

Emergent flocking in mixtures of antialigning self-propelled particlesRüdiger Kürsten 

*Departament de Física de la Matèria Condensada, [Universitat de Barcelona](#), Martí i Franquès 1, 08028 Barcelona, Spain;
[Universitat de Barcelona](#) Institute of Complex Systems (UBICS), 08028 Barcelona, Spain;
 and Institut für Physik, [Universität Greifswald](#), Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany*

Jakob Mihatsch  and Thomas Ihle 

Institut für Physik, [Universität Greifswald](#), Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany



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We observe a flocking mechanism, the emergence of a state with global polar order, in mixed systems of self-propelled particles with purely antialigning interactions, i.e., the ground state for any pair of particles is to be oppositely oriented. In binary mixtures, we find that flocking can be realized by cross-species antialigning that is dominant compared to intraspecies antialignment. While the key mechanism can be understood within a mean-field description, beyond mean-field we develop an asymptotically exact Boltzmann-scattering theory from first principles. This theory yields analytical predictions for the flocking transition and shows excellent quantitative agreement with simulations of dilute systems. For large systems, we find either microphase separation or static patterns with patches or stripes that carry different polarization orientations.

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Active matter is characterized by an interplay of directed motion due to the consumption of free energy and dissipation, see, e.g., [1–9] for reviews. Active systems arise naturally or engineered across scales from microtubuli up to humans or robots. Emergent phenomena in active systems are not subject to the laws of equilibrium statistical mechanics due to the constant driving. Nevertheless, collective phenomena and nonequilibrium phase transitions can be observed. One of the typical transitions of large collections of self-propelled particles is the so-called flocking transition. It was first studied in the famous Vicsek model of aligning self-propelled particles [10,11], where the dynamics of the self-propelled particles is formally given by a certain set of rules. Similar models based on Langevin-equations have been studied later, see e.g., [12–17]. Flocking in such models is usually caused by microscopic alignment interactions. However, recently it has been shown that flocking can also appear in non-Markovian models [18] or underdamped dynamics with repulsive interactions [19] without the presence of explicit alignment interactions. The origin of aligning interactions might be social in case of animals, a combination of electromagnetic and hydrodynamic in case of Quincke-rollers [15], or purely hydrodynamic for some type of micro-swimmers.

For model systems of microswimmers, it has been shown that hydrodynamic interactions can lead to both, aligning and antialigning interactions, depending on the properties of the swimmers as well as on the collision parameters, see, e.g., [20–22]. For strong pushers, restricted to two

dimensions, but subject to three-dimensional hydrodynamical interactions, it has been shown that interactions are mainly antialigning [22]. References [23,24] considered long range antialigning hydrodynamic interactions together with direct short range particle-particle interactions that, in combination with self-propulsion, can lead to alignment interactions. Here, we consider a dilute solution of pushers, where direct particle-particle interactions are negligible and only binary hydrodynamic antialignment interactions are relevant.

Due to the mesoscopic to macroscopic size of self-propelled particles they are not perfectly identical but certain properties of the dynamics differ across the population. An important class of nonuniform collections of active particles are binary mixtures of two species of particles with different properties that can be found, e.g., in mixed bacterial swarms [25,26]. For aligning self-propelled particles, binary mixtures have been studied, e.g., in [27–31], where particles of the same species always align. Between particles of different species, also antialignment has been considered.

In this Letter, we study binary mixtures of purely antialigning "dry" [32] self-propelled particles by means of kinetic theory and agent-based simulations. Surprisingly, we find that there is a flocking transition toward a globally polarized state despite the microscopic interactions favoring antialignment. We show that the flocking state can be qualitatively understood in mean field theory. Mean field theories are the standard approach in the study of flocking, see, e.g., [12,33–39], even though predictions of these theories for homogeneous states never depend on the self-propulsion speed which is the key feature that makes the model active at all.

Here, however, we go beyond mean field. Adopting a recently developed scattering theory [40,41] based on one-sided molecular chaos, we are able to achieve an analytical description. Remarkably, the correct analytical dependence of the

flocking transition on the self-propulsion speed is predicted by this asymptotically exact theory. For very large system sizes, various spatially structured states arise within the flocking state, that are analyzed by means of linear stability analysis of the homogeneous flocking states.

