

Mapping Nonequilibrium onto Equilibrium: The Macroscopic Fluctuations of Simple Transport Models

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We study a simple transport model driven out of equilibrium by reservoirs at the boundaries, corresponding to the hydrodynamic limit of the symmetric simple exclusion process. We show that a nonlocal transformation of densities and currents maps the large deviations of the model into those of an open, isolated chain satisfying detailed balance, where rare fluctuations are the time reversals of relaxations. We argue that the existence of such a mapping is the immediate reason why it is possible for this model to obtain an explicit solution for the large-deviation function of densities through elementary changes of variables. This approach can be generalized to the other models previously treated with the macroscopic fluctuation theory.

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Systems driven by reservoirs at the borders are possibly the first step in complication as one enters the nonequilibrium realm. They are already not solvable in general, but many elegant and striking results have been obtained in recent years (for a review, see [1] and references therein). Recently, Derrida, Lebowitz, and Speer [2] (DLS) obtained an exact expression for the large-deviation function of the density profile in the symmetric simple exclusion model (SSEP)—a one-dimensional transport of particles—using a matrix method that had been developed previously [3]. This is a major achievement, as large-deviation functions are a natural extension of free energy to out-of-equilibrium situations.

For the sake of generality, it is desirable to have a purely macroscopic approach, that does not rely on the strong symmetries of the microscopic model. This was done within the macroscopic fluctuation theory [4,5]. This is a version of WKB theory, valid in the limit of large coarse-graining scale N : in the usual manner of semiclassical theory and geometric optics, the logarithm of wave functions evolving with the Fokker Planck operator obey a Hamilton-Jacobi equation whose characteristics are trajectories satisfying Hamilton's equations.

For the hydrodynamic limit of the SSEP, Bertini *et al.* [4] were able to integrate explicitly the corresponding Hamilton-Jacobi equations and recovered the large-deviation function. They thus showed that such a solution is in principle logically independent of the exact microscopic solution. Their derivation amounts to a series of carefully chosen changes of variables, each of one yielding a miracle, whose cause and degree of generality one may still wish to ascertain.

In this Letter we uncover a transformation of the large deviations of densities and currents of the original driven model into those of a “dual” isolated, equilibrium chain. 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. Moreover, emergences of rare fluctuations in the dual model are the time reverse of relaxations to the average profile, but this symmetry is lost in the mapping back to the original model. This accounts in this case for the lack of Onsager-Machlup symmetry [6] between birth and death of a fluctuation, which has received considerable interest [4,7,8] over the past few years.

In what follows, we shall first rephrase the macroscopic fluctuation theory in a path integral language, then single out the specific properties which enable one to compute the large-deviation function for the system (1) and finally encapsulate them in the existence of a dual model with detailed balance.

Hydrodynamic model.—We consider the fluctuating hydrodynamic limit of the SSEP in contact with two reservoirs [9]

$$\begin{aligned} \dot{\rho} &= -\nabla J; & J &= -\frac{1}{2}\nabla\rho - \sqrt{\sigma_\rho}\eta, \\ \rho(0, t) &= \rho_0; & \rho(L, t) &= \rho_L. \end{aligned} \quad (1)$$

Here η is a white noise of variance $1/N$ and $\sigma_\rho = \rho(1 - \rho)$. The probability of a trajectory is given by [10]

$$\begin{aligned} P &\sim \int \mathcal{D}[\rho, \eta] \delta(\dot{\rho} + \nabla J) e^{-N \int dt dx (\eta^2/2)} \\ &\sim \int \mathcal{D}[\rho, \hat{\rho}, \eta] e^{-N \int dt dx \{\hat{\rho}[\rho - (1/2)\Delta\rho - \nabla(\sqrt{\sigma_\rho}\eta)] + (\eta^2/2)\}}. \end{aligned}$$

