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Einstein Relation for Nonequilibrium Steady States

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The Einstein relation, relating the steady state fluctuation properties to the linear response to a perturbation, is considered for steady states of stochastic models with a finite state space. We show how an Einstein relation always holds if the steady state satisfies detailed balance. More generally, we consider non-equilibrium steady states where detailed balance does not hold and show how a generalisation of the Einstein relation may be derived in certain cases. In particular, for the asymmetric simple exclusion process and a driven diffusive dimer model, the external perturbation creates and annihilates particles thus breaking the particle conservation of the unperturbed model.

KEY WORDS: Einstein relation; nonequilibrium steady state; asymmetric exclusion process.

1. INTRODUCTION

A guiding principle of equilibrium statistical mechanics is provided by the fluctuation-dissipation theorem, which relates the fluctuation properties of a system in equilibrium to the response of the system to an external perturbation. Its simplest form—the zero-frequency limit—is the Einstein relation which relates linear transport coefficients to spontaneous equilibrium fluctuations. For example the mobility μ and diffusion constant Δ of a Brownian particle interacting with its environment are related by

$$\mu = \beta \Delta, \tag{1}$$

where β is the inverse temperature. This is a deep result with many implications. It enables one to reduce the calculation of response and transport coefficients (mobility, susceptibility, etc.) to a zero-field calculation. Further,

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one can formally consider that spontaneous equilibrium fluctuations are caused by fictitious random forces. In particular the Einstein relation dictates the forms of dissipative terms and noise in a phenomenological description of, for example, dynamic critical behaviour.

A standard derivation of the Einstein relation (in the above form) comes from the Langevin equation describing Brownian motion. Here, the relation implies that diffusion is a direct consequence of the fluctuations of a Brownian particle, and, conversely, the existence of a frictional drag on the Brownian particle implies spontaneous equilibrium fluctuations of a random force. Because of the general applicability of the Einstein relation, one can make such statements for any transport problem,[1] for example, the existence of an electrical impedance implies spontaneous fluctuations of the voltage difference across its terminals.[2]

The most general formulations, applicable to quantum and classical models of equilibrium statistical mechanics, are due to Kubo,[3–5] and Kadanoff and Martin.[5, 6] The former relies on formal perturbation arguments for the linear response of a system near equilibrium; the latter approach is based on correlation functions. These approaches have been employed to derive the linearised hydrodynamics for the KLS model—a driven diffusive system and nonequilibrium generalisation of the Ising model—where the steady state satisfies detailed balance and the applied perturbation is the drive.[7]

Some attempts have been made to generalise the fluctuation-dissipation theorem to models without detailed balance.[8–10] These consider the relationship between dissipation and spontaneous steady state fluctuations and have found most success for steady states where the system can be divided into cells small on the macroscale, in each of which the dynamics satisfy detailed balance with respect to a local fixed density product measure. The global steady state can then be written in terms of these local product measure states. Such steady states are relevant when boundary driving breaks the global detailed balance of an equilibrium model. Also, a fluctuation theorem for nonequilibrium steady states has been demonstrated by Gallavotti and Cohen.[11, 12]

However, it is not known in general how to derive an Einstein relation for steady states of driven nonequilibrium systems where detailed balance is not satisfied. Since no such guiding principle exists in nonequilibrium statistical mechanics, we seek here to generalise the Einstein relation to nonequilibrium steady states of lattice-based stochastic models governed by a Master equation.

In what follows, we review in Section 2 the approach introduced by Derrida[13] that yields general expressions for a current and diffusion constant for systems described by a Master equation. We consider stochastic models with a finite state space and use this approach to investigate the existence of Einstein relations. In Section 3 we consider steady states where detailed balance is satisfied and show generally that an Einstein relation holds. In Section 4 we consider nonequilibrium steady states where detailed balance is not obeyed and discuss the conditions under which an Einstein relation holds. We show that the usual Einstein relation holds for a simple class of models that includes boundary-driven symmetric exclusion (diffusing particles with hard-core interaction). Beyond this class, we consider bulk-driven models such as the asymmetric simple exclusion process (ASEP) and driven dimer diffusion. In particular, we obtain an Einstein relation for the ASEP that relates the diffusion constant to the response of the current to an applied field that creates and annihilates particles. We conclude in Section 5.

