Dynamics of a line under tension in an active bath

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We study the dynamics of a line under tension in a two-dimensional bath of Active Brownian Particles. Numerical observations indicate that as the bath activity or line tension is varied, the system transitions from a "low temperature" regime in which the line remains localized, to a "high temperature" regime in which the line becomes space-filling. We show that the low-temperature phase exhibits dynamic scaling properties consistent with the Edwards-Wilkinson model. We explore an equilibrium field theory that mimics some features of the space-filling phase but displays important inconsistencies with numerical results.

INTRODUCTION

Active matter systems display a rich phenomenology at boundaries [1, 2]. Self propelled particles accumulate at walls in a manner that depends on wall curvature, leading to a nonuniform mechanical pressure on a curved boundary. Elastic filaments in an active bath display modulational instabilities and spontaneous self-propulsion [3]. Despite this, little work has been done on the statistical mechanics of a fluctuating phase interface in an active bath [4, 5]. This problem is relevant to bacterial swarming, where a 2D bath of active bacteria deforms a water-air interface into a complex space-filling pattern [6]. As a preliminary step towards such problems, we consider here the dynamics of a line under tension in a bath of active particles in $d = 2$.

A line of length l with tension γ has an energy $\mathcal{H}(l) = \gamma l$. On a lattice, it is straightforward to show that the number of paths of length l between two points is asymptotically exponential in l. This means that both the energy and entropy of the line are proportional to its length, and in equilibrium there is a critical temperature T_c beyond which entropic effects are dominant. The average line length $\langle l \rangle$ is finite below T_c but divergent above it. If we restrict to self-avoiding lines, the counting of paths is more complicated, but can be carried out exactly in $d = 2$ [7]. This counting problem emerges naturally in high-temperature expansions of the two-dimensional (2-D) Ising model as well as the "loop-model" of the $O(n)$ universality class, and has been used to obtain exact solutions for these models [7, 8]. It can be shown that the equilibrium partition function of a self-avoiding line under tension falls in the $n \to 0$ limit of the $O(n)$ universality class [8]. The phase transition is similar to the non self-avoiding case, except that the high temperature phase is space-filling and has an average length that is limited by system area.

The case of a line under tension in an *active* bath is not amenable to such exact solutions. The question arises as to whether the active case exhibits a similar phase transition and whether the activity is important. To this end, we consider a 2-D microscopic model in which an overdamped zero-temperature line under tension is placed in a bath of Active Brownian Particles (ABPs). The active particles interact repulsively with the line and cannot cross it, which in turn precludes the line from crossing itself. We find evidence for a similar transition from a localized to a space-filling regime, each characterized by distinct dynamical scaling properties. We discuss potential mappings to equilibrium theories.

NUMERICAL PHENOMENOLOGY

To simulate a line under tension in an active bath, we represent the line by a chain of beads $\{\mathbf{r}_i\}$ which interact with their nearest neighbors through a pairwise potential of the form $V(r \equiv |\mathbf{r}|) = \gamma r$. The beads interact with the ABPs through a repulsive Weeks-Chandler-Andersen (WCA) potential $V(r) = \epsilon\left[(r_0/r)^{12} - (r_0/r)^6\right] + \epsilon/4$, where r_0 defines the effective interaction radius and sets our unit of length. To ensure that particles do not pass through the line, the spacing of the beads is set to approximately 1/5th of the ABP diameter. This spacing is maintained by dynamically adding and removing beads when the spacing fluctuates outside the range $(r_0/8, r_0/4)$. Unless indicated otherwise, the self-propulsion velocity and rotational diffusivity of the ABPs were set to $v = 4$ and $D_r = 1$, respectively. The mobilities of the particles and the beads were both set to unity. Simulations were carried out in a square domain of linear dimension L. Periodic boundary conditions were used on the left and right boundaries for both the ABPs and the line. For numerical reasons, only the ABPs follow periodic boundary conditions on the upper and lower boundaries (i.e. the line is simulated on a cylinder oriented along the y axis). All simulations were started from a horizontally flat initial condition $\mathbf{r}_i = (ir_0/5, 0)$.