After an integration by parts (which shall be frequent and unannounced in the following), the integration over η gives

$$\int \mathcal{D}[\hat{\rho}, \rho] e^{-NS[\hat{\rho}, \rho]} = \int \mathcal{D}[\hat{\rho}, \rho] e^{-N \int dt dx \{\hat{\rho} \dot{\rho} - \mathcal{H}\}}, \quad (2)$$

where we have introduced the Hamiltonian density defined by $H = \int \mathcal{H} dx$:

$$\mathcal{H} \equiv \frac{1}{2}[\sigma_\rho(\nabla\hat{\rho})^2 + \hat{\rho}\Delta\rho]. \quad (3)$$

Large deviations: general strategy.—In the large- N limit, the probability of observing a profile $\rho^*(x)$ in the steady state scales as $P(\rho^*) \sim e^{-N\mathcal{F}[\rho^*(x)]}$. We wish to calculate the large-deviation function \mathcal{F} , which is given by the action of the “instanton.” This is the trajectory starting in a neighborhood of the stationary profile $\bar{\rho}$ that extremizes the action (2), converges to $\rho^*(x)$ at a large time T (and thus has at all times $H = 0$) and satisfies the spatial boundary conditions. The problem then reduces to solving the equations of motion:

$$\begin{aligned}\dot{\rho} &= \frac{\delta H}{\delta \hat{\rho}(x)} = \frac{1}{2} \Delta \rho - \nabla[\sigma_\rho \nabla \hat{\rho}], \\ \dot{\hat{\rho}} &= -\frac{\delta H}{\delta \rho(x)} = -\frac{1}{2} \Delta \hat{\rho} + (2\rho - 1) \frac{(\nabla \hat{\rho})^2}{2},\end{aligned}\quad (4)$$

with the space and time constraints

$$\begin{aligned}\rho(x, 0) &= \bar{\rho}(x) = \rho_0 + x \frac{\rho_L - \rho_0}{L}; & \rho(x, T) &= \rho^*(x); \\ \rho(0, t) &= \rho_0; & \rho(L, t) &= \rho_L; & \hat{\rho}(0, t) &= \hat{\rho}(L, t) = 0.\end{aligned}\quad (5)$$

The last equality simply says that no fluctuations are allowed at the contact with the reservoir [4,9]. Alternatively, one can solve the classical Eqs. (4) via the Hamilton-Jacobi formalism [11] and that amounts to the strategy followed by Bertini *et al.*

Mapping the problem into a downhill one. Detailed balance.—The fact that Eqs. (4) derive from a stochastic problem implies that there is a family of explicit “downhill” (zero noise) solutions: $\hat{\rho}(t) = C^{\text{st}}$ and $\dot{\rho} = \frac{1}{2} \Delta \rho$. For $C^{\text{st}} = 0$, the corresponding action $S[\rho, \hat{\rho}]$ is zero. Such a solution is not what we are looking for, as it relaxes into and not out of the stationary state and hence does not satisfy the boundary conditions in time (5).

A strategy to find solutions of equations like (4) is to make a change of variables that maps the original problem into another one of the same form—i.e., that formally derives from some *other* stochastic problem, but such that the downhill solutions of the new problem obey the correct boundary conditions in time and in space [12].

For a chain at equilibrium, a simple procedure can be followed to do so, taking advantage of the detail balance relation of Hamiltonian (3), which can be made explicit by writing

$$\begin{aligned}\mathcal{H} &= \frac{1}{2} \nabla \hat{\rho} \sigma_\rho \nabla \left[\hat{\rho} - \log \frac{\rho}{1 - \rho} \right] \\ &= \frac{1}{2} \nabla \hat{\rho} \sigma_\rho \nabla \left[\hat{\rho} - \frac{\delta V_\rho}{\delta \rho} \right],\end{aligned}$$

with $V_\rho = \int dx [\rho \log \rho + (1 - \rho) \log(1 - \rho)]$. At the level of the action [13], detailed balance means that this form is left invariant by a succession of two transformations

$$\hat{\rho} \rightarrow \hat{\rho} + \log \frac{\rho}{1 - \rho} = \hat{\rho} + \frac{\delta V_\rho}{\delta \rho}; \quad (\hat{\rho}, t) \rightarrow (-\hat{\rho}, T - t).\quad (6)$$

