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LETTER TO THE EDITOR

Condensation and coexistence in a two-species driven model

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Online at stacks.iop.org/JPhysA/38/L523**Abstract**

Condensation transition in two-species driven systems in a ring geometry is studied in the case where the current–density relation of a domain of particles exhibits two degenerate maxima. It is found that the two maximal-current phases coexist both in the fluctuating domains of the fluid and in the condensate, when it exists. This has a profound effect on the steady-state properties of the model. In particular, phase separation becomes more favourable, as compared with the case of a single maximum in the current–density relation. Moreover, a selection mechanism imposes equal currents flowing out of the condensate, resulting in a neutral fluid even when the total numbers of particles of the two species are not equal. In this case, the particle imbalance shows up only in the condensate.

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Many properties of the phase diagram of driven systems are known to be determined by some overall features of the current–density relation. For example, this relation serves as a starting point for analysing models of vehicular traffic [1], where it is termed the fundamental diagram. It is also a useful tool for analysing boundary-induced phase transitions in one-dimensional systems [2, 3], and stability of shocks [4]. The aim of this paper is to investigate how these global features affect the properties of condensation transitions in driven diffusive systems (DDS) on a ring. To this end, we analyse in detail the case where the current–density relation has two degenerate maxima. This is found to have far-reaching consequences on the emergence of phase separation. It results in new features which are not present in the previously studied case of a current–density relation with a single maximum [5–7].

Condensation transitions in one-dimensional DDS have been studied in detail in recent years [8]. In particular, it was suggested that on a mesoscopic level one can describe the dynamics of a broad class of two-species DDS by a zero-range process (ZRP) [5, 7]. In this description one views the microscopic configuration of the model as a sequence of particle

domains, bounded by vacancies. Each domain is defined as a stretch of particles of both types. Neighbouring domains exchange particles through their currents. The existence of condensation in these models, analogous to Bose–Einstein condensation (BEC), was found to be related to the dependence of these currents on the length of the domains. A quantitative criterion for the existence of a condensation transition in a ring geometry was thus suggested. According to this criterion, if the asymptotic form of the current for large domains of length n behaves as $j_n \sim j_\infty(1 + b/n)$, with $b > 2$, a condensation transition takes place at a sufficiently high overall particle density. This form of the current implies that, at criticality, the steady-state domain-size distribution scales as $p_n \sim n^{-b}$ for large n . The condensed phase is composed of a critical fluid of fluctuating domains coexisting with a single macroscopically large condensate. This is analogous to BEC, where condensation takes place in momentum space rather than real space.

The criterion has previously been applied to models where the current–density curve $j_\infty(\eta)$ in the bulk of a domain exhibits a single maximum [5–7]. Here we apply this approach to a model where $j_\infty(\eta)$ has two degenerate maxima, and examine the condensation transition in cases where, on average, the density within the domains lies between the two extremal values corresponding to the two maxima. A simple physical picture for the dynamics inside a domain is inferred from numerical simulations of the model. This picture is substantiated by analysing the properties of a two-species ZRP for modelling the collective dynamics of domains. Our main findings are: (i) the density in each particle domain (whether a fluid or a condensate) is not homogeneous. The two maximal-current phases coexist within each domain, with a sharp interface separating the two. The density profile of each of these phases is algebraic, as expected for maximal-current phases. (ii) The non-homogeneous density profile affects the finite-size correction of the current, leading to a finite-size correction coefficient B which is larger than the expected b of homogeneous domains. For example, when the numbers of particles of both species are equal, we find $B \gtrsim 2b$. This makes phase separation in this model more favourable. Exact solution of the ZRP in mean-field geometry and numerical simulations of the one-dimensional ZRP support this finding. (iii) In the condensed phase, the fluid domains are neutral, even in systems with non-equal numbers of particles of the two species, leaving the condensate as the only imbalanced domain. This is in contrast with the case in which the current–density curve has a single maximum, where all domains, fluid and condensate, have the same average density.

