

Driven Diffusive Systems of Active Filament Bundles

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The cytoskeleton is an important subsystem of cells that is involved for example in cell division and locomotion. It consists of filaments that are cross-linked by molecular motors that can induce relative sliding between filaments and generate stresses in the network. In order to study the effects of fluctuations on the dynamics of such a system we introduce here a new class of driven diffusive systems mimicking the dynamics of active filament bundles where the filaments are aligned with respect to a common axis. After introducing the model class we first analyze an exactly solvable case and find condensation. For the general case we perform a mean-field analysis and study the behavior on large length scales by coarse-graining. We determine conditions for condensation and establish a relation between the hopping rates and the tension generated in the bundle.

KEY WORDS: Cytoskeleton, motor filament systems, stochastic dynamics, hopping models

1. INTRODUCTION

Our current understanding of non-equilibrium systems owes a lot to the studies of driven diffusive systems⁽¹⁾. These are models of particles hopping from site to site on a lattice where the hopping rates do not fulfill the condition of detailed balance. Even though the rules governing the stochastic dynamics are often very simple, these models show a variety of phenomena that are unknown to systems at thermodynamic equilibrium. In particular, even in one spatial dimension they can exhibit phase separation and phase transitions.

Biology provides ample examples of systems that are maintained out of thermodynamic equilibrium and physical studies of these systems are essential for

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understanding their behavior. In contrast to the driven diffusive systems mentioned before, they in general do not follow simple rules. This can be illustrated by the cytoskeleton which is a network of filamentous proteins, mainly actin-filaments and microtubules⁽²⁻⁴⁾. The cytoskeleton plays an essential role in many vital cellular processes as, for example, cell division and locomotion. Cytoskeletal filaments are polar objects, because they have two structurally distinguishable ends. Other proteins associated with the cytoskeleton control filament assembly and disassembly. Furthermore, they can form cross-links between filaments. In addition to passive cross-links there are active cross-links formed by motor proteins. These are molecules that can move directionally along filaments. Their motion is driven by the hydrolysis of Adenosine-Tri-Phosphate during which a phosphate group is cleaved from the molecule. The chemical energy thus liberated is then transformed by the motor proteins into mechanical work. The direction of their motion is determined by the orientation of the filament. If a motor protein connects two filaments its motion results in relative motion between the filaments and creates stresses in the filament network.

Now each of the proteins involved in the dynamics of the cytoskeleton is already a complicated system on its own, consisting of many atoms. However, the separation of time scales allows phenomenological descriptions of the slow modes. Essential features of cytoskeletal dynamics can be studied using simple models. For example, driven diffusive systems have been used to study the growth of filaments against external forces⁽⁵⁾, the motion of single motors on a filament^(6,7), as well as collective effects of motor molecules interacting through excluded volume effects⁽⁸⁻¹⁰⁾.

Motivated by the dynamics of bundles of polar filaments interacting with molecular motors, we study in this work a new class of driven diffusive systems. In contrast to commonly studied models, elementary events consist here of a correlated motion of two particles reflecting the effects of filament motor interactions. After defining the model class we study a sub-class that allows for an exact solution of the steady state. We identify criteria for condensation in these models. In a filament bundle, condensation corresponds to bundle shortening. We then analyze cases without exact solution by employing a mean-field approximation. Finally, we look at a coarse-grained version and relate the model to phenomenological descriptions of active filament bundles. In this way we can connect the kinetic hopping rates defining the driven diffusive system to the stress generated in a filament bundle.

2. ACTIVE FILAMENT BUNDLES

We will now briefly review a microscopic physical model of the filament dynamics in a bundle induced by motor molecules. Motivated by this model we

will then define the processes that determine the class of driven diffusive systems to be studied below.

2.1. The Minimal Model

Consider a bundle of polar filaments in which all filaments are aligned with respect to a common axis. Each filament has one of two possible orientations which in the following will be referred to as “plus” and “minus”, respectively. Filament pairs are set into relative motion by the action of molecular motors which form active cross-links. As a consequence, the bundle can shorten and filaments can be separated according to their polarity^(11,12).

For sufficiently large filament densities, the state of the bundle can be represented by two densities corresponding to the distributions of filaments oriented in one way and the other. They are denoted c^+ and c^- , respectively. Due to mass conservation, the time evolution of the densities is governed by continuity equations

$$\partial_t c^\pm + \partial_x j^\pm = 0 \quad (1)$$

The currents j^\pm reflect various active processes in the bundle, for example the action of motors connecting filament pairs. If filaments are created and destroyed or change their orientation, then source terms have to be added on the right hand side of Eq. (1). In the following, these processes will be neglected such that the numbers of plus- and minus-filaments are both conserved independently.

