Jamming at the laning-flocking transition in systems of self-propelled rods

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Non-equilibrium active matter made up of self-driven particles exhibits collective motion and nonequilibrium order-disorder transitions. Self-propelled rod models with short-range repulsive interactions are a useful minimal system to study active matter. We simulated high-aspect-ratio self-propelled rods with varying packing fraction and driving. Two characteristic phases, the flocking and laning phases, occupy much of the phase diagram. We study the laning-flocking transition and the emergence of the laning state from the equilibrium nematic. For low packing fraction, driving induces formation of a clustered flocking phase, as observed previously. In flocks the average pressure is high and structural and mechanical relaxation times are long. These results suggest that rods in flocks are in a translating jammed state with an internal structure similar to a jammed solid despite overall flock motion. For higher packing fraction, a laning state emerges in response to driving, with polar domains that vary in size with the driving force. The average pressure is relatively low and structural and mechanical relaxation times are short, showing fluid-like behavior. Both structural and mechanical properties vary rapidly upon lowering the packing fraction from the laning to flocking regime, suggesting an abrupt dynamic phase transition occurs in this system. We propose that the laning-flocking transition is a type of jamming transition which, in contrast to other jamming systems, occurs as density is decreased. In contrast, the laning state appears to emerge continuously from the equilibrium nematic as driving is increased.

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Active matter is made up of self-driven particles and raises questions outside our understanding of equilibrium materials. Understanding active matter may aid the development of new technologies including autonomous motile and self-healing synthetic materials. Active matter is diverse in length scale and composition; examples include animal flocks \cite{1}, crawling cells and swimming bacteria \cite{2}, vibrated granular materials \cite{3,4}, self-propelled colloidal particles \cite{5,6}, and the cellular cytoskeleton and cytoskeletal extracts \cite{7}. Novel physical properties exhibited by active matter include collective motion, nonequilibrium order-disorder transitions, and anomalous fluctuations and mechanical properties \cite{8}.

Self-propelled rods (SPR) provide a useful minimal model to interrogate behavior of active matter. In these typically 2D models self-propulsion and excluded volume interactions via a short-range repulsive potential are the only ingredients; rod alignment occurs through collisions. Experiments which may be approximated as SPR include animal flocks \cite{1}, crawling cells and swimming bacteria \cite{2}, vibrated granular materials \cite{3,4}, self-propelled colloidal particles \cite{5,6}, and the cellular cytoskeleton and cytoskeletal extracts \cite{7}. Novel physical properties exhibited by active matter include collective motion, nonequilibrium order-disorder transitions, and anomalous fluctuations and mechanical properties \cite{8}.

For SPR and for active matter in general, we have only a limited ability to predict the dynamic phase diagram and the nature of dynamic phase transitions. While the transition to collective motion \cite{4,21,26} and the emergence of clusters \cite{10,14,15,18,19,20,27} in aligning self-propelled particle systems have been extensively studied, other dynamic phases and transitions have seen less work.

Further understanding the dynamic phases and transitions of SPR as well as the relationship between dynamic and equilibrium phases is needed to improve our understanding of active matter.

Previous work on SPR has made clear that rod shape, density, and driving are important in determining the dynamic behavior \cite{12,14,20}. For low driving, equilibrium-like isotropic and nematic liquid crystal phases are recovered \cite{19,20}. For higher driving, dynamic states characterized by the appearance of flocks, stripes, and swirls appear \cite{12,14,17,20}. Baskaran and Marchetti derived a hydrodynamic model from the kinetics of SPR with two-rod collisions and determined a phase diagram from linear stability analysis of homogeneous states. They found that no global polar state is possible and that activity lowers the isotropic-nematic transition density \cite{20}. In simulation work, Wensink and Löwen varied rod aspect ratio and packing fraction in the high-activity limit (thermal fluctuations were neglected) \cite{17}. They observed a laning phase for high density and aspect ratio similar to the one characterized here. Both McCandlish et al. \cite{18} and Abkenar et al. \cite{19} studied SPR over a wide range of packing fraction and driving, and observed a similar set of dynamic phases to those we present but did not focus on dynamic phase transitions. As described below, our work differs from previous papers in our detailed structural and mechanical characterization of the laning-flocking transition and the emergence of the laning state from the equilibrium nematic.

