Einstein's fluctuation relation and Gibbs states far from equilibrium

Alexandre Lazarescu[1]

[1] *Institut de Recherche en Mathématiques et Physique, UCLouvain, Louvain-la-Neuve, Belgium*

We examine a class of one-dimensional lattice-gases characterised by a *gradient condition* which is a necessary and sufficient condition for the existence of Gibbs-type homogeneous stationary states. We show how, defining appropriate boundary conditions, this condition leads to a novel fluctuation relation under reservoir exchange, unrelated to the Gallavotti-Cohen symmetry. We show that it can be interpreted as a nonequilibrium and nonlinear generalisation of Einstein's relation, leading to Onsager reciprocity relations in the limit of a small reservoir imbalance. We illustrate these results with two examples.

Understanding the structure of nonequilibrium stochastic processes is one of the great challenges of modern statistical physics. A particularly interesting question is whether lattice models, such as interacting particle gases, can be described by fluctuating hydrodynamics in some appropriate scaling limit. For models close to equilibrium, this is known to be the case, as formalised by the macroscopic fluctuation theory [1]: an extended system can be split into mesoscopic regions, each converging rapidly to an equilibrium Gibbs state with a local average value of each conserved quantity [2], with the slow part of the dynamics describing how those quantities are exchanged between adjacent regions through a noisy diffusion equation. A particular property of such an equation, due to it describing the linear regime around equilibrium, is Einstein's relation: the diffusion can be cast as an entropic force deriving from a local entropy, and relates to the variance of the noise felt by the system [3]. Moreover, the noise variance matrix being symmetric, this implies the famed Onsager reciprocity relations [4, 5].

Far from equilibrium, things are much less clear, and although a few isolated result seem to suggest that such a structure should also exist [6, 7], they often come from very specific models, with methods and proofs that cannot be generalised. A promising approach is to build nonequilibrium processes in a way that guarantees local Gibbs-type stationary states [8–11] ; one way to achieve this is to impose a so-called *gradient condition* on the dynamics [10, 12], which turns out to be also useful in carrying out proofs at or near equilibrium [2, 3, 13].

In this paper, we present a new class of models, verifying a gradient condition less restrictive than the one mentioned above, that have many desirable properties. We show that their bulk dynamics allow for stationary Gibbs states, and that we can define reservoirs that maintain these states. Moreover, we can construct a finite-size version of the models with unbalanced reservoirs, whose dynamics shows a new fluctuation relation distinct from the Gallavotti-Cohen symmetry , which exchanges those reservoirs. We then show how this symmetry reduces to a non-equilibrium Einstein's relation (with the corresponding Onsager relations) in the limit of a small unbalance, and give two illustrative examples.

Bulk dynamics and the gradient condition

We will define the models under consideration in a semi-general way, to allow for interesting and varied examples while keeping heavy notations to a minimum. In particular, we will focus on translation-invariant finite-range versions of the models with only a finite number of nearest-neighbour exchanges, though most of our results can easily be made space-dependent with short-range interactions and continuous families of longer jumps.

Let us consider a 1D infinite lattice, with each site carrying a vector of quantities $n_i = \{n_i^\alpha\}$, each conserved by the dynamics, i.e. exchanged between neighbouring sites but not created or destroyed. These exchanges occur through various channels denoted by l, where a vector $d^l = \{d^l_\alpha\}$ is transferred from a site i to the next $i+1$, with a rate $r^l_i(C)$, taking the system from configuration $C = \{n_j\}$ to $C^{l,i} = \{n_j + d^l(\delta_{j,i+1} - \delta_{j,i})\}$. We assume that the rates from site i to $i+1$ depend only on the sites in $[\![i-K, i+1+K]\!]$, and we note that the exchanged quantities d^l can be negative. Moreover, we treat the backward transition from l as a different channel l' with $d^{l'} = -d^l$, and we do not impose anything on the corresponding rate, which can for instance be zero.

Let us now define a local potential with the same range K, i.e. of the form $U(C) = \sum_i u_i(C)$, where each term u_i is the same function applied to C around site i, and depending on at most K subsequent neighbours. This allows us to define rates $\hat{r}^l_i$ dual to r_i with respect to U:

$$\hat{r}^l_i(C^{l,i}) = r^l_i(C)\mathrm{e}^{U(C^{l,i}) - U(C)} \tag{1}$$

which also have the same range K by construction. We will call our original dynamics the *forward process*, and these dual dynamics the *backward process*. Note that we have kept the channel label l for this transition for simplicity, so that the same label corresponds to transitions in opposite directions in the forward and backward process. We can now state the property on which all our results are based: if there exists a function $w_i(C)$ such that the rates satisfy the *gradient condition*

$$\sum_l r_i^l(C) - \hat{r}_i^l(C) = w_i(C) - w_{i+1}(C), \tag{2}$$

then the system has local Gibbs stationary states with potential U, and the backward rates $\hat{r}_i^l$ are those of the time-reversed process, with the same stationary states. As above, the index i on w means that it is applied to C as centered on site i. Also note that this gradient condition is less restrictive than the one found in [3, 10, 12], where the forward and backward rates are gradients separately.

