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LETTER

The distribution function of entropy flow in stochastic systems

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Abstract. We obtain a simple direct derivation of the differential equation governing the entropy flow probability distribution function of a stochastic system first obtained by Lebowitz and Spohn. Its solution agrees well with the experimental results of Tietz *et al* (2006 *Phys. Rev. Lett.* **97** 050602). A trajectory-sampling algorithm allowing us to evaluate the entropy flow distribution function is introduced and discussed. This algorithm turns out to be effective at finite times and in the case of time-dependent transition rates, and is successfully applied to an asymmetric simple exclusion process.

Keywords: dynamical processes (theory), fluctuations (theory)

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The concept of entropy is usually associated with probability distributions (ensembles) via Gibbs' formula. However, it has been recently emphasized that in non-equilibrium systems one can consistently define the entropy production along a single trajectory [1]–[3], and that the fluctuation theorems [1], [3]–[12] can be interpreted as giving connections between the probability of entropy-generating trajectories with respect to that of entropy-annihilating trajectories. Since the entropy flow along a given trajectory is experimentally accessible (see, e.g., [13]), it is of some interest to investigate the distribution function of the entropy production and flow in a non-equilibrium system. The distribution of entropy flow in a stochastic system satisfies a differential equation derived by Lebowitz and Spohn in [8]. They made use of this equation to investigate the large deviation function of entropy production in the long time limit, thus obtaining a form of the Gallavotti–Cohen symmetry [5]. In the present paper, we provide a new direct derivation of this differential equation in a general non-equilibrium system with discrete states, and show that its solution satisfies more general fluctuation relations also at finite times. This derivation highlights its connection with the entropy production along a single trajectory. We exploit it to evaluate the entropy flow in experiments on an optically driven defect centre in diamond [13]. We suggest a practical computational scheme for evaluating the distribution of entropy flow. We illustrate the feasibility of the method by applying it to the simple asymmetric exclusion process (ASEP) [14].

We consider a system with a discrete phase space, whose states are denoted by $i = 1, \dots, N$. We assume that the evolution of the system is described by a Markovian stochastic dynamics

$$\frac{dp_i(t)}{dt} = \sum_{j (\neq i)} [W_{ij}(t)p_j(t) - W_{ji}(t)p_i(t)], \quad (1)$$

where $p_i(t)$ is the probability that the system is found in state i at time t , and $W_{ij}(t)$ is the rate of transition from the state j to the state i at time t . We consider a generic path ω defined by $\omega(t) = i_k$ iff $t_k \leq t < t_{k+1}$, with $k = 0, 1, \dots, M$, with $t_{M+1} = t_f$, and define the time-reversed path $\tilde{\omega}$ by $\tilde{\omega}(t) = i_k$ iff $t \in [\tilde{t}_{k+1}, \tilde{t}_k)$, where $\tilde{t} = t_0 + t_f - t$. Let $Q(\omega)$ be defined in terms of the ratio between the probability $\mathcal{P}(\omega)$ of the forward path ω (conditioned by its initial state i_0) and the probability $\tilde{\mathcal{P}}(\tilde{\omega})$ of the time-reversed path $\tilde{\omega}$, conditioned by its initial state $i_M \equiv i_f$ and subject to the time-reversed protocol $\tilde{W}_{ij}(t) = W_{ij}(\tilde{t})$ [1, 3, 8]:

$$Q(\omega) = -\ln \left[\frac{\mathcal{P}(\omega)}{\tilde{\mathcal{P}}(\tilde{\omega})} \right] = -\sum_{k=1}^M \ln \left[\frac{W_{i_k i_{k-1}}(t_k)}{W_{i_{k-1} i_k}(t_k)} \right]. \quad (2)$$

