} \partial_t \rho = \frac{\delta \mathcal{H}}{\delta H} = \frac{1}{2} \nabla \cdot (D(\rho) \nabla \rho) - \nabla \cdot (\chi(\rho) \nabla H) \\ \partial_t H = -\frac{\delta \mathcal{H}}{\delta \rho} = -\frac{1}{2} \sum_{1 \leq i, j \leq d} [\chi'_{i,j}(\rho) \partial_{u_i} H \partial_{u_j} H + D_{i,j}(\rho) \partial_{u_i} \partial_{u_j} H] \end{cases} \quad (2.28)$$

where $\rho(t, u)$ satisfies the same boundary conditions as in the hydrodynamical equation (1.1) $H(t, u)$ vanishes at the boundary, and $\chi'(\rho)$ is the derivative of $\chi(\rho)$ with respect to ρ .

We note that $(\bar{\rho}, 0)$ is an equilibrium solution of (2.28) belonging to the zero energy manifold $\mathcal{H}(\rho, H) = 0$. Any solution $\rho(t)$ of the hydrodynamical equation (1.1) corresponds to a solution $(\rho(t), 0)$ of the Hamilton equation (2.28) which converges asymptotically, as $t \rightarrow +\infty$, to the equilibrium point $(\bar{\rho}, 0)$. The action J evaluated on this solution is identically zero; this corresponds to the trivial solution $S = 0$ of the Hamilton–Jacobi equation (2.12) and is consistent with the vanishing of the conjugate moment H . Furthermore, if we take the time reversal of any solution of the adjoint hydrodynamics, i.e., $\partial_t \rho(t) = -\mathfrak{D}^*(\rho(t))$ we find a solution of the Hamilton equations given by $(\rho(t), (\delta S / \delta \rho)(\rho(t)))$ which converges asymptotically, as $t \rightarrow -\infty$, to the equilibrium point $(\bar{\rho}, 0)$; the action J evaluated on this solution, as a function of the final state ρ , is the macroscopic entropy $S(\rho)$. Both these trajectories live on the zero energy manifold. Similar properties hold for the Hamiltonian flow of \mathcal{H}^* .

Let us introduce the involution Θ on the phase space (ρ, H) defined by

$$\Theta(\rho, H) = \left(\rho, \frac{\delta S}{\delta \rho}(\rho) - H \right)$$

If we denote by Φ_t , resp. Φ_t^* , the Hamiltonian flow of \mathcal{H} , resp. \mathcal{H}^* , then, by using (2.25), as easy computation shows that Θ acts as the time reversal in the sense that

$$\Theta \Phi_t = \Phi_{-t}^* \Theta \quad (2.29)$$

equivalently, in terms of the Liouville operators, we have

$$\Theta \{f, \mathcal{H}\} = -\{\Theta f, \mathcal{H}^*\}$$

where f is a function on the phase space and $\{\cdot, \cdot\}$ is the Poisson bracket.

The relationship (2.29) is nontrivial also for reversible processes, i.e., when $\mathcal{H} = \mathcal{H}^*$, in such a case it tells us how to change the momentum under time reversal. This definition of time reversal in a Hamiltonian context agrees with the one given in ref. 23.

3. BOUNDARY DRIVEN ZERO RANGE PROCESS

We consider now the so called zero range process which models a nonlinear diffusion of a lattice gas, see, e.g., ref. 24. The model is described by a positive integer variable $\eta_x(\tau)$ representing the number of particles at site x and time τ of a finite subset A_N of the d -dimensional lattice, $A_N = \mathbb{Z}^d \cap N\mathcal{A}$ where \mathcal{A} is a bounded open subset of \mathbb{R}^d . The particles jump with rates $g(\eta_x)$ to one of the nearest-neighbor sites. The function $g(k)$ is increasing and $g(0) = 0$. We assume that our system interacts with particle reservoirs at the boundary of A_N whose activity at site x is given by $\psi(x/N)$ for some given smooth strictly positive function $\psi(u)$. The microscopic dynamics is then defined by the generator (see ref. 12 for the one dimensional case)

$$L_N = L_{N, \text{bulk}} + L_{N, \text{bound.}}$$

where

$$L_{N, \text{bulk}} f(\eta) = \frac{1}{2} \sum_{\substack{x, y \in A_N \\ |x-y|=1}} g(\eta_x) [f(\eta^{x,y}) - f(\eta)]$$

$$L_{N, \text{bound.}} f(\eta) = \frac{1}{2} \sum_{\substack{x \in A_N, y \notin A_N \\ |x-y|=1}} \{g(\eta_x) [f(\eta^{x,-}) - f(\eta)] + \psi(y/N) [f(\eta^{x,+}) - f(\eta)]\} \quad (3.1)$$

in which

$$\eta_z^{x,y} = \begin{cases} \eta_z & \text{if } z \neq x, y \\ \eta_z - 1 & \text{if } z = x \\ \eta_z + 1 & \text{if } z = y \end{cases} \quad (3.2)$$

is the configuration obtained from η when a particle jumps from x to y , and

$$\eta_z^{x,\pm} = \begin{cases} \eta_z & \text{if } z \neq x \\ \eta_z \pm 1 & \text{if } z = x \end{cases} \quad (3.3)$$

is the configuration where we added (resp. subtracted) one particle at x . Note that, since $g(0) = 0$, the number of particles cannot become negative.

We also remark that if $g(k) = k$ the dynamics introduced represents simply non-interacting random walks on A_N (with the appropriate boundary conditions) in terms of the occupation numbers η_x .

3.1. Invariant Measure

Since the generator L_N is *irreducible* (we can go with positive probability from any configuration to any other), under very general hypotheses on the function $g(k)$ there exists a unique invariant measure. It is however remarkable that such invariant measure can be constructed explicitly (see ref. 12 for the one dimensional case).

Let $\lambda_N(x)$ be the solution of the discrete Laplace equation with boundary condition ψ , namely

$$\begin{cases} \frac{1}{2} A_N \lambda_N(x) \equiv \frac{1}{2} \sum_{\substack{y \in \mathbb{Z}^d \\ |x-y|=1}} [\lambda_N(y) - \lambda_N(x)] = 0 & \text{for any } x \in A_N \\ \lambda_N(x) = \psi(x/N) & \text{for any } x \notin A_N \text{ such that} \\ & \exists y \in A_N \text{ for which } |x-y|=1 \end{cases} \quad (3.4)$$

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

$$\mu_{x,N}(\eta_x = k) = \frac{1}{Z(\lambda_N(x))} \frac{\lambda_N^k(x)}{g(1) \cdots g(k)} \quad (3.5)$$

where

$$Z(\varphi) = 1 + \sum_{k=1}^{\infty} \frac{\varphi^k}{g(1) \cdots g(k)} \quad (3.6)$$

is the normalization constant.

The fact that μ_N is an invariant measure can be verified by showing that

$$\sum_{\eta} \mu_N(\eta) L_N f(\eta) = 0$$

for any bounded observable f . The above identity can be easily checked taking into account that, since λ_N solves (3.4), it is an harmonic function; in particular we have

$$\sum_{\substack{x \in A_N, y \notin A_N \\ |x-y|=1}} [\lambda_N(y) - \lambda_N(x)] = 0 \quad (3.7)$$

We emphasize that, if ψ is not constant, the generator L_N is not self-adjoint with respect to the invariant measure so that the process is different from its time reversal and detailed balance does not hold.

3.2. Hydrodynamic Limit

Let us introduce now the macroscopic time $t = \tau/N^2$ and space $u = x/N$. For $u \in A$, $t \geq 0$, we introduce the empirical density as

$$\rho_N(t, u) = \frac{1}{N^d} \sum_{x \in A_N} \eta_x(N^2 t) \delta\left(u - \frac{x}{N}\right) \quad (3.8)$$

where δ denotes the Dirac function. Note that

$$\int_A du \rho_N(t, u) = \frac{1}{N^d} \sum_{x \in A_N} \eta_x(N^2 t)$$

is the average density of particles at (macroscopic) time t .

Let $G(u)$, $u \in A$ be a smooth function and consider

$$\langle \rho_N(t), G \rangle = \int_A du \rho_N(t, u) G(u)$$

To compute the time evolution of $\langle \rho_N(t), G \rangle$ we first note that, according to the general theory of Markov processes, see, e.g., ref. 10, Chap. X, we have

$$\frac{d}{dt} \mathbb{E}_\eta^N(\langle \rho_N(t), G \rangle) = \mathbb{E}_\eta^N(N^2 L_N \langle \rho_N(t), G \rangle) \quad (3.9)$$

where \mathbb{E}_η^N denotes the expectation with respect to the microscopic process with initial configuration η .

