

# Nonequilibrium stationary states and equilibrium models with long range interactions

Richard Brak<sup>1</sup>, Jan de Gier<sup>1</sup> and Vladimir Rittenberg<sup>2</sup>

<sup>1</sup> Department of Mathematics and Statistics, University of Melbourne, VIC 3010, Australia

<sup>2</sup> Physikalisches Institut, Nußallee 12, Bonn University, 53115 Bonn, Germany

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## Abstract

It was recently suggested by Blythe and Evans that a properly defined steady state normalization factor can be seen as a partition function of a fictitious statistical ensemble in which the transition rates of the stochastic process play the role of fugacities. In analogy with the Lee–Yang description of phase transition of equilibrium systems, they studied the zeros in the complex plane of the normalization factor in order to find phase transitions in nonequilibrium steady states. We show that like for equilibrium systems, the ‘densities’ associated with the rates are nondecreasing functions of the rates and therefore one can obtain the location and nature of phase transitions directly from the analytical properties of the ‘densities’. We illustrate this phenomenon for the asymmetric exclusion process. We actually show that its normalization factor coincides with an equilibrium partition function of a walk model in which the ‘densities’ have a simple physical interpretation.

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## 1. Introduction

The extension of concepts used in equilibrium statistical mechanics, such as the free energy, to nonequilibrium steady states is a subject of great interest [1, 2]. That a simple extension is not possible can be seen in [3] where it was shown that in certain cases, the free energy functional is not a convex function of the density. On the other hand, Arndt [4] has shown in the example of the totally asymmetric simple exclusion model (TASEP) that applying the Lee–Yang description using the zeros of an *ad hoc* definition of a grand-canonical partition function gives the correct phase transition. Further applications of this idea can be found in [5–7]. In a very interesting new development, Blythe and Evans [8] considered the normalization of the stationary state of several stochastic systems as a function of the transition rates and applied the Lee–Yang approach in the same way as one would for an equilibrium partition function. While a normalization may seem to be defined ambiguously, it was noted

in [9, 10] that in a formal way, a unique definition of this normalization can be made using the matrix-tree theorem, which has a long history in graph theory going back to Sylvester [11], see also [12, 13] and sections 2 and 4. This connection explicitly relates the normalization of a stationary state to the combinatorial problem of counting weighted spanning trees on graphs, which implies a direct interpretation of the normalization as a statistical mechanical partition sum. Can we learn anything about the steady state phase diagram from the spanning trees? There are a few problems with that. For example, it is generically unclear how the order parameters describing the spanning trees relate to those describing the steady state, and vice versa. Secondly, the normalization as defined above may not be ‘minimal’ in the sense that it may contain an overall nontrivial polynomial factor which is common to each of the stationary state weights. Such a polynomial factor cannot contribute to the phase behaviour of the stationary state. We will call the normalization as defined via the matrix-tree theorem but with common factors removed the *reduced* normalization.

The purpose of this paper is to try to bring a better understanding of the Blythe–Evans approach which is summarized in section 2. In this section, we also show that to each transition rate one can formally associate ‘particle numbers’ the same way one relates particle numbers to fugacities. Moreover, like in thermodynamics, one can prove that the ‘particle numbers’ are nondecreasing functions of the transition rates. This important observation allows us to detect the existence of phase transitions from the behaviour of the ‘particle numbers’ in the space of transition rates. At this point the physical meaning of the ‘particles’ is completely obscure (there are as many kinds of ‘particles’ as the number of independent transition rates minus one). Moreover, the thermodynamic potential defined through the (reduced) normalization factor is not necessarily an extensive quantity. The volume, defined by the leading asymptotic behaviour of the normalization, and therefore the definition of the ‘densities’ might change in the space of transition rates. This allows for phase transitions not encountered in equilibrium models with local interactions. This phenomenon appears in the following way. In a certain domain of the fugacities, the ‘densities’ span the entire interval between zero and one. This defines a ‘phase’ (inside this domain one can have, like in equilibrium, several phase transitions). The boundary of the domain separates it from another domain (‘phase’) where one has to take another definition of the ‘densities’ because of the change of the volume. In this second phase the ‘densities’ are not necessarily finite.

The fact that the reduced normalization factor might have a direct physical interpretation is known from the raise and peel model [14]. This is a one-dimensional stochastic model with nonlocal transition rates and its reduced normalization factor (whose logarithm is proportional to the square of the system size) coincides with the number of configurations of the two-dimensional ice model with domain-wall boundary condition—an equilibrium problem. In a different context [2], it was shown that certain nonequilibrium expectation values in the boundary sine-Gordon model coincide with associated equilibrium state expectation values. It is our aim to show that a similar mapping exists for the TASEP.

In section 3, we define the one-transit walk (OTW) model. This model, which is not parity invariant, depends on two parameters which are the Boltzmann weights or fugacities of contact points. We compute the partition function of this model as well as the two densities corresponding to the two fugacities. The two densities have a clear physical meaning. The phase diagram of the OTW model is obtained from the expressions for these densities. It is the same as that of the TASEP [15–19] if we replace the two fugacities with the boundary rates of TASEP. As we are going to show, the derivation of the phase diagram of the TASEP model from the analytic properties of the number of ‘particles’ as a function of fugacities will give a better understanding of the nature of the phase transitions. In section 3.5, we discuss the microscopic properties of the OTW model making clear the connection with the TASEP. The

connection between the TASEP normalization calculation and a random walk was first noted in [16] and further developed in [28]. We conclude with a discussion of the phase diagram obtained from the ‘densities’ of the partially asymmetric simple exclusion process (PASEP) [20, 21]. In this case we have three kinds of ‘particle’ numbers: two associated with the boundary rates and one associated with the back hopping rate  $q$ . At the symmetric point  $q = 1$  a new kind of phase transition occurs. The number of ‘particles’  $N(q)$  associated with the rate  $q$  is proportional to the length  $n$  of the system for  $q < 1$  and to  $n^2$  for  $q > 1$ .

Our conclusions are presented in section 5.

