

Mapping out-of-equilibrium into equilibrium in one-dimensional transport models

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Received 19 August 2008, in final form 7 October 2008

Published 3 November 2008

Online at stacks.iop.org/JPhysA/41/505001

Abstract

Systems with conserved currents driven by reservoirs at the boundaries offer an opportunity for a general analytic study that is unparalleled in more general out-of-equilibrium systems. The evolution of coarse-grained variables is governed by stochastic *hydrodynamic* equations in the limit of small noise. As such it is amenable to a treatment formally equal to the semiclassical limit of quantum mechanics, which reduces the problem of finding the full distribution functions to the solution of a set of Hamiltonian equations. It is in general not possible to solve such equations explicitly, but for an interesting set of problems (the driven symmetric exclusion process and the Kipnis–Marchioro–Presutti model) it can be done by a sequence of remarkable changes of variables. We show that at the bottom of this ‘miracle’ is the surprising fact that these models can be taken through a non-local transformation into isolated systems satisfying detailed balance, with probability distribution given by the Gibbs–Boltzmann measure. This procedure can in fact also be used to obtain an elegant solution of the much simpler problem of non-interacting particles diffusing in a one-dimensional potential, again using a transformation that maps the driven problem into an undriven one.

PACS numbers: 05.70.Ln, 02.70.-c, 05.20.-y, 05.40.-a

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Transport models are systems with conserved currents. In certain cases, they are such that their evolution leads to equilibrium when they are isolated or in contact with a thermal bath. The probability distribution is then of the Gibbs–Boltzmann form. Coupling the boundaries

to several external sources may induce currents across the bulk, driving the system out of equilibrium. In that case we do not have any general explicit formula for the distribution of probability of configurations, even in the stationary regime reached after long times.

In order to make progress, one strategy has been to study systems that, due to their specific symmetries, admit a complete solution. Thus, in recent years a number of remarkable analytic results have been found for simple transport models (see [11], and references therein). Two important examples are the simple symmetric exclusion process (SSEP)—a one-dimensional system of particles, and the Kipnis–Marchioro–Presutti model (KMP) [27], a model of energy transport. For the former, Derrida, Lebowitz and Speer [10] (DLS) obtained an exact expression for the large-deviation function of density using a matrix method that had been developed previously [9].

An alternative strategy is to restrict the calculation to the probability distributions of coarse-grained variables. If one considers conserved quantities, then the macroscopic fluctuations obey hydrodynamic equations with noise, the latter a manifestation of the microscopic chaos or stochasticity. Clearly, the more coarse-grained the description, the lower the level of noise, because fluctuations tend to average away. One is thus led, in the macroscopic limit, to deterministic equations perturbed by stochastic terms whose variance is of the order of the inverse of coarse-graining box size N . As usual, one can recast the problem in terms of the evolution in time of the probability distribution. This is given by the Fokker–Planck equation, which is closely analogous to a Schrödinger equation in imaginary time, with the small parameter N^{-1} playing the role of \hbar . The ‘semiclassical’ treatment of these equations [16] follows the same lines as the derivation of classical from quantum mechanics, or geometric optics from wave dynamics. The logarithm of the transition probability obeys a Hamilton–Jacobi equation whose characteristics are trajectories satisfying Hamilton’s equations. Macroscopic fluctuation theory developed by Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim (BDGJL) [1, 3] is the resulting classical Hamiltonian field theory describing coarse-grained fluctuations.

Up to this point the formalism is completely general. However, an analytic expression for the solutions of the classical equations is not possible for every model, so that even in the coarse-grained limit the problem has no closed solution. Remarkably, for the hydrodynamic limit of the driven SSEP [1], BDGJL were able to integrate explicitly the corresponding Hamilton–Jacobi equations and recover the large-deviation function. They thus followed a path that is in principle logically independent of the one used to obtain the exact microscopic solution. Their derivation amounts to rewriting the problem in a carefully chosen set of variables. An analogous strategy subsequently allowed Bertini, Gabrielli and Lebowitz [3] to do the same for the hydrodynamic limit of KMP.

One is left wondering what is the underlying reason for the existence of changes of variable that allows one to completely solve the Hamiltonian equations, and how general their applicability is. In this paper, we show that *in the cases where this has been possible, there exists a non-local mapping taking the hydrodynamic equations of the model in contact with reservoirs into those of an isolated, equilibrium system*. Large deviations and optimal trajectories are easily obtained in this representation using the detailed-balance property, and can then be mapped back to the original setting in which detailed balance was broken by the boundary conditions. In the transformed, isolated model, spontaneous rare fluctuations are the time reverse of relaxations to the average profile, but this symmetry is lost (as it should be) in the mapping back to the original model. This accounts in this case for the breaking of the Onsager–Machlup symmetry [31] between birth and death of a fluctuation, which has received considerable interest [6, 29] over the past few years. A short account of this work has appeared elsewhere [38].

The layout of this paper is as follows. In section 2, we review the expression of particle exclusion problem in terms of spin operators. We construct a (coherent-state) path integral for the transition probability and derive from it the hydrodynamic limit. This route to the hydrodynamic limit is conceptually simple, and in addition has the advantage that the spin notation makes the symmetries and integrability properties of the hydrodynamic limit explicit. Perhaps more surprisingly, the coherent-state representation yields directly a set of (Doi–Peliti) variables in terms of which the problem can be explicitly solved.

In section 3, we take the more direct route starting directly from fluctuating hydrodynamics, and deriving from it the coarse-grained hydrodynamic equations. The reader may skip section 2 and start here, the only loss is that the symmetries of the hydrodynamic equations are not explicit and the boundary conditions less straightforward.

In section 4, we review how the original stochastic dynamics for a single density field $\rho(x)$ leads, in the low-noise limit, to a classical Hamiltonian field theory in a phase space with *two* fields $\rho(x)$ and $\hat{\rho}(x)$. The large-deviation function—the logarithm of the probability of a configuration in the stationary regime—is given by the action of a ‘classical’ trajectory $[\rho(x, t), \hat{\rho}(x, t)]$ reaching the configuration at very long times. The formalism is a variant of the low-noise Freidlin–Wentzell formalism, itself an implementation of the usual WKB semiclassical theory.

For an undriven system with detailed balance (section 5) the dynamics has a symmetry between ‘downhill’ relaxations and ‘uphill’ excursions. Using this symmetry one obtains the uphill trajectories as the time reversed of the downhill ones, and this allows us to compute explicitly the large-deviation function. In the case of driven transport models, the boundary terms violate detailed balance, and there is no obvious symmetry playing the role of time reversal, no general method to find the uphill trajectories, and hence no explicit solution for the large-deviation function.

In section 6, a paraphrase of the solution of BDGJL, we show that in the particular case of the SSEP, there is a very special set of variables that allows one to solve completely the driven problem. The main result of this paper, in section 7, is to show that at the bottom of this possibility is the fact that there is a non-local mapping converting the driven chain into an isolated, undriven one. In section 8, we briefly show that one can apply the same arguments to solve the KMP model.

To conclude, in section 9 we discuss how the method can be applied to the much simpler case of non-interacting particles diffusing in a generic potential, driven out-of-equilibrium by boundary terms.

1.1. Mapping a driven into an undriven problem

Let us consider here the simplest example of a mapping from out-of-equilibrium to equilibrium. This exercise will help to fix ideas, and to see how much one gets out of such an approach.

Consider a diffusion process given by a Fokker–Planck equation driven by boundary conditions $P(0) = p_o$ and $P(L) = p_L$,

$$\dot{P} = \frac{d}{dx} \left(T \frac{d}{dx} + \frac{dV}{dx} \right) P. \quad (1)$$

Because of the boundary conditions, the current $J = \left(-T \frac{d}{dx} - \frac{dV}{dx} \right) P$ is in general nonzero.

Now let us introduce $e^{\beta V} P = P_1$. Equation (1) maps to the backward Fokker–Planck equation

$$\dot{P}_1 = \left(T \frac{d}{dx} - \frac{dV}{dx} \right) \frac{d}{dx} P_1. \quad (2)$$

Defining $P' = \frac{d}{dx} P_1$, we get

$$\dot{P}' = \frac{d}{dx} \left(T \frac{d}{dx} - \frac{dV}{dx} \right) P'. \quad (3)$$

This takes the form of a probability P' describing an evolution in a potential $-V$. The remarkable fact is that the original boundary condition on P expresses in the new variables just a normalization for P' ,

$$\int_0^L P' dx = e^{\beta V(L)} p_L - e^{\beta V(0)} p_0. \quad (4)$$

Furthermore, it also implies that the current J' associated with P' vanishes at the ends $\Lambda = (0, L)$, since

$$\dot{P}(\Lambda) = 0 \rightarrow \frac{d}{dx} \left(T \frac{d}{dx} + \frac{dV}{dx} \right) P(\Lambda) = 0 \rightarrow \left(T \frac{d}{dx} - \frac{dV}{dx} \right) P'(\Lambda) = -J'(\Lambda) = 0. \quad (5)$$

P' thus evolves with a Fokker-Planck equation with potential $-V$ and no current at the boundaries; the integral of P' is conserved and the process satisfies detailed balance. The stationary measure is thus $P'_{\text{stat}}(x) \propto e^{\beta V(x)}$,

$$P'_{\text{stat}} \propto e^{\beta V} \rightarrow P_{\text{stat}}(x) = p_0 e^{-\beta[V(x)-V(0)]} + c \int_0^x e^{-\beta[V(x)-V(x')]} dx', \quad (6)$$

where the constant c is fixed by the right boundary condition $P(L) = p_L$. The overall distribution then reads

$$P_{\text{stat}}(x) = \frac{p_0 e^{-\beta[V(x)-V(0)]} \int_x^L e^{\beta V(x')} dx' + p_L e^{-\beta[V(x)-V(L)]} \int_0^x e^{\beta V(x')} dx'}{\int_0^L e^{\beta V(x')} dx'}. \quad (7)$$

This result could have been obtained from the beginning by quadratures [25]. Actually, we have obtained much more, since we have mapped the evolution operator into the one of an equilibrium problem and we now understand the time evolution of the primed variable as the relaxation of an isolated system: even without calculating anything, we have an intuition of the qualitative behavior.

To see that the transformation is non-local, we may consider the expectation value of a function $O(x)$,

$$\begin{aligned} \langle O \rangle(t) &= \int_0^L dx O(x) P(x) = \int_0^L dx O(x) e^{-\beta V(x)} P_1(x) \\ &= \int_0^L dx O'(x) P'(x) - O'(L) p_L e^{\beta V(L)}. \end{aligned} \quad (8)$$

All the time dependence is given by the expectation value of the new operator

$$O'(x) \equiv - \int_0^x dy O(y) e^{-\beta V(y)}, \quad (9)$$

which is a non-local function of the original one.

In section 9, we shall show that actually one can use the same non-local transformation to map *any* single-particle diffusion model in a one-dimensional potential with sources at the ends into the same equilibrium diffusion problem with no sources.

In the rest of the paper, we shall meet an analogous situation, for models with many interacting particles. The main difference is that we shall be making a *transformation at the level of fields, not of their probability* (P here is a probability of the zero-dimensional 'field' x).

2. Path-integral representations of exclusion processes

In this section we introduce the exclusion processes. We write their evolution matrix in terms of (quantum) spin operators. This makes explicit the fact that the problem has more symmetries than mere particle conservation. Using standard spin coherent state techniques we present a novel derivation of the path integral and then take the hydrodynamic limit. We also obtain a natural set of variables F, \hat{F} (related to the stereographic representation of the spins) which are often implicitly used in the literature. Finally, we write the hydrodynamic equations in terms of the average particle density ρ , and its conjugate variable $\hat{\rho}$.

The main result of this section is the construction of an hydrodynamic action which gives the logarithm of the transition probability between two smooth density profiles, together with the associated spatio-temporal boundary conditions. It is given by equations (46)–(49). The reader familiar with these representations of exclusion processes may skip this section, and find the more standard approach in the next one.

2.1. Partial exclusion process

Let us consider the symmetric partial exclusion process, a generalization of simple symmetric exclusion processes introduced in [35]. It consists of a one-dimensional lattice gas, for which all sites can be occupied by at most $2j$ particles. The probability of a jump between a site and its neighbor is proportional to both the occupation number of the starting site and the proportion of vacancies of the target one⁴,

$$\begin{aligned} W(\dots, n_k, n_{k+1}, \dots \rightarrow \dots, n_k + 1, n_{k+1} - 1, \dots) &= \frac{p}{2j} (2j - n_k) n_{k+1} \\ W(\dots, n_k, n_{k+1}, \dots \rightarrow \dots, n_k - 1, n_{k+1} + 1, \dots) &= \frac{p}{2j} n_k (2j - n_{k+1}). \end{aligned} \quad (10)$$

We fix a timescale by choosing $p = 1/2$. The system can be put in contact at sites 1 and L with reservoirs of densities ρ_0 and ρ_1 . This is usually done by introducing four rates α, δ and γ, β which correspond to deposition and evaporation of particles at site 1 and L , respectively. We thus have the added rates of interchange with the reservoirs

$$\begin{aligned} W(n_1, \dots \rightarrow n_1 + 1, \dots) &= \alpha(2j - n_1) & W(\dots, n_L \rightarrow \dots, n_L + 1) &= \delta(2j - n_L) \\ W(n_1, \dots \rightarrow n_1 - 1, \dots) &= \gamma n_1 & W(\dots, n_L \rightarrow \dots, n_L - 1) &= \beta n_L. \end{aligned} \quad (11)$$

Though the bulk diffusion is symmetric, and the system thus satisfies a local detail balance relation, it can be driven out-of-equilibrium by the boundaries, if the densities imposed by the reservoirs are different,

$$\rho_0 = \frac{\alpha}{\alpha + \gamma} \neq \rho_1 = \frac{\delta}{\delta + \beta}. \quad (12)$$

These models are amongst the simplest interacting many-particle systems driven out-of-equilibrium by the boundary sources. A schematic representation of the partial exclusion process is shown in figure 1. For $j = 1/2$, we recover the usual SSEP, which is known to be related to the $1/2$ representation of the $SU(2)$ group, whereas the partial exclusion processes correspond to the spin j representation [35]. For the sake of completeness, we give the details of the relations with the spin operators in the following subsections and use the $SU(2)$ coherent states to construct a path-integral representation afterward.

⁴ The prefactor $1/(2j)$ ensures that the rate at which a fixed number of particles jump to an empty site does not diverge with j .

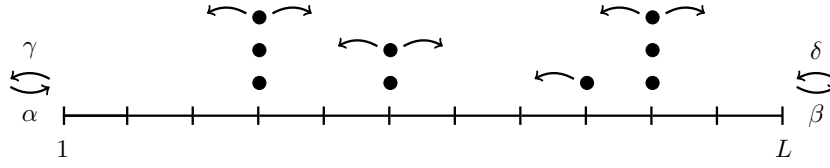


Figure 1. Schematic representation of a partial exclusion process for $j = 3/2$. There can be at most three particles per site. Particles are injected at site 1 and L with rate α and δ and can jump to the corresponding reservoirs with rate δ and β .

2.2. Master equation and spin representation

The evolution of the probability $P(\mathbf{n})$ of observing a configuration defined by the vector of occupation numbers $\mathbf{n} = (n_1, \dots, n_L)$ is given by the master equation

$$\frac{\partial P(\mathbf{n})}{\partial t} = \sum_{\mathbf{n}' \neq \mathbf{n}} W(\mathbf{n}' \rightarrow \mathbf{n})P(\mathbf{n}') - W(\mathbf{n} \rightarrow \mathbf{n}')P(\mathbf{n}), \tag{13}$$

where $W(\mathbf{n}' \rightarrow \mathbf{n})$ is the transition rate from configuration \mathbf{n}' to configuration \mathbf{n} . To keep the notation as compact as possible, we introduce $n_k^+ = n_k + 1$ and $n_k^- = n_k - 1$. From (10) and (11), the master equation reads

$$\begin{aligned} \frac{\partial P(\mathbf{n})}{\partial t} = & \frac{1}{4j} \sum_{k=1}^{L-1} [(2j - n_k^-)n_{k+1}^+ P(\dots, n_k^-, n_{k+1}^+, \dots) + n_k^+(2j - n_{k+1}^-)P(\dots, n_k^+, n_{k+1}^-, \dots) \\ & - [(2j - n_k)n_{k+1} + n_k(2j - n_{k+1})]P(\dots, n_k, n_{k+1}, \dots)] \\ & + \alpha(2j - n_1^-)P(n_1^-, \dots) + \gamma n_1^+ P(n_1^+, \dots) + \delta(2j - n_L^-)P(\dots, n_L^-) \\ & + \beta n_L^+ P(\dots, n_L^+) - [\gamma n_1 + \alpha(2j - n_1) + \delta(2j - n_L) + \beta n_L]P(n_1, \dots, n_L). \end{aligned} \tag{14}$$

The two first lines correspond to the dynamics in the bulk whereas the last ones stand for the interaction with the reservoirs.

