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Single-file diffusion far from equilibrium

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Abstract

The stationary states of driven diffusive single-file systems, connected to boundary reservoirs with fixed particle density are shown to be selected by an extremal principle for the macroscopic current. Given the current one obtains the exact first- and second-order non-equilibrium phase transition lines for the bulk density as a function of the boundary densities. The basic dynamical mechanism behind the extremal principle is an intriguing generic interplay between the motion of shocks and localized perturbations. Two-component driven systems exhibit unexpected and fascinating critical phenomena.

1 Introduction

Many materials exhibit a phenomenon generally termed single-file diffusion. This refers to a diffusive random motion of particles which is confined to essentially only one spatial degree of freedom. Such a situation arises typically if particles move under the influence of a random force in a tube-like geometry where the tube diameter is of the order of the particle size, but the length of the tube is much larger. Well-known examples of such single-file systems are molecules diffusing in the channels of certain types of zeolites [1], or colloidal particles in narrow tubes [2]. Sometimes effectively one-dimensional dynamics appears in disguise, e.g. in the reptation of entangled polymers [3] where the transverse dynamical degrees of a freedom of a polymer chain is suppressed by the surrounding chains, or in the motion of the one-dimensional boundary of a thin surface layer [4]. Last, but not least, quasi-one-dimensional random motion plays a crucial role in some non-physical systems, notably automobile traffic flow and the motion of motor proteins along microtubuli or actin filaments in a biological cell.

Most of these systems are kept permanently far from equilibrium by boundary density gradients or external driving fields, or, in the case of the non-physical examples, by being self-driven. In either case there is no equilibrium steady state given by the Boltzmann distribution. Instead, a current flows in the system which is described by a nonequilibrium stationary distribution for which no general macroscopic theory analogous to equilibrium thermodynamics exists [5, 6, 7]. Therefore stationary behaviour cannot be deduced from any known general principle, but has to be derived from the system dynamics of each system separately. This unfortunate situation calls for the study, both theoretical and experimental, of simple model systems. The objective is the identification of generic mechanisms which shed light on general features of the emergence of macroscopic nonequilibrium behaviour from the microscopic laws of interaction. In this paper we review some of the theoreti-

cal progress that has been achieved in the past decade for a wide class of driven diffusive systems and which is amenable to verification with present-day experimental equipment.

The study of single-file diffusion is motivated not only by its ubiquitity indicated above. The investigation of interacting particle systems far from equilibrium has shown that one-dimensional driven diffusive systems with short-range interactions exhibit a remarkably rich variety of critical phenomena. Unlike in thermal equilibrium one observes spontaneous symmetry breaking, long-range order and phase coexistence in the steady state if the system evolves under certain microscopic kinetic constraints or has more than one conservation law, i.e., in two-component many-body systems [8]. Most of these phenomena are not well-understood yet and a matter of current research. For systems with only one conserved particle species, however, it has turned out that parts of the program of deriving macroscopic non-equilibrium behaviour from microscopic stochastic dynamics can be carried out to a very satisfactory degree. Despite their simplicity, these systems exhibit a rich and rather non-trivial dynamical and stationary behaviour. For an exactly solvable paradigmatic model, the asymmetric simple exclusion process (ASEP, see below) not only the macroscopic nonlinear hydrodynamics have been derived rigorously [9, 12] but also detailed microscopic information about *universal* phenomena, including formation and diffusion of shocks [10, 11], the microscopic origin of the stability of shocks [5] and the dynamical structure function [13, 14] could be obtained in the past decade.

For one-species systems with open boundaries where particles can exit and enter this has led to a theory of boundary-induced phase transitions which provides a general framework for a quantitative description of the steady-state selection in driven diffusive systems which are in contact with particle reservoirs at their boundary. Unlike in equilibrium, boundary conditions determine the bulk behaviour of driven diffusive systems in a decisive fashion which can be captured in terms of an extremal principle for the current [15, 16]. The resulting phase diagram for the nonequilibrium steady state is determined by the interplay of localized excitations and shocks. This theory is reviewed in the following three sections and some suggestions are made how the theory could be confirmed experimentally (Sec. 5). In the final two sections we review some recent intriguing work on two-component systems. In particular, we derive a quantitative criterion for phase separation and thus show how the occurrence of phase separation can be understood dynamically in terms of a classical nonequilibrium analogue of Bose-Einstein condensation.

2 Steady state selection in open driven systems

Imagine an interacting driven particle system – it may be *any* system such as ribosomes moving along a m-RNA, ions diffusing in a narrow channel, or even cars proceeding on a long road – where classical objects move with preference in one direction and which is coupled at its two ends to external reservoirs. The simplest model which captures the three basic features of biased random motion with short-ranged interactions is the totally asymmetric simple exclusion process (TASEP) where particles hop on a 1-d lattice with constant rate to the right, provided the neighbouring lattice site is vacant. Otherwise an attempted move is rejected. In a finite, open system particles are injected with rate α at

the left boundary site 1. At the right boundary site L particles leave the system with rate β. This corresponds to a coupling to reservoirs of constant densities $\rho_L = \alpha = \rho_L^{true}$ and $\rho_R = 1 - \beta = \rho_R^{true}$. This model was first introduced in 1968 to describe the kinetics of protein synthesis [17, 18] and has since then obtained paradigmatic status as an interesting and exactly solvable model for a many-body system out of equilibrium [7, 5]. It even serves as a very simple toy model for traffic flow [19, 20], exhibiting stable shocks analogous to traffic jams.

