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Abstract

Active matter is the study of collective motion of systems of particles that are able to consume energy in order to perform systematic motion. Such systems are abundant in nature and come on a large range of scales: from animal herds and bird flocks, to bacterial colonies, to active polymer suspensions. In this Thesis, we focus on the so-called wet active matter, where interactions between an active particle and its environment (usually a surrounding fluid, as in bacterial or active polymer suspensions) conserve momentum.

Dilute suspensions of motile bacteria are one of the best-studied examples of wet active matter. When the density of the suspension is sufficiently high enough, it exhibits a phenomenon often referred to as bacterial turbulence. When it occurs, the suspension exhibits strong orientational and velocity and correlations on large length scales, enhanced diffusion and mixing of the suspending fluid, and reduced apparent viscosity that vanishes at the onset of collective motion. While the transition to bacterial turbulence is reasonably well-understood, the properties of the turbulent phase are largely unknown.

The purpose of this Thesis is to study theoretically aspects of collective motion of self-propelled particles in the presence of hydrodynamic interaction. Motivated by previous work on the onset of bacterial turbulence, first we develop and study a lattice model of the collective phase. Since the transition to bacterial turbulence was previously shown to be driven by the orientational degrees of freedom alone, we confine model microswimmers to a regular lattice and fix their positions. The dynamics of each microswimmer then comprise re-orientations in the velocity fields created by other microswimmers and random orientational changes representing bacterial tumble event. We observe that in the absence of tumbling, all dynamics cease after some initial time, yielding a frozen configuration. For sufficiently strong tumbling, these configurations melt, and we discuss the implications of this scenario for bacterial turbulence.
As the next step, we study partially filled lattices of microswimmer. In addition to the dynamical rules presented above, each swimmer can now hop on the lattice with a hopping rate dependent on the surrounding velocity field. This hopping simultaneously represents self-propulsion, advection, and spatial diffusion exhibited by real microswimmers. The model also incorporates excluded volume interactions as only a single microswimmer is allowed to occupy a single lattice site. In the absence of hydrodynamic interactions, the model exhibits a motility-induced phase separation, typical of dry active systems. In the presence of hydrodynamic interactions, the system exhibits microphase separation instead, leading to a total disappearance of clusters. The latter state is shown to be hyperuniform and we discuss how hydrodynamic interactions affect the phase diagram of such systems.

Finally, we study another example of collective motion in active fluids. We consider the active liquid crystalline model that is often referred to as active gel or active nematic model, that is widely used in studying mechanics of biological tissues, bacterial colonies, cell mechanics, etc. Previous work on these systems mostly focussed on the case of a highly packed suspension with a constant density of active agents. Here, motivated by our work above, we introduce an analogous model that allows for local density variations. We study the onset of spontaneous flows in this model and discuss how our observations differ from their constant-density counterparts.
Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

(Renato Assante, April 2023)
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Chapter 1

Active Matter

With the word *Active Matter* we describe a system of particles that does not respect the principle of detailed balance. Some mechanism, usually some form of self propulsion, injects energy into the system at a local level, maintaining the system out of equilibrium. Opposite to more classic systems, that are driven out of the equilibrium by some global large scale mechanism (like an external flow or field gradient), the fact that the energy input is at the particle level is what makes active systems behave differently. We can divide active systems in two big categories, based on how the particles interact with their surrounding.

We talk of *Dry Active Matter* when total momentum is not conserved in the system, because the background medium in which particles move acts only as a momentum sink through friction. Examples of dry active systems can be found in nature when we look at bird flocks or animal herds. In these systems, the interaction between animals is only dictated by the rules that each element of the flock follows to move respect to the others surrounding it, and not mediated by any fluid. Conversely, we talk of *Wet Active Matter* when we have self propelled particles that are suspended in a fluid that mediates their interactions with hydrodynamics. In bacterial suspensions for example, each bacterium swims creating a fluid flow that acts as a background flow for every other swimmer in the suspension. This creates momentum-conserving long range hydrodynamic interactions that, added to the bacteria swimming and decorrelation mechanisms, contribute to the characteristic collective motion that we observe in these systems.

Since the most common active matter system are usually living ones, their
evolution is not only determined by physics, but often the biological nature of its elements comes into play with driving forces dictated by the need of nutrients, mating, a more favourable environment, or simply escaping predators.

Thanks to their peculiar out of equilibrium nature, active systems exhibit a wide range of interesting collective behaviours, such as ordered/disordered phase transitions, modified rheological properties and phase separation.

In all its declinations, active matter is able to describe an incredible number of phenomena with a wide range of nature nature and scale: from kilometre-wide animal herds and bird flocks to bacterial colonies and active polymers in the micron scale, including also man-engineered systems.

### 1.1 Dry Active Matter

As introduced before, in Dry Active Systems the medium in which particles move does not take part in the interaction between them, but rather acts at most on the single particle physics, usually as a momentum sink. In these systems, interaction are usually short ranged and mediated via communication between nearest neighbours or spatial exclusion. A first theory of dry active system was developed by Vicsek et al. [83], while working on a model to describe a bird flock. He compared this system to the non-equilibrium equivalent of a ferromagnetic system, with the only difference laying in the motility of the single particles. Further work on developing a continuous minimal model for dry active systems was pursued by Toner and Tu [80], Bertin, Droz, and Grégoire [8].

#### 1.1.1 Flocking and Vicsek Model

In his discrete model for simulating flocking, Vicsek considered a group of particles moving in space at constant speed. The rule each particle follows is that, at each timestep, it tries to align its velocity vector to the average direction of motion of its neighbours, fighting the random noise present to disturb the alignment.

We can summarise the model with these discrete equations for position $x$ and
orientation $\theta$:

$$
\theta_i(t + 1) = \langle \theta_j(t) \rangle_R + \xi, \quad (1.1)
$$

$$
x_i(t + 1) = x_i(t) + v_i(t + 1), \quad (1.2)
$$

where the $v_i(t + 1)$ has the direction of $\theta_i(t + 1)$ and constant modulus $v_0$. Averages are taken over particles in a circle of radius $R$ and $\xi$ represents a random orientational noise chosen in the interval $[-\eta \pi; \eta \pi]$. Parameters of the system are only: particle density $\rho$, speed $v_0$, and the noise level $\eta$.

It is worth to notice that for $v_0 = 0$ the system is essentially the XY-model, and therefore analogue to a ferromagnetic material. For a non-zero velocity and small densities (or high noise) particles will move around in random directions trying to form small comoving clusters. If we raise the density and lower the noise enough, we will witness a transition from chaotic to ordered motion as particles will start moving in the same average direction.

This spontaneous symmetry breaking is what differentiate active systems from ferromagnetic ones. As stated by Mermin-Wagner theorem [50], it is impossible for an equilibrium 2d system with short range interaction to develop a long range spontaneous breaking in the system’s symmetry. Flock’s property of being able to "decide" a common direction to follow reside in their nonequilibrium nature. Since each particle is moving consuming energy, the system is able to convey this energy in creating and maintaining long range fluctuations that break rotational invariance.

To describe it we utilise the average velocity normalised with single particle velocity $v_0$ as the order parameter for the system.

$$
\phi = \frac{1}{N v_0} \left| \sum_N v_i \right|. \quad (1.3)
$$

Using $\phi$ we can clearly distinguish between a completely disordered state, where every particle moves in a random direction keeping rotational symmetry ($\phi = 0$), and a fully ordered state, where all the particles in the system are coherently moving in the same direction ($\phi = 1$) breaking the isotropic symmetry of the former case. The transition between the two phases occurs when changing the density (or the noise level) of the flock. This phase transition is observed to be comparable to continuous transitions in equilibrium systems,
described by:

\[
\varphi \sim [\eta_c(\rho) - \eta]^\beta, \quad (1.4)
\]

\[
\varphi \sim [\rho - \rho_c(\eta)]^\delta. \quad (1.5)
\]

Here \(\eta_c(\rho)\) and \(\rho_c(\eta)\) are critical values for noise and density in the thermodynamic limit. Chatè et al. [19] showed that transition to collective motion in flocks is not always continuous. They show evidence that, if the system size is larger than a "crossover" value, the transition will be discontinuous. It is important to notice that this system size diverges for many limits of the system parameters, such as small velocity and extreme densities (both high and low).

1.1.2 Minimal Continuum Model

Following Vicsek work, Toner and Tu [79] developed a continuum model for the collective motion of flocks. To achieve this result, they treated the flock as a fluid using the coarse grained variables density \(\rho(r,t)\) and polarisation vector \(p(r,t)\). It is important to notice that, since particles move at constant speed, the polarisation vector works both as the orientation order parameter and as fluid velocity.

Starting from Navier-Stokes equations, keeping only the terms that remain consistent with the general symmetries and conservation laws of the system, it is possible to build a continuum theory for dry active systems. A similar result was derived by Bertin, Droz, and Grégoire [8], by coarse graining Vicsek’s model.

The most striking difference between active and ferromagnetic systems is due to the double nature of the order parameter. Since \(p\) is both the orientation and the velocity, changes in \(p\) will be advected by \(p\) itself, generating convection in the flock. This suppress velocity fluctuations at long wavelength, helping the formation and the stabilisation of the ordered phase.

Following the derivation shown by Marchetti et al. [42], we can write the equation of motion for density \(\rho\) and order parameter \(p\) as:

\[
\partial_t \rho + v_0 \nabla \cdot (\rho p) = 0, \quad (1.6)
\]

\[
\partial_t p + \lambda_1 (p \cdot \nabla) p = -\frac{1}{\gamma} \frac{\delta F_p}{\delta p} + f. \quad (1.7)
\]
Second terms on the left-hand side of each equation describe advection \( (v_0 \) being the self-propulsion velocity of each bird in the flock), and the order parameter evolution is driven by the functional derivative of the free energy \( F \).

In general, on the right-hand side of the \( \rho \) equation there should be a diffusive current depending on \( \delta F/\delta \rho \) and noise. For the sake of this derivation we ignore this term since, in both the ordered and disordered phase that the flock will present, its effects will be negligible compared to the effective diffusion due to activity.

The two advection terms have different constants (respectively \( v_0 \) and \( \lambda_1 \)) because of the double nature of \( p \), that is both orientational order parameter and current. In the density equation it acts only as an advective term, while in the order parameter equation acts on itself via advection and flow alignment as well. This leads to density and orientation fluctuations being advected at different speeds and the second term of the \( p \) equation having a phenomenological constant \( (\lambda_1 \neq v_0) \) that depends on microscopical properties of the specific system we are considering. The noise term that generate fluctuations in birds orientation is described by \( f \) and is gaussian, with zero average and delta-correlated in position, time and element of the flock.

\[
\langle f_\alpha(r, t) f_\beta(r', t') \rangle = 2\Delta \delta_{\alpha\beta} \delta(r - r')\delta(t - t'). \tag{1.8}
\]

The free energy functional in the order parameter equation is given by:

\[
F_p = \int dr \left[ \frac{\tilde{\alpha}(\rho)}{2} |p|^2 + \frac{\tilde{\beta}}{4} |p|^4 + \frac{\tilde{K}}{2} (\partial_\alpha p_\beta) (\partial_\alpha p_\beta) + \right.
\]
\[\left. + \frac{w}{2} |p|^2 \nabla \cdot p - w_1 \nabla \cdot p \frac{\delta \rho}{\rho_0} + \frac{A}{2} \left( \frac{\delta \rho}{\rho_0} \right)^2 \right]. \tag{1.9}
\]

The continuous transition from disordered to ordered phase is dictated by the \( \tilde{\alpha} \) and \( \tilde{\beta} \) terms. In particular occurs when \( \tilde{\alpha} = 0 \) and for stability \( \tilde{\beta} \) is always positive. We can model how \( \tilde{\alpha} \) changes with density around the transition using the heuristic equation:

\[
\tilde{\alpha}(\rho) = a_0 (1 - \rho/\rho_c), \tag{1.10}
\]

so that it changes sign at \( \rho = \rho_c \). A more detailed derivation is given by Bertin et al. [8] with their microscopical approach, where \( \tilde{\alpha} \) is found to be dependent also by the noise strength. If we divide the constant \( a_0 \) by \( \gamma \) we
obtain a rotational diffusion rate $D_r$ that we set to unity to scale time in our
equations. In the second term we use the one-constant approximation and take
the same elastic constant for splay and bend deformations, to describe spatial
deformations of the order parameter. The $w$ and $w_1$ terms give density and $|p|^2$
contributes to spontaneous splay ($\rho_0$ and $\delta \rho$ are respectively the average density
and the local fluctuations over the average). After integration, they generate a
local alignment field for the order parameter. Alternatively, merging the $w$ and
$\tilde{\alpha}$ terms, the former can be interpreted as a splay dependent correction to the
local order term $\tilde{\alpha}$. Finally, $A$ is a compression modulus that opposes to density
variations.

Plugging the free energy in the $p$ equation (1.7) we obtain the complete
equation of motion for the order parameter of the flock:

$$\partial_t p + \lambda_1 (p \cdot \nabla) p = - [\alpha(\rho) + \beta|p|^2] p + \nabla^2 p$$
$$- v_1 \nabla \frac{\rho}{\rho_0} + \frac{\lambda}{2} \nabla |p|^2 - \lambda \rho (\nabla \cdot p) + f. \quad (1.11)$$

The driving term is now expanded and we can identify how each part acts on
the evolution of $p$. Writing the equation of motion in this form we hid $\gamma$ in each
one of the constants: every letter without a tilde is equal to its correspondent
divided by gamma. The two new constants are $\lambda = w/\gamma$, $v_1 = w_1/\gamma$. These are
the coupling between density fluctuations and local order, same as we would
see in an equilibrium polar liquid crystal. An effective pressure gradient that
acts on $p$ is given by the sum of the third and fourth terms on the right-hand
side of the equation, using the approximation $P \sim v_1 \rho - \lambda/2 \rho_0 |p|^2$. A striking
difference between a passive system and an active one is that here the pressure
depends on density and particle’s propelling velocity instead of density and
temperature. Note how, in a more general derivation the $\lambda$ coefficients are not
all the same for every term, although deriving the equation from the free energy
functional we do not distinguish between them.

As we noted before, the system undergoes a transition between ordered and
disordered phases when $\alpha$ crosses zero. In particular, when $\alpha > 0$ it means that
the system will have a density smaller than the critical value ($\rho_0 < \rho_c$) and it
will be in a homogeneous disordered isotropic state, with $|p| = 0$ and therefore
null average velocity and preserved rotational symmetry.

When density rises over $\rho_c$, $\alpha$ becomes negative and the rotational symmetry
breaks creating an ordered state where every particle follow the same average
direction $|\mathbf{p}_0| = \sqrt{-\alpha_0/\beta}$, being $\alpha_0 = \alpha(\rho_0)$. Because of the non null average orientation, the system will now move at an average velocity $v = v_0 \mathbf{p}$.

The dilute isotropic state

We can focus first on the homogeneous isotropic state ($\alpha > 0$), studying how it behaves under small perturbations in density and polarisation around their averages ($\rho_0 < \rho_c$ and $p_0 = 0$). Linearizing the equation of motion we get:

$$
\partial_t \delta \rho = -v_0 \rho_0 \nabla \cdot \mathbf{p} \quad (1.12)
$$

$$
\partial_t \mathbf{p} = -\alpha_0 \mathbf{p} - \frac{v_1}{\rho_0} \nabla \delta \rho + K \nabla^2 \mathbf{p} + f. \quad (1.13)
$$

Searching for dispersion relations in the Fourier space we find that polarisation fluctuations transverse to the wave vector $\mathbf{q}$ decouple and decay at a rate $\alpha_0 + K q^2$, while polarisation fluctuations parallel to $\mathbf{q}$ and density fluctuations have coupled modes with frequency:

$$
\omega(\mathbf{q}) = -\frac{i}{2}(\alpha_0 + K q^2) \pm \frac{i}{2} \sqrt{(\alpha_0 + K q^2)^2 - 4v_0 v_1 q^2}. \quad (1.14)
$$

As long $v_0 v_1$ is positive, the disordered state will be linearly stable for every parameter value. With the aid of microscopic models [8] it is possible to derive that $v_1 = v_0/2$ at small densities, thus the isotropic state will be stable. For higher densities (still below transition level $\rho_c$), a dependency on density of $v_1$ arises, that brings instability effects in the isotropic phase of dry active systems.

Cates and Tailleur first studied this phenomenon, naming it motility induced phase separation, or MIPS for short [18]. We will expand further about this phenomenon in coming sections of this thesis, but for now we keep focusing on the case where the disordered phase remains stable.

When $\alpha_0$ decreases, bringing the system close to transition to the ordered phase, dispersion relations acquire a real part when $\alpha_0 \leq v_0 v_1/K$ and $q_{c-} \leq q \leq q_{c+}$ with:

$$
q_{c+}^2 = \frac{2v_0 v_1}{K^2} \left[ 1 - \frac{K \alpha_0}{2v_0 v_1} \pm \sqrt{1 - \frac{K \alpha_0}{v_0 v_1}} \right]. \quad (1.15)
$$

In this situation, density fluctuations don’t diffuse, but propagate like waves. In particular, close to transition, in the limit of $\alpha_0 \to 0^+$ also $q_{c-}$ vanishes, $q_{c+} \approx 2\sqrt{v_0 v_1}/K$ and $\omega \approx \pm q \sqrt{v_0 v_1}$ similarly to sound waves.
The dense polarised state

We now look at linear stability and properties of the system past transition, hence in the ordered state. Here average density is higher than the critical value \( \rho_0 > \rho_c \) (so \( \alpha < 0 \)) and the order parameter has a non-null average \( p_0 = p_0 \hat{n} \), where \( \hat{n} \) is the directional unit vector for the order parameter. Without loss of generality we will work in two dimensions and align \( \hat{n} \) with the \( \hat{x} \) direction in our lab reference frame. Fluctuations of the order parameter of the type \( \delta p = \hat{n} \delta p + p_0 \delta n \) will then be written as:

\[
\delta n = \delta n \hat{y}, \tag{1.16}
\]

\[
\delta p = \delta p \hat{x} + p_0 \delta n \hat{y}, \tag{1.17}
\]

and consequently the linearized equations of motion are:

\[
(\partial_t + v_0 p_0 \partial_x) \delta \rho = -v_0 \rho_0 \nabla \cdot \delta p, \tag{1.18}
\]

\[
(\partial_t + \lambda_1 p_0 \partial_x) \delta p = -2|\alpha_0| \hat{x} \delta p + a p_0 \delta \rho + \lambda_2 p_0 (\nabla \cdot \delta p) - \frac{v_1}{\rho_0} \nabla \delta \rho + \lambda_3 p_0 \nabla \delta p + K \nabla^2 \delta p + f, \tag{1.19}
\]

with \( a = - (\partial_\rho \alpha + \partial_\rho \beta p_0^2) \). This time we approach the transition from the order phase, so \( \alpha_0 \to 0^- \) and \( p_0 \to 0^+ \). Since fluctuations in magnitude of \( p \) decay with a rate proportional to \( |\alpha_0| \), near transition their timescale diverges, and we can neglect coupling to \( \delta n \). The decay of the director’s fluctuations has a stable propagating mode with frequency:

\[
\omega_n = - q \lambda_1 p_0^2 - i K q^2 \tag{1.20}
\]

For small wave vectors, the density and order parameter magnitude fluctuations are governed by:

\[
\text{Im}[\omega_n^p] = -(s_2 q^2 + s_4 q^4 + O(q^6)), \tag{1.21}
\]

\[
s_2 = \frac{v_0 v_1}{2 |\alpha_0|} \left( 1 - \frac{v_0 a^2 p_0^2}{4 v_1 |\alpha_0| \beta} \right). \tag{1.22}
\]

Instability at small \( q \) therefore occurs when \( |\alpha_0| < v_0 a^2 p_0^2 / 4 v_1 \beta \). From microscopic derivation emerges that both \( \alpha_0 \approx v_0 \) and \( v_1 \approx v_0 \), so there is a range of densities \( \rho_0 > \rho_c \) for which the ordered state is unstable at small velocities. Numerical simulations show that without noise, in this instability
region, the system is no longer completely polarised, but it is possible to see bands perpendicular to the direction of broken symmetry that travel along $\hat{x}$, similarly to what is possible to observe using the discrete Vicsek model.