Different approaches have been developed to derive expressions for the filament currents. Phenomenological equations have been derived based on systematic expansions of the currents in terms of the filament densities and their derivatives respecting the symmetries of the system^(13–17). The same approach has been used for describing the hydrodynamics of actively propelled particles like bacteria which share a number of essential features with active filament systems^(19,20). The virtue of these approaches is that they are independent of many microscopic details of the active processes, most of which are only partially known at present. In more microscopic descriptions, expressions for the currents follow from an analysis of the action of active cross-links formed by motor molecules^(21–25).

We will now discuss further the approach presented in Ref. 22 as it will form the basis for the driven diffusive systems discussed later. It is based on an analysis of the momentum flux in the bundle. Since the motion of filaments in a bundle typically occurs with velocities in the order of $\mu\text{m}/\text{min}$, the dynamics is dominated by friction and inertial terms can be neglected. The conservation of momentum is thus expressed by a balance of forces. Summing up all the forces acting on a filament connected to other filaments by active motors and moving against an immobile fluid leads to a general expression for the currents in terms of the internal forces. Within the framework developed in Ref. 22 it is assumed that

the dominant contributions to the currents result from filament pair-interactions, which is for example valid in the case of a low motor density. In the simplest case, the motor density is not considered as a dynamic variable, such that it only enters in the parameters describing the dynamics.

For a simple model of the internal forces between filament pairs, the current of plus-filaments is given by^(21,22)

$$j^+(x) = -\alpha \partial_x \int_0^\ell d\xi [c^+(x+\xi) - c^+(x-\xi)]c^+(x) \\ + \beta \partial_x \int_{-\ell}^\ell d\xi c^-(x+\xi)c^+(x) - D\partial_x c^+(x) + v_{tr}c^+(x) \quad (2)$$

This current defines the minimal model of active filament bundles. The first term describes the contribution to the current resulting from interactions between filaments of the same orientation, while the second term accounts for interactions between filaments of opposite orientation. The corresponding coupling constants are α and β , respectively. The integrals reflect that filaments can interact whenever they overlap, where ℓ is the filament length which is taken to be the same for all filaments. The terms resulting from the action of active cross-links have a simple interpretation. The interaction of filaments of the same orientation is such that, for $\alpha > 0$, a filament pair tends to increase its overlap, while for filaments of opposite orientation the distance between their plus ends decreases if $\beta > 0$, see Fig. 1.

The following term is a diffusion current that captures effects of fluctuations in the system. Since the fluctuations are not only thermal, the effective diffusion constant D does not satisfy an Einstein-relation. Finally, the convective part $v_{tr}c^+$ of the current has been introduced in Ref. 25 to describe filament treadmilling. In this process filament subunits are added at the plus-end and removed with the same rate at the minus-end. This leads to an apparent motion of the filament in the direction of the plus-end while the length of the filament remains constant.

The expression for the current of minus-filaments is obtained from expression (2) by interchanging the superscripts $+$ and $-$ and by replacing β with $-\beta$ as well as v_{tr} by $-v_{tr}$. This assures that the currents transform correctly under space inversion which also transforms plus filaments into minus filaments and vice versa. Furthermore, the currents respect the conservation of momentum.

An analysis of the dynamic equations reveals that the important parameter for the dynamics is α , the coupling between filaments of the same orientation. If it exceeds a critical value, a homogeneous distribution of filaments becomes unstable^(21,22). Provided that $\beta = 0$, filaments then aggregate at some position. If on the contrary $\beta \neq 0$, then oscillatory solutions in the form of traveling waves can be generated⁽²⁶⁾. The critical value α_c is inversely proportional to the filament density c_0 of the homogeneous state, $\alpha_c \propto c_0^{-1}$.