We now define the model. Consider a one-dimensional ring with L sites. Each site i can be either vacant (0) or occupied by a positive (+) or a negative (–) particle. Positive particles are driven to the right while negative particles are driven to the left. In addition to the hard-core repulsion, particles are subjected to short-range interactions through a potential

$$V = -\frac{\epsilon}{4} \sum_i s_i s_{i+1}, \quad (1)$$

where $s_i = +1$ (–1) if site i is occupied by a + (–) particle and $s_i = 0$ if site i is vacant. The interaction parameter ϵ satisfies $-1 < \epsilon < 1$ to ensure positive transition rates. The evolution of the model is defined by a random-sequential local dynamics, whereby a pair of nearest-neighbour sites is selected at random, and particles are exchanged with the following rates:

$$\begin{aligned} +- &\rightarrow -+, && \text{with rate } 1 - \Delta V, \\ +0 &\rightarrow 0+, && \text{with rate } 1, \\ 0- &\rightarrow -0, && \text{with rate } 1. \end{aligned} \quad (2)$$

Here ΔV is the difference in the potential V between the final and initial configurations. This dynamics conserves the numbers of particles of each species, N_+ and N_- , or, equivalently,

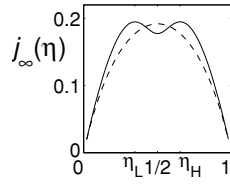


Figure 1. The current–density relation $j_\infty(\epsilon, \eta)$ for $\epsilon = 0.5$ (dashed line) and $\epsilon = -0.9$ (solid line).

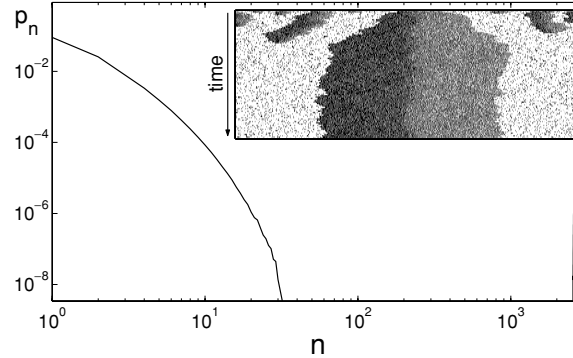


Figure 2. Domain-size distribution for the case $\epsilon = -0.9$. Simulation was performed on a system of size $L = 5000$ with $N_+ = N_- = 1500$. Configurations of the model during coarsening towards the steady state are presented in the inset. Positive particles are marked in black, negative particles in white and vacancies in grey. A configuration is presented every 500 Monte Carlo sweeps. The system size is $L = 1000$, $N_+ = N_- = 300$ and $\epsilon = -0.9$.

the overall particle densities in the system, $\rho_\pm = N_\pm/L$. For a given domain, i.e., a sequence of positive and negative charges confined by vacancies, the relative density η is simply the fraction of positive particles in that domain. This is a fluctuating quantity, both in time and from domain to domain. Model (2) was studied on a ring geometry for positive ϵ in [6, 7]. Here we focus on the negative ϵ region, where the current–density relation exhibits two degenerate maxima, and study mainly the case $\rho_+ = \rho_-$. The non-equal density case is briefly considered at the end of this letter, and is studied in detail in [9].

The region $\epsilon < 0$ was studied in [3] in open systems with the purpose of analysing boundary-induced phase transitions. The current–density relation of a domain of particles, $j_\infty(\epsilon, \eta)$, was found to display a single maximum at $\eta = 1/2$ for $\epsilon \geq -0.8$ and two degenerate maxima at $\eta_{H,L} = \frac{1}{2}\{1 \pm [3 - 2((\epsilon - 1)/\epsilon)^{1/2}]^{1/2}\}$ for $\epsilon < -0.8$, as depicted in figure 1.

We carried out direct numerical simulations of the model for $\epsilon < -0.8$. In figure 2 we present the domain-size distribution and typical configurations for $\epsilon = -0.9$ at high densities $\rho_+ = \rho_-$. This figure suggests the existence of a pronounced macroscopic domain. Examining the configurations it is evident that the relative density within the domains is not homogeneous. Rather, it exhibits two coexisting regions, corresponding to the two maximal-current phases. Indeed, the densities of the two coexisting phases are equal to $\eta_{H,L}$, and the current in the system is $j_\infty(\eta_H) = j_\infty(\eta_L)$. This should be compared with an open system driven with large boundary rates, where the system assumes its maximal current and a similar coexistence takes place [2].