Let us now introduce a non-Hermitian representation of the $SU(2)$ group to write the master equation in an operatorial form. A configuration of the system can be written as the tensor product of states of each sites i : $|\psi\rangle = \otimes_i |\psi_i\rangle$, where each state $|\psi_i\rangle$ is given by a $2j + 1$ components vector, such that an occupation number equal to n is represented by

$$|n\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{15}$$

where the 1 is on the $(n+1)$ th line, starting from the top. One then defines the $(2j+1) \times (2j+1)$ matrices

$$\begin{aligned}
 S^+ &= \begin{pmatrix} 0 & \cdots & \cdots & \cdots & 0 \\ 2j & \ddots & & & \vdots \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix} & S^- &= \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ \vdots & & & \ddots & 2j \\ 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix} \\
 S^z &= \begin{pmatrix} -j & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & j \end{pmatrix},
 \end{aligned} \tag{16}$$

whose action on the state $|n_i\rangle$ are given by

$$\begin{aligned}
 S_i^+ |n_i\rangle &= (2j - n_i) |n_i + 1\rangle & S_i^- |n_i\rangle &= n_i |n_i - 1\rangle & S_i^z |n_i\rangle &= (n_i - j) |n_i\rangle \\
 S_i^x &= \frac{1}{2} [S_i^+ + S_i^-] & S_i^y &= \frac{1}{2i} [S_i^+ - S_i^-].
 \end{aligned} \tag{17}$$

Direct computations show that they satisfy the commutation relations

$$[S^z, S^\pm] = \pm S^\pm \quad [S^+, S^-] = 2S^z \quad [S^i, S^j] = i\epsilon^{ijk} S^k \quad \forall i, j, k \in \{x, y, z\}. \tag{18}$$

They thus form a $(2j + 1)$ -dimensional representation of the $SU(2)$ group, that is a representation of spin j , the usual magnetic number m_i being related to the occupation number n_i through $m_i = n_i - j$. This is a non-unitary representation as S^+ is not the adjoint of S^{-5} .

The evolution operator of the partial exclusion process can now be written using these spin operators. To make this explicit, let us introduce the vector $|\psi\rangle = \sum_{\mathbf{n}} P(\mathbf{n}) |\mathbf{n}\rangle$ where the sum runs over all the possible configurations $\mathbf{n} = (n_1, \dots, n_L)$. Using the master equation, the time derivative of $|\psi\rangle$ is given in terms of the spin operators by

$$\begin{aligned}
 \frac{\partial |\psi\rangle}{\partial t} &= -\hat{H} |\psi\rangle; & \hat{H} &= \hat{H}_1 + \hat{H}_B + \hat{H}_L; \\
 \hat{H}_B &= \frac{1}{4j} \sum_{k=1}^{L-1} [-S_{k+1}^- S_k^+ + (j + S_{k+1}^z)(j - S_k^z)] + [-S_{k+1}^+ S_k^- + (j - S_{k+1}^z)(j + S_k^z)]; \\
 \hat{H}_1 &= -\alpha [S_1^+ - (j - S_1^z)] - \gamma [S_1^- - (j + S_1^z)]; \\
 \hat{H}_L &= -\delta [S_L^+ - (j - S_L^z)] - \beta [S_L^- - (j + S_L^z)],
 \end{aligned} \tag{19}$$

where \hat{H}_B corresponds to the dynamics in the bulk, whereas \hat{H}_1 and \hat{H}_L result from the coupling with the reservoirs on the sites 1 and L . Introducing spin vectors $\vec{S}_k = (S_k^x, S_k^y, S_k^z)$, \hat{H}_B can be written in a more compact way as

$$\hat{H}_B = -\frac{1}{2j} \sum_{i=1}^{L-1} (\vec{S}_i \cdot \vec{S}_{i+1} - j^2). \tag{20}$$

This is the usual connexion between exclusion processes and spin chains [12, 14, 18, 35].

⁵ Note that a similar path could be followed with the usual unitary representation of $SU(2)$, see appendix C. It would however lead to additional temporal boundary terms in the path integral, which makes the analysis of the action less straightforward.

2.3. Path integral representation in the hydrodynamic limit

The hydrodynamic limit of lattice-gas models is usually achieved through the definition of a coarse-grained density field ρ , averaged over macroscopic boxes, the size of which is then sent to infinity [37]. Here, each site of the lattice already contains up to $2j$ particles. We can thus obtain a hydrodynamic limit by taking the limit of j, L going to infinity. In the macroscopic limit, all the spin representations are equivalent, j and L enter through the combination jL . This is just the manifestation of the fact [14] that the hydrodynamic variables represent the total spin in a box, whatever the spin of the elementary sites.

2.3.1. Coherent states. To construct a path-integral representation of \hat{H} , we shall use, for each site k of the lattice, the following right- and left-spin coherent states [33]:

$$\begin{aligned} |z_k\rangle &= \frac{1}{(1 + \bar{z}_k z_k)^j} e^{z_k S_k^+} |0_k\rangle = \frac{1}{(1 + \bar{z}_k z_k)^j} \sum_{0 \leq n_k \leq 2j} \binom{2j}{n_k} z_k^{n_k} |n_k\rangle, \\ \langle z_k| &= \frac{1}{(1 + \bar{z}_k z_k)^j} \langle 0_k| e^{\bar{z}_k S_k^-} = \frac{1}{(1 + \bar{z}_k z_k)^j} \sum_{0 \leq n_k \leq 2j} \langle n_k| \bar{z}_k^{n_k}. \end{aligned} \quad (21)$$

For an extended system of k sites, one introduces the tensor product

$$|z\rangle = \bigotimes_k |z_k\rangle. \quad (22)$$

Due to the non-Hermiticity of the representation (16), $|z_k\rangle$ is not the adjoint of $\langle z_k|$. The construction of the path integral relies on the following representation of the identity:

$$\int d\mu(z_k) |z_k\rangle \langle z_k| = \hat{1} \quad \text{with} \quad d\mu(z_k) = \frac{2j+1}{\pi} \frac{d^2 z_k}{(1 + z_k \bar{z}_k)^2}. \quad (23)$$

2.3.2. Action functional in the large spin limit. The functional approach for spin operators has some subtleties [17] (see Solarì [36], Kochetov [28], Vieira and Sacramento [39] for a derivation of the action and of the associated time boundary conditions). For the sake of clarity, most of the technical details are presented in appendix A and we simply outline below the main steps in the path-integral construction.

Keeping in mind that we ultimately want to describe a continuum theory, we replace number occupations by ‘discrete’ densities,

$$\rho_k = \frac{n_k}{2j}. \quad (24)$$

We would like to compute $P(\rho^f, T; \rho^i, 0)$, the probability of observing the system in state $(\rho_1^f, \dots, \rho_L^f)$ at time T , starting from $(\rho_1^i, \dots, \rho_L^i)$ at time 0, that is the propagator between two states $\langle \rho^f|$ and $|\rho^i\rangle$ with fixed initial and final number of particles in each site. Using $2L$ representations of the identity (23), we write

$$P(\rho^f, T; \rho^i, 0) = \langle \rho^f| e^{-T\hat{H}} |\rho^i\rangle = \int \prod_k d\mu(z_k^f) d\mu(z_k^i) \langle \rho^f| z^f \rangle \langle z^f| e^{-T\hat{H}} |z^i\rangle \langle z^i| \rho^i\rangle. \quad (25)$$

Because we are interested in the hydrodynamic limit (large jL), we may first take a large j limit and then send L to ∞ . In this ‘large spin’ limit, (25) reads (see details in appendix A)

$$P(\rho^f, T; \rho^i, 0) = \int \prod_k d\mu(z_k^f) d\mu(z_k^i) \int D\bar{z} Dz \prod_{e=i,f} \delta\left(\frac{\bar{z}_k^e z_k^e}{1 + \bar{z}_k^e z_k^e} - \rho_k^e\right) \exp[-S], \quad (26)$$

$$S = 2j \sum_k \left[\frac{z_k \bar{z}_k}{1 + z_k \bar{z}_k} \log \bar{z}_k - \log(1 + z_k \bar{z}_k) \right]_i^f + 2j \int dt \left[\sum_k \frac{\bar{z}_k \dot{z}_k}{1 + \bar{z}_k z_k} - \mathcal{H}(\bar{z}, z) \right]. \quad (27)$$

The role of the Hamiltonian $\mathcal{H}(\bar{z}, z)$ is played by the quantity $-\frac{1}{2j} \langle z | \hat{H} | z \rangle$ which is computed using [17]

$$\langle z_k | S_k^+ | z_k \rangle = 2j \frac{\bar{z}_k}{1 + z_k \bar{z}_k}; \quad \langle z_k | S_k^- | z_k \rangle = 2j \frac{z_k}{1 + z_k \bar{z}_k}; \quad \langle z_k | S_k^z | z_k \rangle = j \frac{z_k \bar{z}_k - 1}{z_k \bar{z}_k + 1}. \quad (28)$$

Explicitly, this yields

$$\begin{aligned} \mathcal{H}(\bar{z}, z) &= \mathcal{H}_B(\bar{z}, z) + \mathcal{H}_0(\bar{z}, z) + \mathcal{H}_L(\bar{z}, z) \\ \mathcal{H}_B(\bar{z}, z) &= - \sum_{k=1}^{L-1} \frac{z_k}{1 + \bar{z}_k z_k} \frac{z_{k+1}}{1 + \bar{z}_{k+1} z_{k+1}} \frac{(\bar{z}_{k+1} - \bar{z}_k)^2}{2} \\ &\quad + \left(\frac{z_{k+1}}{1 + z_{k+1} \bar{z}_{k+1}} - \frac{z_k}{1 + z_k \bar{z}_k} \right) \frac{\bar{z}_{k+1} - \bar{z}_k}{2} \\ \mathcal{H}_0(\bar{z}_1, z_1) &= \alpha \frac{\bar{z}_1 - 1}{1 + z_1 \bar{z}_1} + \gamma \frac{z_1(1 - \bar{z}_1)}{1 + z_1 \bar{z}_1}; \quad \mathcal{H}_L(\bar{z}_L, z_L) = \delta \frac{\bar{z}_L - 1}{1 + z_L \bar{z}_L} + \beta \frac{z_L(1 - \bar{z}_L)}{1 + z_L \bar{z}_L}. \end{aligned} \quad (29)$$

Initial and final conditions on the fields z, \bar{z} are imposed by the delta functions in (26) and read

$$\frac{\bar{z}_k^i z_k^i}{1 + \bar{z}_k^i z_k^i} = \rho_k^i, \quad \frac{\bar{z}_k^f z_k^f}{1 + \bar{z}_k^f z_k^f} = \rho_k^f. \quad (31)$$

2.3.3. Density field. To get more insight on the physics of this field theory, we introduce a new parametrization

$$z_k = \frac{\rho_k}{1 - \rho_k} e^{-\hat{\rho}_k}, \quad \bar{z}_k = e^{\hat{\rho}_k}, \quad (32)$$

so that

$$\rho_k = \frac{z_k \bar{z}_k}{1 + z_k \bar{z}_k} = \frac{1}{2j} \langle z_k | j + S_k^z | z_k \rangle \quad (33)$$

plays the role of a density. The transformation (32) is such that $\hat{\rho}$ is canonically conjugated to ρ . The time boundary conditions (31) on the field can be written, as expected, as

$$\rho_k(0) = \rho_k^i, \quad \rho_k(T) = \rho_k^f, \quad (34)$$

whereas $\hat{\rho}_k(0)$ and $\hat{\rho}_k(T)$ are unconstrained (for details, see appendix A). This highlights the correspondence between the field ρ and the actual density of the system, as do (33). From (28) and (32), one sees the correspondence between spins and densities,

$$\langle z_k | S_k^+ | z_k \rangle = 2j(1 - \rho_k) e^{\hat{\rho}_k}, \quad \langle z_k | S_k^- | z_k \rangle = 2j\rho_k e^{-\hat{\rho}_k}, \quad \langle z_k | S_k^z | z_k \rangle = j(2\rho_k - 1). \quad (35)$$

This yields for the Hamiltonian

$$\begin{aligned} \mathcal{H}(\hat{\rho}, \rho) &= \frac{1}{2} \sum_{k=1}^{L-1} \{ (1 - \rho_k) \rho_{k+1} [e^{\hat{\rho}_k - \hat{\rho}_{k+1}} - 1] + \rho_k (1 - \rho_{k+1}) [e^{\hat{\rho}_{k+1} - \hat{\rho}_k} - 1] \} \\ &\quad + \{ \alpha (1 - \rho_1) (e^{\hat{\rho}_1} - 1) + \gamma \rho_1 (e^{-\hat{\rho}_1} - 1) \\ &\quad + \delta (1 - \rho_L) (e^{\hat{\rho}_L} - 1) + \beta \rho_L (e^{-\hat{\rho}_L} - 1) \}. \end{aligned} \quad (36)$$

Making the change of variables in the action gives

$$P(\mathbf{n}_f, T; \mathbf{n}_i, 0) = \int \mathcal{D}\hat{\rho} \mathcal{D}\rho \exp\{-S[\hat{\rho}, \rho]\} \quad (37)$$

$$S[\hat{\rho}, \rho] = 2j \int_0^T dt \left[\sum_k \hat{\rho}_k \dot{\rho}_k - \mathcal{H}(\hat{\rho}, \rho) \right], \quad (38)$$

where one integrates over fields ρ satisfying the temporal boundary conditions (34).

2.3.4. Connection with Doi–Peliti variables. In the previous subsections, we took advantage of the $SU(2)$ coherent states to construct the path-integral representation of the evolution operator. A more standard approach, based on Doi–Peliti formalism, could have been followed. Starting from the density fields $\rho, \hat{\rho}$, the usual bosonic coherent states can be obtained through a Cole–Hopf transformation [4],

$$\rho = \phi\phi^*; \quad \hat{\rho} = \log \phi^*, \quad (39)$$

which in the z, \bar{z} variables reads

$$\phi^* = \bar{z}; \quad \phi = \frac{z}{1 + z\bar{z}}. \quad (40)$$

From (29) one sees that the bulk Hamiltonian \mathcal{H}_B reads in these variables

$$\mathcal{H}_B(\phi, \phi^*) = -\frac{1}{2} \sum_k \phi_k \phi_{k+1} (\phi_{k+1}^* - \phi_k^*)^2 + (\phi_{k+1} - \phi_k)(\phi_{k+1}^* - \phi_k^*). \quad (41)$$

To understand the meaning of the ϕ, ϕ^* variables, we recall the action of the spin operators in the coherent-state representation,

$$\begin{aligned} \langle z_k | S_k^+ | \psi \rangle &= \left[2j\bar{z}_k - \bar{z}_k^2 \frac{\partial}{\partial \bar{z}_k} \right] \langle z_k | \psi \rangle \\ \langle z_k | S_k^- | \psi \rangle &= \frac{\partial}{\partial \bar{z}_k} \langle z_k | \psi \rangle \\ \langle z_k | S_k^z | \psi \rangle &= \left[\bar{z}_k \frac{\partial}{\partial \bar{z}_k} - j \right] \langle z_k | \psi \rangle. \end{aligned} \quad (42)$$

The matrix elements used to construct the path integral (28) are given in terms of ϕ, ϕ^* by

$$\begin{aligned} \langle z_k | S_k^+ | z_k \rangle &= 2j\phi_k^* - (\phi_k^*)^2 (2j\phi_k); & \langle z_k | S_k^- | z_k \rangle &= 2j\phi_k; \\ \langle z_k | S_k^z | z_k \rangle &= \phi_k^* (2j\phi_k) - j, \end{aligned} \quad (43)$$

and one sees by comparing (42) and (43) that

$$\phi^* = \bar{z}; \quad \phi = \frac{1}{2j} \frac{\partial}{\partial \bar{z}}. \quad (44)$$

ϕ and ϕ^* satisfy the usual bosonic commutation relation. They correspond to the usual Doi–Peliti [13, 32] representation of bosons. We thus see that one can construct a path integral in terms of the variables ϕ and ϕ^* either by a Cole–Hopf transformation, or by directly expressing the spin operators in the representation (42) and then constructing the path-integral treating \bar{z} and $\frac{1}{2j} \frac{\partial}{\partial \bar{z}}$ as conjugate bosons⁶. In what follows, however, it will be useful not to lose sight of the $SU(2)$ symmetry.

⁶ One must however proceed with care as states with more than $2j$ particles are not physical and are difficult to handle using bosonic coherent state. See for instance [40].

2.3.5. *Hydrodynamic limit.* So far, the action is still a discrete sum over the whole lattice. We shall now take the full hydrodynamic limit to describe the evolution of smooth profiles on diffusive timescales. We thus introduce a space parametrization $x_k = \frac{k}{L}$ and rescale the time $t \rightarrow L^2 t$. At the macroscopic level, the density profiles are smooth functions and discrete gradients can be replaced by continuous ones,

$$\rho_{k+1} - \rho_k \rightarrow \frac{\nabla \rho(x_k)}{L}, \quad \hat{\rho}_{k+1} - \hat{\rho}_k \rightarrow \frac{\nabla \hat{\rho}(x_k)}{L}, \quad \frac{1}{L} \sum_{k=1}^{L-1} \rightarrow \int_0^1 dx. \quad (45)$$

For a more rigorous approach, see [2, 37]. The first order in a $\frac{1}{L}$ expansion of the action then reads

$$P(\rho^f, t_f; \rho^i, 0) = \int \mathcal{D}\hat{\rho} \mathcal{D}\rho e^{-2jLS[\rho, \hat{\rho}]} \quad (46)$$

$$S[\rho, \hat{\rho}] = \int_0^{t_f} \int_0^1 dx dt \{ \hat{\rho} \partial_t \rho - \mathcal{H}[\rho, \hat{\rho}] \}; \quad \mathcal{H}[\rho, \hat{\rho}] = \frac{1}{2} \sigma (\nabla \hat{\rho})^2 - \frac{1}{2} \nabla \rho \nabla \hat{\rho}, \quad (47)$$

where $\sigma = \rho(1 - \rho)$.

In appendix B we show that fields ρ and $\hat{\rho}$ are constrained, in the hydrodynamic limit, to satisfy the spatio-temporal boundary conditions

$$\forall t, \quad \rho(0, t) = \rho_0 = \frac{\alpha}{\alpha + \gamma}, \quad \rho(1, t) = \rho_1 = \frac{\delta}{\delta + \beta}, \quad \hat{\rho}(0) = \hat{\rho}(L) = 0 \quad (48)$$

$$\rho(x, 0) = \rho_i(x), \quad \rho(x, T) = \rho_f(x). \quad (49)$$

If $\alpha, \beta, \gamma, \delta \sim \mathcal{O}(1)$ at the microscopic level, these conditions are strict, in the sense that the fields do not fluctuate in the borders⁷, whereas $\alpha, \beta, \gamma, \delta \sim \mathcal{O}(L^{-1})$ would also allow fluctuations of ρ and $\hat{\rho}$ at the boundaries.