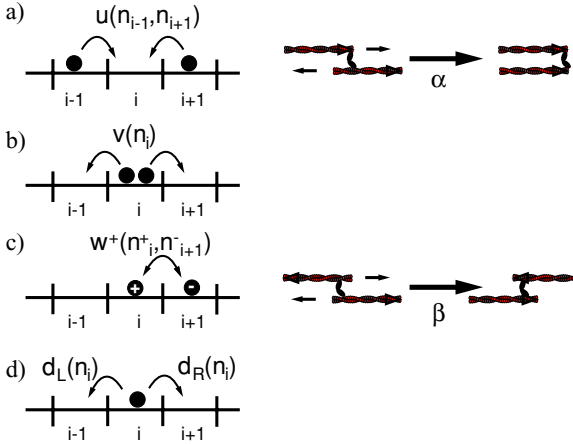


Fig. 1. The three processes governing the particle dynamics. (a) Particles of the same kind separated by one site, hop simultaneously to the middle site with rate u . On the right the corresponding process of two filaments with the same orientation aligning their plus-ends is illustrated; the coupling parameter in the minimal model is α . (b) The opposite event of two particles of the same kind leaving a site to different neighboring sites occurs with rate v . (c) Two neighboring particles of different kinds exchange their position with rates w^\pm . On the right the corresponding process of sliding two filaments of opposite orientation is illustrated; the corresponding coupling parameter in the minimal model is β . (d) Particles hop to the left or right neighboring sites with rates $d_{L,R}$.

We will now use these elementary processes as a motivation for defining a class of driven diffusive systems capturing essential parts of the dynamics of active filament bundles.

2.2. Stochastic Dynamics of Interacting Particles

Consider a one-dimensional lattice of L sites. On the lattice there are two kinds of particles, referred to as “plus” and “minus”, which represent the two possible orientations of the filaments in a bundle. Each site i with $i = 1, \dots, L$ accommodates $n_i^+ + n_i^- \geq 0$ particles, where n_i^\pm are the occupation numbers of plus- and minus-particles. The dynamics of the particles is determined by processes corresponding to the different terms appearing in the current (2), see Fig. 1.

First of all, two particles of the same kind located respectively on sites $i - 1$ and $i + 1$ can simultaneously hop to site i . This process corresponds to the dynamics of a pair of equally oriented filaments in a bundle that are cross-linked by a motor. The action of the motor tends to increase the overlap of the filaments, see Fig. 1a, right. The rate of such an event depends on the number of particles on sites $i - 1$ and $i + 1$ and is denoted by $u(n_{i-1}^\pm, n_{i+1}^\pm)$ with $u(n, m) = u(m, n)$. Note, that

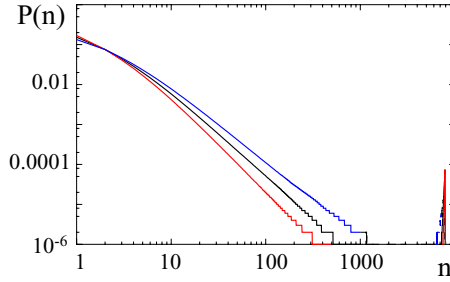


Fig. 2. Probability $P(n)$ of finding in the steady state a site with n particles obtained from stochastic simulations. The different curves correspond to different models within the general class where the non-zero rates are specified by Eqs. (5)-(8). Top: ZRP ($u = v = 0$), Middle: Exactly solvable case (all rates non-zero), and Bottom: $v = 0$. In all cases, the probability distribution shows first an algebraic decay and then a high probability for finding a site containing a high fraction of the particles. The non-vanishing parameters are in all cases $r = 0.24$, $p = 0.6$, $q = 0.4$ and $w(n) = 1 + 2.5/n$. The length of the system was $L = 2000$ and the number of particles were $N = 6L$.

the function u is the same for both kinds of particles³. For the following analysis, it will turn out to be convenient to allow also for the opposite events to occur even though there is no direct analog in the minimal model: Two particles on site i can separate and move to sites $i - 1$ and $i + 1$, respectively. The corresponding rate v depends on the number of particles at i , i.e. $v(n_i)$.

The next process reflects the action of a motor on a pair of oppositely oriented filaments, illustrated in Fig. 1c right. A plus particle at i will exchange its position with a minus particle at $i + 1$ with a rate w^+ that depends on n_i^+ and n_{i+1}^- , i.e. $w^+(n_i^+, n_{i+1}^-)$. The opposite process occurs with rate $w^-(n_i^-, n_{i+1}^+)$. Motivated by the behavior of the term proportional to β in Eq. (2) under the combined operation $+\leftrightarrow-$ and space inversion, we require $w^\pm(m, n) = w^\mp(n, m)$.