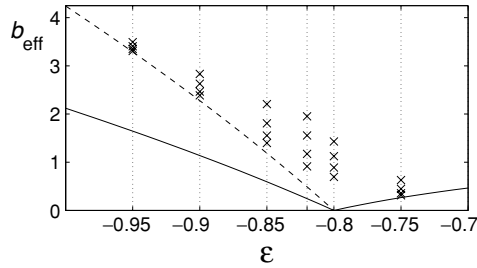


Figure 3. The effective coefficient $b_{\text{eff}}(\epsilon)$ measured in open systems of size $L = 400, 800, 1600$ and 3200 (from top to bottom). The lines correspond to $b(\epsilon, \eta)$ (solid line) and $2b(\epsilon, \eta)$ (dashed line), with $\eta = 1/2$ for $\epsilon > -0.8$ and $\eta = \eta_{\text{H,L}}$ for $\epsilon < -0.8$.

By itself, the appearance of a macroscopic domain in numerical simulations of finite systems does not prove that condensation takes place, as the presence of such a domain could result from a finite-size crossover [10]. The real question is whether the macroscopic domain survives in the thermodynamic limit and becomes a genuine condensate. To answer this question we use the criterion for phase separation, and calculate the finite-size correction to the current of large domains. When the current–density relation has a single maximum, the current of a domain of length n takes the asymptotic form $j_n \sim j_\infty [1 + b(\epsilon, \eta)/n]$, where $b(\epsilon, \eta)$ is explicitly known [7], and where in all domains η is given by $N_+/(N_+ + N_-)$. In the present case b must be computed at the values of the density corresponding to the two maxima of the current, $\eta = \eta_{\text{H}}$ or $\eta = \eta_{\text{L}}$. For example we find $b(\epsilon = -0.9, \eta = \eta_{\text{H,L}}) \simeq 1.14$. Applying the criterion with this value of b would then lead to the conclusion that the existence of a macroscopic domain in figure 2 is merely a finite-size effect. However, as explained below, when a domain is composed of two coexisting phases, the real finite-size correction coefficient which enters the expression of the current is not b , but an enhanced coefficient $B \gtrsim 2b$, making phase separation more favourable. In other words, $j_n \sim j_\infty [1 + B(\epsilon)/n]$, with $j_\infty = j_\infty(\epsilon, \eta = \eta_{\text{H,L}})$. In particular, this yields $B(\epsilon = -0.9) > 2$, implying that figure 2 corresponds to a genuine phase separation.

We first provide numerical evidence that indeed $B \gtrsim 2b$. It is convenient to calculate the finite-size correction to the current $B(\epsilon)$ by simulating an isolated open domain of a fixed length n [5]. The coefficient B is then extracted by measuring the effective coefficient at finite length $b_{\text{eff}}(n) = n(j_n/j_\infty - 1)$ and extrapolating to $n \rightarrow \infty$. In figure 3 we present $b_{\text{eff}}(n)$ for various values of ϵ and system lengths. It is found that, while for $\epsilon > -0.8$ the quantity b_{eff} approaches $b(\epsilon, \eta = 1/2)$ at large n , it is larger than $b(\epsilon, \eta = \eta_{\text{H,L}})$ by a factor $\gtrsim 2$ for $\epsilon < -0.8$. We note that higher order corrections become significant as one approaches $\epsilon = -0.8$, where the leading finite-size correction, $b(\epsilon, \eta = 1/2)/n$, vanishes.

We now present a physical explanation of these observations. For a domain of length n , each of the two coexisting phases occupies, on average, only a length $n/2$. This effectively reduces the length of the domain by a factor 2, and thus the finite-size correction is expected to be about $\simeq 2b/n$ rather than b/n . Quantifying this intuitive picture leads to an estimate of the enhancement factor $A \equiv B(\epsilon)/b(\epsilon, \eta_{\text{H,L}})$. We analyse the current emitted from a domain of length n in the fluid, composed of two coexisting maximal-current phases. A schematic density profile in such a domain is given in figure 4. At the left side of the domain, a fraction x of its length is occupied by a phase with high bulk density η_{H} , while the remaining right side is occupied by the other maximal-current phase, with low density η_{L} . The position of the interface fluctuates in time around the midpoint, i.e., on average, $\langle x \rangle = 1/2$. Numerical