We simulated high-aspect-ratio SPR in 2D with short range repulsive interactions, and characterized the dy-
where the random displacements $\delta r_i(\tau)$ and $\delta u_i(\tau)$ are Gaussian-distributed, $\mathbf{\Gamma}_i^{-1}(t)$ is the inverse friction tensor, $\gamma_r$ is the rotational drag coefficient, and $\mathbf{T}_i(t)$ and $\mathbf{F}_i(t)$ are the deterministic force and torque on particle $i$. Excluded-volume interactions between particles are modeled by the WCA potential as a function of the minimum distance $s_{ij}$ between the two finite line segments of length $L$ that define the axes of particles $i$ and $j$. The self-propulsion force is directed along the particle axis with $\mathbf{F}_{\text{drive}} = F_D \mathbf{u}_i$. In the absence of nonequilibrium driving, this model has been well-characterized both in 2D and 3D.

We nondimensionalize using the length $\sigma$, energy $k_B T$, and time $\tau = D/\sigma^2$, where $D$ is the diffusion coefficient of a sphere of diameter $\sigma$. The three dimensionless control parameters are the rod aspect ratio $R = L/\sigma$, fixed at 40 for this study, the packing fraction $\phi = N_{\text{rods}}/N_{\text{system}}$ (the ratio of the total area of rods to the system area), and the Peclet number $\text{Pe} = F_D L/(k_B T)$. We varied $\phi$ between 0.01 and 0.6, and Pe between 0 and 320. We simulated $N = 4000$ rods in a square, periodic box. Most simulations were initialized in an equilibrium isotropic or nematic initial condition, then nonequilibrium activity was turned on and the system was allowed to equilibrate for $10^7 \tau$. The simulation measurement run was $10^7 \tau$, and the time step $\Delta t = 0.25 \tau$.

At zero or low driving, we observe an equilibrium isotropic phase for low packing fraction (fig. 1). As the Peclet number is increased, lower packing fractions roughly corresponding to the equilibrium isotropic phase typically show flocking behavior characterized by collective motion of dense clusters interacting with a low-density vapor (fig. 1), as observed previously. While the flocking phase remains globally isotropic (consistent with previous predictions), the formation of clusters in the flocking phase is characterized by short-range density correlations that lead to peaks in the pair distribution function and the emergence of polar and nematic orientational correlations that persist over a cluster-size length scale due to alignment of rods within clusters (fig. 1 inset, and other data not shown). Rod mean-squared displacements are ballistic at short times, turning over to diffusive at long times due to flock reorientation. The long-time angular mean-squared displacement is diffusive.

At higher packing fraction and zero or low Peclet number, we observe an equilibrium nematic phase. While we did not map the equilibrium phase transition in detail, the IN transition we observe is consistent with previous work. As the Peclet number is increased, higher packing fractions typically show laning behavior characterized by the formation of polar lanes of upward- and downward-moving particles (fig. 1). Unlike the flocking phase, in the laning phase the density is approximately constant. The laning phase appears to be globally nematic in most cases with polar correlations on the scale of the system size in the alignment direction and on the scale of a typical lane width perpendicular to the alignment direction (fig. 1 inset and data not shown). Rod mean-squared displacements are ballistic in the alignment direction and diffusive perpendicular, while the angular mean-squared displacement is bounded due to the maximum angular deviation of rods.

![FIG. 1. Snapshots and phase diagram of self-propelled rods of aspect ratio 40. In (a–b), rods are colored by orientation as shown in the colorwheel and the red line denotes the border of the 2D periodic simulation box. (a) Snapshot of the flocking phase, with zoomed view of the front edge of a flock at inset. (b) Snapshot of the laning phase, with zoomed view of the boundary between two lanes at inset. (c) Dynamic phase diagram as a function of Peclet number and packing fraction, where yellow denotes the isotropic phase, green the flocking phase, and blue the nematic-laning phase. Points indicate parameter sets for which simulations were run.](image-url)
flocking phases, we performed expansion and compression runs in which the packing fraction was changed by Δφ = 0.02, the simulation was run for 10^7τ to reach a dynamic steady state, and then measurements were performed over an additional 10^7τ. During expansion runs, the isotropic system pressure \( P_s \) shows an abrupt jump in pressure by a factor of 2–10 at the transition from laning to flocking under expansion (fig. 2a).