Let us assume that G has compact support $K \subset \mathcal{A}$, so that only $L_{N, \text{bulk}}$ gives a non-zero contribution; by summing by parts, we get

$$\begin{aligned} N^2 L_N \langle \rho_N(t), G \rangle &= \frac{1}{2} \frac{1}{N^d} \sum_{x \in \mathcal{A}_N} g(\eta_x(N^2 t)) N^2 \Delta_N G(x/N) \\ &\approx \frac{1}{2} \frac{1}{N^d} \sum_{x \in \mathcal{A}_N} g(\eta_x(N^2 t)) \Delta G(x/N) \end{aligned} \quad (3.10)$$

where we recall that Δ_N denotes the discrete Laplacian.

At this point we face the main problem in the hydrodynamical limit: Equation (3.10) is not closed in $\rho_N(t)$ (its r.h.s. is not a function of $\rho_N(t)$). In order to derive the macroscopic hydrodynamic equation we need to express $g(\eta_x(N^2 t))$ in terms of the empirical density $\rho_N(t)$. This will be done by assuming a “local equilibrium” state (which can be rigorously justified in this context). Let us consider a microscopic site x which is at distance $O(N)$ from the boundary and introduce a volume Q , centered at x , which is very large in microscopic units, but still infinitesimal at the macroscopic level. The time evolution in Q is essentially given only by the bulk dynamics $L_{N, \text{bulk}}$; since the total number of particles in Q changes only via boundary effects and we are looking at what happened after $O(N^2)$ microscopic time units, the system in Q has relaxed to the canonical state corresponding to the density $\rho_N(t, x/N)$.

Let us construct first the grand-canonical measure in Q with constant activity $\varphi > 0$, namely the product measure $\mu_Q^\varphi = \prod_{x \in Q} \mu_x^\varphi$ with marginal given by

$$\mu_x^\varphi(\eta_x = k) = \frac{1}{Z(\varphi)} \frac{\varphi^k}{g(1) \cdots g(k)}$$

where $Z(\varphi)$, which has been defined in (3.6), is the normalization constant. Let now ν_Q^α be the associated canonical measure at density α , i.e.,

$$\nu_Q^\alpha(\eta) = \mu_Q^\varphi \left(\eta \left| \sum_{x \in Q} \eta_x = \alpha |Q| \right. \right)$$

We introduce a function $\phi(\alpha)$ by

$$\phi(\alpha) = \lim_{Q \uparrow \mathbb{Z}^d} E^{\nu_Q^\alpha}(g(\eta_x)) \quad (3.11)$$

where we recall that $E^{\nu_Q^\alpha}$ denotes the expectation with respect to the probability ν_Q^α .

According to the previous discussion, the system in the volume Q is well approximated by a canonical state with density $\rho_N(t, x/N)$; we can thus replace, for N large, $g(\eta_x(N^2t))$ on the r.h.s. of (3.10) by $\phi(\rho_N(t, x/N))$ thus obtaining

$$\frac{d}{dt} \mathbb{E}_\eta^N(\langle \rho_N(t), G \rangle) \approx \frac{1}{2} \mathbb{E}_\eta^N(\langle \phi(\rho_N(t)), \Delta G \rangle) \quad (3.12)$$

To see which are the boundary conditions satisfied by $\rho_N(t)$ we need to consider the boundary dynamics, $L_{N, \text{bound.}}$. In contrast to the bulk dynamics, this is a non-conservative, Glauber-like, dynamics. Since we are looking after $O(N^2)$ microscopic time units the density at the boundary has well thermalized to its equilibrium value which impose

$$\mathbb{E}_\eta^N(\phi(\rho_N(t, u))) \approx \psi(u) \quad u \in \partial A \quad (3.13)$$

where the function ϕ has been defined above.

Assume the initial configuration η of the process is such that for any smooth function G we have

$$\lim_{N \rightarrow \infty} \langle \rho_N(0), G \rangle = \lim_{N \rightarrow \infty} \frac{1}{N^d} \sum_{x \in A_N} \eta_x G(x/N) = \int_A du \gamma(u) G(u) \quad (3.14)$$

for some function γ . By the law of large numbers, $\rho_N(t)$ becomes a deterministic function in the limit $N \rightarrow \infty$, so that we can eliminate the expectation values in (3.12) and (3.13). In conclusion we have obtained, for any smooth function G , that

$$\lim_{N \rightarrow \infty} \langle \rho_N(t), G \rangle = \int_A du \rho(t, u) G(u)$$

where the convergence is in probability. Recalling (3.12), the limiting density $\rho = \rho(t, u)$ solves

$$\begin{cases} \partial_t \rho(t, u) = \frac{1}{2} \Delta \phi(\rho(t, u)) & u \in A \\ \phi(\rho(t, u)) = \psi(u) & u \in \partial A \\ \rho(0, u) = \gamma(u) \end{cases} \quad (3.15)$$

which is the hydrodynamic equation for the boundary driven zero range process.

We finally show that, by the equivalence of ensembles, we can express the function $\alpha \mapsto \phi(\alpha)$ introduced in (3.11), in a more convenient way, in

terms of the grand-canonical measure μ_Q^φ . By exploiting the product structure of μ_Q^φ and choosing the activity $\varphi(\alpha)$ so that $\mu_x^{\varphi(\alpha)}(\eta_x) = \alpha$, we have

$$\phi(\alpha) = E^{\mu_x^{\varphi(\alpha)}}(g(\eta_x))$$

A straightforward computation shows now that $\phi(\alpha) = \varphi(\alpha)$ so that the function $\alpha \mapsto \phi(\alpha)$ is the inverse of the function $\varphi \mapsto R(\varphi)$ given by

$$R(\varphi) = E^{\mu_x^\varphi}(\eta_x) = \varphi \frac{Z'(\varphi)}{Z(\varphi)} \quad (3.16)$$

i.e., $R(\varphi)$ is the equilibrium density corresponding to the activity φ . From the assumptions on g it follows that $R(\varphi)$ is strictly increasing.

3.3. Dynamical Large Deviations

In order to compute the probability of deviation from the typical behavior described by Eq. (3.15), namely the action functional $J(\hat{\rho})$, we follow the classical strategy in large deviation theory: we need “only” to consider a perturbation of the system which makes the deviation $\hat{\rho}$ the typical behavior and write the probability in the unperturbed system in terms of the perturbed one. From this computation we shall extract, asymptotically in N , the factor $\exp\{-N^d J(\hat{\rho})\}$.

We consider the zero range process in a (space time dependent) external field $H(t, u)$ which is a smooth function of the macroscopic variables vanishing outside Λ , i.e., $H(t, u) = 0$ for $u \notin \Lambda$, $t \geq 0$. The perturbed dynamics is specified by the time dependent generator $L_{N, \tau}^H = L_{N, \tau, \text{bulk}}^H + L_{N, \tau, \text{bound}}^H$, where

$$\begin{aligned} L_{N, \tau, \text{bulk}}^H f(\eta) &= \frac{1}{2} \sum_{\substack{x, y \in \Lambda_N \\ |x-y|=1}} g(\eta_x) e^{H(\tau/N^2, y/N) - H(\tau/N^2, x/N)} [f(\eta^{x, y}) - f(\eta)] \\ L_{N, \tau, \text{bound}}^H f(\eta) &= \frac{1}{2} \sum_{\substack{x \in \Lambda_N, y \notin \Lambda_N \\ |x-y|=1}} \{g(\eta_x) e^{H(\tau/N^2, y/N) - H(\tau/N^2, x/N)} [f(\eta^{x, -}) - f(\eta)] \\ &\quad + \psi(y/N) e^{H(\tau/N^2, x/N) - H(\tau/N^2, y/N)} [f(\eta^{x, +}) - f(\eta)]\} \end{aligned} \quad (3.17)$$

The interpretation of the perturbed dynamics is the following: in the macroscopic scale, we simply introduced a small space-time dependent drift $N^{-1} \nabla H(t, u)$ in the motion of the particles.