If we look away from transition, at higher density and values of $\alpha_0 << 0$, fluctuations of $\delta p$ will decay at very short timescales. Assuming they already decayed (and $p_0 = 1$), and including the previously neglected diffusive terms in the $\rho$ equation, we find stable hydrodynamic modes that propagate like sound waves, with dispersion relation:

$$\omega_\pm^2 = qc_\pm(\theta) - iq^2K_\pm(\theta) + O(q^3),$$

(1.23)

Where $c_\pm(\theta)$ is the speed and $K_\pm(\theta)$ the damping of the propagating wave, depending on the angle $\theta$ that describes the direction of the wave vector. In contrast with a standard fluid, in active systems sound waves propagate at different velocities depending on the direction in which the wave is travelling. This is, of course, an effect of the missing rotational invariance and momentum conservation that is typical of active systems.

Another weird behaviour of active system consists in how density fluctuations scale with density itself. To analyse this, is useful to consider the static structure factor $S(q)$:

$$S(q) = \frac{\langle \delta \rho_q(t) \delta \rho_{-q}(t) \rangle}{\rho_0 V} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(q, \omega),$$

(1.24)

$$S(q, \omega) = \frac{1}{\rho_0 V} \int_0^\infty dt \langle \delta \rho_q(0) \delta \rho_{-q}(t) \rangle e^{i\omega t}.$$  

(1.25)

In the linearly stable regime, far from transition, we can integrate over frequencies to find $S(q)$ being proportional to $1/q^2$ and depending on the angle $\theta$. The static structure factor diverges then in the limit of large wavelength.

This has an important effect on number density fluctuations, since $S(q \to 0)$ becomes

$$\lim_{q \to 0} S(q) = \frac{\Delta N^2}{\langle N \rangle^2},$$

(1.26)

where $N$ is the number density (number of particles in a volume $V$), $\langle N \rangle$ is averaged over time, and $\Delta N^2$ is the variance of number fluctuations. In equilibrium systems $\Delta N \approx \sqrt{\langle N \rangle}$, and $S(q)$ vanishes as $1/\sqrt{\langle N \rangle}$ when $\langle N \rangle \to \infty$. In active systems, the dependence on $1/q^2$ changes things. The smallest
wave vector has to be of the order of $V^{-1/d}$ (with $d$ as the number of spatial dimensions), being $V$ directly proportional to $\langle N \rangle$, we have $S(q\to 0)\approx \langle N \rangle^{2/d}$. We can now write:

$$\Delta N \approx \sqrt{\langle N \rangle S(q \to 0)} \approx \langle N \rangle^{\frac{1}{2} + \frac{1}{d}}. \quad (1.27)$$

This implies that fluctuations in number will always grow faster regular equilibrium systems. In particular, in two dimensions systems, the exponent will be unitary bringing the fluctuations to grow at the same rate of $\langle N \rangle$. This significative enhancement of density fluctuations manifests in active systems because of how orientational fluctuations generate curvature, and curvature, being a form of local polarity, leads to a current in the flock that generate the changes in density.

1.1.3 Active Nematics

Another important example of flocking can be observed in active nematic systems. Nematic is the most fundamental orientational symmetry, where all particles are aligned on one axis, with nothing to differentiate positive from negative orientation along this direction. A common example of systems that exhibit nematic symmetry are of course any collection of elongated particles with no particular front-back distinction, such as liquid crystals. Such system is described by the conservation of number density $\rho(r, t)$ and the Q-tensor as the orientational order parameter:

$$Q_{\alpha\beta}(r, t) = \frac{1}{\rho(r, t)} \sum_i \left( \hat{\nu}_{i\alpha}(t) \hat{\nu}_{i\beta}(t) - \frac{\delta_{\alpha\beta}}{d} \right) \delta(r - r_i(t)), \quad (1.28)$$

where $\hat{\nu}_i$ is the orientation unit vector of the i-th particle and $d$ the dimensionality of the system. The Q-tensor main property is the capability of describing the local nematic order (local alignment without distinction between front and back). The free energy that drives the motion is:

$$F_Q = \int_r \left[ \frac{\alpha Q(\rho)}{2} Q : Q + \frac{\beta Q(\rho)}{4} (Q : Q)^2 + \frac{K_Q}{2} (\nabla Q)^2 + C_Q Q : \nabla \nabla \frac{\delta \rho}{\rho_0} + \frac{A}{2} \left( \frac{\delta \rho}{\rho_0} \right)^2 \right]. \quad (1.29)$$
Where we used the notation for the double dot product \((A : B = A_{ij}B_{ij})\).
The system leans towards nematic order when \(\alpha_Q < 0\) and \(\beta_Q > 0\), and we can recognize the elasticity module in \(K_Q\), a bilinear coupling for \(Q\) and \(\rho\) in the \(C_Q\) term, and the compression term \(A\) that works against variations in density \(\delta \rho\).

Finally from the expression (1.28) we notice that for 2-dimensional \(Q\)-tensors, every cubic term \(Q^3\) always vanishes. This would not hold true working in three-dimensional systems.

We can write the equation of motion for \(Q\) and \(\rho\) as usual:

\[
\begin{align*}
\partial_t Q & = -\frac{1}{\gamma Q} \frac{\delta F_Q}{\delta Q} + f_Q & (1.30) \\
\partial_t \rho & = -\nabla \cdot \left( \frac{1}{\gamma \rho} \nabla \delta F_Q \delta \rho + J_{\text{active}} \right) & (1.31)
\end{align*}
\]

Aside from the usual mobility and noise terms, we have to look closely at the density conservation equation. The density current is split in two different contributions: a passive current ruled by the mobility parameter \(1/\gamma\), and an active one due to the combined effects of activity and the geometry of the system.

The collection of particles we are considering is composed of strictly apolar elements, meaning that the whole system can have a preferred direction but, even when tightly packed, will not distinguish between front and back on this direction. A non-zero divergence of the \(Q\)-tensor generates a local curvature that will be the only form of polarity allowed in the system, and since the particles are active, this will generate a current. We can then write \(J_{\text{active}}\) as:

\[
J_{\text{active}} = \xi_Q \nabla \cdot Q. \tag{1.32}
\]

It is then possible to write a complete equation of motion for \(\rho\) as:

\[
\partial_t \rho = D \nabla^2 \rho + B \nabla^2 \nabla \cdot Q + \xi_Q \nabla \nabla \cdot Q + \nabla \cdot f_\rho. \tag{1.33}
\]

We added a random current \(f_\rho\) to generate fluctuations that are number-conserving, and grouped the constants \(D = A/\rho^2_0 \gamma_\rho\) and \(B = C_Q/\rho_0 \gamma_\rho\). We approach the study of density fluctuations only in the fully ordered state (where \(\alpha_Q < 0\), \(\beta_Q > 0\)), and we set the nematic order to be along \(\theta = 0\). To linearise the previous equation of motion, we can write the two-dimensional \(Q\)-tensor...
as:

\[ Q = \begin{pmatrix} S \cos 2\theta & S \sin 2\theta \\ S \sin 2\theta & -S \cos 2\theta \end{pmatrix}. \]  

(1.34)

We can now write \( \rho \) and \( Q \) with respect to their average value and fluctuations as:

\[ \rho = \rho_0 + \delta \rho(\mathbf{r}, t), \quad Q = \text{diag}(S, -S) + \delta Q. \]  

(1.35)

Small fluctuations in \( Q \) will have negligible diagonal elements: \( \delta Q_{xx} = -\delta Q_{yy} = O(\theta^2) \) and off-diagonal elements proportional to the angle formed with respect to the nematic order \( \delta Q_{xy} = \delta Q_{yx} \approx 2S\theta \). In Fourier space it is possible to find the correlation functions:

\[ S_{q\omega}^\rho = \frac{1}{\rho_0 V} \langle |\delta \rho_{q\omega}|^2 \rangle, \]  

(1.36)

\[ S_{q\omega}^\theta = \frac{1}{V} \langle |\theta_{q\omega}|^2 \rangle, \]  

(1.37)

\[ S_{q\omega}^{\rho \theta} = \frac{1}{V} \langle |\delta \rho_{q\omega} \theta_{q\omega}^*| \rangle. \]  

(1.38)

From the linearised equations we can observe that \( C_Q \) terms are subdominant in wave number, so they bring only a finite renormalisation in the Q-tensor equation. Dynamics of \( Q \) and \( \rho \) are then decoupled. The second term containing \( Q \) in the density equation can be viewed as noise with variance \( \propto q_x^2 q_y^2 / q^2 \) and relaxation time \( \propto 1/q^2 \). This is because the term \( \nabla \nabla : Q \) can be rewritten as \( \partial_x \partial_y \theta \), and \( \theta_q \) correlations and lifetime are proportional to \( 1/q^2 \). This noise term, purely generated by activity, is analogue to a non-number-conserving noise and with its long-time and distance effects overweighs the random current noise \( f_Q \) that has a zero-frequency weight vanishing proportionally to \( q^2 \).

### 1.1.4 MIPS

It is possible for active particle systems to undergo spontaneous liquid-gas phase separation when the activity (speed) depends directly on particle density. This phenomenon, first discovered by Cates and Tailleur [71] takes the name of motility induced phase separation (MIPS). In particular, if active particle’s speed decreases fast enough when density rises, the system can engage a positive feedback loop, in which dense regions make particle go slower, and slower particles tend to accumulate increasing local density. Thanks to this loop, an
homogeneous system can become unstable and spontaneously phase separate into a slow dense phase with highly reduced motility and a fast dilute one. It can be shown [18] that a system of swimmers having speed $v(\rho)$ that decrease with increasing density can be described at a mean field level similarly to a system of a passive Brownian particles with attractive interactions. Due to the irreversible dynamics of the active system the mapping between active and passive cases holds only under specific conditions, for instance when we assume that $\rho$ is varying slowly and we can ignore gradient contributions on the expansion of the particle velocity.

To properly treat this problem we have to resort to a modified version of the generalised Cahn-Hillard equation for phase separation, expanding the free energy at first order in gradients:

$$ F[\rho] = \int f(\rho) + c(\rho)|\nabla \rho|^2 d\rho, \quad (1.39) $$

$$ \partial_t \rho = -M(\rho)\nabla \frac{\delta F}{\delta \rho}. \quad (1.40) $$

This brings to a non-equilibrium chemical potential of the form:

$$ \mu = g_0(\rho) - \kappa(\rho)\nabla^2 \rho + \lambda(\rho)|\nabla \rho|^2. \quad (1.41) $$

We can now restore the thermodynamic treatment if we use an effective density $R(\rho)$ that obeys:

$$ \kappa R'' = -(2\lambda + \kappa')R'. \quad (1.42) $$

From this treatment we can grasp the main difference with the equilibrium phase separation. In equilibrium systems, the phase separation depends only on bulk properties. If activity enters the picture, it is necessary to take into account gradient terms where the activity appears, so physics at the interfaces takes a leading role in the dynamics of phase separation.

### 1.2 Wet Active Matter

When we look at active particles inside a fluid considering it as a proper medium, and not just a substrate, the main source of particle interaction changes from the one seen in dry systems. In dry flocking models each
particle spontaneously tries to align to others around it. When the particles are suspended in a fluid medium, what drives them to change their orientation is prevalently hydrodynamic interactions. Just by swimming, each element of the system will push fluid around it and will contribute to create the background fluid flow in which all other swimmers will move. Two main differences with the dry case arise when we look at wet systems: momentum is conserved by hydrodynamic interactions, and secondly interactions become long range.

1.2.1 Introducing Hydrodynamics

If we suspend active particles inside a fluid, these will exert an active stress on their surroundings. In most cases this active stress is caused by particles swimming and it is the mechanism through which the system breaks detailed balance (e.g. the burning of chemicals inside the cell that gives the energy to power flagella or other cellular motors). This stress is what couples the motion of active particles with the fluid equations, generating the collective dynamics that we are going to observe.

To add hydrodynamics to the system, we have to couple the concentration and orientation equations for the swimmers with a Navier-Stokes equation for the fluid velocity. We have to bear in mind that in the wet case the order parameter doesn’t parallel as the velocity field of the swimmers anymore. Now the complete velocity field will be the sum of the actual swimming velocity in the p direction plus the advection due to the background fluid velocity \( u \). To allow the coupling between swimmers and fluid equation, we have to treat swimmers as force densities acting on the fluid. The minimal model for a swimmer, as we will see in the next section, is a force dipole.

1.2.2 Swimming Mechanisms

In nature we find two main categories of swimmers, that differ in the way they propel themselves: we call pushers organisms that move pushing the fluid behind them (e.g. E. Coli, Sperm Cells), and pullers the ones that move pulling the fluid towards them (e.g. Chlamydomonas). In both cases the simplest organisms that are able to swim are composed of a main body and a propulsion
organ (typically one or more flagella) located at the back of the organism in pushers or in the front in pullers. Having pointed out the main differences between pushers and pullers we will now omit explicitly mentioning the puller case for the sake of readability, being straightforward the switch between one and the other.

Since our main goal is to study collective motion of a large number of particles, on length scales much larger than the single bacterium, it is pointless to delve further on the details of swimming mechanisms. The highlight of what is needed to continue is that pushing the fluid behind him with the flagellum, the organism will move forward, with the side effect of pushing the fluid ahead of it, since the swimmer is force-free.

We can then model both using force-free dipoles acting on the fluid around them. The only difference in modelling pushers or pullers is their dipolar strength: this will be positive for pushers, and negative for pullers. The last thing to consider to fully explain how microorganisms swim, is the run-and-tumble mechanism. Until now we only described straight motion. To change direction, bacteria undergo what is called tumbling: after a short period of linear swimming, they unbundle their flagella, with the effect of stopping abruptly and changing their orientation. These events happen in a time interval negligible with respect to the time spent swimming, so we can consider tumbling instantaneous. After the tumbling happens, the bacteria will reform its flagella bundle and start again swimming at constant speed in the new direction. In our model we can treat this similarly to a random walk, with a characteristic time and length, dictated by the average tumbling frequency and the speed of the swimmer. In the framework of collective motion, the run-and-tumble takes the role of a decorrelation mechanism and is the main source of rotational diffusion of the system.

### 1.2.3 Hydrodynamic Equations

We look at a suspension of particles described by \( \Psi(x, p, t) \), a distribution function of position \( x \) and orientation \( p \) (where \( p \) is a unit vector). The time evolution of such distribution will be regulated by:

\[
\frac{\partial_t \Psi(x, p, t)}{} = -\nabla_x \cdot (\dot{x}\Psi) - \nabla_p \cdot (\dot{p}\Psi),
\]

(1.43)
with $\Psi(x, p, t)$ normalised as $\frac{1}{V} \int_V dx \int_S dp \Psi = n$ ($V$ being the volume of space we are considering and $S$ the surface of the unit sphere). We used the notation $\nabla_p = (I - pp) \partial_p$ to represent the gradient operator on the unit sphere. Denoting propulsion speed as $U_0$, we can assert that particles oriented along $p$ will swim with velocity $U_0 p$ with respect to the background fluid. For a more complete description of the single particle equations of motion we can write:

$$
\dot{x} = U_0 p + u - D \nabla_x (\ln \Psi),
$$

(1.44)

$$
\dot{p} = (I - pp) \cdot [(\gamma E + W) \cdot p - d_r \nabla_p (\ln \Psi)].
$$

(1.45)

The three terms on the right-hand side of the translational velocity equation are respectively: self propulsion, background fluid flow ($u(x, t)$) and translational diffusion with a constant coefficient $D$. The angular velocity instead is generated by local flow only, through the tensorial terms $E = 1/2(\nabla u + \nabla u^\dagger)$ (fluid rate of strain) and $W = 1/2(\nabla u - \nabla u^\dagger)$ (vorticity). The coefficient $\gamma$ is a shape parameter for the swimmer that takes values between $-1$ and $1$ ($\gamma \approx 1$ for slender rods). Finally, as for the previous equation, we model rotational diffusion with a constant coefficient $d_r$.

From the distribution function, we can define the local concentration field and the director field respectively:

$$
c(x, t) = \int_S \Psi(x, p, t) dp,
$$

(1.46)

$$
n(x, t) = \frac{1}{c(x, t)} \int_S p \Psi(x, p, t) dp.
$$

(1.47)

We look now at the evolution equation for $c(x, t)$, derived integrating the conservation equation for $\Psi$ over orientations and using the incompressibility condition for the fluid ($\nabla_x u = 0$):

$$
\partial_t c + u \cdot \nabla_x c - D \nabla_x^2 c = -U_0 \nabla_x \cdot (cn).
$$

(1.48)

On the left-hand side we have an advective term that originates from fluid flow and a diffusive term that contrasts the advection. On the right-hand side we can see how concentration evolution is directly driven by a $cn$ term, that acts as a source and involves the director field and self propulsion $U_0$.

Having described the particle evolution, now we can write down the mass and
momentum conservation for the fluid, resulting in:

\[
\nabla \cdot \mathbf{u} = 0, \quad (1.49)
\]

\[
-\mu \nabla^2 \mathbf{u} + \nabla_x q = \nabla_x \cdot \Sigma_p. \quad (1.50)
\]

The first of these two equations is the condition for an incompressible fluid that we already took advantage of, while in the second we denote the viscosity as \(\mu\), pressure as \(q\) and the active stress that drives the motion as:

\[
\Sigma_p(x, t) = \sigma_0 \int_S \Psi(x, p, t) \left( pp - \frac{1}{3} \right) \, dp. \quad (1.51)
\]

As we mentioned before a single swimmer can be modelled as a force dipole, and we are now denoting with \(\sigma_0\) its dipole strength. The active stress tensor in the position \(x\) is the configuration average over all the orientations of all the force dipoles that the particles at that position exert on the fluid. Scaling distances by the swimmer length \(l\), velocities by the swimming speed \(U_0\) and times by \(l/U_0\) we can reduce the dipole strength \(\sigma_0\) to a constant \(\alpha\) that depends purely on the swimming mechanism:

\[
\frac{\sigma_0}{U_0 \mu l} = \alpha, \quad (1.52)
\]

Being \(\alpha < 0\) for pushers and \(\alpha > 0\) for pullers.

Making the right choice of units it is possible to make the evolution equations dimensionless, and consequently eliminate every constant except for those related to shape of the particles and swimming mechanism (\(\gamma\) and \(\alpha\)). In particular, using \(u_c = U_0\), \(l_c = 1/nt^2\) and \(t_c = l_c/u_c\) we get the new normalisation as:

\[
\frac{1}{V} \int_V \, dx \int_S \, dp \Psi = 1, \quad (1.53)
\]

the dimensionless equations for particle motion

\[
\dot{x} = \mathbf{p} + \mathbf{u} - D \nabla_x (\ln \Psi), \quad (1.54)
\]

\[
\dot{\mathbf{p}} = (\mathbf{I} - \mathbf{pp}) \cdot [(\gamma \mathbf{E} + \mathbf{W}) \cdot \mathbf{p} - d_r \nabla_p (\ln \Psi)], \quad (1.55)
\]
(with $D$ and $d_r$ dimensionless), and the continuity and momentum equations

$$\nabla \cdot \mathbf{u} = 0, \quad (1.56)$$
$$-\nabla^2 \mathbf{u} + \nabla x q = \nabla x \cdot \Sigma^p. \quad (1.57)$$

with dimensionless active stress tensor $\Sigma^p(x, t) = \alpha \int_S \Psi(x, p, t) \left( pp - \frac{1}{3} \right) dp$. We can now look at stability of an active suspension, and to do that we look first at the entropy of the system:

$$S = \int_V dx \int_S dp \frac{\Psi}{\Psi_0} \ln \left( \frac{\Psi}{\Psi_0} \right). \quad (1.58)$$

For $\Psi(x, p, t) = \Psi_0 = 1/4\pi$ the system is in a homogeneous isotropic state that minimises entropy ($S = 0$). Through some algebra using conservation equation for $\Psi$ and momentum equation we find that changes in entropy are described by:

$$4\pi \dot{S} = -\frac{6\gamma}{\alpha} \int_V dx \int_S dp \frac{\Psi}{\Psi_0} \ln \left( \frac{\Psi}{\Psi_0} \right) \left( d_r |\nabla x \ln \Psi|^2 + d_r |\nabla_p \ln \Psi|^2 \right) \Psi, \quad (1.59)$$

where the first term in the right-hand side is a flux term generated from the active stress tensor, and the second term is clearly translational and rotational diffusion. The diffusion terms (both translational and rotational) are always contributing negatively to $\dot{S}$, lowering the entropy and pushing the system towards the homogeneous and isotropic state. The global sign of the entropy change depends then on the sign of $\alpha$, and therefore on the swimming mechanism of the particles that propel in the fluid.