Simulations reveal that as the line tension γ is decreased or the self-propulsion velocity v is increased, the system transitions from a regime in which the line fluctuations are localized to one in which the line is space filling (Figure 1). This is reminiscent of the corresponding phase transition in the equilibrium case, and we will

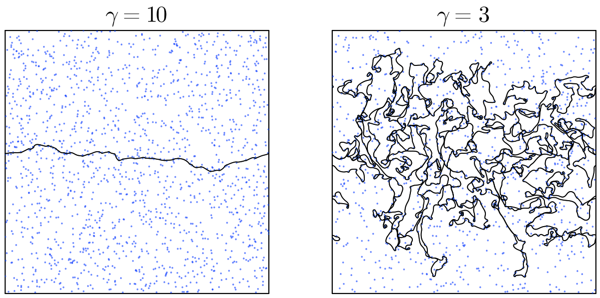

FIG. 1. Low- and high- temperature regimes of the line under tension in an active bath. The line tension γ is indicated.

therefore refer to these regimes as "low-" and "high-temperature". More detailed numerical studies would be necessary to verify that this is in fact a critical phase transition and not a smooth transition. Our preliminary results display hallmarks of a singular phase transition, including critical slowing down.

In the low-temperature regime, we find that the particle density field remains uniform, except for a layer of accumulation near the fluctuating line. The width of the layer is on the order of a particle diameter. Such wall accumulation is a known behavior of active particles [1]. In the space filling regime, the line width increases until it approaches system size. Figure 2 shows position histograms for the ABPs (blue) and the line beads (red) projected onto the y axis. A region of high line density is excited and expands until it approaches a steady-state distribution. This distribution is approximately uniform, except for regions of depletion near the top and bottom boundaries. These regions are due to a boundary effect and their width does not scale with system size.

We see from Figure 2 that the particle density is enriched in regions of high line density. This is a consequence of both the boundary accumulation behavior of ABPs as well as an additional entrapment effect where particles become confined by the tangled line. The enrichment along the line leads to a slight depletion of particle density beyond the expanding front (Figure 2, $t = 200$).

Numerical observations strongly suggest that in the space-filling phase, the average length of the line $\langle l\rangle(L,t)$ obeys a dynamic scaling relation of the form

$$\langle l\rangle(L,t) \sim L^2 f\left(\frac{t}{L^2}\right) \tag{1}$$

where $f(u)$ is an undetermined function satisfying $f(0) = 1/L$ and $f(\infty)$ is equal to some constant. This is shown in Figure 3, where we have plotted $\langle l\rangle(t)$ for different system sizes. Rescaling $\langle l\rangle(t) \to \langle l\rangle(t)/L^2$ and $t \to t/L^2$ collapses the results from different L onto a single curve. The scaling of $\langle l\rangle$ with system area at large times is consistent with the steady-state line density profile being uniform in space. The dynamical exponent $z = 2$ is characteristic of a diffusive process.

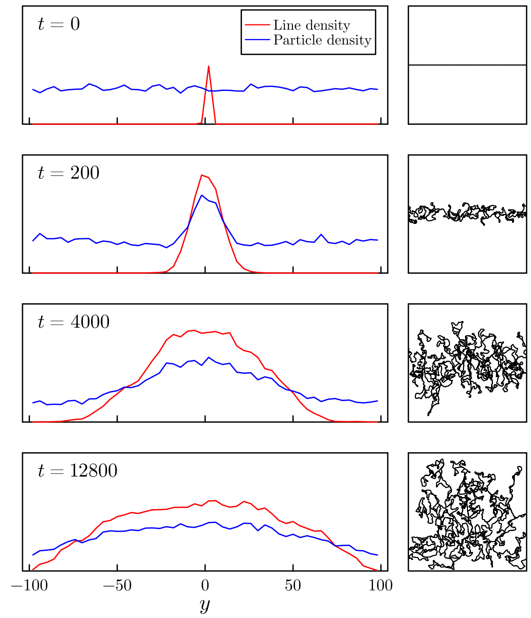

FIG. 2. Time evolution of the density profiles. Left: Ensemble-averaged line and particle density histograms projected onto the y-axis. Right: simulation snapshots.