We have assumed that, if $W_{ij}(t) > 0$ at any time t , one also has $W_{ji}(t) > 0$. In order to interpret this quantity, let us consider the Gibbs entropy of the system $S(t) = -\sum_i p_i(t) \ln p_i(t)$ (we take the Boltzmann constant $k_B = 1$ throughout). Using (1), the time derivative of S_S reads

$$\frac{dS}{dt} = -\sum_{i \neq j} W_{ij} p_j \ln \left(\frac{W_{ji} p_i}{W_{ij} p_j} \right) - \sum_{i \neq j} W_{ij} p_j \ln \frac{W_{ij}}{W_{ji}}. \quad (3)$$

By exploiting the relation $\ln x \leq x - 1$, one sees that the first sum is non-negative, and can thus be interpreted as the entropy production rate [8, 10]. The second sum defines the

entropy S_f which flows into the reservoir: $dS_f/dt = \sum_{i \neq j} W_{ij} p_j \ln(W_{ij}/W_{ji})$. It is easy to verify that, if we define $\langle Q \rangle_t$ as the average of the quantity $Q(\omega)$, defined by (2), over all possible paths up to time t , the following equality holds: $d\langle Q \rangle_t/dt = dS_f/dt$, and thus $\langle Q \rangle_{t_f} = \Delta S_f = \int_{t_0}^{t_f} dt dS_f/dt$. Notice that if the detailed balance conditions hold for the transition rates $W_{ij}(t)$, and the energy $E_i(t)$ is associated with the state i of the system, we have $W_{ji}(t)/W_{ij}(t) = \exp\{[E_i(t) - E_j(t)]/T\}$, and thus $T \ln[W_{ji}(t)/W_{ij}(t)]$ represents the heat exchanged with the reservoir in the jump from state j to state i . Thus the quantity $Q(\omega)$, defined by (2), is the entropy which flows into the reservoir as the system evolves along the path ω (see, e.g., [3]). We now introduce the joint probability distribution $\phi_i(Q, t)$, for the system being found at time t in state i , having exchanged a total entropy flow Q with the thermal bath. The entropy which flows into the reservoir as a result of the jump of the system from state j to state i is given by $\Delta s_{ij} = \log[W_{ji}(t)/W_{ij}(t)]$. In a small time interval τ the variation of $\phi_i(Q, t)$ is given by

$$\begin{aligned} \phi_i(Q, t + \tau) &\simeq \phi_i(Q, t) + \tau \sum_{j (\neq i)} W_{ij} \phi_j(Q - \Delta s_{ij}, t) - W_{ji} \phi_i(Q, t) \\ &= \phi_i(Q, t) + \tau \sum_{j (\neq i)} \left\{ W_{ij} \left[\sum_{n=0}^{\infty} \frac{(-\Delta s_{ij})^n}{n!} \frac{\partial^n \phi_j(Q, t)}{\partial Q^n} \right] - W_{ji} \phi_i(Q, t) \right\}, \end{aligned} \quad (4)$$

and thus we obtain the differential equation governing the time evolution of the distribution function $\phi_i(Q, t)$:

$$\frac{\partial \phi_i(Q, t)}{\partial t} = \sum_{j (\neq i)} \left\{ W_{ij} \left[\sum_{n=0}^{\infty} \frac{(-\Delta s_{ij})^n}{n!} \frac{\partial^n \phi_j(Q, t)}{\partial Q^n} \right] - W_{ji} \phi_i(Q, t) \right\}. \quad (5)$$

By introducing, for each i , the generating function

$$\psi_i(\lambda, t) = \int dQ e^{\lambda Q} \phi_i(Q, t), \quad (6)$$

and taking into account the expression for Δs_{ij} , we obtain the master equation

$$\begin{aligned} \frac{\partial \psi_i(\lambda, t)}{\partial t} &= \sum_{j (\neq i)} \left[W_{ij} \left(\frac{W_{ji}}{W_{ij}} \right)^{\lambda} \psi_j(\lambda, t) - W_{ji} \psi_i(\lambda, t) \right] \\ &= \sum_j H_{ij}(\lambda) \psi_j(\lambda, t). \end{aligned} \quad (7)$$

This last equation was first derived by Lebowitz and Spohn in [8].