## 2. The normalization as a positive polynomial

Let us start by considering an arbitrary Markov process in continuous time on a state space spanned by the states  $\{|a\rangle\}_{a=1}^n$ , whose master equation is given by

$$\frac{d}{dt} \bar{P}_t(a) = \sum_{b \neq a} (r_{ab} \bar{P}_t(b) - r_{ba} \bar{P}_t(a)). \quad (1)$$

The  $r_{ab}$  are the transition rates from state  $|b\rangle$  to  $|a\rangle$  and  $\bar{P}_t(a)$  is the (unnormalized) probability to find the system at time  $t$  in state  $|a\rangle$ . Equation (1) can be conveniently rewritten as

$$\frac{d}{dt} |\bar{P}_t\rangle = -H |\bar{P}_t\rangle \quad |\bar{P}_t\rangle = \sum_{a=1}^n \bar{P}_t(a) |a\rangle \quad (2)$$

where  $H$  is the matrix with off-diagonal elements  $H_{ab} = -r_{ab}$  and whose columns add up to zero. One of the main properties of interest of such a Markov process is its long time behaviour. In the limit  $t \rightarrow \infty$  the system approaches its stationary state  $|\bar{P}_\infty\rangle$ , which we will assume to exist and for simplicity to be unique, given by

$$H |\bar{P}_\infty\rangle = 0. \quad (3)$$

The stationary state is thus given by the right eigenvector of the matrix  $H$  corresponding to its eigenvalue 0. This equation can be solved in the following formal way, see e.g. [22]. Let  $H(a, b)$  be the matrix corresponding to  $H$  with the  $a$ th row and  $b$ th column removed. The cofactor  $X(a, b)$  is then defined by,

$$X(a, b) = (-1)^{a+b} \det H(a, b). \quad (4)$$

If the eigenvalue 0 is unique,

$$0 = \det H = \sum_b H_{ab} X(a, b) = \sum_b H_{ab} X(b, b) \quad (5)$$

where we have used  $X(a, b) = X(b, b)$  for all  $a$  (see appendix A). We see that the eigenvalue equation (3) is solved by the cofactors of  $H$ ,

$$H |P\rangle = 0 \quad P(b) = X(b, b). \quad (6)$$

This solution fixes a particular normalization of the eigenvector for all system sizes. This normalization is uniquely defined up to an overall rescaling of  $H$ , or equivalently a rescaling of time (which can vary with the system size). To be able to interpret  $P(b)$  as a probability distribution, we write

$$\bar{P}_\infty(b) = P(b)/Z_n \quad Z_n = \sum_{b=1}^n P(b) = \sum_{b=1}^n X(b, b). \quad (7)$$

It can be shown using the matrix-tree theorem [12, 13] that the normalization  $Z_n$  of a stationary state of any stochastic (Markov) process is always given by a homogeneous

polynomial in the rates  $r_{ab}$  (some of which might be equal or be zero), of degree  $n - 1$  and with positive coefficients, i.e. it has the form of a generating function. A simple proof of this important statement is for example given in [22], which we have included in appendix A.

We would like to identify the rates  $r_{ab}$  as generalized Boltzmann factors or fugacities  $r_{ab} = z_{ab}$ , and  $Z_n(\{z_{ab}\})$  as a generalized partition sum for nonequilibrium systems. Since the normalization  $Z_n$  is a polynomial in the variables  $z_{ab}$  with positive coefficients, by the Cauchy–Schwartz inequality its negative logarithm,

$$F_n = -\log Z_n \quad (8)$$

is therefore a convex function in all its arguments  $z_{ab}$ . In analogy with equilibrium statistical mechanics, we will associate with each rate  $r_{ab} = z_{ab}$  a ‘particle number’  $N_{ab}$ ,

$$N_{ab} = -z_{ab} \frac{\partial F_n}{\partial z_{ab}}. \quad (9)$$

These numbers are positive and increasing functions of the fugacities for any size of the system but they are linearly dependent. One can arbitrarily choose one rate equal to one which fixes the time scale and leaves the remaining rates dimensionless. In this way we are left with one fugacity less. In the large  $n$  limit,

$$N_{ab} = V(n)\rho_{ab} \quad (10)$$

where  $V(n)$  is the volume and  $\rho_{ab}$  are the ‘densities’. One can now use the equilibrium approach to the theory of phase transitions and apply it to the densities  $\rho_{ab}$ . A ‘first-order phase transition’ corresponds to a discontinuity of the fugacity as a function of the density and a ‘second-order phase transition’ corresponds to the vanishing of the derivative of the fugacity. The physical meaning of these phase transitions is not obvious. Does a ‘second-order phase transition’ for example, correspond to an infinite correlation length? This remains as an open question. In section 3 we will show, in the case of TASEP, that using our procedure one recovers the known phase diagram.

It may happen however, as it will in our example below, that all cofactors  $X(b, b)$  contain a common nontrivial polynomial factor. Such a common factor will cancel out in  $\bar{P}_\infty(b)$  and hence cannot contribute to the nonequilibrium phase behaviour. In (8), however, it could give rise to spurious singularities that are not related to the physical phase transitions. In the example of section 3 no such spurious phase transitions appear (see section 4).

There is another major difference, however, between equilibrium systems with short-range interactions and the present problem: the ‘particle numbers’ are not necessarily extensive quantities (see the examples in sections 3.3 and 3.6). This implies that in the parameter space, the  $\rho_{ab}$  might diverge and we have to change the definition of the factor  $V(n)$  in (10). Actually such a phenomenon is also known in equilibrium problems with nonlocal interactions (see [23]) in the theory of special surface phase transitions [24]. As we are going to show in section 3.6 the analogy goes deeper.

The philosophy we adopt in this paper is to assign a physical meaning to the purely formally defined normalization factor and ‘densities’ by looking at simple weighted walk problems for which we can compute the partition functions. The weights of the configurations depend on parameters which correspond to the rates of the stochastic processes and the partition function coincides with the normalization factor defined in (7) if a common factor to all the cofactors is removed. In the following sections we illustrate this approach with the help of an example. We first consider a combinatorial problem which is interesting on its own. This is the one-transit walk model. We will compute its partition function and obtain the phase diagram of the model from the properties of the densities. We also show that the same partition function coincides with the normalization factor of the TASEP model.

### 3. The OTW model versus the TASEP

The TASEP has grown to be one of the main theoretical models of nonequilibrium statistical physics. This is not only due to its simplicity and general applicability, but also because its stationary probability distribution (SPDF) and other properties can be calculated exactly [15–19]. In this paper, we show that this SPDF can be regarded as an equilibrium probability distribution of a simple model of a walk near an interface. Since the walk model is an equilibrium system, it can be described thermodynamically using standard methods. The phase behaviour of the TASEP can be explained in terms of adsorption transitions of the walk on the interface.

In section 3.1 we briefly review the TASEP model with open boundaries. We furthermore present the DEHP algebra which is going to be used in section 3.4. In section 3.2, we introduce a model of a walk in the vicinity of a fixed interface. The walk is allowed to penetrate the interface once. Both ends of the walk are fixed but the point of penetration is free. An excess interface fugacity  $1/z_1$  is associated for contacts above the interface, and a fugacity  $1/z_2$  for contacts below. We call this model the OTW. The walk model without penetration was used as a simple model for polymer adsorption in [23]. After discussing the thermodynamics of the walk model, we show in section 3.4 that it is closely related to the TASEP with open boundaries. We show that the statistical mechanical partition function  $Z(z_1, z_2)$  of the OTW is equal to the reduced normalization of the stationary state of the TASEP if the interface fugacities in the walk model are equal to the input and output rates of the two reservoirs. After discussing the thermodynamics of the OTW we calculate the phase diagram exactly, see section 3.3. In section 3.4 we give the matrix algebra behind the OTW and its relation to the DEHP algebra.