Due to the correspondence (20), (35) with the spin operators, the whole process described here simply amounts to taking the classical limit of a Heisenberg spin chain with some particular boundary conditions. One can indeed check that the Hamiltonian (47) corresponds to

$$\mathcal{H}_B = -\frac{1}{2} \int dx \nabla S \cdot \nabla S, \quad (50)$$

where the classical spins⁸ are defined as $S^{x,y,z} = \lim_{j \rightarrow \infty} (2j)^{-1} \langle z | S^{x,y,z} | z \rangle$. The spatial boundary conditions in terms of classical spins are then given by

$$\begin{aligned} S^z(0) &= \rho_0 - \frac{1}{2} & S^z(1) &= \rho_1 - \frac{1}{2} \\ S^x(0) &= \frac{1}{2} & S^x(1) &= \frac{1}{2} \\ S^y(0) &= \frac{1 - 2\rho_0}{2i} & S^y(1) &= \frac{1 - 2\rho_1}{2i} \\ S^+(0) &= 1 - \rho_0 & S^+(1) &= 1 - \rho_1 \\ S^-(0) &= \rho_0 & S^-(1) &= \rho_1. \end{aligned} \quad (51)$$

⁷ The probability to observe a smooth profile such that $\rho(0) \neq \rho_0$ scales as e^{-jL^2} .

⁸ Note that with this convention the spin normalization is $S \cdot S = \frac{1}{4}$ instead of the usual $S \cdot S = 1$.

3. Fluctuating hydrodynamics

Let us briefly review in this section the construction of the action starting from fluctuating hydrodynamics and using the Martin–Siggia–Rose [30], DeDominicis–Janssen [7, 22] formalism.

In terms of the instantaneous current $J(x)$ at site x , defined by the continuity equation, the evolution of the density is given by the stochastic equation

$$\dot{\rho} = -\nabla J; \quad J = -\frac{1}{2}\nabla\rho - \sqrt{\sigma}\eta; \quad \rho(0) = \rho_0; \quad \rho(1) = \rho_1 \quad (52)$$

where η is a white noise of variance $1/(2jL)$ and $\sigma = \rho(1 - \rho)$. This is the usual formula for the fluctuating hydrodynamics of the exclusion process [37]. We write this as a sum over paths and noise realizations with a delta function imposing the equations of motion and a Gaussian weight for the noise,

$$P(\rho^f, t_f; \rho^i, 0) = \int \mathcal{D}\eta \mathcal{D}\rho \delta[\dot{\rho} + \nabla J] e^{-2jL \int_0^{t_f} \int_0^1 dx dt \frac{1}{2}\eta^2(x,t)}. \quad (53)$$

Exponentiating the functional delta function with the aid of a function $\hat{\rho}(x, t)$,

$$P(\rho^f, t_f; \rho^i, 0) = \int \mathcal{D}\eta \mathcal{D}\rho \mathcal{D}\hat{\rho} e^{-2jL \int_0^{t_f} \int_0^1 dx dt \{\hat{\rho}(\dot{\rho} + \nabla J) + \frac{1}{2}\eta^2(x,t)\}}, \quad (54)$$

where $\hat{\rho}$ is integrated along the imaginary axis. Integrating by parts, we obtain

$$P(\rho^f, t_f; \rho^i, 0) = \int \mathcal{D}\eta \mathcal{D}\rho \mathcal{D}\hat{\rho} e^{-2jL \int_0^{t_f} \int_0^1 dx dt \{\hat{\rho}(\dot{\rho} + \nabla \hat{\rho}(\frac{1}{2}\nabla\rho + \sqrt{\sigma}\eta)) + \frac{1}{2}\eta^2(x,t)\}}. \quad (55)$$

We can now integrate away the noise

$$P(\rho^f, t_f; \rho^i, 0) = \int \mathcal{D}\rho \mathcal{D}\hat{\rho} e^{-2jL \int_0^{t_f} \int_0^1 dx dt \{\hat{\rho}(\dot{\rho} + \frac{1}{2}\nabla\hat{\rho}\nabla\rho - \frac{1}{2}(\nabla\hat{\rho})^2\sigma\}}, \quad (56)$$

which reads

$$P(\rho^f, t_f; \rho^i, 0) = \int \mathcal{D}\rho \mathcal{D}\hat{\rho} e^{-2jL \int_0^{t_f} \int_0^1 dx dt \{\hat{\rho}(\dot{\rho} - \mathcal{H})\}} \quad (57)$$

to obtain

$$\mathcal{H} = \frac{1}{2}[\sigma(\nabla\hat{\rho})^2 - \nabla\hat{\rho}\nabla\rho], \quad (58)$$

which is equivalent to (46). The paths are constrained to be $\rho_i(x)$ and $\rho_f(x)$ at initial and final times, respectively. The values of $\hat{\rho}$ are unconstrained, which is in agreement with the fact that this is a Hamiltonian problem with two sets of boundary conditions. The construction above can thus be seen as a formal Hubbard–Stratonovich transformation to introduce the $\hat{\rho}$ field.

Let us finally note that from equation (52) and (56), one sees that

$$P(\rho^f, t_f; \rho^i, 0) = \int \mathcal{D}\rho \mathcal{D}\hat{\rho} e^{-2jL \int_0^{t_f} \int_0^1 dx dt \{J\nabla\hat{\rho} + \frac{1}{2}\nabla\hat{\rho}\nabla\rho - \frac{1}{2}(\nabla\hat{\rho})^2\sigma\}}. \quad (59)$$

Formally integrating over $\nabla\hat{\rho}$ gives back the usual fluctuating hydrodynamics [1, 24, 34]

$$P(\rho^f, t_f; \rho^i, 0) = \int \mathcal{D}\rho \exp\left[-2jL \int_0^{t_f} \int_0^1 dx dt \frac{(J + \nabla\rho/2)^2}{2\sigma}\right]. \quad (60)$$

In all this we have been very sloppy about the spatial conditions $\hat{\rho}$ should satisfy; see appendix B.2 for details.

4. Large deviations in the coarse-grained limit

In this section, we review the steps leading from the fluctuating theory to a non-fluctuating Hamiltonian dynamics, valid in the low-noise limit—itsself arising in the large coarse-graining limit.

4.1. Classical solutions

In order to calculate a probability we have to evaluate

$$P(\rho^f, T) = \int d\rho^i P(\rho^f, T; \rho^i, 0) P(\rho^i, 0), \quad (61)$$

which is true for any time T . Using the path-integral expressions of the previous sections (cf (26)), one then gets the sum of the exponential of the action

$$P(\rho^f, T) = \int d\rho^i \int \mathcal{D}[\rho, \hat{\rho}] e^{-2jLS[\rho, \hat{\rho}]} P(\rho^i, 0) \quad (62)$$

over trajectories with initial and final profiles ρ^i and ρ^f . To leading order in jL , we have that $P(\rho^f, T; \rho^i, 0)$ is dominated by the trajectories extremalizing the action (46)

$$S = \int dx dt [\hat{\rho} \dot{\rho} - \mathcal{H}], \quad (63)$$

i.e. satisfying Hamilton's equations

$$\dot{\rho}(x, t) = \frac{\delta}{\delta \hat{\rho}(x, t)} \int dx' dt' \mathcal{H}[\rho(x', t'), \hat{\rho}(x', t')] \quad (64)$$

$$\dot{\hat{\rho}}(x, t) = -\frac{\delta}{\delta \rho(x, t)} \int dx' dt' \mathcal{H}[\rho(x', t'), \hat{\rho}(x', t')]. \quad (65)$$

These are completely determined (at least up to a discrete set of trajectories) by the initial and final values of $\rho(x)$. What we have outlined is the exact analogue of the way classical trajectories dominate the path integral in the semi-classical limit $\hbar \rightarrow 0$ in quantum mechanics. Similar approaches have been used many times, as for instance to analyze the noisy Burgers equation [15] or in reaction diffusion systems [26].

In the case of the SSEP, Hamilton's equations read

$$\dot{\rho}(x) = \frac{1}{2} \Delta \rho - \nabla[\sigma \nabla \hat{\rho}] \quad (66)$$

$$\dot{\hat{\rho}}(x) = \left(\rho - \frac{1}{2}\right) (\nabla \hat{\rho})^2 - \frac{1}{2} \Delta \hat{\rho}. \quad (67)$$

Equation (66) is a conservation equation and thus defines a current through $\dot{\rho} = -\nabla J_\rho$, where

$$J_\rho[\rho, \hat{\rho}] = -\frac{1}{2} \nabla \rho + \sigma \nabla \hat{\rho}. \quad (68)$$

To determine the probability of a transition between a profile ρ^i and another profile ρ^f in a time T , one thus has to find the trajectory $(\rho(x, t), \hat{\rho}(x, t))$ that solves (66) and satisfies the appropriate boundary conditions. The action of this trajectory then yields the logarithm of the probability of the transition.

We are thus led to solving a classical Hamiltonian *field* problem, where initial and final positions are fixed and momenta unknown. This is in general very difficult—even numerically,

where one has to solve a ‘shooting’ problem to reach the desired final configuration at the right time⁹.

For completeness, let us write the equations of motion in terms of classical spins satisfying the Poisson bracket algebra¹⁰,

$$\{S^z(x), S^\pm(y)\} = \pm S^\pm(x)\delta(x - y); \quad \{S^+(x), S^-(y)\} = 2S^z\delta(x - y), \quad (69)$$

which corresponds to the quantum commutations (18) and yields the equation of motion in terms of spin variables through

$$\dot{S} = \{S, H\} = i\Delta S \wedge S. \quad (70)$$

4.2. Downhill trajectories

For classical equations deriving from a stochastic problem, there always exists a class of trajectories which are easy to find: those that are overwhelmingly the most likely in the low-noise limit. Here and in what follows, we shall call these ‘downhill’ trajectories. If one remembers that the dynamical action corresponds to the stochastic equation (52), one obtains these solutions by directly putting $\eta = 0$. They correspond to the following solutions of the system (66):

$$\dot{\rho}(x) = \frac{1}{2}\Delta\rho \quad \hat{\rho}(x, t) = 0. \quad (71)$$

The solution corresponds to diffusive relaxation toward the linear stationary profile $\bar{\rho}(x) = (1 - x)\rho_0 + x\rho_1$. The corresponding action is zero, in agreement with the fact that the corresponding probability is 1, which simply means that an initial configuration $\rho(x)$ almost surely relaxes toward the stationary state. The stationary profile $\hat{\rho} = 0, \rho = \bar{\rho}$ is a *hyperbolic* fixed point of the dynamics in the full phase space, since it is missed as soon as $\hat{\rho} \neq 0$ in the initial condition.

4.3. Large deviation function from extremal trajectories

As shown by equation (61), the probability $P(\rho^*) \sim e^{-N\mathcal{F}(\rho^*)}$ to observe a profile ρ^* is the average probability of going from an initial profile ρ_i to the profile ρ^* . The logarithm of this transition probability is given in the large- N limit by the ‘classical’ action of a trajectory starting in ρ^i and arriving in a time T in the configuration $\rho^f = \rho^*$, and satisfying (66).

How can a trajectory just reach a generic configuration ρ^* at a very large time $T \rightarrow \infty$? The only possibility is that it takes a hyperbolic trajectory that falls in a finite time in the vicinity of the stationary profile, stays there almost all the time, and then goes to the profile ρ^* in a finite time. This is illustrated in figure 2: trajectories that matter at long times are thus near misses of the stationary points. The first part of such a trajectory (essentially the diffusive relaxation toward the stationary profile) has almost zero action. Thus $P(\rho^i, 0 \rightarrow \rho^*, T) = P(\bar{\rho}, \rho^*, T')$ where T' is a time which differs from T by a finite contribution, not relevant in the $T \rightarrow \infty$ limit: the transition probability $P(\rho^i, 0 \rightarrow \rho^*, T)$ is independent of ρ^i in the long-time limit and equation (61) becomes

$$P(\rho^*, T \rightarrow \infty) = \int d\rho^i P(\rho^i, 0)P(\bar{\rho}, \rho^*, T' \rightarrow \infty) = P(\bar{\rho}, \rho^*, T' \rightarrow \infty). \quad (72)$$

⁹ Note that the same kind of formalism can be used to compute moment generating functions rather than large-deviation functions. In certain cases, the shooting problem thus obtained is easier to solve as it implies nicer boundary conditions. See [26] for an example.

¹⁰ This can be checked using expressions (35) in the continuum space limit and the Poisson bracket $\{A(x), B(y)\} = \int dz \left\{ \frac{\delta A(x)}{\delta \rho(z)} \frac{\delta B(y)}{\delta \bar{\rho}(z)} - \frac{\delta B(y)}{\delta \rho(z)} \frac{\delta A(x)}{\delta \bar{\rho}(z)} \right\}$.

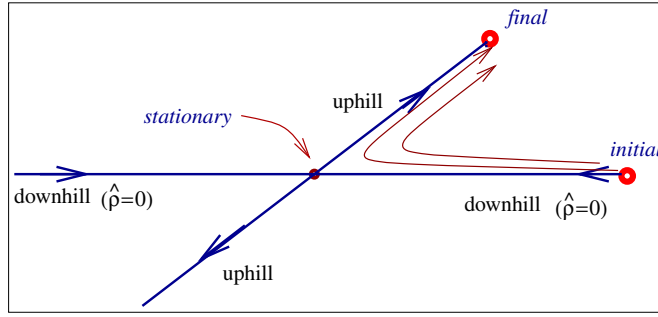


Figure 2. ‘Downhill’ (noiseless) trajectories have $\hat{\rho}(t) = 0$. Trajectories reaching an arbitrary point at long times are ‘near misses’ from the stationary point, and can be decomposed in the long-time limit in a ‘downhill’, followed by an ‘uphill’ trajectory flowing into, and out of the stationary point, respectively.

To determine the probability to observe a given profile ρ^* , one thus has to find the extremal trajectory which starts at $t = -\infty$ in the stationary profile and arrives at $t = 0$ in the desired profile ρ^* . Its action then yields the large-deviation function $\mathcal{F}[\rho^*]$,

$$P(\rho^*) = P(\bar{\rho}, t = -\infty, \rho^*, t = 0). \tag{73}$$

We have assumed here that there are no metastable states. The cases in which many such states exist, one has to consider trajectories falling into each one of them, and also making jumps between them before reaching the final point.

5. Detailed-balance relation, relaxation–excursion symmetry

Finding the trajectory that reaches a given density profile starting from the vicinity of the stationary one is in general a difficult task. There is however a class of systems for which this calculation greatly simplifies: those for which there is a *detailed-balance* symmetry—playing the role of a time reversal—that relates the paths followed by the system in a rare (noise-induced) excursion with the relaxation back to equilibrium. This *Onsager–Machlup* symmetry allows one to compute the rare excursions (in general difficult) from the sole knowledge of the relaxations (easy, as explained in the previous section). This is for instance the case for a SSEP in contact with reservoirs of equal densities $\rho_0 = \rho_1$, as we shall see below.

At the level of operators, detailed balance simply says that the evolution operator and its adjoint are related by a similarity transformation. Here, we are only interested in symmetries at the level of the action, which can be read as a canonical transformation followed by time reversal, leaving the action invariant up to boundary terms (see appendix D).

To make this explicit in our case, we write the Hamiltonian density as

$$\mathcal{H}[\rho, \hat{\rho}] = \frac{1}{2} \nabla \hat{\rho} \sigma \nabla \left(\hat{\rho} - \log \frac{\rho}{1 - \rho} \right) = \frac{1}{2} \nabla \hat{\rho} \sigma \nabla \left(\hat{\rho} - \frac{\delta V_\rho}{\delta \rho} \right), \tag{74}$$

where V_ρ is the equilibrium entropy

$$V_\rho = \int dx [\rho \log \rho + (1 - \rho) \log(1 - \rho)]. \tag{75}$$

The transformation we are looking for is given in two steps [23]: (i) the canonical transformation

$$\hat{\rho} \rightarrow \hat{\rho} + \frac{\delta V_\rho}{\delta \rho}; \quad \rho \rightarrow \rho \quad (76)$$

followed by (ii) a time reversal

$$(\hat{\rho}, \rho, t) \rightarrow (-\hat{\rho}, \rho, T - t). \quad (77)$$

In terms of the current (68), this reads

$$[\rho(x, t), J(x, t)] \rightarrow [\rho(x, -t), -J(x, -t)] \quad (78)$$

the meaning of which is transparent. The new, ‘time-reversed’ variables are

$$\rho_{\text{TR}}(x, t) = \rho(x, -t); \quad \hat{\rho}_{\text{TR}}(x, t) = -\hat{\rho}(x, -t) + \frac{\delta V_\rho}{\delta \rho}(x, -t). \quad (79)$$

It is easy to check that (76), (77) map the action into

$$S[\hat{\rho}, \rho] \rightarrow [V_\rho]_0^T + \int dt dx \{ \hat{\rho}_{\text{TR}} \dot{\rho}_{\text{TR}} - \mathcal{H}[\hat{\rho}_{\text{TR}}, \rho_{\text{TR}}] \}. \quad (80)$$

The space and time boundary conditions are transformed from (48) and (49) to

$$\rho_{\text{TR}}(x, 0) = \rho^*(x) \quad \rho_{\text{TR}}(x, T) = \bar{\rho}(x) \quad (81)$$

$$\begin{aligned} \rho_{\text{TR}}(0, t) &= \rho_0 & \rho_{\text{TR}}(1, t) &= \rho_1 \\ \hat{\rho}_{\text{TR}}(0, t) &= \log \frac{\rho_0}{1 - \rho_0} & \hat{\rho}_{\text{TR}}(1, t) &= \log \frac{\rho_1}{1 - \rho_1}. \end{aligned} \quad (82)$$

The problem is thus recast into finding a trajectory starting in ρ^* and relaxing toward the stationary profile. When the system is at equilibrium, in contact with two reservoirs imposing the same density on the two boundaries ($\rho_0 = \rho_1$), the zero-noise diffusive trajectory

$$\hat{\rho}_{\text{TR}}(x, t) = C^{st} = \log \frac{\rho_0}{1 - \rho_0} \quad \dot{\rho}_{\text{TR}} = \frac{1}{2} \Delta \rho_{\text{TR}} \quad (83)$$

is a legitimate solution of the classical equations which satisfies the new boundary conditions in space and time. The action of such a trajectory is

$$\int dt dx \{ \hat{\rho}_{\text{TR}} \dot{\rho}_{\text{TR}} - \mathcal{H} \} = \log \frac{\rho_0}{1 - \rho_0} \int dx (\rho_0 - \rho^*). \quad (84)$$

Together with the boundary terms of (80), one gets for the large-deviation function, *in terms of the original variables*,

$$S[\rho^*] = \int dx \left[(1 - \rho) \log \frac{1 - \rho}{1 - \rho_0} + \rho \log \frac{\rho}{\rho_0} \right], \quad (85)$$

which is the usual equilibrium entropy [2]. The computation of the extremal trajectory going from $\bar{\rho}$ to ρ^* has thus been made possible by the time-reversal connection between excursion and relaxation induced by the detailed-balance relation. Thanks to the mapping (76) and (77), one just has to find a trajectory going from ρ^* to $\bar{\rho}$ —a relaxation—and from it obtain an excursion.

