Nonequilibrium Phase Transition in the Sedimentation of Reproducing Particles

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We study numerically and analytically the dynamics of a sedimenting suspension of active, reproducing particles, such as growing bacteria in a gravitational field. In steady state we find a nonequilibrium phase transition between a "sedimentation" regime, analogous to the sedimentation equilibrium of passive colloids, and a "uniform" regime, in which the particle density is constant in all but the top and bottom of the sample. We discuss the importance of fluctuations in particle density in locating the phase-transition point, and report the kinetics of sedimentation at early times.

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About a century ago, Einstein showed theoretically and Perrin demonstrated experimentally that in a dilute colloidal suspension, the particle density ρ as a function of height z is given by the barometric distribution: $\rho(z) = \rho(0)\exp(-z/z_0)$, where z_0 is the sedimentation height. This distribution results from a subtle interplay between thermal diffusion, hydrodynamics, and gravity. Diffusion and hydrodynamics are related via the Stokes-Einstein formula, a form of the fluctuation-dissipation theorem for equilibrium systems, while balancing gravity and Brownian motion gives $z_0 = D/v_s$, where D is the particles' diffusion coefficient and v_s their sedimentation speed. The barometric distribution applies when the suspension is so dilute that interparticle potential interactions (excluded volume, Coulomb, etc.) can be neglected. Modern colloid physics has focused on the behavior of *concentrated* suspensions [1].

An equally interesting avenue to explore is that of *active* particles (APs) [2]. Specifically, we consider APs able to propel themselves in such a way that their long-time motion is diffusive, i.e., each particle's mean-squared displacement from an initial position $\langle r^2(t)\rangle$ increases linearly with time t so that (in three dimensions) $\langle r^2\rangle = 6D_{\mathrm{eff}}t$, where D_{eff} is an effective diffusion coefficient. The swim-tumble-swim motion of an *Escherichia coli* bacterium ($\sim 2\ \mu\mathrm{m} \times 1\ \mu\mathrm{m}$ spherocylinder, average density $\rho_b = 1.08\ \mathrm{g/cm^3}$) is an example [3], for which experiments give $D_{\mathrm{eff}} \sim \mathcal{O}(10^2\ \mu\mathrm{m}^2\,\mathrm{s}^{-1})$ [4]. An equivalent passive colloid has $D \sim 0.5\ \mu\mathrm{m}^2\,\mathrm{s}^{-1}$ at 300 K, so that an *Escherichia coli* functions at an effective temperature of $\mathcal{O}(10^4\ \mathrm{K})$: it is far from equilibrium. Mimicking bacteria, we assume our APs can also "reproduce" and "die." Both motility and reproduction require energy intake, although this is nowhere explicit in what follows.

In this Letter, we study the behavior of (effectively) diffusing and reproducing, noninteracting APs *in a gravitational field*. This may model, for instance, a dilute suspension of motile *E. coli* that are growing but not responding to chemical gradients (i.e., nonchemotactic). Such a system is, arguably, the simplest example of "active soft matter." Does this paradigmatic AP system differ significantly from its passive counterpart (dilute colloidal sedimentation equilibrium), and if so how?

We first report stochastic simulations of the dynamics of diffusing and reproducing APs in a gravitational field. We then interpret these results by analyzing a continuum equation describing the evolution of a density profile of a dilute sedimenting AP fluid. We find the steady-state profile, as well as the dynamic pathway leading to it. Even a mean-field description reveals a much richer phenomenology for APs than passive colloids. We find a nonequilibrium phase transition between a "sedimentation" regime with exponential profile, and another regime showing essentially constant density in the bulk of the suspension. Using realistic parameter values, we predict that one may switch between the two phases by modifying the growth rate of a real system of bacteria. Close to this transition, there exist novel "sedimentation bands" in which a region of uniform AP density coexists with an AP-depleted region. This may usefully be compared to the phenomenon of shear banding. We also show that the presence of noise shifts the transition point. Finally, we relate our results to real bacterial suspensions.

We use a stochastic algorithm to simulate the coupled biased diffusion and reproduction or death of APs. We consider a column of sedimenting APs as a discrete lattice of sites $i = 1, \ldots, L$ with the number of AP occupying each lattice site specified as $n_i(t)$. Gravity acts towards $i = 0$. At each time step $t \to t + \Delta t$ the array of occupation numbers is updated according to a "multiply" step or a "move" step chosen with probabilities $w/(1+w)$ or $1/(1+w)$, respectively, where $w = \alpha\{1 + \sum_{i=1}^{L} n_i^2/[\rho_0 \sum_i n_i(t)]\}$ is the ratio of the total rate of reproduction or death per particle to the total rate of moving per particle, and α, ρ_0 are parameters to be discussed below [5].

