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Phase separation in one-dimensional stochastic particle systems?

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Abstract. A class of interacting particle systems modelling driven diffusive systems with short range interactions has been suggested to exhibit macroscopic phase separation in $d = 1$ dimensions. Unlike all previously studied models exhibiting similar phenomena, there the phase separated state is fluctuating in the bulk of the macroscopic domains. We discuss a recently introduced sufficient criterion for the existence of such phase separation and point out some assumptions which require rigorous proof. We also introduce a new model for strong phase separation into essentially nonfluctuation states. We informally describe its exact invariant measure.

Keywords: phase separation, ergodicity, exclusion process, zero-range process.

Mathematical subject classification: 82C22, 82C26, 60K35.

For a very long time it was generally believed that in translation invariant noisy one-dimensional systems with short-range interaction and finite local state space one has a unique invariant measure unless judiciously chosen local transitions have zero probability. This is the essence of the so-called positive rates conjecture which is a more precise version of the well-known statistical physics verdict "No phase transition in one dimension at positive temperature". Only very recently a rigorous proof has been given (by providing a counterexample) that the positive rates conjecture is not true in such generality [1].

Nevertheless there are reasons why the positive rates conjecture continues to intrigue. Firstly, the counterexample constructed by Gacs is rather complicated. It is a lattice model requiring either a very large local state space of the order of $m = 10^6$ or a correspondingly large range R (in lattice units) of interaction [2].

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Therefore there is interest in finding more natural models motivated by physical problems that would contradict the positive-rates conjecture. "Nice" models could be fairly straightforward generalizations of the exclusion process [3, 4]. Secondly, the main argument in favor of the conjecture is quite generic and, as factual evidence tells us, rather robust: In order to have a phase transition (i.e., at least two invariant measures for the same set of parameters of the model) one needs a mechanism that suppresses the growth of islands of the minority phase inside the majority phase. In two and more dimensions such a suppresion can be taken care of by the interplay of entropy and surface energy of the minority islands. However, in one dimension the "surface" are just two points and thus the surface energy does not depend on the size of the "island". Hence surface energy cannot limit island growth if interactions are local, unless forbidden transitions (zero rates) would somehow dynamically restrict the accessibility of the state space.[1]

This argument is so simple that it is tempting to apply it to conservative stochastic particle systems and argue that no phase transition is expected to occur, unless one makes very elaborate assumptions on either local state space or range of interaction as in the model of Gacs. Since, however, conservative particle systems have a build-in violation of the positive rates assumption we first have to clarify what we mean. Let us assume a particle system with conserved particle number. Clearly, the conservation law imposes zero rates since transitions that change the particle number are not permissible. Nevertheless, in a finite system (i.e. with finite local state space and a periodic lattice with L lattice points) which allows for all local transitions that do preserve particle number, one has ergodicity for each sector of fixed particle number. If one demands positive rates for all transitions compatible with the conservation law then the island growth argument suggests that this ergodicity survives in the thermodynamic limit $L \to \infty$.

A violation of this modified positive rates conjecture in a translation invariant conservative system – if it exists – would manifest itself in macroscopic phase separation, somewhat analogous to what happens in the two-dimensional zero-field Ising model below criticality. Recently a general criterion for the existence of phase separation in driven one-dimensional models has been introduced [6]. The criterion relates the existence of phase separation in a given model to the rate at which domains of various sizes exchange particles with each other. Assuming that for a domain of length n this rate is given by the steady state current J_n which

[1] Such zero rates would keep the system "frozen" within some domain of state space and are not subject of the positive rates conjecture. See e.g. [5] for a nontrivial example of this kind for which some precise information is known about a system which, like the model of Gacs, is not defined in terms of a Hamiltonian but in terms of transition rates.

flows through it, phase separation was suggested to exist only in the following cases: either the current vanishes in the thermodynamic limit,

$$J_n \to 0 \text{ as } n \to \infty \qquad (\textbf{Case I}) \tag{1}$$

or the behavior of the current for large domains is of the form

$$J_n \sim J_\infty (1 + b/n^\sigma) \qquad (\textbf{Case II}) \tag{2}$$

for either $\sigma < 1$ and $b > 0$, or for $\sigma = 1$ and $b > 2$. This conjecture has been applied with some success to various exclusion processes with two conserved species of particles.

