Mean field approach of dynamical pattern formation in underdamped active matter with short-ranged alignment and distant anti-alignment interactions

Dominic Arold and Michael Schmiedeberg

Institut für Theoretische Physik I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

E-mail: michael.schmiedeberg@fau.de

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Abstract

Many active matter systems, especially on the microscopic scale, are well approximated as overdamped, meaning that any inertial momentum is immediately dissipated by the environment. On the other hand, especially for macroscopic active systems but also for many mesoscopic systems the time scale of translational inertial motion can become large enough to be relevant for the dynamics. This raises the question how collective dynamics and the resulting states in active matter are influenced by inertia. Therefore, we propose a coarse-grained continuum model for underdamped active matter based on a mean field description for passive systems. Furthermore, as an example, we apply the model to a system with interactions that support an alignment on short distances and an anti-alignment on longer length scales as known in the context of pattern formation due to orientational interactions. Our numerical calculations of the under- and overdamped dynamics both predict a structured laneing state. However, activity induced convective flows that are only present in the underdamped model destabilize this state when the anti-alignment is weakened, leading to a collective motion state which does not occur in the overdamped limit. A turbulent transition regime between the two states can be characterized by strong density fluctuations and the absence of global ordering.

Keywords: active matter, underdamped dynamics, collective motion

(Some figures may appear in colour only in the online journal)

1. Introduction

Active matter denotes a whole plethora of biological and artificial many-body systems composed of self-propelled, interacting particles [1–3]. Often, microscopic systems are considered in which the constituents move in a viscous environment. Typical examples include protein filaments in motility assays [4], cell colonies [5–7], biological or artificial microswimmers [8–10], all surrounded by a viscous background fluid at low Reynolds numbers or binding to an adhesive substrate. These systems are overdamped, meaning the motion of particles is solely governed by the momentary forces acting on them. However, Newton’s first law formulates that massive objects resist any change in momentum due to their inertia. While not relevant on the microscopic length scale in solution, inertial effects become relevant in typical macroscopic realizations of active matter like flocks of birds.
or artificially made massive robots moving on a two-
dimensional plate [13–15]. For the latter, the influence of iner-
tia on the long time statistics was observed recently for a one
particle system [16]. Another interesting study proposes that
the pressure of active particles exerted on a moving wall varies
with inertia [17].

There is a wide range of particle based active matter mod-
els which explicitly incorporate the microscopic interactions
[18–22]. Another approach to such systems is the formulation of
continuum models which typically describe systems on a
length scale above the particle resolution. Such coarse-grained
models are already able to predict experimental observa-
tions of microscopic systems like bacterial colonies [23], ensembles
of microswimmers [9, 24] or active nematics [3, 25, 26]. How-
ever, for other systems where the time scale of inertial motion
becomes relevant an extended underdamped description of the
dynamics becomes necessary.

In this article, we propose a continuum model for classical
underdamped active matter by including activity to a dynam-
cal density functional theory for underdamped passive systems
[27]. Then we use the model to investigate an example sys-
tem where we capture the consequences of introducing trans-
lational inertia by comparing the found states to those of the
corresponding overdamped limit system. The interaction rules
of particle orientations we specify on the continuum level are
derived from microscopic interactions and discussed in detail in
[21, 22]. Consequently, we find in our system several of the
states reported there. However, as discussed later on, differ-
ences arise due to the varying dynamics. Specifically, we note
that in our approach the actual velocity of a particle that is the
case of inertia effects does not have to coincide with the orien-
tation of a particle that determines the direction of the intrinsic
self-propulsion.

The article is structured as follows: in section 2 we derive
the model and specify the system. Simulation results on the
latter are discussed in section 3 and concluded in section 4.

2. Model

2.1. Derivation

In this section, we outline the derivation of the general model
which follows [27] concerning the calculation steps and coinci-
cides with it when active components are neglected. These
additional active terms do not change the principal calculation
but give additional contributions in each step. The inclusion of activity
follows similar approaches used for overdamped active systems [10, 28]. Afterward, we introduce the specific
system which is investigated later on.

We consider a general system which consists of \(N\) iden-
tical polar particles of mass \(m\) with position and momentum
coordinates \(\mathbf{r}^N = \{\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\}\) and \(\mathbf{p}^N = \{\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N\}\).
All particles self-propel with an active force \(f_0\) into the
direction of their orientation given by the unit vectors
\(\hat{\mathbf{u}}^N = \{\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, \ldots, \hat{\mathbf{u}}_N\}\). For convenience, we restrict
the derivation to effectively two dimensional systems where an
angle \(\varphi\) determines the orientation \(\hat{\mathbf{u}} = (\cos(\varphi), \sin(\varphi))^{T}\).
A particle’s phase space coordinates are summarized as
\(\mathbf{x}_i = \{\mathbf{r}_i, \mathbf{p}_i, \varphi_i\}\). The force \(\mathbf{F}_i = F^{(1)}(\mathbf{r}_i) + F^{(2)}(\mathbf{r}_i)\)
summarizes an external potential force \(F^{(1)}(\mathbf{r}_i) = -\nabla_n V^{(1)}(\mathbf{r}_i)\) and
particle interactions \(F^{(2)}(\mathbf{r}_i) = -\sum_j \nabla_n V^{(2)}(\mathbf{r}_i, \mathbf{r}_j)\)
with the pair interaction potential \(V^{(2)}(\mathbf{r}_i, \mathbf{r}_j)\). Analogously to these
translational forces particles change their orientation due to
the torque \(G_i(t, \varphi_i) = G^{(1)}(\mathbf{r}_i, \varphi_i) + G^{(2)}(\mathbf{r}_i, \varphi_i)\) with
a one particle contribution \(G^{(1)}(\mathbf{r}_i, \varphi_i)\) and a pairwise interaction
torque \(G^{(2)}(\mathbf{r}_i, \varphi_i)\). The corresponding Langevin equations
for the underdamped motion of the particle ensemble then
read