It is remarkable that in the OTW model one can define a current density operator, whose average values coincide with those of the TASEP, see section 3.5. We also show that the thermodynamic TASEP density  $\rho$  and current  $J$  are related to the contact densities  $\rho_1$  and  $\rho_2$ , conjugate to  $z_1$  and  $z_2$  respectively, as

$$\frac{2\rho - 1}{J} = \frac{1 - \rho_2}{z_2} - \frac{1 - \rho_1}{z_1} \quad (11)$$

where

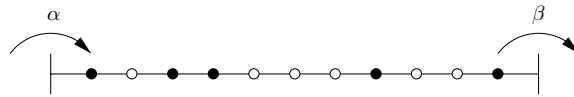
$$\omega = - \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n(z_1, z_2) \quad \rho_i = -z_i \frac{\partial \omega}{\partial z_i}. \quad (12)$$

These equations show that one may derive the thermodynamic behaviour of quantities for a nonequilibrium model from those of an equilibrium model. We hope to make contact between our approach and the formulation of a free energy functional for the TASEP from large deviation functions as adopted in [25, 26]. We would also like to point out that the walk model has an appealing analogy with a continuous model for the dynamics of shocks in terms of which the TASEP phase diagram can be explained quantitatively [27].

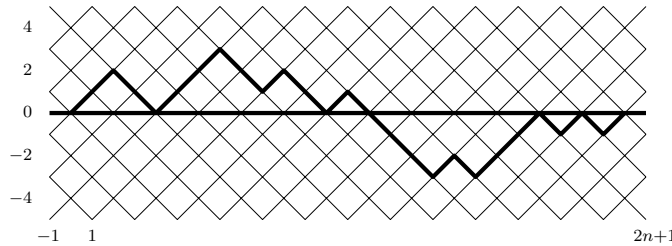
#### 3.1. The TASEP revisited

The asymmetric simple exclusion process in continuous time is a particle hopping model with excluded volume in one dimension, where particles hop from the left to the right with rate 1. In the presence of open boundaries, the input rate of particles on the left of the system is  $\alpha$  and the output rate on the right is  $\beta$ , see figure 1.

If the  $\tau_i \in \{0, 1\}$  denotes the presence or absence of a particle, one would for example like to know the probability  $P(\tau_1, \tau_2, \dots, \tau_n)$  to find a system in configuration  $\{\tau_1, \tau_2, \dots, \tau_n\}$  in the



**Figure 1.** Sample TASEP configuration. Particles enter the system from the left with rate  $\alpha$  and leave from the right with rate  $\beta$ . Particles hop in the bulk from left to right with rate 1.



**Figure 2.** An example of a one-transit walk starting at  $(0, 0)$  and ending at  $(2n, 0)$  crossing the  $x$ -axis only once.

long time limit. In this limit, all these probabilities are stationary, and in [15] this stationary state was calculated exactly. In [16] it was shown that this solution can be conveniently expressed in a matrix product form,

$$P(\tau_1, \dots, \tau_n) = \frac{1}{\tilde{Z}_n} \langle W | \prod_{i=1}^n (\tau_i D + (1 - \tau_i) E) | V \rangle \tag{13}$$

where the normalization  $\tilde{Z}_n$  is given by

$$\tilde{Z}_n = \langle W | (D + E)^n | V \rangle \tag{14}$$

and the matrices  $D$  and  $E$ , and the vectors  $\langle W |$  and  $|V\rangle$  are a representation of the so-called DEHP algebra,

$$DE = D + E \quad D|V\rangle = \frac{1}{\beta}|V\rangle \quad \langle W|E = \frac{1}{\alpha}\langle W|. \tag{15}$$

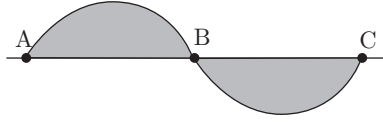
We will show that (14) is related to the partition function of the OTW model.

### 3.2. The one-transit model

Consider a statistical model of a path on the rotated square lattice. Paths start at  $(0, 0)$  and end at  $(2n, 0)$ , can only move in the North-East (NE) or in the South-East (SE) direction and cross the  $x$ -axis exactly once, see figure 2. We call such a path a OTW. Paths of this form that do not cross the  $x$ -axis are called Dyck paths. We associate energies  $-\varepsilon_1$  and  $-\varepsilon_2$  with the returns (or contact points) of the path above and below the  $x$ -axis, respectively. To make contact with section 2 we implement this in the following way. A fugacity  $z_1 = e^{\varepsilon_1/kT}$  is given to each down step, and  $z_2 = e^{\varepsilon_2/kT}$  to each up step, except those ending on the  $x$ -axis. This model is directly related to the canonical model of [28].

By reflecting the last part of the OTW in the  $x$ -axis, it can be easily seen that the total number of possible OTW paths is equal to the number of Dyck paths of length  $2n$ . It is known, see e.g. [29], that the number of Dyck paths with  $p$  returns is given by Ballot numbers,

$$B_{n,p} = \frac{p}{n} \binom{2n - p - 1}{n - 1} = \frac{p(2n - p - 1)!}{n!(n - p)!}. \tag{16}$$



**Figure 3.** The OTW always factorizes into two Dyck paths—one from A to B and above  $y = 0$ , and one from B to C and below  $y = 0$ .

The total number  $C_n$  of Dyck paths of length  $2n$  can be obtained by summing over  $p$  in (16), or by noting that it is equal to the number of Dyck paths of length  $2n + 2$  with exactly one return (for such a path the first and last step are fixed to be up and down, respectively),

$$C_n = \sum_{p=1}^n B_{n,p} = B_{n+1,1} = \frac{1}{n+1} \binom{2n}{n} \quad (17)$$

which is the Catalan number. The partition function of the one-transit model is simply given by

$$Z_n(z_1, z_2) = (z_1 z_2)^n \tilde{Z}_n(z_1, z_2) \quad (18)$$

where

$$\tilde{Z}_n(z_1, z_2) = \sum_{p=0}^n B_{n,p} \sum_{q=0}^p z_1^{-q} z_2^{-p+q}. \quad (19)$$

An OTW always factorizes into two Dyck paths as illustrated in figure 3.

It follows from this factorization that the partition sum of the OTW can also be written as

$$Z_n(z_1, z_2) = (z_1 z_2)^n \sum_{p=0}^n \tilde{Z}_p(z_1, \infty) \tilde{Z}_{n-p}(\infty, z_2). \quad (20)$$

This formula shows that we can also interpret our model as the combination of two contact models with a movable but impenetrable wall in between them at a random position, each position being equally probable. Equation (20) thus defines the partition function of an annealed system, i.e. where the partition sum is averaged over the random position of the wall.