Model. We consider two species (A particles and B particles) of self-propelled point particles in two dimensions subject to periodic boundary conditions. The particle positions are denoted by $\mathbf{r}_i = (x_i, y_i)$ and the directions of self-propulsion are described by angles $\phi_i \in [-\pi, \pi]$. We denote the number of A particles, the number of B particles, and the total number of particles by N_A, N_B , and N , respectively. The indices of A and B particles are $\{1, \dots, N_A\}$ and $\{N_A + 1, \dots, N\}$, respectively. The time evolution is following the Langevin dynamics

$$\begin{aligned} \dot{x}_i &= v \cos \phi_i, \quad \dot{y}_i = v \sin \phi_i, \\ \dot{\phi}_i &= \sum_{j \in \Omega_i} \Gamma_{ij} \sin(\phi_j - \phi_i) + \sigma \xi_i, \end{aligned} \quad (1)$$

where $\Omega_i = \{k : |\mathbf{r}_i - \mathbf{r}_k| < R\}$ denotes the set of indices of neighbors of particle i , that is, the indices of all particles that are closer to particle i than distance R . The angular dynamics is subject to independent Gaussian white noise terms ξ_i with noise strength $\sigma \geq 0$. The coupling matrix Γ_{ij} is symmetric and consists only of three different entries: Γ_A if both particles, i and j are from species A, Γ_{AB} if exactly one of i and j is from species A and the other one is from species B and Γ_B if both; i and j are from species B. In this letter, we consider only antialigning couplings $\Gamma_A, \Gamma_B, \Gamma_{AB} \leq 0$.

Mean field theory. The Langevin dynamics (1) is equivalent to the Fokker-Planck equation

$$\begin{aligned} \partial_t P &= -v \sum_{i=1}^N \cos \phi_i \partial_{x_i} P - v \sum_{i=1}^N \sin \phi_i \partial_{y_i} P \\ &\quad - \sum_{i=1}^N \partial_{\phi_i} \sum_{j \in \Omega_i} \Gamma_{ij} \sin(\phi_j - \phi_i) P + \sum_{i=1}^N \frac{\sigma^2}{2} \partial_{\phi_i}^2 P, \end{aligned} \quad (2)$$

where P denotes the probability density of the full system that depends on all spatial and angular coordinates $\{\mathbf{r}_i, \phi_i\}$ (arguments omitted for short notation). For further simplifications, we assume that the N -particle probability density factorizes into a product of N_A identical and independent one-particle probabilities of A particles and N_B identical and independent one-particle probabilities of B particles $P = P_A(\mathbf{r}_1, \phi_1) \cdots P_A(\mathbf{r}_{N_A}, \phi_{N_A}) \cdot P_B(\mathbf{r}_{N_A+1}, \phi_{N_A+1}) \cdots P_B(\mathbf{r}_N, \phi_N)$. Furthermore, we assume that the particles are distributed homogeneously, that is $P_{A/B}(\mathbf{r}, \phi) = \frac{1}{\mathcal{A}} P_{A/B}(\phi)$, where $\mathcal{A}$ is the area of the domain the particles move in. For simplicity, we consider only solutions that satisfy the symmetry $\phi \leftrightarrow -\phi$.

Plugging the above assumptions into Eq. (2), integrating over all degrees of freedom but ϕ_1/ϕ_{N_A+1} and renaming ϕ_1/ϕ_{N_A+1} into ϕ , we obtain

$$\begin{aligned} \partial_t P_{A/B}(\phi) &= \Gamma_{A/B} M_{A/B} \langle \cos \rangle_{A/B} \partial_\phi \sin \phi P_{A/B}(\phi) \\ &\quad + \Gamma_{AB} M_{B/A} \langle \cos \rangle_{B/A} \partial_\phi \sin \phi P_{A/B}(\phi) \\ &\quad + \frac{\sigma^2}{2} \partial_\phi^2 P_{A/B}(\phi), \end{aligned} \quad (3)$$