\[
\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m} \\
\frac{d\mathbf{p}_i}{dt} = -\gamma \mathbf{p}_i + \mathbf{F}_i(\mathbf{r}_i^N) + f_0 \hat{\mathbf{u}}_i + \sqrt{2D} \Gamma_i(t) \\
\frac{d\varphi_i}{dt} = G_i(\mathbf{r}_i^N, \varphi_i) + \sqrt{2D_R} \xi_i(t)
\]

where \(\gamma = \alpha/m\) is the damping constant with friction \(\alpha\)
and \(D, D_R\) are translational and rotational diffusion constants.
\(\Gamma_i(t), \xi_i(t)\) are independent \(\delta\)-correlated white noises
meaning \(\langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t - t')\) and analogously for
the components of \(\Gamma_i\). Note that the damping \(\gamma\) and diffusion \(D\) are not
necessarily related via the Stokes–Einstein relation since they might
describe, e.g., the interaction with a substrate instead of a ther-
mal bath. We also want to point out that here we only consider
translational inertia but that we neglect inertia effects in angu-
lar direction, i.e. we consider a case where the inertia time scale
of the rotation is negligible while the inertia time scale of the
translational motion still is considered. In case of particles that
have to be rotated in order to change the orientation, this is
the case if the mass of the particle is mainly located close to
the center of the particle or in the limit of point particles as in
[21, 29].

These microscopic equations of motion for the stochas-
tic state variables are converted into the corresponding
Fokker–Planck equation of the \(N\) body phase space probability
density \(f^{(N)}(\mathbf{x}^N, t)\) which gives us the probability of finding
the system in a configuration \(\mathbf{x}^N = \{\mathbf{r}_i^N, \mathbf{p}_i^N, \hat{\mathbf{u}}^N\}\) at time \(t\) [30].

The resulting dynamical equation reads

\[
\frac{\partial f^{(N)}}{\partial t} = \sum_{i=1}^{N} \left[ -\frac{\mathbf{p}_i}{m} \cdot \nabla_{\mathbf{r}_i} f^{(N)} + \gamma \nabla_{\mathbf{p}_i} \cdot \left( \mathbf{F}_i f^{(N)} \right) \\
- \mathbf{F}_i \cdot \nabla_{\mathbf{p}_i} f^{(N)} - f_0 \hat{\mathbf{u}}_i \cdot \nabla_{\mathbf{p}_i} f^{(N)} \\
+ D \nabla_{\mathbf{p}_i}^2 f^{(N)} - \partial_{\varphi_i} \left( G_i f^{(N)} \right) + D_R \partial_{\varphi_i}^2 f^{(N)} \right]
\]

This \(N\) body problem is simplified by defining the \(n\) body
reduced phase space distribution functions

\[
f^{(n)}(\mathbf{x}^n, t) = \frac{N!}{(N-n)!} \int d\mathbf{r}^{(N-n)} \int d\mathbf{p}(N-n) \\
\times \int d\varphi^{(N-n)} f^{(N)}(\mathbf{x}^N, t)
\]

where \(N-n\) of the \(N\) bodies’ state variables are integrated out.
Equivalently, integrating the \(N\) body Fokker–Planck equation
over \( N - 1 \) sets of particle variables yields the dynamical equation for the one body distribution

\[
\frac{\partial f^{(1)}}{\partial t} = - \frac{p_i}{m} \cdot \nabla_{r_i} f^{(1)} + \gamma \nabla_{p_i} \cdot (p_i \cdot f^{(1)}) - F^{\text{ext}} \cdot \nabla_{p_i} f^{(1)} - \int dr_2 \int dp_2 \int d\varphi_2 \frac{\partial F^{(2)}}{\partial \varphi_1}(r_1, r_2, f^{(2)}) - \int dr_2 \int dp_2 \int d\varphi_2 \partial_{\varphi_1} \varphi_2 (G^{(2)} f^{(2)})
\]

where we assume that the \( N \) body density and its first derivatives decay to zero for all \( r_i, p_i \to \infty \) and are periodic in \( \varphi_i \). The latter assumption is also used for the torques \( G_1, G_2 \). The reduced one body phase space density \( f^{(1)}(x_1, t) \) gives the probability of finding a particle at the position \( r_1 \) with momentum \( p_1 \) and orientation \( u_1 \) at time \( t \). Note that due to particle interactions, (4) still depends on the two body density \( f^{(2)}(x_1, x_2, t) \).