2. CALCULATION OF THE CURRENT AND DIFFUSION CONSTANT

In this section, we outline how to obtain general expressions for a current J and diffusion constant Δ, for stochastic models defined on a finite state space. The approach is given in detail by Derrida *et al.*;[13–15] here we just present the key equations.

We consider a random variable Y_t which increases and decreases according to specified dynamical events. For example, for a system of random walkers, if we take Y_t as the total displacement, then Y_t increases when a walker steps to the right and decreases when one steps to the left. In the long-time limit, the mean and variance of Y_t increase linearly in time, and the constants of proportionality are interpreted respectively as a current (sometimes referred to as a velocity) and a diffusion constant. This is always true for finite systems, regardless of whether or not the infinite system exhibits anomalous diffusion, i.e., when the mean or variance of Y_t increases nonlinearly in time.

The moments of Y_t are obtained from $P_t(\mathscr{C}, Y)$, which is the probability that at time t the system is in a configuration $\mathscr{C}$ and the random variable takes the value $Y_t = Y$. The time evolution of $P_t(\mathscr{C}, Y)$ is governed by a Master equation

$$\begin{aligned}\frac{d}{dt} P_t(\mathscr{C}, Y) = \sum_{\mathscr{C}'} [\{&M_0(\mathscr{C}, \mathscr{C}')\, P_t(\mathscr{C}', Y) + M_1(\mathscr{C}, \mathscr{C}')\, P_t(\mathscr{C}', Y-1) \\ &+ M_{-1}(\mathscr{C}, \mathscr{C}')\, P_t(\mathscr{C}', Y+1)\} \\ &- \{M_0(\mathscr{C}', \mathscr{C})\, P_t(\mathscr{C}, Y) + M_1(\mathscr{C}', \mathscr{C})\, P_t(\mathscr{C}, Y) \\ &+ M_{-1}(\mathscr{C}', \mathscr{C})\, P_t(\mathscr{C}, Y)\}], \qquad (2)\end{aligned}$$

where $M_0(\mathscr{C},\mathscr{C}')$ is a transition rate from the configuration $\mathscr{C}'$ to the configuration $\mathscr{C}$ without contributing to Y_t, $M_1(\mathscr{C},\mathscr{C}')$ contains transitions from $\mathscr{C}'$ to $\mathscr{C}$ which increase Y_t by one and $M_{-1}(\mathscr{C},\mathscr{C}')$ contains transitions from $\mathscr{C}'$ to $\mathscr{C}$ which decrease Y_t by one. The diagonal elements $M_0(\mathscr{C},\mathscr{C})$, $M_1(\mathscr{C},\mathscr{C})$ and $M_{-1}(\mathscr{C},\mathscr{C})$ are defined to be zero. It is straightforward to obtain evolution equations for the first two moments of Y_t, $\langle Y_t\rangle$ and $\langle Y_t^2\rangle$, by multiplying both sides of (2) by Y and Y^2. The angled brackets here denote an average over steady state initial conditions and all histories of the dynamics. (The formalism can be extended to include other initial conditions.[16]) These evolution equations are expressed in a compact fashion in terms of $p_t(\mathscr{C})=\sum_Y P_t(\mathscr{C},Y)$ and $q_t(\mathscr{C})=\sum_Y YP_t(\mathscr{C},Y)$: $p_t(\mathscr{C})$ is the probability of being in configuration $\mathscr{C}$ at time t; $q_t(\mathscr{C})/p_t(\mathscr{C})$ is the average value of Y_t given the system is in configuration $\mathscr{C}$ at time t. These quantities tend toward the asymptotic steady-state forms[13]

$$p_t(\mathscr{C})\to p(\mathscr{C}) \qquad \text{and} \qquad q_t(\mathscr{C})\to Jtp(\mathscr{C})+r(\mathscr{C}), \tag{3}$$

in the long-time limit.