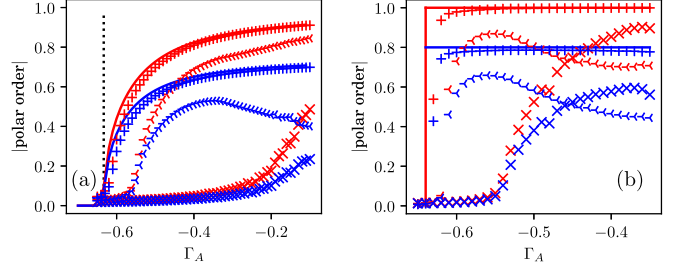


FIG. 1. Absolute value of polar order parameter of A (red) and B particles (blue) for high densities and small system size ($N_A = N_B = 2400$) with (a) and without noise (b). A and B particles are polarized in opposite directions. Agent-based simulations (symbols) are compared to mean field theory (solid line) [solution of Eq. (S4) of [42], Eq. (5)]. The dashed vertical black line in (a) displays the mean field onset of flocking according to Eq. (4). Parameters are (a) $M_{A/B} = N_{A/B} \pi R^2 / L^2 = 5$, $R = \sigma = 1$, $\Gamma_B = \Gamma_{AB} = -1$. (b) $M_{A/B} = N_{A/B} \pi R^2 / L^2 = 20$, $R = 1$, $\sigma = 0$, $\Gamma_B = -1$, $\Gamma_{AB} = -0.8$. $v = 1$ (cross markers), $v = 10$ (y-shaped markers), $v = 100$ (plus markers). Simulations have been performed by AAPPP simulation package [43]. See [42] for numerical details.

where $M_{A/B} := \pi R^2 N_{A/B} / \mathcal{A}$ is the expected number of neighboring A or B particles and for any function f , $\langle f \rangle_{A/B} := \int_0^{2\pi} f(\alpha) p_{A/B}(\alpha) d\alpha$ is the expectation value of that function with respect to $p_{A/B}$.

Following the standard approach for this type of nonlinear Fokker-Planck equations, we explicitly find the von Mises distribution as the exact steady state solution. Depending on parameters, the steady state is either disordered or polarly ordered. The transition toward polar order occurs at [42]

$$\frac{1}{4} M_A M_B (\Gamma_A \Gamma_B - \Gamma_{AB}^2) - \frac{\sigma^2}{4} (\Gamma_A M_A + \Gamma_B M_B) + \frac{\sigma^4}{4} = 0. \quad (4)$$

Note that this transition condition was obtained in [27] (considering positive A-A and B-B couplings) from the dynamics of the zeroth and first angular Fourier modes only, without actually solving for the steady state distribution. Obviously, there is no solution to (4) for identical particles $\Gamma_A = \Gamma_B = \Gamma_{AB} < 0$. For the binary mixture, however, we find that there is a transition toward polar order even in the case of pure antialigning interactions, $\Gamma_{A/B}, \Gamma_{AB} < 0$. For nonzero noise, the transition phenomenology is continuous within mean field theory, see Fig. 1(a).

Zero noise limit. Remarkably, for zero noise, the transition condition (4) depends only on the ratio $\Gamma_{AB}^2 / (\Gamma_A \Gamma_B)$. That means it is independent on the densities $M_{A/B}$. The zero noise limit allows to solve for the polar order parameters within the ordered phase exactly, leading to

$$|\langle \cos \rangle_{A/B}| = \min \left(1, \frac{\Gamma_{AB} M_{B/A}}{\Gamma_{A/B} M_{A/B}} \right). \quad (5)$$

Thus, within the ordered state, there is always at least one species that is perfectly aligned while the other species is von Mises distributed with width given by (5). That implies in particular that mean-field theory predicts the transition phenomenology to be discontinuous in the case of zero noise.

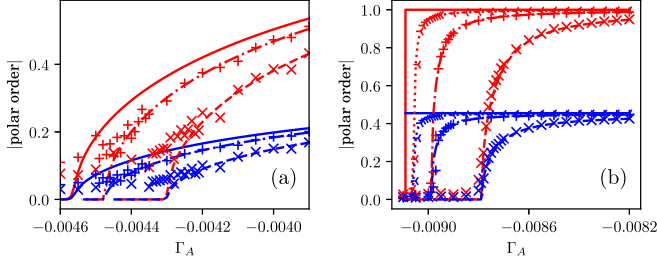


FIG. 2. Polar order parameter of A (red) and B particles (blue). Agent-based simulations (symbols) are compared to mean field theory (solid line) [solution of Eq. (S4) of [42], Eq. (5)] and one-sided molecular chaos based scattering theory [Eq. (7)] for $v = 1$ (dashed line), $v = 3$ (dash-dotted line), and $v = 10$ (dotted line). (a) $\sigma = 0.01$, (b) $\sigma = 0$. Parameters: $M_A = N_A \pi R^2 / L^2 = 0.03$, $M_B = N_B \pi R^2 / L^2 = 0.06$, $\Gamma_B = -0.011$, $\Gamma_{AB} = -0.01$, $v = 1$ ($\times$), $v = 3$ ($+$), $v = 10$ [y-shaped marker, only in (b)]. System size in simulations is given by $N_A = 1600$. See [42] for numerical details.