For the next step, we define the mean field quantities number density \( \rho \), momentum current \( j \) and orientation current \( \rho \mathbf{P} \) with the mean orientation field \( \mathbf{P} \) as

\[
\rho(r_1, t) = \int dp_1 \int d\varphi_1 f^{(1)}(x_1, t), \quad j(r_1, t) = \int dp_1 \int d\varphi_1 \frac{p_1}{m} f^{(1)}(x_1, t), \quad \rho \mathbf{P}(r_1, t) = \int dp_1 \int d\varphi_1 \frac{p_1}{m} u_1 f^{(1)}(x_1, t).
\]

Our goal is now to reduce the equation for \( f^{(1)} \) to equations for the mean fields and simplify the problem further from there. Equation (4) may be integrated over \( p_1 \) and \( \varphi_1 \) which yields the continuity equation for the number density

\[
\frac{\partial \rho}{\partial t} + \nabla_{r_1} \cdot j = 0.
\]

Similarly, an equation for \( j \) is found by multiplying (4) with \( p_1/m \) and then integrating over \( p_1 \) and \( \varphi_1 \) to obtain

\[
\frac{\partial j}{\partial t} = - \frac{1}{m} \int dp_1 \int d\varphi_1 p_1 \varphi_2 f^{(1)}(x_1, t) - \gamma j + \int dr_2 \int dp_2 \int d\varphi_2 F^{(2)}/\rho + \frac{f_0}{m} \rho \mathbf{P}.
\]

Here, the two body number density

\[
\rho^{(2)}(r_1, r_2, t) = \int dp_1 \int dp_2 \int d\varphi_1 \int d\varphi_2 f^{(2)}(r_1, r_2)
\]

is used in the interaction integral.

Now, we effectively make the same two approximations as in [27] to proceed further. The only difference is the dependence of \( f^{(1)} \) on \( \varphi_1 \). First, we approximate the interaction integral containing the two body number density via

\[
\int dr_2 F^{(2)}(r_1, r_2) \rho^{(2)} = -\rho \nabla_{r_1} \frac{\delta F^{\text{exc}}[\rho]}{\delta \rho}
\]

which is exact only in equilibrium. Therefore, the commonly used approximation is to use this expression also in the non-equilibrium case [31]. \( F^{\text{exc}} \) is the excess free energy which contains energy contributions due to particle interactions. The second approximation is to assume that the \( \varphi_1 \) dependencies in \( f^{(1)} \) decouple from dependencies on \( p_1 - p_{\text{ext}} \) where \( p_{\text{ext}} = m \mathbf{v}(r_1, t) \) with the local average particle velocity \( \mathbf{v} \) that is analogous to the local mean orientation \( \mathbf{P} \). To be specific, we assume \( p_1 \) approximately is Gaussian distributed [32] around \( p_{\text{ext}} \) in a way that is independent of \( \varphi_1 \). Therefore, we write the one body density as

\[
f^{(1)}(x_1, t) = \frac{\varPhi(r_1, \varphi_1, t)}{2\pi mkT} \exp \left( -\frac{(p_1 - m \mathbf{v})^2}{2mkT} \right)
\]

where \( \varPhi(r_1, \varphi_1, t) \) contains the orientational dependence and \( kT \) gives the width of the Gaussian distribution and in equilibrium systems would correspond to the equilibrium thermal energy. With this form of the one body density it follows from the definition of the mean field densities

\[
\rho(r_1, t) = \int d\varphi_1 \varPhi(r_1, \varphi_1, t), \quad j(r_1, t) = \rho(r_1, t) \mathbf{v}(r_1, t).
\]

Applying now the approximations (9) and (10) to the current equation in (7) results in a dynamical equation for \( \mathbf{v} \) which only depends on the other mean fields. This calculation is done and described in [27] and therefore not rewritten here. All terms originating from the additional particle orientation vanish up to a coupling term in the momentum equation which does not change the principal calculation but is also found again in the resulting mean velocity equation

\[
\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\gamma \mathbf{v} - \frac{1}{m} \nabla \frac{\delta F[\rho]}{\delta \rho} + \frac{f_0}{m} \mathbf{P}.
\]

Diffusion, interactions with other particles and external fields are summarized here under the Helmholtz free energy functional [32]

\[
F[\rho] = kT \int dr \rho \ln(\Lambda \rho) - 1 + F^{\text{exc}}[\rho] + \int dr \rho \mathbf{v}^{\text{ext}}(r).
\]

The first term is the ideal gas free energy with the thermal wave length \( \Lambda = h/(2\pi mkT)^{1/2} \) where \( h \) is the Planck constant and the so called excess free energy \( F^{\text{exc}}[\rho] \) denotes whatever is left after the ideal gas contribution and the contribution due to an external potential \( \mathbf{v}^{\text{ext}}(r) \) have been subtracted from the free energy \( F[\rho] \).