Here J is a current defined by $J=\partial_t\langle Y_t\rangle$ and is found, by substituting the asymptotics into the evolution equation for $\langle Y_t\rangle$, to be

$$J=\sum_{\mathscr{C},\mathscr{C}'}[M_1(\mathscr{C},\mathscr{C}')-M_{-1}(\mathscr{C},\mathscr{C}')]\,p(\mathscr{C}'). \tag{4}$$

The diffusion constant Δ associated with the current J is defined as $\Delta=\partial_t(\langle Y_t^2\rangle-\langle Y_t\rangle^2)$. Then substituting the asymptotics (3) into the evolution equations for $\langle Y_t\rangle$ and $\langle Y_t^2\rangle$ yields

$$\begin{aligned}\Delta=&\sum_{\mathscr{C},\mathscr{C}'}[M_1(\mathscr{C},\mathscr{C}')+M_{-1}(\mathscr{C},\mathscr{C}')]\,p(\mathscr{C}')\\ &+2\sum_{\mathscr{C},\mathscr{C}'}[M_1(\mathscr{C},\mathscr{C}')-M_{-1}(\mathscr{C},\mathscr{C}')]\,r(\mathscr{C}')-2J\sum_{\mathscr{C}}r(\mathscr{C}).\end{aligned} \tag{5}$$

The quantities $p(\mathscr{C})$ and $r(\mathscr{C})$ are determined by substituting the asymptotic forms (3) into the evolution equations for $p_t(\mathscr{C})$ and $q_t(\mathscr{C})$, which are obtained from (2): $p(\mathscr{C})$ satisfies

$$\sum_{\mathscr{C}'}[M(\mathscr{C},\mathscr{C}')\,p(\mathscr{C}')-M(\mathscr{C}',\mathscr{C})\,p(\mathscr{C})]=0, \tag{6}$$

where the total transition matrix $M = M_0 + M_1 + M_{-1}$, and $r(\mathscr{C})$ satisfies

$$\sum_{\mathscr{C}'} [M(\mathscr{C}, \mathscr{C}')\, r(\mathscr{C}') - M(\mathscr{C}', \mathscr{C})\, r(\mathscr{C})] = J p(\mathscr{C}) - \sum_{\mathscr{C}'} [M_1(\mathscr{C}, \mathscr{C}') - M_{-1}(\mathscr{C}, \mathscr{C}')]\, p(\mathscr{C}'). \tag{7}$$

Although (7) only fixes $r(\mathscr{C})$ up to a term proportional to $p(\mathscr{C})$, this term will cancel from (5), so we take without loss of generality

$$\sum_{\mathscr{C}} r(\mathscr{C}) = 0. \tag{8}$$

3. EINSTEIN RELATION FOR SYSTEMS SATISFYING DETAILED BALANCE

We now illustrate how one may exploit the approach outlined in Section 2 in order to obtain an Einstein relation in the case where the dynamics obey detailed balance.

Firstly, the condition under which detailed balance holds is

$$M(\mathscr{C}, \mathscr{C}')\, p(\mathscr{C}') = M(\mathscr{C}', \mathscr{C})\, p(\mathscr{C}). \tag{9}$$

Under the assumption that if Y_t increases by one on going from $\mathscr{C}$ to $\mathscr{C}'$, then Y_t decreases by one on going from $\mathscr{C}'$ to $\mathscr{C}$, (9) implies

$$M_1(\mathscr{C}, \mathscr{C}')\, p(\mathscr{C}') = M_{-1}(\mathscr{C}', \mathscr{C})\, p(\mathscr{C}), \tag{10}$$

$$M_{-1}(\mathscr{C}, \mathscr{C}')\, p(\mathscr{C}') = M_1(\mathscr{C}', \mathscr{C})\, p(\mathscr{C}). \tag{11}$$

Using these in Eq. (4) implies that the current $J = 0$. Therefore, from (7), we find that $r(\mathscr{C})$ satisfies

$$\sum_{\mathscr{C}'} [M(\mathscr{C}, \mathscr{C}')\, r(\mathscr{C}') - M(\mathscr{C}', \mathscr{C})\, r(\mathscr{C})] = -\sum_{\mathscr{C}'} [M_1(\mathscr{C}, \mathscr{C}') - M_{-1}(\mathscr{C}, \mathscr{C}')]\, p(\mathscr{C}'). \tag{12}$$