The appearance of the laning phase is dependent on initial conditions; lanes with equal numbers of up- and down-moving rods result from initialization with an equilibrium nematic state and the high rod packing fraction which prevents rod reorientation between up and down. Compression simulations which started in the laning phase and increased density in steps of Δφ = 0.02 showed no transition back to the laning phase for a range of packing fractions (in fig. 2c, the red Pe=160 curve is one example). This strong hysteresis is another signature of an abrupt dynamic transition between the laning and flocking states.

McCandlish et al. found the laning state to be unstable to break up [13]. We did not observe this instability above the laning-flocking transition boundary. While we cannot rule out the possibility that our apparent laning phase is a long-lived metastable state, our expansion simulations effectively extended our simulation times up to 2 × 10^8τ in the laning state, and upon reaching the transition boundary we typically see break up of the lanes into flocks within the 10^7τ equilibration run. Therefore in our system the laning phase appears stable, consistent with other work [12, 17, 19].

To characterize structural relaxation we measured the normalized structure-factor autocorrelation function \( C(t)/C(0) \), where \( C(t) = ⟨δS(k, t)δS(k, 0)⟩ \). k is the magnitude of the wavevector and \( δS(k, t) = S(k, t) − ⟨S(k, t)⟩ \) is the fluctuation in the the angle-averaged structure factor \( S(k, t) = \frac{1}{2πN} \int_0^{2π} dϕ ρ(k, t)ρ(−k, t) \) [29]. Because the angle-averaged structure factor is rotationally invariant, its autocorrelation probes internal structural relaxation of flocks and lanes but is insensitive to flock reorientation. We determined the location of the peak nearest to wave number \( k = 2π/σ \), corresponding to side-by-side filaments separated by approximately one diameter. In the laning phase (φ = 0.4, light blue curve in fig. 2b), the structure-factor autocorrelation rapidly relaxes to zero. In the flocking phase (φ = 0.1 – 0.3), the structure-factor autocorrelation exhibits a nonzero plateau value after the initial relaxation, indicating slow structural relaxation at this wave number. For lower densities in the flocking phase, corresponding to smaller flocks, this plateau is more prominent. This occurs because larger packing fraction in the flocking phase is associated with larger flocks and eventually one giant flock, for which the angle-averaged structure factor is typically closer to its mean value and so the fluctuations are less prominent.

Similar behavior occurs for mechanical relaxation, measured by the autocorrelation function of the off-diagonal stress tensor \( ⟨Π_{xy}(t)Π_{xy}(0)⟩ \) [29]. In the laning phase (φ = 0.4, light blue curve in fig. 2c), the stress autocorrelation drops to zero around t = 1. In the flocking phase (φ = 0.1 – 0.3), the stress autocorrelation function relaxes to a long-lived plateau. Consistent with this, the effective shear viscosity measured via the Green-Kubo relation \( η_{eff} = \frac{3}{k_BT} \int_0^∞ ⟨Π_{xy}(t)Π_{xy}(0)⟩ dt \) shows a factor of 10^3 increase upon transition from the laning to the flocking phase for Pe=80 (fig. 2d).

Based on the large increase in pressure and shear viscosity and slowed structural and mechanical relaxation that occurs at the transition from laning to flocking, we propose that this is a type of jamming transition in which flocks, although collectively moving, have an internally jammed, solid-like structure. Related observations were made in an experimental system with self-propelled colloids, for which nonequilibrium driving promoted formation of small, dense, mobile crystalline clusters [6]. Jamming in self-propelled systems has also been observed in systems of self-propelled disks or spheres, where increasing the density of particles leads to the formation of static jammed clusters. Phase separation between a low-density gas and high-density jammed clusters or crystals...
FIG. 3. The onset of laning behavior from the nematic phase for a simulation with $\phi = 0.5$. (a) Snapshots with Peclet number 0, 4, 8, 12, and 28. (b) Global polar order parameter $P$ versus Peclet number. (c) Average number of rods per lane. (d) Average lane width versus Peclet number. (e) Average lane height versus Peclet number.

has been observed both in experiments [6] [33] and theory and simulations [34]. In contrast to both recent active jamming work and classic granular jamming [35], in our SPR system the increased importance of aligning interactions at higher packing fraction means that the fluid laning state occurs at high density, and the transition to the translating jammed flocking state occurs as density is lowered. This appears to be a novel feature of this transition in systems of self-propelled rods.