Next, we find a dynamical equation for the mean orientation \( \mathbf{P} \) by first multiplying equation (4) with \( \mathbf{u}_1 \) and then integrating over \( p_1 \) and \( \varphi_1 \). The terms of the resulting dynamical equation of \( \mathbf{P} \) are calculated separately in the following. First, we rewrite the left hand side of equation (4) by using (6) and the expression for the current in equation (11) to obtain
\[
\frac{\partial (\rho P)}{\partial t} = \rho \frac{\partial P}{\partial t} - \rho P \nabla \cdot v - P (v \cdot \nabla \rho). \tag{14}
\]

Afterward, we simplify the first term on the right hand side with the approximation (10) to

\[
\frac{1}{m} \int dp_1 \int dp_2 \int d\varphi_2 G_2^0(r_1, r_2, \varphi_1, \varphi_2) f^{(1)} = \rho (v \cdot \nabla) P + P (v \cdot \nabla \rho) + \rho P \nabla \cdot v. \tag{15}
\]

Like the pair interaction in the current dynamics (7) we now approximate the interaction term for the orientation via an equilibrium excess functional

\[
\int dr_2 \int dp_2 \int d\varphi_2 G_2^0(r_1, r_2, \varphi_1, \varphi_2) f^{(2)} = -f^{(1)} \frac{\partial f^{(1)}}{\partial \varphi_1} \delta f^{(1)} = -f^{(1)} \frac{\partial f^{(1)}}{\partial \varphi_1} \frac{\delta F_{xc}^0}{\delta \Phi} \tag{16}
\]

leading to the expression for the orientational interaction

\[
- \int dr_2 \int dp_1 \int dp_2 \int d\varphi_1 \int d\varphi_2 \int d\varphi_2 \varphi_1 \varphi_2 (G_2 f^{(2)}) = - \int d\varphi_1 (\varphi_1 \hat{u}) \Phi \frac{\delta F_{xc}^0[\Phi]}{\delta \Phi} = - \rho \frac{\delta F_{xc}^0[P]}{\delta \Phi}. \tag{17}
\]

To arrive at the second line, the momentum integrations on the two body density are carried out, partial integration on \( \varphi_1 \) is used, and the approximation (16) is inserted. In the last step, the excess functional \( F_{xc}^0[\Phi] = F_{xc}^0[P[\Phi]] \) is expressed via the mean orientation \( \Phi \) by applying the chain rule for functional differentiation

\[
\frac{\delta F_{xc}^0[P[\Phi]]}{\delta \Phi(r, \varphi, t)} = \int dr' \int dr'' \frac{\delta F_{xc}^0[P]}{\delta \Phi(r', t')} \frac{\delta P[\Phi]}{\delta \Phi(r, \varphi, t)} = \delta F_{xc}^0[r, t] \hat{u}(\varphi). \tag{18}
\]

Here, \( P[\Phi] \) is given by inserting the approximation (5) into the definition of \( P \) in equation (5) which yields

\[
P[\Phi] = \int d\varphi \hat{u} \Phi(r, \varphi, t). \tag{19}
\]

All other terms in the resulting dynamical equation of \( P \) ever vanish or are dealt with via partial integration. A resulting non-vanishing term is the average one particle torque

\[
\overline{G^{(1)}} = \frac{1}{\rho} \int d\varphi (\partial_\varphi \hat{u}) G^{(1)} \Phi \tag{20}
\]

which describes a particle’s behavior of orienting independently of other particles’ orientations. Together with equations (6) and (12) we can now write down the final form of our model for underdamped active systems

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho v)
\]

\[
\frac{Dv}{Dt} = -\gamma v - \frac{1}{m} \nabla \frac{\delta F}{\delta \rho} + \gamma \nu_0 P \tag{21}
\]

\[
\frac{DP}{Dt} = -D_R P - \frac{\delta F_P}{\delta P} + \bar{G}^{(1)}
\]

with the convective derivative \( \frac{D}{Dt} = \frac{\partial}{\partial t} + (v \cdot \nabla) \). The self-propulsion velocity \( \nu_0 = f_0 / \alpha \) corresponds to the steady state velocity of a particle in an environment with friction constant \( \alpha \) and accelerated by the active force \( f_0 \). Although closure relations for particle interactions do not need to be formulated in a functional form this conceptual connection to equilibrium physics proves to be a useful and instructive ansatz in the context of active matter models \cite{3, 28}. Equation (21) represents the starting point for many possible mean field approaches for various active systems with underdamped translational motion. In the next section, we will study one specific example, where translational and orientational interactions are given by simple free energy approaches.