Next, we consider a perturbation which couples only to dynamics which evolve the random variable Y_t, i.e., the perturbed transition matrix is written

$$M(\mathscr{C}, \mathscr{C}') = M_0(\mathscr{C}, \mathscr{C}') + e^{\gamma} M_1(\mathscr{C}, \mathscr{C}') + e^{-\gamma} M_{-1}(\mathscr{C}, \mathscr{C}'), \tag{13}$$

where γ, which measures the strength of the perturbation, is small (and where $M(\mathscr{C},\mathscr{C})=0$). Then, to first order in γ, the steady-state Master equation (6) requires that

$$\sum_{\mathscr{C}'}\left[M(\mathscr{C},\mathscr{C}')\frac{\partial p(\mathscr{C}')}{\partial\gamma}-M(\mathscr{C}',\mathscr{C})\frac{\partial p(\mathscr{C})}{\partial\gamma}\right]$$
$$=-\sum_{\mathscr{C}'}\left[\frac{\partial M(\mathscr{C},\mathscr{C}')}{\partial\gamma}p(\mathscr{C}')-\frac{\partial M(\mathscr{C}',\mathscr{C})}{\partial\gamma}p(\mathscr{C})\right] \tag{14}$$

We can use (13) in the r.h.s. of this equation along with the detailed balance conditions (10), (11) to write

$$\sum_{\mathscr{C}'}\left[M(\mathscr{C},\mathscr{C}')\frac{\partial p(\mathscr{C}')}{\partial\gamma}-M(\mathscr{C}',\mathscr{C})\frac{\partial p(\mathscr{C})}{\partial\gamma}\right]$$
$$=-2\sum_{\mathscr{C}'}\left[M_1(\mathscr{C},\mathscr{C}')-M_{-1}(\mathscr{C},\mathscr{C}')\right]p(\mathscr{C}'). \tag{15}$$

By comparing Eqs. (12) and (15) we deduce

$$2r(\mathscr{C})=\frac{\partial p(\mathscr{C})}{\partial\gamma}. \tag{16}$$

Therefore we can express the diffusion constant, given by (5), in terms of the response of the steady state to the applied field:

$$\Delta=\sum_{\mathscr{C},\mathscr{C}'}\left[M_1(\mathscr{C},\mathscr{C}')+M_{-1}(\mathscr{C},\mathscr{C}')\right]p(\mathscr{C}')$$
$$+\sum_{\mathscr{C},\mathscr{C}'}\left[M_1(\mathscr{C},\mathscr{C}')-M_{-1}(\mathscr{C},\mathscr{C}')\right]\frac{\partial p(\mathscr{C}')}{\partial\gamma}. \tag{17}$$

From (4) the expression of the response $\partial J/\partial\gamma$ of the current to the perturbation (13), to first order in γ, is the same as the r.h.s. of (17). Thus,

$$\Delta=\frac{\partial J}{\partial\gamma}, \tag{18}$$

which is the usual equilibrium Einstein relation.

Thus we have demonstrated an Einstein relation for all finite-state stochastic models which obey detailed balance (in the absence of the perturbing field). Previously Einstein relations have been derived for particular models in this class. For example, the symmetric exclusion process[17] and the zero-field repton model of polymer dynamics.[18]

4. EINSTEIN RELATION FOR NONEQUILIBRIUM STEADY STATES

In the absence of detailed balance, the structure of the steady state is not known in general and it is not known how to formulate an Einstein relation.

For the case of detailed balance we showed in the previous section that the Einstein relation resulted from the simple relationship given in Eq. (16), between $r(\mathscr{C})$ and the response of $p(\mathscr{C})$ to the applied field. Inspired by this, in the following in cases where detailed balance doesn't hold, our aim is to find a perturbation, parameterised by a rate γ, such that

$$2r(\mathscr{C}) = \Omega \frac{\partial p(\mathscr{C})}{\partial \gamma}, \tag{19}$$

where Ω is a constant of proportionality.

4.1. Simple Case of Usual Einstein Relation

For a perturbation of the form (13), it is clear by comparing (7) and (14) that (19) holds for the class of models which satisfies the condition

$$J = \sum_{\mathscr{C}'} [M_1(\mathscr{C}', \mathscr{C}) - M_{-1}(\mathscr{C}', \mathscr{C})], \tag{20}$$

for all configurations $\mathscr{C}$. Using the condition (8), the diffusion constant for this class of models can be written

$$\Delta = \sum_{\mathscr{C}, \mathscr{C}'} [M_1(\mathscr{C}, \mathscr{C}') + M_{-1}(\mathscr{C}, \mathscr{C}')]\, p(\mathscr{C}'), \tag{21}$$

which using the expression for J (4) yields the usual Einstein relation (18). Thus (20) is a simple condition for the usual Einstein relation to hold for nonequilibrium systems.