First we consider Case I. It corresponds to strong phase separation characterized by coexistence of pure domains, each consisting of a single type of particles [7, 8, 9, 10]. Thus, the particle density in the interior of a domain is non-fluctuating like in a zero-temperature Ising system. The noisy dynamics is reflected only in density fluctuations that are limited to finite regions around the domain boundaries. Moreover, in this case phase separation is expected to take place at *any* density, no matter how small. Interestingly all the models where strong phase transition has so far been established have two conserved currents. Not much is known about dynamics in such systems on a rigorous level. With a view on dynamical phenomena in strong phase separation it would thus be of great interest to establish this phenomenon in a one-component system. For such systems the hydrodynamic theory is quite developed [11] and it may be possible to study such a system under Eulerian scaling.

To this end we propose a generalized asymmetric exclusion process with next-nearest neighbor interaction and period boundary conditions as follows: (1) Particles move with rate p (q) to the right (left) across the bond $(x, x+1)$, provided that the target site $x+1$ (x) is empty and that there is either a vacancy on site $x-1$ or a particle on site $x+2$. The invariant measure can be explicitly computed. For $p = q$ it is a product measure, corresponding to disordered state with finite mean cluster size given by the particle density. For $p \neq q$ the nature of the invariant measure is more easily described in terms of an associated anchored growth process. In this process the bonds of the exclusion process becomes sites in an interface model where each site carries a height variable h_x. A particle on site x corresponds to a negative local height gradient $h_{x+1} - h_x = 1$ while a vacancy corresponds to a positive unit gradient. For particle number $N = L/2$ the height model is periodic, for $N \neq L/2$ one has $h_{x+L} = h_x - (N - L/2)$. (We assume L to be even.) The particle configuration then defines a height profile, with its minimum always defined to be at height 0. The hopping dynamics thus turn into a growth dynamics such that the interface remains anchored on a substrate at height 0. The invariant measure is a translation invariant sum of measures which give exponential weight to the area under the interface, with a parameter determined by the logarithm of the hopping asymmetry. This can be proved by direct computation [12]. For $p > q$ the interface tries to grow, but cannot grow indefinitely due to the anchoring. Thus it reaches (almost) maximal height before growth stops. In particle language this corresponds to strong phase separation with mean domain size N where N is the number of particles in the system.

This observation is in agreement with the criterion (1) since the current inside a cluster is exponentially small in the size of the cluster. It would be interesting to investigate whether a hydrodynamic limit at least for weak hopping asymmetry could be proved. Unlike the two-component ABC model of Ref. [13] this model has a genuine transition from the phase-separated state through a disordered state into a state that corresponds to an interface attracted by the substrate. Notice, however, that this model is not quite in the spirit of the introduction, since it has vanishing local rates compatible with particle conservation. In interface language this constraint ensures anchoring. If this constraint would be relaxed the interface would be able to grow and one would expect strong phase separation to disappear.

On the other hand, in Case II the phase separated state is expected to be fluctuating in the bulk of the macroscopic domains, as is normally expected in a noisy system. It exists only at high enough densities $\rho > \rho_c$, while at low densities $0 < \rho < \rho_c$ the system is homogeneous. This phase was termed *condensed* as the mechanism of the transition is similar to that of the Bose-Einstein condensation. We refer to this phenomenon as soft phase separation. We note that in many models which carry a non-zero current in the thermodynamic limit the current of a finite domain of size n takes the form $J_n = J_\infty(1 + b/n)$ to leading order in $1/n$ and we shall focus here on this case. 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. This is clearly a necessary condition for phase separation. According to the criterion (2) phase separation may take place only for $b > 2$. This is motivated by a careful analysis of condensation in the zero-range process [14].