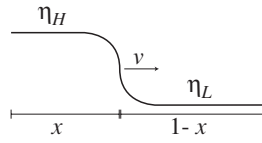


Figure 4. A schematic picture of a typical snapshot of the density profile within a particle domain.

simulations strongly suggest that the position x varies on time scales which are much longer than the equilibration time of the local density within each phase [9]. We thus consider the dynamics of the system on time scales which are short enough such that the position of the interface x and the size of the domain n are fixed. On these time scales the currents of, say, positive particles $j_H(x)$ and $j_L(x)$ in the high- and low-density phases, respectively, are given by

$$j_H(x) = j_\infty \left(1 + \frac{b}{nx} \right), \quad j_L(x) = j_\infty \left(1 + \frac{b}{n(1-x)} \right). \quad (3)$$

Thus, as a result of the flow of particles through the domain, the interface moves with a velocity v , such that $j_H(x) - j_L(x) = v(\eta_H - \eta_L)$. The outflow of particles from the domain is therefore given by

$$j_H(x) - v\eta_H = j_L(x) - v\eta_L = j_\infty [1 + A(x)b/n], \quad (4)$$

where, using the expressions above, one has

$$A(x) = \frac{1}{\eta_H - \eta_L} \left(\frac{\eta_H}{1-x} - \frac{\eta_L}{x} \right). \quad (5)$$

On longer time scales where the position of the interface x fluctuates, one has to average (4) in order to get the current emitted from the domain, leading to $A = \langle A(x) \rangle$. If the fluctuations in the position of the interface do not scale with the domain size, then $\langle 1/x \rangle = 1/\langle x \rangle = 2$ and hence $A = 2$. On the other hand, if these fluctuations scale like the domain length, then $\langle 1/x \rangle > 1/\langle x \rangle$ and $A > 2$. In the following we explore this question in more detail. Our analysis suggests that indeed the width of the interface scales with the domain length leading to $B > 2b$.

Motivated by the discussion presented above, we introduce a two-species ZRP which captures the main features of the collective dynamics of the evolving domains. Consider a ring of M boxes, where box i contains n_i particles, k_i of which are positive and l_i are negative: $n_i = k_i + l_i$. The dynamics of the model is such that a box i is chosen at random and a positive charge is moved to its right neighbouring box with rate $u_{k,l}$ and a negative charge moves to its left neighbouring box with rate $v_{k,l}$. In this model, a box represents a generic domain of the original DDS and the rates u and v correspond to the outflow of particles from this domain, as found in (4). We thus take $u_{k,l} = 1 + A(x)b/n$ and $v_{k,l} = 1 + A(1-x)b/n$. The variable x is expressed in terms of the relative density η by $x\eta_H + (1-x)\eta_L = \eta = k/n$. In what follows, we analyse for simplicity the case $\eta_H = 1$ and $\eta_L = 0$, which yields

$$u_{k,l} = 1 + \frac{b}{l}, \quad v_{k,l} = 1 + \frac{b}{k}. \quad (6)$$

With this choice of rates the steady state of the model is not a product measure [11], implying that no explicit description of the stationary state is known. We first consider the model in the mean-field geometry, where all sites are connected. We denote by $f_{k,l}$ the probability for a

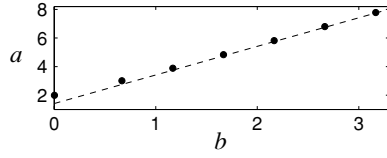


Figure 5. The decay exponent a for different values of b , as obtained from numerical integration of (9). The line is given by the large b asymptotic form $2b + \sqrt{2}$.