We now show that the condition (20) holds for the boundary driven symmetric exclusion process. This is a stochastic model defined on a lattice of N sites, where each site i is either occupied by a particle (indicated by the variable n_i taking value 1) or vacant (indicated by $n_i = 0$). In one dimension, the dynamics in the bulk are defined such that particles hop to the right (which we represent as the process $1\ 0 \to 0\ 1$) or the left (the process $0\ 1 \to 1\ 0$) with rate 1. At the left-hand boundary site, particles are injected with rate $1-\rho_L$ and removed with rate ρ_L and at the right-hand boundary site, particles are removed with rate ρ_R and injected with rate $1-\rho_R$. Thus the system is in contact with boundary reservoirs at densities

ρ_L at the left-hand boundary and ρ_R at the right-hand boundary. This forces a current through the system (provided $\rho_L \neq \rho_R$) and in the steady state the density profile is linear.

We define Y_t such that it is increased (decreased) every time a particle is added (removed) at the left-hand boundary, every time a particle hops to the right (left), or every time a particle is removed (added) at the right-hand boundary. In the absence of the perturbation, the exact current is[19]

$$J = \rho_R - \rho_L. \tag{22}$$

(Note that the current across a bond is $J/(N+1)$.) To verify that (20) holds, this is to be compared with

$$\begin{aligned} \sum_{\mathscr{C}'} [M_1(\mathscr{C}', \mathscr{C}) - M_{-1}(\mathscr{C}', \mathscr{C})] \\ &= (1-\rho_L)(1-n_1) - \rho_L n_1 + \rho_R n_N - (1-\rho_R)(1-n_N) \\ &\quad + \sum_{i=0}^{N-1} [n_i(1-n_{i+1}) - (1-n_i)\, n_{i+1}]. \end{aligned} \tag{23}$$

For any configuration $\mathscr{C} = \{n_i\}$, the terms in the sum over i cancel except near the boundaries, and one obtains

$$\sum_{\mathscr{C}'} [M_1(\mathscr{C}', \mathscr{C}) - M_{-1}(\mathscr{C}', \mathscr{C})] = \rho_R - \rho_L, \tag{24}$$

for every configuration $\mathscr{C}$. Therefore the condition (20) holds and the Einstein relation (18) follows.

The class of models for which (20) holds includes the boundary driven symmetric zero-range process and other models where detailed balance is broken by the boundary dynamics, i.e., models which would satisfy detailed balance if periodic boundary conditions were imposed.

4.2. Einstein Relation for the ASEP

We now consider the asymmetric simple exclusion process (ASEP). In one dimension the model, with periodic boundary conditions, is defined such that particles hop only to the right with rate 1 (i.e., the process $1\ 0 \to 0\ 1$). In the steady state, all configurations occur with equal likelihood, so $p(\mathscr{C})$ is given by the binomial coefficient,

$$p(\mathscr{C}) = \left[\binom{N}{M}\right]^{-1} \equiv Z_{N,M}^{-1}, \tag{25}$$

for a ring of N sites containing M particles. For the ASEP neither detailed balance nor the condition (20) are satisfied. However, by considering a perturbation which creates and annihilates particles, an Einstein relation can be derived in the following way.

We define Y_t such that it is incremented every time any particle performs a hop, so the current (4) is given by

$$J = N Z_{N,M}^{-1} Z_{N-2,M-1}, \tag{26}$$

and using Eq. (7), $r(\mathscr{C})$ must satisfy

$$\sum_{\mathscr{C}'} [M(\mathscr{C},\mathscr{C}')\, r(\mathscr{C}') - M(\mathscr{C}',\mathscr{C})\, r(\mathscr{C})] = (N Z_{N,M}^{-1} Z_{N-2,M-1} - l_{10})\, p(\mathscr{C}), \tag{27}$$

where $l_{10} = \sum_{i=1}^{N} n_i(1-n_{i+1})$ is the number of 1 0 configurations across all bonds in the system configuration $\mathscr{C}$.