Furthermore, we allow for processes similar to diffusion: particles can spontaneously hop to the left or right neighboring site with rates d_L^\pm and d_R^\pm , respectively, each of which can depend on the number of particles at the site. Motivated by the behavior of the filament system under space inversion, we require $d_L^+ = d_R^-$ and $d_R^+ = d_L^-$. Note, that if $d_R^+ \neq d_L^+$ then there is a spontaneous flux of particles similar to the convective term $v_{tr}c^+$ in Eq. (2). Finally, the rates have to respect that a process can only take place if there is a particle at the donating site(s), i.e., $u(n, n') = 0$ if either $n = 0$ or $n' = 0$, $v(0) = v(1) = 0$, and $d_{L,R}^\pm(0) = 0$.

If only one kind of particles is present and if $u = v = 0$, the model reduces to a class of hopping models known as Zero Range Process (ZRP)⁽²⁷⁾. In these models, the rate of a particle leaving a site depends on its occupation number but

³ This process is similar to the one introduced in Ref. 21 where the “interaction range” was larger and u was chosen to be constant.

is otherwise unconstrained. In spite of this simplicity, phase transitions are found in this class even in one dimension. The ZRP allows for an analytical solution of the steady state. This property is intimately linked to the factorization of the steady state probability distribution $P(\{n_i\})$ of having a certain configuration with n_i particles at site $i = 1, \dots, L$. Explicitly,

$$P(\{n_i\}) = Z^{-1} \prod_{j=1}^L f(n_j), \quad (3)$$

where $f(n)$ depends on the hopping rate. The factor Z assures normalization of the probability distribution, depends on the length of the lattice L and the number of particles N in the system. For example, if $d_L(n) = pd(n)$ and $d_R(n) = qd(n)$ with arbitrary $p > 0$ and $q > 0$, then

$$f(n) = \prod_{m=1}^n \frac{1}{d(m)}. \quad (4)$$

If the rate $d(n)$ goes to zero as $n \rightarrow \infty$, the system shows condensation, i.e., in the steady state there will be a finite number of sites with a macroscopic occupation number⁽²⁷⁾.

We will now analyze the case of non-vanishing u and v , where we focus on the case of one kind of particles. First, we will study a case that allows for an analytic solution of the steady state probability distribution and shows that the the model can exhibit condensation. Then we discuss the general case by using a mean-field approximation.

3. FACTORIZED STEADY STATE

Consider the case of N particles of one kind that move on a periodic lattice of L sites. The hopping rates are specified by

$$u(m, n) = rw(m)w(n) \quad (5)$$

$$v(n) = rw(n)w(n-1) \quad (6)$$

$$d_L(n) = qw(n) \quad (7)$$

$$d_R(n) = pw(n) \quad (8)$$

where w is an arbitrary function of n with $w(0) = 0$ and p, q , and r are positive parameters. As can easily be checked, these rates fall into the class introduced in the previous section. For this process, the steady state probability distribution factorizes and has the form (3). Indeed, the steady state of the probability distribution

P is determined by

$$\begin{aligned}
 & \sum_{i=1}^L [2u(n_{i-1} + 1, n_{i+1} + 1)P(\dots, n_{i-1} + 1, n_i - 2, n_{i+1} + 1, \dots) \\
 & \quad - \{u(n_{i-2}, n_i) + u(n_i, n_{i+2}) + 2v(n_i)\}P(\dots, n_{i-1}, n_i, n_{i+1}, \dots) \\
 & \quad \quad + v(n_{i-1} + 2)P(\dots, n_{i-2} - 1, n_{i-1} + 2, n_i - 1, \dots) \\
 & \quad \quad + v(n_{i+1} + 2)P(\dots, n_i - 1, n_{i+1} + 2, n_{i+2} - 1 \dots) \\
 & \quad + d_R(n_{i-1} + 1)P(\dots, n_{i-1} + 1, n_i - 1, \dots) - d_L(n_i)P(\dots, n_{i-1}, n_i, \dots) \\
 & \quad + d_L(n_{i+1} + 1)P(\dots, n_i - 1, n_{i+1} + 1, \dots) - d_R(n_i)P(\dots, n_i, n_{i+1}, \dots)] = 0.
 \end{aligned} \tag{9}$$

This condition is clearly fulfilled if each process occurs with the same rate as the corresponding opposite process. Inserting the ansatz (3), this detailed balance yields $3L$ conditions

$$\begin{aligned}
 u(n_{i-1} + 1, n_{i+1} + 1)f(n_{i-1} + 1)f(n_i - 2)f(n_{i+1} + 1) &= v(n_i)f(n_{i-1})f(n_i)f(n_{i+1}) \\
 d_L(n_{i+1} + 1)f(n_{i+1} + 1)f(n_i - 1) &= d_L(n_i)f(n_{i-1})f(n_i) \\
 d_R(n_{i-1} + 1)f(n_{i-1} + 1)f(n_i - 1) &= d_R(n_i)f(n_i)f(n_{i+1})
 \end{aligned} \tag{10}$$

with $i = 1, \dots, L$. For the special choices (5)–(8), they are solved by

$$w(n + 1) \frac{f(n + 1)}{f(n)} = \text{const.} \tag{11}$$

Without loss of generality we choose the constant to be 1 and find

$$f(n) = \prod_{m=1}^n \frac{1}{w(m)} \tag{12}$$

which formally is the same expression as for the ZRP.