2.2. Example system

By orienting on minimal ingredients for phenomenological models on the microscopic scale \cite{9, 23, 24, 33–35} we now use equation (21) to specify a concrete system by choosing

\[
F[\rho] = \int dr \frac{c}{2} \rho^2
\]

\[
F_P[\rho] = \int dr \frac{P}{2} \left[ -a + \lambda (q_0^2 + \nabla^2)^2 \right] P + \frac{\beta}{4} |P|^4
\]

\[
\bar{G}^{(1)} = 0.
\]

Our model allows density variations which occur preferably in dilute systems. We consider repulsive interactions with an effective finite compressibility of the system described by \( F \) where \( c \) is the compressibility parameter. The interaction of orientations given by \( F_P \) has the form of a Swift–Hohenberg functional \cite{36} with the preferred wave number for structure formation \( q_0 \) and additional free parameters \( a, \lambda, \beta \). Its physical meaning becomes more evident when inserting equation (22) into (21) resulting in

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho v)
\]

\[
\frac{Dv}{Dt} = -\frac{1}{m} \left( -a v - c \nabla \rho + \alpha \nu_0 P \right) \tag{23}
\]

\[
\frac{DP}{Dt} = (\kappa - \beta |P|^2) P - \lambda (q_0^2 + \nabla^2)^2 P.
\]

The \( \kappa = a - D_R \) and \( \beta \) terms were introduced before by Toner and Tu \cite{37} for the description of flocking in active systems. For \( \kappa < 0 \), the system evolves into the isotropic state \( v = 0 \). We restrict to the non-trivial case \( \kappa > 0 \) where the local alignment strength of orientations \( a \) outweighs rotational diffusion \( D_R \), resulting in a preferred net velocity amplitude \( \sqrt{\kappa / \beta} \). The second term in the orientation dynamics is interpreted as an anti-alignment interaction with strength \( \lambda \) at a preferred
particle distance $l_0/2 = \pi/q_0$ [21, 22]. This type of interaction supports the formation of dynamical patterns that are aligned at short distances, but usually do not favor a globally aligned state due to the preference of the anti-alignment on longer distances. Additional one body torques $G^{(1)}$ are not considered. A detailed discussion of the physical background and consequences of the orientational interactions can be found in [21, 22]. However, in these works the particles move with an artificially fixed velocity, while the velocity in our approach can vary in amplitude and direction with respect to the orientation of self-propulsion. The orientational interaction in equation (23) corresponds to the one used in [21, 22] where results of particle-based simulations are presented. Inserting these orientational interaction rules into our underdamped dynamics equation (1) one arrives at a particle-based model ready for simulations to compare to our corresponding mean field example in equation (23). We note that in [38], we also use equation (21) to investigate another system with different free energy interactions.

We are especially interested in the consequences of introducing translational inertia into active systems. Therefore, as an important reference case, we determine the overdamped limit of (23) by taking a low-mass limit. The convective derivative of the velocity equation can then be neglected leading to a quasi-stationary velocity dynamics. Additionally, we neglect convection of $\mathbf{P}$ which also results from the inclusion of translational inertia. With this, we simplify the dynamics in the overdamped limit to

$$\frac{\partial \rho}{\partial t} = \frac{c}{2\alpha} \nabla^2 \rho^2 - v_0 \nabla \cdot (\rho \mathbf{P})$$

$$\frac{\partial \mathbf{P}}{\partial t} = (\kappa - \beta |\mathbf{P}|^2) \mathbf{P} - \lambda (q_0^2 + \nabla^2)^2 \mathbf{P}. \quad (24)$$

We rescale and numerically implement equations (23) and (24) as described in appendix A. This reduces the set of dimensionless and independent parameters to $v_0$, $\lambda$ for the overdamped and to $m$, $v_0$, $\lambda$ for the underdamped model. From now on we solely refer to the dimensionless form of these parameters.

3. Results

We investigate the role of translational inertia by comparing predicted states along different regimes of the anti-alignment strength $\lambda$ in the under as well as the overdamped model. The influence of the active drive $v_0$ and mass $m$ on the state diagram is discussed afterward.

We distinguish qualitatively different states from changes of observables for density fluctuation and velocity alignment. First, we use the variance of the space averaged density

$$\Delta \rho^2 = \bar{\rho}^2 - \bar{\rho}^2$$

and determine its time average

$$\langle \Delta \rho \rangle = \frac{1}{T} \int_0^T dt \, \Delta \rho(t) \quad (26)$$

for a time interval $T$ that is chosen long enough such that the average does not depend on $T$. We use the mean value $\langle \Delta \rho \rangle$ to quantify density fluctuations in space while the corresponding variance is a measure for temporal fluctuations.

Second, we measure velocity alignment with the space averaged polar orientational order of the normalized velocity field

$$p_v = \left| \frac{\nabla}{|\nabla|} \right| \quad (27)$$

where $||\cdot||$ denotes the Cartesian norm. A value near one indicates global orientational order of the velocity field while zero indicates the absence of global ordering. In the overdamped model the velocity field for $p_v$ is given from the density dynamics in equation (24) which has the form of a continuity equation. Thus, we have