Assuming the initial configuration η is associated to a density profile γ in the sense of (3.14), by similar computations as the ones given for $H = 0$, we get that the hydrodynamic equation for the perturbed system is

$$\begin{cases} \partial_t \hat{\rho}(t, u) = \frac{1}{2} \Delta \phi(\hat{\rho}(t, u)) - \nabla \cdot (\phi(\hat{\rho}(t, u)) \nabla H(t, u)) & u \in \Lambda \\ \phi(\hat{\rho}(t, u)) = \psi(u) & u \in \partial \Lambda \\ \hat{\rho}(0, u) = \gamma(u) \end{cases} \quad (3.18)$$

If we regard $\hat{\rho}(t, u)$ as given and consider $H(t, u)$ as the unknown, the above equation tells us which is the perturbation for which $\hat{\rho}(t, u)$ is the typical behavior. Note (3.18) is precisely the relationship (2.27) between $\partial_t \hat{\rho}$ and the conjugate momentum H .

Let us denote by \mathbb{P}_η^N , resp. $\mathbb{P}_\eta^{N,H}$, the probability for the unperturbed, resp. perturbed, process with initial configuration η . We then have

$$\frac{d\mathbb{P}_\eta^{N,H}(\eta(N^2t), t \in [0, T])}{d\mathbb{P}_\eta^N(\eta(N^2t), t \in [0, T])} = \exp\{\mathcal{J}_{[0,T]}^N(\eta(\cdot), H)\} \quad (3.19)$$

where

$$\begin{aligned} \mathcal{J}_{[0,T]}^N(\eta(\cdot), H) &= \sum_{x \in \Lambda_N} [H(T, x/N) \eta_x(N^2T) - H(0, x/N) \eta_x(0)] \\ &\quad - \int_0^T dt \sum_{x \in \Lambda_N} \partial_t H(t, x/N) \eta_x(N^2t) \\ &\quad - \frac{N^2}{2} \int_0^T dt \sum_{\substack{x \in \Lambda_N, y \in \mathbb{Z}^d \\ |x-y|=1}} g(\eta_x(N^2t)) [e^{H(t, y/N) - H(t, x/N)} - 1] \\ &\quad - \frac{N^2}{2} \int_0^T dt \sum_{\substack{x \in \Lambda_N, y \notin \Lambda_N \\ |x-y|=1}} \psi(y/N) [e^{H(t, x/N) - H(t, y/N)} - 1] \end{aligned} \quad (3.20)$$

See Appendix A for a derivation of the above formula (another proof can be found in ref. 24, Prop. A1.7.3).

With the help of Eq. (3.19) we can write the probability that $\rho_N(t)$ is close to $\hat{\rho}(t)$ for the unperturbed system as follows

$$\mathbb{P}_\eta^N(\rho_N(t) \sim \hat{\rho}(t), t \in [0, T]) = \mathbb{E}_\eta^{N,H}(e^{-\mathcal{J}_{[0,T]}^N(\eta(\cdot), H)} \mathbb{1}_{\rho_N \sim \hat{\rho}}) \quad (3.21)$$

where $\mathbb{E}_\eta^{N,H}$ denotes the expectation with respect to the perturbed process. Using the explicit expression (3.20), by Taylor expansion, we get

$$\begin{aligned} & \mathcal{J}_{[0,T]}^N(\eta(\cdot), H) \\ & \approx N^d \left\{ \langle \rho_N(T), H(T) \rangle - \langle \rho_N(0), H(0) \rangle - \int_0^T dt \langle \rho_N(t), \partial_t H(t) \rangle \right. \\ & \quad - \frac{1}{2} \int_0^T dt \frac{1}{N^d} \sum_{x \in \Lambda_N} g(\eta_x(N^2 t)) [\Delta H(t, x/N) + |\nabla H(t, x/N)|^2] \\ & \quad \left. + \frac{1}{2} \int_0^T dt \int_{\partial A} du \psi(u) \partial_{\hat{n}} H(t, u) \right\} \end{aligned} \quad (3.22)$$

where $\partial_{\hat{n}} H(t, u)$ is the normal derivative of $H(t, u)$ (\hat{n} being the outward normal to A).

If $\eta(N^2 t)$ is a typical trajectory for the perturbed process, by the same argument given in derivation of the hydrodynamical equation, we can replace $g(\eta_x(N^2 t))$ above by $\phi(\rho_N(t, x/N))$. Since $\rho_N(t)$ is close to $\hat{\rho}(t)$, and

$$\lim_{N \rightarrow \infty} \mathbb{P}_\eta^{N,H}(\rho_N(t) \sim \hat{\rho}(t), t \in [0, T]) = 1$$

from (3.21) we get

$$\mathbb{P}_\eta^N(\rho_N(t) \sim \hat{\rho}(t), t \in [0, T]) \approx \exp\{-N^d J_{[0,T]}(\hat{\rho})\} \quad (3.23)$$

where

$$\begin{aligned} J_{[0,T]}(\hat{\rho}) &= \langle \hat{\rho}(T), H(T) \rangle - \langle \hat{\rho}(0), H(0) \rangle - \int_0^T dt \langle \hat{\rho}(t), \partial_t H(t) \rangle \\ & \quad - \frac{1}{2} \int_0^T dt \langle \phi(\hat{\rho}(t)), \Delta H(t) + |\nabla H(t)|^2 \rangle \\ & \quad + \frac{1}{2} \int_0^T dt \int_{\partial A} du \psi(u) \partial_{\hat{n}} H(t, u) \end{aligned} \quad (3.24)$$

Recalling that H and $\hat{\rho}$ are related by (3.18), we finally get, after an integration by parts (recall that $H(t, u)$ vanishes at the boundary ∂A)

$$J_{[0,T]}(\hat{\rho}) = \frac{1}{2} \int_0^T dt \langle \phi(\hat{\rho}(t)), |\nabla H(t)|^2 \rangle \quad (3.25)$$

The action functional J is defined to be infinite if $\hat{\rho}$ does not satisfy the boundary conditions in (3.18). From (3.25) and (3.18) we see that $J_{[0,T]}$ is of the form (2.10) with $D_{i,j}(\hat{\rho}) = \phi'(\hat{\rho}) \delta_{i,j}$ and $\chi_{i,j}(\hat{\rho}) = \phi(\hat{\rho}) \delta_{i,j}$.

The rigorous derivation of the action functional J requires some difficult estimates. In fact, while in the proof of the hydrodynamic limit it is enough to show that we can replace $g(\eta_x(N^2t))$ by $\phi(\rho_N(t, x/N))$ with an error vanishing as $N \rightarrow \infty$, in the proof of the large deviations we need such an error to be $o(e^{-N^d})$. This can be proven by the so called super exponential estimate, see refs. 3 and 24, which is the key point in the rigorous approach.

3.4. Macroscopic Entropy and Adjoint Hydrodynamics

From the expression (3.25) for J it follows that the Hamilton–Jacobi equation (2.12) for the boundary driven zero range process is

$$\left\langle \nabla \frac{\delta S}{\delta \rho}, \phi(\rho) \nabla \frac{\delta S}{\delta \rho} \right\rangle + \left\langle \frac{\delta S}{\delta \rho}, \Delta \phi(\rho) \right\rangle = 0 \quad (3.26)$$

Let us consider the functional

$$S(\rho) = \int_A du \left[\rho(u) \log \frac{\phi(\rho(u))}{\lambda(u)} - \log \frac{Z(\phi(\rho(u)))}{Z(\lambda(u))} \right] \quad (3.27)$$

where $Z(\varphi)$ has been defined in (3.6) and $\lambda(u)$ is the stationary activity profile, namely $\lambda(u) = \phi(\bar{\rho}(u))$ where $\bar{\rho}$ is the stationary solution of the hydrodynamic equation (3.15). Note that λ is also the macroscopic limit of λ_N , solution of (3.4). By using that $\varphi \mapsto R(\varphi)$ given in (3.16) is the inverse function of $\rho \mapsto \phi(\rho)$, we get

$$\frac{\delta S(\rho)}{\delta \rho(u)} = \log \phi(\rho(u)) - \log \lambda(u) \quad (3.28)$$

We remark that the functional S given in (3.27) is uniquely characterized by (3.28) once we impose the normalization $S(\bar{\rho}) = 0$.

