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Steady States of Dynamically Coupled Two-Species Systems*

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Abstract

We study the steady states of two stochastic lattice models with two species of particles, where the local mobility of one species depends on the spatial distribution of the other. The eigenvalues of a 2×2 matrix of couplings can develop imaginary parts, and the question arises whether this implies an instability to a macroscopically different steady state. In the first model, where the mobility depends on the local density of the other species, we show that the system undergoes macroscopic phase separation. In the second model, where the mobility depends on the second derivative of the density of the other species, there is a finite correlation length and the density is homogeneous on macroscopic scales.

1. Introduction

Interesting effects arise when the time evolutions of two different statistical fields are coupled, and fluctuations of one field feed into the dynamics of the other. Such effects arise in several physical systems, for instance, coupled interfaces [1], drifting polymers [2] and sedimenting colloidal crystals [3, 4]. In this paper, we focus on instabilities that can arise in coupled-field systems in which the mobility of one species depends on the spatial distribution of the other.

The instabilities in question arise within a linearized hydrodynamic description, and we seek to clarify the circumstances under which the final steady state is macroscopically

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different. To this end, we study two lattice models with two species of particles, one on each sublattice of a one-dimensional lattice. In the first model, the local mobility of one species depends on the local density of the other, while in the second model the mobility of one species depends on the second derivative of the density of the other species. We find that the first model exhibits macroscopic phase separation of an exceptionally robust sort [4], while in the second model there is a finite correlation length and a homogeneous macroscopic density.

Before turning to the two-species problem, we briefly recapitulate some well-known properties of single-species driven diffusive systems.

1.1. Single-Species Driven Diffusive Systems

The simplest models of driven systems consist of lattice gases evolving through probabilistic update rules. A configuration of the system is specified by giving the set of occupation numbers $\{n_i\}$ for all lattice sites i of a one-dimensional lattice, where $n_i = 1$ if site i is occupied and 0 if it is not; double occupancy of a site is disallowed. The dynamics is stochastic: for example, in the well-studied asymmetric exclusion process, each particle attempts a rightward (leftward) hop to a neighbouring site at rate $p(q)$, but the hop is actually completed only if the neighbouring site is unoccupied. Other rules for particle movement (e.g. next neighbour hops, or leapfrogging moves) specify alternative models.

With periodic boundary conditions, the system reaches a steady state which supports a macroscopic current J_0 through the system. J_0 depends on the hopping rules and is a nonlinear function of the overall density ρ_0 of particles. For instance, in the asymmetric exclusion process referred to above, $J = (p-q)\rho_0(1-\rho_0)$. To learn about the properties of fluctuations on large length and time scales, we turn to a continuum hydrodynamic description. An approximate equation of motion for coarse-grained density fluctuations $\delta\rho(x,t) \equiv \rho(x,t) - \rho_0$ can be derived starting from the continuity equation $\partial\rho/\partial t + \partial J/\partial x = 0$. It is assumed that J can be written as the sum of three contributions [5]: a systematic part given by $J_0(\rho(x))$, a diffusive part $-D\partial\rho/\partial x$, and a noisy part $\eta(x)$ with $\langle\eta(x,t)\eta(x't')\rangle = \Gamma\delta(x-x')\delta(t-t')$. Then expanding $J_0(\rho(x))$ up to quadratic order in $\delta\rho(x)$, we obtain

$$\frac{\partial(\delta\rho)}{\partial t} = \frac{\partial}{\partial x}\left[c\delta\rho + \frac{D\partial(\delta\rho)}{\partial x} + \lambda(\delta\rho)^2 + \eta\right] \tag{1}$$

with $c = (\partial J/\partial\rho)_{\rho_0}$ and $\lambda = \frac{1}{2}(\partial^2 J/\partial\rho^2)_{\rho_0}$. On defining $h(x,t) = \int^x dx'\ \delta\rho(x',t)$, Eq. (1) may be rewritten as

$$\frac{\partial h}{\partial t} = c\frac{\partial h}{\partial x} + D\frac{\partial^2 h}{\partial x^2} + \lambda\left(\frac{\partial h}{\partial x}\right)^2 + \eta. \tag{2}$$

This form of the evolution equation also describes a different physical problem, namely the dynamics of a driven interface [6], in which case $h(x,t)$ represents the height of interface.