5.1. System driven out-of-equilibrium—violation of detailed balance and loss of Onsager–Machlup symmetry

Let us now consider why this ‘trick’ does not work when the system is driven out-of-equilibrium by the boundaries. One can still make the transformation (76) and (77), as the bulk dynamics satisfies detailed balance. However, if $\rho_1 \neq \rho_0$, (83) is not acceptable as $\hat{\rho} = C^{st}$ does not satisfy the spatial boundary conditions. We conclude that the most probable excursion from $\bar{\rho}$ to ρ^* is consequently not the time reversed of a diffusive relaxation: the Onsager–Machlup symmetry is broken by the boundaries.

6. Driven exclusion process: remarkable changes of variables

As we have seen, in out-of-equilibrium systems detailed balance is violated—for example by the boundary conditions—and there is no simple relation between excursions and relaxations. One thus cannot, in general, compute easily the rare excursions away from the stationary state, and from it the large-deviation function. Even if we have been able to reduce the computation of large-deviation functions to the solution of a problem of classical dynamics, we are not able to solve for its trajectories in a closed way. It may then come as a surprise that BDGJL [1, 2] were able to uncover what amounts to a series of changes of variables, which end up by mapping the driven problem into one where there is a simple time-reversal symmetry between excursions and relaxations. This allowed them to compute the excursions in terms of the relaxations in the new variables, and then work their way back to the original variables in which the symmetry does not hold.

In this section we shall paraphrase their derivation, to emphasize how surprising it is. In the following section, we shall argue that at the bottom of this is the (also very surprising) fact that the SSEP driven out-of-equilibrium by the boundaries can be mapped back through a change of variables, in the hydrodynamic limit, to an equilibrium SSEP.

Let us first note that the choice of axes we have used to write the hydrodynamic limit Hamiltonian (50) in terms of spin variables $\mathcal{H}_B = -\frac{1}{2} \int dx \nabla S \cdot \nabla S$ is arbitrary. Only the boundary conditions (51) break the rotation invariance.

Let us make a transformation

$$S'_x = S_z \quad S'_z = -S_x \quad S'_y = -S_y; \tag{86}$$

a rotation of angle $\pi/2$ around the y -axis followed by a reflexion with respect to the x' - z' plane. In terms of the coherent-state coordinates—the stereographic representation of classical spins—this transformation is given by the simple homography

$$\bar{z}' = \frac{z - 1}{z + 1} \quad z' = \frac{\bar{z} - 1}{\bar{z} + 1}. \tag{87}$$

In this set of variables, the action reads after a lengthy but straightforward computation

$$S = \int dx \left[\rho \log \frac{\rho}{\frac{1+z'}{2}} + (1 - \rho) \log \frac{(1 - \rho)}{\frac{1-z'}{2}} \right] + S[z', \bar{z}']. \tag{88}$$

As this change of variable corresponds to a symmetry of the Hamiltonian, the action $S[z', \bar{z}']$ is the same as the original one where z and \bar{z} have been replaced by z' and \bar{z}' . It is thus obtained by taking the continuum limit of (26),

$$S[z', \bar{z}'] = \int dx dt \left\{ \frac{\dot{\bar{z}}' z'}{1 + z' \bar{z}'} + \frac{1}{2} (\nabla \bar{z}')^2 \left(\frac{z'}{1 + z' \bar{z}'} \right)^2 + \frac{1}{2} \nabla \bar{z} \nabla \left(\frac{z'}{1 + z' \bar{z}'} \right) \right\}. \tag{89}$$

Of course, we could have arrived at the same point by defining at the outset the coherent states in terms of the rotated operators.

As previously, we can make a Cole–Hopf transformation to introduce Doi–Peliti-like variables,

$$\phi' = \frac{z'}{1 + z'\bar{z}'} \quad \phi^{*'} = \bar{z}'. \quad (90)$$

Surprisingly, as we shall show below, this change of variables greatly simplifies the problem. To stay as close as possible to the solution introduced by BDGJL, we rather introduce a slightly different set of variables

$$F = \frac{1 + \phi^{*'}}{2}, \quad \hat{F} = 2\phi' \quad (91)$$

with which the same simplification occurs. In the F, \hat{F} variables, the action is given by

$$S = \int dx \left[\rho \log \frac{\rho}{F} + (1 - \rho) \log \frac{(1 - \rho)}{1 - F} \right] + S_F[F, \hat{F}] \quad (92)$$

$$S_F[F, \hat{F}] = \int dt dx \left[\hat{F} \dot{F} + \frac{1}{2} \hat{F}^2 \nabla F^2 + \frac{1}{2} \nabla F \nabla \hat{F} \right]. \quad (93)$$

The overall change of variables from $\rho, \hat{\rho}$ to F, \hat{F} reads

$$F = \frac{\rho}{\rho + (1 - \rho)e^{\hat{\rho}}}; \quad \hat{F} = (1 - \rho)(e^{\hat{\rho}} - 1) - \rho(e^{-\hat{\rho}} - 1). \quad (94)$$

In terms of these, the spatial boundary conditions read

$$F(0) = \rho_0 \quad F(1) = \rho_1 \quad \hat{F}(0) = 0 \quad \hat{F}(1) = 0 \quad (95)$$

while the equations of motion become

$$\dot{F} = \frac{1}{2} \Delta F - \hat{F} (\nabla F)^2; \quad \dot{\hat{F}} = -\frac{1}{2} \Delta \hat{F} - \nabla [\hat{F}^2 \nabla F]. \quad (96)$$

In particular, by analogy with the ‘downhill’ zero-noise solutions of the previous sections, we can try $\hat{F}(t) = 0$, which corresponds to

$$\dot{F} = \frac{1}{2} \Delta F. \quad (97)$$

In the original variables, this solution reads

$$\hat{\rho} = 0; \quad \dot{\rho} = \frac{1}{2} \Delta \rho, \quad (98)$$

which is nothing but the diffusive relaxation to the linearly stationary profile $\bar{\rho}$. Diffusion in F, \hat{F} variables thus corresponds to relaxation in $\rho, \hat{\rho}$.

6.1. A second detailed-balance-like symmetry

Remarkably, the action (92) has a detailed-balance-like symmetry, which is unrelated to the original physical one. To see this, integrate the last term of S_F by parts¹¹, so that the action becomes

$$S_F[F, \hat{F}] = \int dt dx \left\{ \hat{F} \dot{F} + \frac{1}{2} \hat{F} \nabla F^2 \left[\hat{F} - \frac{\Delta F}{\nabla F^2} \right] \right\}, \quad (99)$$

¹¹ None of the spatial integrations by parts done in this paper produce any spatial boundary terms thanks to the boundary conditions $\hat{\rho} = \hat{F} = 0$.

which can also be written as

$$S_F[F, \hat{F}] = \int dt dx \left[\hat{F} \dot{F} + \frac{1}{2} \hat{F} \nabla F^2 \left[\hat{F} - \frac{\delta V_F}{\delta F} \right] \right], \quad (100)$$

where we have introduced the potential

$$V_F = \int dx \log \nabla F. \quad (101)$$

The composition of the transformations

$$\hat{F} \rightarrow \hat{F} + \frac{\delta V_F}{\delta F} = \hat{F} + \frac{\Delta F}{\nabla F^2}; \quad (\hat{F}, t) \rightarrow (-\hat{F}, T - t) \quad (102)$$

is thus a symmetry of the action. Note the analogy with (76), (77). The new variables read

$$F_{\text{TR}}(x, t) = F(x, -t); \quad \hat{F}_{\text{TR}}(x, t) = -\hat{F}(x, -t) + \frac{\Delta F}{\nabla F^2}(x, -t). \quad (103)$$

Once again, rather than looking for excursions in the variables F, \hat{F} , the problem is reduced to searching relaxations in the variable $F_{\text{TR}}, \hat{F}_{\text{TR}}$.

Because the system is driven out-of-equilibrium, it would be natural to expect, as in section 5, that this symmetry is broken. Remarkably, we shall show below that this symmetry is not violated by the spatial boundary conditions, in spite of the system being driven. Transformation (102) indeed maps the spatial boundary condition (95) into

$$F_{\text{TR}}(0) = \rho_0; \quad F_{\text{TR}}(1) = \rho_1; \quad \hat{F}_{\text{TR}}(0) - \frac{\Delta F_{\text{TR}}}{(\nabla F_{\text{TR}})^2} \Big|_{x=0} = \hat{F}_{\text{TR}}(1) - \frac{\Delta F_{\text{TR}}}{(\nabla F_{\text{TR}})^2} \Big|_{x=1} = 0. \quad (104)$$

Contrary to what happened in section 5, the ‘zero-noise solution’ $\dot{F}_{\text{TR}} = \Delta F_{\text{TR}}/2; \hat{F}_{\text{TR}} = 0$ this time satisfies (104). From (95), one indeed sees that

$$\dot{F}|_{x=0,1} = \hat{F}|_{x=0,1} = 0. \quad (105)$$

Together with (96), this shows that any extremal trajectory satisfies

$$\Delta F|_{x=0,1} = 2[\dot{F} + \hat{F}(\nabla F)^2]|_{x=0,1} = 0. \quad (106)$$

Furthermore, $\hat{F}_{\text{TR}} = 0$ reads in the initial F, \hat{F} variables

$$\hat{F} - \frac{\Delta F}{(\nabla F)^2} = 0, \quad (107)$$

which is indeed compatible with (105) and (106). Zero-noise diffusive relaxations in the variables $F_{\text{TR}}, \hat{F}_{\text{TR}}$ thus correspond to the excursion in the initial variables. The action of such a solution is

$$S_F = [V_F]_0^T = \left[\int dx \log \nabla F \right]_0^T \quad (108)$$

and the corresponding large-deviation function is given, in the original variables, by

$$S[\rho^*] = \int dx \left[\rho \log \frac{\rho}{F} + (1 - \rho) \log \frac{(1 - \rho)}{1 - F} + \log \nabla F \right]_0^T. \quad (109)$$

F is determined from ρ by solving the equation $\hat{F}_{\text{TR}} = 0$ which reads

$$\rho = F + F(1 - F) \frac{\Delta F}{\nabla F^2}. \quad (110)$$

Injecting the temporal boundary conditions in (109), one gets

$$S[\rho^*] = \int dx \left[\rho^* \log \frac{\rho^*}{F} + (1 - \rho^*) \log \frac{(1 - \rho^*)}{1 - F} + \log \frac{\nabla F}{\rho_1 - \rho_0} \right]. \quad (111)$$

This is indeed the solution of the problem, initially found by Derrida, Lebowitz and Speer [10] and later recovered by BDGJL [1]. Let us stress however that the existence of a potential functional V_F is a mystery, as nothing guarantees that such a function exists out-of-equilibrium. Yet another mystery is the fact that the symmetry related to V_F is unbroken by the reservoirs. We shall show below that these surprises are deeply related to the fact that this model can be brought back to equilibrium.

7. Non-local mapping to equilibrium

In the previous section we have shown that if one rotates the axes, and expresses everything in terms of variables F, \hat{F} associated with the spin operators in the coherent-state representation (or, in the classical limit, with the stereographic projection of the spins), a new, surprising detailed-balance symmetry becomes explicit. It is unrelated to the original one and is not broken by the source terms at the boundaries. In this section, we show that this sequence of miracles can be condensed into only one: at the hydrodynamic level the chain driven out of equilibrium can be mapped onto a free equilibrium chain with no sources at the boundaries. The transformation that does this is, however, non-local in space, and is the analogue of the one we discussed in the introduction for non-interacting particles in a potential.

Starting from the action S_F (99), one introduces the *non-local* variables

$$\hat{F}' = \nabla F; \quad \nabla F' = \hat{F} - \frac{\Delta F}{(\nabla F)^2}, \quad (112)$$

where the second equation can also be written as

$$\hat{F} = \nabla \left[F' - \frac{1}{\hat{F}'} \right] = \nabla F' + \frac{\nabla \hat{F}'}{\hat{F}'^2}. \quad (113)$$

This change of variables takes the action into itself, apart from temporal boundary terms,

$$S = \int dx \left[\rho \log \frac{\rho}{F} + (1 - \rho) \log \frac{1 - \rho}{1 - F} + \log \hat{F}' - F' \hat{F}' \right]_0^T \\ + \int dx dt \left\{ \hat{F}' \dot{F}' + \frac{1}{2} \hat{F}'^2 (\nabla F')^2 + \frac{1}{2} \nabla F' \nabla \hat{F}' \right\}. \quad (114)$$

Equation (112) thus describes a non-local symmetry of the Hamiltonian. This suggests that we continue the succession of changes of variables done up to here

$$(\rho, \hat{\rho}) \rightarrow (F, \hat{F}) \rightarrow (F', \hat{F}') \quad (115)$$

by a further transformation $(F', \hat{F}') \rightarrow (\rho', \hat{\rho}')$, where ρ' and $\hat{\rho}'$ are related to F', \hat{F}' in the same way as are the unprimed counterparts of (94)

$$\rho' = F' + F'(1 - F')\hat{F}'; \quad \hat{\rho}' = \log \left(1 + \frac{\hat{F}'}{1 - F'\hat{F}'} \right). \quad (116)$$

One thus ends up with

$$S = \int dx \left[\rho \log \frac{\rho}{F} + (1 - \rho) \log \frac{1 - \rho}{1 - F} + \log \nabla F - \frac{\rho' - F'}{1 - F'} \right. \\ \left. - \rho' \log \frac{\rho'}{F'} - (1 - \rho') \log \frac{1 - \rho'}{1 - F'} \right]_0^T + S', \quad (117)$$

where $S' = \int dt dx \{\hat{\rho}' \dot{\rho}' - \mathcal{H}'\}$ and \mathcal{H}' is formally equivalent to the initial Hamiltonian density \mathcal{H} but for the primed variables,

$$S' = \int dt dx \left\{ \hat{\rho}' \dot{\rho}' - \frac{1}{2} \sigma_{\rho'} \nabla \hat{\rho}'^2 + \frac{1}{2} \nabla \rho' \nabla \hat{\rho}' \right\}. \quad (118)$$

The overall change of variables, which reads

$$\nabla \left[\frac{1}{1 - e^{\hat{\rho}'}} \right] = (1 - \rho)(e^{\hat{\rho}} - 1) - \rho(e^{-\hat{\rho}} - 1) \quad (119)$$

$$\nabla \left[\frac{\rho}{\rho + (1 - \rho) e^{\hat{\rho}}} \right] = (1 - \rho')(e^{\hat{\rho}'} - 1) - \rho'(e^{-\hat{\rho}'} - 1) \quad (120)$$

thus maps the action of the hydrodynamic limit of the SSEP into another SSEP.

What we shall now prove is that this new process corresponds to an isolated chain, and consequently possesses a detailed-balance relation, induced by its equilibrium entropy, which is not violated by the boundaries. Last, we shall show that this detailed-balance relation, mapped back to the original $\rho, \hat{\rho}$ variables is the non-local symmetry (102).

