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Collective Motion in Microswimmer Suspensions

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What is true for *E. coli* is true for the elephant.
– Jacques Monod
Abstract

The main distinction of active matter from its passive counterpart is the ability to extract energy from the environment (consume food) and convert it into directed motion. One of the most striking consequences of this distinction is the appearance of collective motion in self-propelled particles suspended in a fluid observed experiments and simulations: at low densities particles move around in an apparently uncorrelated fashion, while at higher densities they organise into jets and vortices comprising many individual swimmers. Although this problem received significant attention in recent years, the precise origin of the transition is poorly understood.

In this work, we develop theoretical tools, both analytical and numerical, to address this problem. We will study the minimal model of self-propelling particles immersed in an incompressible viscous fluid. Our approach is based on Kinetic theory – a probabilistic description of many-particle systems with both positional and orientational degree of freedom. The emphasis is put on the rôle of hydrodynamic interactions, which are long-ranged in nature and result in nematic alignment between the individual particles. We aim to understand the properties of microswimmer suspensions when passing through the instability threshold leading to collective motion, as well as the collective motion itself.

Our results, although derived for a minimal model, can be directly tested in experiments, and numerical simulations. We carry out detailed linear stability analysis, and show that the exact type of instability in microswimmer suspensions depends on the geometry of the system. The collective motion regime is assessed at the mean-field level, where statistical properties of this highly non-linear state are measured using large-scale pseudo-spectral simulations. Moreover, we develop Kinetic theory that goes beyond the commonly assumed mean-field approximation, and directly incorporates both correlations stemming from the tumbling effects, as well as the self-propulsion mechanism. The results presented in this work shed light on the collective behaviour of large number of microorganisms, and serve as a solid basis for further research.
Bacteria constitute the bulk of the biomass of our planet. As they are invisible to the naked eye, we often forget about their existence. Still, they are present in our bodies and play a key role in our metabolic system. Understanding the collective behaviour of large number of microorganisms is essential for broad spectrum of fields ranging from medicine, and pharmaceutical industry, to biotechnology.

The life of bacteria is relatively simple. They live in a viscous fluid, move towards regions with higher number of nutrients essential for their survival, and reproduce. The physics at the level of microscale is, however, very different from our own human experience. Due to the relatively small size of bacteria compared to the fluid molecules, the friction forces of the environment overcome any inertial effects. The resulting physics is nicely concluded in *Scallop theorem* introduced by Purcell in 1977, which states that a time-symmetric motion cannot achieve any net displacement under such conditions. Hence, in order to self-propel some bacteria have evolved flagella – one or more tails bundled together the rotation of which drives locomotion.

Even more interesting phenomena appear when two or more microorganisms swim together. Due to their non-spherical shape, they always tend to align with the surrounding fluid flow. The more bacteria in the fluid, the stronger the flow exerted by their flagella, and hence the stronger the alignment. This effects leads to exotic macroscopic behaviour at moderate densities known as *collective motion*, which has become one of the most studied phenomena in the modern biophysics.

When discussing macroscopic properties, we are often not interested in exact microscopic structure of individual microorganisms, but seek an effective description with small number of variables that still accurately predicts observables. Most of the macroscopic physical systems, such as solids, gases, and fluids can be well described as continuum. The same idea can be applied to microbiology, where a field theory for bacterial suspension can be constructed; Since bacteria are free to swim in the environment, they can be regarded as a fluid of particles where standard methods of non-equilibrium statistical physics can be applied.

In this work, we will present an effective description for a collection of swimming microorganisms. The microswimmers are considered to be ellipsoidal in shape, and immersed in an incompressible fluid. Their self-propulsion mechanism exerts hydrodynamic flow, which in turn leads to their mutual alignment. The main aim is to understand the conditions under which macroscopic collective motion appears, and what are the statistical properties of the collective motion. We will apply both theoretical, as well as numerical tools to answer these questions.
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 processional qualification except as specified.