More precisely, considering that the sum of each n_i^α over the whole lattice is constant, we can include potentials $\phi = \{\phi^\alpha\}$ conjugate to each one, and define the formal (un-normalised) distribution

$$\mathrm{P}_\phi(C) = \mathrm{e}^{-U(C)+\sum_i \phi\cdot n_i}. \tag{3}$$

Let us also define the biased generator of transitions from site i with current-counting virtual forces $\mu = \{\mu^\alpha\}$:

$$m_i(\mu) = \sum_{C,l} r_i^l(C)\Big(\mathrm{e}^{\mu\cdot d^l}|C^{l,i}\rangle - |C\rangle\Big)\langle C|, \tag{4}$$

and a similar definition for $\hat{m}_i(\mu)$. The gradient condition can then be rewritten as a local quasi-duality relation

$$\mathrm{P}_\phi^{-1} m_i(\mu)\mathrm{P}_\phi = {}^t\hat{m}_i(-\mu) + W_{i+1} - W_i \tag{5}$$

with W_i being the diagonal matrix with entries $w_i(C)$ and P_ϕ being the diagonal matrix with entries $\mathrm{P}_\phi(C)$. Summing over i cancels the gradient part, leading to the global duality of the two generators. We can then project the equality on the uniform vector to the right or on the vector $\langle \mathrm{P}_\phi|$ to the left for $\mu = 0$ to find that the distribution P_ϕ is stationary for both processes. We therefore have generically non-equilibrium processes with a family of well-defined local stationary Gibbs states indexed by ϕ, and the gradient condition essentially generalises the detailed balance of equilibrium systems. In particular, any detail-balanced process verifies the gradient condition with $W = 0$, though the reverse is not true. Note that all of this also applies to the case of periodic boundary conditions as long as the system has more than $2K$ sites.

We can in fact show that the gradient condition is not only sufficient to have such stationary states, but also necessary. Let us consider a periodic system with $L > 2K$ sites and nearest-neighbour transitions with a finite range K, and let us assume that there exists a potential U with the same range K such that the states 3 are stationary. We can then define the backward rates 1, which are the rates of the time-reverse process $\hat{M}$ and have the same range K by construction. Because M and $\hat{M}$ are similar matrices, their diagonals are identical: for any configuration C, we have

$$\sum_{i,j} r_i^l(C) - \hat{r}_i^l(C) = 0. \tag{6}$$

Let us now define a function $w_i(C)$ as

$$w_i(C) = \sum_{j=1}^{i}\sum_l r_j^l(C) - \hat{r}_j^l(C) = -\sum_{j=i+1}^{L}\sum_l r_j^l(C) - \hat{r}_j^l(C), \tag{7}$$

which is a sum of the differences of local escape rates between the forward and backward process, over the first i sites of the system, and which is equal to minus its complement as per the previous relation. Given that both r and $\hat{r}$ have range K, $w_i(C)$ cannot depend on the occupancies of the sites in $[\![i+K+1, LK]\!]$ due to the first equality, nor on those in $[\![K+2, iK1]\!]$ due to the second, and the part depending on sites $[\![LK, K+2]\!]$ does not depend on i and can be removed from each w_i. We then have the gradient condition 2 by construction, with a function $w_i(C)$ that only depends on the neighbourhood of site i.

This last result provides a useful condition for the existence of local homogeneous stationary states in one-dimensional lattice models, which can for instance serve to exclude certain types of solutions if they are incompatible with the gradient condition (e.g. solutions with a specific range).

Gibbs-compatible boundaries

The next step is to define reservoirs and associated transition rates that preserve the structure above. This can be done quite simply by tracing over half of the infinite system in a chosen distribution P_ϕ [14]. For instance, we define a leftward reservoir with potential ϕ by restricting our configurations to $\mathbb{N}$ and defining averaged rates

$$r^{l,+}_{i,\phi}(C) = \sum_{j\leq 0}\sum_{n_j} r^l_i(C)\mathrm{P}_\phi(C) \Big/ \sum_{j\leq 0}\sum_{n_j} \mathrm{P}_\phi(C) \quad \text{with} \quad \mathrm{P}^+_\phi(C) = \sum_{j\leq 0}\sum_{n_j} \mathrm{P}_\phi(C), \tag{8}$$

with a potential $U_\phi(C) = \sum_i u_{i,\phi}(C)$. The traced Gibbs state P^+_ϕ is stationary under the new dynamics by construction. Note that, because of the range K of the original dynamics, if $i > K$, the traced rates and local potential $u_{i,\phi}$ are equal to the original bulk ones, and in particular are independent of ϕ. Corresponding definitions are implied for a rightward reservoir with potential ϕ, rates $r^{l,-}_{i,\phi}$, and a traced distribution P^-_ϕ, as well as reservoirs for the backwards process. If we now choose a size $L > 2K$, we are able to define those left and right reservoirs independently, and have our original bulk rates in between. Moreover, by construction, the corresponding doubly-traced Gibbs states P^L_ϕ are stationary for the restricted dynamics. Note that we now have a single stationary state for our system, as ϕ has to be fixed to define both reservoirs.

