

Critical Motility-Induced Phase Separation Belongs to the Ising Universality Class

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A collection of self-propelled particles with volume exclusion interactions can exhibit the phenomenology of a gas-liquid phase separation, known as motility-induced phase separation (MIPS). The nonequilibrium nature of the system is fundamental to the phase transition; however, it is unclear whether MIPS at criticality contributes a novel universality class to nonequilibrium physics. We demonstrate here that this is not the case by showing that a generic critical MIPS belongs to the Ising universality class with conservative dynamics.

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Active matter is an extreme kind of nonequilibrium system in that detailed balance is broken at the microscopic scale [1]. A typical active system can be a collection of particles that continuously exert mechanical forces on their surrounding environment, and systems of interacting active particles can display novel phenomena, ranging from the emergence of collective motion in two dimensions (2D) [2–4] when the active particles are aligning, to motility-induced phase separation (MIPS) when the particles interact solely via volume exclusion interactions [5–9]. However, even though active matter breaks detailed balance in a fundamental way, it remains unclear whether the hydrodynamic, universal behavior of active matter necessarily differs from that of equilibrium systems. Indeed, the ordered phase of a generic incompressible polar active fluid in 2D, and in 3D with an easy-plane, belong to the universality classes of equilibrium smectics in 2D [10] and the equilibrium sliding columnar phase [11], respectively. The investigation of universal behavior, besides being of central interest to physics, allows us to transfer knowledge of a well-known system to a different system of novel interest. Here, we do exactly that by demonstrating that the critical behavior of MIPS belongs to the Ising universality class with conservative dynamics. We do so using three approaches: hydrodynamic argument, field-theoretic description of a microscopic model, and simulation of a lattice model.

Hydrodynamic argument.—The generic system we are interested in consists of a collection of self-propelled particles in a frictional medium (i.e., no momentum conservation) with volume exclusion interactions (e.g., see Fig. 1). As such it may be viewed as a typical compressible polar active fluid system [2–4,12] with the alignment interactions switched off. In other words, a system undergoing MIPS constitutes a subclass of an active fluid system that is described by the Toner-Tu equations in the hydrodynamic limit [3,4,13]. Another way to view this is that since the symmetries underlying MIPS systems are

the same as polar active fluids, the hydrodynamic equations, which are derived from symmetry consideration alone, must be the same. We therefore start with the Toner-Tu equations:

$$\partial_t \rho + \nabla \cdot \mathbf{g} = 0, \quad (1a)$$

$$\partial_t \mathbf{g} = -\zeta \nabla \rho - \kappa \mathbf{g} + \mu \nabla^2 \mathbf{g} + \mathbf{f}, \quad (1b)$$

where only terms linear in the mass density field ρ and the momentum density field \mathbf{g} , together with their lowest order of spatial derivatives, are shown above since these terms suffice for our discussion. In Eq. (1b), \mathbf{f} is a Gaussian noise with spatiotemporal statistics:

$$\langle \mathbf{f}(t, \mathbf{r}) \rangle = 0, \langle \mathbf{f}(t, \mathbf{r}) \mathbf{f}(t', \mathbf{r}') \rangle = 2D \delta(t - t') \delta(\mathbf{r} - \mathbf{r}'), \quad (2)$$

where D is the noise strength.

Without the alignment interactions, collective motion is impossible. As a result, the momentum field has to go to zero in the hydrodynamic limit, implying that the coefficient κ has to be always positive. Therefore, the field \mathbf{g} is *not* a soft mode, namely, the momentum field is slaved to

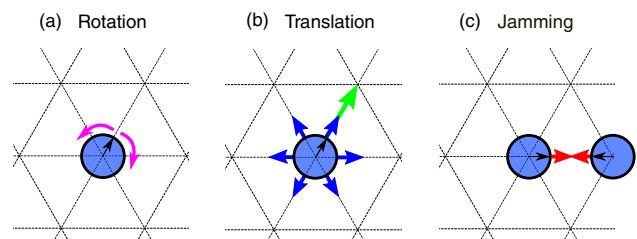


FIG. 1. Active Brownian particles on a planar hexagonal lattice in our simulation. Particle behavior is restricted to (a) rotational diffusion, (b) ballistic motion (green arrow), and translation diffusion (blue arrows), and (c) disallowed translation due to attempting to move to an occupied lattice site. This minimal model generically exhibits MIPS.