7.1. Boundary conditions—currents

From (112) one sees that the spatial boundary conditions (95) read in the new variables

$$\nabla \left[F' - \frac{1}{\hat{F}'} \right]_{x=0,L} = 0; \quad \int_0^L \hat{F}' = \rho_1 - \rho_0. \quad (121)$$

In the language of spin variables, the hydrodynamic Hamiltonian (50) presents three conserved quantities in the bulk—the components of the spins—which can be written as

$$Q_1 = 2\rho' - 1 = 2S'_z; \quad Q_2 = \hat{F}' = 2(S'_z + iS'_y); \quad Q_3 = \hat{F}'(1 - 2F') = 2S'_x - 1. \quad (122)$$

Their continuity equations read

$$\dot{Q}_i = -\nabla J_i, \quad (123)$$

where the currents J_i are given by

$$\begin{aligned} J_{Q_1} &= -\nabla \rho' + 2\sigma_{\rho'} \nabla \hat{\rho}'; & J_{Q_2} &= \frac{1}{2} \nabla \hat{F}' + \hat{F}'^2 \nabla F' \\ J_{Q_3} &= (1 - 2F') \frac{\nabla \hat{F}'}{2} + [\hat{F}' + \hat{F}'^2(1 - 2F')] \nabla F'. \end{aligned} \quad (124)$$

Let us show that these currents vanish at the boundaries for all extremal trajectories. Such trajectories satisfy the equation of evolution (96) and the boundary condition (95). This implies that ΔF vanishes at the boundary (lhs of (96) together with $\hat{F} = 0$). From definition (112) one then gets that $\nabla \hat{F}'$ also vanishes, which implies, together with the lhs of (121), that $\nabla F'$ also vanishes. Last, from the mapping $F', \hat{F}' \rightarrow \rho', \hat{\rho}'$ one sees that if both $\nabla F'$ and $\nabla \hat{F}'$ vanish, so do $\nabla \rho'$ and $\nabla \hat{\rho}'$. All in all, one gets that at the boundaries

$$\nabla F' = \nabla \hat{F}' = \nabla \rho' = \nabla \hat{\rho}' = 0. \quad (125)$$

We then see from (124) that the three currents J_{Q_i} vanish at the boundary: *the transformed model in the primed variables is an isolated chain*. This condition alone, supplemented with the rhs of (121), encompasses all the original boundary conditions.

7.2. Profiles and trajectories

When the dust sets, we see that all that has been used is the fact that the original variables $(\rho, \hat{\rho})$ or, more physically (ρ, J) , have been mapped by a non-local transformation into new densities and currents

$$(\rho(x, t), J(x, t)) \rightarrow (\rho'(x, t), J'(x, t)). \quad (126)$$

The original detailed-balance symmetry (78) that maps a trajectory into its time reversed

$$(\rho(x, t), J(x, t)) \rightarrow (\rho(x, -t), -J(x, -t)) \quad (127)$$

is broken by the source terms driving the system out-of-equilibrium. Miraculously, the transformed chain is isolated, so that time-reversed trajectories are related through

$$(\rho'(x, t), J'(x, t)) \rightarrow (\rho'(x, -t), -J'(x, -t)). \quad (128)$$

Coming back to the original variables via (126) mixes the density ρ' (symmetric in time) with the current J' (antisymmetric in time), thus making the pair of transformed trajectories expressed in ρ and J neither symmetric nor antisymmetric.

Let us now describe ‘uphill’ and ‘downhill’ trajectories. The stationary profile $\bar{\rho}$ maps to a flat profile $\bar{\rho}' = C^{st}$. The precise value of C^{st} is arbitrary, due to dilation invariance of the model, contrary to \hat{F}' which is constrained by the rhs of (121).

- *Relaxations.* Diffusive trajectories of the initial model satisfy

$$\dot{\hat{\rho}} = \frac{1}{2} \Delta \rho, \quad \hat{\rho} = 0. \quad (129)$$

From (119), one sees that $\hat{\rho} = 0$ implies $\nabla \hat{\rho}' = 0$. As the primed variables also satisfy the equations of motion (66), the resulting trajectories evolve with

$$\dot{\rho}' = \frac{1}{2} \Delta \rho'. \quad (130)$$

Relaxations thus map into relaxations.

- *Excursions.* The instanton equations (107) imply $\nabla F' = 0$ (cf (112)). Using the relation of F, \hat{F} (94), as applied to the primed variables, one gets

$$\nabla \hat{\rho}' - \frac{\nabla \rho'}{\sigma_{\rho'}} = 0. \quad (131)$$

Injected back in the equations of motion (66), this shows that densities evolve with

$$\dot{\rho}' = -\frac{1}{2} \Delta \rho'. \quad (132)$$

Excursions of the initial model, once mapped back to equilibrium through (119), are given by time reversal of the isolated chain’s relaxations. The action $S'[\hat{\rho}', \rho']$ of such an uphill trajectory is $\int_0^L dx [\rho' \log \rho' + (1 - \rho') \log(1 - \rho')]_0^T$. As F' is constant along the instanton and $\int_0^L \rho'$ is a constant of motion, the overall action (117) reduces to the large-deviation function (111), as it should.

7.3. Detailed-balance symmetry

Let us now show in terms of spin variables how the detailed-balance relation of the isolated chain accounts for the miraculous transformation (102) which allowed BDGJL to compute the large-deviation function. In the spin variables, the original detailed-balance symmetry (76) and (77) amounts to a reflexion of all the spins with respect to the x - z plane

$$(S_x, S_y, S_z) \rightarrow (S_x, -S_y, S_z); \quad T \rightarrow T - t. \quad (133)$$

Because the bulk Hamiltonian is also invariant with respect to any simultaneous rotation of all the spins, any composition of (133) with a rotation gives another ‘detailed-balance-like’ symmetry. These symmetries are all broken by the boundary conditions of the original model. Once mapped to the isolated chain, the boundary conditions (121) reduce to fixing the value of an integral of motion

$$2 \int_0^L (S'_z + iS'_y) = \int_0^L \hat{F}' = \rho_1 - \rho_0. \quad (134)$$

Among all the ‘detailed-balance-like’ symmetries of the isolated chain, only one preserves (134). We are thus left with the transformation

$$(S'_x, S'_y, S'_z) \rightarrow (-S'_x, S'_y, S'_z); \quad t \rightarrow T - t. \quad (135)$$

From the expression of Q_3 in (122), one sees that $S_x^{\text{TR}'} = -S'_x$ can be written as

$$1 + \hat{F}'_{\text{TR}}(1 - 2F'_{\text{TR}}) = -1 - \hat{F}'(1 - 2F'). \quad (136)$$

Using $\hat{F}' = \nabla F$ and looking for $F_{\text{TR}} = F$, this reads

$$F' + F'_{\text{TR}} = 1 + \frac{1}{\nabla F}. \quad (137)$$

Differentiating once and using $\nabla F' = \hat{F} - \frac{\Delta F}{(\nabla F)^2}$, one gets

$$\hat{F}'_{\text{TR}} + \hat{F}' = \frac{\Delta F}{(\nabla F)^2}, \quad (138)$$

which is nothing but the non-local mapping (103) between ‘downhill’ diffusive solutions and the instantons. One thus sees that the miraculous solution of the initial model is simply induced by the detailed-balance-like relation (135) of the isolated chain, which does not violate the boundary conditions (121).

8. KMP

The Kipnis–Marchioro–Presutti model (KMP) was introduced in [27] as a one-dimensional model of energy transport satisfying Fourier law. Bertini, Gabrielli and Lebowitz recently computed the large-deviation function of the energy profile using an approach similar to the one used previously for the SSEP [3]. We shall show below that once again a mapping back to equilibrium explains this success.

The functional expression for the fluctuating hydrodynamics of KMP is very similar to that of SSEP,

$$\int \mathcal{D}[\hat{\rho}, \rho] e^{-N S[\hat{\rho}, \rho]} = \int \mathcal{D}[\hat{\rho}, \rho] e^{-N \int dt dx (\hat{\rho} \dot{\rho} - \mathcal{H})}, \quad (139)$$

where we have introduced the Hamiltonian density

$$\mathcal{H} \equiv \frac{1}{2}[\rho^2 \nabla \hat{\rho}^2 - \nabla \hat{\rho} \nabla \rho]. \quad (140)$$

To compute the large-deviation function $\mathcal{F}(\rho^*)$, one has to solve the corresponding Hamilton equations

$$\dot{\rho} = \frac{1}{2} \Delta \rho - \nabla[\rho^2 \nabla \hat{\rho}]; \quad \dot{\hat{\rho}} = -\frac{1}{2} \Delta \hat{\rho} - \rho(\nabla \hat{\rho})^2 \quad (141)$$

with the boundary conditions

$$\rho(x, 0) = \bar{\rho}(x) = (1 - x)\rho_0 + x\rho_1; \quad \rho(x, T) = \rho^*(x) \quad (142)$$

$$\rho(0, t) = \rho_0; \quad \rho(1, t) = \rho_1; \quad \hat{\rho}(0, t) = \hat{\rho}(1, t) = 0. \quad (143)$$

Once again, the last equality simply says that no fluctuations are allowed at the contact with the reservoir.

8.1. Connection with the $SU(1, 1)$ spin chain

KMP is related to $SU(1, 1)$ spin chains in a rather subtle way [19, 20]. Starting from the $SU(1, 1)$ coherent states for spin k ,

$$|z\rangle = \frac{1}{(1 - z\bar{z})^k} e^{zK^+} |0\rangle, \quad (144)$$

one gets the following expression for the pseudo-spin operators:

$$\langle z|K^+|z\rangle = 2k \frac{\bar{z}}{1 - z\bar{z}}; \quad \langle z|K^-|z\rangle = 2k \frac{z}{1 - z\bar{z}}; \quad \langle z|K^z|z\rangle = k \frac{1 + z\bar{z}}{1 - z\bar{z}} \quad (145)$$

of the $SU(1, 1)$ group. By analogy with equation (40) for the $SU(2)$ case, the Doi–Peliti variables are defined through

$$\phi^* = \bar{z}; \quad \phi = \frac{z}{1 - z\bar{z}}. \quad (146)$$

The difference with the $SU(2)$ case stems from the fact that the energy-density variables $\rho, \hat{\rho}$ have to be identified directly with the Doi–Peliti variables,

$$\rho = \phi = \frac{z}{1 - z\bar{z}}; \quad \hat{\rho} = \phi^* = \bar{z}. \quad (147)$$

In particular, from (145) and (147), one sees that ρ corresponds to K^- and not to the z -component of the spins as was the case for the SSEP and the $SU(2)$ representation¹². Defining the classical spin

$$K^{x,y,x} = \frac{1}{2k} \langle z|K^{x,y,z}|z\rangle, \quad (148)$$

one then checks that the Hamiltonian (140) corresponds to the continuous pseudo-spin chain $\mathcal{H} = -\frac{1}{2}[(\nabla K_x)^2 + (\nabla K_y)^2 - (\nabla K_z)^2] = -\frac{1}{2}[\nabla K^+ \cdot \nabla K^- - (\nabla K_z)^2]$. (149)

8.2. Remarkable change of variables

As we did in section 6 for the SSEP, we shall use the symmetry of the evolution operator under simultaneous $SU(1, 1)$ ‘rotation’ of all ‘spins’ to find a basis where a non-local mapping to equilibrium is easily revealed. Making a reflexion with respect to the $x - z$ plane maps K^y in $-K^y$ and lets (149) invariant. As expected, it is thus a symmetry of the action. In the (z, \bar{z}) coordinates it reads

$$z' = \bar{z}; \quad \bar{z}' = z. \quad (150)$$

By analogy with (146), one defines

$$\phi' = \frac{z'}{1 - z'\bar{z}'}; \quad \phi^{*'} = \bar{z}'. \quad (151)$$

The transformation then reads in density variables

$$\rho = \phi^{*'}(1 + \phi\phi^{*'}); \quad \hat{\rho} = \frac{\phi'}{1 + \phi'\phi^{*'}}; \quad \Leftrightarrow \quad \phi' = \hat{\rho}(1 + \rho\hat{\rho}); \quad \phi^{*'} = \frac{\rho}{1 + \rho\hat{\rho}}. \quad (152)$$

As for the SSEP, we could now work with these new ‘Doi–Peliti’ like variables, but to make contact with the solution of BDGJL we use slightly different notations

$$F = \phi^{*'}; \quad \hat{F} = \phi', \quad (153)$$

¹² If one wants to understand S^z as a density particle in (149), one gets the dual model of KMP [3, 20], for which there also exist a non-local mapping back to equilibrium.

so that the overall mapping of the action reads

$$S[\rho, \hat{\rho}] = \int dx \left[\frac{\rho}{F} - \log \frac{\rho}{F} \right]_0^T \quad (154)$$

$$+ \int dx dt \left\{ \hat{F} \dot{\hat{F}} - \frac{1}{2} \hat{F}^2 (\nabla F)^2 + \frac{1}{2} \nabla \hat{F} \nabla F \right\}. \quad (155)$$

The fields F, \hat{F} are related to energy densities through

$$F = \frac{\rho}{1 + \rho \hat{\rho}}; \quad \hat{F} = \hat{\rho}(1 + \rho \hat{\rho}), \quad (156)$$

so that the spatial boundary conditions (142) are given by

$$\hat{F}(0) = \hat{F}(1) = 0; \quad F(0) = \rho_0; \quad F(1) = \rho_1. \quad (157)$$

8.3. Non-local mapping back to equilibrium

Let us introduce the non-local variables

$$\hat{F}' = \nabla F; \quad \hat{F} = \nabla \left[F' + \frac{1}{\hat{F}'} \right], \quad (158)$$

which maps the action into

$$S[\rho, \hat{\rho}] = \int dx \left[\frac{\rho}{F} - \log \frac{\rho}{F} - \log \hat{F}' - F' \hat{F}' \right]_i^f \quad (159)$$

$$+ \int dx dt \left\{ \hat{F}' \dot{\hat{F}}' - \frac{1}{2} \hat{F}'^2 (\nabla F')^2 + \frac{1}{2} \nabla \hat{F}' \nabla F' \right\}. \quad (160)$$

Comparison of (159) and (154) reveals that (158) is a non-local symmetry of the action. The boundary conditions (157) now reads

$$\int_0^L \hat{F}' = \rho_L - \rho_0 \quad \nabla F' - \frac{\nabla \hat{F}'}{\hat{F}'^2} = 0. \quad (161)$$

As the classical trajectories in the original F, \hat{F} variables satisfy

$$\dot{\hat{F}} = \frac{1}{2} \Delta F + \hat{F} \nabla F^2 \quad (162)$$

$$\dot{\hat{F}} = -\frac{1}{2} \Delta \hat{F} + \nabla [\hat{F}^2 \nabla F], \quad (163)$$

we see that on the boundaries, $\dot{\hat{F}} = 0$ and $\hat{F} = 0$ implies $\Delta F = \nabla \hat{F}' = 0$. Together with the rhs of (161), this implies

$$\nabla F' = \nabla \hat{F}' = 0 \quad (164)$$

and all the currents vanish on the boundaries. Equation (158) thus maps the chain into an isolated one. One can continue the mapping $\rho, \hat{\rho} \rightarrow F, \hat{F} \rightarrow F', \hat{F}'$ to introduce new energy densities $\rho', \hat{\rho}'$,

$$\rho' = F'(1 + F' \hat{F}'); \quad \hat{\rho}' = \frac{\hat{F}'}{1 + F' \hat{F}'}. \quad (165)$$

One then gets an overall action

$$S[\rho, \hat{\rho}] = \int dx \left[\frac{\rho}{F} - \log \frac{\rho}{F} - \log \hat{F}' - F' \hat{F}' - \frac{\rho'}{F'} + \log \frac{\rho'}{F'} \right]_i^f \quad (166)$$

$$+ \int dx dt \left\{ \hat{\rho}' \dot{\rho}' - \frac{1}{2} \rho'^2 (\nabla \hat{\rho}')^2 + \frac{1}{2} \nabla \hat{\rho}' \nabla \rho' \right\}, \quad (167)$$

which shows that the hydrodynamic limit of the KMP model driven out-of-equilibrium can be mapped back to equilibrium through a non-local change of variables. This chain has a detailed-balance symmetry, and as before its instantons are time reversal of relaxations and are thus given by

$$\dot{\rho}' = -\frac{1}{2} \Delta \rho'. \quad (168)$$

From the equations of motion (141), one sees that this corresponds to

$$\rho^2 \nabla \hat{\rho} = \nabla \rho. \quad (169)$$

In the F' , \hat{F}' variables, this reads

$$\nabla F' = 0. \quad (170)$$

Mapped back to the initial variables, one gets the instanton equation

$$\hat{F} = -\frac{\Delta F}{(\nabla F)^2} \quad (171)$$

or, for the density variables,

$$\rho = F - F^2 \frac{\Delta F}{\nabla F^2}. \quad (172)$$

This is the counterpart for KMP of the instanton equation (110) for the SSEP, and corresponds to the equation found by BDGJL. The action of this trajectory is

$$S[\rho, \hat{\rho}] = \int dx \left[\frac{\rho}{F} - \log \frac{\rho}{F} - \log \hat{\nabla} F \right]_0^T, \quad (173)$$

which is precisely the large-deviation function obtained in [3]. One sees that once again a non-local mapping back to equilibrium enables one to find the instanton equation and thus compute the large-deviation function. This result can be extended to the whole class of systems defined by a Hamiltonian density $H(\rho, \hat{\rho}) = \sigma (\nabla \hat{\rho})^2 / 2 - \nabla \rho \nabla \hat{\rho} / 2$ where σ is a second-order polynomial in ρ .

9. Non-interacting particles in an arbitrary potential driven out of equilibrium

Apart from the simple example addressed in the introduction, the mappings to equilibrium we have presented so far only apply at the level of large deviations. We shall show below that such a mapping can also be constructed for the full probability distribution, without coarse graining, of a model of *non-interacting* particles driven out-of-equilibrium. We shall do the mapping in two ways: at the level of probabilities in subsection 9.1, and at the level of evolution operators in subsection 9.2.

We consider an open chain of L sites (index $1 \leq k \leq L$) in contact with two reservoirs. Each particle at site k can jump to a neighboring site $k \pm 1$ with rates $W_{k \rightarrow k \pm 1}$. The system is coupled to reservoirs at the two boundaries (sites 1 and L) through transition rates $W_{0 \rightarrow 1}$, $W_{1 \rightarrow 0}$, $W_{L \rightarrow L+1}$, $W_{L+1 \rightarrow L}$ (see figure 3).