What is missing is a rigorous proof of the existence of soft phase separation. In order to prepare the ground that may serve as starting point for achieving this goal we explain in this work the mechanism that leads to the criterion for soft phase with $\sigma = 1$ and discuss some related open questions that we hope can be proved rigorously with some generality. To keep the exposition simple we consider two specific two-component exclusion processes, defined on a one-dimensional ring with L sites. Each site i can be either vacant (0) or occupied by at most one positive (+) or at most one negative (−) particle (or charge). Hence a configuration $\mathbf{s} = \{s_1, \ldots, s_L\} \in \{-1, 0, 1\}^L$ is given in terms of local states $s_i = +1$ (-1) if site i is occupied by a + (−) particle, and $s_i = 0$ if site i is vacant. We impose periodic boundary conditions by identifying site $L+1$ with site 1. We shall see that both models have zero rates for some local transitions, but unlike in the one-component model for strong phase separation this is not believed to relevant for the qualitative properties of these models.

For defining the stochastic continuous-time dynamics of the process we follow standard probabilistic notation and define $\mathbf{s}^{ij}$ as the configuration with s_i and s_j interchanged, i.e.,

$$\mathbf{s}_k^{ij} = \begin{cases} s_k & \text{if} \quad k \neq i, j \\ s_j & \text{if} \quad k = i \\ s_i & \text{if} \quad k = j \end{cases} \tag{3}$$

Then the infinitesimal generator $\mathcal{L}$ acting on functions $f(\mathbf{s})$ is given by

$$\mathcal{L} f(\mathbf{s}) = \sum_{i=1}^{L} c(i, i+1; \mathbf{s}) \left[f(\mathbf{s}^{i,i+1}) - f(\mathbf{s}) \right] \tag{4}$$

Here $c(i, i+1; \mathbf{s})$ are the particle exchange rates which are different in the two models. In both models positive particles are driven to the right while negative particles are driven to the left. The dynamics conserves the number of particles of each species, N_+ and N_-. The total density of particles in the system is $\rho = (N_+ + N_-)/L$. We consider the case where the number of positive and negative particles is equal, $N_+ = N_- =: N$.

In model A, known as AHR model [8], particles have asymmetric hopping dynamics with mutual hard-core repulsion and hopping rates

$$\begin{aligned} c(i, i+1; \mathbf{s}) \;\; = \;\; & \frac{\alpha}{2} \left[\left(s_i^2 + s_i\right)\left(1 - s_{i+1}^2\right) + \left(1 - s_i^2\right)\left(s_{i+1}^2 - s_{i+1}\right) \right] \\ & + \frac{1}{4} \left[q\left(s_i^2 + s_i\right)\left(s_{i+1}^2 - s_{i+1}\right) + \left(s_i^2 - s_i\right)\left(s_{i+1}^2 + s_{i+1}\right) \right]. \end{aligned} \tag{5}$$

More intuitively the nonvanishing jump rates can be represented as follows

$$\begin{array}{lcll} +0 & \rightarrow & 0+ & \text{with rate} \quad \alpha \\ 0- & \rightarrow & -0 & \text{with rate} \quad \alpha \\ +- & \rightarrow & -+ & \text{with rate} \quad 1 \\ -+ & \rightarrow & +- & \text{with rate} \quad q \end{array} \tag{6}$$

The invariant measure of the process is rather complicated but known explicitly [15].

In model B [16] particles are subject to short-range interactions in addition to the hard-core repulsion. These interactions are "ferromagnetic", in the sense that particles of the same kind attract each other. They are not given in terms of a Hamiltonian, but are encoded in the hopping rates

$$\begin{aligned} c(i,i+1;\mathbf{s}) &= \frac{\alpha}{2}\left[\left(s_i^2+s_i\right)\left(1-s_{i+1}^2\right)+\left(1-s_i^2\right)\left(s_{i+1}^2-s_{i+1}\right)\right] \\ &\quad + \frac{1}{4}\left(s_i^2+s_i\right)\left(s_{i+1}^2-s_{i+1}\right)\left[1-\frac{\epsilon}{4}\left(s_{1+1}-s_i\right)\left(s_{i+2}-s_{i-1}\right)\right]. \end{aligned} \tag{7}$$