The linear term $c\delta\rho \equiv c\partial h/\partial x$ describes the movement of the pattern of fluctuations at speed c through the system [7]. It can be eliminated by the Galilean shift $x \to x + ct$,

$t \to t$, tantamount to moving into a frame of reference in which the wave is stationary. The remaining terms give rise to the decay of the fluctuation wave in time. A fluctuation of spatial extent Δx survives for a time $\tau \sim (\Delta x)^z$ where z is a dynamical critical exponent. When $\lambda = 0$, one finds $z = 2$ [8], whereas if $\lambda \neq 0$, the decay is more rapid and $z = \frac{3}{2}$ [5, 6].

1.2. Two-Species Driven Diffusive Systems

We now turn to the case of two driven coupled fields. The development of approximate hydrodynamic equations proceeds much as before, but as we will see below, the linear first derivative terms can have much more drastic consequences.

Let $n_\sigma(x,t)$ and $n_\tau(x,t)$ be local densities, and let $J_\sigma(x,t)$ and $J_\tau(x,t)$ be the corresponding local currents. The coupling between the fields implies that the systematic parts of J_σ and J_τ depends on both $\delta n_\sigma(x,t)$ and $\delta n_\tau(x,t)$. Proceeding as in the single-component case, we obtain the coupled equations

$$\begin{aligned}
\frac{\partial h_1}{\partial t} &= c_{11}\frac{\partial h_1}{\partial x} + c_{12}\frac{\partial h_2}{\partial x} + D_1\frac{\partial^2 h_1}{\partial x^2} \\
&\quad + \lambda_1\left(\frac{\partial h_1}{\partial x}\right)^2 + \mu_1\left(\frac{\partial h_2}{\partial x}\right)^2 + \nu_1\left(\frac{\partial h_1}{\partial x}\right)\left(\frac{\partial h_2}{\partial x}\right) + \eta_1(x,t) \\
\frac{\partial h_2}{\partial t} &= c_{21}\frac{\partial h_1}{\partial x} + c_{22}\frac{\partial h_2}{\partial x} + D_2\frac{\partial^2 h_2}{\partial x^2} \\
&\quad + \lambda_2\left(\frac{\partial h_1}{\partial x}\right)^2 + \mu_2\left(\frac{\partial h_2}{\partial x}\right)^2 + \nu_2\left(\frac{\partial h_1}{\partial x}\right)\left(\frac{\partial h_2}{\partial x}\right) + \eta_2(x,t)
\end{aligned} \tag{3}$$

where $\partial h_1/\partial x = \delta n_\sigma(x,t)$ and $\partial h_2/\partial x = \delta n_\tau(x,t)$.

Let us first examine the effect of keeping only the first derivative terms on the right hand side of the above equations [9]. Let the eigenvectors of the 2×2 matrix $\begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}$ be e_+ and e_-, and let the corresponding eigenvalues be c_+ and c_-. There are two cases to consider:

(A) If c_+ and c_- are real (i.e. if $\Delta \equiv (c_{11} - c_{22})^2 + 4c_{12}c_{21} > 0$), they represent the speeds of two waves. The two waves involve e_+ and e_-, each composed of a linear combination of h_1 and h_2. To proceed, rewrite Eqs. (3) in terms of $e_+(x,t)$ and $e_-(x,t)$. Notice that in the rest frame of each wave, the other wave moves with a finite speed $|c_+ - c_-|$; the two waves are coupled through nonlinear terms. It would be interesting to clarify how this coupling affects the dissipation of the waves.

(B) There is a much more drastic effect — an instability — if c_+ and c_- pick up an imaginary part (i.e. if $\Delta < 0$). The solutions of the linear equations then no longer describe a pattern of fluctuations moving as a wave, but rather an unbounded exponential growth of fluctuations. This instability signals the advent of a new state which is qualitatively different from the statistically homogeneous state assumed at the outset. To be able to describe this state, it is essential to include appropriate nonlinear terms. We turn to this in Section 2, by studying a lattice model in the unstable regime where we find that the system undergoes macroscopic phase separation.

Finally, in order to understand better the occurrence of putative instabilities, we study a related but different lattice model in Section 3. The hydrodynamic description of this model involves linear *third* derivative terms in place of the first derivative terms in Eq. (3). In this case, we show that even when the eigenvalues of the corresponding 2×2 matrix are complex, there is no macroscopic instability.

2. Two-Species Lattice Model with Coupling to Density

In this section, we study a lattice model which involves two species of Ising spins evolving under dynamical rules which make the mobility of one species dependent on the local density of the other. This model was introduced by Lahiri and Ramaswamy (LR) [3] to study coupled-field systems such as the density and tilt fields in a sedimenting colloidal crystal.