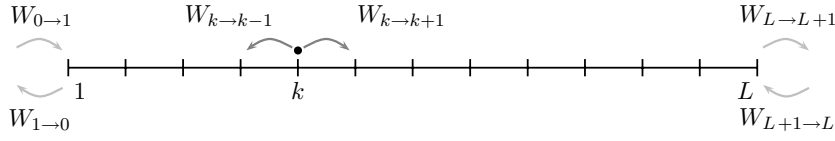


Figure 3. Open chain in contact with reservoirs: generic rates for individual particles.

A simple case for which the steady state is known is that of equilibrium systems, where probability currents vanish. For non-interacting particles, the corresponding detailed-balance relation is equivalent to balancing the stationary mass fluxes over each bond. Introducing the average occupancies P_k^{eq} , it reads

$$W_{0 \to 1} = P_1^{\text{eq}} W_{1 \to 0} \quad P_k^{\text{eq}} W_{k \to k+1} = P_{k+1}^{\text{eq}} W_{k+1 \to k} \quad W_{L \to L+1} P_L^{\text{eq}} = W_{L+1 \to L}. \quad (174)$$

The first two equations imply that P_k^{eq} takes the form

$$P_k^{\text{eq}} = \prod_{\ell=0}^{k-1} \frac{W_{\ell \to \ell+1}}{W_{\ell+1 \to \ell}} \quad \text{for } 1 \leq k \leq L. \quad (175)$$

Combining the last equation of (174) and (175), we see that this solution is consistent as long as

$$\frac{W_{0 \to 1} W_{1 \to 2} \dots W_{L \to L+1}}{W_{L+1 \to L} \dots W_{1 \to 0}} = 1. \quad (176)$$

This condition can be violated in many physical situations as for instance when a current is forced by the reservoirs. In such cases, the steady-state occupancies are not the P_k^{eq} 's and one has to resort to other methods for their determination, as has been done for instance by Derrida in [8] for a particle hopping in a periodic potential. To our knowledge, the case of open systems with non-vanishing steady current has not been considered in the literature and could be interesting in the context of non-equilibrium disordered media [5].

In the following section, we show how to map our open system back to equilibrium, allowing us to get an explicit expression for the steady-state distribution.

9.1. Transformation of probabilities

Let us consider a probability distribution obtained as a product of Poisson distribution in each site

$$P(n_1, \dots, n_L) = \prod_{k=1}^L \frac{P_k^{n_k}}{n_k} e^{-P_k}. \quad (177)$$

Its form is preserved by the time evolution and the P_k 's evolve with the conservation equation

$$\partial_t P_k = -(J_{k+1} - J_k), \quad (178)$$

where one has introduced the currents

$$J_k = -P_k W_{k \to k-1} + P_{k-1} W_{k-1 \to k} \quad (\text{for } 2 \leq k \leq L) \quad (179)$$

$$J_1 = -P_1 W_{1 \to 0} + W_{0 \to 1} \quad J_{L+1} = -W_{L+1 \to L} + P_L W_{L \to L+1}. \quad (180)$$

In general, the steady state is not given by canceling all currents J_k , as this takes us back to the detailed-balance conditions (174). In the spirit of previous sections, our aim here is to map our model to an isolated system, for which currents vanish at the boundaries. The

construction of the equilibrium model follows closely the one of the Fokker–Planck equation presented in the introduction. We introduce primed occupancies

$$\begin{aligned} P'_k &= (P_{k+1}^{\text{eq}})^{-1} P_{k+1} - (P_k^{\text{eq}})^{-1} P_k; & (\text{for } 1 \leq k \leq L-1) \\ P'_0 &= (P_1^{\text{eq}})^{-1} P_1 - (P_0^{\text{eq}})^{-1}; & P'_L = (P_{L+1}^{\text{eq}})^{-1} - (P_L^{\text{eq}})^{-1} P_L, \end{aligned} \quad (181)$$

where one has extended definition (175) of P_k^{eq} to P_{L+1}^{eq} and set $P_0^{\text{eq}} = 1$. Defining the new rates

$$W'_{k \rightarrow k+1} = W_{k+1 \rightarrow k}; \quad W'_{k+1 \rightarrow k} = W_{k+1 \rightarrow k+2}, \quad (182)$$

we now have the evolution for a chain of $L+1$ sites ($0 \leq k \leq L$),

$$\partial_t P'_k = -(J'_{k+1} - J'_k), \quad (183)$$

where the currents are defined by

$$J'_0 = J'_{L+1} = 0; \quad \text{and} \quad J'_k = -P'_k W'_{k \rightarrow k-1} + P'_{k-1} W'_{k-1 \rightarrow k}; \quad (\text{for } 1 \leq k \leq L). \quad (184)$$

Strikingly, the currents J'_0 and J'_{L+1} vanish and the primed chain is thus isolated.

Note that although we mapped our initial open chain of L sites into an isolated chain of $L+1$ sites, there is no contradiction when counting degrees of freedom. Indeed, from definition (181), we see that the primed occupancies satisfy

$$\sum_{k=0}^L P'_k = (P_{L+1}^{\text{eq}})^{-1} - (P_0^{\text{eq}})^{-1}, \quad (185)$$

which means that there are only L independent occupancies in the isolated chain.

The (equilibrium) steady state of the primed chain is found by imposing $J'_k = 0$ for all k 's,

$$P'_k \propto P'_{\text{eq}}(k) = \prod_{\ell=0}^{k-1} \frac{W'_{\ell \rightarrow \ell+1}}{W'_{\ell+1 \rightarrow \ell}} = \frac{W_{0 \rightarrow 1}}{W_{k+1 \rightarrow k} P_{k+1}^{\text{eq}}} = \frac{W_{0 \rightarrow 1}}{W_{k \rightarrow k+1} P_k^{\text{eq}}}. \quad (186)$$

Mapping back to the original variables, one obtains the expression of the steady-state occupancies P_k^{st} ,

$$P_k^{\text{st}} = \frac{1}{Z_L} \left[(P_0^{\text{eq}})^{-1} \sum_{\ell=k}^L \frac{P_k^{\text{eq}}}{W_{\ell \rightarrow \ell+1} P_\ell^{\text{eq}}} + (P_{L+1}^{\text{eq}})^{-1} \sum_{\ell=0}^{k-1} \frac{P_k^{\text{eq}}}{W_{\ell \rightarrow \ell+1} P_\ell^{\text{eq}}} \right], \quad (187)$$

where Z_L is a normalization constant given by

$$Z_L = \sum_{\ell=0}^L \frac{1}{W_{\ell \rightarrow \ell+1} P_\ell^{\text{eq}}}. \quad (188)$$

The result (187) is reminiscent of that obtained by Derrida in [8], the differences highlighting the role of the reservoirs.

To highlight the connection with the case treated in introduction, let us consider explicitly particles diffusing in a discrete potential, where the rates $W_{k \rightarrow k \pm 1}$ are given by

$$W_{k \rightarrow k \pm 1} = \beta^{-1} e^{-\frac{1}{2}\beta(V_{k \pm 1} - V_k)}. \quad (189)$$

In the bulk, they obey detailed balance with respect to the Boltzmann weight $P_k^{\text{eq}} \propto e^{-\beta V_k}$, but the system is driven out-of-equilibrium as soon as $V_{L+1} \neq V_0$ (see relation (176)). The averaged occupancies P_k evolve with

$$\beta \partial_t P_k = P_{k+1} e^{-\frac{1}{2}\beta(V_k - V_{k+1})} + P_{k-1} e^{-\frac{1}{2}\beta(V_k - V_{k-1})} - P_k [e^{-\frac{1}{2}\beta(V_{k+1} - V_k)} + e^{-\frac{1}{2}\beta(V_{k-1} - V_k)}]. \quad (190)$$

Taking the continuum limit ($k = xL$ with $0 \leq x \leq 1$, $L \gg 1$) and rescaling time with L^2 (diffusive scaling), one recovers the Fokker–Planck equation (1) with $\beta^{-1} = T$, upon gradient expansion of (190). In particular, taking the continuum limit of the microscopic steady state (187), one recovers as expected the result (7) for the non-equilibrium Fokker–Planck steady state. Last, with the potential V_k defined in (189), the primed equilibrium law reads $P'_{\text{eq}}(k) \propto \exp\left\{\frac{\beta}{2}(V_k + V_{k+1})\right\}$, which is analogous to the sign change of V for Fokker–Planck (see equation (3)), but also induces a smooth averaging of the potential over two neighboring sites.

9.2. Transformation for evolution operators

As shown above, the average occupancies P_k fully determine the steady state of non-interacting particles and can be computed through a mapping to equilibrium. Such approach does not apply for exclusion processes, as exclusion correlates particles. To cast the mapping to equilibrium in a form similar in both cases, we shall now work directly with the evolution operator of non-interacting particles. Beyond the quest for a formalism ultimately applicable to microscopic models of interacting particles, this point of view proves to be much stronger than the one developed in section 9.1, even for non-interacting particles. Indeed, it applies when the initial distribution is not factorized, i.e. not in the form (177), and gives access not only to the steady state, but also to the whole dynamics.

For the system of non-interacting particles considered in this section, the probability $P(\mathbf{n}, t)$ evolves with (we refer to section 2.2 for the notation)

$$\begin{aligned} \partial_t P(\mathbf{n}, t) = & \sum_{k=1}^{L-1} \left\{ n_{k+1}^+ W_{k+1 \rightarrow k} P(n_k^-, n_{k+1}^+) + n_k^+ W_{k \rightarrow k+1} P(n_k^+, n_{k+1}^-) \right. \\ & - [n_k W_{k \rightarrow k+1} + n_{k+1} W_{k+1 \rightarrow k}] P(\mathbf{n}) \left. \right\} + W_{1 \rightarrow 0} [n_1^+ P(n_1^+) - n_1 P(\mathbf{n})] \\ & + W_{0 \rightarrow 1} [P(n_1^-) - P(\mathbf{n})] + W_{L \rightarrow L+1} [n_L^+ P(n_L^+) - n_L P(\mathbf{n})] \\ & + W_{L+1 \rightarrow L} [P(n_L^-) - P(\mathbf{n})]. \end{aligned} \quad (191)$$

Let us introduce the usual Doi–Peliti [13, 32] creation and annihilation operators a_k^\dagger, a_k , defined by

$$a_k^\dagger |n_k\rangle = |n_k + 1\rangle; \quad a_k |n_k\rangle = n_k |n_k - 1\rangle. \quad (192)$$

The master equation can then be written as $\partial_t |\psi\rangle = -\mathbb{H} |\psi\rangle$, where $|\psi\rangle = \sum_{\mathbf{n}} P(\mathbf{n}) |\mathbf{n}\rangle$, and the evolution operator \mathbb{H} reads

$$\begin{aligned} \mathbb{H} = & \sum_{k=1}^{L-1} (a_{k+1}^\dagger - a_k^\dagger) \{ a_{k+1} W_{k+1 \rightarrow k} - a_k W_{k \rightarrow k+1} \} \\ & - (a_1^\dagger - 1) (W_{0 \rightarrow 1} - W_{1 \rightarrow 0} a_1) - (a_L^\dagger - 1) (W_{L+1 \rightarrow L} - W_{L \rightarrow L+1} a_L). \end{aligned} \quad (193)$$

Because of the boundary terms, this operator does not correspond to an equilibrium dynamics. We know however that its ground state can be mapped to that of an equilibrium operator (see section 9.1) and it is thus quite natural to investigate the question as to whether this mapping extends to the whole operator.

For the exclusion process, the equilibrium model was constructed at macroscopic coarse-grained level through the use of canonical transformations, which mapped the action onto that of an equilibrium, isolated system. At the level of operators, canonical transformations correspond to similarity transformations $\mathbb{H}' = Q^{-1} \mathbb{H} Q$ (see appendix D). We will now show that using such transformations, one can map \mathbb{H} to an equilibrium operator. As these

transformations do not modify the spectrum, the determination of the eigenstates reduces to the determination of the spectrum of an equilibrium operator.

We first translate the a_k^\dagger 's by 1, using the transformation obtained from $Q_0 = e^{-\sum_{k=1}^L a_k}$ (one has $Q_0^{-1} a_k^\dagger Q_0 = a_k^\dagger + 1$). Rearranging the sum, we get for $\mathbb{H}_0 = Q_0^{-1} \mathbb{H} Q_0$

$$\begin{aligned} \mathbb{H}_0 = & - \sum_{k=2}^{L-1} a_k^\dagger \{ (W_{k+1 \rightarrow k} a_{k+1} - W_{k \rightarrow k+1} a_k) - (W_{k \rightarrow k-1} a_k - W_{k-1 \rightarrow k} a_{k-1}) \} \\ & - a_1^\dagger \{ (W_{2 \rightarrow 1} a_2 - W_{1 \rightarrow 2} a_1) - (W_{1 \rightarrow 0} a_1 - W_{0 \rightarrow 1}) \} \\ & - a_L^\dagger \{ (W_{L+1 \rightarrow L} - W_{L \rightarrow L+1} a_L) - (W_{L \rightarrow L-1} a_L - W_{L-1 \rightarrow L} a_{L-1}) \}. \end{aligned} \quad (194)$$

Then, we use the similarity transformation induced by $Q_1 = \prod_{k=1}^L (P_k^{\text{eq}})^{a_k^\dagger}$, which yields

$$\begin{cases} Q_1^{-1} a_k Q_1 = P_k^{\text{eq}} a_k \\ Q_1^{-1} a_k^\dagger Q_1 = (P_k^{\text{eq}})^{-1} a_k^\dagger \end{cases} \quad (195)$$

and thus for $\mathbb{H}_1 = Q_1^{-1} \mathbb{H}_0 Q_1$,

$$\begin{aligned} \mathbb{H}_1 = & - \sum_{k=2}^{L-1} a_k^\dagger \{ W_{k \rightarrow k+1} (a_{k+1} - a_k) - W_{k \rightarrow k-1} (a_k - a_{k-1}) \} \\ & - a_1^\dagger \{ W_{1 \rightarrow 2} (a_2 - a_1) - W_{1 \rightarrow 0} (a_1 - (P_0^{\text{eq}})^{-1}) \} \\ & - a_L^\dagger \{ W_{L \rightarrow L+1} ((P_{L+1}^{\text{eq}})^{-1} - a_L) - W_{L-1 \rightarrow L} (a_L - a_{L-1}) \}. \end{aligned} \quad (196)$$

Noting that the boundary terms (second and third lines of (196)) look like the bulk term (first line), with $(P_0^{\text{eq}})^{-1}$ playing the role of an operator a_0 , and $(P_{L+1}^{\text{eq}})^{-1}$ the role of an operator a_{L+1} , we add two sites $k = 0$ and $k = L + 1$, with their corresponding creation and annihilation operators $a_0^{(\dagger)}, a_{L+1}^{(\dagger)}$. We also define two vectors $|L\rangle$ and $|R\rangle$, satisfying $a_0 |L\rangle = (P_0^{\text{eq}})^{-1} |L\rangle$, $a_{L+1} |R\rangle = (P_{L+1}^{\text{eq}})^{-1} |R\rangle$.¹³ Defining, on the extended space (of $L + 2$ sites)

$$\mathbb{H}_2 = - \sum_{k=1}^L a_k^\dagger \{ W_{k \rightarrow k+1} (a_{k+1} - a_k) - W_{k \rightarrow k-1} (a_k - a_{k-1}) \}, \quad (197)$$

we observe from (196) that

$$\mathbb{H}_2 (|L\rangle \otimes |n_1, \dots, n_L\rangle \otimes |R\rangle) = |L\rangle \otimes (\mathbb{H}_1 |n_1, \dots, n_L\rangle) \otimes |R\rangle. \quad (198)$$

In other words, the action of the extended operator \mathbb{H}_2 on states of the form $|L\rangle \otimes |n_1, \dots, n_L\rangle \otimes |R\rangle$ reduces to that of \mathbb{H}_1 on the physical state $|n_1, \dots, n_L\rangle$.

A last transformation brings \mathbb{H}_2 into an equilibrium form; it is generated by the non-local operator

$$Q_2 = \exp \sum_{0 \leq p < q \leq L+1} \frac{a_p^\dagger a_q}{q - p}, \quad (199)$$

which transforms the $(L + 2)$ creation and annihilation operators according to

$$Q_2^{-1} a_k Q_2 = \sum_{p=k}^{L+1} a_p; \quad Q_2^{-1} a_k^\dagger Q_2 = a_k^\dagger - a_{k-1}^\dagger (1 - \delta_{k,0}). \quad (200)$$

¹³ $|L\rangle$ and $|R\rangle$ correspond to bosonic coherent states $|z\rangle = \sum_{n=0}^{\infty} e^{-z} (z^n/n!) |n\rangle$ with $z = (P_0^{\text{eq}})^{-1}$ and $z = (P_{L+1}^{\text{eq}})^{-1}$, respectively.

These relations are analogous to the non-local primed variables we have introduced for exclusion processes. Moreover, the operator $\mathbb{H}_3 = Q_2^{-1} \mathbb{H}_2 Q_2$ reads

$$\mathbb{H}_3 = \sum_{k=0}^{L-1} (a_{k+1}^\dagger - a_k^\dagger) \{W'_{k+1 \rightarrow k} a_{k+1} - W'_{k \rightarrow k+1} a_k\}. \quad (201)$$

This expression corresponds to an *isolated* equilibrium process of primed rates W' , given in (182). We have thus shown that the evolution operator \mathbb{H} can be mapped to an equilibrium operator \mathbb{H}_3 acting on a larger space. We shall now explain how to use this mapping to determine the spectrum of \mathbb{H} from that of \mathbb{H}_3 .