If the particles are pullers ($\alpha > 0$) the flux term will have the same sign of the diffusion, contributing to lower $S$, so that any fluctuation will dissipate into the isotropic and homogeneous state where the entropy assumes its minimum value ($S = 0$). If we are dealing with pushers instead ($\alpha < 0$), the system will undergo a positive feedback loop where fluctuations and velocity gradients are sustaining themselves mutually, giving a positive contribute to the entropy growth, in contrast with the diffusion term that tries to slow down this growth. The two terms will at some point reach a stable balance and the system will reach its steady state. It is possible to address better this problem studying linear stability for the two cases of aligned and isotropic states.

Take a system that is almost uniform and aligned along $\hat{z}$ axis with some
deviation:

\[ c(x, t) = 1 + \epsilon \delta c(x, t), \quad (1.60) \]
\[ n(x, t) = \hat{z} + \epsilon \delta n(x, t). \quad (1.61) \]

In this notation \( \epsilon \) is an arbitrary small constant (\(|\epsilon| \ll 1\)) and \( \delta n \cdot \hat{z} = 0 \) in order to keep \( n \) a unit vector. Solving the linearised equations of motion in the Fourier space and looking for plane wave solutions of the type \( \delta c = \tilde{c}(k) \exp \left[ ik \cdot x + \sigma t \right] \), following the steps of [60] we find the dispersion relation:

\[ \lambda_\pm = \frac{1}{2} f(\theta) \cos 2\theta \left[ 1 \pm \left( 1 + 4ik \frac{\sin^2 \theta \cos \theta}{f(\theta \cos^2 2\theta)} \right)^{1/2} \right], \quad (1.62) \]

where \( \lambda = \sigma \pm ik \cos \theta \), being \( \theta \) the angle the plane wave travels at with respect to \( \hat{z} \), and \( f(\theta) = -\alpha[(\gamma + 1) \cos^2 \theta - (\gamma - 1) \sin^2 \theta]/2 \) is a function that stores all the information about shape and swimming mechanism. Looking at the growth rate \( \Re(\lambda) \) we can confirm that the aligned case is always unstable, since for \( k > 0 \), independently of swimmer’s type there is always a fluctuation growth rate greater than zero, no matter what angle the wave travels. Note that if concentration is high enough to force the modelling of steric interaction to describe the system correctly, it is possible for it to overcome the instability and lead to a stable aligned case.

In the second case we have an isotropic and non uniform system, described by:

\[ \Psi(x, p, t) = \frac{1}{4\pi} \left[ 1 + \epsilon \delta \Psi(x, p, t) \right]. \quad (1.63) \]

Solving for plane wave solutions of the form \( \delta \Psi(x, p, t) = \tilde{\Psi}(p, k) \exp [ik \cdot x + \sigma t] \), we find the dispersion relation:

\[ \frac{3i\alpha \gamma}{4k} \left[ 2a^3 - \frac{4}{3}a + (a^4 - a^2) \log \left( \frac{a - 1}{a + 1} \right) \right] = 1, \quad (1.64) \]

with \( a = (i\sigma + Dk^2)/k \). Solving numerically the dispersion relation for a system of pushers, it is possible to see how, for small values of \( k \) \( \Re(\sigma) > 0 \) and \( \Im(\sigma) = 0 \), meaning that shear stress fluctuations will grow. For higher wavenumbers, \( \Re(\sigma) \) decreases until it reaches zero, where the fluctuations become damped. Different values of translational diffusion contribute with a term \( Dk^2 \), therefore only helping the dampening appear at lower values of \( k \). For pullers the fluctuation growth rate is always negative, resulting in the
suspension being always stable.

1.3 Conclusions

In this Chapter we described the state of the art of the study of active matter. Active matter began as a simple model to describe how bird flocks fly in the sky, but rapidly grew up to current models that lay the ground for new research in many scientific fields: from pure statistical mechanics, to applications in better understanding biological phenomena or technical improvements in medicine and engineering.

We described the basic theory for dry active matter, introducing the continuum model and the concepts of active nematics and motility-induced phase separation that we will encounter in future chapters. Most importantly for the purpose of this thesis, we introduced the effect of hydrodynamic interactions in a active system, to describe what is then called wet active matter, meaning that the medium on which particles move is not just a momentum sink as in dry active matter, but acts as the medium through which single particles interact. We here described the ideas behind the swimming mechanisms of wet active particles and the hydrodynamic equations we will need in the future Chapters of this thesis.
Chapter 2

Swimming Crystals

In this chapter we will lay down the basic lattice model for simulations that we developed to study the collective evolution of microswimmer suspensions.

As we saw in the previous Chapter, when concentration is above a certain threshold, active suspensions undergo a phase transition. At lower concentrations, swimming particles move independently, making the whole suspension homogeneous and isotropic. Above the density threshold, particles in the suspension start moving collectively, forming coherent flows and vortices at bigger length scales than the typical swimmer’s size.

Even though in bacterial suspensions swimmers have a very low Reynolds number, when the collective motion sets in we can observe a chaotic pattern of vortices and jets, that reminds of turbulent flows we see in systems with high Reynolds numbers. For this reason the collective motion phase in bacterial suspension is also known as bacterial turbulence.

In previous papers [68] it was hinted that bacterial turbulence is obtainable not only in suspensions of swimmers, but also in suspensions of microorganisms that push the fluid without propelling themselves in any direction (we call these shakers). Following the idea behind this information, we wanted to check whether active turbulence was possible when the particles in the suspension are stripped completely of any translational degree of freedom.

To pursue this idea we created a model for swimmers suspensions where each swimmer, modelled as a force dipole acting on the surrounding fluid, is free to rotate but its position is fixed on a rigid lattice. This led to an interesting result:
without rotational decorrelation, the suspension quickly reached a frozen stable steady state configuration, that we found fundamentally different in pushers and pullers.
The former tried to reach a tetradic configuration, where each swimmer tends to be perpendicular to its neighbours, while the latter arrange themselves to be in a local nematic configuration. Since in our model we witnessed that without decorrelation the isotropic state is always linearly unstable and decaying in the frozen state mentioned above, we identified the latter with collective motion in the active suspension.

2.1 Model Swimmer

Our model consists of N swimmers modelled, as we stated previously, as a point dipole located at position \( \mathbf{r} \) with orientation \( \mathbf{p} \) and length \( L \). Being the i-th swimmer fixed in position, its evolution is only dictated by the equation:

\[
\dot{p}_i^\alpha = \left( \delta^{\alpha\beta} - p_i^\alpha p_i^\beta \right) p_i^\gamma \nabla_\gamma U^\beta(\mathbf{r}_i),
\]  
(2.1)

where \( \delta^{\alpha\beta} \) is the Kronecker delta, and \( U(\mathbf{r}_i) \) is the fluid velocity at the position of the i-th swimmer. In this treatment the fluid velocity at \( \mathbf{r}_i \) will be generated by all the other dipoles in the system. To implement this equation in the simulations, we can write Eq.(2.1) up to the first order in \( \Delta t \) as:

\[
p_* = p_i + z_i \Delta t,
\]  
(2.2)

\[
p_i(t + \Delta t) = \frac{p_*}{|p_*|},
\]  
(2.3)

with \( z_i^\beta = p_i^\gamma \nabla_\gamma U^\beta(\mathbf{r}_i) \). Anticipating Chapter 3, we will add tumbling changing the dipole orientation randomly with a frequency \( \lambda \): at each timestep of our simulation every dipole will have a chance \( 1/\lambda \) to reorient in a new direction picked randomly from a uniform distribution. Each dipole interacts with the fluid applying two point forces of the same magnitude \( F \): \( F\mathbf{p}_i \) at the head of the swimmer positioned at \( \mathbf{r}_i \), and an opposite one \( -F\mathbf{p}_i \) at its tail at \( \mathbf{r}_i + L\mathbf{p}_i \). The sign of the force modulus will determine if the swimmer is a pusher (\( F > 0 \)) or a puller (\( F < 0 \)). The dipole acts then on the fluid via two stokeslets, of the
form:

\[ G_{\alpha\beta}(\mathbf{r}) = \frac{\delta_{\alpha\beta}}{r} + \frac{x_{\alpha}x_{\beta}}{r^3}, \]  

(2.4)

with \( x_{\alpha/\beta} \) being the cartesian component of \( \mathbf{r} \) and \( r \) its modulus. The fluid velocity field generated by the i-th dipole at position \( \mathbf{r} \) will then be:

\[ V^\alpha_i(\mathbf{r}) = \frac{F}{8\pi\mu} \left[ G_{\alpha\beta}(\mathbf{r} - \mathbf{r}_i - Lp_i)p_i^\alpha - G_{\alpha\beta}(\mathbf{r} - \mathbf{r}_i)p_i^\alpha \right] \]

\[ \approx \frac{F}{8\pi\mu} \left[ G_{\alpha\beta}(\mathbf{r} - \mathbf{r}_i) + \nabla_\gamma G_{\alpha\beta}(\mathbf{r} - \mathbf{r}_i)(-Lp_i^\gamma) - G_{\alpha\beta}(\mathbf{r} - \mathbf{r}_i)p_i^\alpha \right] \]

\[ = -\frac{FL}{8\pi\mu}p_i^\alpha p_i^\gamma \nabla_\gamma G_{\alpha\beta}(\mathbf{r} - \mathbf{r}_i). \]  

(2.5)

### 2.2 Swimmers on a Lattice

We consider a square lattice of size \( N = M \times M \), and spacing \( a \). At each lattice point we locate a single swimmer as described in the previous section. Knowing the distribution of all the swimmers on the lattice now we can compute the total value of \( U(\mathbf{r}_i) \) by summing all the \( V_i(\mathbf{r}) \) contributions from the other swimmers in the system:

\[ U^\beta(\mathbf{r}_i) = \sum_{i=1}^{N} V^\beta_j(\mathbf{r}) = -\frac{FL}{8\pi\mu} \sum_{i=1}^{N} p_j^\alpha p_j^\delta \nabla^\delta G_{\alpha\beta}(\mathbf{r}_i - \mathbf{r}_j), \]

(2.6)

making it possible to write down the expression for the update step \( z_i \):

\[ z_i^\beta = p_i^\gamma \nabla_\gamma U^\beta(\mathbf{r}_i) = -\frac{FL}{8\pi\mu} \sum_{i=1}^{N} \sum_{i \neq j} p_j^\gamma p_j^\delta \nabla_\gamma \nabla^\delta G_{\alpha\beta}(\mathbf{r}_i - \mathbf{r}_j). \]

(2.7)

Evaluating the term inside the summation, and removing the terms parallel to \( \mathbf{p}_i \), since they will disappear anyway after the action of the projector operator \( (\delta_{\alpha\beta} - \mathbf{p}_i^\alpha \mathbf{p}_i^\beta) \) in Eq.2.1, we obtain the following equation for \( z_i \):

\[ z_i^\beta = -\frac{FL}{8\pi\mu} \sum_{i=1}^{N} \sum_{i \neq j} \frac{3(\mathbf{p}_i \cdot \mathbf{\hat{x}}_{ij}) + 6(\mathbf{p}_i \cdot \mathbf{p}_j)(\mathbf{p}_j \cdot \mathbf{\hat{x}}_{ij}) - 15(\mathbf{p}_i \cdot \mathbf{\hat{x}}_{ij})(\mathbf{p}_j \cdot \mathbf{\hat{x}}_{ij})^2}{|x_{ij}|^3} x_{ij}^\beta, \]

(2.8)
where $x_{ij} = r_i - r_j$ is the distance between $i$-th and $j$-th lattice points, and
\[ \hat{x}_{ij} = x_{ij} / |x_{ij}|. \]
As a last step in this derivation we can use dimensionless units by scaling distances with lattice spacing $a$ and times with
\[ \tau = FL/(8\pi\mu a^3) \]
resulting in:
\begin{equation}
  z_i^\beta = \text{sgn}(F) \sum_{i=1}^{N} \frac{3(p_i \cdot \hat{x}_{ij}) + 6(p_i \cdot p_j)(p_j \cdot \hat{x}_{ij}) - 15(p_i \cdot \hat{x}_{ij})(p_j \cdot \hat{x}_{ij})^2}{|x_{ij}|^3} x_{ij}^\beta. \tag{2.9}
\end{equation}

This expression is of great use for computational purposes, since reduces the update step for the dipole orientation to being dependent only on distances between lattice points and the relative unit vectors. Those values can be precomputed at the start of the simulation and save a great amount of computational time and resources.

### 2.3 Frozen lattice

Simulating systems of pushers and pullers on our lattice without rotational diffusion we can see in detail the patterns formed when the system reaches the frozen state. In figure [2.1] we can see how pushers and pullers arrange themselves in a tetradic and nematic configuration respectively. It is shown on the right side of the figure how for a single run (of $N=400$ swimmers) some defects appear on the configuration, while on the left is the most probable distribution of swimmers. We suspect that these defects are a finite-size effect and will disappear in the thermodynamic limit with larger systems.

To show when the frozen state is effectively reached we introduce the quantity $\bar{Z}(t)$ to represent the average magnitude squared of dipoles’ angular velocity:
\begin{equation}
  \bar{Z}(t) = \frac{1}{N} \sum_{i=1}^{N} \left[ \left( \delta^{\alpha\beta} - p_i^\alpha p_i^\beta \right) z_i^\beta \right]^2. \tag{2.10}
\end{equation}

In figure [2.2] we can see an example of the temporal evolution of $\bar{Z}(t)$ for a lattice of $N = 400$ pullers on a squared lattice, as the one showed in figure [2.1].

Here $\bar{Z}(t)$ rapidly decays to $10^{-2}$ and briefly oscillates around those values. After that small period of time $\bar{Z}(t)$ reaches $10^{-14}$ and remains stable in this state, where we can consider the system frozen in a static state.

The next question to address is whether the frozen states are always reached...
eventually. To answer this we performed a large number of runs for a single lattice size recording the freezing time, namely the first instant when the value of $\bar{Z}(t)$ falls below $10^{-10}$. Using the resulting freezing times distribution we can define the survival probability:

$$S(t) = 1 - \frac{\sum_{j=1}^{N_{\text{runs}}} \theta(t - t_j)}{N_{\text{runs}}} ,$$

(2.11)

where $\theta(t)$ is the step function, $0 < t < T_{\text{max}}$ is a time value between zero and the total simulation time $T_{\text{max}}$, and $N_{\text{runs}}$ is the number of runs performed. The quantity $S(t)$ represents then the probability that the system is not in a frozen state after time $t$. In figure 2.3 we show the decay of the survival probability with time in a system of swimmers (pushers) for increasing lattice sizes. Times are here normalized as mentioned in the previous section ($\tau = FL/(8\pi \mu a^3)$). The calculation for $S(t)$ has been performed with $N_{\text{runs}} = 10^4$. We can see
Figure 2.2 Evolution of $\bar{Z}(t)$ against time for a square lattice of $N = 400$ swimmers (pushers). It is noticeable how the rotational dynamic dies after a short time that, even if survival probability at the same time instant increases with system size, the curves appear to get closer to each other when the system grows bigger, hinting a convergence in the shape of $S(t)$ that is reached for very large systems.

Figure 2.3 Survival probability of a system of pushers of different lattice linear sizes.

For a more quantitative measure of this convergence we can also plot the average stopping time $\bar{t}_0$ for each lattice against the system size. In figure 2.4 we show these data along with a function we used to fit them.
The best fit the data shown in figure 2.4 we found to be:

$$\bar{t}_0 = 274.189 - 353.349 \exp\left(-0.0186788 \sqrt{N}\right).$$

With the growth of system size, the average stopping time approaches a convergence value with an exponential slowdown. Already for systems with $\sqrt{N} = 400$ we would reach a $\bar{t}_0$ within 0.1% of the convergence value. Although these plots are not strict proof of the actual convergence of the freezing time with lattice size, we were not able to run these tests for systems bigger than $N = 50 \times 50$ because of the limit imposed by the long computational times needed to make enough runs to get an accurate statistics on bigger systems.

2.4 Tumbling

In active suspensions, when no orientational decorrelation mechanisms are involved in the system dynamics, the homogeneous and isotropic state is always linearly unstable. After it evolves for enough time without such decorrelations, the system always reaches a state where collective motion sets in. As described in the previous section, starting simulations using our model with the same premises of no decorrelations allowed in the evolution, the
system always reaches the frozen states (tetradic or nematic). Inferring from this consideration, we can then interpret the frozen states in our model as a corresponding representation of the active collective motion.

After having acknowledged this analogy, and given a physical interpretation to the frozen states, we can study how the system reacts to decorrelation. We decided to look at two different mechanisms for orientational decorrelations: tumbling and rotational diffusion. As mentioned in the first chapter, microswimmers move with the so-called run and tumble motion: they normally swim on a straight line with constant speed (run state) until they suddenly stop to abruptly change their direction in a random new one (tumble event). This is the main mechanism microorganisms use to autonomously change their orientation in order to swim towards favourable environments (more food, light or other energy sources) or away from unfavourable ones.

While tumbling is a discrete change in direction that happens with a specific frequency during the swimmer’s motion, rotational diffusion is a continuous effect that forces the swimmer to smoothly change its direction, and it’s typically due to thermal effects.

In our model we denote with $\Lambda$ the dimensionless tumbling rate, which is related to its dimensional counterpart $\lambda$ by the expression:

$$\Lambda = \frac{8\pi mu^3}{FL}.$$  

**Figure 2.5** Different decorrelation mechanisms. On the left, run-and-tumble motion is characterised by the swimmer moving in a straight line (run) until a sudden reorientation event (tumble) changes its direction of motion. On the right instead, rotational diffusion is represented; here the direction of motion changes smoothly and continuously.
We can reshape this equation by using reduced units for dipolar strength ($\kappa = FL/\mu$) and substituting $1/a^2$ with $n_{2D}$, the area density of dipoles, obtaining:

$$\Lambda = \frac{8\pi a \lambda}{\kappa n_{2D}}.$$  \hspace{1cm} (2.14)

Utilising analytical work performed by Škultéty et al.\[87\], we can derive that orientational instability sets in when this relation is satisfied:

$$\left(\frac{\lambda}{\kappa n_{2D}}\right)_{crit} = \frac{k_{max}}{8},$$  \hspace{1cm} (2.15)

or, using dimensionless quantities:

$$\Lambda_{crit} = \pi a k_{max}.$$  \hspace{1cm} (2.16)

In previous equations, we denoted with $k_{max}$ the highest Fourier wavenumber available in the system. In our case this is the inverse of lattice spacing $a$, so we obtain $\Lambda_{crit} = \pi$.

### 2.5 Conclusions

In this Chapter, we discussed the basics behind the first implementation of our lattice model. We chose our minimal swimmer model to be a single force dipole (of positive sign for pushers and negative for pullers) acting on the surrounding fluid and free to rotate affected by the local fluid flow. Fixing these swimmers on a square lattice and leaving them free to rotate, we observed that the system, without decorrelation, always incurred in freezed states both for pushers and pullers suspensions, leading us to identify these states with collective motion in the active suspension.