An easy computation shows that the functional S given in (3.27) solves the Hamilton–Jacobi equation (3.26). Recalling that $\phi(\rho(u)) = \lambda(u) = \psi(u)$ for $u \in \partial A$ we have indeed

$$\begin{aligned}
 & \left\langle \nabla \log \frac{\phi(\rho)}{\lambda}, \phi(\rho) \nabla \log \frac{\phi(\rho)}{\lambda} \right\rangle + \left\langle \log \frac{\phi(\rho)}{\lambda}, \Delta \phi(\rho) \right\rangle \\
 &= - \left\langle \nabla \log \frac{\phi(\rho)}{\lambda}, \phi(\rho) \frac{\nabla \lambda}{\lambda} \right\rangle \\
 &= \left\langle \phi(\rho), \frac{|\nabla \lambda|^2}{\lambda^2} \right\rangle - \left\langle \nabla[\phi(\rho) - \lambda], \frac{\nabla \lambda}{\lambda} \right\rangle - \left\langle \nabla \lambda, \frac{\nabla \lambda}{\lambda} \right\rangle \\
 &= \left\langle \phi(\rho), \frac{|\nabla \lambda|^2}{\lambda^2} \right\rangle - \left\langle \nabla \lambda, \frac{\nabla \lambda}{\lambda} \right\rangle + \left\langle [\phi(\rho) - \lambda], \nabla \cdot \frac{\nabla \lambda}{\lambda} \right\rangle = 0 \quad (3.29)
 \end{aligned}$$

since $\Delta \lambda(u) = 0$ for $u \in A$.

From the fluctuation-dissipation relationship (2.15) we get that the adjoint hydrodynamic equation for the boundary driven zero range process is

$$\begin{cases} \partial_t \rho^*(t, u) = \frac{1}{2} \Delta \phi(\rho^*(t, u)) - \nabla \cdot (\phi(\rho^*(t, u)) \nabla \log \lambda(u)) & u \in A \\ \phi(\rho^*(t, u)) = \psi(u) & u \in \partial A \\ \rho^*(0, u) = \gamma(u) \end{cases} \quad (3.30)$$

Recalling that $\lambda(u) = \phi(\bar{\rho}(u))$, the density profile $\bar{\rho}$ is also a stationary solution of (3.30). Since $\phi'(\alpha) > 0$, the right hand side of (3.30) is dissipative; therefore we have that $\rho^*(t) \rightarrow \bar{\rho}$ as $t \rightarrow \infty$; so that we meet the criterion (2.23).

Since in this model we know explicitly the invariant measure μ_N we can check whether the predictions (3.27) on the macroscopic entropy and (3.30) on the adjoint hydrodynamics of the general theory are correct.

Given a smooth function $h(u)$ let us introduce the pressure $G(h)$ corresponding to the chemical potential profile h as

$$\begin{aligned}
 G(h) &= \lim_{N \rightarrow \infty} \frac{1}{N^d} \log E^{\mu_N}(\exp\{N^d \langle \rho_N, h \rangle\}) \\
 &= \lim_{N \rightarrow \infty} \frac{1}{N^d} \log \sum_{\eta} \mu_N(\eta) \exp \left\{ \sum_{x \in A_N} h(x/N) \eta_x \right\} \\
 &= \lim_{N \rightarrow \infty} \frac{1}{N^d} \sum_{x \in A_N} [\log Z(\lambda_N(x) e^{h(x/N)}) - \log Z(\lambda_N(x))] \\
 &= \int_A du [\log Z(\lambda(u) e^{h(u)}) - \log Z(\lambda(u))] \quad (3.31)
 \end{aligned}$$

where $Z(\varphi)$ has been defined in (3.6) and $\lambda_N(x)$ is the solution of (3.4).

By a standard computation due to Cramer we have that the Legendre transform of the pressure $G(h)$, i.e., the macroscopic entropy, is the rate functional for the asymptotic probability of large deviations of the density profile in the invariant measure μ_N . Let us in fact introduce a perturbed measure μ_N^h by

$$\mu_N^h(\eta) = \prod_{x \in A_N} \frac{Z(\lambda_N(x))}{Z(\lambda_N(x) e^{h(x/N)})} \exp\{h(x/N) \eta_x\} \mu_{x,N}(\eta_x)$$

and, for a fixed density profile $\rho(u)$, choose the chemical potential profile h so that

$$E^{\mu_N^h}(\eta_x) = \rho(x/N) \quad (3.32)$$

namely $h(x/N) = \log[\phi(\rho(x/N))/\lambda_N(x)]$. We then have

$$\begin{aligned} \mu_N(\rho_N \sim \rho) &= E^{\mu_N^h}(e^{-\sum_{x \in A_N} [h(x/N) \eta_x - \log Z(\lambda_N(x) e^{h(x/N)}) + \log Z(\lambda_N(x))]} \mathbb{1}_{\rho_N \sim \rho}) \\ &\approx E^{\mu_N^h}(e^{-N^d[\langle \rho_N, h \rangle - G(h)]} \mathbb{1}_{\rho_N \sim \rho}) \approx e^{-N^d[\langle \rho, h \rangle - G(h)]} \end{aligned} \quad (3.33)$$

since, by the law of large numbers, $\lim_{N \rightarrow \infty} \mu_N^h(\rho_N \sim \rho) = 1$. From (3.32) we have that $\delta G/\delta h = \rho$. We therefore have obtained precisely that S is the Legendre transform of G . A computation, which is left to the reader, shows now that the Legendre transform of the right hand side of (3.31) gives indeed the functional $S(\rho)$ defined in (3.27).

We want to stress a main difference between the macroscopic computation (3.29) and the microscopic one just given. While the former depends on the action functional J , which involves only macroscopic quantities, the latter depends on the explicit expression of the invariant measure μ_N . In particular the macroscopic computation is independent of the specific way the interaction with reservoirs is modeled (provided of course the functional J is not affected).

We now discuss the adjoint hydrodynamics from a microscopic point of view. Since the invariant measure μ_N is explicitly known we can obtain the adjoint generator L_N^* which is defined by the identity (1.3). Recalling that λ_N solves (3.4) and that (3.7) holds, we have that $L_N^* = L_{N, \text{bulk}}^* + L_{N, \text{bound}}^*$ where

$$\begin{aligned} L_{N, \text{bulk}}^* f(\eta) &= \frac{1}{2} \sum_{\substack{x, y \in A_N \\ |x-y|=1}} g(\eta_x) \frac{\lambda_N(y)}{\lambda_N(x)} [f(\eta^{x,y}) - f(\eta)] \\ L_{N, \text{bound}}^* f(\eta) &= \frac{1}{2} \sum_{\substack{x \in A_N, y \notin A_N \\ |x-y|=1}} \left\{ g(\eta_x) \frac{\psi(y/N)}{\lambda_N(x)} [f(\eta^{x,-}) - f(\eta)] \right. \\ &\quad \left. + \lambda_N(x) [f(\eta^{x,+}) - f(\eta)] \right\} \end{aligned} \quad (3.34)$$

Notice that the form of (3.34) is the same as (3.1) with the rates modified in such a way to invert the particle flux. The generator L_N^* can also be interpreted as the original system perturbed by a time independent external field $H(t, x/N) = \log \lambda_N(x)$, compare (3.17) to (3.34). In particular we have that the adjoint hydrodynamic equation is indeed given by (3.30).

By repeating the same argument given in Section 3.3, it is not difficult to show that the action functional J^* describing the probability of large deviations from the hydrodynamic behavior for the adjoint process is given by

$$J_{[0, T]}^*(\hat{\rho}) = \frac{1}{2} \int_0^T dt \langle \phi(\hat{\rho}(t)), |\nabla K(t)|^2 \rangle \tag{3.35}$$

where $K(t) = K(t, u)$ is to be obtained from $\hat{\rho}$ by solving the equation

$$\begin{cases} \partial_t \hat{\rho}(t, u) = \frac{1}{2} \Delta \phi(\hat{\rho}(t, u)) - \nabla \cdot (\phi(\hat{\rho}(t, u)) \nabla [\log \lambda(u) + K(t, u)]) & u \in A \\ \phi(\hat{\rho}(t, u)) = \psi(u) & u \in \partial A \\ \hat{\rho}(0, u) = \gamma(u) \end{cases} \tag{3.36}$$

A computation now allows us to check that the identity (2.2), which has been obtained only by a time symmetry argument, holds for the boundary driven zero range process.

4. BOUNDARY DRIVEN SIMPLE EXCLUSION PROCESS

The simple exclusion process is a model of a lattice gas with an exclusion principle: a particle can move to a neighboring site, with rate 1/2 for each side, only if this is empty. Let, as in the previous section, $A_N = \mathbb{Z}^d \cap N A$ and denote by $\eta_x(\tau) \in \{0, 1\}$ the number of particles at the site x at (microscopic) time τ . The system is in contact with particle reservoirs at the boundary of A_N whose activity at site x is given by $\psi(x/N)$ for some given strictly positive smooth function $\psi(u)$.