The similarity of the steady state probability distribution with that of the ZRP allows us to immediately carry over a number of results to our system. Of particular interest in the present context are the conditions for which the particles condensate. Condensation means that in the “thermodynamic limit”, where $N, L \rightarrow \infty$ with $\rho = N/L = \text{constant}$, a single site is occupied by macroscopic number of particles. Three cases can be distinguished as follows:

1. $w(n) \rightarrow \infty$ as $n \rightarrow \infty$: No condensation, the distribution of particles will be homogeneous in the limit $N \rightarrow \infty$.
2. $w(n) \rightarrow 0$ as $n \rightarrow \infty$: Condensation occurs for any density.

3. $w(n) \rightarrow \gamma > 0$ as $n \rightarrow \infty$: Condensation depends on the first order correction to $w(n)$. For example⁴, if

$$w(n) = \gamma \left(1 + b/n + O(1/n^2) \right) \quad (13)$$

then condensation occurs for large enough densities iff $b > 2$.

Let us discuss case 3 further. First of all we note that the leading term of w implies that the process (a), see Fig. 1, occurs with a rate proportional to $n_{i-1}n_{i+1}$. This is reminiscent of the filament current (2) which is proportional to the product of the filament density at two different locations. To discuss this case further, we will first consider

$$w(n) = \gamma \left(1 + \frac{b}{n} \right) \quad (14)$$

where the higher order terms are exactly 0. Then

$$f(n) = \prod_{k=1}^n \frac{n\gamma^{-1}}{n+b} \quad (15)$$

which is asymptotically $f(n) \approx \gamma^{-n} n^{-b}$.

The distribution must respect the global conservation of particles, i.e., $\sum_i n_i = N$. It is helpful to consider the system in the grand canonical ensemble, where the density ρ is controlled by the fugacity z . The grand partition function is

$$F(z) = \sum_n \left(\frac{z}{\gamma} \right)^n f(n) \quad (16)$$

which is well-defined for $0 \leq z \leq z_c$, where z_c is the radius of convergence of $F(z)$. For the rate (14) one gets $z_c = \gamma^{(27)}$. Knowing that the density of particles in the grand canonical ensemble is $\rho(z) = \langle n \rangle = z \frac{d \ln Z}{dz}$, the condensation can be understood as follows: if ρ diverges for $z \rightarrow z_c$ then one can obtain any arbitrary density by tuning z . However, if $\rho(z_c) < \infty$ then the maximum achievable macroscopic density is just $\rho_c = \rho(z_c)$. Thus, in a system having density $\rho > \rho_c$, the extra particles, in total $(\rho - \rho_c)L$, must form the macroscopic condensate. For the rate (14) it can be shown analytically⁽²⁷⁾ that $\rho_c = \frac{1}{b-2}$ is finite for $b > 2$. For any other form of $w(n)$ which asymptotically reduces to Eq. (14), for example $\tilde{w}(n) = \gamma(1 + b/(n+c))$, b_c is still 2 whereas ρ_c is in general different from $\frac{1}{b-2}$. When $b \geq 2$ and $\rho > \rho_c$, the probability of finding n particles at a site decays as n^{-b} with average density ρ_c . The condensate occurs on top of this ‘‘critical fluid.’’ See Fig. 2 for an example.

⁴In general, the first order correction to γ is not $O(1/n)$. A detailed study of these non-trivial cases can be found in Ref. 27.

Thus, b is the important parameter of the model which decides if the system can possibly phase separate. Physically, in the ZRP, b can be interpreted as the escape rate of particles from the condensate⁽²⁷⁾. Note that the mean rate at which particles hop from the “critical fluid” is given by $\langle w \rangle = \gamma$ and thus particles escape from the condensate with a rate $w(n) - \langle w \rangle = \gamma b/n$.

Comparing these results to the minimal model of active filament bundles we thus find a remarkable difference. While condensation depends in both cases on a critical density, in the hopping model the value of this critical density does not depend on the leading order term, but on the first order correction b . In contrast, the critical value of the minimal model depends on α which corresponds to the leading order term as will be shown below.