(Viktor Škultéty, February 2023)

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Chapter 1

Introduction

1.1 Active matter

In recent years active systems emerged as a new state of matter with unique properties that are absent from their passive counterparts [11, 12]. Such systems comprise particles that are capable of extracting energy from their environment and using it to exert forces on their surroundings or generating physical fields. The resulting motion, and interactions between particles break detailed balance at the microscopic level, often leading to steady states that are not invariant under time reversal and exhibit macroscopic currents [13]. Such currents, or collective motion, have been reported in a variety of systems [14], including Vicsek particles [15], mixtures of microtubules and molecular motors [16], light-activated colloids [17], Quincke rollers [18, 19], bacterial colonies [20], sperm cells [21], locusts [22], birds, and fish [23]. The omnipresence of collective motion raises the need to classify various active systems according to common features of their phenomenological behaviour. Marchetti et al. [12] recently introduced two broad classes for active systems, ‘dry’ and ‘wet’, depending on whether the system can be described by models without or with momentum conservation. In practice these two classes correspond to a collection of particles dominated either by friction with their surroundings or long-ranged hydrodynamic interactions, respectively. Each class is expected to be defined by a few, relatively simple model systems, and significant effort has been invested into finding such models. For dry active matter, these include Vicsek-like models [14, 24], that describe cases where alignment interactions are dominant, and Active Brownian Particles [25, 26] or Run and Tumble particles [27], that describe systems dominated by steric forces randomising their self-propulsion direction either smoothly or in a discontinuous manner. In this thesis, we study a minimal model for dilute suspensions of motile bacteria that, arguably, play the same rôle for wet active matter [28, 29].

Figure 1.1: Swarming P. vortex bacteria [10]. Breaking of the time-reversal symmetry at the microscopic level can lead to stunning macroscopic behaviour.
1.2 The rôle of Hydrodynamics

The survival of bacteria heavily depends on their ability to search for a food source. To move through viscous fluids, motile micro-organisms exert forces and torques on their environment [32–34]. Due to their relatively small size and low propulsion speed, the resulting motion is dominated by the viscous stresses in the fluid, and is well-described by Stokes equation [35]. Historically, the early attempts to model motile bacteria can be tracked back to Lighthill, who in 1972 proposed the Squirmer model – a spherically symmetric body generating self-propulsion using small oscillations of its surface [32]. A couple of decades later the model was applied by Blake to describe the fluid flow generated by a carpet of beating cilia on the surface of an eukaryotic cell Paramecium [33].

Unlike Paramencium, locomotion of prokaryotic cells is caused by periodic motion of their flagella [36]. The hydrodynamic flow created by these micro-organisms can be described by a combination of the singular solutions of Stokes equation, which decay algebraically in space [37]. The leading singularity for force- and torque-free microswimmers suspended in an infinite viscous fluid is given by a force dipole, which exhibits slow spatial decay, $r^{-d+1}$, where $r$ is the distance from the microorganism, and $d$ is the dimensionality of space. Such velocity fields are long-ranged, and even rather dilute suspensions of microorganisms exhibit significant fluid motion far away from microorganisms. Such ‘self-stirring’ in the absence of an external forcing is a strongly non-equilibrium phenomenon characteristic of active matter [12].

Depending on the symmetry of their hydrodynamic flow, microswimmers can be divided into two distinct classes: i) ‘pushers’, which accurately describe most swimming bacteria such as E. coli [38], and ii) ‘pullers’, whose reversed hydrodynamic flow field is typically exemplified by the alga C. reinhardtii [39]. Moreover, it is well known that microorganisms tend to randomly change the direction of their self-propulsion (so-called run-and-tumble motion), which is essential while searching for the food source [36]. These ingredients result in a unique set of transport and mechanical properties of microswimmer suspensions, such as enhanced diffusivity of tracer particles [40, 41], and significant changes of the apparent suspension viscosity [29].