We now introduce the total probability distribution $\phi(Q, t) = \sum_i \phi_i(Q, t)$, and the total generating function $\psi(\lambda, t) = \sum_i \psi_i(\lambda, t)$. In the case of time-independent transition rates W_{ij} , or of transition rates which depend periodically on the time, it can be useful, in order to evaluate the distribution function $\phi(Q, t)$, to introduce the large deviation function. In the long time limit, the generating function $\psi(\lambda, t)$ is dominated by the maximum eigenvalue $g(\lambda)$ of the matrix $H(\lambda) = (H_{ij}(\lambda))$, which appears in the master equation (7). Therefore, we have, for long times t ,

$$\psi(\lambda, t) \propto \exp[t g(\lambda)]. \quad (8)$$

By using the last equation and inverting (6), one obtains the probability distribution of the entropy flow in the long time limit as

$$\phi(Q, t) = \int \frac{d\lambda}{2\pi i} e^{-\lambda Q} \psi(\lambda, t) \propto e^{t g(\lambda^*) - \lambda^* Q}, \quad (9)$$

where λ^* is the saddle point value implicitly defined by $\partial g / \partial \lambda|_{\lambda^*} = Q/t$. If we introduce the entropy flow per unit time $q = Q/t$, we obtain the large deviation function

$$f(q) \equiv g(\lambda^*) - \lambda^* q = \lim_{t \rightarrow \infty} \frac{1}{t} \log \phi(Q, t). \quad (10)$$

Note that the functions $g(\lambda)$ and $f(q)$ are Legendre transforms of each other, and can be thus interpreted in terms of path thermodynamics: $g(\lambda)$ can be viewed as a path Gibbs free energy, while $f(q)$ is the corresponding Helmholtz free energy. This analogy was first pointed out in [15, 16] where work probability distributions of systems driven out of equilibrium were studied. The Gallavotti–Cohen theorem [5] $\phi(Q)/\phi(-Q) = \exp(Q)$ is immediately recovered by considering that $H(-\lambda + 1) = H^T(\lambda)$, where H^T is the transpose of H , and thus has the same eigenvalues as H [8].

Another remarkable fluctuation relation has been recently proposed by Seifert [3]. Since the path probability densities $\mathcal{P}(\omega)$ and $\tilde{\mathcal{P}}(\tilde{\omega})$ must be normalized, one obtains from (2), for any distribution of initial states p_i^0 and any distribution of final states p_i^f , the following fluctuation relation:

$$\begin{aligned} \left\langle \exp \left[Q(\omega) + \ln \left(\frac{p_{i_f}^f}{p_{i_0}^0} \right) \right] \right\rangle &\equiv \sum_{i_0, i_f} \int_{\omega(t_0)=i_0}^{\omega(t_f)=i_f} \mathcal{D}\omega \, p_{i_0}^0 \mathcal{P}(\omega) e^{Q(\omega)} \frac{p_{i_f}^f}{p_{i_0}^0} \\ &= \sum_{i_0, i_f} \int_{\tilde{\omega}(t_0)=i_f}^{\tilde{\omega}(t_f)=i_0} \mathcal{D}\tilde{\omega} \, p_{i_f}^f \tilde{\mathcal{P}}(\tilde{\omega}) = 1. \end{aligned} \quad (11)$$