4. ABSENCE OF PARTICLE REPULSION $v = 0$: MEAN-FIELD ANALYSIS

In order to further investigate the last point we will now consider the case $v = 0$ when there is no repulsion of particles. In this case an analytic solution is out of reach. Numerical solution reveals condensation for $b > 2$. As an example in Fig. 2 we show the steady state distribution of particles for $b = 2.5$. It shows a clear peak at high particle numbers similar to the corresponding distributions for exactly solvable cases. For smaller particle numbers, the distributions show a power law with an exponent $\xi = 2.4 \pm 0.05$. The exponent is thus close to b , which is the value obtained in the exactly solvable case.

Some insight into the condensation behavior of the model can be gained by using a mean-field approximation. To this end we first write the dynamic equations for the expectation values $v_i = \langle n_i \rangle$ for $i = 1, \dots, L$. These equations depend on expectation values of products of occupation numbers of different sites. The mean-field approximation then consists of approximating these by products of the expectation values such that the dynamic equations are closed. Following this procedure we find

$$\begin{aligned} \frac{dv_i}{dt} = & d_R(v_{i-1})v_{i-1} - d_R(v_i)v_i - d_L(v_i)v_i + d_L(v_{i+1})v_{i+1} \\ & + v(v_{i-1})v_{i-1} - 2v(v_i)v_i + v(v_{i+1})v_{i+1} \\ & - u(v_{i-2}, v_i)v_{i-2}v_i + 2u(v_{i-1}, v_{i+1})v_{i-1}v_{i+1} - u(v_i, v_{i+2})v_i v_{i+2} \end{aligned} \quad (17)$$

First, consider again the rates (5)–(8) with w given by Eq. (14), but now with $v = 0$ and $p = q = r = 1$. It is easy to check that $v_i = \rho_0 = \text{const.}$ is a solution of (17). Because of the global conservation of particles $L\rho_0 = N$, thus ρ_0 must be the density of the system. Stability of this homogeneous state $v_i = \rho_0$ can be checked by adding a small perturbation δv_i . Representing the density by a Fourier-series

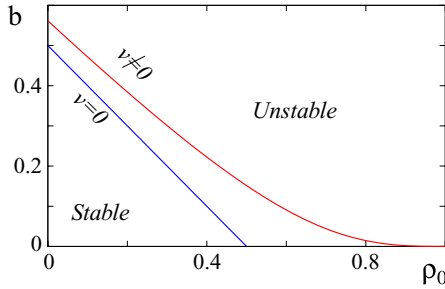


Fig. 3. Mean-field analysis of the stochastic model with rates specified in Eqs. (5)–(8) with $w(n) = 1 + b/n$. The homogeneous state is stable for values of b below the blue line if $v = 0$ and below the red line if $v \neq 0$. The parameter values are $p = q = r = 1$, $\gamma = 1$, and the limit $L \rightarrow \infty$ is considered.

we find for the dynamic equations in linear order in the perturbation

$$\frac{d\delta v_k}{dt} = \epsilon_k \delta v_k \quad (18)$$

where

$$\epsilon_k = 2\gamma(\cos(2\pi k/L) - 1)(1 - 2\gamma(b + \rho_0)\cos(2\pi k/L)) \quad (19)$$

and δn_k are the Fourier coefficients of the perturbation, $k = 1, \dots, L$. Thus, the perturbation $\delta v_k(t) = e^{\epsilon_k t} \delta v_k(0)$ decays if $\epsilon_k > 0$ and grows in the opposite case. Since $\cos(2\pi k/L) - 1 < 0$ for all k , modes can only become unstable if $2(b + \rho_0)\gamma > 1$. In the limit $L \rightarrow \infty$ the instability occurs at $b_c = 1/2\gamma - \rho_0$. The minimal model discussed in section 2.1 is equivalent to the $b = 0$ case of Eq. (14), where the critical value of γ is inversely proportional to the density ρ_0 .

In the case when v is chosen according to Eq. (6) the critical value of b is given by

$$b_c = -(A^2 + 1/2) + \sqrt{(A^2 + 1/2)^2 - 2A^3 + (1 - \gamma^{-1})A^2}, \quad (20)$$

where $A = \rho_0 - 1$. Figure 3 describes the phase diagram in (b, ρ_0) -plane for $\gamma = 1$. Inclusion of the v -process shifts the critical line to larger values of b , that is, it increases the stability region of homogeneous state.