In general, any system with open boundaries where particles can enter and leave will settle into a non-equilibrium steady state characterized by some bulk density and the corresponding particle current. We pose the following fundamental question: Which stationary bulk density will the system assume as a function of the boundary densities?

At first glance this appears to be an ill-posed question as undoubtedly the answer to this problem of steady state selection (first considered in general terms by Krug [15]) depends on the system under investigation. However, guided by the insights gained from the exact solution [21, 22] (see below) of the totally asymmetric simple exclusion process (TASEP), we have developed a dynamical theory of boundary-induced phase transitions for homogeneous one-species driven particle systems with a single conserved density [16, 23]. The phase diagram for the bulk density is governed by an extremal principle for the current – *irrespective of the local dynamics*. As a function of non-universal effective right and left boundary densities $\rho_{R,L}$ the steady-state current j is given by the macroscopic current-density relation

$$j = \begin{cases} \max\limits_{\rho\in[\rho_R,\rho_L]} j(\rho) & \text{for } \rho_L > \rho_R \\ \min\limits_{\rho\in[\rho_L,\rho_R]} j(\rho) & \text{for } \rho_L < \rho_R. \end{cases} \tag{1}$$

The structure of the phase diagram which exhibits a variety of first- and second-order non-equilibrium transitions is determined by the number of extrema of the current. The microscopic details of the system enter only in so far as they determine the functional form of the current $j(\rho)$ and the effective boundary densities which depend on the true boundary densities through the details of the coupling mechanism. At the second-order phase transition lines the intrinsically non-universal properties of the boundary layer are dominated by a universal power law decay of the density profile to its bulk value [15, 24]. The extremal principle (1) and hence the various phases and the nature of the transitions can be understood dynamically by the interplay of local fluctuations (which lead to an overfeeding effect [21, 23]) with the branching and coalescence of shocks [16] (see below).

3 Exact solution of the TASEP with open boundaries

In the simplest non-trivial case the current is a convex function with a local extremum. This is realized in the TASEP with the current-density relation

$$j = \rho(1 - \rho) \tag{2}$$

which has a single maximum of the current at the density $\rho^* = 1/2$.

Employing probabilistic tools, Liggett [25] obtained a recursion relation for the stationary distribution of the TASEP in system size L from which he could extract the bulk density as a function of α and β and hence the phase diagram. However, in order to understand the physical origin of the phase transitions, one has to study the local density profile. From the steady-state recursion for the 2^L configurational probabilities one obtains closed recursions for the unnormalized string weights

$$Y_{L,k} \quad \propto \quad \langle \ldots 00000 \rangle \atop k \ldots L. \tag{3}$$

These quantities are the probability of finding the last $L-k+1$ sites empty. Furthermore, one finds

$$X^p_{L,k} \quad \propto \quad \langle \ldots 1 \ldots 00000 \rangle \atop p \ldots k \ldots L \tag{4}$$

resp. [26] for the probability to find the last $L-k+1$ sites empty, but a particle at site p. These quantities satisfy

$$\begin{aligned}
Y_{L,k} &= Y_{L,k-1} + \alpha\beta Y_{L-1,k} \quad \text{for } 1 < k < L+1 && (5)\\
Y_{L,1} &= \beta Y_{L-1,1} \quad \text{with } Y_{0,1} = 1 && (6)\\
X^p_{L,k} &= X^p_{L,k-1} + \alpha\beta X^p_{L-1,k} \quad \text{for } p+1 < k < L+1 && (7)\\
X^p_{L,L+1} &= X^p_{L,L} + \alpha X^p_{L-1,L} \quad \text{with } X^p_{L,p+1} = \alpha\beta Y_{L-1,p+1}. && (8)
\end{aligned}$$

For general α, β these recursion relations are not straighforward to solve with standard approaches. However, solving explicitly for small system size, guessing the pattern behind the expressions and verifying the guess by cross-checking with the recursion relations yields the bulk density ρ as well as the density profile $t_p = \rho_p - \rho_{p-1}$ for $1 \le p \le L$ [21]. One finds in agreement with the extremal principle (1)

$$\rho = \begin{cases} \alpha = \rho_L & \text{for} \quad \beta < \alpha < 1/2 \\ \beta = 1 - \rho_R & \text{for} \quad \alpha < \beta < 1/2 \\ 1/2 = \rho^* & \text{for} \quad \alpha, \beta > 1/2. \end{cases} \tag{9}$$

and

$$t_p = A(\alpha,\beta)\Phi_p(\alpha)\Phi_{L-p}(\beta) \tag{10}$$

with

$$\Phi_n(x) = \frac{1-2x}{2[x(1-x)]^n} + 2 \begin{pmatrix} 2n \\ n \end{pmatrix} {}_2F_1(1, n+1/2, 1/2; (1-2x)^2) \tag{11}$$

involving the standard hypergeometric function ${}_2F_1(1, n+1/2, 1/2; (1-2x)^2)$. In an alternative matrix product approach [22] the same exact results were obtained.