The microscopic dynamics is defined by the generator $L_N = L_{N, \text{bulk}} + L_{N, \text{bound}}$ where

$$\begin{aligned} L_{N, \text{bulk}} f(\eta) &= \frac{1}{2} \sum_{\substack{x, y \in A_N \\ |x-y|=1}} \eta_x (1-\eta_y) [f(\eta^{x,y}) - f(\eta)] \\ L_{N, \text{bound}} f(\eta) &= \frac{1}{2} \sum_{\substack{x \in A_N, y \notin A_N \\ |x-y|=1}} \{ \eta_x [f(\eta^{x,-}) - f(\eta)] \\ &\quad + \psi(y/N) (1-\eta_x) [f(\eta^{x,+}) - f(\eta)] \} \end{aligned} \tag{4.1}$$

where $\eta^{x,y}$ and $\eta^{x,\pm}$ have been defined in (3.2) and (3.3).

In contrast to the zero range model the invariant measure μ_N is not known explicitly; we shall see that it carries long range correlations making the entropy nonlocal.

4.1. Hydrodynamic Equation and Dynamical Large Deviations

The hydrodynamic equation for the simple exclusion process can be derived by the same argument given for the zero range process; in fact it is easier in this case because a computation analogous to (3.10) leads directly to a closed equation in the empirical density. We find that the limiting density evolves according to the linear heat equation

$$\begin{cases} \partial_t \rho(t, u) = \frac{1}{2} \Delta \rho(t, u) & u \in \Lambda \\ \rho(t, u) = \frac{\psi(u)}{1 + \psi(u)} & u \in \partial \Lambda \\ \rho(0, u) = \gamma(u) \end{cases} \quad (4.2)$$

where γ is the initial density profile, associated to the initial microscopic configuration η in the sense (3.14). In this case the density of particles ρ takes values in $[0, 1]$. The hydrodynamic limit for more general boundary driven models has been discussed in ref. 13. As in the previous section we shall denote by $\bar{\rho} = \bar{\rho}(u)$ the unique stationary solution of (4.2).

The action functional J describing the probability of large deviations from the hydrodynamic behavior can be obtained as for the zero range process. In this case the perturbed dynamics is defined by the time dependent generator $L_{N, \tau}^H = L_{N, \tau, \text{bulk}}^H + L_{N, \tau, \text{bound}}^H$ where

$$\begin{aligned} L_{N, \tau, \text{bulk}}^H f(\eta) &= \frac{1}{2} \sum_{\substack{x, y \in A_N \\ |x-y|=1}} \eta_x (1 - \eta_y) e^{H(\tau/N^2, y/N) - H(\tau/N^2, x/N)} [f(\eta^{x, y}) - f(\eta)] \\ L_{N, \tau, \text{bound}}^H f(\eta) &= \frac{1}{2} \sum_{\substack{x \in A_N, y \notin A_N \\ |x-y|=1}} \{ \eta_x e^{H(\tau/N^2, y/N) - H(\tau/N^2, x/N)} [f(\eta^{x, -}) - f(\eta)] \\ &\quad + \psi(y/N) (1 - \eta_x) e^{H(\tau/N^2, x/N) - H(\tau/N^2, y/N)} [f(\eta^{x, +}) - f(\eta)] \} \end{aligned} \quad (4.3)$$

and the external field $H(t, u)$ vanishes for $u \notin \Lambda$.

The hydrodynamic equation for the perturbed dynamics is then given by

$$\begin{cases} \partial_t \hat{\rho}(t, u) = \frac{1}{2} \Delta \hat{\rho}(t, u) - \nabla \cdot \{ \hat{\rho}(t, u) [1 - \hat{\rho}(t, u)] \nabla H(t, u) \} & u \in \Lambda \\ \hat{\rho}(t, u) = \frac{\psi(u)}{1 + \psi(u)} & u \in \partial \Lambda \\ \hat{\rho}(0, u) = \gamma(u) \end{cases} \quad (4.4)$$

For the simple exclusion process the functional $\mathcal{J}_{[0, T]}^N$ defined in (3.19) is given by

$$\begin{aligned} & \mathcal{J}_{[0, T]}^N(\eta(\cdot), H) \\ &= \sum_{x \in \Lambda_N} [H(T, x/N) \eta_x(N^2 T) - H(0, x/N) \eta_x(0)] \\ & \quad - \int_0^T dt \sum_{x \in \Lambda_N} \partial_i H(t, x/N) \eta_x(N^2 t) \\ & \quad - \frac{N^2}{2} \int_0^T dt \sum_{\substack{x, y \in \Lambda_N \\ |x-y|=1}} \eta_x(N^2 t) [1 - \eta_y(N^2 t)] [e^{H(t, y/N) - H(t, x/N)} - 1] \\ & \quad - \frac{N^2}{2} \int_0^T dt \sum_{\substack{x \in \Lambda_N, y \notin \Lambda_N \\ |x-y|=1}} \eta_x(N^2 t) [e^{H(t, y/N) - H(t, x/N)} - 1] \\ & \quad - \frac{N^2}{2} \int_0^T dt \sum_{\substack{x \in \Lambda_N, y \notin \Lambda_N \\ |x-y|=1}} \psi(y/N) [1 - \eta_x(N^2 t)] [e^{H(t, x/N) - H(t, y/N)} - 1] \end{aligned} \quad (4.5)$$

we refer again to Appendix A for the derivation of the above formula.

By Taylor expansion, summation by parts, the replacements $\eta_x(N^2 t) \times [1 - \eta_y(N^2 t)] \approx \rho_N(t, x/N) [1 - \rho_N(t, x/N)]$ in the bulk and $\eta_x(N^2 t) \approx \psi(t, x/N) / [1 + \psi(t, x/N)]$ at the boundary (which can be heuristically justified by the same argument given for the zero range process) we get

$$\begin{aligned} \mathcal{J}_{[0, T]}^N(\eta(\cdot), H) &\approx N^d \left\{ \langle \rho_N(T), H(T) \rangle - \langle \rho_N(0), H(0) \rangle \right. \\ & \quad - \int_0^T dt \left\langle \rho_N(t), \partial_i H(t) + \frac{1}{2} \Delta H(t) \right\rangle \\ & \quad - \frac{1}{2} \int_0^T dt \langle \rho_N(t) [1 - \rho_N(t)], |\nabla H(t)|^2 \rangle \\ & \quad \left. + \frac{1}{2} \int_0^T dt \int_{\partial \Lambda} du \frac{\psi(u)}{1 + \psi(u)} \partial_{\bar{n}} H(t, u) \right\} \end{aligned} \quad (4.6)$$

Recalling that the hydrodynamic equation for the perturbed dynamics is given by (4.4), after an integration by parts, we finally get the action functional J

$$J_{[0, T]}(\hat{\rho}) = \frac{1}{2} \int_0^T dt \langle \hat{\rho}(t)[1 - \hat{\rho}(t)], |\nabla H(t)|^2 \rangle \quad (4.7)$$

which is of the form (2.10) with $D_{i,j}(\hat{\rho}) = \delta_{i,j}$ and $\chi_{i,j}(\hat{\rho}) = \hat{\rho}[1 - \hat{\rho}] \delta_{i,j}$. As for the zero range, the functional $J_{[0, T]}(\hat{\rho})$ is defined to be infinite if $\hat{\rho}$ does not satisfy the boundary condition in (4.4).

4.2. Reduction of Hamilton–Jacobi to a Nonlinear Differential Equation ($d=1$)

We consider here the boundary driven simple exclusion process in one space dimension. In a very interesting paper, by using a matrix representation of the microscopic invariant measure and combinatorial techniques, Derrida *et al.*⁽¹⁴⁾ have recently shown that the action functional S (which we called the macroscopic entropy) can be expressed in terms of the solution of a nonlinear ordinary differential equation. We show next how this result can be recovered in our approach by following the dynamical/variational route explained in Section 2. Namely, we consider the variational problem (2.5) for the one-dimensional simple exclusion process and show that the associated Hamilton–Jacobi equation which, taking into account (4.7) and (4.4), is the functional derivative equation

$$\left\langle \nabla \frac{\delta S}{\delta \rho}, \rho(1 - \rho) \nabla \frac{\delta S}{\delta \rho} \right\rangle + \left\langle \frac{\delta S}{\delta \rho}, \Delta \rho \right\rangle = 0 \quad (4.8)$$

can be reduced to the nonlinear ordinary differential equation first obtained in ref. 14.