The partition sum (20) is equal to  $(\alpha\beta)^n$  times the reduced normalization (14) of the TASEP [15–19] if the fugacities  $z_1$  and  $z_2$  are replaced by the boundary input and output rates  $\alpha$  and  $\beta$ . This result is important since it will allow us to associate the ‘densities’ defined formally from the reduced normalization of the TASEP with the physical densities of the OTW model. In section 3.4, we will go deeper into the relation between the OTW model and the TASEP, but before that we first describe the phase diagram of the OTW model.

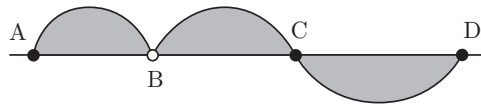
### 3.3. The phase diagram of the OTW model

We define the grand potential per site for the gas of contacts as

$$\omega = - \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_n. \quad (21)$$

Note that to get rid of spurious factors of 2 in subsequent formulae we divide by  $n$  instead of the system size  $2n$ . The potential  $\omega$  can be easily calculated from (20) once we know the asymptotic properties of  $\tilde{Z}_n(z, \infty) = \tilde{Z}_n(\infty, z)$ . This is well known, see e.g. [16, 23], and can for example be derived from the differential equation it satisfies,

$$-(1-z)(1-2z)\tilde{Z}'_n(z, \infty) + z(z+n(1-2z)^2)\tilde{Z}_n(z, \infty) = 2z^2 \frac{(2n-1)!}{n!^2}. \quad (22)$$



**Figure 4.** The OTW with one contact marked (the white circle at B), factorizes into a Dyck path from A to B, and an OTW from B to D.

Analysing the large  $n$  behaviour of this equation for the regions  $z > 1/2$ ,  $z = 1/2$  and  $z < 1/2$  we immediately obtain

$$\tilde{Z}_n(z, \infty) \approx \begin{cases} \frac{z}{(1-2z)^2} \frac{4^n}{\sqrt{\pi n^{3/2}}} & z > 1/2 \\ \frac{4^n}{\sqrt{\pi n^{1/2}}} & z = 1/2 \\ \frac{1-2z}{1-z} \frac{1}{z^n(1-z)^n} & z < 1/2. \end{cases} \tag{23}$$

The grand potential  $\omega$  is given by minimizing over the position of the domain wall, and is therefore given by

$$\omega(z_1, z_2) = -\log 4z_1z_2 + \inf_{0 \leq x \leq 1} \omega_x(z_1, z_2) \tag{24}$$

where

$$\omega_x(z_1, z_2) = \begin{cases} 0 & z_1, z_2 \geq 1/2 \\ x \log 4z_1(1-z_1) + (1-x) \log 4z_2(1-z_2) & \text{elsewhere.} \end{cases} \tag{25}$$

From (24) one finds the grand potential in all regions of the phase diagram,

$$\omega(z_1, z_2) = \begin{cases} -\log 4z_1z_2 & z_1, z_2 \geq 1/2 \\ -\log z_2 + \log(1-z_1) & z_1 < 1/2, z_2 > z_1 \\ -\log z_1 + \log(1-z_2) & z_2 < 1/2, z_1 > z_2. \end{cases} \tag{26}$$

We now turn to the calculation of the contact densities, which are the order parameters of the OTW model. From the definition of the walk model it immediately follows that the probabilities  $\langle \hat{a}_i \rangle_n$  and  $\langle \hat{b}_i \rangle_n$  to have a contact at site  $2i$  above or below the  $x$ -axis, are given by,

$$\langle \hat{a}_i \rangle_n = (z_1z_2)^i \frac{\tilde{Z}_i(z_1, \infty) Z_{n-i}(z_1, z_2)}{Z_n(z_1, z_2)} \tag{27}$$

$$\langle \hat{b}_i \rangle_n = (z_1z_2)^{n-i} \frac{Z_i(z_1, z_2) \tilde{Z}_{n-i}(\infty, z_2)}{Z_n(z_1, z_2)}. \tag{28}$$

The easiest way of seeing this is the fact that the OTW with a single contact marked—as illustrated in figure 4—factorizes into a Dyck path and a OTW.

We define the average number of contacts at  $x$  by

$$\langle \hat{a}_x \rangle = \langle \hat{a}_{xn} \rangle_n \quad \langle \hat{b}_x \rangle = \langle \hat{b}_{xn} \rangle_n \tag{29}$$

and find in the thermodynamic limit  $n \rightarrow \infty$ ,

$$(\langle \hat{a}_x \rangle, \langle \hat{b}_x \rangle) = \begin{cases} (0, 0) & z_1, z_2 \geq 1/2 \\ (\rho(z_1), 0) & z_1 < 1/2 \quad z_2 > z_1 \\ (0, \rho(z_2)) & z_2 < 1/2 \quad z_1 > z_2 \end{cases} \tag{30}$$

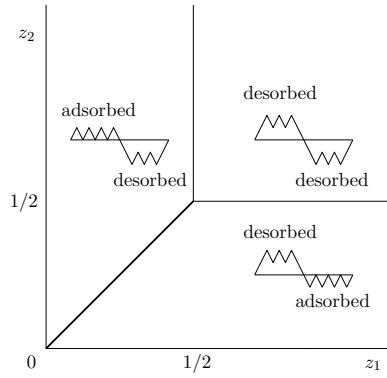


Figure 5. Phase diagram of the walk model.

with

$$\rho(z) = \frac{1 - 2z}{1 - z}. \quad (31)$$

In this limit, these numbers are independent of  $x$  except on the line  $z_1 = z_2 = z$  where we find

$$(\langle \hat{a}_x \rangle, \langle \hat{b}_x \rangle) = (\rho(z)(1 - x), \rho(z)x). \quad (32)$$

The total number of contacts above and below are denoted by  $\langle \hat{a} \rangle$  and  $\langle \hat{b} \rangle$ , respectively, and the corresponding thermodynamic densities can be calculated through derivatives of the grand potential,

$$a = \lim_{n \rightarrow \infty} \frac{\langle \hat{a} \rangle}{n} = 1 + z_1 \frac{\partial \omega}{\partial z_1} \quad b = 1 + z_2 \frac{\partial \omega}{\partial z_2}. \quad (33)$$

Note that  $\omega$  is not everywhere differentiable. If  $\omega$  is not differentiable in a point  $z_*$  we define

$$z_* \frac{\partial \omega}{\partial z}(z_*) = \lim_{\varepsilon \rightarrow 0} \frac{1}{2} \left( (z_* - \varepsilon) \frac{\partial \omega}{\partial z}(z_* - \varepsilon) + (z_* + \varepsilon) \frac{\partial \omega}{\partial z}(z_* + \varepsilon) \right). \quad (34)$$