It is also straightforward to check what becomes of the duality (5) by directly tracing the relation. We define

$$w^\phi_i(C) = \sum_{j\leq 0}\sum_{n_j} w_i(C)\mathrm{P}_\phi(C) \Big/ \sum_{j\leq 0}\sum_{n_j} \mathrm{P}_\phi(C) \tag{9}$$

and its rightward equivalent. Conveniently, it turns out that $w^\phi_i = \langle w\rangle_\phi \equiv w(\phi)$, which is the average of w in the distribution P_ϕ, for $i < 1$ *and* $i > L$. This leads to a cancellation from one reservoir to the other when summing the averaged version of (5). We also get that the trace of the backward process is the dual of the traced forward process with respect to P^L_ϕ.

Patchwork states and process duality

The final step is to examine what happens when we mix boundaries with different potentials ϕ_a and ϕ_b. The process may be defined by parts by using $r^{l,+}_{i,\phi_a}$ for $i \in [\![1, K]\!]$, $r^{l,-}_{i,\phi_b}$ for $i \in [\![L-K+1, L]\!]$, and r^l_i otherwise. The first thing to note is that we no longer know the stationary state of the system: the left part of the system verifies a quasi duality relation with respect to $\mathrm{P}^+_{\phi_a}$, but the right part has one with respect to $\mathrm{P}^-_{\phi_b}$. This incites us to define a *patchwork Gibbs state* $\mathrm{P}_{\phi_a,\phi_b}$ (the letter L will be implied from now on), by fixing $i \in [\![K+1, L-K]\!]$ and constructing

$$\mathrm{P}_{\phi_a,\phi_b}(C) = Z^{-1}_{\phi^a,\phi^b} \exp\!\left(\sum_{j\leq i} -u_{j,\phi_a}(C) + \phi_a\cdot n_j + \sum_{j>i} -u_{j,\phi_b}(C) + \phi_b\cdot n_j\right) \tag{10}$$

with the obvious normalisation. We then define a biased generator with a virtual force on the edge separating the two parts of our patchwork states, which is able to “catch” the twist produced by the conjugation by $\mathrm{P}_{\phi_a,\phi_b}$:

$$M_{\phi_a,\phi_b}(\mu) = \sum_{j<i} m^+_{j,\phi_a}(0) + m_i(\mu) + \sum_{j>i} m^-_{j,\phi_b}(0) \tag{11}$$

Conjugating this expression with $\mathrm{P}_{\phi_a,\phi_b}$ and applying the gradient condition on each part yields the process duality

$$\begin{aligned}&\mathrm{P}^{-1}_{\phi_a,\phi_b} M_{\phi_a,\phi_b}(\mu + \phi_b - \phi_a)\mathrm{P}_{\phi_a,\phi_b}\\ &\quad = {}^t\hat{M}_{\phi_a,\phi_b}(-\mu) + w(\phi_b) - w(\phi_a).\end{aligned} \tag{12}$$

A special case of this duality was observed in [15] and generalised in [16] in the case of the ASEP.

Einstein’s fluctuation relation

This last relation implies identities between the eigenelements of both matrices, of which one is particularly interesting: let us call $E_{\phi_a,\phi_b}(\mu)$ the largest eigenvalue of $M_{\phi_a,\phi_b}(\mu)$, known to be equal to the generating function of stationary currents of conserved quantities [17]. To go any further, we need to make an additional assumption on the structure of our dynamics, namely than the backward rates $\hat{r}$ are the same as r under space reversal:

$$\hat{r}^l_i(C) = r^l_i(\hat{C}) \tag{13}$$

where $\hat{C}$ is the configuration C flipped around the edge between sites i and $i+1$. Under that condition, we can flip the system left to right, and obtain that $\hat{E}_{\phi_a,\phi_b}(-\mu) = E_{\phi_b,\phi_a}(\mu)$. This yields

$$E_{\phi_a,\phi_b}(\mu + \phi_b - \phi_a) = E_{\phi_b,\phi_a}(\mu) + w(\phi_b) - w(\phi_a). \tag{14}$$

For the large deviations function of the currents $g_{\phi_a,\phi_b}(j)$, which is the Legendre transform of $E_{\phi_a,\phi_b}(\mu)$, we get

$$g_{\phi_a,\phi_b}(j) = g_{\phi_b,\phi_a}(j) + j(\phi_b - \phi_a) - w(\phi_b) + w(\phi_a). \tag{15}$$

This is a new and surprising fluctuation symmetry for open driven systems, which relies on reverting time and space simultaneously, and does not require microreversibility. It can be understood as a nonlinear and nonequilibrium generalisation of Einstein's relation [3], which can be seen by making the difference $\phi_b - \phi_a$ small, as we show in the next section.