This generator describes a hopping process with the following jump rates:

$$\begin{array}{lclll} +0 & \to & 0+ & \text{with rate} & \alpha \\ 0- & \to & -0 & \text{with rate} & \alpha \\ +- & \to & -+ & \text{with rate} & 1-\Delta H \end{array} \tag{8}$$

The quantity ΔH is the difference in the "ferromagnetic" interactions between the final and the initial configurations given by

$$H = -\epsilon/4 \sum_i s_i s_{i+1} \,. \tag{9}$$

The interaction parameter ϵ satisfies $0 \leq \epsilon < 1$ to ensure positive transition rates. The model is a generalization of the Katz-Lebowitz-Spohn (KLS) model, introduced in [17] and studied in detail in [18, 19], in which the lattice is fully occupied by particles and no vacancies exist. Notice that the process is not reversible and hence the quantity H is not simply related with the invariant measure of the process. This measure is expected to have a complicated structure for $N \neq 0, 1, L$, known explicitly only for $\epsilon = 0$ where it coincides with the AHR model with $q = 0$.

In the context of these models we define as a (particle) cluster of size n a consecutive set of n occupied sites, bounded by vacancies on each side. No assumption on the distribution of $\pm$-particles inside the domain is implied in this definition. Macroscopic phase separation between a condensed phase and a homogeneous phase then manifests itself by an invariant measure that is concentrated on configurations which have (at least) one cluster of size $n = cL$ with $0 < c \leq \rho$ as L tends to infinity. This means that a finite fraction of particles condenses into a macroscopic cluster. Anticipating the arguments given below one expects a single cluster, hence $c = \rho - \rho_c$. Strong phase separation

($c = \rho$ and further separation inside the macroscopic cluster) is included in this definition but is not envisaged here.

Based on numerical simulations and mean field approximation in which the true invariant measure of the process is approximated by a product measure it was suggested that the AHR model exhibits a condensed phase separated state at sufficiently high densities [8]. However, a subsequent exact computation of the invariant measure [15] shows that what numerically seems like a condensed state is in fact homogeneous, with a very large but finite mean cluster size. Further analysis of this model along the lines discussed below shows that the currents J_n corresponding to this model are given by the form II, with $\sigma = 1$ and $b = 3/2$ [6]. Therefore, according to the criterion and in agreement with the exact result, no phase separation takes place.

On the other hand, model B has a parameter range ($\epsilon > 0.8$ and sufficiently large α) where $\sigma = 1$ and $b > 2$. According to the criterion (2) a condensation transition occurs as the density ρ is increased above a critical density ρ_c. To our knowledge, this is the first example of a genuine transition of this type in one-dimensional driven systems. Typical configurations obtained during the time evolution of the model starting from a random initial configuration are given in Fig. 1. This figure suggests that a coarsening process takes place, leading to a phase separated state as described above. However, this by itself cannot be interpreted as a demonstration of phase separation in these models. The reason is that this behavior may very well be a result of a very large but finite correlation length, as is the case in the AHR model [8, 15].

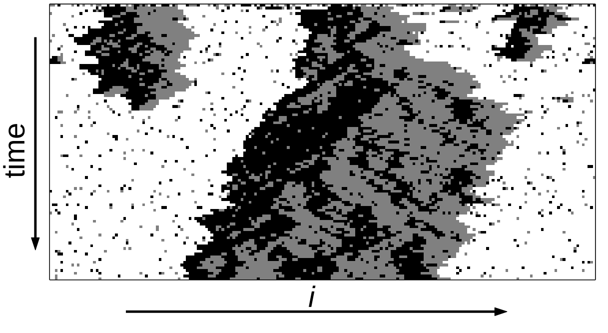

Figure 1: Evolution of a random initial configuration of model (8) with nearest-neighbor interactions, on a ring of 200 sites. Here $\epsilon = 0.9$, $\alpha = 2$, and the particle density is $\rho = 0.5$. Positive particles are colored black, and negative particles are colored grey. One hundred snapshots of the system are shown every 100 Monte-Carlo sweeps.