Now consider the perturbed transition matrix for the ASEP,

$$M(\mathscr{C},\mathscr{C}') = M_1(\mathscr{C},\mathscr{C}') + M_\gamma(\mathscr{C},\mathscr{C}'), \tag{28}$$

where the elements of $M_1(\mathscr{C},\mathscr{C}')$ describe the unperturbed ASEP and the elements of $M_\gamma(\mathscr{C},\mathscr{C}')$ describe the following processes that occur at all pairs of nearest neighbour sites

$$\begin{aligned} 1\ 1 &\xrightarrow{\gamma\epsilon_1} 1\ 0, \qquad & 1\ 1 &\xrightarrow{\gamma\epsilon_3} 0\ 1,\\ 0\ 0 &\xrightarrow{\gamma\epsilon_2} 1\ 0, \qquad & 0\ 0 &\xrightarrow{\gamma\epsilon_4} 0\ 1, \end{aligned} \tag{29}$$

where γ is a rate and $\{\epsilon_i\}$ measure the relative strengths of the four processes. Since this perturbation creates and annihilates particles, the different particle sectors (i.e., configurations with the same number of particles) are now connected by the dynamics. This modifies the steady state: if we define $P(M)$ to be the (normalised) probability that the system is in the sector containing M particles, then, for $\gamma \to 0$, the probability that the system is in the configuration $\mathscr{C}$ in the M-particle sector, $p_M(\mathscr{C})$, can be written as

$$p_M(\mathscr{C}) = P(M)\, p(\mathscr{C}) \tag{30}$$

where $p(\mathscr{C})$ is the steady state probability in the absence of the perturbation. $P(M)$ is determined by the following balance condition with respect to transitions between particle sectors in the limit $\gamma \to 0$:

$$(\epsilon_1 + \epsilon_3)\, \langle 1\ \ 1 \rangle_{M+1}\, P(M+1) = (\epsilon_2 + \epsilon_4)\, \langle 0\ \ 0 \rangle_M\, P(M), \tag{31}$$

where $\langle \cdot \rangle_M$ represents a correlation function calculated with the respect to the steady state (25) in the M-particle sector. Since in the limit $\gamma \to 0$ all configurations within each sector are equally likely, these correlation functions are easily found to be $\langle 1\ 1 \rangle_{M+1} = Z_{N,M+1}^{-1} Z_{N-2,M-1}$ and $\langle 0\ 0 \rangle_M = Z_{N,M}^{-1} Z_{N-2,M}$. Consequently the solution of (31) is readily obtained as

$$P(M) = \Lambda_N^{-1} \left(\frac{\epsilon_2 + \epsilon_4}{\epsilon_1 + \epsilon_3} \right)^M Z_{N,M} Z_{N-2,M-1}, \tag{32}$$

leading to the modified steady state $p_M(\mathscr{C})$ given by

$$p_M(\mathscr{C}) = \left(\frac{\epsilon_2 + \epsilon_4}{\epsilon_1 + \epsilon_3} \right)^M \Lambda_N^{-1} Z_{N-2,M-1}, \tag{33}$$

where Λ_N is a normalisation, fixed by the requirement that $\sum_M P(M) = 1$.

For the ASEP, (19) is shown to hold as follows. By (14),

$$\sum_{\mathscr{C}'} \left[M(\mathscr{C}, \mathscr{C}') \frac{\partial p_M(\mathscr{C}')}{\partial \gamma} - M(\mathscr{C}', \mathscr{C}) \frac{\partial p_M(\mathscr{C})}{\partial \gamma} \right]$$

$$= (\epsilon_1 + \epsilon_3)\, l_{11}\, p_M(\mathscr{C}) + (\epsilon_2 + \epsilon_4)\, l_{00}\, p_M(\mathscr{C}) - \epsilon_1 l_{10}\, p_{M+1}(\mathscr{C}) - \epsilon_3 l_{01}\, p_{M+1}(\mathscr{C})$$
$$- \epsilon_2 l_{10}\, p_{M-1}(\mathscr{C}) - \epsilon_4 l_{01}\, p_{M-1}(\mathscr{C}). \tag{34}$$