Note that this fluctuation symmetry is in general distinct from the Gallavotti–Cohen symmetry based on time-reversal alone, which does require the system to be microscopically reversible but not to obey the gradient condition. This symmetry requires a different biased generator

$$m_i(\lambda) = \sum_{C,l} r_i^l(C)\Big(\mathrm{e}^{\lambda_i^l}|C^{l,i}\rangle - |C\rangle\Big)\langle C|, \tag{16}$$

where the exponent in the bias now involves a space-dependent variable λ_i^l. The symmetry can then generally be written as

$$E(-\lambda) = E(\lambda - s) \quad \text{and} \quad g(-\mathrm{j}) = g(\mathrm{j}) + \mathrm{j}\cdot s \tag{17}$$

for an antisymmetric variable $\lambda_i^{-l} = -\lambda_i^l$, with j_i^l being a probability current defined independently from the transported quantities α, s being the stationary edge-wise entropy production in the system

$$s_i^l = \ln\left(\frac{r_i^l(C)}{r_i^{-l}(C^{l,i})}\right), \tag{18}$$

and the backward transition l now being part of the real dynamics of the system. The only case where the two symmetries coincide is when the total entropy production of the system reduces to a per-particle contribution $\phi_a\phi_b$ from the boundaries, i.e. when the system is detail-balanced in the bulk (so that $w=0$), and has boundary transition rates such that $s_0^l = \phi_a \cdot d^l$ and $s_L^l = -\phi_b \cdot d^l$, in which case we can define

$$\lambda_i^l = \sum_\alpha \mu^\alpha d_\alpha^l, \qquad j_\alpha = \sum_{i,l} \mathrm{j}_i^l d_\alpha^l, \tag{19}$$

and obtain

$$\mathrm{j}\cdot s = j(\phi_a - \phi_b), \qquad w(\phi_a) - w(\phi_b) = 0, \qquad E_{\phi_b,\phi_a}(\mu) = E_{\phi_a,\phi_b}(-\mu), \qquad g_{\phi_b,\phi_a}(j) = g_{\phi_a,\phi_b}(-j), \tag{20}$$

from which the identity of the two symmetries follows immediately.

Near-Gibbs regime

To illustrate this last statement, let us choose $\phi_b = \phi + \varepsilon/2$ and $\phi_a = \phi - \varepsilon/2$. For $\mu = 0$ in particular, we have $E_{\phi_a,\phi_b}(0) = 0$, so that the symmetry becomes

$$E_{\phi-\varepsilon/2,\phi+\varepsilon/2}(\varepsilon) = w(\phi + \varepsilon/2) - w(\phi - \varepsilon/2). \tag{21}$$

Expanding it to second order in ε, with $\hat{\partial}_\phi = \partial_{\phi^b} - \partial_{\phi^a}$, we get the following relations:

$$\partial_\mu E_\phi(0) = \partial_\phi w(\phi) \tag{22}$$

$$\hat{\partial}_{\phi_\alpha}\partial_{\mu_\beta} E_\phi(0) = -\partial_{\mu_\alpha}\partial_{\mu_\beta} E_\phi(0). \tag{23}$$

This implies that the stationary current in the system, which is the first derivative of $E_{\phi_a,\phi_b}(\mu)$, is equal to

$$J(\phi,\varepsilon) = \partial_\mu E_{\phi^a,\phi^b}(0) \approx \partial_\phi w(\phi) - \partial_\mu \frac{(\varepsilon\cdot\partial_\mu)}{2} E_\phi(0) \tag{24}$$

In order to interpret this equation, it is useful to define the average density of conserved quantities in the homogeneous Gibbs states, which we can express as

$$\rho(\phi) = \langle n \rangle_\phi = L^{-1}\partial_\phi \ln(Z_{\phi,\phi}) \tag{25}$$

and can be computed generically using transfer matrix techniques. We can also define the compressibility matrix σ and the linear response matrix R as

$$\sigma_{\alpha\beta}(\rho) = \partial_{\phi_\alpha}\rho_\beta(\phi(\rho)), \qquad R(\rho) = (\frac{\partial_\mu^2}{2}E_{\phi(\rho)})(\mu = 0). \tag{26}$$

Writing the potential difference as $\varepsilon = \nabla\phi = \sigma^{-1}(\rho)\nabla\rho$ (which is not a real local gradient in this context), we get

$$J(\rho, \nabla\rho) = \sigma(\rho)\partial_\rho w(\phi(\rho)) - R(\rho)\sigma^{-1}(\rho)\nabla\rho \tag{27}$$

which is readily interpretable as a diffusion equation with a diffusion matrix $D(\rho) = R(\rho)\sigma^{-1}(\rho)$ typically proportional to L^{-1}. The average drift $\partial_\phi w(\phi)$ is the same as in the linear regime around equilibrium: the process $pM_{\phi_a,\phi_b} + q\hat{M}_{\phi_a,\phi_b}$ for $(p-q)$ small has a gradient function $(p-q)w(\phi)$.