$$\mathbf{v} = -\frac{c}{\alpha} \nabla \rho + v_0 \mathbf{P}. \quad (28)$$

We measure average density fluctuation $\langle \Delta \rho \rangle$ and velocity order $p_v$ for varying $\lambda$. From the shown results in figure 1 three states can be distinguished within the underdamped model which are discussed later in more detail. First, for high anti-alignment strengths the average density fluctuation is close to the reference value $\Delta \rho_0$ and the temporal variance is negligible. The system shows no global ordering of velocities. In this regime we observe alternating high and low density lanes along which particles move in opposite directions which we refer to as laneing [18–20, 39]. This is the only state which is equally predicted by the overdamped model. Second, near the critical value $\lambda = 0.2$, $\langle \Delta \rho \rangle$ and its temporal variance spontaneously increase which is accompanied by an onset of global orientational velocity ordering in $p_v$. We refer to this transition state as turbulent due to its non-steady character. And third, in the low $\lambda$ regime $\langle \Delta \rho \rangle$ continuously decreases again relative to the turbulent state and even below the value of the laneing state. The temporal variance stays high. In this regime global ordering of velocities is observed with $p_v$ close to one leading to the identification of this state as collective motion. We now first discuss the laneing state in the overdamped case in order to compare with the underdamped model afterward.

3.1. Laneing in the overdamped model

The interaction of particle orientations given by $\mathcal{F}_p$ in (22) has two contributions. The Toner–Tu local alignment and the anti-alignment at distance $l_0/2$. In figure 2(a) we observe that for a high anti-alignment strength $\lambda$ the system favors a periodic modulation of orientations. Such emergent structures due to competing interactions are for example also observed in Ising models with ferromagnetic and anti-ferromagnetic couplings on different length scales [40]. The resulting orientation field accumulates density in bands with the same periodicity. This process is balanced by the compressibility of the system which counteracts along the arising density gradients. In the shown steady state the density and orientation fields may be approximated by harmonic modulations around their mean along one spatial direction. From inserting these expressions in the steady state force balance condition we predict the amplitude of the density variation and the corresponding...
spatial variance to

\[ \rho_0 = \sqrt{\frac{\rho}{\beta}} \frac{v}{q_0 c} \]

\[ \Delta \rho_0 = \frac{\rho_0}{\sqrt{2}} \tag{29} \]

which is in accordance with our numerically found global stripe pattern and its spatial fluctuation in figure 1(a). Along the maxima and minima of the density bands the active drive is not balanced by the compressibility of the system and therefore induces particle fluxes organized in lanes. Due to the preferred anti-alignment particles in neighboring high and low density lanes propel in opposite directions with the same self-propulsion velocity \( v_0 \) which explains the observed absence of global velocity ordering in figure 1(b). However, we emphasize that the density difference between the opposite propulsion directions leads to a net current in the direction of movement within high density lanes. For high enough active drive we expect all particles might accumulate in the high density lanes and move in the same direction, thereby maximizing the current, which is however not explicitly tested. Such unidirectional laning states are observed in particle simulations with orientational alignment [18]. There, the maximum distance of local alignment coincides with the resulting lane distance. In this reference the formation of lanes is explained as an overreaction of the alignment interaction. This differs from the laning mechanism observed here since alignment of particles happens only locally and an anti-alignment rule dominates at further distances thereby determining the lane spacing. In other active systems laning structures form due to a combination of crowding effects and flocking [41, 42].

When the anti-alignment strength \( \lambda \) is lowered the orientation field becomes more likely to locally form vortices with diameter \( k_0/2 \). Seeing the orientational interactions as the derivative of the vectorial phase field crystal model (PFC) functional \( \mathcal{F}_p \) the increasing occurrence of vortices between laning domains can be seen as a transition from the stripe to the crystal phase. The difference to a typically used one component PFC interaction [43–45] is the coupling of the two vector components of \( \mathbf{P} \). So instead of a clear transition from laning (stripe phase) to a regular lattice of vortices (crystal phase) we observe in figure 2(b) that the system is typically stuck in metastable states of laning domains which are separated by defects in the form of vortices in the orientation field. Those defects increase the functional free energy of the \( \lambda \) term relative to the global laning state as anti-parallel alignment is only locally given.

For the lowest tested \( \lambda \) values the number of vortices in the orientation field steadily increases until clear laning domains are absent. Instead, the density pattern varies locally depending on the metastable states of the orientation field. Additionally, we find several vortices in the orientation field which arrange in local lattices of alternating clockwise and anticlockwise motion like illustrated in figure 2(c). Different to the hexagonal lattice symmetry arising for one component PFC functionals we solely observe square lattices which enable a frustration free arrangement of the vortices’ orientation of circular motion. We finally note that local square lattices are typically distorted by their surrounding leading to inward and outward spiraling vortices in the orientation field instead of perfectly circular ones. Inward spiraling orientations accumulate density while outward spiraling ones spread density. In the steady state the resulting density variations between contrary rotating vortices are balanced by the compressibility of the system resulting in square lattices of perfectly circular vortices in the velocity field.