![Image](image1.png)

Figure 1.2: Left: The locomotion in Eukaryotic cells is due to beating cilia at the surface of their body [30]. Right: Prokaryotic cells undergo locomotion due to rotation of their flagella [31].
1.3 Collective motion

Arguably, the most profound effect of the long-range velocity fields self-generated by a suspension of motile microorganisms is the transition to a large-scale, collective motion in elongated pusher-like microswimmers such as bacteria. Driven by the mutual advection and re-orientation of the microswimmers, the ensuing fluid motion exhibits chaotic behaviour, often referred to as bacterial turbulence, see Fig. 1.3 [42, 43]. Even below the onset of collective motion, the long-ranged hydrodynamic interactions result in strong correlations between microswimmers, present at any microswimmer density [5, 44]. The mechanism of the transition to bacterial turbulence is usually rationalised based on mean-field kinetic theories that take into account the presence of long-range hydrodynamic interactions between microswimmers [45]. For pusher bacteria, these theories predicts the onset of large-scale flows above a well-defined critical microswimmer volume fraction, and identifies mutual particle reorientation as the main mechanism behind the instability.

Collective motion in bacteria has been extensively studied in dilute [46–48] and dense [42, 43, 49–54] suspensions. These studies reveal the following sequence of dynamical states. At very low densities, bacterial suspensions appear featureless and disordered [48, 50]. At higher, yet still, sufficiently low densities, collective motion sets in on the scale of the system. In this state, bacterial motion takes the form of large-scale jets and vortices with typical speeds that are larger than the swimming speeds of individual organisms [46–48]. At significantly higher densities, there emerges a typical lengthscale of the vortices, which is comparable to about 5 – 10 times the bacterial size [43, 54, 55]. Although this sequence of dynamical states has never been simultaneously observed in a single systematic bulk experiment, with the exception of Sokolov et al. [52], the transition scenario is supported by computer simulations of self-propelled particles interacting through various forms of long-ranged hydrodynamic fields and short-ranged steric repulsion [44, 56–69].

Figure 1.3: Experimental snapshot of highly concentrated homogeneous suspension of *B. subtilis* in a quasi two-dimensional geometry (left), and the corresponding flow streamlines and vorticity fields (right). The pictures are taken from [42].
Bulk experiments with *E. coli* [48] and *B. subtilis* [47] show that the transition to collective motion occurs around a volume fraction of bacterial bodies of about 1 − 2%. At such densities, the typical distance between organisms is about 5 − 8 times their body length, collisions are rare, and the far-field hydrodynamic interactions are thought to be dominant [28, 29]. The latter are well-described by a ‘pusher’-like Stokesian dipolar field [35, 38], generated when two point forces of equal magnitude and pointing away from each other are applied to a viscous fluid. Self-propelled pusher-like dipolar particles thus form a minimal model for dilute bacterial suspensions. In practice, observations of such bulk collective flows are complicated by the unavoidable presence of boundaries in experimental setups used to study motile microorganisms. Importantly, motile organisms accumulate in close vicinity of solid boundaries, significantly depleting the bulk in-between [70]. Therefore, from the experimental perspective, it is sometimes more convenient to study the ensuing collective motion in a layer of microswimmers confined by either one or two boundaries.

The transition to collective motion in dilute bacterial suspensions can be understood in terms of a mean-field kinetic theory [28, 29] incorporating the minimal ingredients discussed above. Such theory identifies re-orientation of bacteria in the velocity field created by other organisms as the key ingredient leading to a global isotropic-nematic transition. The globally ordered state is, however, linearly unstable through a long-wavelength generic instability [12, 71], and there ensue never-settling dynamics as a compromise between the two instabilities. The critical density of bacteria at the onset of collective motion is determined by the strength of their dipolar interactions, their shape, and the way individual organisms change their orientation: either by occasionally re-orienting in a random way (tumbling), or by rotational diffusion [45, 63, 72–74]. Typically, the critical threshold density is significantly lower in the latter case, and going to zero in the absence of a decorrelation mechanism for individual bacterium orientation. The mean-field kinetic theory has also been extended to systems with steric interactions [55, 75–77] and to microswimmers suspended in non-Newtonian fluids [78–80].