The phase diagram (Fig. 1) has three phases, a maximal-current phase C in the domain $\rho_L > \rho^*, \rho_R < \rho^*$ (bulk density $\rho = \rho^*$), with second-order transitions to the low-density

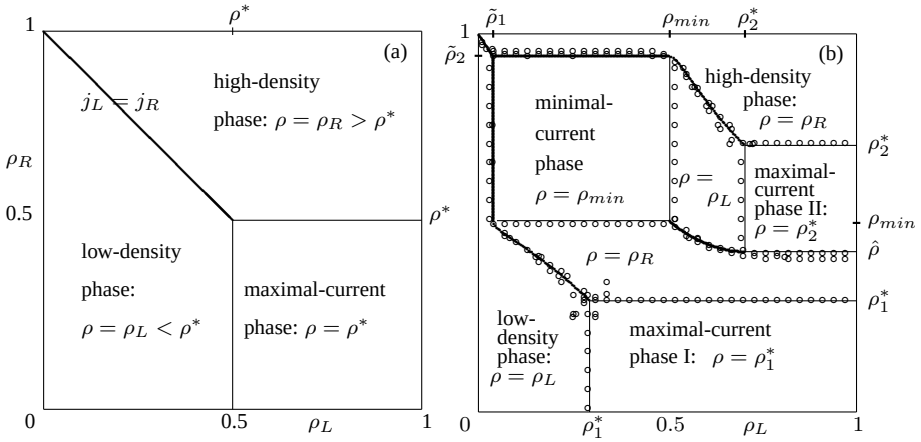

Figure 1: Exact phase diagram of the TASEP (a) and of a lattice gas model with two maxima at $\rho^*_{1,2}$ and a minimum at $\rho_{min} = 0.5$ in the current density relation (b). Full (bold) lines indicate phase transitions of second (first) order. Circles show the results of Monte-Carlo simulations of a system with 150 sites [16].

($\rho = \rho_L < \rho^*$) and the high-density phase ($\rho = 1 - \rho_R > \rho^*$) resp. These phases are separated by a first-order transition along the line $j_L = j_R$ in the domain $\rho_L < \rho^*, \rho_R > \rho^*$. The phase diagram of the TASEP is generic for all systems with a single maximum in the current-density relation in that the phase transition lines are given by the same relations in terms of the current. For a system with two maxima of the current the phase diagram consists of seven distinct phases, including two maximal current phases with bulk densities corresponding to the respective maxima of the current and a minimal current phase in a regime defined by

$$j(\rho_R), j(\rho_L) > j(\rho_{min}); \;\; \rho_L < \rho_{min} < \rho_R. \tag{12}$$

Somewhat contrary to intuition the system organizes itself into a state with bulk density ρ_{bulk} corresponding to the local minimum of the current even though both boundaries support a higher current [16].

4 Shocks and overfeeding

To understand the origin of the extremal principle for the current we first note that in the absence of detailed balance stationary behavior cannot be understood in terms of a free energy, but has to be derived from the system dynamics. Following Kolomeisky et al. [23] there are two basic dynamical phenomena to consider. A density wave, i.e. a localized perturbation in a stationary region of background density ρ (Fig. 2), spreads out in the

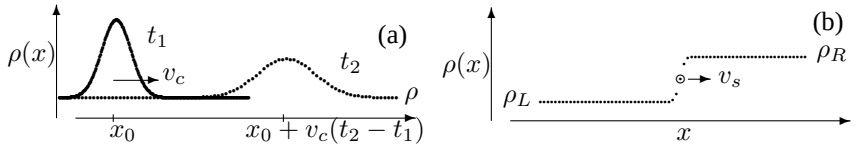

Figure 2: (a) Diffusive spreading of a density perturbation in the steady state at two times $t_2 > t_1$. The collective velocity describes the motion of the center of mass of the perturbation. (b) Motion of a shock. To the left (right) of the domain wall particles are distributed homogeneously with an average density ρ_L (ρ_R).

course of time, but keeps a constant center-of-mass velocity v_c. Under mild assumptions on the nature of the steady state this collective velocity is given by the derivative

$$v_c = \frac{d}{d\rho} j \tag{13}$$

of the current [5].

In a driven system with non-linear current-density relation one observes shocks, i.e. abrupt changes in the local density (Fig. 2). Shocks are stable collective excitations which travel with a mean velocity v_s determined by the boundary densities of the shock. Irrespective of the specific system mass conservation yields

$$v_s = \frac{j_L - j_R}{\rho_L - \rho_R}. \tag{14}$$

In equilibrium phenomena a domain wall is a localized region where the order parameter interpolates between degenerate ground states. In driven non-equilibrium systems a shock is like a domain wall, separating two possible *stationary* states of the system. A first-order transition between these states takes place when the shock velocity changes sign. Since the shock velocity is determined by boundary conditions a first-order (discontinuous) transition in the bulk density may be induced by boundary effects. This picture is well-supported by the linear increase of the local density (10) exactly at the first-order transition which corresponds to an average over all shock positions resulting from an unbiased random walk.

The factorized form of the density profile (10) suggests to study the two boundaries separately from each other. An overfeeding occurs when the collective velocity with which variations of the boundary density penetrate into the bulk changes sign. Injected particles create a localized increase of the density which cause back-moving density waves for boundary densities where the current has negative slope. These waves block further injection attempts and thus prevent a change in the stationary bulk current. The result is a second-order (continuous) phase transition in the bulk density.