With this definition, (33) is valid everywhere. Because we average over the position of the domain wall, the densities  $a$  and  $b$  are not independent. Their values can be easily calculated and are given by,

$$(a, b) = \begin{cases} (0, 0) & z_1, z_2 \geq 1/2 \\ (\rho(z_1), 0) & z_1 < 1/2 \quad z_2 > z_1 \\ (0, \rho(z_2)) & z_2 < 1/2 \quad z_1 > z_2 \\ (\rho(z)/2, \rho(z)/2) & z_1 = z_2 = z \leq 1/2. \end{cases} \quad (35)$$

Note that either both densities are equal or only one of the two does not vanish. This means that effectively one sees only one density. We thus find that for  $z_1, z_2 > 1/2$  the walk is entirely desorbed from the interface. When  $z_1 < 1/2$  and  $z_2 > z_1$  the walk is adsorbed above the interface, the contact density  $a$  is nonzero, while it is desorbed below and vice versa when  $z_2 < 1/2$  and  $z_1 > z_2$ , see figure 5.

The grand potential (26) is nonanalytic at the lines  $z_1 = 1/2$  when  $z_2 \geq z_1$  and  $z_2 = 1/2$  when  $z_1 \geq z_2$ . There is also a singularity at the line  $z_1 = z_2 = z$  when  $z < 1/2$ . These lines therefore indicate phase boundaries. There is a first-order phase transition along the line  $z_1 = z_2 = z$  for  $z < 1/2$  along which the mirror symmetry of the system is spontaneously broken. The sum of the two densities  $r = a + b$  varies continuously across the line but their difference  $d = a - b$  is discontinuous.

Above the line  $z_2 = 1/2 (z_1 \geq z_2)$  the densities of contact points  $a = \langle \hat{a} \rangle / n$  and  $b = \langle \hat{b} \rangle / n$  vanish as  $n \rightarrow \infty$ . Approaching the line  $z_2 = 1/2$  from above, the number of contacts  $\langle \hat{b} \rangle$  diverges like

$$\langle \hat{b} \rangle \sim \frac{1}{2z_2 - 1} \quad (36)$$

where we have used (23). Using the same equation, on the critical line  $z_2 = 1/2$  we get

$$b \sim n^{-1/2} = n^{-\phi} \quad (37)$$

and below the critical line

$$b \sim 1 - 2z_2 = (1 - 2z_2)^{1/\phi-1}. \quad (38)$$

A similar behaviour is obtained for the line  $z_1 = 1/2$  when  $z_2 \geq z_1$  and if we replace the density  $b$  by  $a$ . The critical behaviour (36) and (38) as well as the finite-size scaling behaviour (37) characterize a special surface phase transition [24] with a single critical exponent  $\phi = 1/2$ . A similar exponent is found in other equilibrium problems with long range interactions [23]. The interest in discussing the phase diagram comes from the fact that it gives another physical interpretation of the phase transitions observed in TASEP.

We conclude this section with a description of the model using the canonical ensemble. We now consider  $a$  and  $b$  as free parameters. The canonical free energy per site for given values of  $a$  and  $b$  can be calculated from the grand potential  $\omega(z_1, z_2)$ ,

$$f(a, b) = \sup_{z_1, z_2} ((1-a) \log z_1 + (1-b) \log z_2 + \omega(z_1, z_2)) \quad (39)$$

from which we find

$$f(a, b) = \max\{g(a, b), g(b, a)\} \quad (40)$$

$$g(a, b) = (1-a-b) \log(1-a) - (2-a-b) \log(2-a). \quad (41)$$

This result can be conveniently rewritten using  $r = a + b$  and  $d = a - b$  as

$$f(a, b) = \tilde{f}(r, d) = (1-r) \log \left( 1 - \frac{r+|d|}{2} \right) - (2-r) \log \left( 2 - \frac{r+|d|}{2} \right). \quad (42)$$

The phase diagram in figure 5 can then be rederived by minimizing

$$\tilde{f}(r, d) - (1-r) \log z_1 z_2 - d \log z_1 / z_2 \quad (43)$$

with respect to  $r$  and  $d$ . The first-order phase transition along the line  $z_1 = z_2 < 1/2$  is immediately apparent in (42) because of the discontinuity of the first derivative of  $|d|$ . Because  $r$  has to be positive, we find a second-order phase transition to the region  $z_1, z_2 > 1/2$  where  $r = 0$ . The canonical free energy per site can be used to calculate large deviations.

### 3.4. Connection with the totally asymmetric simple exclusion process

In [16], the stationary state of the TASEP was constructed using equivalent representations of the DEHP algebra given by (15). The reduced normalization calculated using this method is equal to the partition sum of the OTW model, given by (19), if the boundary rates of the TASEP are replaced by the contact fugacities of the OTW model. In this section we show more precisely how the OTW model of section 3.2 is related to the TASEP.

Following an observation by Brak and Essam [28] (see also [30]) that the different equivalent representations of the DEHP algebra can be interpreted as transfer matrices for various lattice walk models, we construct a new representation which will give the transfer

matrix for the OTW model. We will show that the partition function  $\tilde{Z}_n(z_1, z_2)$  can be written in the following form:

$$\tilde{Z} = \langle L|T^n|R \rangle \quad (44)$$

where  $T$  is the transfer matrix. We introduce a two-step transfer matrix  $T = T^o T^e$ , where

$$T^o = \begin{pmatrix} D_1 & S \\ 0 & D_2 \end{pmatrix} \quad T^e = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}. \quad (45)$$

The matrices  $D_1$  and  $E_1$  will act as transfer matrices for the walk above the  $x$ -axis, and  $D_2$  and  $E_2$  for the walk below the  $x$ -axis. The upper triangular form of  $T^o$  then ensures that the walk can cross the  $x$ -axis only once. We will now describe the transfer matrices in detail.