Starting from (7), this relation is recovered as follows. Let $\psi_j^{i_0}(\lambda, t)$ be the solution of (7) with the initial condition $\psi_j^{i_0}(\lambda, t=0) = \delta_{j, i_0}$, and let $\bar{\psi}_j(\lambda, t) = \sum_{i_0} \psi_j^{i_0}(\lambda, t)$. The function $\bar{\psi}_j(\lambda=1, t) = 1, \forall t$, is the solution of (7) with the initial condition $\bar{\psi}_j(\lambda=1, t=0) = 1$. Thus, (11) reads

$$\begin{aligned} \left\langle \exp [Q + \ln (p_{i_f}^f / p_{i_0}^0)] \right\rangle &= \sum_{i_0, j} p_{i_0}^0 \psi_j^{i_0}(\lambda=1, t) \exp [\ln (p_j(t) / p_{i_0}^0)] \\ &= \sum_j p_j(t) \bar{\psi}_j(\lambda=1, t) = 1, \end{aligned} \quad (12)$$

for any value of t . This result is a generalization of equation (2.20) of [8] and has been recently applied to a specific case in [17].

If the system is characterized by a small number of states, one can explicitly solve the equations (7), and thus obtain the total generating function $\psi(\lambda, t) = \sum_i \psi_i(\lambda, t) = \langle e^{\lambda Q} \rangle$.

As an example, we consider an optically driven defect centre in diamond, which can be viewed as a two-state system [13]. If excited by a red light laser, the defect exhibits fluorescence. By superimposing a green light laser, the rate of transition from the non-fluorescent to the fluorescent state (W_+ in the following) and that from the fluorescent to the non-fluorescent state (W_-) turn out to depend linearly on the green

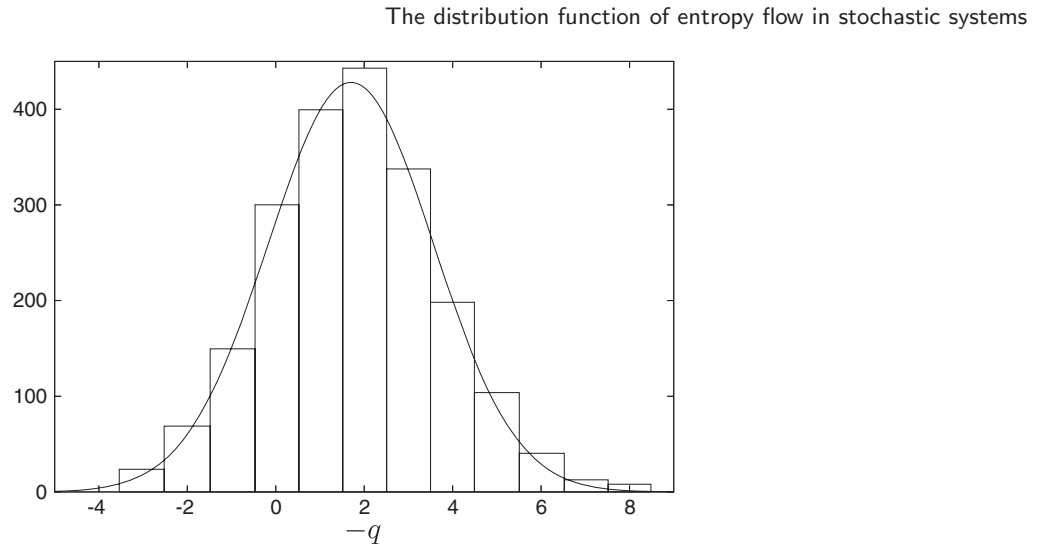


Figure 1. Entropy production of a two-state system: a defect centre in diamond is optically driven from a fluorescent to a non-fluorescent state. The experimental histogram is taken from [13]; the full line corresponds to the entropy flow distribution function $\phi(Q, t = 20 t_m)$ as obtained from (5) to (9). Note that the definition of q in [13] is the negative of ours.

and red light intensity, respectively. In [13], the experimental set-up was such that the rate $W_- = (21.8 \text{ ms})^{-1}$ was kept constant, and the rate W_+ was modulated according to the sinusoidal function $W_+(t) = W_0[1 + \gamma \sin(2\pi t/t_m)]$, with $W_0 = (15.6 \text{ ms})^{-1}$, $\gamma = 0.46$, $t_m = 50 \text{ ms}$. In the same reference, the histogram of the entropy flux, as defined by (2), was measured, over 2000 trajectories of time length $20 t_m$. By solving (7) for this system, we obtain the generating function $\psi(\lambda, t)$, and using (9) we obtain the probability distribution of the entropy flow $\phi(Q, t = 20 t_m)$, which is found to agree very well with the measured histogram; see figure 1.