These velocities and the underlying single-shock picture are sufficient to understand the phase diagram of systems with a single maximum in the current. If the current has a local minimum a single shock may branch into two distinct shocks, moving away from each other. This phenomenon follows from the stability criterion [5]

$$v_c(\rho_L) > v_s(\rho_L, \rho_R) > v_c(\rho_R) \tag{15}$$

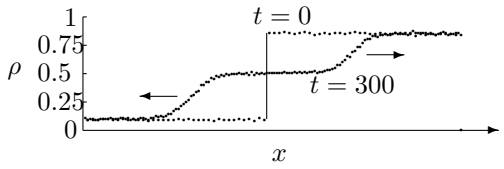

Figure 3: Monte-Carlo simulation of the particle density distribution in a lattice gas in the initial state (one shock) and after 300 Monte-Carlo sweeps, showing branching into two shocks. 3000 histories are averaged over [16].

for a single shock which one obtains by considering the flow of fluctuations in the neighbourhood of the shock. This behaviour which explains the emergence of the minimal current phase can be checked numerically (Fig. 3).

With these observations the dynamical origin of all phase transition lines can be understood by considering the time evolution of judiciously chosen shock initial states. Because of ergodicity, the steady state does not depend on the initial conditions and a specific choice involves no loss of generality. Thus one constructs the complete phase diagram and obtains the extremal principle (1).

5 Measuring boundary-induced phase transitions

We have shown above that the interplay of density fluctuations and shock diffusion, coalescence and branching resp. determines the steady state selection of driven diffusive systems with a single conserved density and leads to the extremal principle (1). In the absence of bulk phase transitions we expect this scenario to remain valid also in higher dimensions. A surprising phenomenon is the occurrence of a self-organized minimal current phase. Since little reference is made to the precise nature of the dynamics we argue that the phase diagram is generic and hence knowledge of the macroscopic current-density relation of a given physical system is sufficient to calculate the exact nonequilibrium phase transition lines.

It would be interesting to investigate these theoretical predictions for colloidal particles dragged down in a liquid in a narrow tube under the influence of gravitation. A difference to the models described above is the presence of hydrodynamic interaction between particles. However, according to the theory, the crucial property is a nonlinear flow-density relation, but not the microscopic origin of that relation. Experimental evidence for such a nonlinear relation has been provided by a three-dimensional setting. Hence one expects boundary-induced phase transitions of the nature discussed here when tuning entrance and exit rates for the colloidal particles in the tube. It is essential to avoid essentially ballistic motion where the flow is simply proportional to the density.

So far, empirical evidence for the first-order transitions has been found in automobile traffic flow data close to an on-ramp [27, 28]. However, the theory developed above does not explicitly incorporate non-conserved internal degrees of freedom of the particles which would correspond to velocity changes of cars. As a result, the behaviour of real traffic may

be more complex.

It is worthwhile to consider in some more detail the kinetics of biopolymerization on nucleic acid templates, as studied by MacDonald et al.[17, 18] using the TASEP. The mechanism they try to describe is (in a very simplified manner) the following: Ribosomes attach to the beginning of a messenger-RNA chain and "read" the genetic information which is encoded in triplets of base pairs by moving along the m-RNA.[1] At the same time the ribosome adds monomers to a biopolymer attached to it: Each time a unit of information is being read a monomer is added to a biopolymer attached to the ribosom and which is in this way synthesized by the ribosom. After having added the monomer the ribosom moves one triplet further and reads again. So in each reading step the biopolymer grows in length by one monomer. Which monomer is added depends on the genetic information read by the ribosom. The ribosoms are much bigger than the triplets on the m-RNA, they cover 20-30 of such triplets. Therefore neighbouring ribosomes sitting at the same time on the m-RNA cannot simultaneously read the same information. Furthermore they cannot overtake each other: If a ribosom sits at a particular place on the m-RNA and does not (temporarily) proceed further (e.g. because no appropriate monomer has been found in the surrounding medium for the polymerization process), then an oncoming ribosom from behind will stop until the first has eventually moved on. In order to describe the kinetics of this process MacDonald et al. introduced the following simple model. The m-RNA is represented by one-dimensional lattice of L sites where each lattice site represents one triplet of base pairs. The ribosom is a particle covering r neighbouring sites (for real systems $r = 20 \ldots 30$) but moving by only one lattice site in each (infinitesimal) time step with a constant rate p. These particles interact via hard-core repulsion, i.e. there is no long range interaction, but there is also no overlap of ribosomes. At the beginning of the chain particles are added with rate αp and at the end of the chain they are removed with rate βp.

The idealized case $r = 1$ corresponds to the ASEP with open boundary conditions. Its steady state was first studied using a mean-field approach [17]. Then in a following paper [18] the generalized case $r > 1$ was studied numerically and compared to experimental data on the stationary density distribution of ribosomes along the chain. These were found to be consistent with the results obtained from the model with $q = 0$ and $\alpha = \beta < p/2$. Furthermore it turned out that the mean field phase diagram for general r is similar to the much simpler case $r = 1$ in the sense that there are three distinct phases, a low density phase, a high density phase and a maximal current phase as discussed above. These observations encourage to use the asymmetric exclusion process as a simple but in certain aspects realistic model for this biological system.