The first shift maps

$$\begin{aligned}\mathcal{H} &\rightarrow \tilde{\mathcal{H}} = \frac{1}{2} \nabla \hat{\rho} \sigma_\rho \nabla \left[\hat{\rho} + \frac{\delta V_\rho}{\delta \rho} \right], \\ S[\hat{\rho}, \rho] &\rightarrow [V_\rho]_0^T + \int dt dx \{ \hat{\rho} \dot{\rho} - \tilde{\mathcal{H}} \}.\end{aligned}\quad (7)$$

The new $\tilde{\mathcal{H}}$ has the form of a stochastic problem, and the equations of motion associated to (7) admit a downhill solution $\hat{\rho} = C^{\text{st}}$, which in the old variables reads

$$\dot{\rho} = -\frac{1}{2} \Delta \rho, \quad \hat{\rho} = \log \frac{\rho}{1 - \rho} + C^{\text{st}},\quad (8)$$

and corresponds to the optimal uphill trajectory. The second shift in (6) shows that this trajectory is the time reverse of a diffusive trajectory. For a chain driven out of equilibrium by the boundaries, this simple strategy fails: (8) is not compatible with the spatial boundary conditions (5) for $\hat{\rho}$.

Before going on, let us note a striking property, specific to the problem (1). Rearranging the Hamiltonian density

$$\begin{aligned}\mathcal{H} &= -\rho \frac{(\nabla \hat{\rho})^2}{2} \left[\rho - 1 - \frac{\Delta \hat{\rho}}{(\nabla \hat{\rho})^2} \right] \\ &= -\rho \frac{(\nabla \hat{\rho})^2}{2} \left[\rho - 1 - \frac{\delta V_\rho}{\delta \hat{\rho}} \right],\end{aligned}\quad (9)$$

where $V_\rho = \int dx [\log \nabla \hat{\rho}]$, \mathcal{H} can formally now be seen as deriving from another stochastic dynamics: $\dot{\hat{\rho}} = -\frac{1}{2} \Delta \hat{\rho} - \frac{1}{2} (\nabla \hat{\rho})^2 + \eta \nabla \hat{\rho}$ with a further detailed balance symmetry, induced by the two transformations

$$\rho \rightarrow \rho + \frac{\delta V_\rho}{\delta \hat{\rho}}; \quad (\rho, t) \rightarrow (1 - \rho, T - t).\quad (10)$$

As in the previous paragraph, two further classes of solutions can be directly read in (9): $\rho = 0$, $\dot{\hat{\rho}} = -\frac{1}{2} \Delta \hat{\rho} - \frac{1}{2} \nabla \hat{\rho}^2$ and $\rho - 1 = \frac{\delta V_\rho}{\delta \hat{\rho}}$, $\dot{\hat{\rho}} = \frac{1}{2} \Delta \hat{\rho} + \frac{1}{2} \nabla \hat{\rho}^2$, respectively. However, none of these solutions satisfies the boundary conditions. This additional symmetry is a signature of the existence of the dual model, as we shall see below. This is the first time the specific form of the model (in particular its one-dimensional nature) plays a role.