As shown in Figs. 1(b) and 2(b) this is in contradiction with agent-based simulations in small systems and the scattering theory to be developed below.

Beyond mean field: one-sided molecular chaos. Within mean field theory, we assume that all particles are statistically independent at all times. Due to the interactions this is obviously not strictly true. However, the concept of molecular chaos gives an argument that correlations are vanishing fast due to collisions with many different particles. Nevertheless, correlations can not be neglected on a quantitative level, cf., e.g., [44,45].

In order to incorporate the most relevant correlations in our theory, we apply the concept of one-sided molecular chaos [46]. The idea is that two particles are assumed to be completely independent before they collide because they have most likely collided with many different particles before and lost almost all memory of a potential previous collision. The collision between two particles, however, lasts a finite period of time. During this collision time, particles clearly build up correlations that can not be neglected on a quantitative level. Following [40,41], we take these collision correlations rigorously into account. Here, we focus on dilute systems such that collisions between more than two particles at the same time can be neglected. Furthermore, we assume that $v/R \gg \sigma^2$ such that the impact of noise on the particle trajectory during the short collision time is negligible. In particular, using Eq. (1) the microscopic evolution of two particles can be analytically backtraced in time from the end of their collision to the start of the encounter where the factorization of the two-body probability is admissible. In that way the collision dynamics is a two-body problem that is analytically manageable. Using these ingredients, we derive a Boltzmann-like scattering theory from first principles in complete analogy to [40,41] where the corresponding theory was derived for a single-species system using an asymptotically exact solution of the second member of the BBGKY hierarchy. As a result we obtain a Boltzmann-equation similar to (3). Note, that in contrast to previous kinetic approaches [33,36], our active Boltzmann equation was explicitly derived from the N -particle Fokker-Planck equation using an exact

representation of correlated two-particle collisions during binary encounters. To proceed, we Fourier transform the angular degrees of freedom according to

$$p_{A/B}(\phi) = \sum_k \hat{p}_k^{A/B} \exp(ik\phi), \quad (6)$$

yielding

$$\begin{aligned} \partial_t \hat{p}_m^{A/B} = & M_{A/B} \Gamma_{A/B} \left[\pi m (\hat{p}_{m-1}^{A/B} \hat{p}_1^{A/B} - \hat{p}_{m+1}^{A/B} \hat{p}_{-1}^{A/B}) \right. \\ & \left. + \Gamma_{A/B} \frac{R}{\pi v} \sum_n \hat{p}_{m-n}^{A/B} \hat{p}_n^{A/B} g_{mn} \right] \\ & + M_{B/A} \Gamma_{AB} \left[\pi m (\hat{p}_{m-1}^{A/B} \hat{p}_1^{B/A} - \hat{p}_{m+1}^{A/B} \hat{p}_{-1}^{B/A}) \right. \\ & \left. + \Gamma_{AB} \frac{R}{\pi v} \sum_n \hat{p}_{m-n}^{A/B} \hat{p}_n^{B/A} g_{mn} \right] - m^2 \frac{\sigma^2}{2} \hat{p}_m^{A/B}, \quad (7) \end{aligned}$$

where

$$g_{mn} = \frac{8}{3} m \left(\frac{\frac{3}{2}m - n}{n^2 - \frac{9}{4}} + \frac{\frac{1}{2}m + n}{n^2 - \frac{1}{4}} \right). \quad (8)$$

The terms that come with the mode-coupling matrix g_{mn} are nontrivial corrections compared to mean field.

A linear stability analysis of the disordered state (considering only the leading order modes $\hat{p}_{\pm 1}^{A/B}$ close to the onset of flocking) yields the transition condition

$$\begin{aligned} 0 = & \left(\Gamma_A - \frac{128}{45\pi^2} \Gamma_A^2 \frac{R}{v} - \frac{64}{9\pi^2} \Gamma_{AB}^2 \frac{M_B R}{M_A v} - \frac{\sigma^2}{M_A} \right) \\ & \times \left(\Gamma_B - \frac{128}{45\pi^2} \Gamma_B^2 \frac{R}{v} - \frac{64}{9\pi^2} \Gamma_{AB}^2 \frac{M_A R}{M_B v} - \frac{\sigma^2}{M_B} \right) \\ & - \left(\Gamma_{AB} + \frac{64}{15\pi^2} \Gamma_{AB}^2 \frac{R}{v} \right)^2 \quad (9) \end{aligned}$$

that is the analog to Eq. (4).