The experimentally relevant case is the phase transition line from the low-density phase to the high density phase. On this phase transition line the mean-field calculation predicts a region of low density of ribosomes from the beginning of the chain up to some point where the density suddenly jumps (over a few lattice sites) to a high density value. The exact solution confirms the three phases predicted by mean field, but gives a linearly increasing density profile rather than the sharp shock predicted by mean field [21]. Within the theory developed above this can be explained by assuming that a sharp shock exists, but, due to

[1] The m-RNA is a long molecule made up of such consecutive triplets.

current fluctuations, performs a random walk along the lattice. What one therefore expects for an experimental sample is indeed a region of low density of ribosoms followed by a sharp transition to a region of high density of ribosoms as found experimentally. This rapid increase can be anywhere on the m-RNA, but with an exponential probability distribution with localization length $\xi = 1/(\ln[\alpha(1-\alpha)/\beta(1-\beta)])$ for $\alpha \neq \beta$ and constant distribution for $\alpha = \beta$ [21]. Thus the shock known from the exclusion process corresponds to a traffic jam of ribosomes which explains an experimentally observed slowing down of the ribosomes as they approach the terminal point of the m-RNA where they are released after completion of the protein synthesis [29, 30, 31, 32]. It would be interesting to reexamine the kinetics of biopolymerization in the light of these predictions.

In another biological setting it has been suggested that exclusion particles may describe molecular motors such as kinesins moving along microtubuli or actin filaments in a cell [45, 46]. Due attachment and detachment during the motion a description with non-conservative dynamics is required where particles are annihilated and created with a small rate also in the bulk. This leads to the model of Ref. [47] with open boundaries which yields interesting new phenomena, in particular localization of shocks [48, 49] and ergodicity breaking [50] even though the non-conservative bulk reactions increase the randomness of the dynamics.

6 Two-component systems

Somewhat surprisingly, numerical evidence shows that driven diffusive systems with two distinct particle species cannot be understood by straightforward generalization of the ideas developed above for one-component systems. Rather it was found that there is exciting new physics, including spontaneous symmetry breaking and phase separation phenomena, even in translation invariant systems [8, 33, 34]. Neither the hydrodynamic behaviour of systems with more than one conservation law nor the microscopic conditions for the occurrence of critical phenomena are well-understood. In order to describe a system with two different conserved species A, B of identical particles (or alternatively: tagged particles or particles with two internal states which do not affect its dynamics) one needs a model where each lattice site can be found in at least three different states: empty, or occupied by either an A-particle or a B-particle. The most simple extension of the exclusion process that accounts for the possibility of two particle species may hence be described by the six hopping rates

$$\begin{array}{rcrlll} A0 & \to & 0A & \text{with} & \text{rate} & D_{A0} \\ 0A & \to & A0 & \text{with} & \text{rate} & D_{0A} \\ B0 & \to & 0B & \text{with} & \text{rate} & D_{B0} \\ 0B & \to & B0 & \text{with} & \text{rate} & D_{0B} \\ AB & \to & BA & \text{with} & \text{rate} & D_{AB} \\ BA & \to & AB & \text{with} & \text{rate} & D_{BA}. \end{array} \tag{16}$$

There is no established name for this generic process and we shall refer to it as two-species ASEP. Associated with the two conservation laws there are two currents defined by

$$\frac{d}{dt}\rho_k^A = j_{k-1}^A - j_k^A \tag{17}$$

$$\frac{d}{dt}\rho_k^B = j_{k-1}^B - j_k^B . \tag{18}$$

Notice that in general j^A and j^B depend on both occupation numbers n_k^A, n_k^B respectively. Hence one has two coupled lattice continuity equations. The stationary distribution of this process and hence the current-density relation is known only on certain parameter manifolds. The natural order parameter that describes the macroscopic state of the system is the particle density of each species. In order to illustrate the significance of these models we give some examples of quasi one-dimensional two-component systems.

Tracer diffusion: The simplest way of obtaining a system with two conservation laws consists in considering tagged particles in the usual ASEP. Tagged particles (= particles of type B) have the same physical properties as usual particles, except that they carry a marker which allows for their identification, but does not affect the dynamics. Thus one gets the two-species ASEP (16) with

$$\begin{aligned} D_{B0} &= D_{A0} \\ D_{0B} &= D_{0A} \\ D_{AB} &= D_{BA} = 0. \end{aligned} \tag{19}$$

In the unbiased case $D_{A0} = D_{0A}$ a single tracer particle in a stationary system of density ρ is predicted to perform anomalous diffusion with a mean square displacement $\langle X^2(t) \rangle \propto (1-\rho)/\rho\sqrt{t}$ [35, 36, 37]. Recently this was confirmed experimentally in the investigation of tracer diffusion in zeolites [1] using pulsed field gradient NMR [38] and in the study of single-file diffusion of colloidal particles [2].

In the driven case (19) the situation is more complex. When averaging over random initial states of the system according to the weights given by the stationary distribution, the mean square displacement was proved to grow linearly in time with a diffusion coefficient $D = (D_r - D_\ell)(1-\rho)$ [39]. On the other hand, for fixed initial states (averaging only over realizations of the process) the variance is expected to grow subdiffusively with power $t^{2/3}$ [40, 41]. In a finite system with periodic boundaries the variance in the number of hops made in the totally asymmetric process ($D_{0A} = 0$) has been calculated exactly in the infinite-time limit [22, 42] and been found to decrease asymptotically $\propto 1/\sqrt{L}$ in system size. This is to be expected from dynamical scaling with the well-known dynamical exponent $z = 3/2$ of the asymmetric exclusion process [43, 44].

Biophysics: A two-species exclusion process has been introduced to describe the motion of ants along ant trails [51]. While crawling along a trail, the ants – modelled by A-particles hopping along a lattice – produce pheromones (B-particles) which serve as a marker of the traversed path for other ants which again produce pheromones for subsequent ants.