This Chapter lays the ground for the understanding of our lattice model for motility-induced phase separation in a swimmer suspension. In the next Chapter we will re-introduce translational degrees of freedom to our model, giving swimmers the ability to move between lattice points, and implement decorrelation mechanisms in the form of tumbling and diffusion. This will lead us to understand how the presence of hydrodynamic interactions affects the motility-induced phase separation in swimmers suspensions.
Chapter 3

A lattice model of motility-induced phase separation in the presence of hydrodynamic interactions

As mentioned in the Introduction, active matter comprises systems that are strongly out-of-equilibrium. Self-propelled particles break the detailed balance principle at the microscopic scale [15], and do not obey the laws of equilibrium statistical mechanics. As the consequence, the observed state of active systems in the absence of any external forcing is not given the minimum of the corresponding free energy and can involve large-scale macroscopic currents. Often such currents take the form of large-scale collective motion of the particles, where a finite number of particles exhibiting the same type of motion in the thermodynamic limit [42, 55, 84].

One of the most striking example of such a non-equilibrium phenomenon is the motility-induced phase separation (MIPS) [18]. Similar to the Ising model in equilibrium statistical physics, it requires a small number of physical ingredients to generate a novel non-equilibrium phase transition. In its simplest form, MIPS can be observed with self propelled particles that interact with each other through an excluded volume potential (see [58], for example). A small amount of spatial diffusion is often required to prevent kinematic trapping in intermediate, metastable states [65]. At low volume fractions and/or for slowly
moving particles, the system can be described as a disordered collection of run-and-tumble particles. At sufficiently high volume fractions and self-propulsion speeds, the system separates into a dense cluster embedded into a low-density gas phase. As in a true phase separation, the volume fractions of the particles in the high- and low-density phases are set by the system’s parameters (self-propulsion speed, volume fraction and spatial diffusivity) and is independent of the system size; this implies that the size of the clusters is growing linearly with the system size and this is often used to prove the nature of the transition in question.

The minimal number of ingredients required to study this transition ensured that it received a lot of attention in the community. There is now a very large number of theoretical and numerical studies confirming the phenomenology described above [41, 51, 52, 57, 58, 69, 82, 92]. Its experimental confirmation is significantly less developed with the main difficulty being associated with creating particles that can self-propel autonomously. The most popular choices utilised in this context are phoretic [13, 36, 53, 75] or light-controlled particles [5] and motile organisms [38]. Both systems differ fundamentally from the minimal ingredients described above as both types of particles require the presence of a suspending viscous fluid to operate. Such a fluid mediates long-range hydrodynamic interactions and it is unclear whether the phenomenology described above can at all be observed under these conditions. Moreover, experiments on motility-induced phase separation in these systems are further complicated by the unavoidable presence of confining boundaries. With motile organisms known to accumulate in a close vicinity of solid [7] and liquid [85] boundaries, and with synthetic microswimmers being sufficiently heavier than the surrounding fluid to sediment to the bottom of the confining geometry, experimental studies of motility-induced phase separation necessarily involve these two additional ingredients: the presence of a viscous fluid and of a confining boundary. Under these conditions, experiments seem to confirm the existence of dense clusters of self-propelled particles [13, 36, 53]. However, their size appears to be set by an unknown mechanism and not depend trivially on the system size.

Here, we study how hydrodynamic interactions influence motility-induced phase separation. This question has already been studied in numerical simulations with the emerging consensus being that the presence of fluid-mediated interactions suppresses MIPS [1, 10, 48, 93]. These works, however, either
focused on truly two-dimensional systems or a layer of microswimmers tightly confined between two solid boundaries. Here we argue that these arrangements miss an important aspect of the emerging hydrodynamic interactions.

To illustrate the point, consider a force dipole - the simplest model for the velocity field generated by a microswimmer far away from its surface \cite{35}. Let us assume that the dipole is positioned parallel to a solid wall at a distance \( h \) away from it. The fluid velocity component \( u_\parallel \) parallel to the wall can be deduced from the image system developed by \cite{9} for a point force next to a solid boundary with vanishing boundary conditions \( u_\parallel(z = h) = 0 \), and is given by \cite{66}:

\[
\begin{align*}
  u_\parallel(x) &= \frac{\kappa}{8\pi \left| x \right|^3} \left[ 3 \frac{(x \cdot p)^2}{\left| x \right|^2} - 1 \right] + \frac{x}{R^3} \\
  &\quad - \frac{3(x \cdot p)^2 + 6h^2 \{x + 2p(x \cdot p)\}}{R^5} + \frac{30h^2(x \cdot p)^2 x}{R^7}.
\end{align*}
\]

(3.1)

Here, \( p \) and \( x \) are two-dimensional vectors that lie in the plane parallel to the wall and denote respectively the dipole orientation and the point where the velocity is evaluated relative to the position of the swimmer. Furthermore, \( R = \sqrt{|x|^2 + 4h^2} \), and \( \kappa \) is the strength of the dipole. In the limit \( h \to \infty \), this expression reduces to the well-known result for the force dipole in an infinite three-dimensional fluid.

Now we calculate the total flux of the fluid through a circle of radius \( X \) centred on the microswimmer with the plane of the circle being parallel to the wall. This calculation yields

\[
\int_{|x|=X} d\mathbf{x} \cdot \mathbf{u}_\parallel = \frac{\kappa}{8X} \left[ 1 - \frac{X^4 - 10X^2h^2 + 64h^4}{(X^2 + 4h^2)^{7/2}} X^3 \right].
\]

(3.2)

A similar result can be obtained next to liquid-liquid interface. This observation has profound implications for hydrodynamic interactions in the vicinity of a boundary. Since the total flux through an arbitrary circle around a microswimmer is non-zero, the velocity components parallel to the boundary behave as if the fluid is effective compressible. Furthermore, the sign of the expression for the flux derived above is determined by the sign of \( \kappa \), as its prefactor is strictly positive. Thus, on average, microswimmers with \( \kappa > 0 \)
(pushers) act as hydrodynamic sources in the plane parallel to the boundary, while microswimmers with $\kappa < 0$ (pullers) act as hydrodynamic sinks. When averaged over all orientations, two pusher microswimmers advect each other away, while two pullers effectively attract each other. This argument illustrates that hydrodynamic interactions between dipolar microswimmers moving next to a boundary have a very different nature than their bulk counterparts, which has previously been shown to promote dynamic self-assembly and crystallisation in active particle systems [64, 77].

In this Chapter, we study the effect of such effectively compressible in-plane hydrodynamic interactions on motility-induced phase separation. We choose to study this effect in the simplest possible setting and consider a layer of microswimmers confined to move on a two-dimensional plane surrounded by a three-dimensional fluid, far away from any boundary. We assume that the velocity field of each microswimmer is given by a dipolar field. This setting still has the effective compressibility of the in-plane fluid velocity as can be seen from Eq. (3.2) in the limit $h \to \infty$. To take into account the excluded volume interactions in its most rudimentary form, we constraint the microswimmers to move on a square lattice with only a single microswimmer being allowed to occupy a given lattice site. Below we will show that this simple model generates a rich variety of predictions. First, we observe that hydrodynamic interactions suppress MIPS, in line with the previous studies. Importantly, we demonstrate that they also change the nature of the transition leading to a microphase separation. At very high values of the dipolar fields, we observe a novel hyperuniform state, specific to systems with effectively compressible hydrodynamic interactions.

3.1 Model

3.1.1 Equations of motion

We consider a collection of model microswimmers confined to move on a two-dimensional (2D) square lattice. As discussed in the introduction, the lattice is embedded in a three-dimensional (3D) fluid and all hydrodynamic interactions are assumed to take a form suitable for 3D. The lattice consists of $H \times H$ sites, where $H$ is an integer, with the lattice spacing being $a$. The
microswimmers are modelled as $N$ point dipoles with their spatial positions being confined to the lattice sites, while their orientations are continuous and can point anywhere on the microswimmer plane. The microswimmer dynamics consist of the following ingredients: the spatial position of a microswimmer changes due to its self-propulsion, advection by the velocity field generated by all other microswimmers at its position, and translational diffusion; its orientation changes due to its aligning in the velocity field created by the other microswimmers at its position, and random tumbling. We now discuss all these ingredients in turn.

We assume that the dipolar microswimmers are located at the lattice positions $\mathbf{r}_i$ and have instantaneous orientations $\mathbf{p}_i$, where $i = 1 \ldots N$ enumerates the microswimmers. Each microswimmer obeys the following Jeffrey’s equation

$$\dot{\mathbf{p}}_i^\alpha = \left( \delta^{\alpha\beta} - \mathbf{p}^\alpha_i \mathbf{p}^\beta_i \right) z^\beta_i,$$  \hspace{1cm} (3.3)

where

$$z^\beta_i = \mathbf{p}^\gamma_i \nabla^\gamma U^\beta_i (\mathbf{r}_i),$$  \hspace{1cm} (3.4)

that treats each microswimmer as an infinitely slender object, i.e. strongly aligning in an external flow. Here, $\delta^{\alpha\beta}$ is the Kronecker delta, $U_i(\mathbf{r}_i)$ is the velocity field generated by all other dipoles at the position of dipole $i$, and indices refer to the Cartesian components the vectors.

To evaluate $z^\beta_i$, we start from the velocity field of a dipole $j$ comprising two point forces: $-F \mathbf{p}_j$ applied at $\mathbf{r}_j$ and $F \mathbf{p}_j$ applied at $\mathbf{r}_j + L \mathbf{p}_j$, where $F$ is the magnitude of the force and $L$ is the dipolar length. The velocity field generated by such an arrangement far away from the dipole is given by

$$V^\alpha_j (\mathbf{r}) = \frac{F}{8\pi \mu} \left[ G^{\alpha\beta} (\mathbf{r} - \mathbf{r}_j - L \mathbf{p}_j) p^\beta_j - G^{\alpha\beta} (\mathbf{r} - \mathbf{r}_j) p^\beta_j \right]$$

$$\approx \frac{F}{8\pi \mu} \left[ G^{\alpha\beta} (\mathbf{r} - \mathbf{r}_j) + \nabla^\gamma G^{\alpha\beta} (\mathbf{r} - \mathbf{r}_j) (-L p^\gamma_j) - G^{\alpha\beta} (\mathbf{r} - \mathbf{r}_j) \right] p^\beta_j$$

$$= -\frac{FL}{8\pi \mu} p^\gamma_j p^\beta_j \nabla^\gamma G^{\alpha\beta} (\mathbf{r} - \mathbf{r}_j),$$  \hspace{1cm} (3.5)

where

$$G^{\alpha\beta}(\mathbf{r}) = \frac{\delta^{\alpha\beta}}{r} + \frac{x^\alpha x^\beta}{r^3},$$  \hspace{1cm} (3.6)
is the Stokeslet, \( r = |\mathbf{r}| \), \( x^\alpha \) are Cartesian components of \( \mathbf{r} \), and \( \mu \) is the viscosity of the suspending fluid. The total velocity field at the position of dipole \( i \) is then

\[
U^\beta(\mathbf{r}_i) = \sum_{j=1}^{N} V^\beta_j(\mathbf{r}_i) = -\frac{FL}{8\pi\mu} \sum_{j=1}^{N} \begin{vmatrix} \hat{x}_{ij}^\beta \end{vmatrix} \left[ 3 (\mathbf{p}_j \cdot \hat{x}_{ij})^2 - 1 \right], \quad (3.7)
\]

and

\[
z^\beta_i = \hat{p}_i^\gamma \nabla^\gamma U^\beta(\mathbf{r}_i) = -\frac{FL}{8\pi\mu} \sum_{j=1}^{N} \hat{p}_i^\gamma \hat{x}_{ij}^\delta \nabla^\delta \nabla^\gamma \nabla^\beta (\mathbf{r}_i - \mathbf{r}_j). \quad (3.8)
\]

This expression can either be evaluated directly, using Eq. (3.6), which gives a result similar to the equations are (2.6) and (A.3) from [66]. This yields

\[
p_i^\gamma p_j^\alpha p_j^\delta \nabla^\gamma \nabla^\delta \nabla^\beta (\mathbf{r}_i - \mathbf{r}_j)
\]

\[
= \frac{1}{\begin{vmatrix} \mathbf{x}_{ij} \end{vmatrix}^3} \left[ p_i^\beta - 3 p_i^\beta (\mathbf{p}_j \cdot \hat{x}_{ij}) \right] + \hat{x}_{ij}^\beta \left\{ 15 (\mathbf{p}_i \cdot \hat{x}_{ij}) (\mathbf{p}_j \cdot \hat{x}_{ij})^2 - 3 (\mathbf{p}_i \cdot \hat{x}_{ij}) - 6 (\mathbf{p}_i \cdot \mathbf{p}_j) (\mathbf{p}_j \cdot \hat{x}_{ij}) \right\}, \quad (3.9)
\]

where we introduced \( \mathbf{x}_{ij} = \mathbf{r}_i - \mathbf{r}_j \), \( |\mathbf{x}_{ij}| \) denotes its length, and \( \hat{x}_{ij} = \mathbf{x}_{ij}/|\mathbf{x}_{ij}| \).

We now observe that the projection operator \( (\delta^{\alpha\beta} - p_i^\alpha p_i^\beta) \) in Eq. (3.3) removes all vectors parallel to \( \mathbf{p}_i \), and therefore the first two terms in the equation above do not contribute to the dynamics as they are changing the length of \( \mathbf{p}_i \). Therefore,

\[
z^\beta_i = \frac{FL}{8\pi\mu} \sum_{j=1}^{N} \begin{vmatrix} \mathbf{x}_{ij} \end{vmatrix}^3 \left[ 3 (\mathbf{p}_i \cdot \hat{x}_{ij}) + 6 (\mathbf{p}_i \cdot \mathbf{p}_j) (\mathbf{p}_j \cdot \hat{x}_{ij}) - 15 (\mathbf{p}_i \cdot \hat{x}_{ij}) (\mathbf{p}_j \cdot \hat{x}_{ij})^2 \right] \hat{x}_{ij}^\beta. \quad (3.10)
\]
Finally, the orientation obeys

$$\dot{p}_i^\alpha = \frac{F \ell}{8\pi\mu} \left( \delta^{\alpha\beta} - p_i^\alpha p_i^\beta \right) \sum_{j=1 \atop j \neq i}^N \frac{3 (p_i \cdot \hat{x}_{ij}) + 6 (p_i \cdot \hat{x}_{ij}) (p_j \cdot \hat{x}_{ij}) - 15 (p_i \cdot \hat{x}_{ij}) (p_j \cdot \hat{x}_{ij})^2}{|x_{ij}|^3} \hat{x}_{ij}. \quad (3.11)$$

As mentioned above, the position of each microswimmer changes due to self-propulsion and advection, and is encoded in the following equation

$$\dot{x}_i^\alpha = v_s p_i^\alpha + U^\alpha (r_i), \quad (3.12)$$

where $v_s$ is the self-propulsion speed, and the velocity $U$ created by all other dipoles at the position of the dipole $i$ is given by Eq. (3.7).

The other two ingredients, spatial diffusion and tumbling, are stochastic in nature and need to be treated separately. While spatial diffusion can be represented by a noise term in Eq. (3.12), tumbling is a set of discrete events and cannot be represented by a continuous in time random process. Below, we outline how these are implemented in our lattice model.

### 3.1.2 Numerical implementation of the equations of motion

To solve the equations of motion numerically, we cast them in a dimensionless form. We choose the lattice spacing $a$ as the unit of space, and $\lambda^{-1}$ as a unit of time, where $\lambda$ is the tumble frequency. Rescaling the equations leads to the following dimensionless quantities

$$L = \frac{v_s}{\lambda a}, \quad \tilde{D} = \frac{D}{a^2 \lambda}, \quad K = \frac{F \ell}{8\pi \mu a^3 \lambda}, \quad \phi = \frac{N}{H^2}. \quad (3.13)$$

Here, $L$ is the dimensionless persistence length, $\tilde{D}$ is the dimensionless spatial diffusivity, and $K$ is the dimensionless strength of the hydrodynamic interactions; it is positive for pushers and negative for pullers. Note, in this units the tumble rate is unity. Finally, $\phi$ is the filling fraction, defined as number
of swimmers $N$ divided by the total number of lattice sites $H^2$.

To solve equations numerically, we discretise time with a timestep $\Delta t$. The orientations, which are treated as continuous vectors, are updated through the following rule

$$p_*(t) + \Delta t K \sum_{j=1, j \neq i}^N \frac{3 (p_i \cdot \hat{x}_{ij}) + 6 (p_i \cdot p_j) (p_j \cdot \hat{x}_{ij}) - 15 (p_i \cdot \hat{x}_{ij}) (p_j \cdot \hat{x}_{ij})^2}{|x_{ij}|^3} \hat{x}_{ij}, \quad (3.14)$$

$$p_i(t + \Delta t) = \frac{p_*}{|p_*|}.$$  \quad (3.15)

While it might appear that these update rules lack the projection operator from Eq.(3.3), we note that the two sets of equations are identical to first order in $\Delta t$. We have opted for this implementation instead of utilising Eq.(3.3) directly to ensure that the length of all orientation vectors is strictly unity at every timestep. To model tumbling, the orientation of every microswimmer is changed to a new direction, chosen randomly from a uniform distribution with the rate $\Delta t$.

The dimensionless version of Eq.(3.12) is implemented as a two-step process. First, each swimmer hops along one of the lattice directions with the rate $\tilde{D} \Delta t$, provided the target site is free. Upon coarse-graining, this leads to the usual spatial diffusion with the correct dimensionless diffusivity on an empty lattice, while for finite values of $\phi$ this leads to an effective diffusivity that decreases as a function of the local density of microswimmers. Second, we model self-propulsion and advection as hopping along the lattice direction which is the closest to the direction of its instantaneous velocity $V_i$. The hopping rate is chosen to be

$$\frac{\tilde{V}_i \Delta t}{1 + \Delta t (\tilde{V}_i - L)}, \quad (3.16)$$

where

$$\tilde{V}_i^\alpha = L p_i^\alpha + K \sum_{j=1, j \neq i}^N \frac{\hat{x}_{ij}^\alpha}{|x_{ij}|^2} \left[ 3 (p_j \cdot \hat{x}_{ij})^2 - 1 \right], \quad (3.17)$$

and $\tilde{V}_i = |\tilde{V}_i|$. Trivially, the hopping rate is zero when $\tilde{V}_i = 0$. More importantly,
due to the presence of hydrodynamic interactions, $\tilde{V}_i$ can become significantly larger than the bare propulsion speed of a single microswimmer. This choice of the hopping rate ensures that every microswimmer hops by at most one lattice site every timestep. When the advection contribution is zero ($K = 0$), the rate above reduces to $L \Delta t$, corresponding to self-propulsion with the dimensionless speed $L$ upon coarse-graining. Again, no hop can occur if the target site is occupied.

### 3.2 Results

#### 3.2.1 Motility-induced phase separation

![Figure 3.1](image-url)  
Figure 3.1 Snapshots from a simulation with $\tilde{D} = 10$, $L = 30$, and $\phi = 0.25$ on a $400 \times 400$ lattice in the absence of hydrodynamic interactions, $K = 0$. The dimensionless simulation time is a) 0, b) 50, c) 500, d) 2500, e) 5000, f) 48000.

Before studying what our model predicts in the presence of hydrodynamic interactions between the particles, here we analyse the well-established case of $K = 0$, that corresponds to a collection of run-and-tumble particles with an effective excluded volume interaction. In Fig[3.1], we present the results of a simulation with $\tilde{D} = 10$, $L = 30$, and $\phi = 0.25$ on a $400 \times 400$ lattice. We observe
rapid formation of a high-density cluster phase that slowly coarsens towards one large cluster. These observations are in line with the motility-induces phase separation (MIPS) previously reported in run-and-tumble particles with repulsive interactions \[41, 51, 52, 58, 69, 82, 92\].

![Figure 3.2](image)

**Figure 3.2** Time evolution of the typical cluster size \(L(t)\) with \(\bar{D} = 10\), \(L = 30\), \(\phi = 0.25\), and \(K = 0\) on lattices of various sizes. (left) Linear-linear scale, (right) log-log scale. The dashed line in the right panel indicates the slope \(1/3\), previously linked to phase separations with diffusive transport of the order parameter and neglectable hydrodynamic interactions \[69\].