In a "move" update each AP moves independently up or down with probability p or $1-p$. In a "multiply" update, at each site i each particle is replaced by two particles with probability $\rho_0/[\rho_0 + n_i(t)]$ or removed with probability $n_i(t)/[\rho_0 + n_i(t)]$. We impose no flux, or reflecting, boundary conditions at the top and the bottom of the container ($i = 0$ and $i = L$).

If Δz, Δt represent, respectively, the spatial and temporal steps, then the continuum limit of our Markov process leads to a diffusion constant $D = \frac{\Delta z^2}{2\Delta t}$ and sedimentation velocity $v = (1 - 2p)\frac{\Delta z}{\Delta t}$. The parameter p controls the strength of the gravitational force, α controls the rate of reproduction or death, and ρ_0 gives the value of the occupation in which reproduction and death are balanced. In a real bacterial suspension, α will be the growth rate (medium dependent, but $\gtrsim \mathrm{hour}^{-1}$ for *E. coli*) and ρ_0 is the saturation cell density ($\sim 10^9$ cells/cm^3 for *E. coli* [6]).

Note that the state where the lattice is devoid of APs is an absorbing state of the dynamics in the algorithm, which we call model I. We also considered a variation, model II, in which a depopulated site is allowed to be repopulated spontaneously (during the "multiply" update).

Our simulations suggest that there is a phase transition between two different regimes. If the APs reproduce slowly (α small), we obtain a steady-state density profile which decays sharply with z [Fig. 1(a)]. We call this the "sedimentation regime" in analogy with the similar behavior of passive colloids under gravity. If the growth rate exceeds a threshold α_c, the steady state is one with a uniform density throughout the bulk of the sample, with depleted and enriched layers in the top and the bottom of the container [Fig. 1(b)]. In model II, we find that the critical value is close to $\alpha_c = \frac{v^2}{4D}$; whereas in model I, the presence of an absorbing state widens the sedimentation regime, shifting α_c to slightly larger values.

To understand the simulations, we take a continuum approach and coarse grain our discrete model by defining a 1-dimensional profile of AP density $\rho(z, t)$ (gravity acts along the negative z axis). To make contact with the numerical simulations, and on general grounds, we may assume that the density profile obeys the following dynamic equation of motion:

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial z^2} + v\frac{\partial \rho}{\partial z} + \alpha\rho\left(1 - \frac{\rho}{\rho_0}\right) + \Gamma(\rho)\eta(t). \quad (1)$$

The first term represents diffusion, the second term represents the sedimentation due to gravity and the third term represents reproduction or death. Here, D and v have the same meaning as in the numerical simulations. An important dimensionless control parameter is $\theta = v/\sqrt{D\alpha}$. The last term in (1) represents noise, and $\eta(t)$ is a white noise with unit variance, while $\Gamma(\rho)$ is a function to be specified. We first consider the deterministic case $\Gamma(\rho) = 0$ which reduces to a mean field description. We also take $\rho_0 = 1$.

Considering the steady state ($t \rightarrow \infty$), if $\alpha = 0$, we get back passive colloid sedimentation equilibrium $\rho(z) \propto \exp(-vz/D)$. However, for $\alpha > 0$ one obtains a nonlinear equation for which an exact solution is not available. Therefore we perform a perturbation expansion for small α using the first 30 terms of a series expansion $\rho(z) = \sum_n \alpha^n \rho^{(n)}(z)$. The series converges for $\alpha < \alpha_c = \frac{v^2}{4D}$ and diverges otherwise. This corroborates the simulation results and suggests that indeed a phase transition occurs as the $\theta = v/\sqrt{D\alpha}$ goes through 2.