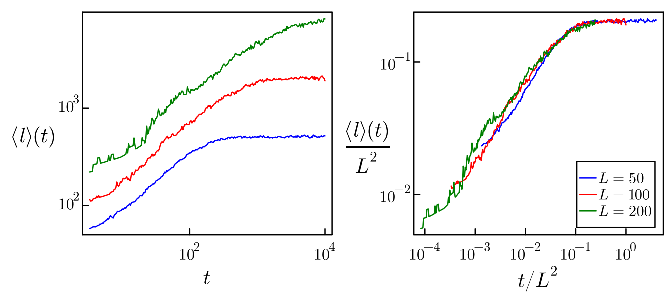

FIG. 3. Dynamic scaling of the line length in the space-filling phase. Left: Average line length over time. Right: data collapse after rescaling t and $\langle l\rangle$ by L^2.

DYNAMIC SCALING IN THE LOW TEMPERATURE PHASE

In the low temperature phase, the width fluctuations of the line are much smaller than the linear dimension of the system, and so the line path can be approximated by a univalued function $h(x,t)$ at long wavelengths. We seek a local equation of motion for $h(x,t)$ consistent with the symmetries of the problem. Invariance under translation in x and t implies the form

$$\partial_t h = F[h, \nabla h, \nabla^2 h, \dots] + \eta(x,t),$$

where F is a function of $h(x,t)$ and its derivatives, and $\eta(x,t)$ is a Gaussian noise term satisfying

$$\langle \eta(x,t) \rangle = 0, \qquad \langle \eta(x,t)\eta(x',t') \rangle = 2D\delta(x-x')\delta(t-t') \tag{2}$$

for some $D > 0$. The noise represents perturbations to the line from the active bath. Since F must be invariant under $h \to h + a$ and $x \to -x$, it can only depend on derivatives of h, and these must be of even order. The active particles are situated on both sides of the line, and so the system posses an up-down symmetry $h \to -h$. This excludes terms with even powers of h, such as $(\nabla h)^2$. Thus the most general equation of motion admits a gradient expansion of the form

$$\begin{aligned} \partial_t h = c_1 \nabla^2 h + c_2 \nabla^4 h + \cdots + c_n \nabla^{2n} h \\ + c_{lk} \left(\nabla^{2k} h\right) (\nabla h)^{2l} + \cdots + \eta(x,t). \end{aligned}$$

We are interested in the long-wavelength limit, where $h(x,t)$ is expected to be self-affine. Then under rescaling $x \to x' = bx$, we have $h(x,t) \to h'(x,t) = b^{\alpha} h(x,t)$. Using $\nabla^n \to b^{-n}\nabla^n$, we see that the $\nabla^2 h$ term is dominant for large b. The equation of motion can then be written

$$\partial_t h = v\nabla^2 h + \eta(x,t). \tag{3}$$

This is the Edwards-Wilkinson (EW) equation [9], and is derivable from a free-energy of the form

$$F[h(x,t)] \propto \int dx\, (\nabla h)^2.$$

We see that, in the low-temperature phase, the symmetries of the system imply a mapping to an effective equilibrium description in the scaling limit. Equation 3 has well-known dynamic scaling properties that we will review here [10]. Under rescaling of both space $x \to bx$ and time $t \to b^z t$, the noise term will transform as $\eta \to b^{-d/2 - z/2}\eta$ (this follows from equation 2). The full equation 3 thus scales as

$$\partial_t h = v b^{z-2} \nabla^2 h + b^{(z-d)/2 - \alpha} \eta(x,t)$$

This is scale invariant if $z = 2$ and $\alpha = (2-d)/2$. For $d = 1$,

$$z = 2, \qquad \alpha = \frac{1}{2}.$$

These are respectively the *dynamical* and *roughness* exponents of the EW model in 1-D. The exponents determine the scaling properties of the interface width, defined as