However this direct approach becomes rapidly impracticable, as the system phase space size increases. On the other hand, the evaluation of $\phi(Q, t)$ or $\psi(\lambda, t)$ by direct simulation of the stochastic process described by the master equation (1) is a very difficult task. Similarly to what happens when one tries to evaluate free energies differences by using the Jarzynski equality [6], dealing with the probability distribution of the work of a driven system (see, e.g., [15, 16]), the most relevant contributions to the average $\langle \exp(\lambda Q) \rangle$ often come from the tails of the distribution of $\phi(Q, t)$.

In [18], the authors proposed a procedure for evaluating the large deviation function $g(\lambda)$, based on biased dynamics and on the parallel evolution of system clones. Here we discuss how (7) leads to an alternative scheme for the evaluation of the fluctuations in the entropy flow. Differently from what discussed in [18], such a scheme allows one to evaluate correctly the function $\psi(\lambda, t) = \langle \exp(\lambda Q) \rangle$ at any time, and not only in the long time limit, and turns out to be effective also in the case of time-dependent transition rates. In the following we adapt to our problem the concept of weighted trajectory ensemble, introduced by Sun in [19] and extended by Oberhofer *et al* in [20], where it was successfully applied to the Jarzynski equality. The idea is to sample trajectories in the weighted ensemble $\mathcal{P}(\omega_t) \exp[\lambda Q(\omega_t)]$ rather than successions of single states in the unbiased ensemble. Since

$\psi(\lambda, t) = \int \mathcal{D}\omega_t \mathcal{P}(\omega_t) e^{\lambda Q(\omega_t)}$, we have

$$\frac{\partial \psi(\lambda, t)}{\partial \lambda} = \langle Q \rangle_\lambda \psi(\lambda, t), \quad (13)$$

where $\langle \dots \rangle_\lambda$ is the average in the weighted ensemble $\mathcal{P}(\omega_t) \exp[\lambda Q(\omega_t)] / \psi(\lambda, t)$, where $\psi(\lambda, t) = Z_\lambda$ is the ‘partition function’ of this ensemble, which will be called the ‘ λ -ensemble’ in the following. The solution of (13) thus reads

$$\psi(\lambda, t) = \exp \left[\int_0^\lambda d\lambda' \langle Q \rangle_{\lambda'} \right]. \quad (14)$$

While Sun [19] proposes a Monte Carlo procedure for the sampling of trajectories, so as to obtain the average $\langle Q \rangle_\lambda$ in the weighted ensemble, in the present paper we propose a different procedure which generates trajectories in a suitable entropy flow weighted ensemble. The direct simulation of trajectories in the λ -ensemble is hindered by the fact that one should already know the exact expression of the ensemble partition function, i.e., the function $\psi(\lambda, t)$, which is the unknown quantity at issue.

To avoid the problem of the direct evaluation of $\psi(\lambda, t)$, following [20], we introduce a generic functional of the paths $\Pi(\omega)$, and write

$$\langle Q \rangle_\lambda = \frac{\int \mathcal{D}\omega_t (Q(\omega_t) / \Pi(\omega_t)) \Pi(\omega_t) \mathcal{P}(\omega_t) e^{\lambda Q(\omega_t)}}{\int \mathcal{D}\omega_t (1 / \Pi(\omega_t)) \Pi(\omega_t) \mathcal{P}(\omega_t) e^{\lambda Q(\omega_t)}} = \frac{\langle Q / \Pi \rangle_{\lambda, \Pi}}{\langle 1 / \Pi \rangle_{\lambda, \Pi}}, \quad (15)$$

where $\langle \dots \rangle_{\lambda, \Pi}$ indicates the average in the new $\mathcal{P}(\omega_t) \Pi(\omega_t) \exp[\lambda Q(\omega_t)]$ -ensemble (the (λ, Π) -ensemble in the following).