Notably, equation (23) expresses Einstein's relation between the current produced by a force μ (right side) and that produced by a chemical potential difference $\nabla\phi$ (left side). The former being symmetric, this also implies Onsager's reciprocity relations [4, 5], though notably they exclude the drift current (22) in this case.

It is unclear whether equation 27, which involves the global average stationary current in the system in terms of the difference of reservoir densities, can be recast as a local diffusion equation for an extended version of the system. At equilibrium, the response matrix $R(\rho)$ can be computed in terms of a covariance matrix for local currents in a local equilibrium state, independently of boundary conditions:

$$R^{eq}_{\alpha\beta}(\rho) = \sum_{C,l} r_i^l(C) d^l_\alpha d^l_\beta P_{\phi(\rho)}(C), \tag{28}$$

for any i, where the sum is taken over only the forward rates (the backward rates give the same contribution by symmetry, and result in a factor 2 canceling the factor 1/2 above). This allows for a local interpretation of the diffusive term in equation 27 and therefore of the whole equation. In the present case, however, we were only able to derive a global formula involving the eigenvalue $E_{\phi(\rho)}(\mu)$ of the entire biased generator. That being said, encouraged by known results on current large deviations for the ASEP [7], which is one of the few models where the mixed-boundary stationary states are known [18], we conjecture that the nonequilibrium response matrix is in fact the same as the one that may be computed locally at equilibrium, up to a factor $(2L)^1$ due to different dynamical scalings and the absence of backward rates, and that the diffusion matrix can be calculated by similar techniques as those applicable there [19].

One last thing to note before presenting some examples is that the quantity $\mathcal{G}(\phi) = L^{-1}\ln(Z_{\phi,\phi})$ involved in eq.(25) can be interpreted as a thermodynamic potential associated to a free energy $\mathcal{F}(\rho) = \rho \cdot \phi(\rho) - \mathcal{G}(\phi(\rho))$ which is minimised by the stationary density and such that the potential force $\nabla\mathcal{F}'(\rho) = \nabla\phi(\rho)$ drives the diffusive part of (27). However, as far as we can tell, that free energy is not necessarily always decreasing in time and so does not constitute a Lyapunov function for the system.

Example A: multi-velocities exclusion

The first example we consider is a multi-species partial exclusion process with relative velocities, which is a generalisation of the model studied in [20]. Each site carries N particles of K possible species, written as $\{n_i^{(k)}\}_{k\in[\![1,K]\!]}$. Each species is assigned a velocity v_k (which are ordered to be increasing with k), and can only overtake slower particles $l < k$, with a rate

$$r_i^{kl}(n_i^{(k)}, n_{i+1}^{(l)}) = (v_k - v_l)n_i^{(k)}n_{i+1}^{(l)} \quad \text{if} \quad l < k \tag{29}$$

equal to the velocity difference multiplied by the number of choices of particles to exchange. Note that we do not take N to be large, so that we will not be scaling any quantity with it.

Given the simplicity of the model and the absence of interactions other than the hierarchy between the species, it is natural to first look for a solution with a simple on-site potential, i.e. with $u_i(n) = u(n_i)$. In particular, the potential of the stationary state of the the infinite-volume symmetric version of the model is often a good candidate, as it guarantees that the backwards process be the spatial symmetric of the forward process. In this case, the unnormalised stationary distribution is given by a multinomial product state (i.e. a multipoissonian distribution with a cutoff on the total occupancy of a site)

$$\mathrm{P}_\phi(C) = \prod_i \binom{N}{\{n_i^{(k)}\}} \tag{30}$$

for which the symmetrised dynamics is trivially detail-balanced. The backwards rates are then

$$\hat{r}_i^{kl}(n_i^{(k)}+1, n_{i+1}^{(l)}+1) = (v_k - v_l)\left(n_i^{(l)}+1\right)\left(n_{i+1}^{(k)}+1\right) \quad \text{if} \quad l<k \tag{31}$$

with $k>l$, and we can check that they verify the gradient condition with respect to the function

$$w_i(C) = -N\sum_k v_k n_i^{(k)}. \tag{32}$$

The proof is straightforward:

$$\begin{aligned}
\sum_{k,l} r_i^{kl}(C) - \hat{r}_i^{kl}(C) &= \sum_{k>l}(v_k - v_l)\left(n_i^{(k)}n_{i+1}^{(l)} - n_i^{(l)}n_{i+1}^{(k)}\right) \\
&= \sum_{k>l} v_k\left(n_i^{(k)}n_{i+1}^{(l)} - n_i^{(l)}n_{i+1}^{(k)}\right) - \sum_{k<l} v_k\left(n_i^{(l)}n_{i+1}^{(k)} - n_i^{(k)}n_{i+1}^{(l)}\right) \\
&= \sum_{k,l} v_k\left(n_i^{(k)}n_{i+1}^{(l)} - n_i^{(l)}n_{i+1}^{(k)}\right) \\
&= N\sum_k v_k\left(n_i^{(k)} - n_{i+1}^{(k)}\right) = w_{i+1}(C) - w_i(C),
\end{aligned} \tag{33}$$

where we exchanged k and l in part of the sum between the first and second line.