In order to show nonrigourously that phase separation takes place in model B we argue that the current J_n corresponding to a cluster of length n may be determined by studying an open chain of n sites, only occupied by positive and negative particles, with entrance and exit rates α at its ends. This is just the one-dimensional KLS model with open boundaries. We consider α such that the system is in its maximal current state, whereby J_∞ assumes its maximum possible value, and is independent of α.

To evaluate J_n we first consider the KLS model on a periodic chain of n sites with no vacancies. We then extend these results to study the behavior of an open chain. On a ring particle number is conserved and one has a canonical invariant measure for each fixed particle number. From these canonical measures one can construct in standard fashion grandcanonical ensembles parametrized by a chemical potential μ. Under rather general conditions, requiring only a single sharply peaked particle number distribution in the grandcanonical ensemble with finite compressibility $\kappa = \lim_{n\to\infty} n^{-1}\left(\langle n_+^2\rangle - \langle n_+\rangle^2\right)$ at its maximum one can show that expectations of thermodynamic observables in the canonical and grandcanonical ensembles respectively differ by an amount $O(1/n)$ to leading order in particle number n. This is essentially the leading deviation from the law of large numbers. Specifically, the current J_n takes the following form for large n,

$$J_n = J_\infty \left(1 - \frac{\lambda\,\kappa}{2J_\infty}\frac{1}{n}\right) . \tag{10}$$

Here $\lambda = \partial^2 J_\infty/\partial\rho_+^2$ is the second derivative of the current with respect to the density of positive particles ρ_+ in the system.

Hand wavingly this can be derived by considering the current $J_n(n_+)$ for charge densities close to $n_+ = n_- = n/2$. Expanding $J_n(n_+)$ in powers of $\Delta n_+ = n_+ - n/2$ one has

$$J_n(n_+) = J_n\left(\frac{n}{2}\right) + J_n'\,\Delta n_+ + \frac{1}{2}J_n''\,(\Delta n_+)^2 \tag{11}$$

where the derivatives J_n' and J_n'' are taken with respect to n_+ and evaluated at $n/2$. We average (11) over n_+ with the steady state weights of a grand canonical ensemble. This is done by introducing a chemical potential μ which ensures that the average density satisfies $\langle n_+\rangle = n/2$. We find

$$\langle J_n(n_+)\rangle_\mu = J_n\left(\frac{n}{2}\right) + \frac{1}{2}J_n''\,\langle(\Delta n_+)^2\rangle_\mu . \tag{12}$$

Noting that $\langle J_n(n_+)\rangle_\mu$ is J_∞ in the $n \to \infty$ limit, and $J_n(n/2)$ is just J_n, Eq. 10 is obtained.[2]

The result (10) can be used to evaluate J_n for the KLS model. For periodic boundary conditions the grandcanonical invariant measure is an Ising measure with weight [17, 18, 19]

$$P(\{s_i\}) = e^{-\beta\mathcal{H}} \quad ; \quad \mathcal{H} = -\sum_{i=1}^{n} s_i s_{i+1} - \mu \sum_{i=1}^{n} s_i \ , \tag{13}$$

with $s_i = \pm 1$ for positive and negative charges respectively, and $e^{4\beta} = (1-\epsilon)/(1+\epsilon)$. The chemical potential μ controls the density of, say, the positive particles. It vanishes for the case $n_+ = n_-$. Using (13) explicit expressions for $\kappa(\epsilon)$ and $J_\infty(\epsilon)$ of this model have been obtained in [18, 19].

We now consider the KLS model in an open chain, which is the relevant geometry in applying the phase-separation criterion. It has been argued [21] that the finite size correction to the current of an open chain is given by the corresponding correction in a ring geometry, up to a universal multiplicative constant c which depends only on the boundary conditions. In the maximal current phase, c was found to be $3/2$ [22, 23]. Thus the current of an open system is given by (2) with $\sigma = 1$ and

$$b(\epsilon) = -c\frac{\lambda(\epsilon)\kappa(\epsilon)}{2J_\infty(\epsilon)} \ . \tag{14}$$