A solution for the classical problem.—Let us now paraphrase Bertini *et al.*, following a concise but unrigorous Hamiltonian—rather than Hamilton-Jacobi—approach. To make contact with the exact solution, we rewrite the intermediate variable $\hat{\rho}$ appearing in Eq. (7) in terms of the DLS variable F defined by $F = (1 + e^{\hat{\rho}})^{-1}$. To keep the action in a Hamiltonian form, we also introduce the canonically conjugate variable $\hat{F} = \frac{\rho}{F(1-F)}$. This maps the action into

$$S = \int dx \left[\rho \log \rho + (1 - \rho) \log(1 - \rho) + \rho \log \frac{1 - F}{F} \right]_0^T \\ + \int dx dt \left\{ \hat{F} \dot{F} + \frac{1}{2} \hat{F} (\nabla F)^2 \left[\hat{F} - \frac{2}{1 - F} \right] \right. \\ \left. + \frac{1}{2} \nabla \hat{F} \nabla F \right\}.$$

This expression can be further simplified by making the shift $\hat{F} \rightarrow \hat{F} + \frac{1}{1-F}$ to get

$$S = \int dx \left[\rho \log \frac{\rho}{F} + (1 - \rho) \log \frac{1 - \rho}{1 - F} \right]_0^T \\ + \int dx dt \left\{ \hat{F} \dot{F} + \frac{1}{2} \hat{F}^2 (\nabla F)^2 + \frac{1}{2} \nabla \hat{F} \nabla F \right\}. \quad (11)$$

The overall mapping from the initial $(\rho, \hat{\rho})$ to (F, \hat{F}) reads

$$F = \frac{\rho}{\rho + (1 - \rho)e^{\hat{\rho}}}; \quad (12) \\ \hat{F} = (1 - \rho)(e^{\hat{\rho}} - 1) - \rho(e^{-\hat{\rho}} - 1).$$

The boundary conditions (5) are now given by $F(0, t) = \rho_0$, $F(L, t) = \rho_L$ and $\hat{F}(0, t) = \hat{F}(L, t) = 0$ and the equation of motions are

$$\dot{F} = \frac{1}{2} \Delta F - \hat{F} (\nabla F)^2; \quad \dot{\hat{F}} = -\frac{1}{2} \Delta \hat{F} - \nabla [\hat{F}^2 \nabla F]. \quad (13)$$

Modulo an integration by part, the last integral in (11) is of the form $\int dx dt \{ \hat{F} \dot{F} - \mathcal{H}_F \}$, where

$$\mathcal{H} = -\hat{F} \frac{(\nabla F)^2}{2} \left[\hat{F} - \frac{\Delta F}{(\nabla F)^2} \right] \\ = -\hat{F} \frac{(\nabla F)^2}{2} \left[\hat{F} - \frac{\delta V_F}{\delta F(x)} \right].$$

This is very similar to (9), but with $V_F \equiv \int dx \ln(\nabla F)$. Quite surprisingly, we have once again obtained an action formally deriving from a stochastic dynamics, satisfying the detailed balance symmetry induced by

$$\hat{F} \rightarrow \hat{F} + \frac{\Delta F}{(\nabla F)^2}, \quad (\hat{F}, t) \rightarrow (-\hat{F}, T - t). \quad (14)$$

As in all the previous examples, two classes of solutions are immediately available. First, $\hat{F} = 0$, $\dot{F} = \frac{1}{2} \Delta F$ corresponds to a downhill diffusive solution, equivalent to $\dot{\rho} = \frac{1}{2} \Delta \rho$ and which is not what we are looking for. Instead, an uphill trajectory is provided by requiring $\hat{F} = \frac{\delta V_F}{\delta F(x)}$. Together with the equation of motion (13), it implies

$$\dot{F} = -\frac{1}{2} \Delta F; \quad \rho = F + F(1 - F) \frac{\Delta F}{(\nabla F)^2}. \quad (15)$$

Amazingly, this time, its solution satisfies both spatial and temporal boundary conditions, as is easy to check. The corresponding action is the large-deviation function

$$\mathcal{F} = \int dx \left[\rho \log \frac{\rho}{F} + (1 - \rho) \log \frac{1 - \rho}{1 - F} + \log \nabla F \right]_0^T. \quad (16)$$