The r.h.s. is simplified by noting that $l_{10} = l_{01}$ and $l_{11} + l_{10} = M$ and $l_{00} + l_{10} = N - M$, using (33), and exploiting the identity $Z_{N,M} = Z_{N-2,M-2} + 2Z_{N-2,M-1} + Z_{N-2,M}$. Thus, it is straightforward to show that the r.h.s. of (34) is proportional to the r.h.s. of Eq. (27), therefore $r(\mathscr{C})$ is proportional to $\partial p_M(\mathscr{C})/\partial \gamma$ and the constant of proportionality Ω is

$$\Omega = \left(\frac{\epsilon_2 + \epsilon_4}{\epsilon_1 + \epsilon_3} \right)^{-M} \Lambda_N Z_{N,M}^{-2}. \tag{35}$$

Hence the diffusion constant (5) can be expressed in terms of the response of the steady state to the perturbation, leading to an Einstein relation of the form

$$\Delta = J + \Omega \frac{\partial J}{\partial \gamma}. \tag{36}$$

Thus for the ASEP we have shown that an Einstein relation (36) holds which expresses the diffusion constant as the current J plus the response of the current to perturbations (29) that create and annihilate particles. However it should be noted that not all perturbations that create and annihilate particles lead to (19). For example creating and annihilating particles at a site regardless of the occupation of neighbouring sites does not satisfy (19).

It can be shown that a relation of the form (19) holds for several variations of the ASEP under suitable perturbations which we now describe.

(a) Partially asymmetric exclusion: in the partially asymmetric exclusion process (PASEP) particles hop to the left with rate q and to the right with rate p (if the target sites are empty). This model can be treated, as above, by introducing the perturbation (29), leading to an Einstein relation of the form

$$\Delta = \frac{p+q}{p-q} J + (p-q)\, \Omega\, \frac{\partial J}{\partial \gamma}, \tag{37}$$

where the current $J = (p-q)\, Z_{N,M}^{-1} Z_{N-2,M-1}$ and Ω is given by (35).

(b) PASEP in higher dimension: an Einstein relation holds for the PASEP in any dimension, on a hypercubic lattice with fully periodic boundary conditions. To illustrate this, consider a two dimensional square lattice on which particles hop up and to the right with rate p, and down and to the left with rate q. The random variable Y_t is defined such that Y_t increases whenever a particle hops up or to the right and decreases whenever a particle hops down or to the left. By considering a perturbation

$$1\ 1 \xrightarrow{\gamma} 1\ 0, \qquad 1\ 1 \xrightarrow{\gamma} 0\ 1, \qquad 0\ 0 \xrightarrow{\gamma} 1\ 0, \qquad 0\ 0 \xrightarrow{\gamma} 0\ 1,$$

applied to horizontal pairs of nearest neighbour sites, and

$$\begin{matrix}1\\1\end{matrix} \xrightarrow{\gamma} \begin{matrix}0\\1\end{matrix}, \quad \begin{matrix}1\\1\end{matrix} \xrightarrow{\gamma} \begin{matrix}1\\0\end{matrix}, \quad \begin{matrix}0\\0\end{matrix} \xrightarrow{\gamma} \begin{matrix}0\\1\end{matrix}, \quad \begin{matrix}0\\0\end{matrix} \xrightarrow{\gamma} \begin{matrix}1\\0\end{matrix},$$

applied to vertical pairs of nearest neighbour sites, an Einstein relation of the form (37) can be derived, where Ω is given by $\Omega = \Lambda_N Z_{N,M}^{-2}$.

Further, if the dynamics are such that particles hop up and down with the same rate 1, and to the right with rate p and to the left with rate q, then, again, the Einstein relation (37) can be derived. This is achieved by defining Y_t such that Y_t is increased when a particle hops to the right and decreased when a particle hops to the left (i.e., Y_t is unaltered by hops up or down). The perturbation (29) is then applied to pairs of nearest neighbour sites only along the axis of asymmetric hopping.

(c) A marked bond: if Y_t is incremented only whenever a particle hops across a single, specified bond (the "marked" bond), then a perturbation applied across this bond only and defined by the processes

$$1\ 1 \xrightarrow{\gamma} 1\ 0, \qquad 0\ 0 \xrightarrow{\gamma} 1\ 0, \qquad 0\ 1 \xrightarrow{\gamma} 1\ 0, \tag{38}$$

yields a relation of the form (36) with $\Omega = \Lambda_N Z_{N,M}^{-2}$.