The operator \mathbb{H}_3 acts on a space of $L + 2$ sites ($0 \leq k \leq L + 1$) but, as seen from its expression, it only describes hopping among the first $L + 1$ sites ($0 \leq k \leq L$), implying that the last site ($k = L + 1$) is completely isolated. Its eigenstates therefore take the form

$$|P^{3,\lambda}\rangle = \left(\bigotimes_{k=0}^L |P_k^{3,\lambda}\rangle \right) \otimes |f_{L+1}^\lambda\rangle, \quad (202)$$

where f_{L+1}^λ is arbitrary. To determine the eigenstates $|P^\lambda\rangle$ of \mathbb{H} , one maps back the eigenvectors of \mathbb{H}_3 with Q_2 and retains only those which satisfies

$$Q_2 |P^{3,\lambda}\rangle = |L\rangle \otimes |P^{2,\lambda}\rangle \otimes |R\rangle. \quad (203)$$

One then has

$$|P^\lambda\rangle = Q_0 Q_1 |P^{2,\lambda}\rangle. \quad (204)$$

Let us illustrate this procedure to determine the steady state of \mathbb{H} . The degenerate ground state of the equilibrium operator \mathbb{H}_3 takes the form

$$|P^{3,0}\rangle = \left(\bigotimes_{k=0}^L |\mathcal{P}_k\rangle \right) \otimes |f_{L+1}^0\rangle, \quad (205)$$

where $|\mathcal{P}_k\rangle$ is a Poisson distribution of mean density $\mu P_k^{\text{eq}'}$, with μ being an arbitrary constant,

$$|\mathcal{P}_k\rangle = \sum_{n_k} e^{-\mu P_k^{\text{eq}'}} \frac{(\mu P_k^{\text{eq}'})^{n_k}}{n_k!} |n_k\rangle. \quad (206)$$

Forcing that $|P^{3,0}\rangle$ satisfies (203) constrains both μ and $|f_{L+1}^0\rangle$,

$$\mu = \frac{(P_0^{\text{eq}})^{-1} - (P_{L+1}^{\text{eq}})^{-1}}{\sum_{p=0}^L P_k^{\text{eq}'}}; \quad |f_{L+1}^0\rangle = \sum_{n_{L+1}} e^{-(P_{L+1}^{\text{eq}})^{-1}} \frac{(P_{L+1}^{\text{eq}})^{-n_{L+1}}}{n_{L+1}!} |n_{L+1}\rangle. \quad (207)$$

One finally checks that applying further $Q_0 Q_1$ to $|P^{2,0}\rangle$ as in (204) gives back the steady state obtained in section 9.1.

We have thus shown in this section that the evolution operator of non-interacting particles diffusing on a one-dimensional lattice with arbitrary rates can be mapped onto an equilibrium operator. The determination of both steady state and excited states can be mapped to an equilibrium problem. The new microscopic feature of the transformation (200) is that the system has been supplemented with a site at each end, which accounts for the additional constant of motions of the isolated system—the total mass is conserved.

Last, from the knowledge of the mapping to equilibrium for the microscopic dynamics, one can extract its counterpart for the hydrodynamic limit. Indeed, we show in appendix D how similarity transformations for the evolution operator can be read as canonical changes of variables in the action. From the expressions of Q_0 , Q_1 and Q_2 , one can thus construct a mapping to equilibrium at the level of the action and then takes its continuum limit (see section 2.3.5).

10. Conclusions

The macroscopic fluctuation theory, as developed by BDGJL, consists of two distinct steps. The first is the recognition that the coarse-graining level, as measured by the box size, is a parameter playing the role of \hbar in a quantum system: the dynamics, including large deviations, becomes in the hydrodynamic limit a Hamiltonian dynamics. This step is general, and leaves us with a classical field theory to solve.

The second step, that has been followed in a number of systems, is to calculate explicitly the trajectories starting from the stationary situation and ending in a given configuration at long times (i.e., an excursion from equilibrium), and hence obtain the large-deviation function from the action. This can be done trivially in systems satisfying detailed balance, just by reversing the corresponding trajectory that relaxes to equilibrium. In systems driven out of equilibrium, the obvious detailed-balance symmetry is broken. For the driven SSEP and the KMP models, however, a hidden detailed-balance symmetry can be found explicitly, and used to compute the large-deviation functions. In this paper we have shown that the reason for this unexpected symmetry, and hence the solvability, is that these systems can be mapped back into their equilibrium counterparts. This realization suggested to look back at the simpler case of independent particles diffusing in a potential, with sources at the ends. We have found that the same strategy can be applied in this elementary case.

The question that arises is how general this mapping is. The first problem that comes to mind is how ‘one dimensional’ this mechanism is. One can also ask what happens with more general one-dimensional cases. A way to start investigating the first question is to consider the simple case of non-interacting particles, but in higher dimensions. On the other hand, more general one-dimensional models might perhaps admit a mapping back to equilibrium if one is prepared to pay the price of dealing with spatially non-local interactions.

Acknowledgments

We wish to thank H Fogedby and H Spohn for useful discussions. JT acknowledges funding from EPSRC grants EP/030173 and GR/T11753.

Appendix A. Coherent state path integral

The functional expression for spin operators presents a few mathematical subtleties [17]. Recently Solari [36], Kochetov [28], Vieira and Sacramento [39] derived an expression for the action and the associated time boundary conditions. We follow here the clear presentation of Stone, Park and Garg [17].

Usually, one seeks to calculate the ‘propagator’ between two normalized coherent states [28],

$$\langle z^f | e^{-T\hat{H}} | z^i \rangle. \quad (\text{A.1})$$

As usual in the construction of a path integral, the time interval $[0, T]$ is divided into N segments and one inserts at each time interval L representation of the identity (23), one for each site of the lattice. Letting N go to infinity, one ends up with the functional representation of the propagator

$$\langle z^f | e^{-T\hat{H}} | z^i \rangle = \int \mathcal{D}\bar{z} \mathcal{D}z \exp[-\tilde{S}] \quad (\text{A.2})$$

$$\tilde{S} = -j \sum_k \log \frac{(1 + \bar{z}_k^f z_k(T))(1 + \bar{z}_k(0) z_k^i)}{(1 + \bar{z}_k^f z_k^f)(1 + \bar{z}_k^i z_k^i)} + 2j \int_0^T dt \left[\frac{1}{2} \sum_k \frac{\bar{z}_k \dot{z}_k - \dot{\bar{z}}_k z_k}{1 + \bar{z}_k z_k} - \mathcal{H}(\bar{z}, z) \right]. \quad (\text{A.3})$$

Note that the temporal boundary term differs slightly from those in [17, 28] as the representation we used of the $SU(2)$ group is not the usual unitary one (cf appendix C). The role of the Hamiltonian is played by the quantity

$$\mathcal{H}(\bar{z}, z) = -\frac{1}{2j} \langle z | \hat{H} | z \rangle, \quad (\text{A.4})$$

which is computed using (28) or similar expressions for higher powers of the spin operators (see [17]). $\bar{z}_k(t)$ and $z_k(t)$ are two independent complex fields [36]. In the construction of the path integral, one notes that $z_k(0) = z_k^i$ and $\bar{z}_k(T) = \bar{z}_k^f$,¹⁴ while $z_k(T)$ and $\bar{z}_k(0)$ are unconstrained [28, 36].

Here, we rather wish to compute the physical propagator between two states $\langle \mathbf{n}^f |$ and $|\mathbf{n}^i \rangle$, corresponding to fixed initial and final number of particles in each site. The propagator represents the probability $P(\mathbf{n}^f, T; \mathbf{n}^i, 0)$ of observing the system in state (n_1^f, \dots, n_L^f) at time T , starting from (n_1^i, \dots, n_L^i) at time 0. Using $2L$ representations of identity (23), we write

$$P(\mathbf{n}^f, T; \mathbf{n}^i, 0) = \langle \mathbf{n}^f | e^{-T\hat{H}} | \mathbf{n}^i \rangle = \int \prod_k d\mu(z_k^f) d\mu(z_k^i) \langle \mathbf{n}^f | z^f \rangle \langle z^f | e^{-T\hat{H}} | z^i \rangle \langle z^i | \mathbf{n}^i \rangle. \quad (\text{A.5})$$

Keeping in mind that we are aiming to describe a hydrodynamic limit, we introduce the discrete densities

$$\rho_k = n_k / 2j. \quad (\text{A.6})$$

One sees by comparing equations (A.2) and (A.5) that the physical propagator is obtained by subtracting $\log \langle z^i | \mathbf{n}^i \rangle + \log \langle \mathbf{n}^f | z^f \rangle$ to the action (A.3), and by integrating over $z^i, \bar{z}^i, z^f, \bar{z}^f$. As we aim to describe the large j, L limit, we can use Stirling's formula to obtain the asymptotics of $\binom{2j}{n_k^i}$, to get

$$P(\rho^f, T; \rho^i, 0) = \int \prod_k d\mu(z_k^f) d\mu(z_k^i) \int \mathcal{D}\bar{z} \mathcal{D}z \exp[-S] \quad (\text{A.7})$$

$$\begin{aligned} S = & -j \sum_k \log [(1 + \bar{z}_k^f z_k(T))(1 + \bar{z}_k(0) z_k^i)] + 2j \int_0^T dt \left[\frac{1}{2} \sum_k \frac{\bar{z}_k \dot{z}_k - \dot{\bar{z}}_k z_k}{1 + \bar{z}_k z_k} - \mathcal{H}(\bar{z}, z) \right] \\ & + 2j \sum_k \left\{ -\rho_k^i \log \bar{z}_k^i - \rho_k^f \log z_k^f + \rho_k^f \log \rho_k^f + (1 - \rho_k^f) \log (1 - \rho_k^f) \right. \\ & \left. + \log [(1 + \bar{z}_k^f z_k^f)(1 + \bar{z}_k^i z_k^i)] \right\}. \end{aligned}$$

The complex fields $z_k^i, \bar{z}_k^i, z_k^f$ and \bar{z}_k^f have now to be integrated upon, which can be done by saddle point. First, differentiating the action (A.7) with respect to \bar{z}_k^i, z_k^f yields

$$\frac{1}{2j} \frac{\partial S}{\partial \bar{z}_k^i} = \frac{z_k^i}{1 + \bar{z}_k^i z_k^i} - \frac{\rho_k^i}{\bar{z}_k^i} \quad \frac{1}{2j} \frac{\partial S}{\partial z_k^f} = \frac{\bar{z}_k^f}{1 + \bar{z}_k^f z_k^f} - \frac{\rho_k^f}{z_k^f}. \quad (\text{A.8})$$

¹⁴ These fields coincide exactly, not as the result of a saddle point evaluation.

We thus obtain the initial and final conditions

$$\frac{\bar{z}_k^i z_k^i}{1 + \bar{z}_k^i z_k^i} = \rho_k^i \quad \frac{\bar{z}_k^f z_k^f}{1 + \bar{z}_k^f z_k^f} = \rho_k^f. \quad (\text{A.9})$$

Extremalizing with respect to z_k^i and \bar{z}_k^f has to be done carefully as the time integral in the action gives a nonzero contribution (see for instance equation 3.9 of [17]). Such a computation leads to

$$\frac{1}{2j} \frac{\partial S}{\partial z_k^i} = \frac{\bar{z}_k^i}{1 + \bar{z}_k^i z_k^i} - \frac{\bar{z}_k(0)}{1 + \bar{z}_k(0) z_k^i} \quad \frac{1}{2j} \frac{\partial S}{\partial \bar{z}_k^f} = \frac{z_k^f}{1 + \bar{z}_k^f z_k^f} - \frac{z_k(T)}{1 + z_k(T) \bar{z}_k^f}, \quad (\text{A.10})$$

which fixes

$$\bar{z}_k(0) = \bar{z}_k^i \quad z_k(T) = z_k^f. \quad (\text{A.11})$$

Putting everything together, the action reads

$$S[\bar{z}, z; \mathbf{n}_f, \mathbf{n}_i] = 2j \sum_k \left[\frac{z_k \bar{z}_k}{1 + z_k \bar{z}_k} \log \bar{z}_k - \log(1 + z_k \bar{z}_k) \right]_i^f + 2j \int dt \left[\sum_k \frac{\bar{z}_k \dot{z}_k}{1 + \bar{z}_k z_k} - \mathcal{H}(\bar{z}, z) \right]. \quad (\text{A.12})$$

$$\mathcal{H}_B(\bar{z}, z) = -\frac{1}{2} \sum_{k=1}^{L-1} \frac{z_k z_{k+1} (\bar{z}_{k+1} - \bar{z}_k)^2}{(1 + \bar{z}_k z_k)(1 + \bar{z}_{k+1} z_{k+1})} + \left(\frac{z_{k+1}}{1 + z_{k+1} \bar{z}_{k+1}} - \frac{z_k}{1 + z_k \bar{z}_k} \right) (\bar{z}_{k+1} - \bar{z}_k).$$

In the context of quantum mechanics, the coherent state (stereographic) parametrization in terms of $z_k(t)$ and $\bar{z}_k(t)$ is usually transformed into spherical polar coordinates through $z_k = e^{-i\phi_k} \cot \frac{\theta_k}{2}$, $\bar{z}_k = e^{i\phi_k} \cot \frac{\theta_k}{2}$. In our context however, it will prove more convenient to introduce a new parametrization¹⁵

$$z_k = \frac{\rho_k}{1 - \rho_k} e^{-\hat{\rho}_k}, \quad \bar{z}_k = e^{\hat{\rho}_k}. \quad (\text{A.13})$$

Using $\frac{\bar{z}_k z_k}{1 + \bar{z}_k z_k} = \rho_k$, we see from (A.9) and (A.11) that the temporal boundary conditions on the fields can be written as

$$\rho(0) = \rho^i, \quad \rho(T) = \rho^f, \quad \text{with } \hat{\rho}(0), \hat{\rho}(T) \text{ unconstrained.} \quad (\text{A.14})$$

This highlights the correspondence between the field ρ and the actual density of the system. The Hamiltonian (A.12) then reads

$$\mathcal{H} = \mathcal{H}_B + \mathcal{H}_0 + \mathcal{H}_L, \quad (\text{A.15})$$

$$\mathcal{H}_B = \frac{1}{2} \sum_{k=1}^{L-1} \{ (1 - \rho_k) \rho_{k+1} [e^{\hat{\rho}_k - \hat{\rho}_{k+1}} - 1] + \rho_k (1 - \rho_{k+1}) [e^{\hat{\rho}_{k+1} - \hat{\rho}_k} - 1] \} \quad (\text{A.16})$$

$$\mathcal{H}_0 = \alpha (1 - \rho_1) (e^{\hat{\rho}_1} - 1) + \gamma \rho_1 (e^{-\hat{\rho}_1} - 1) \quad (\text{A.17})$$

$$\mathcal{H}_L = \delta (1 - \rho_L) (e^{\hat{\rho}_L} - 1) + \beta \rho_L (e^{-\hat{\rho}_L} - 1), \quad (\text{A.18})$$

where \mathcal{H}_B describes the interaction in the bulk whereas \mathcal{H}_0 and \mathcal{H}_L result from the coupling to the reservoirs. Using

$$\frac{1}{2} \frac{\bar{z}_k \dot{z}_k - \dot{\bar{z}}_k z_k}{1 + \bar{z}_k z_k} = \dot{\rho}_k \hat{\rho}_k - \partial_t \left[\hat{\rho}_k \rho_k + \frac{1}{2} \log(1 - \rho_k) \right], \quad (\text{A.19})$$

¹⁵ In the changes of variable $z, \bar{z} \rightarrow \rho, \hat{\rho}$, the Jacobian $(1 - \rho)^2$ cancel exactly the prefactor of $d\mu(z)$, so that $\int d\mu(z)$ is replaced by $\int \frac{2j+1}{\pi} d\rho d\hat{\rho}$.

we check that all boundary terms cancel so that the classical action reduces to

$$S[\hat{\rho}, \rho; \rho_i, \rho_f] = 2j \int_0^T dt \left[\sum_k \hat{\rho}_k \dot{\rho}_k - \mathcal{H}(\hat{\rho}, \rho) \right]. \quad (\text{A.20})$$

Appendix B. Hydrodynamic limit

B.1. Continuous limit of the action

Let us start from the microscopic Hamiltonian (A.15) for a system of size L . In the large j limit, each site contains a large number of particles, so that the density field tends to self-average. It is thus natural to assume the gradients to be small. Expanding the Hamiltonian up to second order in $(\rho_{k+1} - \rho_k)$, $(\hat{\rho}_{k+1}, \hat{\rho}_k)$, one gets

$$\mathcal{H}_B = \sum_{k=1}^{L-1} \left[\frac{1}{2} \rho_k (1 - \rho_k) (\hat{\rho}_{k+1} - \hat{\rho}_k)^2 - \frac{1}{2} (\hat{\rho}_{k+1} - \hat{\rho}_k) (\rho_{k+1} - \rho_k) \right]. \quad (\text{B.1})$$

One can then introduce a rescaled space variable

$$x_k = \frac{k}{2j}, \quad (\text{B.2})$$

which goes from $1/2j$ to $L/2j$ and becomes continuous in the large j limit. Assuming a diffusive time scale and explicitly rescaling the gradients

$$\begin{aligned} \rho_{k+1} - \rho_k &\rightarrow \frac{1}{2j} \nabla \rho, & \hat{\rho}_{k+1} - \hat{\rho}_k &\rightarrow \frac{1}{2j} \nabla \hat{\rho}, \\ \frac{1}{2j} \sum_{k=1}^L &\rightarrow \int_0^{L/2j} dx, & dt &\rightarrow (2j)^2 dt, \end{aligned} \quad (\text{B.3})$$

transforms the action into

$$\begin{aligned} S[\rho(x), \hat{\rho}(x)] &= (2j)^2 \int dt \left\{ \int_0^{L/2j} dx \left[\hat{\rho} \dot{\rho} - \frac{1}{2} \sigma (\nabla \hat{\rho})^2 + \frac{1}{2} \nabla \rho \nabla \hat{\rho} \right] \right. \\ &\quad \left. - 2j \mathcal{H}_0[\rho, \hat{\rho}] - 2j \mathcal{H}_1[\rho, \hat{\rho}] \right\} \end{aligned} \quad (\text{B.4})$$

$$\mathcal{H}_0[\rho, \hat{\rho}] = \alpha [1 - \rho(0)] (e^{\hat{\rho}(0)} - 1) + \gamma \rho(0) (e^{-\hat{\rho}(0)} - 1)$$

$$\mathcal{H}_1[\rho, \hat{\rho}] = \delta [1 - \rho(1)] (e^{\hat{\rho}(1)} - 1) + \beta \rho(1) (e^{-\hat{\rho}(1)} - 1).$$

It is however more convenient to have a continuous variable x going from 0 to 1, so that the extensivity of the action is explicit. This can be achieved by a further scaling

$$x \rightarrow \frac{L}{2j} x, \quad t \rightarrow \left(\frac{L}{2j} \right)^2 t, \quad (\text{B.5})$$

which maps the action into

$$\begin{aligned} S[\rho(x), \hat{\rho}(x)] &= 2jL \int dt \left\{ \int_0^1 dx \left[\hat{\rho} \dot{\rho} - \frac{1}{2} \sigma (\nabla \hat{\rho})^2 + \frac{1}{2} \nabla \rho \nabla \hat{\rho} \right] \right. \\ &\quad \left. - L \mathcal{H}_0[\rho, \hat{\rho}] - L \mathcal{H}_1[\rho, \hat{\rho}] \right\}. \end{aligned} \quad (\text{B.6})$$

Some comments are in order. First, the bulk integral is proportional to $2jL$, which is consistent with the scaling of a large-deviation function. Then, the boundary terms scale as $2jL^2$ and deserve some further analysis.