Introducing the potentials ϕ_k, the one-site partition function of the homogeneous Gibbs states is simply that of a multinomial distribution

$$Z_N(\phi) = \left(\sum_k \mathrm{e}^{\phi_k}\right)^N. \tag{34}$$

Due to the absence of interactions, the dependence on L of the L-site partition function is simply a power which disappears when computing the average densities, and the average of w is then easily expressed:

$$\rho_k = L^{-1}\partial_{\phi_k}\ln\left(Z_N^L\right) N Z_1^{-1}\mathrm{e}^{\phi_k} \quad \text{and} \quad w(\phi) = -N\sum_k v_k\rho_k = -N^2 Z_1^{-1}\sum_k v_k \mathrm{e}^{\phi_k}. \tag{35}$$

The compressibility is non-diagonal due to the partial exclusion interactions, and is given by

$$\sigma_{kl}(\phi) = \partial_{\phi_l}\rho_k = \rho_k(\delta_{k,l} - \rho_l N^{-1}). \tag{36}$$

We are not able to compute the largest eigenvalue of the biased Markov matrix of the whole system in order to get the response matrix $R(\rho)$. We may instead compute its equilibrium counterpart, consistently with our conjecture, and rescale it with L:

$$\begin{aligned}
R_{\alpha\beta}(\rho) &= (2L)^{-1}\sum_{k>l}\sum_{n_i,n_j} n_i^{(k)}n_j^{(l)}(\delta_{\alpha k} - \delta_{\alpha l})(\delta_{\beta k} - \delta_{\beta l})\mathrm{P}(n_i)\mathrm{P}(n_j)Z_N^{-2}(0) \\
&= -(2L)^{-1}\sum_{n_i,n_j}|v_\alpha - v_\beta| n_i^{(\alpha)}n_j^{(\beta)}\mathrm{P}(n_i)\mathrm{P}(n_j)Z_N^{-2}(0)
\end{aligned} \tag{37}$$

so that

$$R_{kl}(\rho) = -(2L)^{-1}|v_k - v_l|\rho_k\rho_l. \tag{38}$$

Putting all the elements together, the average current vector then reads $J = N\sigma v - R\sigma^{-1}\nabla\rho$.

Example B: finite-range interacting exclusion

This second example is a totally asymmetric simple exclusion process with extra finite-range interactions. The case of first neighbour interactions was treated in [8], so we will consider second neighbour interactions as well.

Let us first fix the stationary states we will consider. We assign a Boltzmann factor ν to pairs of nearest neighbours, and γ to pairs of next-to-nearest neighbours. We can write the formal Gibbs states on the infinite lattice as an infinite product of identical transfer matrices $A = (A_{ij,kl})$ containing the interactions of pairs of neighbours conditioned on the next pair:

$$A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ \mathrm{e}^{\phi} & \mathrm{e}^{\phi}\gamma & \mathrm{e}^{\phi}\nu & \mathrm{e}^{\phi}\gamma\nu \\ \mathrm{e}^{\phi} & \mathrm{e}^{\phi} & \mathrm{e}^{\phi}\gamma & \mathrm{e}^{\phi}\gamma \\ \mathrm{e}^{2\phi}\nu & \mathrm{e}^{2\phi}\gamma\nu & \mathrm{e}^{2\phi}\gamma\nu^2 & \mathrm{e}^{2\phi}\gamma^2\nu^2 \end{bmatrix} \tag{39}$$

in the basis $\{00, 01, 10, 11\}$ for each pair. The two-site partition function is the largest eigenvalue $\Lambda(\phi)$ of that matrix, so that $\mathcal{F}(\phi) = -\ln\left(\sqrt{\Lambda(\phi)}\right)$.

Through trial and error, we find that the following values of w and r verify the gradient condition with respect to P_ϕ (where $*$ denotes arbitrary occupancies):

$$\begin{aligned} &w(000{*}{*}) = w({*}{*}000) = 0, \quad w(111{*}{*}) = w({*}{*}111) = -1 \\ &w(1001{*}) = a, \quad w(01011) = b, \quad w(11011) = \gamma b + a \\ &w(0110{*}) = a - \gamma, \quad w(10100) = b - \nu, \quad w(00100) = a + \gamma(b - \nu) \\ &w(01010) = b - \nu a/\gamma, \quad w(10101) = b - (1 + a)\nu/\gamma \end{aligned}$$

and, sorting the rates in a matrix $r(i10j)$ with i and j in basis $\{00, 01, 10, 11\}$,

$$r = \begin{bmatrix} \gamma(\nu - b) - a & \gamma(\nu - b) & \nu - a/\gamma & \nu \\ \gamma - a & \gamma & \gamma - a + b & \gamma(1 + b) \\ \nu - b & \nu + a - b & \nu/\gamma & \nu/\gamma(1 + a) \\ 1 & 1 + a & 1 + b & 1 + a + \gamma b \end{bmatrix}$$

where the parameters a and b must be chosen such that every rate is positive. The boundary rates corresponding to a given value of z can then be computed by averaging the values above using the dominant left and right eigenvectors $V_{a,b}(z)$ of A as weights.