For notation simplicity, we assume that $\Lambda = (-1, 1)$, so that $\partial\Lambda = \pm 1$. We shall also assume the macroscopic density profile $\rho = \rho(u)$ satisfies the boundary conditions in Eq. (4.2).

We look for a solution of the Hamilton–Jacobi equation (4.8) by performing the change of variable

$$\frac{\delta S}{\delta \rho(u)} = \log \frac{\rho(u)}{1 - \rho(u)} - \phi(u; \rho) \quad (4.9)$$

for some functional $\phi(u; \rho)$ to be determined satisfying the boundary conditions $\phi(\pm 1) = \log \rho(\pm 1) / [1 - \rho(\pm 1)] = \log \psi(\pm 1)$.

Inserting (4.9) into (4.8), we get (note that $\rho - e^\phi / (1 + e^\phi)$ vanishes at the boundary)

$$\begin{aligned}
 0 &= - \left\langle \nabla \left(\log \frac{\rho}{1-\rho} - \phi \right), \rho(1-\rho) \nabla \phi \right\rangle \\
 &= - \langle \nabla \rho, \nabla \phi \rangle + \langle \rho(1-\rho), (\nabla \phi)^2 \rangle \\
 &= - \left\langle \nabla \left(\rho - \frac{e^\phi}{1+e^\phi} \right), \nabla \phi \right\rangle - \left\langle \left(\rho - \frac{e^\phi}{1+e^\phi} \right) \left(\rho - \frac{1}{1+e^\phi} \right), (\nabla \phi)^2 \right\rangle \\
 &= \left\langle \left(\rho - \frac{e^\phi}{1+e^\phi} \right), \left(\Delta \phi + \frac{(\nabla \phi)^2}{1+e^\phi} - \rho (\nabla \phi)^2 \right) \right\rangle \tag{4.10}
 \end{aligned}$$

We obtain a solution of the Hamilton–Jacobi if we solve the following ordinary differential equation which relates the functional $\phi(u) = \phi(u; \rho)$ to ρ

$$\begin{cases} \frac{\Delta \phi(u)}{[\nabla \phi(u)]^2} + \frac{1}{1+e^{\phi(u)}} = \rho(u) & u \in (-1, 1) \\ \phi(\pm 1) = \log \psi(\pm 1) \end{cases} \tag{4.11}$$

A computation shows that the derivative of the functional

$$S(\rho) = \int_{-1}^1 du \left\{ \rho \log \rho + (1-\rho) \log(1-\rho) + (1-\rho) \phi - \log(1+e^\phi) + \log \frac{\nabla \phi}{\nabla \rho} \right\} \tag{4.12}$$

is given by (4.9) when $\phi(u; \rho)$ solves (4.11). According to the discussion in Section 2.6, we will be able to conclude that (4.12) is indeed the macroscopic entropy as soon as we show that it meets the criterion (2.23). This will be done in the next Subsection. By the change of variable $\phi = \log[F/(1-F)]$ Eq. (4.11) becomes the one obtained in ref. 14.

One may be tempted to repeat the same computation in arbitrary dimension; one would obtain a partial differential equation analogous to (4.11). However, in more than one dimension it does not exist, in general, a functional S whose derivative is given by (4.9) with ϕ and ρ related by such partial differential equation.

The equation (4.11), considered as a relationship expressing ρ in terms of ϕ , can be interpreted in the following way. Let

$$S_0(\rho) = \int_{-1}^1 du \{ \rho \log \rho + (1-\rho) \log(1-\rho) \} \tag{4.13}$$

be the equilibrium entropy. Since $\delta S_0/\delta\rho = \log[\rho/(1-\rho)]$ we have

$$\phi(u; \rho) = \frac{\delta S_0}{\delta\rho} - \frac{\delta S}{\delta\rho}$$

If $\mathcal{G}(\phi)$ is the Legendre transform of $S_0 - S$, we find that $\delta\mathcal{G}/\delta\phi = \rho$ which is the relationship (4.11).

We note that the remark after (3.33) for the zero range process also applies to the present context. In particular the macroscopic computation (4.10) depends only on the action functional J and is therefore stable with respect to microscopic perturbations which do not affect the dynamical large deviations.

4.3. Adjoint Hydrodynamics ($d=1$)

By using the fluctuation dissipation relationship (2.15) and the expression (4.9) for $\delta S/\delta\rho$, we find that the adjoint hydrodynamics is given by the equation nonlocal in space

$$\left\{ \begin{array}{l} \partial_t \rho^*(t, u) = \frac{1}{2} \Delta \rho^*(t, u) - \nabla \{ \rho^*(t, u) [1 - \rho^*(t, u)] \nabla \phi(u; \rho^*(t)) \} \\ \quad \quad \quad u \in (-1, 1) \\ \rho^*(t, \pm 1) = \frac{\psi(\pm 1)}{1 + \psi(\pm 1)} \\ \rho^*(0, u) = \gamma(u) \end{array} \right. \quad (4.14)$$

where $\phi(u; \rho^*(t))$ is to be obtained from $\rho^*(t)$ by solving (4.11). Since $\phi(u; \bar{\rho}) = \log[\bar{\rho}/(1-\bar{\rho})]$, we see that $\bar{\rho}$ is also a stationary solution of (4.14).

We now show how (4.14) can be related to the heat equation. Let $\rho^*(t, u)$ be the solution of (4.14) and introduce $F = F(t, u)$ as

$$F(t, u) = \frac{e^{\phi(u; \rho^*(t))}}{1 + e^{\phi(u; \rho^*(t))}} \quad (4.15)$$

it is not too difficult to check (see Appendix B) that $F(t, u)$ satisfies the heat equation

$$\left\{ \begin{array}{l} \partial_t F(t, u) = \frac{1}{2} \Delta F(t, u) \quad u \in (-1, 1) \\ F(t, \pm 1) = \frac{\psi(\pm 1)}{1 + \psi(\pm 1)} \\ F(0, u) = \frac{e^{\phi(u; \gamma)}}{1 + e^{\phi(u; \gamma)}} \end{array} \right. \quad (4.16)$$

Conversely, given $F = F(t, u)$ which solves (4.16), by setting

$$\rho^*(t, u) = F(t, u) + F(t, u)[1 - F(t, u)] \frac{\Delta F(t, u)}{[\nabla F(t, u)]^2} \quad (4.17)$$

a computation (see again Appendix B) shows that ρ^* solves (4.14).

We have thus shown how a solution of the (nonlocal, nonlinear) Eq. (4.14) can be obtained from the linear heat equation by performing the nonlocal transformation (4.15) on the initial datum. In particular, since the solution $F(t, u)$ of (4.16) converges as $t \rightarrow \infty$ to $\bar{\rho}$, we see that the functional $S(\rho)$ given in (4.12) satisfies the criterion (2.23) so that it is indeed the macroscopic entropy.

4.4. Non-Perturbative Lower Bound on the Macroscopic Entropy ($d \geq 1$)

We discuss here a non-perturbative bound for the macroscopic entropy in the boundary driven simple exclusion process in arbitrary space dimension d . Let $S_0(\rho)$ be the equilibrium entropy as defined in (4.13), we shall obtain the following lower bound on $S(\rho)$

$$\begin{aligned} S(\rho) &\geq S_0(\rho) - S_0(\bar{\rho}) - \left\langle \rho - \bar{\rho}, \frac{\delta S_0}{\delta \rho}(\bar{\rho}) \right\rangle \\ &= \int_{\mathcal{A}} du \left\{ \rho \log \frac{\rho}{\bar{\rho}} + (1 - \rho) \log \frac{1 - \rho}{1 - \bar{\rho}} \right\} = \tilde{S}(\rho) \end{aligned} \quad (4.18)$$

with a strict inequality for $\rho \neq \bar{\rho}$. In the one dimensional case the bound (4.18) has been independently obtained in ref. 14.