B.2. Spatial boundary conditions

Let us first note that if the boundary rates $\alpha, \beta, \gamma, \delta$ are of order $1/L$, then the contributions of \mathcal{H}_0 and \mathcal{H}_L to the action are of the same order as that of the bulk term \mathcal{H}_B . This means that trajectories with fluctuations of order 1 at the boundaries give rise to non-vanishing contribution at the level of large deviation, i.e. their action scales as $2jL$. In particular, such rates would *not* lead to the spatial boundary conditions (48).

In the usual case where the rates are of order 1, we shall show below that trajectories with fluctuations at the boundaries are forbidden at the level of large deviations. This accounts for the claim in [1, 3] that trajectories which do not satisfy strictly the boundary condition correspond to infinite values of the large-deviation function.

Let us analyze in details the dynamics at the boundaries. In the large j limit, the probability is dominated by trajectories that extremalize the action (see section 4). Using expression (A.15) for the microscopic Hamiltonian, the classical equations read

$$\begin{aligned}\dot{\rho}_1 &= \frac{\partial(\mathcal{H}_1 + \mathcal{H}_B)}{\partial \hat{\rho}_1} = \frac{1 - \rho_1}{2} \rho_2 e^{\hat{\rho}_1 - \hat{\rho}_2} - \frac{\rho_1}{2} (1 - \rho_2) e^{\hat{\rho}_2 - \hat{\rho}_1} + \alpha(1 - \rho_1) e^{\hat{\rho}_1} - \gamma \rho_1 e^{-\hat{\rho}_1} \\ \dot{\hat{\rho}}_1 &= -\frac{\partial(\mathcal{H}_1 + \mathcal{H}_B)}{\partial \rho_1} = \frac{\rho_2}{2} [e^{\hat{\rho}_1 - \hat{\rho}_2} - 1] - \frac{1 - \rho_2}{2} [e^{\hat{\rho}_2 - \hat{\rho}_1} - 1] + \alpha[e^{\hat{\rho}_1} - 1] - \gamma[e^{-\hat{\rho}_1} - 1].\end{aligned}\tag{B.7}$$

In the large $2jL$ limit, one checks that $\partial_{\rho_1} \mathcal{H}_B$ and $\partial_{\hat{\rho}_1} \mathcal{H}_B$ are of order $1/L$. The rhs of equations (B.7) are thus dominated by the boundary terms so that, at first order, they read

$$\begin{aligned}\dot{\rho}_1 &= \alpha(1 - \rho_1) e^{\hat{\rho}_1} - \gamma \rho_1 e^{-\hat{\rho}_1} \\ \dot{\hat{\rho}}_1 &= \alpha[e^{\hat{\rho}_1} - 1] - \gamma[e^{-\hat{\rho}_1} - 1].\end{aligned}\tag{B.8}$$

For the sake of clarity, we now drop the index ‘1’. Equations (B.8) can be solved and give

$$\begin{aligned}\rho(t) &= [\rho_0(1 - \rho_i)(1 - e^{-\Gamma t}) + \rho_i e^{-\hat{\rho}_i}(\rho_0 + (1 - \rho_0)e^{-\Gamma t})] \\ &\quad \times [(1 - \rho_0)(1 - e^{\Gamma t}) + e^{\hat{\rho}_i}(\rho_0 + (1 - \rho_0)e^{\Gamma t})]\end{aligned}\tag{B.9}$$

$$e^{\hat{\rho}(t)} = \frac{\rho_0 e^{\hat{\rho}_i} + 1 - \rho_0 + (1 - \rho_0) e^{\Gamma t} (e^{\hat{\rho}_i} - 1)}{\rho_0 e^{\hat{\rho}_i} + 1 - \rho_0 - \rho_0 e^{\Gamma t} (e^{\hat{\rho}_i} - 1)},\tag{B.10}$$

where $\Gamma = \alpha + \gamma$, $\rho_0 = \alpha/\Gamma$ and $\rho_i, \hat{\rho}_i$ are the initial conditions of the fields. For such a trajectory, the contribution S_L of the left boundary to the action is

$$S_L = -2jt\Gamma(1 - e^{-\hat{\rho}_i})[\rho_0(1 - \rho_i) e^{\hat{\rho}_i} - \rho_i(1 - \rho_0)].\tag{B.11}$$

In the hydrodynamic limit, the time is rescaled by L^2 so that $S_L \sim 2jL^2$. We know from section 4.3 that the probability to observe a given profile is obtained from the exponential of the action. For nonzero S_L , it is thus of order $\exp(-2jL^2)$ and such profile is even more rare than large deviations, whose probability scale as $\exp(-2jL)$. Quantitatively, such profile has an infinite large-deviation function

$$\mathcal{F}[\rho] = -\lim_{2jL \rightarrow \infty} \frac{1}{2jL} \log P[\rho] = \lim_{2jL \rightarrow \infty} \frac{1}{2jL} S_{\text{traj}} = \infty.\tag{B.12}$$

In addition to an infinite large-deviation function, the trajectories (B.9) can also present a diverging density. Indeed, for large times, one gets

$$\rho(t) \sim e^{\Gamma t} \rho_0(1 - \rho_0)(1 - e^{-\hat{\rho}_i})[\rho_i + (1 - \rho_i) e^{\hat{\rho}_i}].\tag{B.13}$$

To keep the density finite, one thus needs

$$\hat{\rho}_i = 0 \quad \text{or} \quad \rho_i = \frac{1}{1 - e^{-\hat{\rho}_i}}.\tag{B.14}$$

The second solution corresponds to an action $S_L = 2jt\Gamma$ which is once again of order $2jL^2$ in the hydrodynamic limit. Such a trajectory is thus forbidden at the level of large deviations. We are left with $\hat{\rho}_i = 0$, which corresponds to $\rho(t) = \rho_0 + e^{-\Gamma t}(\rho_i - \rho_0)$. The corresponding contribution S_L vanishes exactly and in a macroscopic time of order L^{-2} the density $\rho(t)$ of the first site gets equal to $\rho_0 = \frac{\alpha}{\alpha+\gamma}$.

The same analysis holds for the right boundary and we have thus shown that for boundary rates of order 1, the fields $\rho, \hat{\rho}$ have to satisfy the following boundary conditions at the level of large deviations:

$$\hat{\rho}(0, t) = \hat{\rho}(1, t) = 0; \quad \rho(0, t) = \rho_0 = \frac{\alpha}{\alpha + \gamma}; \quad \rho(1, t) = \rho_1 = \frac{\delta}{\delta + \beta}, \quad (\text{B.15})$$

whereas for rates of order $1/L$, fluctuations are allowed at the level of large deviations.

Appendix C. Unitary and non-unitary representations

C.1. Change of basis

We wish to make the link between the representation of $SU(2)$ matrices we have used (16) and the usual ‘quantum’ representation. In terms of the action of these operators, we start from the action of the matrices (16) on the occupation kets $|n\rangle$,

$$S^+|n\rangle = (2j - n)|n + 1\rangle \quad (\text{C.1})$$

$$S^-|n\rangle = n|n - 1\rangle \quad (\text{C.2})$$

$$S^z|n\rangle = (n - j)|n\rangle \quad (\text{C.3})$$

and perform a similarity transformation to obtain the canonical unitary representation of ‘quantum’ operators, that we denote S_q^\pm, S_q^z ,

$$Q^{-1}S^+Q|n\rangle = S_q^+|n\rangle = \sqrt{(n + 1)(2j - n)}|n + 1\rangle \quad (\text{C.4})$$

$$Q^{-1}S^-Q|n\rangle = S_q^-|n\rangle = \sqrt{n(2j - n + 1)}|n - 1\rangle \quad (\text{C.5})$$

$$Q^{-1}S^zQ|n\rangle = S_q^z|n\rangle = (n - j)|n\rangle. \quad (\text{C.6})$$

The usual magnetic number m is related to the occupation number n through $m = n - j$. We first remark that only S^+ and S^- have to be changed. This suggests we find Q as a function of the number operator $\hat{n} = j + S^z$,

$$Q = q(\hat{n}). \quad (\text{C.7})$$

From (C.4)–(C.5) we have to solve

$$n \frac{q(n)}{q(n - 1)} = \sqrt{n(2j - n + 1)} \quad (\text{C.8})$$

$$(2j - n) \frac{q(n)}{q(n + 1)} = \sqrt{(n + 1)(2j - n)}, \quad (\text{C.9})$$

which is done by choosing

$$Q^{-1} = \sqrt{\binom{2j}{\hat{n}}}. \quad (\text{C.10})$$

C.2. Terms arising from the similarity transformation

We now denote the basis $|n\rangle$ of kets for occupation numbers as $|\theta\rangle$, with $j \cos \theta_k = 2n_k - 1$ on each site. We are interested in the propagator

$$P(n', t|n, 0) = \langle n' | e^{-t\hat{H}} | n \rangle, \tag{C.11}$$

where \hat{H} is expressed in terms of the non-unitary representation (16). However, the field-theoretic construction of the action corresponding to (C.11) is well suited only for ‘quantum’ spin operators acting on kets as in (C.4)–(C.6). To make the bridge between these representations, let us write

$$P(n', t|n, 0) = \langle n' | Q e^{-t\hat{H}_q} Q^{-1} | n \rangle, \tag{C.12}$$

where \hat{H}_q is now expressed in terms of ‘quantum’ spin matrices, that is to say, in terms of the matrices $S_q^{+, -z}$, which act on $|n\rangle$ according to (C.4)–(C.6). Inserting two resolution of the identity yields

$$P(n', t|n, 0) = \int d\xi_f d\bar{\xi}_f d\xi_i d\bar{\xi}_i e^{-S(\theta', \theta)}, \tag{C.13}$$

with

$$S(\theta', \theta) = -\ln \frac{\langle n' | Q | \xi_f \rangle}{\langle \xi_f | \xi_f \rangle} - \ln \frac{\langle \xi_i | Q^{-1} | n \rangle}{\langle \xi_i | \xi_i \rangle} + S(\xi_i, \bar{\xi}_f). \tag{C.14}$$

But Q is diagonal and real valued on the basis $|n\rangle$ so that

$$S(\theta', \theta) = -\ln \frac{\langle \theta' | \xi_f \rangle}{\langle \xi_f | \xi_f \rangle} - \ln \frac{\langle \xi_i | \theta \rangle}{\langle \xi_i | \xi_i \rangle} + \frac{1}{2} \ln \frac{\binom{2j}{n}}{\binom{2j}{n'}} + S(\xi_i, \bar{\xi}_f). \tag{C.15}$$

We thus conclude that using the non-unitary representation of $SU(2)$ yields a new term in the action (the ratio of binomials in (C.15)) that we took into account to obtain (A.3).

Appendix D. From microscopic detailed-balance relation to the symmetry of the action in the path integral

Let us first discuss in detail the relation between similarity transformations of the evolution operator and canonical changes of variable in the action, and then show the consequences of the existence of symmetries for the system. We then analyze the case of the detailed-balance relation. To remain in the context of this paper, we present below the case of the SSEP in the hydrodynamic limit although the results only rely on the existence of the path-integral representation and are thus much more general.

We consider the propagator between two physical states

$$G(\rho_f, \rho_i; T) = \langle \rho_f | e^{-TH} | \rho_i \rangle, \tag{D.1}$$

where H is the evolution operator. We know from section 2.3 that the path-integral representation of this propagator is given by

$$G(\rho_f, \rho_i; T) = \int \mathcal{D}[\hat{\rho}, \rho] e^{-2jLS_H}; \quad S_H = \int dt dx \{ \hat{\rho} \dot{\rho} - \mathcal{H}[\rho, \hat{\rho}] \}, \tag{D.2}$$

where $\mathcal{H}[\rho, \hat{\rho}] = -\frac{1}{2j} \langle z | H | z \rangle$ and we used the relations (32) to introduce densities. Let us introduce the operator obtained after a similarity transformation

$$\tilde{H} = Q^{-1} H Q. \tag{D.3}$$

Equation (D.1) can then be written as

$$G(\rho_f, \rho_i; T) = \langle \rho_f | Q Q^{-1} e^{-TH} Q Q^{-1} | \rho_i \rangle = \langle \rho_f | Q e^{-T\tilde{H}} Q | \rho_i \rangle. \quad (D.4)$$

The path-integral representation of (D.4) leads to

$$G(\rho_f, \rho_i; T) = \int \mathcal{D}[\hat{\rho}', \rho'] e^{-2jLS_{\tilde{H}}}; \quad (D.5)$$

$$S_{\tilde{H}} = -\frac{1}{2jL} [\log Q]_i^f + \int dt dx \{ \hat{\rho}' \dot{\rho}' - \tilde{\mathcal{H}}[\rho', \hat{\rho}'] \},$$

where $\tilde{\mathcal{H}}[\rho', \hat{\rho}'] = -\frac{1}{2j} \langle z | \tilde{H} | z \rangle$ and $Q = \langle z | Q | z \rangle$. It is now simple to check that the actions (D.2) and (D.5) are related via the canonical changes of variables induced by $\log Q$ [21],

$$\int dx \rho' \dot{\rho}' = \frac{1}{2jL} \frac{d}{dt} \log Q + \int dx \dot{\rho} \hat{\rho}. \quad (D.6)$$

If Q is a symmetry of the evolution operator, we see that the commutation relation $[H, Q] = 0$ can also be written $H = Q^{-1} H Q$. At the level of the action, it thus means that $\log Q$ induces a canonical transformation that leaves the action invariant up to boundary terms.

The case of detailed-balance relation is slightly different as it is not a symmetry of the evolution operator but rather a connection between H and its adjoint H^\dagger , as we recall. Indeed, for any configuration ρ_1, ρ_2 it reads

$$\langle \rho_1 | e^{-tH} | \rho_2 \rangle P_{\text{eq}}(\rho_2) = \langle \rho_2 | e^{-tH} | \rho_1 \rangle P_{\text{eq}}(\rho_1). \quad (D.7)$$

Taking the adjoint of the rhs, one gets

$$\langle \rho_1 | e^{-tH} P_{\text{eq}} - P_{\text{eq}} e^{-tH^\dagger} | \rho_2 \rangle. \quad (D.8)$$

As this holds for all ρ_1, ρ_2, t we see by deriving with respect to t and putting $t = 0$ that

$$H^\dagger = P_{\text{eq}}^{-1} H P_{\text{eq}}. \quad (D.9)$$

At the level of the actions, it then reads

$$\int \hat{\rho} \dot{\rho} - \mathcal{H}[\rho, \hat{\rho}] = -\frac{1}{2jL} [\log P_{\text{eq}}]_i^f + \int \hat{\rho} \dot{\rho} - \mathcal{H}^\dagger[\rho, \hat{\rho}]. \quad (D.10)$$

In the case of the SSEP with periodic boundary conditions, one further knows that

$$P_{\text{eq}}[\rho] \propto e^{-2jL \int dx \rho \log \rho + (1-\rho) \log(1-\rho)} \quad (D.11)$$

and

$$\mathcal{H}[\rho, \hat{\rho}] = \frac{1}{2} \sigma \nabla \hat{\rho}^2 - \frac{1}{2} \nabla \rho \nabla \hat{\rho}; \quad \mathcal{H}^\dagger[\rho', \hat{\rho}'] = \frac{1}{2} \sigma \nabla \hat{\rho}'^2 + \frac{1}{2} \nabla \rho' \nabla \hat{\rho}'. \quad (D.12)$$

We thus see that the action of H and H^\dagger are related through the canonical changes of variable induced by (D.6),

$$\rho' = \rho; \quad \hat{\rho}' = \hat{\rho} - \frac{\rho}{1-\rho}. \quad (D.13)$$

By further taking a time-reversal transformation

$$t \rightarrow T - t; \quad \hat{\rho}' \rightarrow -\hat{\rho}', \quad (D.14)$$

one maps back \mathcal{H}^\dagger to \mathcal{H} and thus obtain a symmetry of the action, which finally reads

$$\rho_{\text{TR}}(t) = \rho(T - t); \quad \hat{\rho}_{\text{TR}}(t) = -\hat{\rho}(T - t) + \frac{\rho(T - t)}{1 - \rho(T - t)}. \quad (D.15)$$

We get back the transformation (79), as expected.

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