Dual model.—The above derivation consists of changes of variables that read like a sequence of miracles, at the end of which we are able to find an ‘‘uphill’’ solution that satisfies the boundary conditions. In the following we show that all the surprises can be thought of as deriving from only one: the action for a chain in contact with two reservoirs can be mapped, at the level of large deviations, to that of an open, isolated chain. Starting from the action (11), we introduce the nonlocal variables

$$\hat{F}' = \nabla F; \quad \hat{F} = \nabla \left[F' - \frac{1}{\hat{F}'} \right] = \nabla F' + \frac{\nabla \hat{F}'}{\hat{F}'^2}, \quad (17)$$

which takes the action into

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

Remarkably, the form of this action is, up to boundary terms, the same as (11). This suggests that we complete the mapping

$$(\rho, \hat{\rho}) \rightarrow (F, \hat{F}) \xrightarrow{\text{non-local}} (F', \hat{F}') \rightarrow (\rho', \hat{\rho}'), \quad (18)$$

where the relation between $(\rho', \hat{\rho}')$ and (F', \hat{F}') is of the same form as (12). One then obtains

$$S = \int dx \left[\rho \log \frac{\rho}{F} + (1 - \rho) \log \frac{1 - \rho}{1 - F} + \log \nabla F \right. \\ \left. - \frac{\rho' - F'}{1 - F'} - \rho' \log \frac{\rho'}{F'} - (1 - \rho') \log \frac{1 - \rho'}{1 - F'} \right]_0^T + S', \quad (19)$$

where $S' = \int dt dx \{ \hat{\rho}' \dot{\rho}' - \mathcal{H}' \}$ and \mathcal{H}' is formally equivalent to (3) but for the primed variables:

$$S' = \int dt dx \left\{ \hat{\rho}' \dot{\rho}' - \frac{1}{2} \sigma_{\rho'} (\nabla \hat{\rho}')^2 + \frac{1}{2} \nabla \rho' \nabla \hat{\rho}' \right\}. \quad (20)$$

The overall change of variable (18), which reads

$$\nabla \left[\frac{1}{1 - e^{\hat{\rho}'}} \right] = e^{\hat{\rho}} - 1 - \rho(e^{\hat{\rho}} + e^{-\hat{\rho}} - 2), \\ \nabla \left[\frac{\rho}{\rho + (1 - \rho)e^{\hat{\rho}}} \right] = e^{\hat{\rho}'} - 1 - \rho'(e^{\hat{\rho}'} + e^{-\hat{\rho}'} - 2), \quad (21)$$

thus maps the action of the hydrodynamics limit of the SSEP into another SSEP. We shall next show that the boundary conditions transform in such a way that the dual chain is isolated. Before going on, it is instructive to introduce the classical spins S'

$$S'_z = 2\rho' - 1, \quad S'_+ = 2(1 - \rho')e^{\hat{\rho}'}, \quad S'_- = 2\rho'e^{-\hat{\rho}'}. \quad (22)$$

This is the usual connection between spin chains and particle models [14,15] in the hydrodynamic limit. The Hamiltonian density reads $\mathcal{H}' = -\frac{1}{8} \nabla S' \cdot \nabla S'$ [16]. It is invariant by simultaneous rotation of all the spins, which means that to the three ‘‘charges’’:

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

correspond three currents

$$J_{\rho'} = -\frac{1}{2}\nabla\rho' + \sigma_{\rho'}\nabla\hat{\rho}'; \quad J_{\hat{F}'} = \frac{1}{2}\nabla\hat{F}' + \hat{F}'^2\nabla F', \quad (23)$$

$$J_{\hat{F}'(1-2F')} = (1-2F')\frac{\nabla\hat{F}'}{2} + [\hat{F}' + \hat{F}'^2(1-2F')]\nabla F'$$

that are conserved in the bulk. The boundary conditions read for the primed variables

$$\nabla\left[F' - \frac{1}{\hat{F}'}\right]_{x=0,L} = 0; \quad \int_0^L \hat{F}' = \rho_l - \rho_0. \quad (24)$$