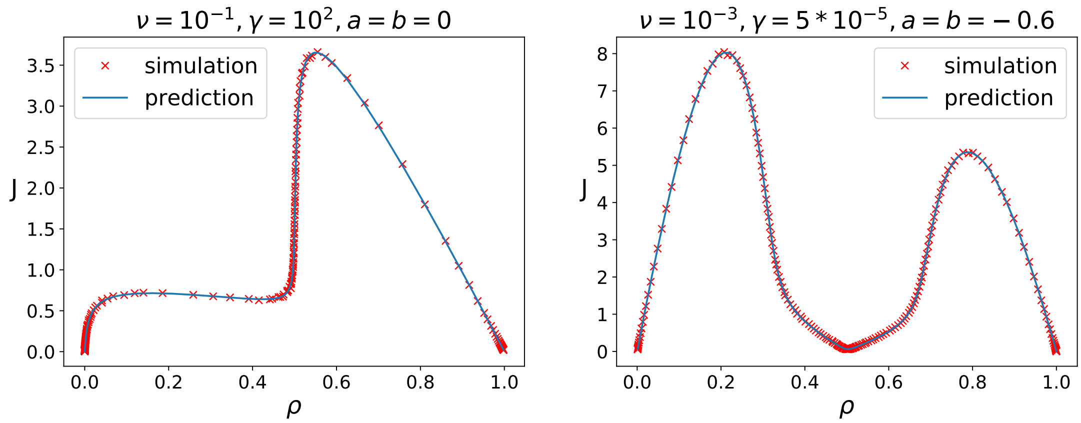

FIG. 1: Comparison between direct simulations and analytical predictions for the average current J (in arbitrary units) as a function of the average density ρ for systems of size $L = 10$.

Except in special cases, it is difficult to compute $\Lambda(z)$ and $V_{a,b}(z)$ analytically, but it is quite easy to obtain them numerically. As a sanity check, we can therefore compute the average current in this model with balanced boundaries, as a function of r, in two ways: firstly through $\partial_\phi w(\phi(z))$ (by computing $\Lambda(z)$ and $V_{a,b}(z)$ numerically, and performing a numerical derivative of $w(\phi)$, which is computationally very cheap and independent of the system size) ; secondly by measuring the current in a direct simulation of the system using the rates given above (by computing $V_{a,b}(z)$ numerically for every z, and running an event-driven simulation of the system from a random initial condition, until the average value of the current has converged, which is numerically much more costly and depends highly on the size of the system). The results of those computations are presented in fig.1, for two choices of the bulk rates showing distinct behaviours, and a system size $L = 10$ which would clearly show any potential finite-size effects.

Discussion

In this letter, we have presented a class of Markov processes far from equilibrium, in which a generalisation of detailed balance called the *gradient condition* which is necessary and sufficient for the existence of homogeneous Gibbs steady states. We discovered in these models a new fluctuation symmetry for the currents of conserved quantities under an exchange of boundary conditions, which can be interpreted as a generalisation of Einstein's relation. This relation involves a non-equilibrium free energy which is minimised at stationarity, and whose derivative drives the diffusion, but does not seem to have all the properties of its equilibrium equivalent such as monotonicity. Examples of models where our results apply include many versions of exclusion processes (with interactions [8], higher occupancies [21], several types of particles [20], longer jumps [22], or longer-range exclusion [23]), as well as asymmetric versions of the inclusion process [24, 25], the KMP model for heat conduction [26], and other models designed to have Gibbs stationary states [10, 11].

Many questions remain open and require further study. First and foremost, we need to determine whether the situation we describe, up to generalisations such as spacial dependence and short-range interactions, is the rule or the exception. Another challenge would be to extend our results to two-dimensional cases, where the gradient condition seems straightforward but the definition of appropriate unbalanced boundary conditions might not be so simple. Finally, the small bias expansion we have performed on a finite system to recover the linear Einstein's relation is not quite equivalent to a coarse-graining of an extended system, as it would be near equilibrium, as we are lacking an additivity principle [27]. Understanding the relation between those two situations could be crucial in building a proper theory of macroscopic fluctuations far from equilibrium.

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[1] L. Bertini, a. De Sole, D. Gabrielli, G. Jona-Lasinio and C. Landim. *Macroscopic fluctuation theory for stationary non-equilibrium states.* Journal of Statistical Physics **107(3-4)**, 635–675 (2002).

[2] P. Gonçalves and M. Jara. *Nonlinear Fluctuations of Weakly Asymmetric Interacting Particle Systems.* Archive for Rational Mechanics and Analysis **212(2)**, 597–644 (2014).