the density field. In the hydrodynamic limit, we can hence ignore the dynamical equation of \mathbf{g} and express \mathbf{g} as a function of ρ and its derivatives:

$$\mathbf{g} = -\nabla[(a_1\phi + a_2\phi^2 + a_3\phi^3) - (\nabla^2(b\phi)) + \text{h.o.t}] + \mathbf{f}, \quad (3)$$

where $\phi(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0$ for some constant ρ_0 , and h.o.t. in Eq. (3) refers to higher order terms in the expansion of \mathbf{g} in powers of ∇ and ϕ . Note that the negative sign in front of the square brackets is for reasons of stability, and the noise term \mathbf{f} is as defined in Eq. (2), albeit with the noise strength rescaled by κ^{-2} .

Substituting this form into Eq. (1a), we have

$$\partial_t\phi = \nabla^2 \frac{\delta H}{\delta \phi} + \text{h.o.t} + \nabla \cdot \mathbf{f}, \quad (4)$$

where $H = (a_1/2)\phi^2 + (a_2/3)\phi^3 + (a_3/4)\phi^4 + (b/2)(\nabla\phi)^2$ is the familiar Landau-Ginzburg Hamiltonian while h.o.t. in Eq. (4) again refers to higher order terms omitted, which include nonequilibrium terms such as $\nabla^4\phi^2$ [14] and $\nabla \cdot [\nabla\phi(\nabla^2\phi)]$ [15]. We note that although the resulting EOM is similar to the active model B introduced in Ref. [14], our approach is completely different—our EOM arises from premises based explicitly on symmetry consideration alone. Practically, our method inevitably leads to the presence of the $\nabla^2\phi^2$ term in the EOM due to the absence of Ising symmetry ($\phi \mapsto -\phi$). Such a term is absent in the active model B . We also note that there is an extensive literature on asymmetric fluid criticality [16–20] and the significance of the higher order odd terms which result from it. It is well established that the presence of such terms will not effect the universality class of the critical transition.

Now, the phenomenology of MIPS indicates that the system can be placed at the critical point by tuning two model parameters, e.g., by tuning the density and the noise strength (Fig. 2). Given this constraint, the only possibility to achieve criticality (i.e., having a divergent correlation length in the system) corresponds to tuning a_1 and a_2 to zero in H . Around this critical point, the standard renormalization group method demonstrates that all higher order terms in Eq. (4) are irrelevant [21,22]. In particular, the dynamical equation (4) is exactly the dynamics of the Ising model with conservative dynamics (model B) [23]. The scaling behavior of MIPS at criticality is thus characterized by three exponents: two static and one dynamic. Our hydrodynamic argument applies in *any* spatial dimension. To verify this conclusion, we will from now on focus on MIPS in 2D, and first look at a field-theoretic formulation of a specific lattice model in 2D to see how the system can be fine-tuned to exhibit critical behavior. We will then demonstrate with simulation results that critical exponents of MIPS show good agreement with our prediction (Fig. 3). We note that in an interesting development, independently