Using the values of J_∞ and κ obtained in [18, 19] and $c = 3/2$ we find

$$b(\epsilon) = \frac{3}{2}\ \frac{(2+\epsilon)\upsilon + 2\epsilon}{2(\upsilon+\epsilon)} \ ; \ \upsilon = \sqrt{\frac{1+\epsilon}{1-\epsilon}} + 1 \ . \tag{15}$$

It is readily seen that for $\epsilon > 0.8$ the value of b is larger than 2. This result – which relies on the identification of the stationary cluster current of fluctuating length n with the stationary current of an open chain with fixed length n – has been confirmed to high accuracy by Monte carlo simulation [16]. The same line of reasoning may be applied to the AHR model. Here the cluster dynamics are that of the partially asymmetric simple exclusion process where $\kappa = \rho(1-\rho)$ and $J'' = -2$, independent of q. In the maximal current phase where $\rho = 1/2$ this yields $b = 3/2$.

[2] The result Eq. 10 has first been obtained with a different argument in the context of interface growth in $1+1$ dimensions using that in these models J_n corresponds to the growth velocity of the interface [20].

This description of the internal cluster dynamics gives the cluster current entering the criterion (2), but does not give the distribution of clusters inside the original three-states model The final step in establishing (nonrigorously) soft phase separation is a description of the cluster dynamics in terms of a non-Markovian zero-range process. This is done by identifying vacant sites with the sites of i a zero-range particle system and a cluster of size n to the right of vacancy i with an occupation number n_i of the zero-range process (Fig. 2). In this mapping zero-range particles hop randomly and strongly correlated in time to neighboring clusters. Approximating these correlated jumps by uncorrelated jumps with exponential waiting time distribution with mean $1/J_n$ one arrives at the usual zero-range process with symmetric jump rate $w_n = J_n$ [24, 25]. Soft phase separation then corresponds to condensation which occurs under the assumptions of (1), (2) [14, 26, 27].

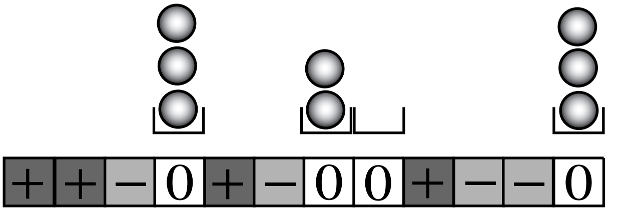

Figure 2: A typical configuration of the three-state model (bottom) and its corresponding configuration in the ZRP (top). Periodic boundary conditions are imposed on the two models.

Surprisingly this seemingly crude picture yields the *exact* invariant measure of the AHR model, i.e., the cluster sizes are distributed independently according to the invariant measure of the zero-range process with jumps rates given by the cluster current of an exclusion process with open boundaries. The distribution of positive and negative particles inside a cluster is equal to that of the particles in the open exclusion process [15].

Apparently the Markovian zero-range process and the highly correlated cluster jump dynamics of the AHR model have the same invariant cluster distribution. Therefore it is conceivable that a prove of soft phase separation is possible in a more general setting. The arguments presented above suggest the following steps:

(1) Identify a family of particle systems with (a) factorized cluster size distribution and (b) such that the distribution of particles inside a cluster is

given by the distribution of the corresponding reduced process with open boundaries.

(2) Prove suitable bounds on current and compressibility in the periodic reduced system

(3) Prove universal relation between current corrections in open and periodic systems

(4) Prove that the non-Markovian zero-range process defined by cluster dynamics has the same invariant measure as the usual zero-range process with rates $w_n = J_n$.

Proving only items (1) and (2) would already constitute substantial progress. The proof of items (3) and (4) would be of great interest in their own right. In order to establish soft phase separation it may be sufficient to prove weaker results than those suggested here.

For further study of strong phase separation it would be interesting to investigate the hydrodynamic limit under Eulerian scaling of the one-component model proposed above. This would shed insight into the far-from equilibrium process of phase separation from a disordered fluctuating state into nonfluctuating domains.

Finally, we remark that even for soft phase separation the vacancy density in the condensed domain does not fluctuate. It would be very interesting to explore the possibility of stationary phase separated states where all conserved quantities fluctuate in all domains.

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