Equation (1) with $v = 0$ and no noise is the well-known Fisher-Kolmogorov-Petrovski-Piskunov equation and admits advancing waves with velocity $v_w = 2\sqrt{D\alpha}$ as solutions [7]. We can understand this phase transition as a competition between gravity forcing the bacteria downwards with velocity v and a traveling wave of proliferation which advances upward. For $v > v_w$, the sedimentation wave wins over the Fisher wave and leads to an exponential profile, while for $v < v_w$ the Fisher wave leads to a uniform bacterial density throughout the sample. However, Eq. (1) actually yields a transient traveling wave for $v > v_w$ only. The transition is reminiscent of transitions in interface depinning [8]; in a branching random walk with an absorbing wall [9], and of extinction transitions in inhomogeneous biological systems [10]. We note that a linearized version of our Eq. (1) with $\Gamma = 0$ and different boundary conditions was considered in Ref. [11] to describe microorganisms advected in a river and resultant extinction. We believe that our analysis should apply to this problem as well. We also stress that the transition would be washed away by translational invariance or periodic boundary conditions, which are usually considered [7,10].

The existence of a nonequilibrium phase transition at $\theta = \theta_c = 2$ is confirmed by numerical solution of the noiseless version of Eq. (1) using a standard finite difference scheme. An example of a series of steady-state solutions for different values of θ is shown for a sample of size $L = 20\sqrt{D/\alpha}$, in Fig. 1(c). Increasing the system size, the segment of the sample at $\rho = 1$ in the uniform regime increases (data not shown), analogous to equilibrium phase transitions. It is interesting to consider the behavior of the decay length of the exponential density profile in the

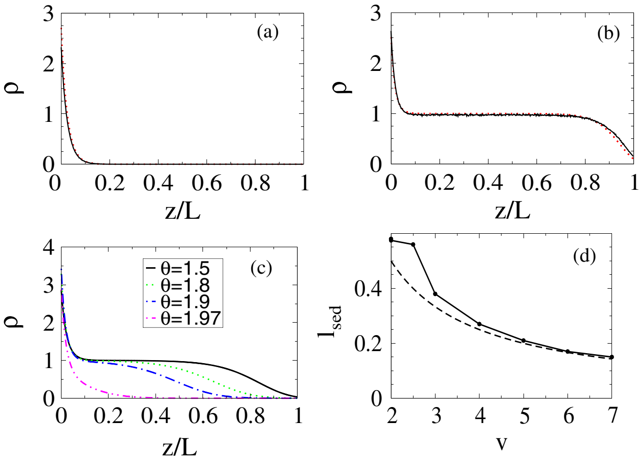

FIG. 1 (color online). The average density ρ versus height z for a suspension of motile and reproducing active particles in gravity. Simulation results (model I), with (a) $\theta = 3.6$, and (b) $\theta = 1.4$. (c) Numerical solutions of the noiseless continuum equation (1). (d) The dependency of the sedimentation length l_{sed} on v (in units of $\sqrt{D\alpha}$; the dashed line gives the colloidal value at $\alpha = 0$, denoted by z_0 in the text).

sedimentation regime (an effective sedimentation length) as a function of $|\theta - \theta_c|$. This sedimentation length is akin to a scaling length in an equilibrium phase transition. We find that after correcting for a small L-dependent shift in θ_c, the sedimentation length does *not* diverge at the transition, and is only at most $\sim$20% larger than the corresponding sedimentation length with no growth ($\alpha = 0$). If we focus on the steady-state concentration value, e.g., in the middle of the sample, it switches abruptly, for $L \to \infty$, from 0, for $\theta > \theta_c$, to 1, for $\theta < \theta_c$. These observations are consistent with a discontinuous phase transition.

For large but finite systems, we find evidence of an intriguing spontaneous banding of the sedimenting APs, which occurs very close to $\theta = \theta_c$. An example is shown in Fig. 2, in which two steady-state regions coexist in the bulk of the sample, one in which ρ is practically 0 and another one in which it is $\sim$1. This kinklike solution, which we call a "sedimentation band," is similar to a *cline*, found in the population biology literature when solving a reaction-diffusion equation, similar to Eq. (1), but with $v = 0$ and a reaction term which is cubic in ρ [12]. In our case, however, the existence of sedimentation bands is more surprising, as without advection the state at $\rho = 0$ is unstable, and bands arise due to the vicinity of a phase transition. In this respect, our sedimentation banding is more akin to shear banding, which is obtained when some complex fluids such as liquid crystals and wormlike micelles in the isotropic or disordered phase, are subjected to a shear, slightly smaller than that needed to order them completely [13]. Sedimentation bands appear in an increasingly small window of θ as L increases, and disappear in the thermodynamic ($L \to \infty$) limit.