$$w(t,L) = \left(\frac{1}{L} \int dx \langle h(x,t)^2 \rangle \right)^{1/2}.$$

where L is the system size (along x). We can write an explicit expression for this quantity by solving equation 3 with the initial condition $h(x,t) = 0$. After Fourier transforming and integrating, the solution is

$$h(q,t) = \int_0^t dt' e^{-vq^2(t-t')} \eta(q,t).$$

Using $\langle \eta(q,t)\eta(q',t') \rangle = 4\pi D\delta(t-t')\delta(q+q')$, we can evaluate $\langle |h(q,t)|^2 \rangle$ to write

$$\begin{aligned} w^2(t,L) &= \frac{1}{L} \int \frac{dq}{2\pi} \langle |h(q,t)|^2 \rangle \\ &= \int_{1/L}^{1/a} \frac{dq}{2\pi} \frac{D(1 - e^{-2q^2 vt})}{q^2 v} \end{aligned} \tag{4}$$

where the integration bounds are set by the system size L and some short-distance cutoff a. In the limit $t \to \infty$ we have

$$w(t,L) = \left(\frac{D}{v}(L-a) \right)^{1/2} \sim L^{1/2} = L^{\alpha},$$

implying that the interface width saturates at a value which scales as $L^{1/2}$. To obtain the behavior prior to saturation, we extend the lower integration bound to 0. The integral can then be evaluated as

$$w^2(t,L) = \left(\frac{2\pi D^2 t}{v} \right)^{1/2} + \mathcal{O}(a) + \mathcal{O}(e^{-2tv/a^2}).$$

We conclude that for times earlier than the saturation time,

$$w(t,L) \sim t^{1/4} \equiv t^{\beta}.$$

where we have defined the *growth* exponent $\beta = 1/4$. In fact, the integral in equation 4 can be evaluated explicitly in terms of special functions to reveal a Family-Vicsek scaling form $w(L,t) \sim L^{\alpha} f(t/L^z)$. This holds in all dimensions, with α and z equal to the values determined earlier through the scaling argument [10, 11].

To numerically verify these predictions, we measured the width of the interface as a function of time and system size. A univalued function $h(x,t)$ was constructed out of the line path by taking the maximum height of the line at each horizontal position x. This was calculated on a uniform grid of points $x_i = (i-1)\Delta x$, and the width was obtained from $w(t,L) = \left(\sum_i \Delta x \langle h(x_i,t)^2 \rangle / L\right)^{1/2}$. The results are shown in Figure 4 (right) and confirm the predictions of the EW theory: For small times, $w(t,L)$ increases as a power law. The growth exponent was estimated by fitting the linear part of $\log w(t)$, yielding

$$\beta = 0.241 \pm 0.007.$$

This is in reasonable agreement with the prediction $\beta = 1/4$. At later times, $w(t,L)$ saturates to a constant value. Rescaling $w(t) \to w(t)/L^{\alpha}$ and $t \to t/L^z$ collapses the data onto a single curve when $\alpha = 1/2$ and $z = 2$ (Figure 4, right).

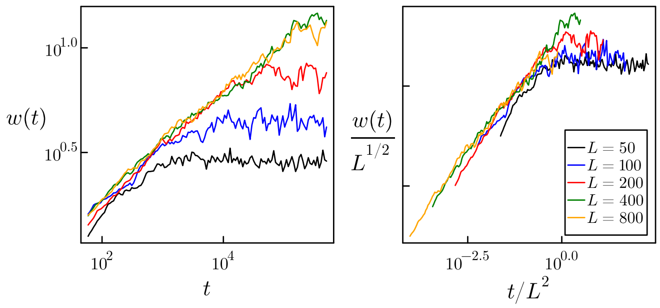

FIG. 4. Dynamic scaling of the interface width in the low-temperature phase. Left: interface width over time. Right: data collapse after rescaling t by L^z and w by L^α, with $z = 2$ and $\alpha = 1/2$ according to EW theory.