3.2. States in the underdamped model

Laning. For high \( \lambda \) values, the laning state found within the overdamped model is equally predicted in the underdamped model. We find the same value of spatial fluctuation \( \Delta \rho_0 \) and absence of global velocity ordering \( p_v = 0 \) (see figure 1). We
Figure 2. Density field predicted by the overdamped model for different anti-alignment strengths. The box size is measured in units of $l_0$ and magnified regions show the orientation field (red) and the velocity field (black). (a) For high anti-alignment strengths, the system is likely to reach a global laning state of alternating high and low density bands along which particles move within lanes. The instability in the density is driven by activity and balanced by the system’s compressibility. Due to the preferred anti-alignment of orientations particles in neighboring lanes self-propel in opposite directions with equal velocity causing a net particle current in the direction of movement of the high density lanes. (b) For intermediate $\lambda$ values, we observe laning domains separated by metastable vortical defect boundaries in the orientation field. (c) In the low $\lambda$ regime, the number of vortical defects in the orientation field increases further thereby preventing the formation of larger laning domains. Several vortices might arrange into a local square lattice where we observe circular motion. Parameters are set to (a) $\lambda = 3$, (b) $\lambda = 0.5$, (c) $\lambda = 0.03$, and $v_0 = 0.2$ for all systems.

Figure 3. Density field predicted by the underdamped model for different anti-alignment strengths. The box size is measured in units of $l_0$ and magnified regions show the orientation field (red) and the velocity field (black). (a) For high anti-alignment strengths, the same laning state as in the overdamped model is found. However, for intermediate values vortex defects in the orientation field are absent when $\lambda$ is lowered as exemplarily shown in figure 3(a). We explain this difference with the convection of orientation. A vortex in the orientation field induces a corresponding circulating flux. Due to their inertia particles radially leave the vortex which gets distorted due to this convection. The anti-alignment interaction counteracts this distortion similar to a centripetal force which holds objects on circular orbits. Consequently, if $\lambda$ is lowered enough the formation of vortices in the orientation field is inhibited. In the steady state the grain boundaries between different laning domains then resolve by branching and linkage of lanes with equivalent orientation at the boundary. In this sense, inertial convection is actually beneficial for the formation of a global laning state at intermediate anti-alignment strengths since it heals out vortical defects in the orientation field.

Turbulence. Lowering $\lambda$ into the turbulent regime suddenly changes the dynamics considerably since now convective flows not only destabilize vortical defects in the orientation field but also the laning structures due to the weakened anti-alignment. As can be seen from the orientation field in figure 3(b) the laning structure evolves only locally. The system does no longer reach a steady state but instead large spatio-temporal fluctuations are self-sustained over time which is reflected by an increase in density fluctuation $\langle \Delta \rho \rangle$ and its temporal variance. The movie in the supplemental materials...
gives an impression of the fluctuating density field. The non-
steady character of the turbulent state results from the contin-
uous interplay of local lane formation and their destabilization
due to convective flows. The sudden increase of density fluc-
tuations coincides with the onset of global velocity ordering
in figure 1. Since convective flows destabilize lane formation
local alignment is no longer restricted to single lanes result-
ing in a small but global drift velocity which is reflected in
a moderate velocity order $v_0$. Our finding that inertial con-
vection destabilizes the laning state is verified by switching
off the convective terms in the dynamical equations of veloc-
ity and orientation within the underdamped model. Then, we
again find local laning structures and vortical defects like in the
overdamped model where otherwise turbulence would arise.

Collective motion. In the turbulent transition state, anti-
alignment is just weak enough so that laning is unstable but
still strong enough to inhibit global velocity ordering. This
changes when $\lambda$ is further lowered since then local align-
ment of orientations increasingly dominates over the weak
anti-alignment resulting in the emergence of global orienta-
tional velocity order as measured in figure 1(b) and shown in
figure 3(c). The homogeneous flow field transports particle
density without accumulating it too much leading to small den-
sity fluctuations in figure 1(a) comparable to the laning state
or even smaller for low enough $\lambda$. Since anti-alignment con-
tinually perturbs the homogeneous velocity field the temporal
variance of $\langle \Delta \rho \rangle$ stays on a high level. We suggest that con-
vective flows stabilize the global collective motion as they do
not influence a homogeneous state of aligned orientations but
mix any arising misaligned clusters with their surrounding due
convective transport of orientation. Hence, the formation of
a larger misaligned cluster is suppressed by convection.

3.3. Remarks

Even for a small mass value in the underdamped model the
predicted states in figure 3 differ from the ones observed in the
overdamped model in figure 2. This seemingly contradictive
observation is explained with the convective term in the under-
damped orientation dynamics. We neglect this term in the over-
damped model to ensure consistency with the corresponding
overdamped microscopic equations of motion, which would
not yield any convective terms on the continuum level when
doing a derivation as in section 2.1. Therefore, we expect the
results within the underdamped model to approach those of
the overdamped limit model when in the low mass regime
also the time scale of convection is negligible compared to
those of interactions. This, for example, happens when we
decrease the active drive $v_0$ in the turbulent regime of the
underdamped model. Then, the values of the order parameters
in figure 1 gradually decrease until the laning state emerges
again since typical particle velocities and therefore the impact
of the convective terms is reduced. We explored the transition
from under- to overdamped dynamics for a different system
in another work [38]. There, we neglect convection of the or-
ientation in the underdamped system and find that its results
approach those of the overdamped limit model for $m \to 0$.