[3] P. Gonçalves and M. Jara. *The Einstein Relation for the KPZ Equation.* Journal of Statistical Physics **158(6)**, 1262–1270 (2015).

[4] D. Andrieux and P. Gaspard. *Fluctuation theorem and Onsager reciprocity relations.* The Journal of Chemical Physics **121(13)**, 6167–6174 (2004).

[5] A. Mielke, D. R. M. Renger and M. A. Peletier. *A Generalization of Onsager's Reciprocity Relations to Gradient Flows with Nonlinear Mobility.* Journal of Non-Equilibrium Thermodynamics **41(2)** (2016).

[6] T. Bodineau and B. Derrida. *Current large deviations for asymmetric exclusion processes with open boundaries.* Journal of Statistical Physics **123(2)**, 277–300 (2006).

[7] A. Lazarescu. *The physicist's companion to current fluctuations: one-dimensional bulk-driven lattice gases.* Journal of Physics A: Mathematical and Theoretical **48(50)**, 503001 (2015).

[8] J. S. Hager, J. Krug, V. Popkov and G. M. Schütz. *Minimal current phase and universal boundary layers in driven diffusive systems.* Physical Review E **63(5)**, 056110 (2001).

[9] J. M. Luck and C. Godrèche. *Nonequilibrium stationary states with Gibbs measure for two or three species of interacting particles.* Journal of Statistical Mechanics: Theory and Experiment **2006(08)**, P08009–P08009 (2006).

[10] L. De Carlo and D. Gabrielli. *Gibbsian Stationary Non-equilibrium States.* Journal of Statistical Physics **168(6)**, 1191–1222 (2017).

[11] A. K. Chatterjee and P. K. Mohanty. *Assisted exchange models in one dimension.* Physical Review E **98(6)**, 062134 (2018).

[12] Y. Nagahata. *The gradient condition for one-dimensional symmetric exclusion processes.* Journal of Statistical Physics **91(3-4)**, 587–602 (1998).

[13] M. Kaiser, R. L. Jack and J. Zimmer. *A variational structure for interacting particle systems and their hydrodynamic scaling limits.* Communications in Mathematical Sciences **17(3)**, 739–780 (2019).

[14] M. Dierl, M. Einax and P. Maass. *One-dimensional transport of interacting particles: Currents, density profiles, phase diagrams, and symmetries.* Physical Review E **87(6)**, 062126 (2013).

[15] P. Torkaman and F. H. Jafarpour. *Effective stochastic generators for conditioned dynamics at an atypical reaction-diffusion current.* Physical Review E **92(6)**, 062104 (2015).

[16] A. Lazarescu. *Generic dynamical phase transition in one-dimensional bulk-driven lattice gases with exclusion.* Journal of Physics A: Mathematical and Theoretical **50(25)**, 254004 (2017).

[17] H. Touchette. *The large deviation approach to statistical mechanics.* Physics Reports **478(1-3)**, 1–69 (2009).

[18] B. Derrida, M. R. Evans, V. Hakim and V. Pasquier. *Exact solution of a 1D asymmetric exclusion model using a matrix formulation.* Journal of Physics A: Mathematical and General **26(7)**, 1493–1517 (1999).

[19] C. Arita, P. L. Krapivsky and K. Mallick. *Variational calculation of transport coefficients in diffusive lattice gases* (2016).

[20] V. Karimipour. *Multispecies asymmetric simple exclusion process and its relation to traffic flow.* Physical Review E **59(1)**, 205–212 (1999).

[21] G. M. Schütz, R. Ramaswamy and M. Barma. *Pairwise balance and invariant measures for generalized exclusion processes.* Journal of Physics A: Mathematical and General **29(4)**, 837–843 (1996).

[22] D. Gabrielli and P. L. Krapivsky. *Gradient structure and transport coefficients for strong particles.* Journal of Statistical Mechanics: Theory and Experiment **2018(4)**, 043212 (2018).

[23] S. Gupta, M. Barma, U. Basu and P. K. Mohanty. *Driven k-mers: Correlations in space and time.* Physical Review E **84(4)**, 041102 (2011).

[24] K. Kuoch and F. Redig. *Ergodic theory of the symmetric inclusion process.* Stochastic Processes and their Applications **126(11)**, 3480–3498 (2016).

[25] Y. Baek, Y. Kafri and V. Lecomte. *Extreme current fluctuations of boundary-driven systems in the large- N limit.* Journal of Statistical Mechanics: Theory and Experiment **2016(5)**, 053203 (2016).

[26] C. Kipnis, C. Marchioro and E. Presutti. *Heat flow in an exactly solvable model.* Journal of Statistical Physics **27(1)**, 65–74 (1982).

[27] T. Bodineau and B. Derrida. *Current fluctuations in nonequilibrium diffusive systems: An additivity principle.* Physical Review Letters **92(18)**, 180601–1 (2004).