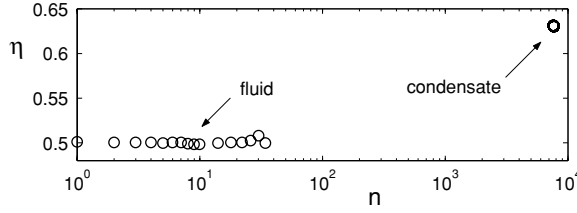


Figure 6. The relative density η of positive particles within a domain, for a system of size 10^4 with $\epsilon = -0.9$. Here $N_+ = 5000$ and $N_- = 3000$.

site to be occupied by k positive particles and l negative particles. In the thermodynamic limit, $f_{k,l}$ obeys the evolution equation

$$\frac{df_{k,l}(t)}{dt} = u_{k+1,l}f_{k+1,l} + v_{k,l+1}f_{k,l+1} + \bar{u}f_{k-1,l}(1 - \delta_{k,0}) + \bar{v}f_{k,l-1}(1 - \delta_{l,0}) - [u_{k,l}(1 - \delta_{k,0}) + v_{k,l}(1 - \delta_{l,0}) + \bar{u} + \bar{v}]f_{k,l}, \quad (7)$$

where $\bar{u} = \sum_{k,l} u_{k,l}f_{k,l}$ and $\bar{v} = \sum_{k,l} v_{k,l}f_{k,l}$ are the (+) and (−) currents, respectively. In the continuum limit the steady-state distribution satisfies the following equation at criticality ($\bar{u} = \bar{v} = 1$):

$$\frac{\partial^2 f_{k,l}}{\partial k^2} + \frac{\partial^2 f_{k,l}}{\partial l^2} + b \left(\frac{1}{l} \frac{\partial f_{k,l}}{\partial k} + \frac{1}{k} \frac{\partial f_{k,l}}{\partial l} \right) = 0. \quad (8)$$

Moving to polar coordinates, and assuming the scaling solution $f(r, \theta) = r^{-a}g(\theta)$, we find an equation for the angular function $g(\theta)$

$$\frac{d^2g(\theta)}{d\theta^2} + \left(a - \frac{2b}{\sin 2\theta} \right) ag(\theta) = 0, \quad (9)$$

with the boundary conditions $g(0) = g(\pi/2) = 0$. The determination of the decay exponent a is obtained by imposing the boundary conditions. This is the quantization condition for this Schrödinger equation. Except for special values of b where a can be determined exactly (e.g. $a = 3$ for $b = 2/3$), the value of a as a function of b is obtained by integrating (9) numerically (figure 5). The large b asymptotic form obtained by the WKB approximation, $a \simeq 2b + \sqrt{2}$, agrees very well with these results down to small b . From the predicted form of the solution $f(r, \theta)$, we deduce that the domain-size distribution p_n , with $n = k + l$, scales as $p_n \sim n^{-(a-1)}$. On the other hand, the rate out of a domain of size n , $j_n \equiv \langle u_{k,l} \rangle_{k+l=n}$, is of the form $j_n \sim 1 + B/n$, and we conclude that $B = a - 1$. Numerical integration of the temporal equation (7) gives a decay exponent a in perfect agreement with the predicted value of the continuum limit. This analysis shows that $B \gtrsim 2b$, supporting the physical picture presented above. This calculation was carried out within the mean-field geometry and should not yield the exact values of B of the one-dimensional model. However, numerical simulations of the

latter indicate that B is well approximated by the mean-field result [9]. Coming back to the DDS, the results above suggest that the position of the interface inside a domain should scale with the domain length. This has been verified by numerical simulations [9].

So far we analysed a neutral system, where $\rho_+ = \rho_-$. We now consider the case of non-equal densities. While this case will be studied in detail elsewhere [9], here we only mention a striking result: as long as $\eta_L < N_+/(N_+ + N_-) < \eta_H$, all domains which reside in the fluid are equally populated with positive and negative particles. The excess numbers of particles of the majority species reside in the condensate. This behaviour is a result of the fact that the two currents emitted from a domain of length n are equal to the maximal current, up to corrections of order $1/n$. The condensate is therefore stationary in the thermodynamic limit even when the densities are not equal. The condensate thus emits equal currents of (+) and (-) particles. Hence, domains in the fluid cannot experience the fact that the overall densities in the system are not equal. Figure 6 depicts the average relative density η of positive particles in domains of various sizes, as measured in a large system for $\epsilon = -0.9$. It is readily seen that, on average, domains in the fluid are neutral, whereas the relative density in the macroscopic domain compensates for the excess of positive particles.

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