Below the onset of collective motion, the mean-field kinetic theory predicts that the suspension is homogeneous and isotropic, as featureless as a suspension of non-interacting microswimmers. These assumptions are widely used when describing rheological properties of very dilute suspensions [2, 81–92] and enhanced diffusivity of tracer particles [40, 41, 59, 93–106]. However, recent large-scale Lattice-Boltzmann simulations of dipolar swimmers [44, 68] revealed the presence of very strong correlations below the onset of collective motion. It was shown that various observables deviate from their mean-field values at any density of microswimmers [44], with the deviation growing rapidly as the system approaches the onset. The origin of such strong correlations can be readily attributed to the slow spatial decay of the dipolar velocity field, implying a simultaneous coupling between all microswimmers in the system. While this argument is intuitive enough, its implementation as a theoretical framework presents major technical challenges, and only simplified cases were studied until now [85, 107]. A systematic account for strong correlations between all microswimmers was achieved by Stenhammar *et al.* [44], who developed a kinetic theory for suspensions of ‘shakers’ – particles that apply forces to the fluid but do not self-propel. However, the general theory for motile bacteria is still lacking.
1.4 Structure of this thesis

In this thesis, we build upon the previous theoretical works of microswimmer suspensions interacting via long-range hydrodynamic interactions, and reveal their statistical properties around the transition to the collective motion. The thesis is organised as follows.

In Chapter 2, we review up-to-date research results regarding modelling microswimmer suspensions. We start with discussing the hydrodynamics at the level of microscale, and how the swimmers interact within each other. We then proceed with discussing modeling a many-particle system using mean-field Kinetic theory. Analytical, as well as numerical results are mentioned, where the onset of the collective motion can be understood on the level of linear stability analysis. Later, we discuss recent theoretical results that take into account correlations in the suspension, showing that the mean-field approximation is inaccurate for the complete description of the suspension. At last, at the end of the sections we point out relevant questions that motivated our work.

We then proceed to our first project – in Chapter 3, we analyse the linear stability of the mean-field kinetic theory. Such a calculation represents the first step towards understanding collective motion. More importantly, collective behaviour of many-particle systems is known to be strongly influenced by the presence of confinement. We therefore consider various geometries to understand the differences between individual instabilities. Our approach is different from the procedures commonly deployed in the literature – instead of guessing the solution to the linearised set of equations, we explicitly derive the solution using Laplace transform. This allows us to directly identify the origin of the instability in a rather simple manner, and show appearance of intriguing instabilities in confined suspensions.

Once the instability threshold is understood, we turn our attention to the collective motion. Due to the rather chaotic nature of the latter state, analytical approaches are inconvenient. Instead, in Chapter 4 we perform large-scale pseudo-spectral simulations in a bulk 2d system, and measure statistical properties of the non-linear regime by averaging the observables over many time steps. We show, that although the instability sets in at the scale of the system size, a finite length-scale emerges within the collective motion regime which sets the typical size of the strongly correlated regions. Moreover, we observe strong finite size effects, and density fluctuations typical for equilibrium systems. The latter is in contrast to fully nematic systems that are expected to show giant number of density fluctuations.

As recent particle-based simulations emphasize the importance of the correlations in the bacterial suspensions, mean-field theory is expected not to fully capture the physics of the collective motion. In Chapter 5 we will test the validity of the mean-field kinetic theory by simultaneously taking into account correlations coming from tumbling effects, and the self-propulsion. Starting with the general N-particle kinetic theory, we calculate the spatial and temporal correlations of the fluid velocity below the onset. We show, that although the correlations decay with increasing self-propulsion speed, their effect remains significant even in the limit of infinitely fast bacteria.

Finally summarise our results in the last Chapter 6, and further details about the mathematical machinery used can be found in the Appendixes A-D.
Chapter 2

Modeling collective motion

This chapter is devoted to summary of current research progress on collective motion in microswimmer suspensions. All the work presented in this thesis follows from the theoretical concepts and experimental results mentioned in the following sections.