A few points resulting from the mean-field analysis merit attention. First, it is interesting that the condensation transition survives in the mean field approximation, which is not the case for ZRP, i.e. when $v = 0 = u$. One can easily check that in this case $\epsilon_k = 2\gamma(\cos(2\pi k/L) - 1) \leq 0$ and thus $b_c = \infty$. Second, although the mean-field equations of our model truly capture the transition, they do not reproduce the exact critical point $b_c = 2$. Also, the density profile obtained in the mean-field approximation is different from the exact results, see Fig. 4. In the stochastic system, the condensate appears on the top of a critical fluid, whereas

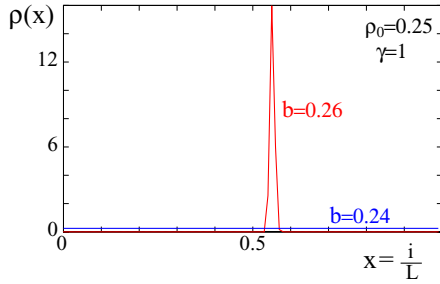


Fig. 4. Steady state density profiles of the mean-field equation (17). Rates are given by (5)–(8) with $p = q = r = 1$ and $w(n) = 1 + b/n$. Density profiles for a super- and a sub-critical value of b are shown. Parameters $\gamma = 1$, $\rho_0 = 0.25$, such that $b_c = 0.25$, and $b = 0.24$ (blue line) and $b = 0.26$ (red line).

the mean-field equations hide the fluctuations coming from the fluid and all the matter is found in the condensate. It is also interesting to note that the mean-field analysis would not change if d is taken to be a constant $d = \gamma$ instead $d = \gamma(1 + b/n)$, because first line of Eq. (17) gives identical results for both cases. This interesting case $d = \gamma$ is further explored in next section.

5. CONNECTION TO PHENOMENOLOGICAL DESCRIPTIONS OF ACTIVE FILAMENT BUNDLES

Having discussed the driven diffusive system introduced in Section 2 for a specific choice of the rates, we now want to return to the general case and to clarify the connection of the stochastic models to the minimal model of active filament bundles which motivated our analysis. This will be done through the intermediate of phenomenological equations governing the dynamics of such bundles on large length scales.

Phenomenological theories of active gels – of which active bundles are a special example – are based on the observation that filament currents are generated by gradients in the stress^(15–18). The system's stress can be expressed in terms of the state variables, that is the dynamic fields describing the system. If all filaments are aligned in a bundle and point all into the same direction, the stress tensor reduces to a scalar σ that depends on the filament density only. Furthermore, if any elastic response of the system is neglected, then the relation between the stress and the filament current j can be written as

$$j = \eta \partial_x \sigma \quad (21)$$

where η is an effective friction coefficient⁽¹⁵⁾. In the phenomenological descriptions, the stress σ is then systematically expanded in terms of the filament density and its gradients with respect to some homogeneous reference state.

We can connect the hopping model to the phenomenological dynamic equation by considering a coarse grained version of the discrete mean-field equations of the hopping model. The coarse-graining procedure amounts to assuming that the occupation numbers of the lattice sites vary only weakly with the site index i . On large length scales the discrete index can then be replaced by a continuous variable x and the occupation numbers v_i can be replaced by a density c such that $c(x = ia) = v_i/a$. Here, a is the lattice spacing. Replacing v_i in the discrete mean-field equations and then expanding terms like $c(x \pm a)$ into a Taylor-series $c(x \pm a) = c(x) \pm c'(x)a + c''(x)a^2 \pm \dots$, which is truncated at some order of a , we arrive at a partial differential equation for the time-evolution of the density.

We now apply this procedure to the mean-field equations of the stochastic model (i.e., Eq. 17), where we focus for simplicity on cases when only particles of one kind are present and when $d_L = d_R = d$. Restricting the expansion to terms of at most 4th order in a we find

$$\begin{aligned} \partial_t c = & \partial_x^2 \left[h(c) + \frac{1}{12} \partial_x^2 h(c) \right] \\ & - \partial_x^2 \left[g(c, c) + \frac{7}{12} \partial_x^2 g(c, c) - 2\partial_1 \partial_2 g(c, c) (\partial_x c)^2 \right] \end{aligned} \quad (22)$$