Note that all trajectories satisfying both the equations of motion (13) and the boundary conditions satisfy also $\Delta F = \nabla\hat{F}' = 0$ on the boundaries. Together with the left-hand side of (24) and the definitions (12), this implies that $\nabla F'$, $\nabla\hat{F}'$, $\nabla\rho'$ and $\nabla\hat{\rho}'$ vanish separately at the boundaries, as do, consequently, all the currents (23): the dual model in the primed variables is an isolated chain. This condition alone, supplemented with the right-hand side (rhs) of (24), encompasses all the original boundary conditions.

Let us now turn to the trajectories. The stationary profile $\bar{\rho}$ maps to a flat profile $\bar{\rho}'$, but whereas \hat{F}' is constrained by the rhs of (24), the precise value of $\bar{\rho}'$ is arbitrary.

Relaxations.—The diffusive trajectories of the initial model correspond to $\dot{\rho} = \frac{1}{2}\Delta\rho$, $\hat{\rho} = 0$, and thus $\hat{F} = 0$, as can be read in (12). Together with (21), this implies $\nabla\hat{\rho}' = 0$. As the primed variables also satisfy the equations of motion (4), the resulting trajectories evolve with $\dot{\rho}' = \frac{1}{2}\Delta\rho'$. Relaxations thus map into relaxations.

Excursions.—The instanton Eqs. (15) imply $\nabla F' = 0$ [cf. (17)]. Using the relation (12) for the primed variable, this yields $\nabla\hat{\rho}' - \frac{\nabla\rho'}{\sigma_{\rho'}} = 0$. Together with the equations of motion (4), this shows that the densities evolve with $\dot{\rho}' = -\frac{1}{2}\Delta\rho'$: excursions are the time reverse of relaxations in the primed variables. The action $S'[\hat{\rho}', \rho']$ of such an uphill trajectory is $\int_0^L dx[\rho' \log\rho' + (1 - \rho') \log(1 - \rho')]$. As F' is constant along the instanton and $\int_0^L \rho'$ is a constant of motion, the overall action (19) reduces to the large-deviation function (16) as it should.

Let us now show how the existence of the primed model accounts for the many nonlocal symmetries of the initial one. The action of the dual, isolated, chain is invariant under a composition of any simultaneous rotation and reflection of all the spins, followed by time-reversal. Written in the original variables, this corresponds to a group of spatially nonlocal symmetries of the out-of-equilibrium chain. Transformations of the primed model which do not conserve $\int_0^L \hat{F}' = \frac{\rho_l - \rho_0}{L}$ correspond to symmetries of the initial model broken by the boundary conditions. This was for instance the case of (10). If we further impose the conservation of $\int_0^L \hat{F}'$, we are left with a trans-

formation that in spin representation amounts to $(S'_x, S'_y, S'_z, t) \rightarrow (-S'_x, S'_y, S'_z, T - t)$. This is in the primed variables the nonlocal mapping (14) between downhill diffusive solutions and the instantons of the initial problem.

Conclusion.—In this Letter we have shown that the remarkable properties of the hydrodynamic model allowing for its direct, explicit solution are attributable to the existence of a dual, equilibrium model. Whereas the derivation we have presented is very specific of the model we studied, it can easily be extended to the other cases recently solved within the macroscopic fluctuation theory, including the Kipnis-Marchioro-Presutti model [5]. A further extension to a larger class of nonequilibrium systems or to microscopic models is still an open and challenging question. The symmetry between excursions and relaxations in the dual model is broken by the mixing of variables due to the nonlocal mapping (17). It would thus be very interesting to see if one can construct nonlocal quantities (like the currents of the dual model) which would be symmetric, and measure them experimentally.

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