In order to simplify the following discussion we consider a stochastic dynamics with a discrete small timescale τ , such that the jumps between states take place at discrete times $t_k = k\tau$. Within this discrete scheme, we want to write the probability of a path in the (λ, Π) -ensemble.

The probability of a given path ω reads

$$\mathcal{P}(\omega) = K_{i_N, i_{N-1}} K_{i_{N-1}, i_{N-2}} \cdots K_{i_1, i_0} p_{i_0}^0, \quad (16)$$

where the transition probabilities K_{ij} are defined as $K_{ij} = \tau W_{ij}$, and $K_{ii} = 1 - \sum_{j(\neq i)} K_{ji}$. We now define the new transition probabilities $\tilde{K}_{ij} = \tau W_{ij} (W_{ji} / W_{ij})^\lambda$, and $\tilde{K}_{ii} = 1 - \sum_{j(\neq i)} \tilde{K}_{ji}$, and choose the functional $\Pi(\omega)$, such that

$$\Pi(\omega) = \prod_{k=1}^M \Pi_{i_k, i_{k-1}}(t_k), \quad (17)$$

with

$$\Pi_{ij}(t) = \begin{cases} 1, & \text{if } i \neq j; \\ \tilde{K}_{jj}(t) / K_{jj}(t), & \text{if } i = j. \end{cases} \quad (18)$$

Recalling the definition of $Q(\omega)$, (2), we obtain that the probability in the (λ, Π) -ensemble is given by

$$\mathcal{P}(\omega) \Pi(\omega) \exp[\lambda Q(\omega)] = \tilde{K}_{i_N, i_{N-1}} \tilde{K}_{i_{N-1}, i_{N-2}} \cdots \tilde{K}_{i_1, i_0} p_{i_0}^0, \quad (19)$$

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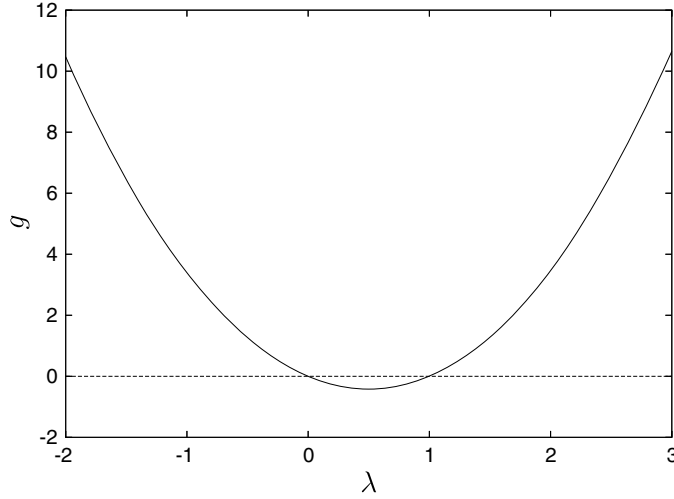


Figure 2. Plot of $g(\lambda)$ as obtained by combining (8) and (14), for the ASEP model. The function $g(\lambda)$ vanishes for $\lambda = 0, 1$ which corresponds to the normalization condition and to Seifert's fluctuation relation (11), respectively.

and thus $\langle Q \rangle_\lambda$ can be evaluated by using (15), for the particular choice of Π , as given by (18). Note that (19) implies that the one can generate a trajectory in the (λ, Π) -ensemble by simply simulating the process with the $\tilde{K}_{ij}(t)$ transition probabilities. Furthermore, the algorithm here described can be used to evaluate the generating function (14) also in the case of time-dependent transition rates. This issue will be addressed in a forthcoming paper.