Furthermore, we note that the value of the particle mass $m$
as a third free parameter is not relevant for the state diagram of
the underdamped model. When choosing the mass two orders
of magnitude higher as in figure 3, we find the same qualitative
states and the same values for the observables in figure 1 in the
long time limit. However, the mass parameter might have an
impact on the relaxation dynamics to the steady state, as we
have shown for another system [38].

The dynamical equations of our overdamped model (24)
and (28) are comparable to those in [21, 22]. Since we employ
the same interaction rules, we find a laning state comparable to
the one in [22] for predominant anti-alignment. More impor-
tantly, for lower anti-alignment strength a transition to collec-
tive motion with a turbulent transition regime is observed in
[21, 22] reminiscent to the findings within our underdamped
model. The authors also explain this with destabilizing con-
vective flows arising from the local alignment. Different to
[21, 22], in our underdamped model vortex array patterns like
in figure 2(c) are absent and instead the laning state is also
observed for intermediate $\lambda$ values. We explain the absence
of vortex patterns in our underdamped model due to convec-
tion in radial direction away from a vortex center which is
enhanced in our model since the actual velocity follows the
active propulsion with an inertial delay. The transient patterns
in the turbulent regime of [21, 22] are described as local vor-
tices or lane like jets in the orientation field while we solely
observe the latter patterns as seen in figure 3(b). This reflects
that the transient structures in the turbulent regime correspond
to the stable states observed for higher anti-alignment strength.
Another mechanism favoring lane structures in our under-
damped model over circular vortices arises due do the imple-
mentation of repulsion. In [21, 22], particles move with con-
stant velocity and actively rotate their orientation to avoid high
density regions while in the present model this repulsion, mod-
eled by the compressibility, is a passive one in the sense that
it lowers a particle’s velocity if it moves to higher densities
instead of turning its orientation.

4. Conclusion

In this work, we have derived the dynamics of a continuum
model for underdamped active matter equation (21) based on
a dynamical density functional theory for passive systems [27].
Further, we applied the model to an example system by speci-
fying the interaction rules equation (22) on the continuum level
which were previously derived in [21] and shown to describe
local alignment and distant anti-alignment of orientations.

Finally, we emphasize here that, especially in fully over-
damped active systems, any effectively convective effects nec-
essarily arise from interactions or noise while in the present
case their physical origin is translational inertia. We stress this
difference by comparing the destabilization of lanes in the
present underdamped model with active turbulence in over-
damped systems. For example, in active nematics the ordered
state generally is unstable for non-vanishing activity due to
hydrodynamic interactions [3]. There is an effective feedback
loop between the nematic relaxing to its aligned state and the
thereby induced flows in the background fluid which again
destabilize this state. In our underdamped system, a similar feedback is present in the turbulent state. The role of the background fluid is replaced by inertial convection of the particles themselves which continually destabilizes lane formation. In polar active systems exhibiting active turbulence one term describing hydrodynamic interactions is even structurally equivalent to convection [23, 35, 46]. Increasing the coupling parameter of this term drives the structured state unstable, leading to the emergence of active turbulence [34].

Appendix A. Rescaling and implementation

We rescale equations (23) and (24) in order to extract physically relevant parameters and for numerical implementation. Independent quantities are rescaled to their dimensionless form according to the rules

\[ r \rightarrow q_0 r, \quad t \rightarrow \kappa^{-1} t, \]
\[ \rho \rightarrow \alpha \kappa \rho, \quad v \rightarrow \kappa v, \]
\[ m \rightarrow \alpha m, \quad v_0 \rightarrow \frac{(\kappa \beta)^{1/2}}{q_0} v_0, \]
\[ P \rightarrow \left( \frac{\kappa}{\beta} \right)^{1/2} P, \quad \lambda \rightarrow \frac{\kappa}{q_0} \lambda \]

which leads to the dimensionless form of the underdamped model in equation (23)

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho v) \\
\frac{Dv}{Dt} = \frac{1}{m} (-v - \nabla \rho + v_0 P) \\
\frac{DP}{Dt} = (1 - |P|^2) P - \lambda \left(1 + \nabla^2 \right)^2 P. \tag{A.2}
\]

And for the overdamped model in equation (24) we have

\[
\frac{\partial \rho}{\partial t} = \frac{1}{2} \omega^2 \rho^2 - v_0 \nabla \cdot (\rho P) \\
\frac{\partial P}{\partial t} = (1 - |P|^2) P - \lambda \left(1 + \nabla^2 \right)^2 P. \tag{A.3}
\]

For numerical implementation, we discretize all fields on a rectangular grid. The simulation box has lengths of multiples of $l_0$ and employs periodic boundary conditions. A pseudospectral algorithm is used for numerical time iteration. For the evaluation of the convective terms in real space a third order upwind scheme is applied [47]. Time stepping is implemented via a semi-implicit Euler discretization with fixed step size. All simulations are started from homogeneous initial conditions. The average density is always set to $\bar{\rho} = 1$.

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