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LETTER TO THE EDITOR

Phase transition in a non-conserving driven diffusive system

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Abstract
An asymmetric exclusion process comprising positive particles, negative particles and vacancies is introduced. The model is defined on a ring and the dynamics does not conserve the number of particles. We solve the steady state exactly and show that it can exhibit a continuous phase transition in which the density of vacancies decreases to zero. The model has no absorbing state and furnishes an example of a one-dimensional phase transition in a homogeneous non-conserving system which does not belong to the absorbing state universality classes.

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One-dimensional driven diffusive systems have been a subject of extensive study in recent years [1–3]. A prototypical model for studying these systems is the asymmetric exclusion process in which particles move stochastically with a preferred direction and hard-core exclusion [4]. In this model the local dynamics conserves the particles. Asymmetric exclusion processes with a single species of particles do not exhibit phase transitions on a ring geometry. On the other hand, open systems in which the particle number is not conserved at the boundaries can exhibit a variety of phase transitions [2, 5]. Generalizations of these models to more than one species of particles have shown that phase transitions and long-range order do exist in these systems even on a ring geometry [6–10].

Generally speaking, one-dimensional models that exhibit phase transitions are either (a) of the asymmetric-exclusion-process type with a drive and conserving bulk dynamics or (b) have non-conserving bulk dynamics with one or more absorbing states. The latter case is related to the directed percolation or other absorbing state universality classes [11]. It is therefore of interest to find a one-dimensional model where the bulk dynamics is not conserving that exhibits a phase transition unrelated to the absorbing state universality classes.

In this letter we introduce such a model and solve for its steady state exactly. The model is defined on a ring of L sites where each site can be occupied by either a positive (+) particle, a negative (−) particle or a vacancy (0). The model evolves through the following conserving rates

$$+\,0 \xrightarrow{1} 0\,+ \qquad 0\,- \xrightarrow{1} -\,0 \qquad +\,- \underset{q}{\overset{1}{\rightleftharpoons}} -\,+ \tag{1}$$

augmented by the following non-conserving rates

$$+\,0 \underset{1}{\overset{w}{\rightleftharpoons}} 0\,0 \qquad 0\,- \underset{1}{\overset{w}{\rightleftharpoons}} 0\,0. \tag{2}$$

Thus, the model generalizes the model of Derrida *et al* [7] and Arndt *et al* [10] through the introduction of the process of creation and annihilation of particles. Note that any configuration can be reached from any other except states with no vacancies which are not dynamically accessible.

The rate w controls the density of vacancies, denoted by θ, in the system. For large w one expects the density of vacancies to be high and for small w it is expected to be low. We will show that for $q < 1$ the dependence of θ on w is not smooth and that for small enough w, θ is zero in the thermodynamic limit. Thus the model exhibits a phase transition from a 'fluid' phase with a finite θ to a 'maximal current' phase where θ is zero (the nomenclature will be explained below). The transition occurs at a critical value $w_c > 0$. The phase transition is found to be continuous with

$$\theta \sim |w - w_c|^\beta \tag{3}$$

where $\beta = 1$. For $q > 1$, on the other hand, the system is always strongly phase separated [8–10] with a single zero and two extensive pure domains of positive and negative particles. Here there is no phase transition as w is varied.

A powerful technique for solving the steady states of asymmetric exclusion processes is the matrix product ansatz [12]. This involves representing the steady-state weights as the trace of a product of matrices which depends on the microscopic configuration. The matrices then obey certain algebraic rules which are derived from the dynamics of the model. This technique has yielded the exact behaviour at the various phase transitions in many asymmetric exclusion models. The transitions solved within the matrix product have been found to be robust for a large class of systems [13]. However, in most models solved so far using the matrix product, particle numbers are conserved in the bulk (two exceptions are [14] and [15]). In this work, we employ the matrix product technique to obtain an exact solution for the steady state and phase transitions of the model defined by (1) and (2). It turns out that despite the non-conserving dynamics of the present model we can use the same matrices that have been previously used to solve models with conserving dynamics.