This is necessary to stabilize the trail as the pheromones evaporate after some time. The pheromones are modelled as an immobile particle species which is deposited when a hopping event has taken place and which disappears with some evaporation rate. The analogy of the flow of ants to traffic flow has been pointed out in Ref. [52] who measured the flow rate versus the density of ants, i.e., the current density relation. The numerical results obtained from the two-species ant trail model yield qualitatively similar results [51]. Essentially the same model (with different parameter values and update rules) has been introduced as a "bus route" model where one observes bunching of particles (="buses") as they travel along lattice ("bus stops") and pick up passengers [53]. Bunching of real buses appears to occur on services which do not run according to fixed schedules, but which stop according to demand. This suggests that phase separation between a region of high density and a region of low density may occur in two-component systems. This question is addressed in detail below.

Polymer dynamics: In polymer networks such as rubber gum or gels, in polymer melts or in dense solutions of macromolecules such as DNA different polymer strands form a complicated topological structure of entanglements somewhat reminiscent of a large portion of spaghetti. The entanglements severely restrict the dynamical degrees of freedom of the polymer chains. In the framework of the celebrated reptation theory developed by Doi, Edwards, and de Gennes [57, 58] the motion of an individual polymer is viewed as being confined by a hypothetical tube which models the collective effect of all entanglements of the neighbouring polymer chains. In an uncrosslinked melt or solution the tube is open at both ends, since at the end points the motion of polymer segments transverse to its own contour is not restricted by topological constraints. This picture results in a snake-like one-dimensional effective dynamics of polymer segments along the tube, with extra orientational degrees of freedom only at its ends.

In a lattice model of Rubinstein [59] the reptation dynamics is modeled by the symmetric exclusion process with open boundaries which describe the extra end point degrees of freedom. With this model exact results for the relaxation of the contour and contour length fluctuations have been obtained. Recent experiments on the dynamics of single entangled DNA-molecules in dense solution confirm the findings [3, 60].

Duke [61] extended the model to allow for tracking the spatial orientation of the tube rather than only its length. This was done in order to introduce a reference axis for describing gel electrophoresis, i.e., the separation of polymer fragments according to their length L. By applying an electric field of strength E (the direction of which is the reference axis) a charged polymer is expected to move through a gel matrix (which provides an entanglement network) according to the rules of reptation. However, standard reptation theory does not allow for a prediction of the drift velocity v beyond the linear response regime of small fields or very long polymers where

$$v \propto DEL. \tag{20}$$

Here D is the diffusion coefficient of an entangled polymer, predicted by reptation theory to scale

$$D \propto 1/L^2 \tag{21}$$

with length. The extended Rubinstein-Duke model is an asymmetric three-states exclusion process (16) with $D_{AB} = D_{BA} = 0$ and open boundaries. Exact and rigorous results [62, 63] confirm the predictions (20), (21). Moreover, simulations at high fields yield the drift velocity in the non-linear regime [64] which are in good agreement with experimental data [65]. At sufficiently high fields the model exhibits spontaneous symmetry breaking in the orientation of the polymer chain [66].

A long-standing mystery in reptation theory has been the asymptotic behaviour of the viscosity η of a polymer melt which is expected to scale asymptotically [57, 58]

$$\eta \propto L^3. \tag{22}$$

However, experiments consistently give higher value ≈ 3.4 of the scaling exponent. Doi had suggested this to be a finite-size effect due to tube-length fluctuations [57]. That tube-length fluctuations lead to an increased effective exponent could be confirmed by a careful numerical analysis of the Rubinstein-Duke model [67]. Also details of the end-segment dynamics were shown to have significant non-universal impact on finite-size behaviour of the viscosity and the diffusion coefficient [68].

Interface growth: It was already realized in the 1980ies that the ASEP describes the dynamics of a fluctuating interface by considering the spin variables as local discrete slopes of an interface on a two-dimensional substrate [69, 70]. Hopping of a particle to the right between sites $k, k+1$ corresponds to the random deposition of a particle on site k of the dual growth lattice, hopping to the left to an evaporation. One thus obtains a growth model in the universality class of the one-dimensional KPZ equation [4], reviewed in [75]. The extension of this mapping to the generalized exclusion process (16) is obvious, one obtains a system where local height differences may take values $0, \pm 1$.

7 Critical Phenomena in one-dimensional two-component systems

It is well-known that in thermal equilibrium one-dimensional systems with finite local state space and short range interactions do not exhibit phase transitions at positive temperatures, only at $T = 0$ long range order may exist. From a dynamical viewpoint there are no thermal fluctuations at $T = 0$ in a classical system. In terms of a stochastic process that means that all transition rates are zero. Conversely, if a transition rate is non-zero, some dynamics – not necessarily satisfying detailed balance – is going on and it has been conjectured that quite generally a system with strictly positive transition rates and local interactions can have at most one stationary distribution, which is often rephrased by saying that there can be no phase transition in a one-dimensional system with strictly positive rates.

To rationalize the conjecture one imagines, in the simplest case, two potentially stationary distributions characterized by a different value of the order parameter. An example is the Ising model where the order parameter is the magnetization, which can take two different values below the critical temperature in two or higher dimensions. The reasoning behind the positive rates conjecture is the difficulty to imagine a local mechanism that

eliminates islands of the minority phase (created constantly by thermal fluctuations in a region where the other phase dominates) since in one dimension energetic effects due to line tension play no role. Since the "boundary" of a one-dimensional island (viz. just the two boundary points) does not grow with the size of the island (as it does in higher dimensions) a local mechanism cannot "detect" the size of a minority island, therefore such an island can grow indefinitely and destroy the majority phase. Since noise (implied by strictly positive rates) can always create such islands there seems to be no possibility to keep the majority phase stable against fluctuations. In a certain "natural" class of systems with nearest-neighbour interaction this conjecture has been proved rigorously some time ago [71].