The matrix element  $(D_1)_{ij}$  for  $j \geq 2$  is the weight of an edge from a point with height  $y = 2i - 2$  to a point with height  $2j - 3$ . The first column of  $D_1$  is auxiliary whose meaning will become clear later. Similarly,  $(D_2)_{ij}$  for  $j \geq 2$  denotes the weight of an edge from a point with height  $y = 2 - 2i$  to a point with height  $3 - 2j$  and the first column is again auxiliary. If the ket  $|n\rangle$  represents the height  $n$ , the matrices  $D_1$ ,  $D_2$  and  $S$  are given in terms of projectors as,

$$D_1 = \sum_{n=0}^{\infty} (|2n\rangle + |2n+2\rangle)\langle 2n+1| \quad (46)$$

$$D_2 = x_1|0\rangle\langle u| + \sum_{n=0}^{\infty} (|-2n\rangle + |-2n-2\rangle)\langle -2n-1| \quad (47)$$

$$S = x_2|0\rangle\langle u| + |0\rangle\langle -1| \quad (48)$$

where  $|u\rangle$  denotes an auxiliary ket vector. Explicitly, the matrices  $D_1$  and  $D_2$  are given by,

$$D_1 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & \ddots \\ 0 & 0 & 0 & 0 & \ddots \end{pmatrix} \quad D_2 = \begin{pmatrix} x_1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & \ddots \\ 0 & 0 & 0 & 0 & \ddots \end{pmatrix} \quad (49)$$

and the matrix  $S$  is given by,

$$S = \begin{pmatrix} x_2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \ddots \\ 0 & 0 & 0 & 0 & \ddots \end{pmatrix}. \quad (50)$$

The parameters  $x_1$  and  $x_2$  are arbitrary and will not enter the partition sum. For simplicity we could therefore set them to zero, but we will need them later for another reason (see equation (58)).

The matrix element  $(E_1)_{ij}$  for  $i \geq 2$  is the weight of an edge from a point with height  $y = 2i - 3$  to a point with height  $2j - 2$ . The first row of  $E_1$  is auxiliary. Similarly,  $(E_2)_{ij}$  for  $i \geq 2$  denotes the weight of an edge from a point with height  $y = 3 - 2i$  to a point with height  $2 - 2j$  and its first row is again auxiliary. In terms of projectors, the matrices  $E_1$  and  $E_2$  are given by,

$$E_1 = x_3|u\rangle\langle 0| + z_1^{-1}|1\rangle\langle 0| + \sum_{n=1}^{\infty} (|2n-1\rangle + |2n+1\rangle)\langle 2n| \quad (51)$$

$$E_2 = z_2^{-1}|-1\rangle\langle 0| + \sum_{n=1}^{\infty} (|-2n-1\rangle + |-2n+1\rangle)\langle -2n|. \tag{52}$$

Explicitly, they are given by,

$$E_1 = \begin{pmatrix} x_3 & 0 & 0 & 0 & 0 \\ z_1^{-1} & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & \ddots & \ddots \end{pmatrix} \quad E_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ z_2^{-1} & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & \ddots & \ddots \end{pmatrix}. \tag{53}$$

Also here, the parameter  $x_3$  is arbitrary and will not enter the partition sum.

To indicate that walks can only start and end at height 0, we furthermore define the vectors  $\langle L| = ({}_1\langle L|, {}_2\langle L|)$  and  $|R\rangle = (|R\rangle_1, |R\rangle_2)$ , such that

$$\begin{aligned} {}_1\langle L| &= \langle 0| = (1, 0, 0, \dots) & {}_2\langle L| &= 0 \\ |R\rangle_1 &= |0\rangle = (1, 0, 0, \dots) & |R\rangle_2 &= |0\rangle = (1, 0, 0, \dots). \end{aligned} \tag{54}$$

It is straightforward to check that the partition sum (19) of all walks of length  $2n$  can be expressed as (44). For future convenience we also define the even and odd identity matrices

$$I^{o,e} = \begin{pmatrix} I_1^{o,e} & 0 \\ 0 & I_2^{o,e} \end{pmatrix} \tag{55}$$

where

$$I_1^o = |0\rangle\langle u| + \sum_{n=1}^{\infty} |2n\rangle\langle 2n-1| \quad I_2^o = |0\rangle\langle u| + \sum_{n=1}^{\infty} |-2n\rangle\langle -2n+1| \tag{56}$$

$$I_1^e = |u\rangle\langle 0| + \sum_{n=1}^{\infty} |2n-1\rangle\langle 2n| \quad I_2^e = |u\rangle\langle 0| + \sum_{n=1}^{\infty} |-2n+1\rangle\langle -2n|. \tag{57}$$

From the result (19) one may already have inferred that the partition sum of the OTW model is equal to the normalization of the stationary state of the asymmetric simple exclusion process (ASEP) with open boundaries [15]. The fugacities  $z_1$  and  $z_2$  are then identified with the input and output rates  $\alpha$  and  $\beta$ , respectively. Indeed, if we set the parameters  $x_i$  to the values,

$$x_1 = z_2^{-1} \quad x_2 = z_2^{-1} \quad x_3 = z_1^{-1} \tag{58}$$

we find that the transfer matrices  $T^o$  and  $T^e$ , and the vectors  $\langle L|$  and  $|R\rangle$  constitute the following representation of the DEHP algebra (15):

$$D = T^o I^e \quad E = I^o T^e \quad |V\rangle = |R\rangle \quad \langle W| = \langle L|. \tag{59}$$

Various representations of [16] for the DEHP matrices were used as transfer matrices in [28] to find bijections between several different path problems. Here we remark that this interpretation of the DEHP matrices allows us to express a stationary nonequilibrium probability distribution in terms of an equilibrium distribution. Among other things, this has the consequence that the thermodynamics of the nonequilibrium model is prescribed by standard equilibrium thermodynamics.

### 3.5. OTW-TASEP relation

In this section, we show how the TASEP current and density can be related to the equilibrium densities of the OTW model.

3.5.1. *Current.* The TASEP current operator is given by,

$$\hat{J} = (T^o I^e)(I^o T^e). \quad (60)$$

The average value,

$$J_{n,i} = \langle \hat{J}_i \rangle_n = \frac{1}{\tilde{Z}_n} \langle L | T^{i-1} \hat{J} T^{n-i-1} | R \rangle_n \quad (61)$$

has the following meaning in the path problem. The two identity matrices in (60) have, above the  $x$ -axis, the effect of forcing an upstep between columns  $2i - 1$  and  $2i$  and a downstep between  $2i$  and  $2i + 1$ . Below the  $x$  axis they have the effect of forcing a downstep between columns  $2i - 1$  and  $2i$  and an upstep between  $2i$  and  $2i + 1$ . Therefore,  $J_i$  is the average number of paths that have a local maximum above or a local minimum below the  $x$ -axis between columns  $2i - 1$  and  $2i + 1$ . The pieces of the path before and after these local extrema can be concatenated to obtain a path of length  $2n - 2$ . Since the local extrema may occur at any height, we thus obtain all paths of length  $2n - 2$  and therefore

$$J_{n,i} = J_n = \frac{\tilde{Z}_{n-1}}{\tilde{Z}_n} \quad (62)$$

independent of  $i$ . In the OTW model, the current corresponds to the pressure, since it is essentially the volume derivative of the grand potential. The value of the current

$$J = \lim_{n \rightarrow \infty} J_n \quad (63)$$

in the various parts of the phase diagram is

$$J = \begin{cases} 1/4 & z_1, z_2 \geq 1/2 \\ z_1(1 - z_1) & z_1 < 1/2 \quad z_2 > z_1 \\ z_2(1 - z_2) & z_2 < 1/2 \quad z_1 > z_2. \end{cases} \quad (64)$$