Recalling that the dynamical action functional J of this model is given by (4.7), a somewhat lengthy but straightforward computation gives

$$\begin{aligned}
J_{[-T, 0]}(\hat{\rho}(\cdot)) &= \frac{1}{2} \int_{-T}^0 dt \left\langle \nabla^{-1} \left(\partial_i \hat{\rho} - \frac{1}{2} \Delta \hat{\rho} \right), \frac{1}{\hat{\rho}[1-\hat{\rho}]} \nabla^{-1} \left(\partial_i \hat{\rho} - \frac{1}{2} \Delta \hat{\rho} \right) \right\rangle \\
&= \tilde{S}(\hat{\rho}(0)) - \tilde{S}(\hat{\rho}(-T)) \\
&\quad + \frac{1}{2} \int_{-T}^0 dt \left\langle \nabla^{-1} \left(\partial_i \hat{\rho} + \frac{1}{2} \Delta \hat{\rho} - \nabla \cdot \left(\hat{\rho}[1-\hat{\rho}] \nabla \log \frac{\bar{\rho}}{1-\bar{\rho}} \right) \right), \right. \\
&\quad \left. \frac{1}{\hat{\rho}[1-\hat{\rho}]} \nabla^{-1} \left(\partial_i \hat{\rho}(t) + \frac{1}{2} \Delta \hat{\rho} - \nabla \cdot \left(\hat{\rho}[1-\hat{\rho}] \nabla \log \frac{\bar{\rho}}{1-\bar{\rho}} \right) \right) \right\rangle \\
&\quad + \frac{1}{2} \int_{-T}^0 dt \int_A du \frac{|\nabla \bar{\rho}(u)|^2}{[\bar{\rho}(u)(1-\bar{\rho}(u))]^2} (\hat{\rho}(t, u) - \bar{\rho}(u))^2 \quad (4.19)
\end{aligned}$$

The last two terms on the right hand side of (4.19) are positive. Therefore, if $\hat{\rho}(t)$ is trajectory connecting $\bar{\rho}$ to ρ , we have

$$S(\rho) = \inf_{\hat{\rho}} J_{[-\infty, 0]}(\hat{\rho}) \geq \tilde{S}(\rho) - \tilde{S}(\bar{\rho}) = \tilde{S}(\rho)$$

Moreover, since the last term on the right hand side of (4.19) is strictly positive as soon as $\hat{\rho} \neq \bar{\rho}$, we have the strict inequality in (4.18) for $\rho \neq \bar{\rho}$.

4.5. Perturbative Solution of the Hamilton–Jacobi Equation ($d \geq 1$)

We show here how the Hamilton–Jacobi equation (2.12) can be used to get a perturbative expansion for the entropy S around the stationary profile $\bar{\rho}$. We discuss only the expansion up to the second order but it will be clear how to generate an iterative approximation scheme.

From a computational point of view it is convenient to expand the pressure $G(h)$ defined in (2.8). Since $\rho(u) = \delta G(h) / \delta h(u)$ and $h(u) = \delta S(\rho) / \delta \rho(u)$, the dual Hamilton–Jacobi equation (2.9) in this model is

$$\left\langle \nabla h, \left[\frac{\delta G}{\delta h} \left(1 - \frac{\delta G}{\delta h} \right) \right] \nabla h \right\rangle = \left\langle \nabla h, \nabla \frac{\delta G}{\delta h} \right\rangle \quad (4.20)$$

where $h(u)$ satisfies the boundary conditions $h(u) = 0$ for $u \in \partial A$.

Recall that $\bar{\rho}(u)$ is the stationary solution of the hydrodynamic equation (4.2) and introduce

$$\tilde{G}(h) = \int_A du \log[1 + \bar{\rho}(u)(e^{h(u)} - 1)] \quad (4.21)$$

Note that $\tilde{G}(h)$ is the Legendre transform of $\tilde{S}(\rho)$ defined in (4.18). We look for a solution of (4.20) in the form

$$G(h) = \tilde{G}(h) + \langle g, h \rangle + \frac{1}{2} \langle h, Bh \rangle + O(h^3) \tag{4.22}$$

for some function $g = g(u)$ and some linear operator B .

Note that $S(\rho)$ has a minimum for $\rho = \bar{\rho}$ and

$$S(\rho) = \frac{1}{2} \langle \rho - \bar{\rho}, C^{-1}(\rho - \bar{\rho}) \rangle + O((\rho - \bar{\rho})^3)$$

where C is the covariance of the density fluctuations with respect to the invariant measure. Therefore

$$G(h) = \langle \bar{\rho}, h \rangle + \frac{1}{2} \langle h, Ch \rangle + O(h^3) \tag{4.23}$$

hence the second derivative of G at $h = 0$ is the covariance of the density fluctuations. By comparing (4.22) to (4.23) we get

$$C = \left. \frac{\delta^2 \tilde{G}}{\delta h^2} \right|_{h=0} + B = \bar{\rho}(1 - \bar{\rho}) \mathbb{1} + B \tag{4.24}$$

Since \tilde{G} is the pressure for the equilibrium system the operator B represents the contribution to the covariance due to the non-equilibrium boundary conditions. For the boundary driven simple exclusion process the covariance of the fluctuation has been derived in refs. 25 and 26 where it is shown that it is nonlocal in space. Therefore the perturbative expansion of the Hamilton–Jacobi equation will give a different derivation of the covariance.

We have

$$\begin{aligned} \frac{\delta \tilde{G}}{\delta h} \left(1 - \frac{\delta \tilde{G}}{\delta h} \right) &= \frac{\bar{\rho}(1 - \bar{\rho}) e^h}{[1 + \bar{\rho}(e^h - 1)]^2} \\ \nabla \frac{\delta \tilde{G}}{\delta h} &= \frac{\bar{\rho}(1 - \bar{\rho}) e^h}{[1 + \bar{\rho}(e^h - 1)]^2} \nabla h + \frac{e^h}{[1 + \bar{\rho}(e^h - 1)]^2} \nabla \bar{\rho} \end{aligned}$$

so that by plugging (4.22) into (4.20) and expanding up to second order in h we get

$$\langle \nabla h, [1 + (1 - 2\bar{\rho}) h] \nabla \bar{\rho} + \nabla g + \nabla Bh \rangle = 0$$

Recalling that h vanishes at the boundary, we thus get $g = 0$ and

$$\left\langle \nabla \left(\frac{h^2}{2} \right), (1 - 2\bar{\rho}) \nabla \bar{\rho} \right\rangle = \langle h, \Delta Bh \rangle$$

which, after an integration by parts, becomes (recall that $\Delta\bar{\rho} = 0$)

$$\langle h, \Delta Bh \rangle = \langle h, |\nabla\bar{\rho}|^2 h \rangle$$

The operator B therefore satisfies

$$\frac{1}{2}[\Delta B + B\Delta] = |\nabla\bar{\rho}|^2$$

In particular, if $\nabla\bar{\rho}$ is constant, B has the kernel

$$B(u, v) = |\nabla\bar{\rho}|^2 \Delta^{-1}(u, v) \quad (4.25)$$

where $\Delta^{-1}(u, v)$ is the Green function of the Laplacian (with Dirichlet boundary conditions). The fact that B is a negative operator can also be obtained as a consequence of the bound $S(\rho) \geq \tilde{S}(\rho)$.

By analogous computation one can obtain also the higher order terms in the expansion of the pressure which are the higher order cumulants. In the one dimensional case $\nabla\bar{\rho}$ is constant and we state below the result of the expansion up to the third order.

$$\begin{aligned} G(h) &= \tilde{G}(h) + \frac{1}{2}|\nabla\bar{\rho}|^2 \langle h, \Delta^{-1}h \rangle \\ &\quad + \frac{1}{3}(\nabla\bar{\rho})^2 [\langle h^2(1 - \frac{2}{3}\bar{\rho}), \Delta^{-1}h \rangle - \langle (\nabla h)^2(1 - 2\bar{\rho}), \Delta^{-2}h \rangle] + O(h^4) \end{aligned}$$

APPENDIX A. DERIVATION OF (3.20) AND (4.5)

Let Ω be a finite set and consider a continuous time jump Markov process X_t on the state space Ω with generator given by

$$Lf(\omega) = \sum_{\omega' \in \Omega} \lambda(\omega) p(\omega, \omega') [f(\omega') - f(\omega)] \quad (A.1)$$

where the rate λ is a positive function on Ω and $p(\omega, \omega')$ is a transition probability. We can construct a realization of X_t as follows. Fix an initial condition $X_0 = \omega_0$. The process waits an exponential time τ_1 with rate $\lambda(\omega_0)$ and then jumps to ω_1 with probability $p(\omega_0, \omega_1)$; the law of τ_1 is

$$P(\tau_1 < t) = \int_0^t ds \lambda(\omega_0) e^{-\lambda(\omega_0)s} \quad (A.2)$$