The flocking-laning transition occurs as density is lowered and rods are able to reorient. In the laning phase the approximately constant rod number density is $n = \phi/(L\sigma)$ and typical spacing between rod centers of mass is $d \sim \sqrt{L\sigma/\phi}$. Rods are able to reorient when this spacing is of order $L$, giving a critical packing fraction $\phi_c \sim \sigma/L$. This is the Onsager criterion for the IN transition, suggesting that near equilibrium the flocking-laning transition should occur at a similar $\phi$ as the IN transition, as we observe. The flocking-laning boundary shifts toward higher packing fraction as the Peclet number is increased because the nonequilibrium driving allows higher local density that can open up space between rods, allowing rod reorientation that starts the process of flock formation.

While the emergence of flocks from the isotropic phase as Peclet number is increased has been studied [10] [14] [15] [18] [19] [20] [27], the nature of the laning phase of SPR and its connection to the equilibrium nematic has not to our knowledge been examined previously. The emergence of lanes in SPR has been observed in previous simulation studies [12] [17] [19], and laning has been studied previously for spherical particles both in experiments [30] and theory/simulation [37] [35]. Laning occurs because of the differences in collisions experienced by rods as a function of their polar environment: a rod moving surrounded by opposite polarity rods will experience more collisions, and therefore more momentum transfer, than when surrounded by rods of similar polarity. A rod surrounded by others of similar polarity will therefore experience reduced lateral movement and be less likely to leave the polar lane [15] [37].

To characterize the emergence of lanes from the equilibrium nematic, we performed simulation runs in which the Peclet number was increased in steps of $\Delta P_e = 2$, the simulation was run for $10^7\tau$ at the new driving to reach a dynamic steady state, and then measurements were performed over an additional $10^7\tau$. Simulation snapshots show a gradual increase with Peclet number in both the parallel and lateral extent of lanes (fig. 3a). To characterize lane formation, we measured a local polar order parameter $p_i$ of rod $i$:

$$p_i = \frac{\sum_{j \neq i} \mathbf{u}_i \cdot \mathbf{u}_j e^{-s_{ij}^2}}{\sum_{j \neq i} e^{-s_{ij}^2}}. \quad (3)$$

The global polar order parameter $P = \langle p_i \rangle$ approaches 1 when lanes are well developed because a typical particle is surrounded by neighbors of the same polarity. The variation of $P$ with Peclet number is shown in fig. 3b. We then identified lanes, defined as contiguous domains of rods with a polar order parameter that exceeds $p_i = 0.9$, and determined the average number of rods per lane, lane width, and lane height (limited by the size of the periodic box) [29] (fig. 3c–e). Our results suggest that the emergence of lanes from the equilibrium nematic is gradual, to the best of our ability to measure it in a finite
system.

The global symmetry of the laning phase as a function of parameters is not clear. In some regimes we observe an apparent stable finite lane width, i.e., global nematic symmetry, while for some parameters it appears that the system approaches just two lanes, an apparent polar demixed state that may reflect global polar symmetry. Further study with larger systems may be necessary to distinguish these cases.

To our knowledge the laning phase has not been predicted from hydrodynamic models of SPR. Baskaran and Marchetti find that no global polar state is possible [20]. However, they find that activity increases the length scale over which polarization fluctuations decay, which perhaps is related to the appearance of lanes in a globally nematic state. In addition, Baskaran and Marchetti as well as others [13] find that activity tends to lower the isotropic-nematic transition density, while we find an increase in the transition density if we assume that the laning phase we observe corresponds to Baskaran and Marchetti’s active nematic. If the hydrodynamic equations are modified to permit a bulk polar state [22] and studied numerically including nonlinear terms, then a stripe phase is predicted but which has the direction of motion perpendicular to the stripe axis [21] [23] [24], unlike our lanes.

Abkenar et al. used a closely related simulation model of SPR, but with the added feature of a penetrable potential that allows rods to cross in 2D [19]. While the overall observations of dynamic phases are similar to ours, their phase diagram shows some differences, including a non-monotonic phase boundary between flocking and laning as a function of Peclet number, and the emergence of large clusters at low driving. In future work it will be of interest to understand which features of the SPR dynamic phase diagram are universal and which reflect specific model choices.

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