where without loss of generality we have set $a = 1$ in the final expression. In this equation, the hopping rates are contained in the functions h and g . Explicitly, $h(c) = d(c)c + v(c)c$ and $g(c, c) = u(c, c)c^2$. Furthermore, $\partial_i g(c, c) = \partial_{c_i} g(c_1, c_2)|_{c_1=c_2=c}$. The dynamic equation for the filament density derived from the discrete mean-field equations of the hopping model are thus of the same form as the corresponding equation for the filament density in the phenomenological descriptions. From this we can deduce the important result that the sum of the hopping rates with appropriate sign multiplied by the filament density equals the tension σ_0 in the homogeneous state

$$\sigma_0 = u(c_0, c_0)c_0^2 - (d(c_0) + v(c_0))c_0. \quad (23)$$

This relation provides a simple link between the kinetic hopping rates, which are microscopic quantities, and the stress generated in the bundle, which is a macroscopic quantity. It should be noted, however, that this relation is in general one way. While for every microscopic model the stress can be determined, the opposite is usually not true.

As an example consider the rates introduced in Section 4, namely $d(c) = D$, $v(c) = 0$, and $g(c, c) = \gamma^2(c + b)^2$. In this case the dynamic equation reads

$$\partial_t c = (D - 2b\gamma^2)\partial_x^2 c + \frac{D - 14b\gamma^2}{12}\partial_x^4 c - \gamma^2\partial_x^2 \left[c^2 - \frac{5}{6}(\partial_x c)^2 + \frac{7}{6}c\partial_x^2 c \right] \quad (24)$$

This equation can be compared to the expression obtained in the phenomenological approach developed in Ref. 15. This comparison shows that all terms appearing in the general expansion are generated by the stochastic model. It can therefore be used to study the effects of fluctuations on the dynamics of a generic active filament bundle. Note, that in Ref. 15 the term $\propto \partial_x^4 c$ was neglected for reasons of simplicity.

A linear stability analysis of Eq. (24) yields a critical value b_c of the parameter b for which the homogeneous distribution loses its stability. This corresponds to condensation in the stochastic model. For the critical value we find $b_c = D/2\gamma^2 - c_0$. This is the same value as obtained in Section 4 for $L \rightarrow \infty$ in the mean-field limit of the discrete hopping model, where $D = \gamma$. The corresponding tension created in the homogenous state at the critical point can be expressed as $\sigma_0 = \gamma^2(c_0 + b)(b + c_0 - 2)$. An instability of the homogenous state leads to a state where filaments condense, i.e., accumulate at one point and can therefore be interpreted as the point where the bundle ruptures. The value of the tension at the critical point is thus the maximal tension that can be generated by a filament bundle before it tears apart.

6. DISCUSSIONS AND CONCLUSIONS

In summary, we have introduced a new class of hopping models on one-dimensional lattices. Motivated by the dynamics of filaments connected by molecular motors, this class is defined by processes in which two particles hop simultaneously; either from adjacent sites to a site in between or away from one site to both adjacent sites. This is, in particular, different from the ZRP where such processes occur in an interval Δt with a probability $\propto (\Delta t)^2$ and are therefore neglected in comparison to processes that occur with a probability $\propto \Delta t$. As a consequence of the two-particle processes the mean-field approximation shows like the stochastic system a condensation transition. This does not hold for the mean-field analysis of the ZRP. Despite these important differences, for rates that have a factorized steady state probability distribution, the steady state distributions of the ZRP and of the class of systems introduced here are identical. This similarity allowed us to transfer results from the ZRP on the conditions of condensation to the new model class. In particular, we found that there is a critical density for condensation, if the rates approach for large occupation numbers a constant different from zero.

Coarse-graining of the mean-field equations allowed us to connect the kinetic hopping rates in the stochastic model to the stress generated in the bundle. The microscopic rates are thus linked to macroscopic physical quantities. Apart from giving the rates a physical meaning, this connection could be used to obtain the strength of the noise term in Langevin equations for the time-evolution of the filament density. As active filament bundles are inherently out of thermodynamic equilibrium there is in general no fluctuation-dissipation theorem that would allow to determine this strength. The coarse-graining also points to limitations of continuum descriptions of active filament bundles. Indeed we find that the criterion for condensation in the exactly solvable case involves only the first order correction of the rates, while the critical value in the mean-field equations depends also on the zeroth order parameter.

Taken these points together, the discrete hopping models introduced here are seen to be a useful tool for analyzing the effects of fluctuations on dynamics of active filament bundles – in spite of their simplicity. In the future it will be in particular interesting to study the case of two different particles present on the lattice. In the corresponding microscopic and phenomenological descriptions, traveling waves were found in this case.

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