We now proceed to outline the matrix product solution for the steady state. The steady-state weight of a configuration $\mathcal{C}$ is represented by the trace of a product of matrices:

$$W_L(\mathcal{C}) = \mathrm{Tr} \prod_{i=1}^{L} \left[\delta_{\tau_i,+} D + \delta_{\tau_i,-} E + \delta_{\tau_i,0} A\right] \tag{4}$$

where L is the system size and $\tau_j = +, -, 0$ if site j is occupied by a +, − or 0, respectively. That is, a matrix D (E) represents a positive (negative) particle and A represents a vacancy. It is easy to show using the technique of [7, 12] that D, E and A should satisfy

$$DE - qED = D + E \qquad DA = AE = A \qquad AA = wA \tag{5}$$

to give the correct steady-state weights. These equations can be satisfied by choosing

$$A = w|V\rangle\langle V| \tag{6}$$

where $\langle V|V\rangle = 1$, $D|V\rangle = |V\rangle$ and $\langle V|E = \langle V|$. Then D, E and $\langle V|$ are identical to the matrices and vectors studied in [16, 17] where they are used to solve the single-species partially asymmetric exclusion process with open boundaries.

We now wish to calculate the normalization, i.e. the partition function, which is given by the sum of the weights (4) of all accessible configurations:

$$\mathcal{Z}_L = \mathrm{Tr}[(A+D+E)^L - (D+E)^L]. \tag{7}$$

Using the form (6) of A we first write the sum of the weights of configurations with exactly M vacancies on a lattice of size L:

$$\mathcal{Z}_{L,M} = w^M \prod_{\mu=1}^{M} \sum_{n_\mu=0}^{\infty} \langle V|C^{n_\mu}|V\rangle \delta_{\sum_\mu n_\mu, L-M} \tag{8}$$

where $C = D + E$. The sum over each n_μ corresponds to the possible number of particles between two consecutive zeros. The delta function enforces the constraint that the total number of particles equals $L - M$ and the factor w^M arises from the M zeros. This form neglects the degeneracy in placing a given configuration $\{n_\mu\}$ on a ring geometry, which is bounded from above by L. It is straightforward to check using bounds on the true partition function that this does not affect any of the results presented here.

In order to calculate the partition function $\mathcal{Z}_L = \sum_{M=1}^{L} \mathcal{Z}_{L,M}$, it is convenient to replace the delta function by a contour integral. Taking the limit of the sum over M to infinity yields

$$\mathcal{Z}_L = \sum_{M=1}^{\infty} \oint \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{w^M}{z^{L-M+1}} \prod_{\mu=1}^{M} \sum_{n_\mu=0}^{\infty} z^{n_\mu} \langle V|C^{n_\mu}|V\rangle \tag{9}$$

$$= \oint \frac{\mathrm{d}z}{2\pi \mathrm{i}\, z^{L+1}} \left[\frac{zwU(z)}{1 - zwU(z)} \right] \tag{10}$$

where $U(z)$ is defined as

$$U(z) = \sum_{n=0}^{\infty} z^n G_n \qquad \text{with} \quad G_n \equiv \langle V|C^n|V\rangle. \tag{11}$$

The weight G_n has been studied before. It is the normalization sum of the single-species partially asymmetric exclusion model on an open lattice of size n and with particle injection rate 1 at the left boundary and removal rate 1 at the right boundary [16, 17].

Below, we shall consider the density of vacancies given by

$$\theta = \lim_{L\to\infty} \frac{\overline{M}}{L} = \lim_{L\to\infty} \frac{w}{L} \frac{\partial \ln \mathcal{Z}_L}{\partial w} \tag{12}$$

where $\overline{M}$ is the average number of vacancies in the system. We shall also consider the current J_L of positive particles (which is equal to that of the negative particles). We define the current in the same way as for the conserving system although here the density is not conserved. Thus taking into account the inaccessibility of configurations with no vacancies we find

$$J_L = \frac{1}{\mathcal{Z}_L} \mathrm{Tr}[(DA + DE - qED)(C+A)^{L-2} - (DE - qED)C^{L-2}] = \frac{\mathcal{Z}_{L-1}}{\mathcal{Z}_L} \tag{13}$$

where we have used the algebraic rules (5) and form (7) of $\mathcal{Z}_L$.