We start with discussing how microswimmers are modeled microscopically. In this thesis, we will primarily focus on microorganisms such as *E. coli*, which self-propulsion mechanism can be approximated with a simple model of two forces that are equal in magnitude and opposite in direction [34]. The ensuing fluid flow in an infinite system is known as hydrodynamic dipole, and plays the fundamental ingredient in the theory of collective motion [35].

Later, we will introduce kinetic theory for microswimmer suspensions – a probabilistic theory for a collection of microswimmers immersed in an incompressible fluid. The crucial assumption, the mean-field approximation, allows us to neglect correlations between the particles which results in a single equation for one-particle phase-space density driven by the mean-field hydrodynamic dipole [45]. Here, the microswimmers will be considered to be self-propelling entities that are ellipsoidal in shape, with the resulting model representing an extension of Doi’s kinetic theory of passive rods [108].

Due to the large number of dependent variables (positional, and orientational), kinetic theory can be inconvenient for practical calculations. Instead, the moment expansion of the phase-space density is commonly used, with leads to equations for the concentration, polar, nematic order etc. [29]. A closure to this infinite series of equations is required, which is normally done by neglecting moments that are higher order than two. The resulting model allows to study the instability leading to the collective motion, as well as the statistical properties of the collective motion itself.

At last, the validity of the mean-field approximation must be verified as well. In the last section of this chapter we review recent work where the role of correlations between the microswimmers have been analysed [44]. The obtained analytical results are in agreement with lattice-Boltzmann simulations developed in the same work, although only the case of vanishing swimming speed was considered.

At the end of all sections we outline the relevant questions appearing in the corresponding topics, which will be discussed in this thesis.
2.1 Life at low Reynolds number

As bacteria swim, they exert forces on the fluid which results in a hydrodynamic flow. At the level of microscale, the viscous forces of the surrounding fluid suppress any inertial effects, so that the resulting flow is accurately described by the Stokes equations. A minimal model for a single microswimmer can be then constructed by considering a small number of forces acting on the fluid. Due to the linearity of the hydrodynamic equations, a many particle system can be derived by simply summing contributions from all particles, as will be now discussed.

2.1.1 Hydrodynamic flow at the microscale

Under any earthly conditions, microorganisms live in an incompressible fluid. In general, the dynamics of an incompressible fluid is given by the incompressible Navier-Stokes equations, accompanied with the incompressibility condition, which have the following form [109]

\[ \rho D_t \mathbf{u} = \nabla \cdot \mathbf{\sigma} + \mathbf{f}, \]  
\[ 0 = \nabla \cdot \mathbf{u}. \]  

Here, \( \mathbf{u} \) is a field describing the velocity of the fluid, \( \rho \) is the (constant) density of the fluid, and \( D_t \equiv \partial_t + \mathbf{u} \cdot \nabla \) is the convective derivative that appears due to self-advection of the velocity field, and describes the inertial effects of the fluid. The stress tensor \( \mathbf{\sigma} \) takes into account all internal forces present in the fluid, and for Newtonian fluids it has two components: the pressure term, \(-P\), that acts as a Lagrange multiplier that enforces the incompressibility condition (2.1.2), and the viscous stress tensor, \( \mathbf{\sigma}_{\text{visc}} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \), with \( \mu \) is the viscosity of the fluid, that is responsible for viscous dissipation due to the internal friction forces. The remaining term \( \mathbf{f} \) stands for all external forces acting on the fluid, which can be used to model any disturbances in the flow due to foreign objects.