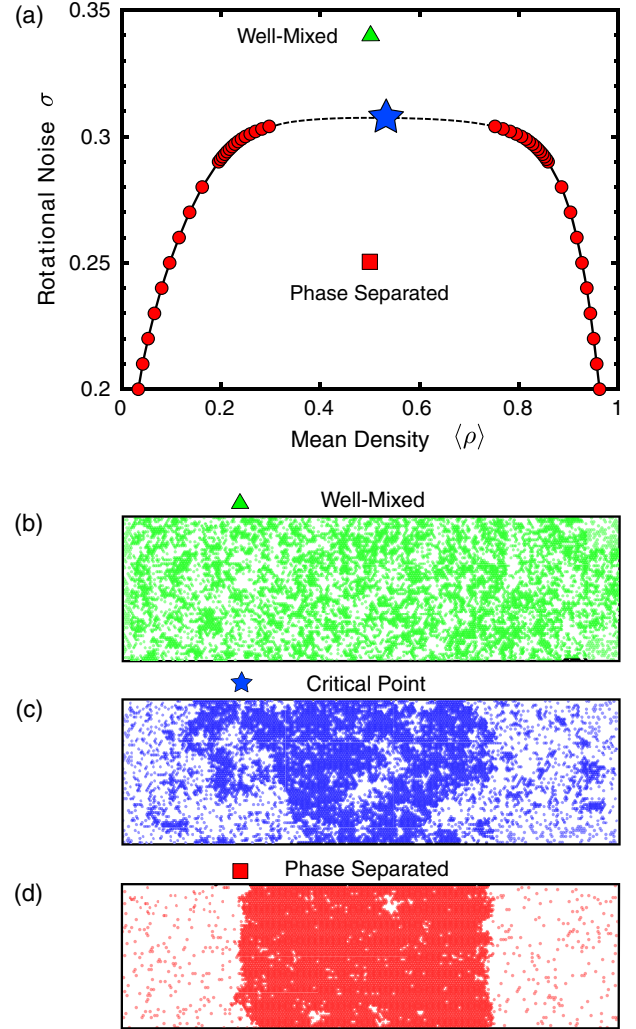


FIG. 2. Phase behavior. (a) The phase diagram resulting from Monte Carlo simulations of the lattice model (Fig. 1) shows the well-mixed region at high rotational noise (σ) and the phase separated region at low noise. Snapshots of the system configuration at the well-mixed region, critical point (estimated to be at $\rho_c \approx 0.522$, $\sigma \approx 0.305$ [25]), and phase separated region are shown in (b), (c), and (d), respectively. The system shown has 72×216 sites.

and concurrently to our work, it has also been concluded [24] that Ising behavior is generically possible. However, the authors also speculate that different, nonequilibrium strong coupling behavior is possible, based on generalizing the perturbative RG analysis beyond the controlled regime. We do not see evidence of such a regime in our simulation results.

Field-theoretic description of a microscopic model.— There have been several notable attempts [33–37]—especially useful in the study of the collective dynamics of bacteria [34,35]—to model clustering and phase separation in active systems on lattice. Here, we consider an active particle model on a 2D hexagonal lattice similar to the one recently introduced in Ref. [38], except here the

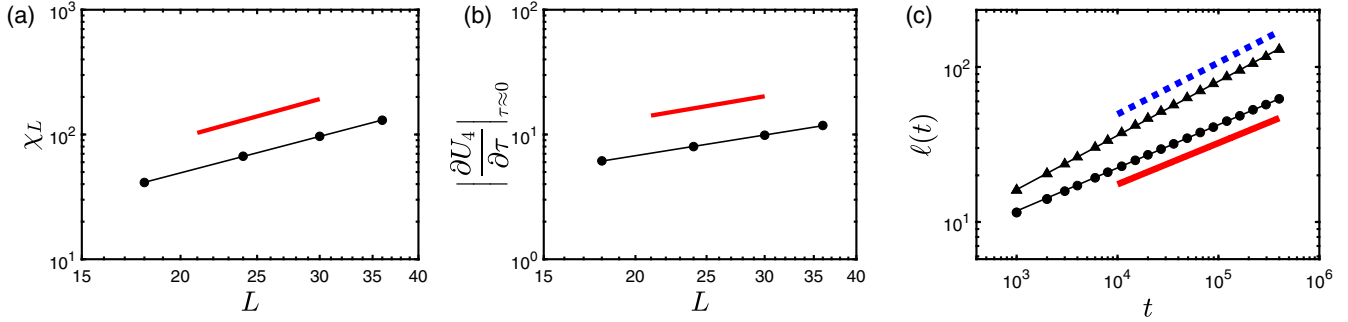


FIG. 3. Static and dynamic exponents estimation from our lattice model simulations. (a) Susceptibility χ_L at criticality as a function of system size L . (b) The Binder cumulant at criticality $(\partial_\tau U_4)_{\tau \approx 0}$, where τ is the dimensionless distance to the critical noise, as a function of L . (c) The average coarsening length scale $\ell(t)$ at criticality (circles) and deep within the phase-separated regime (triangles), as determined by the first intercept of the pair correlation function with the x axis, vs time t as measured by the number of particle sweeps. The red lines show the exact results from the 2D Ising model with conservative dynamics: (a) $\gamma/\nu = 7/4$, (b) $\nu = 1$, and (c) $z = 15/4$. While the dashed blue line in (c) shows the Lifshitz-Slyozov $z = 3$ scaling. In each plot error bars are smaller than the size of the data points. See Ref. [25] for details on simulation procedures and error estimation.