We now discuss the two distinct cases $q < 1$ and $q > 1$ separately:

(i) The case of $q < 1$

Here the normalization $\mathcal{Z}_L$ can be evaluated for large L from integral (10) by the saddle point method. This method amounts to working in the grand canonical ensemble. The term in the square brackets of (10) is then just the grand canonical partition function and $\mathcal{Z}_L \sim (z^*)^{-L}$ where z^* is the saddle point value of z, i.e. the fugacity. Thus, in the thermodynamic limit, we see from (13) that $J_L \to z^* \equiv J$ which identifies the particle current in the system as the fugacity. Also, we see from (12) that the density of vacancies is given by

$$\theta = -w \frac{\partial \ln z^*}{\partial w}. \tag{14}$$

Thus one may identify θ as the order parameter and $-\ln z^* = -\ln J$ as the analogue of the free energy density.

The saddle point equation for integral (10) may be written as

$$L = \frac{1}{1 - wzU(z)} \left[\frac{zU'(z)}{U(z)} + wzU(z) \right]. \tag{15}$$

For $L \to \infty$ this equation is satisfied either by $1 - wzU(z) \sim \mathcal{O}(1/L)$ or by the term inside the brackets being of order L. To analyse which of the two scenarios pertains one needs to consider the properties of the increasing function $U(z)$. Note from (11) that the convergence of $U(z)$ is determined by the large n form of G_n. For $q < 1$ this quantity is known [16, 17] to behave for large n as

$$G_n \simeq a \frac{K^{-n}}{n^{3/2}} \tag{16}$$

where

$$K = \frac{1-q}{4} \qquad \text{and} \qquad a = \frac{4}{\sqrt{\pi}} \left[\prod_{i=1}^{\infty} \frac{(1-q^i)^3}{(1+q^i)^4} \right]. \tag{17}$$

From (16) one deduces that $U(z)$ converges for $z \leqslant K$ and $U'(z)$ diverges as $z \to K$. Thus, when $1 - wzU(z) = 0$ for some $z \leqslant K$ we solve the saddle-point equation (15) by choosing z^* so that $1 - wz^*U(z^*) \sim \mathcal{O}(1/L)$. On the other hand, when $1 - wzU(z) > 0$ for all $z \leqslant K$, the divergence must come from the term in the square brackets of equation (15) and we need $z^* = K(1 - \mathcal{O}(1/L^2))$. This can be deduced by noting that $U'(z) \sim |K - z|^{-1/2}$ for $z \to K$. Thus, in the thermodynamic limit $L \to \infty$, z^* increases to K as w is decreased to w_c, given by

$$w_c = \frac{1}{KU(K)}. \tag{18}$$

Any further decrease in w leaves the value of z^* unchanged. The critical rate $w_c(q)$ obtained from this equation is plotted in figure 1. Using equation (14) one can see that for $w > w_c$, θ decreases as w decreases while for $w < w_c$, $\theta = 0$. Using $U(z) - U(K) \sim |K - z|^{1/2}$ it is easy to show by expanding (15) that $\theta \sim |w - w_c|$ as $w \searrow w_c$, recovering (3).

Since z^* is the current of particles and it saturates at $K = (1 - q)/4$ for $w < w_c$ we refer to this phase as the maximal current phase. We refer to the phase $w > w_c$ as the fluid since the typical configuration is a disordered arrangement of +, $-$ and 0.

(ii) The case of $q > 1$

For $q > 1$ it is known [17] that the n dependence of G_n is given by

$$G_n \sim \left(\frac{q}{q-1} \right)^n q^{n^2/4}. \tag{19}$$

In this case $U(z)$ diverges for all $z > 0$ and we have to impose cut-offs on the sums in equation (9). That is, we write

$$\mathcal{Z}_L = \sum_{M=1}^{L} \oint \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{w^M}{z^{L-M+1}} \left(\sum_{n=0}^{L-M} z^n G_n \right)^M. \tag{20}$$

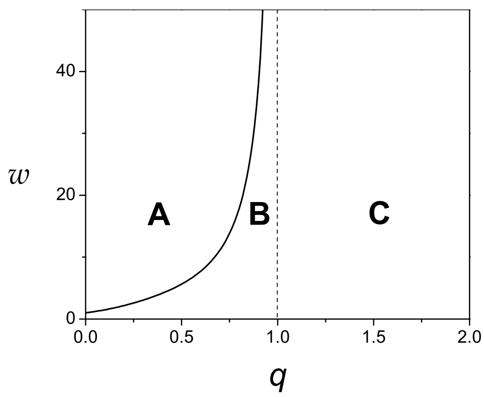

Figure 1. Phase diagram in the q–w plane. The transition line between the fluid phase (A) and the maximal-current phase (B) is given by equation (18). The transition into the strongly phase separated state (C) takes place at $q = 1$.