In order to give an example of the application of the approach described above, we now consider a non-equilibrium system characterized by a large phase space, and evolving according to a stochastic dynamics. Instead of considering systems driven out of equilibrium by manipulation as in [16, 21], we study here a steady-state non-equilibrium system, namely the asymmetric simple exclusion process (ASEP) [14, 22]: it consists in a one-dimensional lattice gas on a lattice of L sites. Each site of the model is either empty or occupied by at most one particle. Each particle can jump into an empty nearest neighbour site with transition rates per time unit W_+ (rightward) and W_- (leftward). The system is kept in an out-of-equilibrium steady state since its first and last site are in contact with two particle reservoirs, at densities ρ_A and ρ_B respectively. By taking $\rho_A > \rho_B$ and $W_+ > W_-$, one observes a net particle current from the left to the right reservoir. We choose the following values of the parameters: $L = 100$, $W_+ = 1$, $W_- = 0.75$, $\rho_A = 0.75$, $\rho_B = 0.25$, which correspond to the maximum current phase [14].

A direct evaluation of the function $g(\lambda)$ by solving the 2^{100} equations (7) is of course impossible. We thus apply our trajectory simulation approach to the ASEP model. We consider trajectories of time length $t_f = 5$, with the elementary time step $\tau = 0.01$: at each time the probability of transition between two states is given by the transition matrix $\tilde{K}_{ij}(t)$. For each value of λ we generate $\mathcal{N} = 1000$ sample trajectories and calculate the entropy flow Q , as defined by (2), for each trajectory. Then, for the given value of λ , by averaging over the \mathcal{N} trajectories, we compute the quantity $\langle Q \rangle_\lambda$ using (15). Finally, by combining (8) and (14), we obtain the function $g(\lambda)$ which governs the long time behaviour of $\psi(\lambda, t)$. This function is plotted in figure 2. It can be seen that it vanishes

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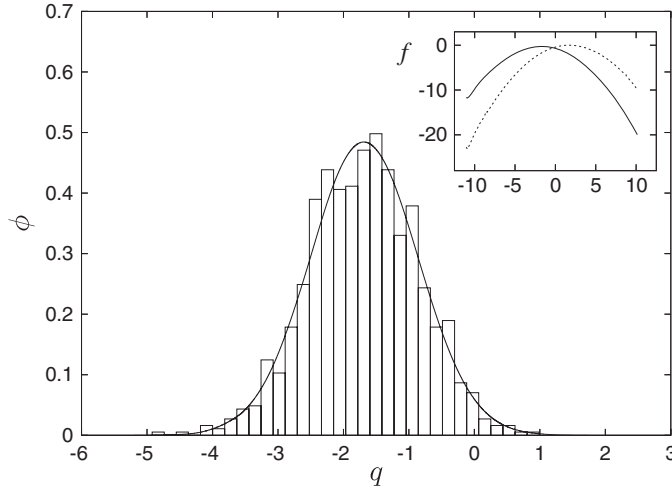


Figure 3. Histogram of the entropy flow per time unit q , corresponding to 1000 unbiased trajectories of the ASEP model. Full line: probability distribution function $\phi(q, t_f)$, obtained with the trajectory-sampling algorithm. Inset: full line, large deviation function f as a function of the entropy per time unit q , as defined by (10); dotted line: plot of $f(q) + q$.