The LR model consists of two sets of spins $\{\sigma_i\}$ and $\{\tau_i\}$ on a one-dimensional lattice, with σ spins on one sublattice, and τ spins on the other. A typical configuration is $\tau_{1/2}\sigma_1\tau_{3/2}\sigma_2\tau_{5/2}\sigma_3\cdots$ where each of σ_i and τ_j take on values $\pm$ 1. Defining $n_\sigma = \frac{1}{2}(1+\sigma)$ and $n_\tau = \frac{1}{2}(1+\tau)$, we may map the Ising spin variables to $(1,0)$ - valued occupation numbers. Pictorially, we denote σ_i by $+$ or $-$, and τ_j by / or \. The local evolution involves Kawasaki exchange of $+\ -$ at a rate which depends on the intervening τ spin. Similarly, the rate of / \ exchanges depend on the intervening σ spin. In other words, the intervening spin sets the direction of a local biasing field, either favouring or disfavouring exchanges of the other species.

Let us label the elementary moves as follows:

$$
\begin{array}{llll}
(a) & + \setminus - & \rightarrow & - \setminus + \\
(b) & - \ / + & \rightarrow & + \ / - \\
(c) & / + \setminus & \rightarrow & \setminus + / \\
(d) & \setminus - / & \rightarrow & / - \setminus
\end{array}
$$

Let $(\bar{a})$, $(\bar{b})$, $(\bar{c})$ and $(\bar{d})$ denote the corresponding reverse moves. The simplest version of the model is defined by taking the rates for moves $(a) - (d)$ to be equal, say U, different from the common rate V for moves $(\bar{a}) - (\bar{d})$.

With $U \neq V$, this model corresponds to the *unstable* case (B) of the previous section, as $c_{11} = c_{22} = 0$ and c_{12} and c_{21} have the same sign; a continum hydrodynamic treatment at the linear level would predict an exponential instability. What then is the final state of the system? An answer can be found in the half-filled case $\Sigma_i \sigma_i = \Sigma_j \tau_j = 0$. Since the details of the analysis have appeared already [4], we only summarize the results here.

(i) The condition of detailed balance is valid with respect to the Hamiltonian

$$\mathcal{H} = \epsilon \sum_{k=1}^{N} h_k\{\tau\}\sigma_k \tag{4}$$

where $h_k\{\tau\}$ is a 'height' field defined by

$$h_k\{\tau\} = \sum_{j=1}^{k} \tau_{j-1/2}. \tag{5}$$

The steady state is thus described by an equilibrium Boltzmann measure, and a configuration $\{\sigma, \tau\}$ has weight $\exp(-\mathcal{H}\{\sigma, \tau\}/T)$ where T is the temperature. This can be seen by noting that the energy change on interchanging neighbouring σ spins is

$$\Delta E_\sigma \equiv \Delta E(\sigma_i \leftrightarrow \sigma_{i+1}) = \epsilon \tau_{i+\frac{1}{2}}(\sigma_i - \sigma_{i+1}), \tag{6}$$

while the change of energy under exchange of τ spins is given by a similar expression with σs and τs interchanged. Thus the ratio of Boltzmann weights of the configurations after and before an interchange of spins, say $\sigma_i \leftrightarrow \sigma_{i+1}$, is $exp(-2\Delta E_\sigma/T)$. This equals the ratio of forward to backward transition rates if the ratio ϵ/T is related to the rates U and V by

$$\frac{V}{U} = e^{-2\epsilon/T} \tag{7}$$

Notice that $\mathcal{H}$ involves long-ranged couplings between spins σ_i and $\tau_{j-1/2}$.

(ii) The ground state exhibits complete *phase separation*, corresponding to all $\sigma = 1$ particles being at the bottom of the potential well formed by the τ spins. Pictorially, the state is

$$- \backslash - \backslash - \backslash - \backslash + \backslash + \backslash + \backslash + / + / + / + / - / - / - /$$

(iii) In an infinite sample, phase separation survives at all T. The effect of any nonzero temperature is only to smear out each of the four interfaces over a finite, T-dependent length, with basically no effect on the bulk of the spins. This unusual behaviour occurs since the energy grows super-extensively ($\sim$ (length)^2), and thus dominates over the entropy at all temperatures.

(iv) When the filling is changed away from $\sum_i \sigma_i = \sum_i \tau_i = 0$, the condition of detailed balance no longer holds, and there is no description in terms of an effective Hamiltonian. Nevertheless, kinetic arguments can be given to show that phase separation survives even when the filling is changed. The extreme robustness of the phenomenon leads us to call it Strong Phase Separation.