![Figure 3.3](image)

**Figure 3.3** The long-time average cluster size \(\overline{L(t)}\) as a function of the system size \(H\) for \(\bar{D} = 10\), \(\phi = 0.25\), \(K = 0\), and several values of \(L\).

To demonstrate that this is indeed a true phase separation, as is expected of MIPS, we now study the time-evolution of the typical cluster size, defined as the first moment of the structure factor:

\[
L(t) = 2\pi \left[ \int d\mathbf{k} S(\mathbf{k}, t) k \right]^{-1}, \tag{3.18}
\]

where \(S(\mathbf{k}, t) = \langle \delta\phi(\mathbf{k}, t) \delta\phi(-\mathbf{k}, t) \rangle\) is the Fourier transform of the instantaneous structure factor, \(\delta\phi\) is the local deviation of the particle area fraction from its average value, \(k\) is the wavevector, \(k = |\mathbf{k}|\), and \(\langle \ldots \rangle\) denote the ensemble
average. In Fig. 3.2 we show the time evolution of $L(t)$ for $\tilde{D} = 10$, $L = 30$, $\phi = 0.25$, and $K = 0$ on lattices of various sizes. For all lattice sizes, we observe that $L(t)$ saturates at its asymptotic value for sufficiently large times. For largest system sizes studied here, the approach to this asymptotic state is governed by $L(t) \propto t^{1/3}$, previously observed in off-lattice simulations of MIPS [69].

![Figure 3.4](image1.png)

**Figure 3.4** The probability distribution function of the cluster size for $\tilde{D} = 10$, $L = 30$, $\phi = 0.25$, and $K = 0$ for various system sizes.

Next, we average $L(t)$ over time in the asymptotic state and denote it by $\overline{L(t)}_t$. In Fig. 3.3, we plot the converged value of the cluster size $\overline{L(t)}_t$ against the system size for $\tilde{D} = 10$, $\phi = 0.25$, and $K = 0$, for several values of $L$. For all cases studied here, we observe a linear scaling of $\overline{L(t)}_t$ with $H$, indicating that the final cluster size is selected by the system size and diverges in the thermodynamic limit, as expected in a true phase separation.

![Figure 3.5](image2.png)

**Figure 3.5** The probability distribution function of the local density of microswimmers for $\tilde{D} = 10$, $L = 30$, $\phi = 0.25$, and $K = 0$ for various system sizes.

Visual inspection confirms that in all cases, simulations in the absence of
hydrodynamic interactions lead to the formation of a single high-density cluster immersed in the low-density surroundings. To confirm this observation, we implemented a linked-list algorithm [70] to identify clusters of various sizes. In Fig.3.4, we plot the probability distribution function to find a cluster of a particular size against the cluster size for the same parameters as in Fig.3.1. We observe that for all system sizes the system comprises a low-density phase that consists of large number of very small clusters (with just a few particles), and small number of very large clusters of a well-selected size that at infinite time leads to the formation of a single high-density cluster. As already noted above, in line with this transition being a true phase separation, we observe that the largest cluster size increases with the system size. This is further supported by Fig.3.5, where we plot the probability distribution function for the local particle density to have a particular value. As can be seen there, the system indeed splits into parts of two different densities. Importantly, while the cluster size linearly increases with the system size, the density inside the cluster and the density of the ‘gas’ phase remain independent of the system size.

![Figure 3.6](image)

**Figure 3.6**  
**MIPS phase diagram for \( \tilde{D} = 10 \) and \( K = 0 \) obtained from simulations on 100 \( \times \) 100 lattices. The colour denotes the average number of nearest and next-to-nearest neighbours of each microswimmer.**

Our final observation in the absence of hydrodynamic interactions pertains to the changes observed as we decrease the persistence length \( L \). As can be seen from Fig.3.3, the typical clusters are smaller for smaller values of \( L \). Simultaneously, the difference between the densities of the low- and high-density phases visible in Fig.3.5 becomes smaller as \( L \) increases (not shown). This behaviour indicates that the decreasing \( L \) leads to the system crossing the phase boundary and leave the phase separated region of the parameter space. To study this systematically, in Fig.3.6, we plot the phase diagram for
the system with $\tilde{D} = 10$ and $K = 0$ obtained from simulations performed on $100 \times 100$ lattices. To distinguish between the phases, we arbitrarily chosen to plot the average number of nearest and next-to-nearest neighbours of each microswimmer as a function of the persistence length $L$ and the particle area fraction $\phi$. We confirmed that a steep rise of that number above 4 is consistent with the appearance of the high-density peak on the density PDF graph, similar to Fig.3.5.

The phase diagram and all other aspects of the phenomenology exhibited by our lattice model is fully in line with the previous lattice [89] and off-lattice [41, 51, 52, 57, 58, 69, 82, 92] simulations of the motility induced phase separation. Having established that our model can reproduce the classical results, we now move to studying its predictions in the presence of hydrodynamic interactions.

### 3.2.2 Motility-induced phase separation in the presence of hydrodynamic interactions

In this section, we study the effect of the (effectively compressible) hydrodynamic interactions on the motility-induced phase separation discussed above. Unless explicitly stated otherwise, below we consider the case with $\tilde{D} = 10$, $L = 30$, and $\phi = 0.25$ for various values of $K$ and the system size $H$. In Fig.3.7 we present the long-time simulation snapshots for various values of $K$ obtained on $200 \times 200$ lattices. At low values of $K$, we observe the formation of a large high-density cluster immersed into a low-density phase, similar to the $K = 0$ case. The size of the cluster, however, seems to be decreasing as $K$ increases, until it entirely disappears around $K = 1$. While the results presented in Fig.3.7 were obtained by starting from a disordered configuration, we confirmed that we obtain the same results if the initial condition was a fully phase-separated state obtained previously for the $K = 0$ case.

To confirm that hydrodynamic interactions suppress the formation of large clusters, in Fig.3.8 study the behaviour of the density probability distribution function as a function of $K$. As $K$ increases from zero, Fig.3.8(left), the high-density peak decreases until it disappears entirely around $K = 1$, while the distribution for the lower-density clusters becomes broader. At yet higher values of $K$, Fig.3.8(right), the low-density peak sharpens until every point
Snapshots from a set of simulations with $\tilde{D} = 10$, $L = 30$, and $\phi = 0.25$ on $200 \times 200$ lattices after 2000 time units for various values of the strength of hydrodynamic interactions: a) $K = 0.1$, b) $K = 0.3$, c) $K = 0.5$, d) $K = 0.7$, e) $K = 1$, f) $K = 100$.

of the system is found to experience the density of the microswimmers that is approximately equal to its nominal value, $\phi = 0.25$. Furthermore, the probability distribution function of the cluster size quickly collapses towards clusters comprising just a few microswimmers, as $K$ increases, see Fig. 3.9. This further confirms that increasing the strength of hydrodynamic interactions leads to the suppression of the phase-separated state and yields a homogeneous suspension consisting almost entirely of single microswimmers.

Next, we demonstrate that hydrodynamic interaction strongly influence the nature of the phase-separated state even below the $K = 1$ threshold. In Fig. 3.10 we plot the time-evolution of the typical cluster size for various values of $K$. As in the case of MIPS, we observe that $L(t)$ plateaus for sufficiently long times, while the plateau value of $L(t)$ decreases with $K$, consistent with the discussion above. In Fig. 3.11 we plot the plateau value averaged in the statistically stationary state $\overline{L(t)}$ as a function of the system size $H$ for selected values of $K$. While MIPS exhibits the linear growth $\overline{L(t)} \propto H$, the typical cluster size scales sub-linearly with the system size for finite values of $K$. In Fig. 3.11 we show that the best fit to the data is obtained by an exponential
Figure 3.8  The probability distribution function of the local density of microswimmers. (top) Small values of $K$, (bottom) larger values of $K$. The vertical dashed line indicates the nominal area fraction of $\phi = 0.25$.

Figure 3.9  The probability distribution function of the cluster size for various values of $K$.

dependence that saturates at a constant value for sufficiently large $H$. This behaviour is followed by both $\overline{L(t)}$ and the maximal cluster size determined by the clustering algorithm discussed above. While we cannot claim that we have discovered the exact functional form for $\overline{L(t)} = \overline{L(t)}(H)$ for finite $K$’s, our results strongly suggest that the presence of hydrodynamic interactions change macroscopic motility-induced phase separation into a microphase separation where the cluster size is an intrinsic property of the system and is not set by
Figure 3.10  *Time evolution of the typical cluster size for different values of $K$.*

Figure 3.11  *Time average over the stationary state of the plateau value of $L(t)$ as a function of system size $H$. Selected values of $K$ are shown.*

the system size. Below, we show how these results can be rationalised with the help of a simple analytical model.
3.3 Discussion

3.3.1 Mean-field theory of cluster formation in motility-induced phase separation

Before attempting to understand how hydrodynamic interactions suppress motility-induced phase separation and change its nature to a microphase separation, we review here a mean-field argument for cluster formation in MIPS, put forward by Redner et al. [58]. While the original argument was made for particles with rotational diffusion, here we adapt it to the case of run-and-tumble particles.

We start by considering a circular cluster of radius $R_0$ surrounded by the low-density (gas) phase. The number of microswimmers that can join the cluster in a time interval $t$ from a shell of width $d\alpha$ and radius $\alpha$, measured from the cluster’s surface, is given by

$$n_G 2\pi (R_0 + \alpha) d\alpha (\lambda t) \frac{2R_0}{2\pi (R_0 + \alpha)}, \quad (3.19)$$

where $n_G$ is the number density of microswimmers in the gas phase, and $\lambda$ is the tumble rate. Here, $n_G 2\pi (R_0 + \alpha) d\alpha$ is the number of particles in the shell, while $2R_0/2\pi (R_0 + \alpha)$ gives the geometric probability for any given microswimmer to be pointed towards the cluster. Finally, $\lambda t$ accounts for the fact that each microswimmer would be re-set after a tumble event and should be considered as an independent attempt to reach the cluster.

Next, we observe that only microswimmers starting at $\alpha \leq \alpha_{max}$ can reach the cluster during a single run. The value of $\alpha_{max}$ is determined from the following equation of motion for a single microswimmer

$$\frac{d\alpha}{dt} = -v_s \quad (3.20)$$

where $\alpha(0) = \alpha_{max}$ and $\alpha(\lambda^{-1}) = a$, and the cluster’s centre is assumed to be located at the origin. Note that $\alpha = a$ is the first available position next to the cluster. Here, $v_s$ is the swimming speed. Solving this problem trivially gives $\alpha_{max} = a + v_s/\lambda$. The total number of particles joining the cluster during time $t$
is thus given by

\[ n_G(\lambda t)2R_0 \int_{0}^{\alpha_{\text{max}}} d\alpha = n_G(\lambda t)2R_0 \left( \frac{v_s}{\lambda} + a \right). \]  \hspace{1cm} (3.21)

To estimate the number of particles leaving the cluster, we assume that the microswimmers at the cluster’s surface will leave it when their orientation points away from the cluster. A typical time for a microswimmer to stay at the cluster’s surface is then \( 2\lambda^{-1} \). During this time, the number of particles leaving the cluster’s surface is given by \( 2\pi R_0a n_L \), where \( a \) is the lattice spacing and \( n_L \) is the number density of the dense phase.

Equating the number of particles leaving the cluster and the number of particles joining it during time \( 2\lambda^{-1} \) gives

\[ 2n_Ga \left( \frac{v_s}{a\lambda} + 1 \right) = \pi a n_L. \]  \hspace{1cm} (3.22)

Introducing \( L = v_s/(\lambda a) \), and assuming that the dense phase is at maximal number density, \( n_L = 1/a^2 \) for our lattice model, we obtain

\[ \phi_G(L + 1) = \frac{\pi}{2}. \]  \hspace{1cm} (3.23)

Redner et al. [58] have introduced a fitting parameter instead of \( \pi/2 \) above and, in terms of our notation, their condition would read \( \phi_G L = 5.55 \).

To determine the size of the cluster to be observed in a particular simulation, we start from the particle conservation

\[ nA = n_L A_L + n_G A_G, \]  \hspace{1cm} (3.24)

where \( n \) is the total particle number density, and \( A_L \) and \( A_G \) are the areas of the liquid and gas phases, respectively. The total area of the system is \( A = a^2 H^2 \), where \( H \) is the number of lattice points in each direction. Assuming that the liquid phase forms a single cluster of radius \( R_0 \), and introducing dimensionless variables, we obtain

\[ \pi R_0^2 = H^2 \frac{\phi - \phi_G}{\phi_L - \phi_G}. \]  \hspace{1cm} (3.25)

Since the area fraction of the dense phase is (visually) close to unity, we use
\( \phi_L = 1 \). Together with the result above, this gives

\[
R_0 = H \sqrt{\frac{1}{\pi} \frac{\phi - \frac{c}{L+1}}{1 - \frac{c}{L+1}}},
\]

(3.26)

where \( c \) is either 5.55, as in Redner et al. [58], or can be seen as a fitting parameter.

### 3.3.2 Velocity fields generated by lattice clusters

As we will see below, to uncover the mechanism of how hydrodynamic interactions affect MIPS, we need to understand the velocity field generated by high-density clusters in our simulations. To this end, here we consider a model arrangement of \((2N + 1)^2\) point dipoles on a 2D regular lattice, see Fig.3.12. Their positions are given by \((m_0, n_0)\), where integers \(m_0, n_0 \in [-N, N]\); all distances are made dimensionless with the lattice spacing \(a\). Due to the spatial symmetries, we are only going to consider the velocity field outside the cluster along Directions (1) and (2), see Fig.3.12.

We consider two types of model clusters. For the first type, Fig.3.13(left), we assume that the dipoles in the cluster are randomly oriented. Performing the angular average over all possible orientation of the microswimmers, we obtain for the velocity field at a point \((m, n)\)

\[
V^\alpha(m, n) = \frac{K}{2} \sum_{m_0, n_0=-N}^{N} \frac{(m-m_0, n-n_0)^\alpha}{[(m-m_0)^2 + (n-n_0)^2]^{3/2}}.
\]

(3.27)
The second type corresponds to a perfectly ordered lattice with a tetradic symmetry, Fig.3.13(middle). Motivation for this arrangement is two fold. First, we observe that such an arrangement of dipoles is a steady-state of the orientational equation of motion, as it leads to the r.h.s. of Eq.(3.3) vanishing exactly. Second, visual inspection of the high-density clusters observed in our simulations with finite $K$ confirms the presence of large patches with such tetradic order. Therefore we include this type of a model cluster in our analysis. For this arrangement, the velocity field at a point $(m, n)$ is given by

$$V^{\alpha}(m, n) = K \sum_{m_0,n_0=-N}^{N} \frac{(m - m_0, n - n_0)^{\alpha}}{[(m - m_0)^2 + (n - n_0)^2]^{3/2}} \times \left\{ 3 \frac{p_{x,m_0,n_0}^x(m - m_0) + p_{y,m_0,n_0}^y(n - n_0)^2}{(m - m_0)^2 + (n - n_0)^2} - 1 \right\}, \tag{3.28}$$

where

$$p_{x,m_0,n_0}^x = \frac{1 + (-1)^{m_0+n_0+1}}{2}, \tag{3.29}$$

$$p_{y,m_0,n_0}^y = \frac{1 + (-1)^{m_0+n_0}}{2}. \tag{3.30}$$

This arrangement assumes that the dipole at centre of the cluster, $(m_0, n_0) = (0, 0)$, is oriented along the $y$-direction. To study whether this choice introduces any bias into the velocity field, we also study a complimentary configuration, Fig.3.13(right), with the expressions for $p_{x,m_0,n_0}^x$ and $p_{y,m_0,n_0}^y$ being swapped in Eq.(3.28).
In Fig. 3.14, we plot the velocity field generated by the cluster evaluated numerically for \( N = 10 \). When considering Direction (1), we plot \( V_x(N + \alpha, 0)/K \) vs \( \alpha \), where \( \alpha \) is the distance from the cluster’s surface; note that \( V_y(N + \alpha, 0) = 0 \) for symmetry reasons. For Direction (2), we plot \( |V(N + \alpha, N + \alpha)|/K \) as a function of \( \alpha \); note that \( \alpha \) is a dimensionless integer that measures the distance from the cluster as a number of the lattice spacings. As can be seen from Fig. 3.14, all model configurations produce indistinguishable velocity fields in the same direction. The difference between the velocity magnitude in Directions (1) and (2) is close to 2.

To understand the structure of this field, we study Eq. (3.27) analytically. (According to Fig. 3.14, ordered configurations produce similar velocity fields while being analytically more involved.) The double sum in Eq. (3.27) cannot be performed analytically and we approximate it by a double integral. For Direction (1) this yields

\[
V_x(N + \alpha, 0) = \frac{K}{2} \sum_{m_0,n_0=-N}^{N} \frac{N + \alpha - m_0}{\left[(N + \alpha - m_0)^2 + n_0^2\right]^{3/2}}
\approx \frac{K}{2} \int_{-N}^{N} \int_{-N}^{N} \frac{d m_0 d n_0}{\left[(N + \alpha - m_0)^2 + n_0^2\right]^{3/2}}
\approx \frac{K}{2} \ln \left[ \frac{\sqrt{\alpha^2 + N^2} + N \sqrt{\alpha^2 + 4\alpha N + 5N^2 - N}}{\sqrt{\alpha^2 + N^2} - N \sqrt{\alpha^2 + 4\alpha N + 5N^2 + N}} \right].
\tag{3.31}
\]

At small distances, \( \alpha \ll N \), Eq. (3.31) predicts

\[
V_x(N + \alpha, 0) \sim K \ln \left[ 2 \sqrt{\frac{\sqrt{5} - 1}{\sqrt{5} + 1}} \frac{N}{\alpha} \right],
\tag{3.32}
\]
while in the opposite limit, $\alpha \gg N$,

$$V^x(N + \alpha, 0) \sim K \frac{2N^2}{\alpha^2},$$

(3.33)

reflecting the dipolar nature of the velocity fields of individual particles. The crossover from one limit to the other takes place for $\alpha \sim N$, since there is no other lengthscale in the problem. In Fig.3.14, we compare the prediction of Eq.(3.31) against the numerical data. We observe that the analytical result correctly reproduces the logarithmic and algebraic decays for small and large distances, respectively. Minor discrepancies at small distances are due to the discrete nature of the cluster absent from the integral used to obtain Eq.(3.31).

Now we assess whether these predictions are compatible with our lattice simulations. In Fig.3.15 we quantify the velocity field in a simulation snapshot with $K = 0.5$ on a $300 \times 300$ lattice. In Fig.3.15(left) we plot the magnitude of the velocity field at the lattice points that are not occupied by particles, while in Fig.3.15(right) we plot the velocity field around a single cluster marked by the red box in Fig.3.15(left). We confirm that the largest velocity magnitude is observed at the cluster surface (bar the odd vacancy inside clusters), and that velocity field points away from the cluster surface everywhere along the cluster’s perimeter. The velocity magnitude at the points marked by the red and blue points in Fig.3.15(right) is $2.82K$ and $5.44K$, respectively. Using $N \sim 40$ in Eq. (3.32), we obtain $V \sim 3.9K$, consistent with the simulations.
3.3.3 Argument *a la* Redner *et al.* in the presence of HI

Having established the nature of the velocity fields generated by high-density clusters of dipolar microswimmers, here we adapt the argument by Redner *et al.* [58] to the case with hydrodynamic interactions. In this case, the argument that leads to Eq. (3.21) requires two modifications.