occupancy of the lattice site is bounded by a constant M . Specifically, we consider a collection of six distinct types of active particles, each type has a specific orientation θ_i and will only jump to the neighboring site along the direction θ_i , with a certain rate that depends on the occupancy of the target site. In addition, the type of a particle will convert, with rate σ , to a different type in the neighboring orientations, which corresponds to the rotational noise of the particle. Enumerating the lattice by the set of vectors \mathbf{R} , and the type (orientation) of the active particle by i , we now denote the number of particles of type i on the lattice site \mathbf{R} by $A_{\mathbf{R}}^{\theta_i}$.

Using the field-theoretic formalism developed in Ref. [39], the action that describes the model is

$$S = \int dt \sum_{\mathbf{R}} \left\{ \sum_i [\hat{A}_{\mathbf{R}}^{\theta_i} \partial_t A_{\mathbf{R}}^{\theta_i} \right. \quad (5a)$$

$$\left. - \gamma (M - N_{\mathbf{R} + \mathbf{e}_{\theta_i}}) A_{\mathbf{R}}^{\theta_i} (e^{\hat{A}_{\mathbf{R} + \mathbf{e}_{\theta_i}}^{\theta_i} - \hat{A}_{\mathbf{R}}^{\theta_i}} - 1) \right\} \quad (5b)$$

$$\left. - \sum_{\langle i, j \rangle} \sigma A_{\mathbf{R}}^{\theta_i} (e^{\hat{A}_{\mathbf{R}}^{\theta_j} - \hat{A}_{\mathbf{R}}^{\theta_i}} - 1) \right\}, \quad (5c)$$

where $\mathbf{e}_\theta \equiv d(\cos \theta \hat{\mathbf{x}} + \sin \theta \hat{\mathbf{y}})$ is a vector pointing along the direction θ with its norm being the lattice spacing d , $\hat{A}_{\mathbf{R}}^{\theta_i}$ are the conjugate fields of $A_{\mathbf{R}}^{\theta_i}$, and $N_{\mathbf{R}} = \sum_j A_{\mathbf{R}}^{\theta_j}$ is the total number of particles on site \mathbf{R} . Specifically, Eq. (5) corresponds to the jumping event with rate $\gamma(M - N_{\mathbf{R} + \mathbf{e}_{\theta_i}})$, which means that the rate of jumping into a lattice decreases with the occupancy of that target lattice and becomes zero if the lattice site has already M particles. This models the volume exclusion interactions between the particles. Equation (5c) corresponds to the interconversion between the particle types and $\langle i, j \rangle$ denotes the pairs of

orientations that are nearest neighbors to each other in angular space.

By first taking the discrete spacing of the lattice to zero ($d \rightarrow 0$), and then the angular space to the continuum limit, we argue in Ref. [25] that the action can be approximated as

$$S = \int dt d^2 r d\theta (\hat{\psi}_\theta [\partial_t \psi_\theta + \hat{\mathbf{e}}_\theta \cdot \nabla_{\mathbf{r}} [\gamma(\rho_M - \rho)\psi_\theta] - \sigma \partial_\theta^2 \psi_\theta] - \sigma \psi_\theta (\partial_\theta \hat{\psi}_\theta)^2), \quad (6)$$

where $\hat{\mathbf{e}}_\theta$ is now a normalized unit vector, $\psi_\theta(\mathbf{r}) \propto A_{\mathbf{R}}^\theta/d^2$ is the density of particles with orientation θ at $\mathbf{r} = \mathbf{R}$, $\hat{\psi}_\theta(\mathbf{r}) = \hat{A}_{\mathbf{R}}^\theta$, $\rho(\mathbf{r}) = (2\pi)^{-1} \int d\theta \psi_\theta(\mathbf{r})$ is the particle density at position \mathbf{r} , and $\rho_M \propto M/d^2$ is the maximal density allowed.