(v) The approach to the steady state is exceptionally slow. It occurs through a coarsening process which involves thermal activation over large barriers, resulting in a coarsening length growing logarithmically in time.

Strong phase separation also occurs in other systems, for instance a 3-species permutation-symmetric model on a 1-d lattice with periodic boundary conditions [10].

3. Two-Species Lattice Model with Second Derivative Coupling

In this section we construct a lattice model which is related to, but ultimately quite different from, the LR model of the previous section. We proceed in a direction opposite to that in Section 2: we define the model through the Hamiltonian and then construct the kinetics using the condition of detailed balance rather than the other way around.

The Hamiltonian is constructed from local terms which explicitly favour the 3 site configuration $C_\sigma \equiv (+/-\ \text{ or }\ -\backslash+)$ over $C'_\sigma \equiv (-/+\ \text{ or }\ +\backslash-)$, and also $C_\tau \equiv (\backslash + /$ and $/ - \backslash)$ over $C'_\tau \equiv (/ + \backslash$ and $\backslash - /)$. To this end, we define 3-spin operators

$$\begin{aligned} h_{i+\frac{1}{2}} &\equiv h(\sigma_i, \sigma_{i+1}, \tau_{i+\frac{1}{2}}) = \frac{1}{2}\tau_{i+\frac{1}{2}}(\sigma_i - \sigma_{i+1}) \\ g_i &\equiv g(\tau_{i-\frac{1}{2}}, \tau_{i+\frac{1}{2}}, \sigma_i) = \frac{1}{2}\sigma_i(\tau_{i+\frac{1}{2}} - \tau_{i-\frac{1}{2}}), \end{aligned} \quad (8)$$

which distinguish between $C_{\sigma,\tau}$ and $C'_{\sigma,\tau}$. The Hamiltonian is then

$$\mathcal{H} = -\epsilon_1 \sum_i h_{i+\frac{1}{2}} - \epsilon_2 \sum_i g_i. \quad (9)$$

If $\epsilon_1, \epsilon_2 > 0$ the configurations C_σ and C_τ have a lower energy than C'_σ and C'_τ. Further, the energy difference on interchanging two spins σ_i and σ_{i+1} is

$$\Delta E_\sigma \equiv \Delta E(\sigma_i \leftrightarrow \sigma_{i+1}) = -\frac{\epsilon_1 + \epsilon_2}{2}\left[(\sigma_i - \sigma_{i+1})(\tau_{i-\frac{1}{2}} + \tau_{i+\frac{3}{2}} - 2\tau_{i+\frac{1}{2}})\right] \quad (10)$$

The expression for ΔE_τ is obtained by interchanging σ's and τ's. These expressions should be contrasted to Eq. (6) for the LR model.

We define the rates of spin interchanges using the condition of detailed balance: for instance, the ratio of the rates of forward and backward σ spin exchanges is given by $\exp(-\Delta E_\sigma/T)$. Interestingly, we see that the local σ current is guided by the discrete second derivative $(\tau_{i-\frac{1}{2}} + \tau_{i+\frac{3}{2}} - 2\tau_{i+\frac{1}{2}})$, in contrast to the $\tau_{i+\frac{1}{2}}$ – guided current in the LR model.

In the continuum limit, this results in a contribution proportional to $\partial^2\tau/\partial x^2$ to the σ current J_σ, and similarly $\partial^2\sigma/\partial x^2$ to J_τ. This results in coupled equations for h_1 and h_2 which resemble Eq. 3, except that the linear *first* derivative terms (e.g. $\partial h_2/\partial x$) are replaced by *third* derivatives (e.g. $\partial^3 h_2/\partial x^3$). Once again, eigenvalues of the corresponding

2×2 matrix pick up an imaginary part, say c_3^{Im}, but this does not signal a macroscopic instability of the sort found for the LR model. This is because the stable second derivative terms dominate the behaviour at low enough wavevectors q (once $Dq^2 > c_3^{Im} q^3$) and correspondingly large distances ($> c_3^{Im}/D$).

Confirmation of this point of view comes from direct consideration of the lattice model. While its ground state

$$\backslash + / - \backslash + / - \backslash + / - \backslash + / - \backslash + / - \backslash + / -$$

exhibits long range order, this cannot be sustained at any finite temperature, as well known arguments militate against an ordered phase in an equilibrium one-dimensional system with short-ranged interactions. The occurrence of phase transitions to an ordered phase in higher dimensions remains an interesting possibility within this lattice model.

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