Finally we note that for symmetric hopping, which satisfies detailed balance, the kinds of perturbations given in this section (i.e., those linking particle sectors without coupling to the original dynamics) do not satisfy the condition (19)—rather, the appropriate perturbation couples only to the hopping dynamics, as discussed in Section 3.

4.3. Einstein Relation for Dimer Diffusion

In a similar way to the ASEP discussed in the previous subsection, we are also able to obtain an Einstein relation for (reconstituting) dimer diffusion: the process

$$1\ 1\ 0 \longrightarrow 0\ 1\ 1, \tag{39}$$

which occurs at all nearest neighbour triples of sites with rate 1. We assume the density is greater than one half so that there are no configurations where all particles are isolated. Again, in the steady state of this model, all configurations are equally likely; we define Y_t such that it increases by one every time the process (39) takes place (anywhere on the lattice), hence the current is given by $J = NZ_{N,M}^{-1} Z_{N-3,M-2}$. The Einstein relation (36) is derived for a perturbation defined by the processes

$$1\ 1\ 1 \xrightarrow{\gamma} 1\ 1\ 0, \qquad 1\ 0\ 0 \xrightarrow{\gamma} 1\ 1\ 0, \qquad 1\ 0\ 1 \xrightarrow{\gamma} 1\ 1\ 0. \tag{40}$$

As before, the steady state distribution is modified to accommodate a balance condition with respect to transitions between particle sectors cf. (31). Using the same reasoning as that applied to the ASEP, $r(\mathscr{C})$ is shown to be proportional the the response of the steady state to the perturbation, where the constant of proportionality Ω is

$$\Omega = \Lambda_N Z_{N-1,M-1}^{-1} Z_{N,M}^{-1}, \tag{41}$$

and the diffusion constant and the response of the current to the perturbation are related by the Einstein relation given in Eq. (36).

4.4. Einstein Relation for the Boundary Driven ASEP

The boundary driven asymmetric simple exclusion process also satisfies an Einstein relation. In this model, particles can hop only to the right, and the multiple occupancy of any site is still forbidden. At the left-hand boundary site particles are injected with rate α and at the right-hand boundary site they are removed with rate β. In this case, Y_t is incremented every time a particle is added at the left-hand boundary site. Along the special line $\alpha+\beta=1$, all configurations in the same particle sector are equally likely in the steady state, and it is known that[16]

$$r(\mathscr{C}) = \alpha(1-\alpha)\,\frac{dp(\mathscr{C})}{d\alpha}, \tag{42}$$

is a solution of (7). This perturbation corresponds to a small increase in α away from the line $\alpha+\beta=1$, thereby changing slightly the density of the left-hand boundary reservoir. Hence, one finds an Einstein relation of the form

$$\Delta = (2\alpha-1)\,J + 2\alpha(1-\alpha)\,\frac{\partial J}{\partial\alpha}. \tag{43}$$

5. CONCLUSION

In this work we have investigated the existence of Einstein relations for stochastic, lattice models. Within the framework reviewed in Section 2 we have shown that an Einstein relation will result if one can express the quantities $r(\mathscr{C})$ as the response of the steady state probabilities $p(\mathscr{C})$ to a perturbation. For the case of detailed balance we showed that this can always be done through the perturbation (13) which yields the usual Einstein relation (18). Further for a class of nonequilibrium steady states where (20) holds one again has the usual Einstein relation. This class includes models where detailed balance is broken only by the boundary dynamics such as boundary-driven symmetric exclusion.[8, 10]

Turning to systems where detailed balance is lacking even under periodic boundary conditions we have found nonequilibrium generalizations of the Einstein relation for some specific models. In these cases the perturbation creates and annihilates particles, breaking the conservation law of the unperturbed dynamics.

The models for which we succeeded in finding an Einstein relation had the simplifying property that in each particle sector all configurations are equally likely. It remains a challenge to establish whether Einstein relations hold for more general nonequilibrium steady states. Natural starting points would be steady states that have a simple structure such as the one dimensional KLS model.[7]

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