First, we need to account for the velocity field created by the cluster advecting swimmers away from the cluster’s surface. The second modification pertains the orientation dynamics of swimmers in the vicinity of the cluster. The radially-symmetric structure of the cluster velocity field and the fact that it decays away from the cluster ensures that a swimmer approaching the cluster along a direction that is not pointing towards the cluster’s centre is rotated further away from the radial direction, see Fig. 3.16. In the absence of HI we assumed that a swimmer can join the cluster as long as its swimming direction points somewhere from the cluster’s centre to its edge. The argument above shows that the velocity field around the cluster makes this range of angles narrower: a swimmer that is pointing sufficiently away from the centre of the cluster and starting sufficiently far from the cluster’s surface, will end up being rotated past the cluster’s edge and will not join it. Thus, the number of particles joining the cluster in the presence of HI is reduced by two mechanisms: by the velocity field ‘blowing’ swimmers away from its surface and by rotating them away from the cluster.
Next, we consider the relative importance of these two mechanisms. To this end, in Fig. 3.17 we study the effect of HI on the average cluster size. We measure $L(t)$ as function of $K$ in our simulations with all other parameters fixed and note the point where the clusters disappear. (We note that this point does not correspond to $L(t) \approx 1$, as small clusters transiently form and disappear in the low-density phase; instead, the disappearance of the high-density cluster is marked by $L(t) \approx 5$ based on visual observations.) We observe that as $K$ is increased from zero, the cluster size becomes smaller until all steady clusters disappear, for sufficiently large values of $K$. To disentangle the two mechanisms mentioned above, we now repeat the same simulations for $L = 30$ with the particle advection being artificially switched off (brown curve) and the particle re-orientation by external flows being switched off (magenta curve). We see that switching off particle advection has only a minor effect on the cluster size behaviour and, therefore, in what follows we focus on the orientational dynamics only. Another argument for the orientational dynamics being the dominant mechanism comes from the dimensionless form of Eq.(3.12): had the advection away from the cluster been the dominant mechanism, one would expect the phase boundary to be approximately given by $K \sim L$, which corresponds to the 'head-wind' being equally strong as the self-propulsion velocity of the microswimmers (in the dimensionless form). The fact that the high-density clusters disappear way before this point, ie $K \approx 1$ and not
\[ K \approx 30 \] in the simulations above, indicates that the advection is a subdominant mechanism here and we ignore it in the following.

In the absence of advection, we assume that the dimensionless distance of the swimmer from the cluster’s surface follows \( \tilde{\alpha}(t) = \tilde{\alpha}_0 - L t \), where \( \alpha_0 \) is the position of the swimmer at the beginning of the run phase. The swimmer’s orientation, given by \( \mathbf{p} = (\cos \phi, \sin \phi) \), where the angle \( \phi \) is measured from the local radial direction (see Fig.3.16), obeys Jeffrey’s equation:

\[
\dot{\mathbf{p}} = (I - \mathbf{pp}) \cdot (\mathbf{p} \cdot \nabla V), \tag{3.34}
\]

where \( V \) is the local velocity field created by the cluster at the position of the swimmer. Since \( V \) only has the radial component, the dynamics of \( \phi \) is given by

\[
\dot{\phi} = \left( \frac{V(\tilde{\alpha}(t))}{\tilde{\alpha}(t) + R_0} - V'(\tilde{\alpha}(t)) \right) \phi, \tag{3.35}
\]

which is valid for small angles \( \phi \). In the following, we are interested in understanding how HI melt the cluster. In that regime, clusters are going to be small and most of the swimmers approaching the cluster would experience its far-field velocity

\[
V = K' \frac{2R_0^2}{\tilde{\alpha}^2} e_r, \tag{3.36}
\]

where \( e_r \) is the unit vector in the radial direction. Solving for the dynamic of the angle yields

\[
\int_{\phi_0}^{\phi_f} \frac{d\phi}{\phi} = 6KR_0^2 \int_0^{t_s} \frac{dt}{(\tilde{\alpha}_0 - L t)^3} \tag{3.37}
\]

where \( t_s = (\tilde{\alpha}_0 - 1)/L \) is the time to reach the cluster’s surface (locate at \( \tilde{\alpha}_0 = 1 \)), while \( \phi_0 \) and \( \phi_f \) are the initial and final values of the orientation angle. Assuming that the final angle should not exceed the cluster’s angular dimensions as seen from \( \tilde{\alpha}_0 \), we set \( \phi_f = R_0/(R_0 + \tilde{\alpha}) \). The range of initial orientations that would lead a swimmer to reach the cluster is thus reduced from \([0, R_0/(R_0 + \tilde{\alpha})]\), as in Redner’s argument, to \([0, \phi_0]\), where \( \phi_0 \) satisfies

\[
\phi_0 = \frac{R_0}{R_0 + \tilde{\alpha}_0} \exp \left[ -\frac{6KR_0^2}{2L} \left( 1 - \frac{1}{\tilde{\alpha}_0^2} \right) \right]. \tag{3.38}
\]
The original Redner’s expression, Eq. (3.19), can now be modified to read

\[
G_n 2\pi (R_0 + \alpha_0) d\alpha_0 (\lambda t) \int_0^{\alpha_m} d\alpha_0 \exp \left[ -\frac{6K R_0^2}{2L} \left( 1 - \frac{1}{\alpha_0^2} \right) \right].
\] (3.39)

The total number of particles joining the cluster is given by the integral

\[
2R_0 n G (\lambda t) \int_0^{\alpha_m} d\alpha_0 \exp \left[ -\frac{6K R_0^2}{2L} \left( 1 - \frac{1}{\alpha_0^2} \right) \right],
\] (3.40)

where \( \alpha_m = L + 1 \) is given by the requirement \( t_s = 1 \). Equating the number of particles moving towards the cluster with the number of particles leaving the cluster during \( 2\lambda^{-1} \) seconds, we obtain to first order in \( K/L \)

\[
(L - \frac{3LR_0^2 K}{L + 1}) \phi_G \approx (L - 3R_0^2 K) \phi_G = c \approx 5.55.
\] (3.41)

In the absence of hydrodynamic interactions, the cluster phase (MIPS) appears at \( L_{MIPS} \) given by \( \phi_G = \phi \) which trivially gives

\[
L_{MIPS} = \frac{c}{\phi}.
\] (3.42)

For larger \( L = L_{MIPS} + \delta L \), the clusters disappear again when \( \phi_G = \phi \), this giving

\[
3R_0^2 K_{crit} = \delta L.
\] (3.43)

At this point the cluster is just a few particles wide, \( R_0 \sim 1 \), and we obtain \( K_{crit} \sim \delta L \) – the strength of hydrodynamic interactions needed to melt all clusters is linear in the distance from the MIPS threshold. This estimate is in a reasonable agreement with our numerical observations.

### 3.3.4 Structure of the low-density phase at high values of \( K \)

In addition to suppressing phase separation and changing the nature of the cluster phase to a microphase separation, here we show that the hydrodynamic interactions strongly affect the structure of the low density phase that we observe at very large values of \( K \). Visual inspection of Fig 3.7(e), for instance,
suggests that the spatial distribution of microswimmers in that case is different from a random homogeneous distribution, and here we assess the nature of the ensuing order. Since the suspension appears to be homogeneous and isotropic, this analysis can be performed analytically. Below we show that the high-$K$ phase corresponds to a hyperuniform state [81].

The starting point of our analysis is the mean-field kinetic theory of dilute suspensions of microswimmers based on the following Smoluchowsky equation

$$\partial_t F + \nabla^a \{ \dot{x}^a F \} + \partial^a \{ \dot{p}^a F \} = 0,$$

Here, $F(x, p, t)$ is the one-particle distribution function that defines the instantaneous probability of finding a particle at a spatial position $x$ with an orientation $p$. Its normalisation condition is given by

$$\int dx \, dp \, F(x, p, t) = 1.$$

The time evolution of the microswimmer positions and orientations are given by Eqs. (3.12) and (3.3) together with the spatial diffusion and tumbling, as discussed above. We note, however, that at the mean-field level tumbling is similar to an effective rotational diffusion with the diffusivity $2D_r = \lambda$, where $\lambda$ is the tumble rate [16]. Since the following calculation is significantly simpler in the case of rotational diffusion than in the case of tumbling, we proceed with the former case keeping in mind that the effective diffusivity $D_r$ is a proxy for the tumble rate $\lambda$.

Since we expect the suspension to be homogeneous and isotropic, we linearise Eq. (3.44) around $F(x, p, t) = F_0 = 1/(2\pi A_0)$, where $A_0$ is the area of the suspension, to obtain

$$\partial_t \delta \hat{f} + iv_s (k \cdot p) \delta \hat{f} + D k^2 \delta \hat{f} - D_r \partial_{\hat{p}}^2 \delta \hat{f} + \frac{n}{\pi} i k^a \delta \hat{U}^a$$

$$- \frac{n}{\pi} i (k \cdot p) p^b \delta \hat{U}^b = \sqrt{2DF_0} i k \cdot \xi(k, p, t) + \sqrt{2D_r F_0} \partial_{\hat{p}} \zeta(k, p, t).$$

Here, $\delta \hat{f}(k, p, t)$ is the Fourier transform of a (small) deviation of $F(x, p, t)$ from $F_0$, $\xi$ and $\zeta$ are Gaussian processes with zero mean and unit variance representing the spatial and rotational Brownian motion, respectively, and $n$ is the number density of the microswimmers. The Fourier transform of the mean-
field velocity field, \( \delta U^\alpha(k,t) \), is given by

\[
\delta U^\alpha(k,t) = \int dp' \hat{u}^\alpha_\alpha(k, p') \delta \hat{f}(k, p', t)
\]

\[
= i \kappa \frac{4}{\delta} \int dp' \left[ \hat{k}^\alpha \left( p' \cdot \hat{k} \right)^2 - 2 p'^\alpha \left( p' \cdot \hat{k} \right) \right] \delta \hat{f}(k, p', t).
\] (3.47)

In two spatial dimensions, the orientation \( p \) can be parametrised by an angle \( \phi \). To proceed, we expand \( \delta \hat{f}(k, p, t) \) in Fourier harmonics and keep the first two modes

\[
\delta \hat{f}(k, p, t) \approx \sum_{n=-2}^{2} \delta \hat{f}_n(k, t) e^{in\phi}.
\] (3.48)

Projecting the original equations onto these Fourier modes yields

\[
\partial_t \delta \hat{f}_0 + \frac{iv_s}{2} \left[ (k_x + ik_y) \delta \hat{f}_1 + \text{c.c.} \right] + Dk^2 \delta \hat{f}_0
\]

\[
+ \frac{nkk}{8} \left[ \delta \hat{f}_0 + \left\{ \frac{1}{2} (k_x + ik_y)^2 \right\} \delta \hat{f}_2 + \text{c.c.} \right] = a_0,
\] (3.49)

\[
\partial_t \delta \hat{f}_1 + \frac{iv_s}{2} \left[ (k_x - ik_y) \delta \hat{f}_0 + (k_x + ik_y) \delta \hat{f}_2 \right] + Dk^2 \delta \hat{f}_1 + D_r \delta \hat{f}_1 = a_1,
\] (3.50)

\[
\partial_t \delta \hat{f}_2 + \frac{iv_s}{2} (k_x - ik_y) \delta \hat{f}_1 + Dk^2 \delta \hat{f}_2 + 4D_r \delta \hat{f}_2
\]

\[
- \frac{nkk}{16} \left[ (k_x - ik_y)^2 \delta \hat{f}_0 + \frac{3}{2} \delta \hat{f}_2 - \frac{1}{2} (k_x - ik_y)^4 \delta \hat{f}_{-2} \right] = a_2.
\] (3.51)

Note that \( \delta \hat{f}_{-1} \) and \( \delta \hat{f}_{-2} \) are not the complex conjugates of \( \delta \hat{f}_1 \) and \( \delta \hat{f}_2 \), respectively. They satisfy equations that are similar to the ones above but they are not c.c.’s of them. The noise terms are given by

\[
a_m = \frac{1}{2\pi} \int_0^{2\pi} d\phi \left[ \sqrt{2DF_0 i} \hat{k} \cdot \hat{\zeta}(k, p, t) + \sqrt{2DF_0} \partial_\phi \hat{\zeta}(k, p, t) \right] e^{-im\phi}.
\] (3.52)

By putting the time derivatives of all Fourier modes with \( n > 0 \) to zero, we enslave their dynamics to that of the density. The equations for \( \delta \hat{f}_{\pm 1} \) and \( \delta \hat{f}_{\pm 2} \) can now be solved to give

\[
\partial_t \delta \hat{f}_0(k, t) + L(k) \delta \hat{f}_0(k, t) = \hat{\chi}(k, t),
\] (3.53)

57
where

$$\hat{\chi}(k, t) = a_0(k, t) - A(k) \left[ a_1(k, t)(i\hat{k}_x - \hat{k}_y) + a_{-1}(k, t)(i\hat{k}_x + \hat{k}_y) \right]$$

$$- B(k) \left[ a_2(k, t)(\hat{k}_x + i\hat{k}_y)^2 + a_{-2}(k, t)(\hat{k}_x - i\hat{k}_y)^2 \right].$$

(3.54)

Here, $L(k)$, $A(k)$ and $B(k)$ are some cumbersome functions of $k$ but not of $k$. Solving this equation formally gives

$$\delta \hat{f}_0(k, t) = \delta \hat{f}_0(k, t = 0) e^{-L(k)t} + e^{-L(k)t} \int_0^t dt' e^{L(k)t'} \hat{\chi}(k, t').$$

(3.55)

In the limit $t \to \infty$, the structure factor can be obtained from

$$S(k) = \langle \delta \hat{f}_0(k, t)\delta \hat{f}_0(-k, t) \rangle = e^{-2L(k)t} \int_0^t dt' dt'' e^{L(k)(t'+t'')} \langle \hat{\chi}(k, t')\hat{\chi}(-k, t'') \rangle.$$

(3.56)

The spectral properties of the noise components are given by

$$\langle \xi^\alpha(k, \phi_1, t_1)\xi^\beta(-k, \phi_2, t_2) \rangle = A_0 \delta^{\alpha\beta} \delta(\phi_1 - \phi_2) \delta(t_1 - t_2),$$

(3.57)

$$\langle \zeta(k, \phi_1, t_1)\zeta(-k, \phi_2, t_2) \rangle = A_0 \delta(\phi_1 - \phi_2) \delta(t_1 - t_2).$$

(3.58)

Again, $A_0$ is the area of the system. Using the definition of $\hat{\chi}(k, t)$ and Eq. (3.52),
we obtain after integration by parts

\[
\hat{\chi}(k, t) = \sqrt{\frac{2DF_0}{2\pi}} \int_0^{2\pi} d\phi_1 \left[ 1 - A(k) \left\{ e^{-i\phi_1(i\hat{k}_x - \hat{k}_y)} + e^{i\phi_1}(i\hat{k}_x + \hat{k}_y) \right\} 
- B(k) \left\{ e^{-2i\phi_1}(k_x + i\hat{k}_y)^2 + e^{2i\phi_1}(k_x - i\hat{k}_y)^2 \right\} \right] ik \cdot \hat{\xi}(k, \phi_1, t)
+ \sqrt{\frac{2DF_0}{2\pi}} \int_0^{2\pi} d\phi_1 \left[ A(k) \left\{ -ie^{-i\phi_1}(i\hat{k}_x - \hat{k}_y) + ie^{i\phi_1}(i\hat{k}_x + \hat{k}_y) \right\} 
+ B(k) \left\{ -2ie^{-2i\phi_1}(\hat{k}_x + i\hat{k}_y)^2 + 2ie^{2i\phi_1}(\hat{k}_x - i\hat{k}_y)^2 \right\} \right] \hat{\zeta}(k, \phi_1, t)
\]

\( = \sqrt{\frac{2DF_0}{2\pi}} \int_0^{2\pi} d\phi_1 \left[ 1 - 2iA(k) \left\{ \hat{k}_x \cos \phi_1 + \hat{k}_y \sin \phi_1 \right\} 
- 2B(k) \left\{ (\hat{k}_x^2 - \hat{k}_y^2) \cos 2\phi_1 + 2\hat{k}_x \hat{k}_y \sin 2\phi_1 \right\} \right] ik \cdot \hat{\xi}(k, \phi_1, t)
+ \sqrt{\frac{2DF_0}{2\pi}} \int_0^{2\pi} d\phi_1 \left[ 2iA(k) \left\{ \hat{k}_y \cos \phi_1 - \hat{k}_x \sin \phi_1 \right\} 
+ 4B(k) \left\{ (\hat{k}_y^2 - \hat{k}_x^2) \sin 2\phi_1 + 2\hat{k}_x \hat{k}_y \cos 2\phi_1 \right\} \right] \hat{\zeta}(k, \phi_1, t) \) (3.59)

The average is then

\[
\langle \hat{\chi}(k, t')\hat{\chi}(\mathbf{-k}, t'') \rangle
= \frac{1}{2\pi^2} \delta(t' - t'') \left[ Dk^2 \left\{ 1 + 2A^2(k) + 2B^2(k) \right\} + 2Dr \left\{ A^2(k) + 4B^2(k) \right\} \right]
\] (3.60)

Substituting this into Eq. (3.56) gives as \( t \to \infty \)

\[
S(k) = \frac{1}{4\pi^2 L(k)} \left[ Dk^2 \left\{ 1 + 2A^2(k) + 2B^2(k) \right\} + 2Dr \left\{ A^2(k) + 4B^2(k) \right\} \right].
\] (3.61)

The resulting expression is a complicated function of \( k \) that is well-approximated by a ratio of two linear polynomials. Introducing the following dimensionless
quantities:

\[ L = \frac{v_s}{2D_r a}, \quad \tilde{D} = \frac{D}{2D_r a^2}, \quad K = \frac{\kappa}{2D_r a^2}, \quad \phi = na^2, \quad (3.62) \]

which are motivated by our lattice dimensionless parameters with \( \lambda \) replaced by \( 2D_r \), we obtain

\[ S(\tilde{q}) \approx \frac{\left[ 256(\tilde{D} + L^2) + \phi^2 K^2 \right] \tilde{q}}{32\phi K + \tilde{q} \left[ 256(\tilde{D} + L^2) - 4\phi^2 K^2 \right]}, \quad (3.63) \]

where \( \tilde{q} \) is the dimensionless wavenumber. For small values of \( \tilde{q} \), we thus obtain \( S(\tilde{q}) \propto \tilde{q} \), which is a hallmark of a hyperuniform state. At higher values of \( \tilde{q} \), \( S(\tilde{q}) \) becomes independent of \( \tilde{q} \). The crossover happens at approximately

\[ \tilde{q} \sim \frac{\phi K}{8(D + L^2)} \quad (3.64) \]

Eq. (3.63) also predicts a divergence at sufficiently high values of \( K \) which seems to be an artefact of the approximations made above.

Figure 3.18 Comparison between the predictions of Eq. (3.63) (on the left) with the structure factor measured in our simulation (on the right) with \( \phi = 0.25, \tilde{D} = 10, L = 30, \) for \( K = 1 \ldots 100 \).

In Fig. 3.18 we compare the predictions of Eq. (3.63) with the structure factor measured in our simulation with \( \phi = 0.25, \tilde{D} = 10, L = 30, \) for \( K = 1 \ldots 100 \). We observe that for very large \( K \) the structure factor indeed scales linearly with \( \tilde{q} \), confirming our prediction that the low-density state at high \( K \) is hyperuniform. At smaller values of \( K \), we do not observe a linear scaling. Since Eq. (3.64) predicts that the linear scaling should be observed up to a value of \( \tilde{q} \)
that is proportional to $K$, we conclude that this is most likely due to the finite size of the simulation box that sets the minimal value of $\tilde{q}$ accessible in our simulations.

### 3.4 Discussion and Conclusion

![Snapshots from simulations at high area fraction of microswimmers, $\phi = 0.6$, with $D = 10$, $L = 30$ on a $250 \times 250$ lattice after 2000 time units for various values of the strength of hydrodynamic interactions: a) $K = 0.0$, b) $K = 0.5$.](image)

**Figure 3.19** Snapshots from simulations at high area fraction of microswimmers, $\phi = 0.6$, with $D = 10$, $L = 30$ on a $250 \times 250$ lattice after 2000 time units for various values of the strength of hydrodynamic interactions: a) $K = 0.0$, b) $K = 0.5$.

In this Chapter, we studied how hydrodynamic interactions between microswimmers affect the motility-induced phase separation. We employed a model where microswimmers move on a square lattice while having a continuously changing orientation. Besides being advected and re-oriented by the velocity fields generated by other microswimmers, each microswimmer is subject to spatial diffusion and tumbling. To describe hydrodynamic interactions, we approximated the velocity fields created by real microswimmers with their far-field, dipolar components. The unique feature of our model is that while the microswimmers are confined to move on a two-dimensional lattice, their hydrodynamic interactions are described by the three-dimensional dipolar fields. We argued that this setting captures the effective in-plane compressibility of the velocity fields exhibited by microswimmers moving close to a boundary.