The process waits now an exponential time τ_2 , independent of τ_1 , with rate $\lambda(\omega_1)$ and then jumps to ω_2 with probability $p(\omega_1, \omega_2)$, and so on. Consider the piecewise constant trajectory $X_s, s \in [0, T]$ with n jumps given by

$$X_s = \begin{cases} \omega_0 & 0 \leq s < t_1 \\ \omega_1 & t_1 \leq s < t_1 + t_2 \\ \vdots & \vdots \\ \omega_{n-1} & t_1 + t_2 + \dots + t_{n-1} \leq s < t_1 + t_2 + \dots + t_n \\ \omega_n & t_1 + t_2 + \dots + t_n \leq s \leq T \end{cases} \tag{A.3}$$

Its probability density is given by

$$dP_{\omega_0}(X_s, s \in [0, T]) = \prod_{i=1}^n (\lambda(\omega_{i-1}) p(\omega_{i-1}, \omega_i) e^{-\lambda(\omega_{i-1}) t_i} dt_i) \cdot e^{-\lambda(\omega_n)[T-\sigma_n]}$$

where $\sigma_n = t_1 + \dots + t_n$

If λ and p depend explicitly on time we can construct a realization X_t by the same procedure; in such a case the law of τ_1 is

$$P(\tau_1 < t) = \int_0^t ds \lambda(\omega_0, s) e^{-\int_0^s ds' \lambda(\omega_0, s')} \tag{A.4}$$

and analogous distributions for τ_i . We thus get

$$dP_{\omega_0}(X_s, s \in [0, T]) = \prod_{i=1}^n (\lambda(X_{\sigma_{i-1}}, \sigma_i) p(X_{\sigma_{i-1}}, X_{\sigma_i}; \sigma_i) dt_i) \cdot e^{-\int_0^T ds \lambda(X_s, s)} \tag{A.5}$$

where $\sigma_k = t_1 + \dots + t_k$ (resp. $\sigma_0 = 0$) are the jump times of X_s .

Let us now consider two processes X_t (resp. X'_t) of this type with rates $\lambda(\omega, t)$ (resp. $\lambda'(\omega, t)$) and transition probability $p(\omega, \omega'; t)$ (resp. $p'(\omega, \omega'; t)$). We can write the formula (A.5) also for the process X' and, by taking the ratio of those expressions, we get the so called Radon–Nikodym derivative

$$\begin{aligned} & \frac{dP'_{\omega_0}}{dP_{\omega_0}}(X_s, s \in [0, T]) \\ &= \exp\{\mathcal{J}_{[0, T]}(X)\} \\ &= \exp\left\{ \sum_{i=1}^n \log \frac{\lambda'(X_{\sigma_{i-1}}, \sigma_i) p'(X_{\sigma_{i-1}}, X_{\sigma_i}; \sigma_i)}{\lambda(X_{\sigma_{i-1}}, \sigma_i) p(X_{\sigma_{i-1}}, X_{\sigma_i}; \sigma_i)} - \int_0^T ds [\lambda'(X_s, s) - \lambda(X_s, s)] \right\} \end{aligned} \tag{A.6}$$

We now consider the special case in which X has generator given by (A.1) and $X' = X^F$ has a time dependent generator

$$L_t^F f(\omega) = \sum_{\omega' \in \Omega} \lambda(\omega) p(\omega, \omega') e^{F(\omega', t) - F(\omega, t)} [f(\omega') - f(\omega)] \quad (\text{A.7})$$

which is of the same form with

$$\begin{aligned} \lambda'(\omega, t) &= \sum_{\omega' \in \Omega} \lambda(\omega) p(\omega, \omega') e^{F(\omega', t) - F(\omega, t)} \\ p'(\omega, \omega'; t) &= \frac{1}{\lambda'(\omega, t)} \lambda(\omega) p(\omega, \omega') e^{F(\omega', t) - F(\omega, t)} \end{aligned}$$

From (A.6) we get that the Radon–Nikodym derivative is given by

$$\frac{dP_{\omega_0}^F}{dP_{\omega_0}}(X_s, s \in [0, T]) = \exp\{\mathcal{J}_{[0, T]}(X, F)\}$$

with

$$\begin{aligned} \mathcal{J}_{[0, T]}(X, F) &= \sum_{i=1}^n [F(X_{\sigma_i}, \sigma_i) - F(X_{\sigma_{i-1}}, \sigma_{i-1})] \\ &\quad - \int_0^T ds \lambda(X_s) \sum_{\omega' \in \Omega} p(X_s, \omega') [e^{F(\omega', s) - F(X_s, s)} - 1] \\ &= \sum_{i=1}^n \left[F(X_{\sigma_i}, \sigma_i) - F(X_{\sigma_{i-1}}, \sigma_{i-1}) - \int_{\sigma_{i-1}}^{\sigma_i} ds \partial_s F(X_{\sigma_{i-1}}, s) \right] \\ &\quad - \int_0^T ds e^{-F(X_s, s)} L e^{F(X_s, s)} \\ &= F(X_T, T) - F(X_0, 0) - \int_0^T ds [\partial_s F(X_s, s) + e^{-F(X_s, s)} L e^{F(X_s, s)}] \end{aligned} \quad (\text{A.8})$$

Formulae (3.20) and (4.5) are special cases of (A.8) obtained by choosing

$$F(\eta, \tau) = \sum_{x \in A_N} H(\tau/N^2, x/N) \eta_x$$

APPENDIX B. ADJOINT HYDRODYNAMICS FOR ONE DIMENSIONAL SIMPLE EXCLUSION

Let $\rho^*(t)$ be a solution of the adjoint hydrodynamics for the one dimensional simple exclusion process (4.14). By the remarks in Section 2.7, $(\rho(t), H(t))$ with

$$\begin{aligned} \rho(t) &= \rho^*(-t) \\ H(t) &= \frac{\delta S}{\delta \rho}(\rho^*(-t)) = \log \frac{\rho^*(-t)}{1-\rho^*(-t)} - \phi(\rho^*(-t)) \end{aligned} \tag{B.1}$$

is a solution of the Hamilton equations (2.28) which for this model read

$$\begin{aligned} \partial_t \rho &= \frac{1}{2} \Delta \rho - \nabla(\rho(1-\rho) \nabla H) \\ \partial_t H &= -\frac{1}{2}(1-2\rho)(\nabla H)^2 - \frac{1}{2} \Delta H \end{aligned} \tag{B.2}$$

By plugging (B.1) into (B.2) and performing the change of variable (4.15), a straightforward computation yields

$$\begin{aligned} \partial_t \rho^* &= \frac{1}{2} \Delta \rho^* - \nabla \left(\frac{\rho^*(1-\rho^*)}{F(1-F)} \nabla F \right) \\ \partial_t F &= -\frac{1}{2} \Delta F + (\rho^* - F) \frac{(\nabla F)^2}{F(1-F)} \end{aligned} \tag{B.3}$$

By writing Eq. (4.11) in terms of $F = e^\phi/(1+e^\phi)$ and ρ replaced by ρ^* we get

$$\begin{cases} (\rho^* - F) = F(1-F) \frac{\Delta F}{(\nabla F)^2} & \text{for any } (t, u) \in [0, \infty) \times (-1, 1) \\ F(t, \pm 1) = \rho^*(t, \pm 1) = \frac{\psi(\pm 1)}{1 + \psi(\pm 1)} \end{cases} \tag{B.4}$$

which inserted in (B.3) concludes the proof that $F(t, u)$ as defined in (4.15) satisfies the heat equation.

The converse statement, namely that if we define $\rho^* = \rho^*(t, u)$ as in (4.17) (with $F = F(t, u)$ the solution of (4.16)) then it satisfies the nonlocal equation (4.14), can be checked without invoking the Hamiltonian formalism. Indeed, from (4.17) we get that

$$\frac{\rho^*(1-\rho^*)}{F(1-F)} = 1 + (1-2F) \frac{\Delta F}{(\nabla F)^2} - F(1-F) \frac{(\Delta F)^2}{(\nabla F)^4} \tag{B.5}$$

recalling (4.16), by a somehow tedious computation of the partial derivatives which we omit, we get

$$\left(\partial_t - \frac{1}{2} \Delta\right) \left[F(1-F) \frac{\Delta F}{(\nabla F)^2} \right] = -\nabla \left(\frac{\rho^*(1-\rho^*)}{F(1-F)} \nabla F \right) \quad (\text{B.6})$$

Therefore, recalling (4.17), the function $\rho^*(t)$ satisfies

$$\partial_t \rho^* = \frac{1}{2} \Delta \rho^* - \nabla \left(\frac{\rho^*(1-\rho^*)}{F(1-F)} \nabla F \right) \quad (\text{B.7})$$

which is precisely (4.14) written in terms of the variable $F = F(\rho^*)$ instead of $\phi = \phi(\rho^*)$.

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