3.5.2. *Density.* The contact operators can be given in terms of projectors,

$$\hat{a}_i = |1\rangle_{2i-1} \langle 0|_{2i} \quad \hat{b}_i = |-1\rangle_{2i-1} \langle 0|_{2i} \quad (65)$$

so that the contact number operators can be rewritten as

$$\hat{a} = \sum_{i=1}^n \hat{a}_i \quad \hat{b} = \sum_{i=1}^n \hat{b}_i. \quad (66)$$

The TASEP density operator  $\hat{\tau}_i$  also has an expression in terms of the projectors of the OTW model. The operator  $\hat{\tau}_i$  is obtained by putting the matrix  $I^e$  instead of  $T^e$  at position  $2i$

$$\hat{\tau}_i = I^e(2i). \quad (67)$$

This has the effect that between columns  $2i - 1$  and  $2i$  each walk above the  $x$ -axis must go up. Walks below the  $x$ -axis must go down between these columns at all heights except  $y = -1$ , where it also may go up. From the result of Derrida *et al* [16], or from a combinatorial argument [28] it follows that the expectation value  $\langle \hat{\tau}_i \rangle$  can be written as

$$\langle \hat{\tau}_i \rangle_n = \frac{1}{\tilde{Z}_n(z_1, z_2)} \left[ \sum_{p=0}^{n-i-1} C_p \tilde{Z}_{n-p-1}(z_1, z_2) + \frac{1}{z_2} \tilde{Z}_{i-1}(z_1, z_2) \tilde{Z}_{n-i}(\infty, z_2) \right] \quad (68)$$

where we have used (17) and (19). Using the expression for the expectation values of the contacts  $\langle \hat{a}_i \rangle_n$  and  $\langle \hat{b}_i \rangle_n$ , see equations (27) and (28), we find

$$\langle \hat{\tau}_i \rangle_n = \sum_{p=0}^{n-i-1} C_p \prod_{j=0}^p J_{n-j} + \frac{1}{z_2} J_{n-1} \langle \hat{b}_{i-1} \rangle_{n-1} \quad (69)$$

and with the particle–hole symmetry of the TASEP this is equivalent to

$$\langle \hat{\tau}_i \rangle_n = 1 - \sum_{p=0}^{i-2} C_p \prod_{j=0}^p J_{n-j} - \frac{1}{z_1} J_{n-1} \langle \hat{a}_{i-1} \rangle_{n-1}. \quad (70)$$

Equations (69) and (70) give the relations between the local densities of the OTW model and the TASEP. Combining (69) and (70) we find

$$\langle \hat{\tau}_i \rangle_n = \frac{1}{2} \left[ 1 + \sum_{p=i-1}^{n-i-1} C_p \prod_{j=0}^p J_{n-j} + J_{n-1} \left( \frac{1}{z_2} \langle \hat{b}_{i-1} \rangle_{n-1} - \frac{1}{z_1} \langle \hat{a}_{i-1} \rangle_{n-1} \right) \right]. \quad (71)$$

In the bulk, the second term on the right-hand side of (71) vanishes in the thermodynamic limit. We thus find that in each part of the phase diagram the following relation between the TASEP bulk density  $\rho$  and current  $J$ , and the equilibrium densities  $a$  and  $b$  is satisfied,

$$\frac{2\rho - 1}{J} = \frac{b}{z_2} - \frac{a}{z_1} \quad (72)$$

where  $z_1 = \alpha$ ,  $z_2 = \beta$  and  $a$  and  $b$  are given by (35).

### 3.6. The partially asymmetric exclusion process

The TASEP can be extended with a nonzero rate  $q$  for back hopping. The resulting model is called the PASEP. Exact results for the symmetric case ( $q = 1$ ) are given in [32] and the stationary state of the general PASEP can also be found using a matrix method [20, 21]. To the rate  $q$  will now correspond a ‘number of particles’  $N(q)$ , not present in the TASEP. For the forward bias regime ( $q < 1$ ) the phase structure is similar to the TASEP model; we are interested in a new phenomenon which occurs in the vicinity of  $q = 1$ . One finds

$$\begin{aligned} N(q) &= \frac{q}{1-q} n + O(\log n) & q < 1 & \quad \alpha, \beta > (1-q)/2 \\ N(q) &= \frac{1}{4} n^2 + O(n) & q > 1. & \end{aligned} \quad (73)$$

This implies a change of the volume when the transition rate  $q$  changes. We note that the density  $\rho(q) = N(q)/n$  defined for  $q < 1$  diverges for a finite value of  $q$ , namely  $q = 1$ . For  $q > 1$  we have to redefine the density as  $\rho(q) = N(q)/n^2$ . This density turns out to be independent of the fugacity. A change of the volume was also observed in TASEP at the phase transition between the disordered state and the maximum current state. The latter phase transition could be interpreted as a special surface phase transition known in polymer physics (the number of ‘particles’ was either proportional to the size of the system or independent of the size of the system). Equation (73) describes a different phase transition since the number of ‘particles’ is either proportional to the size of the system or to the square of the size of the system. We expect therefore that a simple extension of the OTW model could explain what one observes. This is indeed the case. In the new model, a walk gets height-dependent step weights. One can formulate a thermodynamical theory, analogous to that of a heterogeneous gas in a gravitational field [33] using the partition function which is equal to the normalization factor of [21]. For  $q > 1$  the OTW model is genuinely two dimensional, and has therefore a volume of order  $n^2$ . For  $q < 1$  the system undergoes a bulk phase transition and the only contributions to the grand potential now come from the surface, i.e. the system becomes one dimensional. As in the TASEP, for  $q < 1$  the system may undergo further phase transitions through enhancement of the surface chemical potentials. This is indeed what happens and we find the adsorption–desorption transitions discussed in section 3.3.

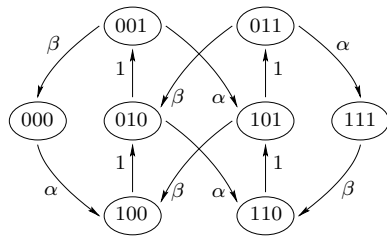


Figure 6. Transition graph of the TASEP for  $L = 3$ .

#### 4. The normalization from cofactors

The TASEP can be formulated using a transition matrix, see e.g. [16]. The normalization as defined by (14) is not equal to that calculated from the cofactors of this transition matrix using the results of section 2. In this approach, for each system size, all the cofactors have a common factor which is a nontrivial polynomial.