Since the action is now quadratic in $\hat{\psi}_\theta$, we can rewrite the dynamics of this field-theoretic model as a Langevin equation

$$\partial_t \psi_\theta + \hat{\mathbf{e}}_\theta \cdot \nabla_{\mathbf{r}} [\gamma(\rho_M - \rho)\psi_\theta] = \sigma \partial_\theta^2 \psi_\theta + \xi_\theta, \quad (7)$$

where ξ_θ are noise terms with statistics:

$$\begin{aligned} \langle \xi_\theta(\mathbf{r}, t) \rangle &= 0 \\ \langle \xi_\theta(\mathbf{r}, t) \xi_{\theta'}(\mathbf{r}', t') \rangle &= 2\sigma \partial_\theta^2 [\psi_\theta \delta(\theta - \theta') \delta(t - t') \delta^2(\mathbf{r} - \mathbf{r}')]. \end{aligned} \quad (8)$$

The set of EOM Eq. (7) constitutes an infinite number of field equations (one for each θ). To reduce these into the hydrodynamic equations of the form (1), we consider the Fourier expansion of ψ with respect to θ [40]:

$$\psi_\theta(\mathbf{r}) = \alpha_0(\mathbf{r}) + 2 \sum_{n \geq 1} [\alpha_n(\mathbf{r}) \cos(n\theta) + \beta_n(\mathbf{r}) \sin(n\theta)]. \quad (9)$$

In particular, $\alpha_0 = \rho$, $\alpha_n = \alpha_{-n}$, and $\beta_n = -\beta_{-n}$. In Ref. [25], we show that in the Fourier transformed space, all modes are massive except for ρ , which is consistent with our previous hydrodynamic argument. Here, we aim to demonstrate how the coefficients in the hydrodynamic equations can in principle be fine-tuned; we will thus simplify the EOM by setting β_n to zero for all n (hence spatial variation is only possible along the x axis), and α_n to zero for all $n > 1$. Note that this kind reduction has been shown to be useful in the study of polar active fluids at the onset of collective motion [40–43].

Going through this reduction procedure [25], we arrive at

$$\partial_t \rho + \frac{\pi\gamma}{2} \partial_x [(\rho_M - \rho)\alpha_1] = 0 \quad (10a)$$

$$\partial_t \alpha_1 + \frac{\pi\gamma}{2} \partial_x [(\rho_M - \rho)\rho] = -\sigma\alpha_1, \quad (10b)$$

where we have also ignored the fluctuating term in α_1 , which we will discuss later.

Solving for α_1 by setting the temporal derivative of α_1 to zero (since it is a fast mode), we have

$$\partial_t \rho + \partial_x \left\{ -\frac{\pi^2 \gamma^2}{4\sigma} (\rho_M - \rho) \partial_x [(\rho_M - \rho)\rho] \right\} = 0. \quad (11)$$

The expression inside the curly brackets corresponds to the x component of \mathbf{g} in Eq. (3). Note that at this level of truncation, the above model equation is similar to other models [15,44]. However, we will show in Ref. [25] how our field-theoretic model leads to other nonequilibrium terms [e.g., $\nabla^4 \phi^2$ and $\nabla \cdot [(\nabla \phi)(\nabla^2 \phi)]$ in Eq. (4)] when higher order modes are incorporated.

Expressing ρ as $\rho_0 + \phi$ for some constant ρ_0 in Eq. (11), we find

$$a_1 = \frac{\pi^2 \gamma^2}{4\sigma} (\rho_M - \rho_0)(\rho_M - 2\rho_0), \quad (12a)$$

$$a_2 = \frac{\pi^2 \gamma^2}{4\sigma} \frac{4\rho_0 - 3\rho_M}{2}. \quad (12b)$$

As aforementioned, the system exhibits Ising critical behavior when both a_1 and a_2 are zero. By tuning ρ_0 , we can either set a_1 to zero (when $\rho_0 = \rho_M/2$), or a_2 to zero (when $\rho_0 = 3\rho_M/4$), but seemingly not both. However, we have not yet incorporated the noise term into the analysis. Indeed, by analyzing the hydrodynamic equation (4) using diagrammatic methods around the critical point, one finds that fluctuation-induced renormalization of the coefficients generically increases a_1 while decreases a_2 [25]. In other words, the fluctuation strength can in principle be fine-tuned so that both a_1 and a_2 are zero. In particular, for this microscopic model, the critical density ρ_c is bounded below by $\rho_M/2$ and above by $3\rho_M/4$. We will see that this bound is

also satisfied by our simulated system [Fig. 2(a)], which we will turn to now.