HIGH TEMPERATURE DYNAMICS

Equilibrium field theory and static analysis

In the space-filling phase, the line path is no longer univalued, and the description as a fluctuating interface is inappropriate. We pursue a coarse-grained theory describing the particles and the line as a pair of coupled fields. The *line density field* $\phi(\mathbf{x}, t)$ is a nonconserved field describing the total length of line within a small area element. The ABPs are described by a conserved *particle density field* $\rho(\mathbf{x}, t)$. The entrapment and accumulation of ABPs near the fluctuating line manifests as an effective attraction between the two fields.

We will look for an equilibrium theory that mimics these dynamics. Since ϕ is both nonconserved and positive-definite, it is useful to choose an order parameter $\psi(\mathbf{x}, t)$ defined by $\psi^2(\mathbf{x}, t) \equiv \phi(\mathbf{x}, t)$. In terms of ψ and ρ, we construct a phenomenological effective free energy

$$F[\psi, \rho] = \int d^2\mathbf{x} \left[\frac{1}{2} r\psi^2 + u\psi^4 + \frac{K}{2}(\nabla\psi)^2 - \lambda\psi^2\rho + \frac{1}{2}s\rho^2 + v\rho^4 + \frac{L}{2}(\nabla\rho)^2 \right] \quad (5)$$

This is related to model C in the theory of dynamical critical phenomena [12], in that it couples a nonconserved model A dynamics for ψ to a conserved model B dynamics for ρ. The coupling $-\lambda\psi^2\rho$ is the lowest order term consistent with up-down symmetry in ψ. Since neither field is spontaneously ordered in absence of coupling, and since the interaction of the fields is attractive, we are interested in the regime $r > 0$, $s > 0$, and $\lambda > 0$. In a mean field approximation $\psi(\mathbf{x}) = \overline{\psi}$, $\rho(\mathbf{x}) = \rho_0$, the effect of the conserved field is simply to alter the coefficient of ψ^2. Minimizing the free energy gives

$$\overline{\psi}^2 = \begin{cases} \frac{2\lambda\rho_0 - r}{4u}, & \text{for} \quad 2\lambda\rho_0 > r, \\ 0, & \text{otherwise.} \end{cases} \quad (6)$$

Thus $\overline{\psi}$ exhibits a continuous phase transition above a critical coupling constant or particle density. The mean-field prediction is that the line density field in the space-filling phase is linear in the particle density.

In the microscopic model, our preliminary numerical results show that the steady-state line density in the space filling phase does indeed increase with particle density. The dependence of the critical tension on the particle density is complicated: when the tension γ is lower than the ABP propulsion velocity v, a single particle can excite the line to a width limited only by the persistence length. In this case, we find that the line is space filling even at very low ρ_0, but that the steady-state line density will also be low. When γ is greater than v, particles must cooperate to excite the line. A space filling regime still exists, but it now requires a sufficiently high ρ_0. Further studies should be directed towards characterizing these different behaviors.

In our field theory, the conservation of the particle density field implies the possibility of phase-coexistence at the mean-field level: To see this, we regard the mean-field line density as a function of ρ, denoted $\overline{\psi}^2(\rho)$ and defined by equation 6 (with ρ in place of ρ_0). The mean-field free energy density is then a single-variable function:

$$f(\rho) = \frac{1}{2} r\overline{\psi}^2(\rho) + u\left[\overline{\psi}^2(\rho)\right]^2 - \lambda\overline{\psi}^2(\rho)\rho + \frac{1}{2}s\rho^2 + v\rho^4.$$