Consider for example the TASEP on three sites, and let  $H$  be its transition matrix. The transition graph, i.e. the graph that has a directed edge from vertex  $b$  to  $a$  with weight  $-H_{ab}$  and no edge if  $a = b$  or  $H_{ab} = 0$ , for the TASEP on a chain of three sites is given in figure 6.

The weighted sum of all directed spanning trees with the vertex (001) as a sink for example is given by  $\alpha\beta^2(1 + \alpha + \beta)$  which is indeed equal to the corresponding cofactor of  $H$ . It turns out that each of the cofactors has a factor  $(1 + \alpha + \beta)$ . The sum of all directed spanning trees on this graph is

$$Z = (1 + \alpha + \beta)(\alpha^3 + \alpha^2\beta + 2\alpha^3\beta + \alpha\beta^2 + 2\alpha^2\beta^2 + 2\alpha^3\beta^2 + \beta^3 + 2\alpha\beta^3 + 2\alpha^2\beta^3) \quad (74)$$

which is indeed  $(\alpha\beta)^3(1 + \alpha + \beta)$  times the TASEP normalization as defined in (14). We observe that the factor  $(1 + \alpha + \beta)$  is never zero for positive real parts of the rates  $\alpha$  and  $\beta$ .

As hinted at in section 2, we believe that in general this common factor will not give rise to additional singularities for positive real rates in the thermodynamic limit. We believe that a common factor is nonzero in the space of complex rates if the real parts of all the rates are positive. This is called the half-plane property, see e.g. [31]. We have checked this for small system sizes in the case of the TASEP. In the spirit of the Lee–Yang theory it implies that the common factor does not develop singularities in the thermodynamic limit for positive real rates and hence it will not influence the phase diagram, except perhaps at the origin. Moreover, upon introduction of inhomogeneities in the transition rates, the cofactors will no longer have a common factor. If these inhomogeneities are small enough the physical properties of the system should remain the same.

#### 5. Conclusion

In a previous paper [14] we have shown that a properly chosen normalization factor of the probability distribution function describing the stationary state of the ‘raise and peel’ one-dimensional model is given by the partition function of the two-dimensional ice model with domain-wall boundary conditions—an equilibrium problem with nonlocal interactions. This connection was proved for small systems but there are good reasons [34] to believe that this conjecture is valid for any size of the system. It turns out that the same way to choose the normalization factor was suggested in a general framework by Blythe and Evans [8] and shown to be useful in order to use the Lee–Yang approach to nonequilibrium problems. This brought us to have a closer look at the problem. We have first noted that the ‘number of particles’

associated with various rates are nondecreasing functions of the rates seen as fugacities. This allows us, as in equilibrium problems, to determine directly the phase diagram of a model, once the normalization factor is known. This observation suggests, obviously, that one can try approximative approaches such as finite-size scaling or power expansions to determine the nature of the phase transition in the case when the normalization factor is not known exactly for all sizes.

We have also shown, in the example of TASEP that, as in the ‘raise and peel’ model, the normalization factor can be understood as a partition function of a two-dimensional equilibrium model: the one-transit walk model. We also think that the correspondence between normalization factors of one-dimensional stationary states and two-dimensional equilibrium problems with nonlocal interactions is of a more general validity.

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### Appendix A. The normalization as a homogeneous polynomial

The normalization of a stationary state of any stochastic (Markov) process can always be interpreted as a polynomial in the rates with positive coefficients, i.e. it has the form of a generating function. By the Cauchy–Schwartz inequality, the negative logarithm of this generating function is therefore convex and its derivatives with respect to the rates are proper ‘particle’ numbers, i.e. the second derivatives are positive.

The above statement is implied by the matrix-tree theorem [11–13]. Here we show a simple proof which can be found in a slightly different version in [22].

**Lemma 1.** *Let  $H$  be a matrix with off-diagonal elements  $H_{ab} = -r_{ab}$  and such that all columns add up to zero,  $\sum_a H_{ab} = 0$ . Assume that  $H$  has a unique largest eigenvalue equal to 0.*

- (a) *The cofactors  $X(a, b)$  are constant for each column, i.e. they do not depend on  $a$ .*
- (b) *The eigenvector corresponding to the largest eigenvalue 0 is a polynomial in the rates  $r_{ab}$  with positive coefficients.*

**Proof.** Let  $H(a, b)$  be the matrix corresponding to  $H$  with the  $a$ th row and  $b$ th column removed. The cofactor  $X(a, b)$  is then defined by,

$$X(a, b) = (-1)^{a+b} \det H(a, b). \quad (\text{A.1})$$

The difference  $X(a, b) - X(a + 1, b)$  of any two successive cofactors is proportional to the sum of determinants of two matrices that differ only in one row, and can thus be expressed as the determinant of the sum of these matrices, which is a zero column-sum matrix. This last determinant therefore vanishes and hence  $X(a, b) = X(b, b)$  for all  $a$ .

Because the eigenvalue 0 is unique and,

$$0 = \det H = \sum_b H_{ab} X(a, b) = \sum_b H_{ab} X(b, b) \quad (\text{A.2})$$

the elements of the eigenvector corresponding to the eigenvalue 0 are given by the cofactors  $X(b, b)$ . Each such cofactor is of the form

$$X(b, b) = \sum_{\pi} N(\pi_1, \dots, \pi_{b-1}, \pi_{b+1}, \dots, \pi_n) \prod_{\substack{c=1 \\ c \neq b}}^n r_{\pi_c, c} \quad (\text{A.3})$$

where the sum is over any permutation  $\pi = \{\pi_1, \dots, \pi_{b-1}, \pi_{b+1}, \dots, \pi_n\}$  of  $\{1, \dots, b-1, b+1, \dots, n\}$  and  $N(\pi) \in \mathbb{Z}$ . We now show that in fact  $N(\pi) \in \{0, 1\}$ , hence proving assertion (b) of lemma 1.

Let  $r_{\rho_a, a} = 1$  for a particular permutation  $\rho$ , and all other  $r_{ac} = 0$ . From (A.3) we then see that  $N(\rho_1, \dots, \rho_{b-1}, \rho_{b+1}, \dots, \rho_n)$  is the determinant of a matrix which we will call  $H(b, b, \rho)$ . If  $\rho_a \neq b$  for all  $a = 1, \dots, b-1, b+1, \dots, n$ , the columns of  $H(b, b, \rho)$  all add up to zero and  $\det H(b, b, \rho) = 0$ . If on the other hand  $\rho_a = b$  for a particular  $a = a^*$ , then  $H(b, b, \rho)$  contains zeros in the column corresponding to  $a^*$  except for the diagonal element which is 1. By deleting the column and row of  $H(b, b, \rho)$  corresponding to  $a^*$  we find again a matrix of the form of  $H(b, b, \rho)$  but with one dimension less. The result thus follows by expanding the determinant with respect to the column corresponding to  $a^*$  and induction on  $n$ .  $\square$

## References

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