at $\lambda = 0, 1$ and is symmetric with respect to $\lambda = 1/2$. The fact that $g(0) = 0$ corresponds trivially to the normalization condition over all the possible trajectories. On the other hand, the fact that the function g vanishes at $\lambda = 1$ is a non-trivial result, and corresponds to Seifert's fluctuation theorem (11). The symmetry around $\lambda = 1/2$ corresponds to the Gallavotti–Cohen fluctuation relation. We are now able to calculate the large deviation function $f(q)$ defined in (10), which is plotted in the inset of figure 3, together with the expression $f(q) + q$, which exhibits the symmetry required by the Gallavotti–Cohen relation. We check as follows that the quantity $f(q)$ actually gives the entropy distribution function $\phi(q, t) \propto \exp[t f(q)]$ for the present model. We simulate the unbiased diffusion process (i.e., we use the transition matrix K_{ij}), and measure the entropy flow along 1000 trajectories. We then plot the histogram of the measured entropy flow per time unit, together with the function $\exp[t f(q)]$, see figure 3. The agreement between the histogram and the predicted entropy distribution $\phi(q, t)$ is excellent. Note that it is hopeless to try to verify the Gallavotti–Cohen and/or the Seifert relation (11) by direct inspection of the histogram, since no single point of the histogram lies in the range $q > 1$, where the function $f(q) + q$ has its maximum. This is the same problem that one faces when trying to exploit the Jarzynski equality to evaluate the free energy of simple microscopic systems [16].

Finally, we consider the dynamic states which contribute most to the function g for each value of λ . We measure the current $J(\lambda)$ of particles that, in the steady state of weighted ensembles, jumps to the right (positive current) or to the left (negative current), in the unit time. This quantity can be easily measured as biased trajectories are generated using the probability \tilde{K}_{ij} . The current J , as measured in both the λ and (λ, Π) -ensemble, is plotted in figure 4, as a function of λ . It can be clearly seen that, as λ goes away from the origin (either in the negative or in the positive direction), the current differs

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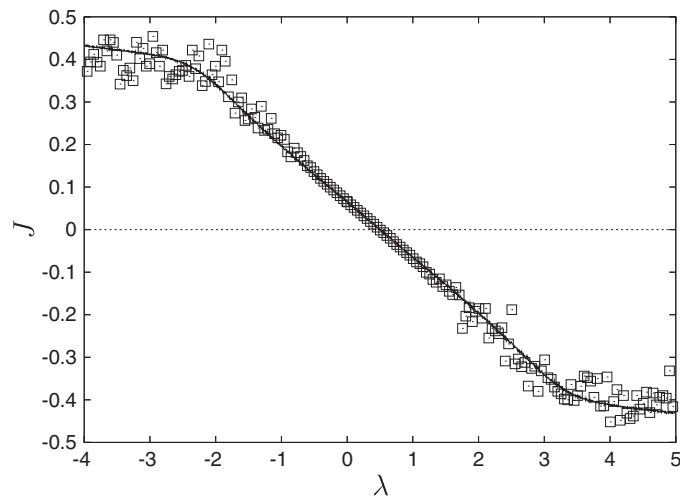


Figure 4. Average particle current J in the weighted trajectory λ -ensemble (full line) and in the (λ, Π) -ensemble (squares), as a function of λ . The current vanishes at $\lambda = 1/2$, and becomes negative for larger values of λ .

more and more from its value in the unbiased dynamics ($\lambda = 0$). Notice that the current vanishes at $\lambda = 1/2$, and that, for larger values of λ , J becomes negative, i.e., the net motion of the particles is opposite to the density gradient. Thus, the parameter λ , which is the thermodynamic conjugate of q , selects dynamical trajectories in the same way as an external field selects states in an ordinary statistical ensemble. Large values of $|\lambda|$ select trajectories which are highly unlikely to appear in an unbiased system. This corroborates the interpretation of the large deviation function as a kind of free energy in the path thermodynamics [15, 16].

We have thus shown how it is possible to evaluate consistently the probability distribution function of the entropy flow in non-equilibrium systems, by solving the differential equation (7) via the simulation scheme for the (λ, Π) -ensemble. In this way the properties of the trajectories which contribute most to the entropy flow in the regime of interest can also be evaluated.

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