Therefore it came as a surprise that P. Gacs constructed a model on the infinite lattice which violates the positive rates conjecture [72, 73]. However, both the model and the proof that there is a phase transition is rather complicated [74], requiring either a very large local state space or a very large interaction range, and the quest for simple models with this property continues to stimulate research.

As a guideline in pursuing this aim we note that the conjecture is clearly true for dynamics satisfying detailed balance with respect to a local interaction energy: In this case the stationary distribution is just the usual equilibrium distribution and the argument underlying the positive rates conjecture applies. Hence from a theoretical perspective one should look for models that either violate detailed balance or have a nonlocal interaction energy, but local dynamics. This would shed insight in critical phenomena that may occur in real complex systems.

By definition, conservative systems have a continuum of stationary states (characterized by the value of the order parameter) and hence the critical phenomena we review concern transitions between different stationary distributions at the same value of the order parameter and coexistence of macroscopic stationary domains where the order parameter takes different values. The domain walls separating these domains are the shocks discussed in the previous section. Hence the stability of domain walls is intimately connected with the existence of phase separation.

The exact and numerical analysis of steady states of one-species systems has revealed that phase separation in periodic systems may occur if one or more of the following conditions are satisfied [8]:

- (I) there are spatially localized defects reducing the mobility of particles
- (II) single particles of a different species act as mobile blockages
- (III) the dynamics have kinetic constraints arising from a nonequilibrium zero-temperature condition.

The last condition leads to *strong phase separation* in the sense that one domain is fully occupied whereas the other domain is entirely empty. The current in the phase separated state vanishes exponentially in the size of the particle domain, the separated state exists at any total particle density. Conditions (I) and (II) may lead to strong phase separation, but allow also for a soft phase separation between domains of different densities. This

phenomenon sets in only for densities above some critical density ρ_c. The steady-state current is nonvanishing and independent of ρ in the phase separated state: Increasing the density leads to an increase of the size of the high-density domain, but not to a change of the current. In analogy to Bose-Einstein condensation we call the high density domain a condensate, the transition at ρ_c is referred to as condensation transition.

Strong phase separation has been found also in homogeneous systems on a ring where neither of the conditions (I) - (III) is satisfied, but where there is a second species of particles with finite density [76, 54, 77]. Hence we add a further condition for the possibility of phase separation

- (IV) the system has two or more conservation laws

We remark that all the conditions (I) - (IV) in some way or other impose local constraints on the dynamics of the driven diffusive system. This appears to be a general requirement for phase separation in generic driven diffusive systems. The size of the local state space and the range of interaction appear to be irrelevant if one of the conditions (I) - (IV) is satisfied.

Using a four-states model which is equivalent to a two-lane model with two conserved densities Lahiri and Ramaswamy [76, 78] address the question of phase separation in terms of the stability of crystals moving steadily through a dissipative medium, e.g., a sedimenting colloidal crystal. In a certain limit (large particle radius or small elastic modulus of the suspension) experiments suggest instability of such a crystal. Numerical analysis of the lattice model, however, reveals a transition to a stable regime, corresponding to strong phase separation. In the 2-species ASEP with rates [77, 79]

$$D_{A0} = D_{0B} = D_{BA} = 1, \quad D_{0A} = D_{B0} = D_{AB} = q \tag{23}$$

the mechanism for strong phase separation for $q < 1$ is very transparent. Here strong phase separation refers into separation of three pure macroscopic domains, each consisting of essentially only one particle species or empty sites. For simplicity we assume $N^A = N^B$, but this is not necessary for the phenomenon to occur. Prepare a phase-separated block which we symbolically represent by $\ldots 000AAAAAABBBBBB000\ldots$. One observes the following: (i) The $0|A$ interface is stable by the criterion (15) since due to the absence of B-particles one has the dynamics of the usual ASEP (with a bias to the right) in the vicinity of this domain wall. (ii) The $B|0$ interface is stable for exactly the same reason (B particles have a bias to the left) (iii) The $A|B$ interface is stable since in the absence of vacancies B-particles act like vacancies w.r.t. the local dynamics of the A-particles and vice versa. (iv) Since each domain wall is stable (only small fluctuations extended over a finite range of lattice sites evolve at the phase boundaries) the assumption used in the argument remains valid for all times.

Exact results have revealed that numerical evidence for soft phase separation may be rather subtle and indeed be misleading [83]. It would thus be of great importance to find other criteria which could distinguish between models supporting phase separation from those which do not. Phase separation is usually accompanied by a coarsening process in which small domains of, say, the high density phase coalesce, eventually leading to

macroscopic phase separation. This process takes place as domains exchange particles through their currents. When smaller domains exchange particles with the environment with faster rates than larger domains, a coarsening process is expected, which may lead to phase separation.