From (19), it is clear that the dominant contribution to the sum is when $M = 1$ and $n = L - 1$. Then $J_L = \mathcal{Z}_{L-1}/\mathcal{Z}_L \simeq (q-1)q^{-L/2-1}$. Thus, the current of particles is exponentially small in the system size and the density of vacancies is zero. This corresponds to a strongly phase-separated state with a single vacancy followed by an extensive block of positive particles (to the right of the vacancy) followed by an extensive block of negative particles (to the left of the vacancy).

Finally, we discuss the transition between $q < 1$ and $q > 1$. Using equations (16) and (17) it is easy to show that as $q \to 1$ from below, $KU(K)$ tends to zero. Thus using equation (18) we see that w_c diverges as $q \to 1$. Therefore at the $q = 1$ transition the system changes from a maximal current phase $J = (1-q)/4$ for $q < 1$ to a strongly phase-separated state with $J = \mathcal{O}(q^{-L/2})$ for $q > 1$. In both of these phases the density of vacancies is zero. Therefore, the transition has no relation to the non-conserving dynamics and is instead related to the reversal of the bias [17]. The phase diagram of the model in the q–w plane is summarized in figure 1.

It is interesting to make a comparison between the transition from the fluid to the maximal current phase and the denaturation transition in DNA where the two strands of the molecule unbind at a certain temperature. In models of this transition [18, 19] one assigns a Boltzmann weight w to bound base pairs and a weight K^{-n}/n^{c} to unbound segments of length n. Here K is a non-universal constant whereas c is a universal exponent depending on the dimension and self-avoidance properties of the unbound DNA. For example, using a random walk model yields $c = 3/2$ in three dimensions [18]. As temperature is raised and w decreases there is an unbinding transition where the fraction of bound base pairs, θ, vanishes. The DNA models and the present model can be related by identifying vacancies with bound pairs and blocks of particles with unbound DNA loops. Then G_n corresponds to the weight of DNA loop of length n and the grand canonical partition functions of the two systems are the same[3].

The difference between the systems is that in the DNA the exponent $c = 3/2$ is a result of the fact that the one-dimensional molecule is embedded in three dimensions. However, for the model considered here the exponent $3/2$ arises from truly one-dimensional phenomena related to the currents flowing in the system. This can be seen from the relation between G_n and

[3] To make the correspondence more explicit one has to identify U and V of the DNA literature with $U - 1$ and $wz/(1 - wz)$ of the present paper.

the current of the single-species partially asymmetric exclusion process. More explicitly, for such a process the current in a system of size n is given by G_{n-1}/G_n. Thus, the n dependence of G_n is related to the n dependence of the current in a single-species system of size n. In the context of the two-species model we have studied here such a system corresponds to an uninterrupted block of particles, of length n, bounded between two vacancies. This picture has recently been used to study the conditions for phase separation in conserving models [20].

The model can easily be generalized to contain two additional parameters α and β by modifying rates (1) to read

$$+\,0 \xrightarrow{\beta} 0\,+ \qquad 0\,- \xrightarrow{\alpha} -\,0 \qquad +\,- \underset{q}{\overset{1}{\rightleftharpoons}} -\,+ \tag{21}$$

and rates (2) to

$$+\,0 \underset{1}{\overset{\beta w}{\rightleftharpoons}} 0\,0 \qquad 0\,- \underset{1}{\overset{\alpha w}{\rightleftharpoons}} 0\,0. \tag{22}$$

Then one can take $A = w|V\rangle\langle W|$ where $\beta D|V\rangle = |V\rangle$ and $\alpha\langle W|E = \langle W|$. This generalization should allow for a richer phase diagram than that presented here.

Finally, we point out that the transition from the fluid to the maximal current phase is lost if particles are not conserved inside a block consisting only of particles. For example, a process where $+ \to 0$ regardless of its neighbours destroys the maximal current phase.

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