This contains a nonanalyticity at $\rho = r/2\lambda$, but is nonetheless once-differentiable with

$$f'(\rho) = \rho(s + 4v\rho^2) - \lambda\left(\frac{2\lambda\rho - r}{4u}\right)\Theta\left[\rho - r/2\lambda\right] \quad (7)$$

where Θ is a step function. For the case of interest $r > 0$, $\lambda > 0$, $f(\rho)$ always has a minimum at $\rho = 0$. This represents a dilute phase in which the particle density is low and the line density field is not excited (note that, in this construction, ρ should be regarded as a reduced density and not the absolute particle density). The condition for phase coexistence is that $f'(\rho) = 0$ has two nonzero solutions, so that $f(\rho)$ possesses a second minimum at a positive value of ρ. An equivalent statement is that the polynomial

$$\rho^3 + \left(\frac{2us - \lambda^2}{8uv}\right)\rho + \frac{\lambda r}{16uv}$$

has three real roots, of which one is greater than $r/2\lambda$. It can be verified that this holds if and only if

$$2\lambda^2 > 6su + 3(2r^2uv\lambda^2)^{1/3}. \quad (8)$$

Notably, this is always satisfied for sufficiently large λ, implying that phase coexistence is possible if the coupling of the fields is large enough. Given a set of parameters satisfying equation 8, one can determine the relative fractions of particles in each phase by minimizing

$\rho_1 f(\rho_1) + \rho_2 f(\rho_2)$ subject to the constraint $\rho_1 + \rho_2 = \rho_0$. This gives rise to the common tangent construction, which can be used to determine a phase diagram.

In the simulation, phase coexistence would manifest as a stable band of high line and particle density, with a width that is a fixed fraction of L. In our preliminary simulations, we were unable to observe such behavior; rather, it appears that the system transitions abruptly from the low temperature phase in which the line is localized to the high temperature phase in which the entire space is filled by the line. This is an important inconsistency between the simulation and the field theory, although further studies are required to map the microscopic phase diagram.

Dynamical field theory

We construct the dynamical equations for $\psi(\mathbf{x}, t)$ and $\rho(\mathbf{x}, t)$ from functional derivatives of $F[\psi, \rho]$.

$$\partial_t \psi(\mathbf{x}, t) = -\mu_\psi \frac{\delta F[\psi, \rho]}{\delta \psi(\mathbf{x}, t)} \tag{9}$$

$$\partial_t \rho(\mathbf{x}, t) = \mu_\rho \nabla^2 \left[\frac{\delta F[\psi, \rho]}{\delta \rho(\mathbf{x}, t)}\right] + \eta(\mathbf{x}, t) \tag{10}$$

where μ_ψ and μ_ρ are mobility coefficients. We have included in $\partial_t \rho$ a Langevin noise source satisfying $\langle \eta_\rho(\mathbf{x}, t)\rangle = 0$, with the Fourier-space correlation function

$$\langle \eta(\mathbf{q}, t)\eta(\mathbf{q}', t')\rangle = 2\mu_\rho q^2 (2\pi)^2 \delta(\mathbf{q} + \mathbf{q}')\delta(t - t').$$

This choice preserves the conservation law and enforces a fluctuation-dissipation theorem. We do not include a noise term in $\partial_t \psi$, as any excitation of the line must be due to interactions with the particles (but note [13]). Explicitly, the equations of motion are

$$\partial_t \psi = \mu_\psi \left[-r\psi - 4u\psi^3 + K\nabla^2\psi + 2\lambda\psi\rho\right] \tag{11}$$

$$\partial_t \rho = \mu_\rho \nabla \cdot \left[s\nabla\rho - L\nabla^3\rho + 4v\nabla\left(\rho^3\right) - \lambda\nabla\left(\psi^2\right)\right] + \eta_\rho(\mathbf{x}, t). \tag{12}$$

We may ask what is the rate at which the excited phase expands to fill the space, and whether this has any universal properties. To determine this, we require a solution of the equations of motion with initial conditions

$$\psi^2(\mathbf{x} = (x, y), t = 0) = L\delta(y), \qquad \rho(\mathbf{x}, t = 0) = \rho_0.$$