We demonstrated that in the absence of hydrodynamic interactions our model reproduces the key features that define the motility-induced phase separation, despite the obvious simplicity of our model. In the presence of hydrody-
namic interactions we observed that the motility-induced phase separation is suppressed, in line with the previous studies \[1, 10, 48, 93\]. Surprisingly, our model predicts that the hydrodynamic interactions result in a change of the transition type, yielding a microphase separation instead of a full phase separation characteristic of MIPS. We explain this result with the help of simple model that studies how a single microswimmer approaches a large cluster and how this approach is influenced by the velocity field generated by the cluster. At sufficiently high strength of hydrodynamic interactions, when the system is outside the phase separated part of the phase diagram, we showed that the suspension of microswimmers is hyperuniform as the result of the source-like velocity fields generated by the microswimmers.

While our results are strikingly similar to the experimental observations often cited as the confirmation of MIPS \[5, 13, 36, 53, 75\], our model has several obvious weaknesses. First, as any lattice model, it biases the formation of structures along the lattice directions and this might be of importance during phase separation. Moreover, the far-field dipolar velocity fields are only expected to faithfully approximate the velocity fields of the microorganisms at distances up to a few microorganism radii. At shorter distances, relevant in the high-density phase, other hydrodynamic singularities need to be taken into account \[35, 66\]. At very short distances, these should be replaced by the lubrication interactions. Nevertheless, the simple model we used to explain how hydrodynamic interactions arrest the cluster formation, implies that the most relevant interactions are those between the microswimmers at the cluster’s surface and the microswimmers in the low-density phase. These interactions should be well-described by the dipolar fields, and we expect our conclusions to apply even to the true suspensions of microorganisms. More work is needed to confirm our observations.

We note that in this work we focused only on a particular part of the phase diagram where the overall density of microswimmers is sufficiently low. To compliment this work, we have performed limited studies of the effect of hydrodynamic interactions on high-density suspensions. In Fig.3.19 we show simulation snapshots from two studies with \(\phi = 0.6\), \(\tilde{D} = 10\), and \(L = 30\) on a \(250 \times 250\) lattice in the absence of hydrodynamic interactions, \(K = 0\), and with \(K = 0.5\). As can be seen there, we observe a phenomenology that is similar to lower-\(\phi\) suspensions with the role of the clusters is being played by the low-density ‘holes’. While for \(K = 0\), the size of the holes scales with the system
size, in the presence of hydrodynamic interactions their growth is arrested (not shown). The question whether this hole-cluster symmetry applies across the whole phase diagram will be the subject of future work.

Finally, here we only focussed on pusher microswimmers that, as we argued in the Introduction, behave as effective sources of fluid when confined to a two-dimensional plane embedded in a three-dimensional fluid. It would be interesting to extend this study to the case of pullers, that act, effectively, as sinks. Naively, one would expect that a suspension of such microswimmers would behave similar to a suspension of run-and-tumble particles with attractive interactions [57]. Whether this is indeed the case, should be studied in the future.
Chapter 4

Active turbulence and spontaneous phase separation in inhomogeneous extensile active gels

4.1 Introduction

Active gels [23, 54, 55] are fascinating examples of non-equilibrium soft matter. Some well-known realisations of these systems include solutions of cytoskeletal filaments, such as actin or microtubules, interacting with molecular motors, such as myosin or kinesin [40, 61]. Other instances come from living materials, and encompass microbial suspensions of algae or bacteria [31, 91]. In an active gel, the constituent particles exert non-thermal forces on their environments. Such forces can be modelled, at the simplest level, as force dipoles, whose direction defines a nematic order parameter, which is a fundamental quantity to describe the emergent physics of these systems [42].

The activity arising from the distribution of force dipoles leads to a phenomenology which is strikingly different from that of passive colloidal particles or polymer suspensions. For instance, these materials harbour a “spontaneous flow” instability, which sets in for sufficiently strong activity, and comprises a non-equilibrium transition between a quiescent suspension and a state where
activity fuels continuous motion \cite{17, 43, 44, 63, 86}. For sufficiently large activity, the flow and orientation patterns of the spontaneously flowing state are seemingly chaotic, and the associated state is known as “active turbulence” \cite{3, 14, 24, 29, 33, 68}. In active turbulence, active gels self-organise into a random arrangement of vortices. Experiments and theories suggest that in the nematic phase these vortices have a typical length scale, arising from the competition between activity and elasticity \cite{29}, while recent work points to important fundamental differences between active turbulence and its more widely studied passive counterpart \cite{2, 14}. Active gels also possess strongly non-Newtonian rheological properties \cite{59}, such as marked activity-induced thinning or thickening \cite{17, 26, 31, 44, 46}, Darcy-like flow \cite{39}, or negative drag in microrheology \cite{26, 27}.

Existing theories and simulations of active gel hydrodynamics typically consider systems with constant composition. In contrast, inspection of active turbulent patterns found with microtubule–kinesin mixtures in the presence of polyethylene-glycol (which causes adsorption to the oil–water interface \cite{47, 61}) shows that the concentration of active material is significantly inhomogeneous. While a linear stability analysis shows that in extensile gels, such as a microtubule–kinesin mixture, the onset of spontaneous flow depends on orientational bend fluctuations and compositional fluctuations should be irrelevant \cite{4}, active turbulence is a highly non-linear phenomenon and the relevance of composition inhomogeneities to its physics remains unclear. We call \textit{lyotropic} a solution which properties are concentration-dependant. Additionally, passive colloidal particles aggregate in active nematics \cite{28}, through a mechanism reminiscent of path coalescence \cite{45, 90} or fluctuation-dominated phase ordering \cite{20}. This nonequilibrium aggregation shows that even a one-way coupling between composition and spontaneous flow (as tracers are affected by the spontaneous flow but do not modify it) can in principle give rise to composition inhomogeneities, and more in general to nontrivial physics outside the reach of a constant-composition approximation.

To understand the role of compositional inhomogeneities in the physics of spontaneous flow and active turbulence, here we study the hydrodynamic equations of motion of a mixture of an isotropic fluid and an active nematic gel by means of computer simulations. While the overall system is always incompressible, the active gel component can change its concentration, as is realistic for the microtubule–kinesin mixtures considered in \cite{47}. With respect
to previous work on Cahn–Hilliard models coupled to active nematics focussing on the crossover between wet and dry systems driven by friction with the substrate [22, 73, 76], here our focus is specifically on the qualitative role of compositional inhomogeneities on the emerging physics and patterns. As in active gels of uniform composition, we find that the system displays a transition between a passive isotropic phase and an active nematic phase. This transition can be triggered either by increasing activity or the nematic tendency of the system (more specifically the coupling between active matter concentration and orientational order). In the active nematic phase, though, compositional inhomogeneities play a fundamental role and give rise to some unique dynamical behaviour. We find three dynamical regimes in this phase. Close to the transition boundary, our lyotropic system settles into regular flowing patterns, with approximately ordered spiral defect arrangements creating a rotational active flow consisting of long-lived and stable vortices. For larger activity, or deeper in the nematic phase, the flow becomes chaotic and we observe active turbulence. Both regular patterns and active turbulence are regimes which can be found in active gels of uniform composition. There are differences though, as in our case the thermodynamic coupling between orientational and compositional order parameters favours a concentration minimum, or relative void of active matter, at defect cores. Additionally, active turbulent patterns are characterised by a very broad distribution of local concentrations. The last regime we observe is unique to inhomogeneous systems, and is found even deeper in the nematic phase with respect to active turbulence, but for low activities. Here the active mixture spontaneously phase separates into low-concentration disordered and high-concentration nematic domains of irregular shape. We show by a semi-analytical theoretical analysis that this phase separation is due to the coupling between composition and nematic ordering and hence is driven thermodynamically. The corresponding coarsening is arrested in our case by the spontaneous active flow, and the size of the steady state domains decreases with activity. We conclude by discussing ways in which our study can be taken forward, both theoretically and experimentally.

4.2 Equations of motion

To describe the equilibrium properties of an inhomogeneous active nematic system in the passive phase (i.e., when the activity parameter defined below is
switched off), we employ a Landau–de Gennes free energy \( F \), whose density we call \( f \). The latter consists of a contribution which characterises the orientational order of the active liquid crystal, measured by a nematic tensor \( Q_{\alpha\beta} \), and of another contribution determining the physics of compositional fluctuations, depending on the compositional order parameter \( \phi \) (which measures the local concentration of active material). The liquid crystalline free energy density we use is a standard one to describe passive nematic liquid crystals \[21\], and is explicitly given by

\[
\begin{align*}
    f_{LC} &= \frac{A_0}{2} \left( 1 - \frac{\gamma(\phi)}{3} \right) Q_{\alpha\beta}^2 - \frac{A_0 \gamma(\phi)}{3} Q_{\alpha\beta} Q_{\beta\gamma} Q_{\gamma\alpha} \\
    &+ \frac{A_0 \gamma(\phi)}{4} (Q_{\alpha\beta}^2)^2 + \frac{K}{2} (\partial_\gamma Q_{\alpha\beta})^2,
\end{align*}
\]

(4.1)

where the first term is a bulk contribution, describing the isotropic–nematic transition, while the second term is an elastic distortion term. In the equation above, \( A_0 \) is a constant, \( \gamma(\phi) \) controls the magnitude of order (so that it may be viewed as an effective temperature or concentration for thermotropic and lyotropic liquid crystals respectively), while \( K \) is an elastic constant — note we are using the (standard in this field) one-constant approximation \[21\]. Here and in what follows Greek indices denote cartesian components and summation over repeated indices is implied. The coupling between concentration and ordering arises through \( \gamma(\phi) \), which equals

\[
    \gamma(\phi) = \gamma_0 + \phi(r, t) \Delta,
\]

(4.2)

where \( \gamma_0 \) and \( \Delta \) are appropriate constants. In our simulations described below, we fix \( \gamma_0 \) and vary \( \Delta \) (see Section 3 for full parameter list).

The free energy density used to describe compositional fluctuations is instead given by a simple function, used to describe binary fluid in the mixed (non-phase-separating) regime, and its form is simply given by

\[
    f_\phi = \frac{a}{2} \phi^2,
\]

(4.3)

where \( a \) is a constant related to the compressibility of the active gel component. Note we do not include a surface-tension-like square gradient term, \( \frac{k_s}{2} (\partial_\alpha \phi)^2 \), required for stabilisation in conventional binary mixture models, as density variations are already penalised thermodynamically by the term proportional to the elastic constant \( K \) in Eq. 4.1. Note also that the total free energy density
The function \( f = f_{\text{LC}} + f_\phi \) has two contributions which depend on \( \phi \): besides the mixing free energy \( f_\phi \), Eq. 4.3, there is also a \( \phi \) dependence in the liquid crystalline free energy \( f_{\text{LC}} \), Eq. 4.1, through the \( \gamma(\phi) \) term.

The fluid velocity, \( u \), obeys the continuity equation and the Navier–Stokes equation,

\[
\partial_\alpha u_\alpha = 0, \tag{4.4}
\]
\[
\rho (\partial_t + u_\beta \partial_\beta) u_\alpha = -\partial_\alpha p_0 + \eta \partial_\beta^2 u_\alpha + \partial_\beta \Pi_{\alpha\beta} - \zeta \partial_\beta (\phi Q_{\alpha\beta}), \tag{4.5}
\]

where \( \rho \) is the fluid density, \( \eta \) is an isotropic viscosity, and

\[
\Pi_{\alpha\beta} = 2\xi (Q_{\alpha\beta} + \frac{1}{3} \delta_{\alpha\beta}) Q_{\gamma\epsilon} H_{\gamma\epsilon} \tag{4.6}
\]
\[
- \xi H_{\alpha\gamma}(Q_{\gamma\beta} + \frac{1}{3} \delta_{\gamma\beta}) - \xi (Q_{\alpha\gamma} + \frac{1}{3} \delta_{\alpha\gamma}) H_{\gamma\beta}
\]
\[
- \partial_\alpha Q_{\gamma\nu} \frac{\partial f}{\partial Q_{\gamma\nu}} + Q_{\alpha\gamma} H_{\gamma\beta} - H_{\alpha\gamma} Q_{\gamma\beta}. \tag{4.7}
\]

is the stress tensor, where \( \zeta \) is the activity \[42\], and measures the strength of active force dipoles. With the sign convention chosen here \( \zeta > 0 \) means extensile rods and \( \zeta < 0 \) means contractile ones \[42\]. The molecular field \( H \) which provides the driving motion is given by

\[
H = -\frac{\delta F}{\delta Q} + (I/3) \text{Tr} \frac{\delta F}{\delta Q}, \tag{4.8}
\]

where \( \text{Tr} \) denotes the tensorial trace.

The equation of motion for \( Q \) is taken to be \[6\]

\[
\partial_t Q + u \cdot \nabla Q = \Gamma H + S, \tag{4.9}
\]

where \( \Gamma \) is a collective rotational diffusion constant. The first term on the left-hand side of Eq. 4.9 is the material derivative describing the usual time dependence of a quantity advected by a fluid with velocity \( u \). This is generalized for rod-like molecules by a second term

\[
S = (\xi D + \omega) \cdot \left( Q + \frac{1}{3} I \right) + \left( Q + \frac{1}{3} I \right) \cdot (\xi D - \omega)
\]
\[- 2\xi \left( Q + \frac{1}{3} I \right) \text{Tr} (Q \cdot \nabla u), \tag{4.10}
\]
where

\[ D = \frac{\nabla u + \nabla u^t}{2}, \quad \omega = \frac{\nabla u - \nabla u^t}{2}, \]

(4.11)

are the symmetric part and the anti-symmetric part respectively of the velocity gradient tensor \( \partial_\beta u_\alpha \). The constant \( \xi \) depends on the molecular details of a given liquid crystal. The first term on the right-hand side of Eq. 4.9 describes the relaxation of the order parameter towards the minimum of the free energy.

Finally, the active material concentration, \( \phi \), obeys a Cahn–Hilliard-like equation,

\[
\partial_t \phi + u \cdot \nabla \phi = M \nabla^2 \mu,
\]

(4.12)

where \( \mu = \frac{\delta F}{\delta \phi} \) is the chemical potential of the active mixture, and \( M \) is a mobility, which for simplicity we consider to be constant.

### 4.3 Numerical method

To study the dynamics of Eqs.(4.4)-(4.12), here we perform direct numerical simulations. Note that in our simulations we assume that the fields are two-dimensional and that the \( Q \) tensor describes nematic order in a 2D plane (i.e., we assume that there is no out-of-plane nematic order). We employ an in-house MPI-parallel code developed within the Dedalus spectral framework [12]. Simulations are performed on a periodic rectangular domain \([0, H] \times [0, H]\) with \( H = 200 \) (here and below, all quantities are given in simulation units).

All fields are represented by de-aliased, double periodic Fourier series with \( 512 \times 512 \) Fourier modes. Our time-iteration scheme employs a 4th-order semi-implicit backward differentiation formula (BDF) scheme [88] with the timestep \( dt = 0.1 \). We have confirmed that our spatial and temporal accuracy is sufficient to obtain numerically converged results. To obtain statistically converged averages, simulations are performed for 30000 time units.

In what follows, we fix \( \rho = 2, \eta = 5/3, \xi = 0.7, A_0 = 0.1, K = 0.01, \gamma_0 = 2, \Gamma = 1, \) and \( a = 0.003 \), and \( M = 4 \). These parameters are chosen as they are in line with those used in previous hybrid lattice Boltzmann simulations of
both constant-composition active nematics \[43, 44\] and self-motile active gel droplets \[78\].

### 4.4 Results

To discuss our results, we first present numerical simulations, and then a semi-analytical discussion of phase separation in the passive limit which sheds light on the phase diagram which we find.

#### 4.4.1 Simulation results

To address the role of compositional inhomogeneities in the hydrodynamics of extensile active gels, we first report numerical simulations (for methodology details, see Section 3). We characterise the dynamical behaviour of the system as a function of two key parameters: activity, quantified by \( \zeta \), and tendency to acquire nematic order, quantified by \( \gamma(\phi_0) = \gamma_0 + \phi_0 \Delta \). In practice, we change \( \zeta \) and \( \Delta \) in our simulations, keeping other parameters fixed (see Section 3 for a full list).

For each set of parameter values, we compute: (i) the average largest eigenvalue of \( Q \), denoted by \( \langle q \rangle \), which we use to quantify the global magnitude of order; (ii) the average fluid velocity, \( \langle |u| \rangle \); and (iii) the average variance of the compositional order parameter. In each case, these averages are computed first spatially, over a configuration, and then over time. We acquire data when the system is in a statistical steady state, removing any initial transient. These quantities allow us to build a phase diagram.

The magnitude of order, \( \langle q \rangle \), is shown in Fig. 4.1 and allows us to map the boundary between the isotropic and nematic phase. The nematic phase can be reached by increasing either \( \Delta \) (thereby \( \gamma(\phi_0) \)) or \( \zeta \). The former is a thermodynamic route, the latter is a non-equilibrium one. The non-equilibrium transition between isotropic and nematic phases arises because activity-induced flows create shear, which in turn generates nematic order. Analogous transitions in systems with constant composition or polar order have been studied in \[30, 62, 73\]. A linear stability calculation analogous to that of \[62\] shows that an isotropic state of constant \( \phi \) is unstable, for sufficiently large \( \zeta \), to an
active nematic state with non-zero flow and order. The critical threshold in the \((\Delta, \zeta)\) plane is described by \(\zeta_c(\Delta)\), where

\[
\zeta_c(\Delta) = \frac{2}{3} \xi A_0 \left( 1 - \frac{\gamma_0 + \phi_0 \Delta}{3} \right) \left( 1 + \frac{9 \Gamma \gamma_2}{2 \xi^2} \right),
\]

(4.13)
corresponding to a straight line on the \((\Delta, \zeta)\) plane. This predicted boundary is shown as a yellow line in Fig. 4.1. It agrees well with our numerics for small \(\Delta\), sufficiently far from the passive isotropic–nematic transition (at \(\zeta = 0\) and \(\Delta = 0.7\)). As the latter is a first-order discontinuous transition, which requires the inclusion of non-linear terms in the equation of motion to be accurately described, it is unsurprising that there is a quantitative discrepancy with our linearised calculation close to this point.

**Figure 4.1** Heatmap of the magnitude of nematic order as a function of \(\zeta\) and \(\Delta\). The plot can be used to define regions in parameter space where the system is in the isotropic passive (bottom left) or active nematic (top right) phase. The prediction for the onset of spontaneous flow (passive–active transition) from linear stability analysis (see text) is shown as a yellow line. Note that the isotropic–nematic transition in the passive limit \((\zeta = 0)\) occurs at \(\gamma(\phi_0) = 2.7\) (corresponding to \(\Delta = 0.7\); cf. section 4.4.2).

Throughout the nematic phase, except at \(\zeta = 0\), we find a non-zero flow in steady state. In other words, the emerging nematic structures are always active in the parameter range which we have explored. To characterise their
behaviour, we show in Fig. 4.2 the dynamical regimes we observe, before discussing the phase diagram quantitatively.