An approach that quantifies this mechanism and yields a criterion for phase separation in terms of the current leaving the domains is proposed by Kafri et al [80]. The current-criterion is readily applicable even in cases which cannot be decided by direct numerical simulations. In order to explicitly state the criterion one distinguishes systems with a vanishing current of a finite domain of size n

$$J_n \to 0 \quad \text{(case A)} \tag{24}$$

from systems finite-size corrections to a finite asymptotic domain current J_∞ of the form

$$J_n = J_\infty(1 + b/n^\sigma) \quad \text{(case B)}. \tag{25}$$

to leading order in $1/n$. For simplicity we assume here domains with vanishing drift velocity in which case the current inside the domains equals the outgoing current. More generally one has to distinguish the two currents leaving the cluster at the right and left boundary respectively.

For $b > 0$ the current of long domains is smaller than that of short ones, which leads to a tendency of the longer domains to grow at the expense of smaller ones. The current criterion asserts that phase separation exists only in the following cases [80]:

$$J_n \quad \to \quad 0 \quad \text{for } n \to \infty \text{ (case A)} \tag{26}$$

$$J_n \quad \to \quad J_\infty > 0 \quad \text{(case B)} \tag{27}$$

for either $\sigma < 1$ and $b > 0$ or $\sigma = 1$ and $b > 2$. In case A one has strong phase separation for any density, whereas in case B one has soft phase separation at any density for $\sigma < 1$ and above a critical density

$$\rho_c \propto \frac{1}{b-2} \tag{28}$$

for $\sigma = 1$. The fluid regime has particles with density ρ_c. Hence in a finite system the macroscopic size of the condensate in the phase-separated regime is determined by the system parameter b. For an asymptotic decay faster than $2/n$ there is no condensed phase, the system is disordered for all densities. The criterion presented above emerges from a careful analysis of the zero-range process [84] which could be viewed as a generic model for domain dynamics in one-dimension [80].

For $J_\infty \neq 0$ (case B) we note that in a system with two conservation laws the current inside a cluster organizes itself to a value determined by the dynamics of the reduced system with only one conservation law resulting from the absence of vacancies. This reduced system has open boundaries with in- and outflow of particles such that the system is in the generic maximal current phase of the reduced system. It is assumed that the current flowing through a block is given by its steady-state value and is independent of its neighboring

blocks. This may be justified by the fact that the coarsening time of large domains is very long, and the domains have a chance to equilibrate long before they coarsen.

In case B one expects generically $\sigma = 1$ for the following reason: (a) In a *periodic system* the leading finite-size corrections to the current J_∞ in a canonical ensemble is given by $J_n - J_\infty = -J''_\infty \kappa/(2n)$ [55, 81]. Here J''_∞ is the curvature of the current-density relation and $\kappa = (\langle N^2 \rangle - \langle N \rangle^2)/L$ is the nonequilibrium analog of the thermodynamic compressibility which is assumed to be finite, i.e., one assumes sufficiently rapidly decaying correlations as was implied above in the derivation of the collective velocity which also requires finite compressibility. (b) There is a universal ratio c^* of the finite-size corrections to the current in the maximal current phase of a driven diffusive system (which describe the dynamics inside the growing domains) and the finite-size corrections of the canonical ensemble of a periodic system [56]. This yields leading finite-size corrections of the form (24) with a parameter b entirely determined by the universal constant c^* and the macroscopic quantities J''_∞ and κ. The value of $c^* = 3/2$ has been obtained from the exact solution of the ASEP with open boundaries [21, 22].

We stress that by definition b is a quantity that itself does not depend on system size. For systems with unknown stationary distribution the reduced dynamics inside a cluster allows for a simple numerical measurement of b by studying the finite-size corrections of the stationary current in the reduced open system of length n. One neither needs huge lattices nor is one faced with the problem of slow relaxation of the phase separation process in the full system. Applying the criterion to the model introduced in Ref. [54] yields the exact value $b = 3/2$ and hence one expects no condensation, in agreement with the exact result [83]. This is important in so far as mean-field analysis and numerical simulations had originally misled the authors of [54] to the conclusion that phase separation should occur in that model. For the two-lane model of Korniss et al [82] one obtains numerically $b \approx 0.8$ [80] and therefore one expects no condensation in contrast to the results of the Monte-Carlo simulation of the full model with 10^4 lattice sites. A three-states model with next-nearest neighbour interaction inside the clusters has been shown to have $b > 2$ [81] which suggests the existence of soft phase separation in driven diffusive systems with two conservation laws.

8 Conclusions

There is hardly a single major field of physics such as biophysics, polymer physics and so on where single-file diffusion plays a dominant role. Yet in many diverse subfields the study of one-dimensional driven diffusive motion provides the conceptual framework to understanding key phenomena in the respective areas, such as polymer reptation, single-file diffusion in zeolites, and so on. Exact analytical tools and numerical investigation of single-component systems has made it possible to bridge the gap between microscopic models and a coarse-grained macroscopic description. Thus we are furnished with a microscopic understanding of macroscopic concepts such as shock motion and steady state selection. A crucial role is played by the macroscopic current-density relation which allows for a quantitative prediction of the phase diagram of boundary-induced bulk phase transitions.

Particle systems with two or more components have proved to exhibit an even richer stationary behaviour, with intriguing critical phenomena that have no analogue in thermal equiilbrium. They have also proved far more challenging from a theoretical viewpoint, with many fundamental issues still under debate. Building on recent experimental work on quasi-one-dimensional diffusive interacting particle systems in equilibrium, the quantitative investigation of driven systems is likely to become feasible in the near future. It will certainly turn out be a rewarding field of research.

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