This corresponds to an initial configuration in which the line lies along the horizontal axis and the particle density is uniform. The boundary conditions are periodic along $x = \pm L/2$ and reflecting along $y = \pm L/2$. With these initial conditions, the system has translational symmetry along x, and so the dynamical equations can be made one-dimensional. Even in the 1-D case, the nonlinearities in the equations of motion preclude their exact solution. As a first approximation, we take a mean-field approach in which the particle density remains uniform at all times, $\rho(\mathbf{x}, t) = \rho_0$. Equation 11 then becomes, in 1-D,

$$\partial_t \psi - \mu_\psi K\, \partial_y^2 \psi = \mu_\psi\, \psi \left(2\lambda\rho_0 - r - 4u\,\psi^2\right). \tag{13}$$

With the definition $\chi^2 \equiv \left(\frac{4u}{2\lambda\rho_0 - r}\right)\psi^2$, this can be written in the form,

$$\partial_t \chi - D\partial_y^2 \chi = \alpha(1 - \chi^2)\chi \equiv G(\chi), \tag{14}$$

where $\alpha = \mu_\psi(2\lambda\rho_0 - r)$ and $D = \mu_\psi K$. The function $G(\chi)$ obeys the condition $G(0) = G(1) = 0$. For $0 \le \chi \le 1$, it satisfies $G(\chi) > 0$, $G'(\chi) \le G'(0) = \alpha > 0$. These conditions place equation 14 within a class of equations studied by Kolmogorov, Petrovskii, and Piskunov [14]. Such equations admit solutions with an asymptotic traveling-wave form $\chi(y, t) = f(y - vt)$, with velocity $v = 2\sqrt{DG'(0)}$, or

$$v = 2\mu_\psi \sqrt{K(2\lambda\rho_0 - r)}.$$

Thus the excited phase expands ballistically in this approximation. This finding is inconsistent with simulations such as that shown in figure 2; we instead find that the expansion velocity slows down over time. This is in part due to the depletion of particle density ahead of the expanding front. Going beyond a mean-field approximation for ρ would likely capture some of this slowdown due to depletion. Whether the form of the slowdown will be consistent with the simulation remains to be determined.

Lastly, we note that the numerical scaling relation in equation 1 (Figure 3) suggests that $\int \psi^2\, d^2\mathbf{x}$ should have a generic scaling form $f(t/L^2)/L^2$ in the space-filling phase, even far from the critical point. The scaling with L^2 as $t \to \infty$ is consistent with the uniform ordered phase of the field theory. The time scaling with $z = 2$ is less trivial; in a field theory such as that described by equations 11 and 12, dynamical scaling is expected only near the critical point and is nongeneric. Away from the critical point, we would instead expect the evolution to have a characteristic time scale. The field theory thus fails to capture this feature of the numerical results.

CONCLUSIONS

We have studied the dynamics of a line under tension in a bath of Active Brownian Particles. We found that the system transitions between two regimes with distinct scaling behavior. In the "low-temperature" regime, the line fluctuations are characterized by a width which scales as $w \sim L^{1/2} f(t/L^2)$. This is consistent with the Edwards-Wilkinson theory of a fluctuating interface, implying a mapping to equilibrium behavior in this regime. As the bath activity is increased or the line tension is decreased, the system transitions to a space-filling phase, in which the interface width scales with system size and the average line length takes the generic form $\langle l \rangle \sim L^2 g(t/L^2)$.

The equilibrium mapping in the low temperature phase is a consequence of up-down symmetry. This symmetry would be broken if the particles had been placed on only one side of the line. The equations of motion would then contain additional terms, including the KPZ term $(\nabla h)^2$ which cannot be derived from a free energy [10, 15]. Only then would the activity of the particles become important to the long-wavelength dynamics. This is in fact the case relevant to bacterial swarming, and future studies should be directed towards characterizing it.

We attempted a description of the space-filling phase in terms of an equilibrium field theory. Although the theory mimics some qualitative features of the numerical model, it fails to capture the dynamic scaling of the line length and erroneously predicts phase coexistence. This may be remedied by a more systematic study in which an equation of motion is constructed from all terms allowed be symmetry, similar to the approach used here in the low-temperature case. It remains to be determined whether the bath activity is relevant in the scaling limit of the space-filling phase.

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