**Figure 4.2** From top to bottom rows represent: snapshots of concentration field, $\{\phi(x, y) \mid x, y \in [0, 200]\}$; director field, $\hat{n}$ (scaled by local magnitude of order, $q$, and coarse grained for visibility), overlaid on concentration (for $x \in [87, 113], y \in [168, 194]$); vorticity ($\omega_z$); largest eigenvalue of $Q$ tensor ($q$); $|Q_{xy}|$, qualitatively corresponding to a Schlieren pattern as could be obtained experimentally with crossed polarisers. Parameters are as in Section except: (a-e) $\zeta = 0.16, \Delta = 0.3$; (f-j) $\zeta = 0.2, \Delta = 1$; (k-o) $\zeta = 0.02, \Delta = 1$. 
Fig. 4.2(a–e) shows an example of regular active patterns. These are found close to the isotropic–nematic transition for moderate values of $\Delta$. The example shown features regular compositional modulations in steady state (Fig. 4.2a), where local minima are collocated with spiral defects in the director field of topological charge 1. The latter are most easily visible through the 4-brush pattern in the Schlieren-like plot of $|Q_{xy}|$ in Fig. 4.2e [21], and also correspond to deep minima in the local nematic order parameter, as shown in Fig. 4.2d. There are also steady vortices associated with the pattern, because spirals continuously rotate as in previous models of defects in constant-composition active nematics [34]. Such vortices can be identified as maxima and minima in the vorticity plot in Fig. 4.2c. This collocation with vortices provides support for the interpretation that these thermodynamically unstable structures are stabilised in steady state by the active flow. It is the thermodynamic coupling (proportional to $\Delta$) between order parameter and concentration in our free energy that drives the local concentration depletion at the centres of spirals, giving rise to a correlation between concentration and order, where larger concentration is associated with larger order, and vice versa. Thus the elastic energy cost associated with defect formation is decreased through proximal depletion, which explains the collocation of defects and voids. Our simulations show that the regular defect patterns we find close to the transition can either be stationary or self-motile (see Suppl. Movie 2 for the dynamics correspondent to the snapshot in Fig. 4.2a–e).

Fig. 4.2(f–j) shows an example of a different dynamical regime, obtained deeper in the nematic phase, for sufficiently large $\zeta$ and $\Delta$ (see also Suppl. Movie 3). Here, the patterns are never stable but display a chaotic dynamics and diffuse around in the system. In line with constant-composition active nematic literature [2, 14, 24], we refer to these spatiotemporally varying patterns as active turbulence. Our simulations show that active turbulent patterns are accompanied by the appearance of defects — mostly of half-integer topological charge, corresponding to two-brush patterns in $|Q_{xy}|$ (Fig. 4.2) — as in active gels of uniform composition. We also find this regime is characterised by large concentration variations (Fig. 4.2f). As in the case of regular patterns, here too the concentration field tends to decrease close to defect cores (Fig. 4.2g). As the active chaotic spontaneous flow moves defects around, streaks of concentration voids form (Fig. 4.2f,g) which follow defect trajectories. While the regimes in Figs. 4.2(a–e) and 4.2(f–j) are qualitatively reminiscent
of those found in the literature for constant-composition active extensile gels [44, 62, 73], we also find a third dynamical regime which is unique to inhomogeneous systems. This regime is found for low activity and sufficiently large $\Delta$, and consists in spontaneous phase separation into active and passive domains (Fig. 4.2(k–o), see also Suppl. Movie 1). Active domains are nematically ordered. Importantly, this is an example of microphase separation, or arrested phase separation, as coarsening does not proceed indefinitely and there are multiple domains in steady state (Figs. 4.2k,l, and S1). In other words, the late-time domain size — computed, for instance, via the inverse first moment of the structure factor — does not scale with system size and decreases with increasing $\zeta$ (see Supplemental Material and Figs. S1, S2). The presence of this spontaneous microphase separation regime is at first sight surprising, as the $\phi$-dependent part of the free energy does not promote demixing by itself. As we show in section 4.4.2, however, phase separation is driven by the coupling between nematic order and local concentration of active matter.

To quantitatively delineate the phase diagram of the system, and the boundaries between the three different dynamical regimes shown in Fig. 4.2, we proceed as follows. We use the plot in Fig. 4.1 to identify the phases as isotropic ($\langle q \rangle \approx 0$) or nematic ($\langle q \rangle \neq 0$). We then classify cases where the kinetic energy reaches a plateau as regular patterns. To discriminate between active turbulence and spontaneous phase separation, we look at probability distribution functions for $\phi$ (calculated over space, and averaged over time, see Fig. 4.3 for examples). If this distribution is bimodal (i.e., it has two maxima), then we classify the pattern as phase separated (Fig. 4.3 yellow curve). A similar identification would arise from analysing the average concentration variance and the average flow magnitude (Fig. 4.4). Flow and concentration variance are highest in the active pattern and spontaneous phase separation regimes respectively. The phase diagram for our inhomogeneous extensile mixture is shown in Fig. 4.5.
Figure 4.3  Probability distribution functions showing frequency versus local concentration at a grid point, for the active pattern (blue curve), the active turbulence (maroon curve) and the spontaneous phase separation (yellow curve) regimes. It can be seen that the distribution corresponding to the active turbulent regime is unimodal, while that associated with the spontaneous phase separated one is bimodal, with peaks at \( \phi \approx 0.19, 1.41 \), cf. binodal points in Fig. 4.6.

Figure 4.4  Combined heatmap of the averaged flow magnitude, \( |u| \) (blue), and variance of \( \phi \) (yellow), as functions of \( \zeta \) and \( \Delta \). The plot can be used to identify the regions of parameter space where phase separation is most prominent (upper left) or where the steady active flow is strongest (right).

The concentration distribution plots show that concentration variations are a generic feature throughout the active nematic phase. First we note that, without such concentration variations, the spontaneous microphase separation regime
could not arise. The existence of this regime in a realisable system depends on
the value of $\Delta$, which will be determined by microscopic parameters. Assuming
an Onsager-like theory for composition-dependent orientational order, we
expect this could be achievable with rod-like active particles of sufficiently large
aspect ratio. Note that we actually observe a bimodal distribution even in
the regular pattern regime, however here the magnitude of the peaks differs
by more than one order of magnitude. This corresponds to a detectable
depletion of active material at the cores of long-lived defects rather than actual
phase separation. A second observation is that the width of the concentration
distributions is remarkably large in the active turbulent regime, as the sampled
values of $\phi$ can vary from $\sim 0$ to $\sim 2$. This range is similar to the spread
observed in the spontaneous phase separation regime, although the distribution
remains peaked at $\phi \simeq \phi_0 = 1$ for active turbulent patterns. This observation
is in line with experimental microscopy of quasi-2D extensile mixtures of
microtubules and molecular motors, which shows a highly inhomogeneous
concentration of active material [47].

![Phase diagram of the system in the $(\zeta, \Delta)$ plane. Each square corresponds to one simulation. Regions A–D correspond respectively to isotropic passive, active patterns, active turbulence, and spontaneous microphase separation regimes.](image)

**Figure 4.5** Phase diagram of the system in the $(\zeta, \Delta)$ plane. Each square corresponds to one simulation. Regions A–D correspond respectively to isotropic passive, active patterns, active turbulence, and spontaneous microphase separation regimes.
4.4.2 Coupling-induced demixing in the passive limit

To shed more light on the physics underlying the occurrence of our spontaneous microphase separated regime, it is instructive to consider the passive limit of our nematic mixture, where the behaviour is solely determined by thermodynamic considerations. In this case, the free energy is minimised in equilibrium, and a full phase diagram can be computed semi-analytically using the common tangent construction (Fig. 4.6).

Recall that our model employs both conserved (composition $\phi$) and non-conserved (nematic tensor $Q_{\alpha\beta}$) order parameters, which are mutually coupled through the free energy given in Eq. 4.1. The resulting mixture is an example of a lyotropic liquid crystal, such as that considered in [49], albeit with an important distinction. Specifically, in the limit of no coupling ($\Delta = 0$ in Eq. 4.2), the system we consider exhibits no phase separation and mixes freely. In what follows, therefore, we shall see that passive phase separation is driven only by the coupling.

To find the equilibrium state, we consider a uniformly aligned (homogeneous) nematic phase, so that the elastic term contribution in Eq. 4.1 vanishes and the total free energy can be written in terms of the magnitude of nematic order, $q$, and of $\phi$ as follows,

$$f_{\text{hom}}(q, \phi) = \frac{A_0}{3} \left( 1 - \frac{\gamma(\phi)}{3} \right) q^2 - \frac{2A_0\gamma(\phi)}{27} q^3 + \frac{A_0\gamma(\phi)}{9} q^4 + \frac{a}{2} \phi^2. \quad (4.14)$$

This homogeneous state has everywhere the same value of the conserved composition. Thus, for each point $(x, y)$ in the system, $\phi(x, y) = \frac{\int dx dy \phi(x, y)}{\int dx dy} \equiv \langle \phi \rangle$. The magnitude of order that minimizes the total free energy for this given homogeneous value of $\phi$ is

$$q_{\text{min}}(\phi) = \begin{cases} 0, & \text{if } \gamma \leq \gamma_c \\ \frac{1}{4} \left( 1 + \sqrt{9 - 24/\gamma(\phi)} \right), & \text{if } \gamma \geq \gamma_c. \end{cases} \quad (4.15)$$

If the homogeneous state is stable against phase decomposition into regions of high and low concentration, then there is no configuration for which $\langle f \rangle$, the spatial average of the free energy density, is less than the value of $f_{\text{hom}}(q_{\text{min}}(\phi), \phi)$. However, as the common tangent construction illustrated
Figure 4.6  Coupling-induced demixing derived semi-analytically from the free energy for a uniformly aligned passive nematic phase given in Eq. 4.14. Panel (a) shows the free energy, $f_{\text{hom}}(q_{\text{min}}(\phi), \phi)$, which, for a given value of $\phi$, is minimized by $q_{\text{min}}(\phi)$ (see Section 4.4.2). The second derivative with respect to $\phi$ is shown with a dashed curve, and is negative in the spinodal region, highlighted in yellow. Here the system is linearly unstable to demixing into regions of high ($\phi_+$) and low ($\phi_-$) concentration, the values of which are given by the respective binodal points, shown in grey. These points are found by the common tangent construction illustrated by the green line, and share the same chemical potential and pressure ($\Pi$, dashed in blue). In this plot $\Delta$ is fixed at 0.7, and the presence of the lower spinodal point at $\phi = 1$ compares well with our simulation results, as illustrated in Fig. 4.5. Panel (b) shows the $\phi$-$\Delta$ plane, which is a phase diagram derived from the loci of the spinodal and binodal points illustrated in panel (a), considered as we vary $\phi$ and $\Delta$. The shaded spinodal and binodal regions are bounded by these loci, and show the parameter combinations for which the system is unstable to phase decomposition. Note that all $\phi$-axis values signify the spatial average over the system, which is dropped from the notation for readability.

in Fig. 4.6a shows, for each homogeneous configuration lying between the binodal points, there exists a corresponding inhomogeneous configuration with the same average composition, $\langle \phi \rangle$, but a lower average free energy density,
\(\langle f_{\text{demixed}}\rangle\), the value of which is given by the tangent line itself. Moreover, for sufficiently large \(\Delta\) and certain values of \(\phi\), we find that \(f_{\text{hom}}(q_{\text{min}}(\phi), \phi)\) is a non-convex function. In this spinodal region, we therefore expect that the nematic mixture is linearly unstable to phase separation. By comparison, in the limit of vanishing activity, our simulation found phase decomposition in the parameter range \(\langle \phi \rangle = 1, \Delta > 0.7\) (see, for instance, the left border of Fig. 4.5). This simulated demixing is highlighted in Fig. 4.6b, and signifies good agreement with our semi-analytic thermodynamic prediction.

In greater detail, the spinodal region — where the system is linearly unstable to phase separation, for any perturbation however small — is precisely where \(f_{\text{hom}}(q_{\text{min}}(\phi), \phi)\) is concave down. Thus it is bounded by the inflexion points, where the second derivative of \(f_{\text{hom}}\) with respect to \(\phi\), \(f_{\phi\phi}(q_{\text{min}}(\phi), \phi)\), crosses the \(\phi\) axis in Fig. 4.6a. The lower spinodal point is simply \(\phi_c = (\gamma_c - \gamma_0)/\Delta\), whereas the upper spinodal point, \(\phi_s\), was found numerically as the only real root of a seventh order polynomial.

This effective free energy also gives, by a common tangent construction, the binodal points, namely the values of the coexisting concentrations of the phase separated systems. Specifically, as coexisting phases must share a common chemical potential \((\mu = f_{\phi}(q_{\text{min}}(\phi), \phi))\) and a common pressure \((\Pi = f_{\text{hom}}(q_{\text{min}}(\phi), \phi) - \mu \phi)\), we have a system of two equations in two unknowns. The two unknowns in question are the two concentrations, \(\phi_-\) and \(\phi_+\), for which a straight line tangentially touches the curve \(f_{\text{hom}}(q_{\text{min}}(\phi), \phi)\) exactly twice, and were found numerically. For values of \(\langle \phi \rangle\) between the binodal points, this tangent represents the average free energy density of the phase separated system, which is visibly lower than the free energy density of the homogeneous system. Thus \(\langle f_{\text{demixed}}\rangle < f_{\text{hom}}(q_{\text{min}}(\phi), \phi)\) for \(\phi_- < \langle \phi \rangle < \phi_+\).

The loci of these spinodal and binodal points as we vary \(\phi\) and \(\Delta\) are the curves plotted in the \(\phi-\Delta\) plane in Fig. 4.6b. Here we can see that, in line with our simulation results shown in Fig. 4.5, there is a spinodal point at \(\Delta = 0.7\) for \(\langle \phi \rangle = 1\).

We stress again that the analysis in this section refers to the \(\zeta = 0\) passive limit of our mixture. In the active case, macroscopic phase separation is generically arrested by the activity-induced spontaneous flow. This leads to microphase separation at steady state, similarly to what has been observed in sheared passive binary mixtures [32, 67, 72] or in active model H [78].
Quantitatively, our theory predicts a spinodal point at $\Delta = 0.7$ for $\langle \phi \rangle = 1$, which compares well with our simulation results (Fig. 4.5). The predicted binodal points for $\Delta = 1$, lie at $\phi = 0.18$ and $\phi = 1.79$ — these values should be compared with the histogram peaks shown in Fig. 4.3, viz. $\phi = 0.19$ and $\phi = 1.41$ — the lower value of the latter peak is likely due to the active flow which drives the system away from thermodynamic equilibrium (assumed in Fig. 4.6). Note our simulations only find phase separation in the spinodal region in Fig. 4.6, as the initial perturbation of the homogeneous state are smaller than the scale required for nucleation.

4.5 Discussion and Conclusions

In summary, we have used computer simulations to study the hydrodynamics of an inhomogeneous active nematic gel. With respect to conventional models for active gels, which only consider the velocity field and Q tensor, our theory also allows for the time evolution of the active matter concentration $\phi$. Previous work has shown by a linear stability analysis that compositional fluctuations are irrelevant for the physics of the “generic instability” of active gels [4], which stands for the transition between the passive (quiescent) and the active (spontaneously flowing) phase. It has however remained unclear what their role is deep in the active phase, where nonlinearities are important; shedding light on this issue has been the focus of our current work.

Our main result is the quantitative characterisation of the phase diagram of inhomogeneous active nematic (Fig. 4.5). We have found that there are three regimes with distinct emergent behaviour in the active phase. First, close to the transition between the passive isotropic and active nematic phase, there are regular patterns typically composed of self-assembled rotating spirals. Second, deeper in the active nematic phase there is an active turbulent regime featuring chaotic dynamics of vortices and half-integer nematic defects. Third, for low activity and large enough nematic tendency ($\Delta$ in our phase diagram in Fig. 4.5), we find spontaneous phase separation into active and passive domains. This latter phase separation is arrested by the active flow, so that domains do not coarsen past a typical size, which decreases with increasing activity.

The regular spiral/vortex patterns we find are reminiscent of those observed with polar active gels in the ordered phase [25, 34]. While polar nematics can
only exhibit defects with integer topological charge, defects in active (apolar) nematics normally have half-integer topological charge, so it is non-trivial that close to the passive-active transitions we observe spirals, whose topological charge is $+1$. Notwithstanding this qualitative resemblance, the patterns we observe also have a non-trivial spatiotemporal dynamics (Suppl. Movie 2). The core of our spirals are also associated with notable concentration minima, or voids, which arise because of the coupling between nematic order and composition in the free energy of the system. The mechanism responsible for this coupling is the same that drives inert colloidal particles or isotropic droplets (with no anchoring on their surface) to the defect cores or disclinations in passive liquid crystals [28, 56].

The chaotic, active turbulent regime we find for sufficiently large $\zeta$ is an analog of the regime of the same name in active gels of uniform composition [2, 14, 37, 74]. An important feature of this regime in our simulations, though, is that there are very large compositional fluctuations (Fig. 4.3a). These are qualitatively in line with experimental observations of active turbulence in microtubule–motor mixtures, which show substantial inhomogeneities in microtubule concentration over a sample [47, 61]. Whether such concentration variations lead to a fundamental change in the scaling properties of active turbulence is an open question which we believe deserves further investigation, for instance by a quantitative detailed analysis of the scaling of velocity–velocity correlations [3, 68, 87].

Regarding the spontaneous microphase separated regime, this is notable especially because there is no term in the free energy density $f_\phi$ which explicitly favours demixing. In other words, in the absence of $f_{LC}$ the system would remain uniform. Phase separation arises due to the coupling between composition and order, measured by the parameter $\Delta$. In this sense, phase separation is not driven by activity but rather thermodynamically, and indeed it can be explained with a theoretical discussion of the free energy in the passive limit (Fig. 4.6). In simulations we observe a microphase separated pattern rather than macroscopic phase separation, as the active flow arrests coarsening, and controls the size of the steady-state domains observed at late times, similarly to the case of active model H [78]. While experimental realisation of active nematics have shown plenty of instances of active turbulence [47, 61],

\[1\] Note that in our geometry integration of the topological charge density, defined as in [11], is conserved and equal to 0.
the spontaneous microphase separation regime appears to not have been found in the lab yet. Our model suggests that the most promising avenue to realise this regime experimentally is to control the composition-order coupling $\Delta$. The latter may be estimated by monitoring how the isotropic–nematic transition point depends on the concentration of nematogenic particles (for instance, microtubules) in the passive limit of no activity.

Looking ahead, we can suggest a few directions in which our work can be carried forward. First, it would be of interest to understand from a more fundamental point of view the universal properties of the dynamical regimes we have identified. For instance, one could quantify the dependence of vortex correlation length and pattern size on physical parameters, and the scaling of the power spectra of the kinetic energy. This would allow to clarify the important theoretical question of whether or not inhomogeneous active turbulence is in the same universality class as turbulence in active gels of uniform composition. Second, from the experimental point of view, it would be desirable to compare more quantitatively concentration distributions in active turbulence with those predicted by our simulations. Third, with regards to computer simulations, it would be highly interesting to explore the phase behaviour and dynamics of inhomogeneous active nematics in 3D, comparing and contrasting it with the one found here in 2D.
Chapter 5

Conclusions

In this work of thesis we have shown the results from computational studies collective motions in active fluids. Most studies (theory and experiments) on active fluids are performed in two-dimensional environments. We developed a minimal model for Bacterial Turbulence, in order to take into account the three-dimensional nature of hydrodynamic interactions in bacterial suspensions, even when swimmers are confined in a two-dimensional plane.

In Chapter 2, we laid down the basics of the minimal lattice model we developed for studying bacterial turbulence, and explored results for fully packed lattices identifying the analogue of collective motion states in what appears to be frozen states in our simulations.

In Chapter 3 we improved on the previous model considering lattices with density $\leq 1$, in order to make the swimmers able to move. On these premises we were able to reproduce Motility Induced Phase Separation (MIPS) and study how hydrodynamic interactions affect it. We found that, other than just suppressing MIPS, hydrodynamic interactions result in a change of transition type, and the system exhibits a microphase separation. We also find that, due to the swimmers being two-dimensional sources in a three-dimensional velocity field, the suspension is hyperuniform when not in a separated phase.

Finally, in Chapter 4 we presented our result for numerical simulations on inhomogeneous active gels. Since it has been shown by linear stability analysis that inhomogeneities do not affect the stability near the transition between passive and active phases, we focused on studying how compositional
fluctuations in the active matter concentration deep in the active phase. In this study we characterised the phase diagram of inhomogeneous active nematics finding three distinct different regimes inside the active phase. In particular the system showed: regular patterns of rotating spirals next to the transition between passive isotropic and active nematic, a turbulent regime deep in the active nematic phase, and spontaneous phase separation for low activity and high nematic tendency.
Bibliography