We compare the onset of flocking between theory and agent-based simulations at high densities in Fig. 1 and at small densities in Fig. 2. We find that mean field theory reproduces the qualitative effect of the presence of a flocking state. Quantitative agreement, however, is only reached at very high velocities, where two distinct particles collide only for a short time and thus build up only little correlations. In the dilute case, the Boltzmann-like scattering theory is applicable and agrees excellently with simulations regarding both, the polar order and the onset of flocking, see Fig. 2. In particular, in contrast to mean field, the predictions based on one-sided molecular chaos reproduce the velocity dependence correctly. Furthermore, not only the steady state is predicted correctly, but also the full dynamics of the orientational distribution, see [42].

Spatially inhomogeneous states. So far, we studied small systems and assumed a homogeneous spatial distribution of particles. For aligning active particles, it is known that the flocking transition is discontinuous and spatial structures are formed within the flocking phase of large systems [35,48–52]. Here, for antialigning active particles, we also

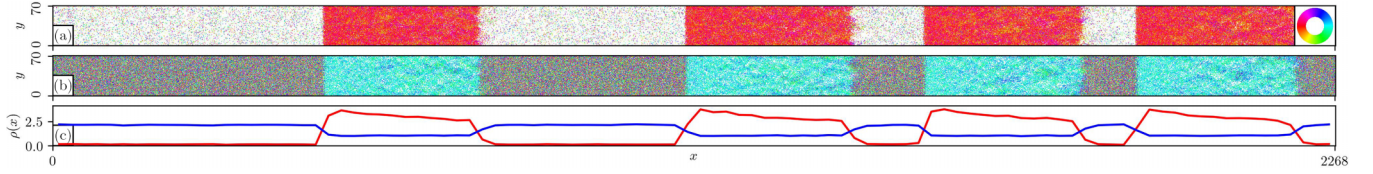


FIG. 3. Snapshot of A particles (a) and B particles (b) in the micro-phase-separated state. Orientations are encoded in color according to the color wheel in (a). The local density of A particles (red) and B particles (blue) are displaced in (c). The system microphase separates into polarly ordered regions with high density of A particles and low density of B particles, and a disordered regions with high density of B particles and low density of A particles. See [42,47] for simulation details.

find spatial structures within the flocking phase for large systems and most likely the flocking transition is discontinuous here as well, however, we did not investigate the nature of the transition in detail here. A mean field linear stability analysis reveals that the homogeneous disordered state is always stable and the homogeneous polarly ordered state is always unstable. However, depending on parameters, there are two kinds of instabilities. The first instability is purely longitudinal with respect to the polarization axis in positional space and it is symmetric with respect to reflections of orientations along the polarization axis, which corresponds for angular modes $\hat{p}_{k_{A/B}}^{A/B}$ and polarization along the x axis to the symmetry $\hat{p}_{k_{A/B}}^{A/B} = \hat{p}_{-k_{A/B}}^{A/B}$. Thus, the instability is not affecting the direction of the polarization. This instability results in the formation of polarized bands, see Fig. 3 (We show simulations on a rectangular domain because in that way the system is very large in one direction and microphase separation can be observed, for the same particle number and the same physical parameters, we observe the same pattern on a square domain, however, in this case there is only one band). The simulation domain microphase separates into stripes of disorder and of high polar order, with A and B particles being polarized in opposite directions. In this phase, particles partially demix: the density of A particles is much higher in the polarized regions whereas the density of B particles is much higher in the disordered regions. The species with larger density within the polarized region dominates the dynamics of the pattern. That means the polarized bands move into the direction of motion of the A particles. It should be mentioned that we observed long living meta stable dynamical patterns that eventually decay into the micro-phase-separated states.