Would it be possible to observe the transition we predict in a real bacterial suspension? For *E. coli* in water, $v \lesssim 0.1\ \mu\mathrm{m\,s}^{-1}$ [14] and is fixed, while $D \gtrsim 10^2 \mu\mathrm{m}^2\,\mathrm{s}^{-1}$ [4]. In rich, well aerated media maintained at the optimal temperature of 37 °C, the population doubles every $\sim$20 min, giving $\alpha \sim 10^{-3}\ \mathrm{s}^{-1}$, and $\theta \approx 0.3$. It is possible to culture the bacterium in what is known as "motility buffer," in which D is maintained, but growth essentially stops ($\alpha \to 0$), allowing the tuning of θ from 0.3 through 2 to arbitrarily large values, thus permitting the observation of our transition in principle.

In this context, it is important to note that the pathway to steady state may be quite slow. This is particularly true close to $\theta_c(L)$, and in the region where sedimentation bands form. In the banding regime for large sample size L, we also find that the behavior of the part of the sample close to the top, or just after the boundary of the band, display nonmonotonic behavior. The density first increases, as if the systems transiently entered the uniform regime, to decay later on to reach equilibrium [see Fig. 3(a)]. The time scale needed to reach equilibrium, t_{eq}, is plotted in Fig. 3(b) as a function of the distance from the transition point. Larger systems take longer to equilibrate, while close to criticality we find that t_{eq} increases as a power law of $|\theta - \theta_c|^{-a}$, with $a \simeq 1$ above the transition, consistent with [9] and confirming the presence of a phase transition at $\theta_c = 2$. These results applied to APs with $\alpha = 10^{-4}\ \mathrm{s}^{-1}$ predict that close to the transition, it may take up to several months for a column of 10 cm height to reach steady state.

Next, we discuss the role of noise, i.e., the case $\Gamma(\rho) \neq 0$ in Eq. (1). If $\rho = 0$ is to be an absorbing state, we need to go beyond the case $\Gamma(\rho) = \Gamma_0 > 0$, and consider instead a density-dependent amplitude Γ. The natural choice is $\Gamma = \Gamma_0\sqrt{\rho}$, which is justified by a central limit argument relating the variance of the noise to the number of active particles [15,16]. Increasing Γ_0 favors large fluctuations and may locally bias the system towards the absorbing state. We observe that as Γ_0 is increased the sedimentation regime is enhanced at the expense of the growth one (see Fig. 4). This is consistent with a negative shift in the Fisher wave velocity due to noise [17]. The nonequilibrium phase

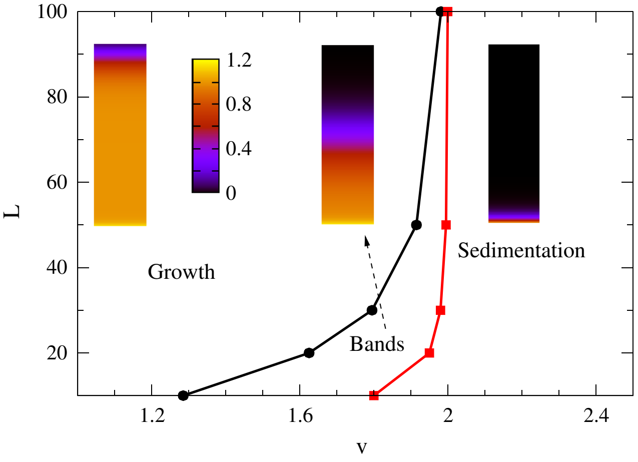

FIG. 2 (color online). Steady-state diagram in the (v, L) plane for the noiseless version of Eq. (1) (with $\alpha = D = 1$). A profile is "banded" if the cline stays in the bottom 75% of the sample. Typical concentration profiles are also shown, together with a color scale for the density.

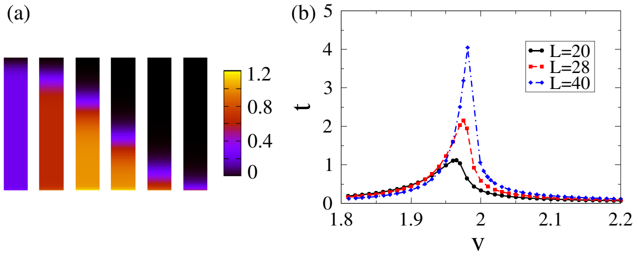

FIG. 3 (color online). (a) Dynamics of the density profile in a system with $L = 30$ (in units of $\sqrt{D/\alpha}$), and with $\theta = 2.1$. The times corresponding to each profile are (from left to right) 0.99, 2.8, 17.5, 62.2, 121.4, 250 (in units of α^{-1}, the bottom 5% of the sample is cut for color readability). (b) Plots of the time needed to get to steady state (in units of $10^3\ \alpha^{-1}$), as a function of v (in units of $\sqrt{D\alpha}$). (L is in units of $\sqrt{D/\alpha}$).