Simulation of a lattice model.—Going beyond our analytical arguments, we will now present simulation results in support of our conclusion. We employ a similar microscopic model as in our field-theoretic formulation (with maximal occupancy $M = 1$), except that we allow the particles to diffuse, with a low probability, in addition to the active movement. Data analysis is adapted from Ref. [45]. Note that based on simulation results in continuum space for the static critical exponents, the authors in Ref. [45] arrived at a different conclusion from us. We speculate that the discrepancy arises because their results are not yet in the scaling regime, potentially due to the limited sizes used in the study. Here, by focusing on a lattice model, we can perform simulations on larger systems and achieve better statistics, enabling us to find good agreement between our analytical predictions and the simulation results for both the static exponents as well as the dynamic exponent (Fig. 3).

In our system, N polar particles move on an elongated hexagonal lattice of size $2L \times 6L$ lattice sites subject to periodic boundary conditions. The system evolves via an iterative Monte Carlo style update scheme in which particles are selected at random and we measure time t in particle sweeps. Specifically, at each time step two stochastic processes per particle are attempted: (i) to implement rotational fluctuations of a particle, a Gaussian random variable with standard deviation σ is drawn and rounded to the nearest integer n , the particle's direction is then rotated by $n \times 60^\circ$; (ii) to implement translation, the particle will attempt to move in a direction prescribed by its orientation with probability $24/30$ (active motion), and in a randomly chosen direction otherwise (diffusive motion). Steric interactions are implemented by disallowing any movement into an occupied site.

Using the sampling method described in Ref. [25] we construct the phase diagram shown in Fig. 2. We then use the Binder cumulant U_4 to locate the asymptotic critical noise strength.

Based on our previous analytical arguments, three independent critical exponents will characterize fully the universal behavior of critical MIPS. Focusing first on the static critical exponents, we use the standard finite-size scaling relations [46]: $\chi_L \sim L^{1/\nu}$ and $|\partial U_4 / \partial \tau| \sim L^{1/\nu}$, where τ is the dimensionless distance to the critical noise and χ_L is the finite-size sub-box susceptibility:

$$\chi_L = \frac{\langle N^2 \rangle_L - \langle N \rangle_L^2}{\langle N \rangle_L}. \quad (13)$$

In the above, $\langle \cdot \rangle_L$ denotes an average taken over a finite system size L . The results of this analysis are shown in Figs. 3(a) and 3(b), which show good agreement with the analytical results for the two-dimensional Ising universality class (red lines).

To estimate the dynamic exponent z for critical MIPS, we adapt a method presented in Ref. [47]: we seed 300 simulation runs from a completely disordered initial state and calculate the characteristic coarsening length $\ell(t)$ of the system for the first 400 000 particle sweeps. We define $\ell(t)$ as the length scale at which the correlation function first becomes negative. Again, we see a good agreement between the data and the Ising result [Fig. 3(c)]. To further ascertain the validity of our simulation method, we repeat this procedure deep within the phase separated regime, where due to the emergence of the Gibbs-Thomson relation at the interface [48,49], we expect that the coarsening dynamics of MIPS at the late stage follows the equilibrium Lifshitz-Slyozov scaling law ($z = 3$), which is indeed the case [Fig. 3(c)].

Conclusion.—We have demonstrated that the critical behavior of MIPS belongs generically to the equilibrium Ising universality class with conservative dynamics. Our hydrodynamic approach is based solely upon consideration of symmetry and conservation law. Therefore, our conclusion applies to all models consistent with these premises. In particular, since neither the mechanism of self-propulsion nor the particularity of the noise can effect the symmetry of the system, a broad class of dry active matter models displaying critical MIPS will belong to the Ising universality class. We also note that novel critical behavior in active matter is indeed possible [50] and it remains an interesting question to see what universality classes unique to active matter await discovery.

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