The second instability is purely transversal with respect to the polarization axis, however the angular modes of the unstable eigenvector are not symmetric with respect to reflections along the polarization axis, that is for angular modes $\hat{p}_{k_{A/B}}^{A/B}$ and polarization along the x axis $\hat{p}_{k_{A/B}}^{A/B} \neq \hat{p}_{-k_{A/B}}^{A/B}$. Exemplary numerical values of the eigenvectors are available in [47]. Thus, the instability causes some bending of the polarization direction. As a result of this instability, we observe patterns of patches with different polarization orientation, see Figs. 4(a) and 4(b), that appear similar to vortices reported, e.g., in [23]. In a few realizations (in 11/30 realizations of the considered parameters from the corresponding phase, see [47]), we also observe a pattern of stripes with different polarization orientations without any vortices.

In Fig. 4(c) we show the mean field phase diagram with the three phases: disorder, microphase separation, and spatially

inhomogeneous polarization patterns (patches or stripes). The corresponding most unstable eigenmodes together with the eigenvectors are available in [47]. We find that the wavelength of both instabilities diverges when approaching the disordered state. We show this behavior exemplary for the transition from microphase separation to disorder in Fig. 4(d). As a result, we observe homogeneous polarized states in simulations of finite size close to the onset of flocking. We did not find a Toner-Tu phase for purely negative couplings, thus we suspect that this phase is only present if at least one of the couplings is positive.

In summary, we study a simplified "dry" model for a binary mixture of pushers in dilute solution, restricted to move in two dimensions, however interacting via antialigning three-dimensional hydrodynamics. Despite antialigning torques between each pair of particles, we find polarized flocking states where particles of different types move in opposite directions. Thus, inhomogeneities of coupling strengths as present here, in the binary mixture, are sufficient to overcome

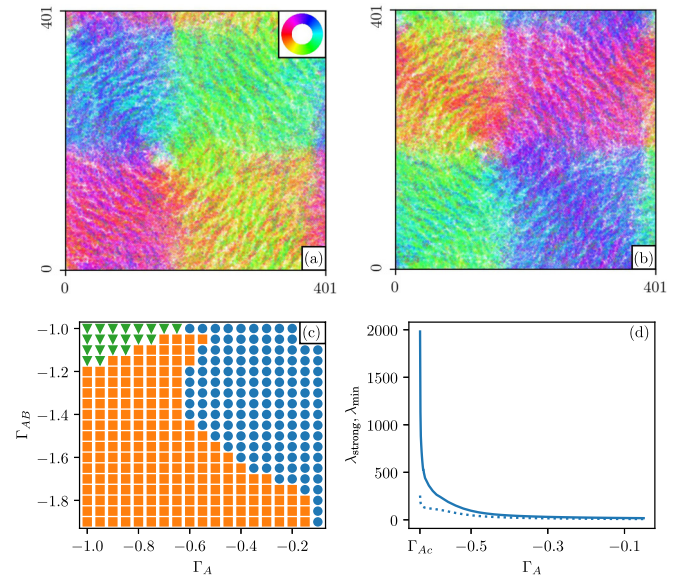


FIG. 4. Snapshots of A particles (a) and B particles (b) in the phase of polarized patches. (c) Mean field phase diagram with disorder (green triangles), polarized moving bands (blue circles), and polarized patches (orange squares). (d) In all considered cases of the polarized homogeneous state we find several unstable modes. We show the wavelength of the most unstable mode (solid line) and the smallest wavelength of all unstable modes (dotted line) within the phase of polarized moving bands. Both wavelengths diverge when approaching the transition toward disorder. See [42,47] for simulation details.

frustration due to the pairwise antialignment interactions. This prediction might be verified in future experiments on microswimmers. Mean field theory correctly predicts the observations from agent-based simulations on a qualitative level. For dilute systems, we develop an asymptotically exact scattering theory based on one-sided molecular chaos. In that way we incorporate the major aspects of pair correlations during collisions. The resulting theory agrees excellently with agent-based simulations on a quantitative level, not only regarding the steady state but it also covers the dynamics of the orientational distribution. In particular, the correct quantitative dependence of the onset of flocking on the velocity is predicted, which is impossible for all mean field theories that have been employed previously in the description of flocking transitions of self-propelled particles.

For very large systems (at the order of magnitude of 10^5 particles for the considered parameters), the flocking

transition goes along with the formation of spatially extended patterns within the flocking state. Depending on parameters, we observe two types of patterns. In the first case, we observe microphase separation between a disordered gas and polarized, moving bands that is known also for aligning active particles. In the second case, we observe patterns of different polarization in different places either organized in quadratic patches or in stripes.

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Data availability. The data that support the findings of this article are openly available [47].

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