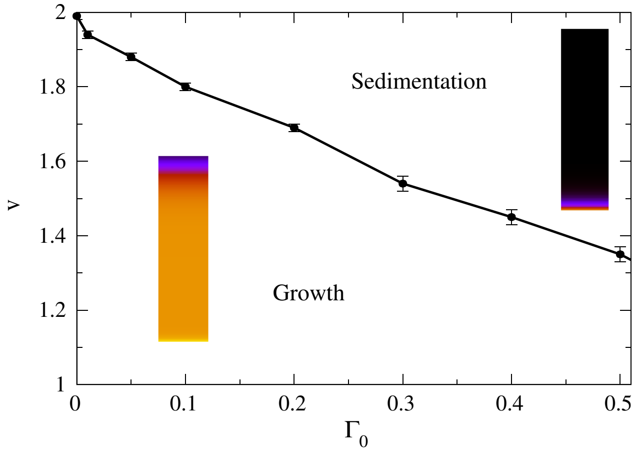

FIG. 4 (color online). The dependence of the critical velocity v_c on the amplitude of noise Γ_0 (with $D = \alpha = 1$).

boundary shown in Fig. 4 is found by locating the maxima of the order parameter fluctuations.

Equation (1) with $v = 0$ describes directed percolation (DP) [15], the generic university class of nonequilibrium transitions from an absorbing state ($\rho = 0$) to a fluctuating state ($\rho > 0$). The dimensionless control parameter is in this case $\Gamma_0/(\rho_0^2 D\alpha)^{1/4}$. Thus Fig. 4 becomes an extension of the DP phase diagram to include a v axis. Intriguingly the transition we have studied for Γ_0 is discontinuous whereas the DP transition at $v = 0$ is continuous. Therefore one may speculate that there is a singular or even tricritical point along the critical curve $v_c(\Gamma_0)$. This scenario might be similar to what occurs in the XY model, where switching the XY spin into a velocity can result in a discontinuous transition [18].

We have already pointed out that with typical values of v and D in a suspension of *E. coli*, it may be possible to "tune" the growth constant α to bring the system from the sedimentation to the uniform regime according to our predictions. In reality, these experiments need stringent controls, e.g., to make sure that the bacteria are not engaged in any form of chemotaxis, which would render D dependent on concentrations of chemical species (nutrient, oxygen, waste products, etc.). The extra level of complexity introduced can be modeled by adding a chemotactic term to Eq. (1), and coupling it to a reaction-diffusion equation, e.g., as in the Keller-Segel model [19]. Moreover, we have shown that the time scales for reaching steady state can be long, reaching $\mathcal{O}(10^3)$ in units of the inverse growth rate α^{-1} in the vicinity of the transition. But in a bacterial culture, α itself is only approximately constant during what is known as the "exponential" growth phase, after which saturation in population density and then death follow. Thus, steady-state experiments at $\theta \approx \theta_c$ are likely impractical.

Clearly, our model also neglects hydrodynamic interactions [20], which may (for example) cause swimmers to attract. Thus, hydrodynamics could have highly nontrivial effects, e.g., concerning the approach to steady states. However, we believe that the qualitative features of the transition we have identified may survive, because these are due to the competition between gravity and Fisher wave fronts, which should be generic. Also, bacterial motility and its hydrodynamic effects can be "turned off" by genetic modification or environmental conditions.

In summary, we have shown that the physics of motile and "reproducing" active particles in a gravitational field yields a surprisingly nontrivial phenomenology. We have found that increasing the growth rate from zero, the system makes an abrupt transition from a sedimentation regime in which the density decays exponentially with the distance from the bottom of the container, to a uniform growth-dominated regime in which the density is practically constant spatially. The essential physics is that of a balancing between a downward gravitational flux, and an upward diffusion-growth flux. Using values appropriate to *E. coli*, we predict it may be possible to tune the growth rate of the bacterium to allow observation of these two types of behavior in a real bacterial suspension, although slow kinetics may preclude detailed study of the transition regime ($\theta \approx \theta_c$) itself.

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