In this thesis, we will be interested in the hydrodynamic flow that is created by the swimming microorganisms. At the relevant spatial scales, the corresponding dynamical equations (2.1.1) can be simplified in the following way. Let us assume that a bacterium with the linear length \( \epsilon \), is swimming through the fluid with the swimming speed \( v_s \). Introducing dimensionless quantities as \( x \to \epsilon x, \ t \to t\epsilon/v_s, \) and \( \mathbf{u} \to v_s \mathbf{u} \), the Navier-Stokes equations (2.1.1) become

\[ \text{Re} \, D_t \mathbf{u} = \nabla^2 \mathbf{u} - \nabla P + \mathbf{f}, \]  

where \( \text{Re} = v_s \epsilon \rho/\mu \) is the Reynolds number, and we have scaled out all other remaining constant prefactors. Eq. (2.1.3) shows that in the absence of any external forces \( \mathbf{f} = 0 \), the only dimensionless number describing the structure of the flow is \( \text{Re} \). For typical microorganisms, \( \epsilon \sim 1\mu m, \ v_s \sim 10\mu m/s \), and considering room-temperature water density, and viscosity \( \rho \sim 10^3\text{kg/m}^3, \ \mu \sim 10^{-3}\text{Pa.s} \) its numerical value is \( \text{Re} \sim 10^{-5} \) [34]. Under these circumstances the viscous forces dominate over the inertial effects which allows us to neglect the convective derivative on the left-hand-side of Eq. (2.1.3). The resulting hydrodynamics is known as the Stokes flow [110], which represents the quintessential hydrodynamical flow in microbiology.
2.1.2 Minimal model of self-propelling microswimmer

The survival of microorganisms crucially depends on their ability to move towards regions containing essential nutrients, such as sugar [34]. In order to self-propel, bacteria are equipped with a flagella – one or more helical filaments bundled together – responsible for a persistent locomotion. For the class of bacteria we will be interested in describing in this thesis, the flagella are composed of several filaments each of which rotates due to molecular motors attached at the surface of the microorganism [36]. This movement exerts forces of the fluid, which are completely balanced by the drag of the fluid, leading to a locomotion with constant swimming speed \( v_s \).

The exact mathematical description of self-propelling microorganisms requires modeling foreign objects immersed in a fluid with nontrivial boundary conditions [111]. The corresponding model can be quite complicated even for a single bacterium, hence a simplified model is needed. In order to capture the large-scale patterns that occur when many swimmers interact, Hernández-Ortiz et al. [56] considered a minimal model of a swimmer, where the self-propulsion is provided by two forces that are equal in magnitude and opposite in direction, thus mimicking the effect of flagellum on the fluid. This model, known as hydrodynamic dipole, is particularly useful for modeling certain class of bacteria that are rather ellipsoidal shape with an orientation \( \mathbf{p} \) [38,43]. Due to the low \( \text{Re} \) nature of the microscale physics, the corresponding hydrodynamic flow is accurately described by the forced Stokes equations [35]

\[
\begin{align*}
0 &= \mu \nabla^2 \mathbf{u} - \nabla P + f \mathbf{p} \left[ \delta(\mathbf{x} - \mathbf{x}_0 - \frac{l}{2}\mathbf{p}) - \delta(\mathbf{x} - \mathbf{x}_0 + \frac{l}{2}\mathbf{p}) \right], \\
0 &= \nabla \cdot \mathbf{u},
\end{align*}
\]

where \( f \) and \( l \) are the amplitude of the force, and the length of the dipole, and \( \mathbf{x}_0 \) is the position of the dipole (see Fig. 2.1). For \( l \ll 1 \), the solution to above set of equations in three spatial dimensions has the following form in the real and Fourier space

\[
\begin{align*}
u_d(r, \mathbf{p}) &= \frac{\kappa}{8\pi} \frac{r}{|r|^3} \left[ 3 \left( \frac{\mathbf{p} \cdot r}{|r|^2} \right) - 1 \right], \\
\mathbf{u}_d(k, \mathbf{p}) &= -\frac{i\kappa}{4\pi} \frac{\mathbf{k} \cdot \mathbf{p}}{k^2} \mathbf{P} \cdot \mathbf{p},
\end{align*}
\]

where \( r = \mathbf{x} - \mathbf{x}_0 \), \( \mathbf{P} = 1 - \mathbf{k}\mathbf{k}/k^2 \) is the transversal projection operator ensuring the incompressibility of the fluid\(^\text{1}\), and \( \kappa = fl/\mu \) is the dipolar strength. The value of the latter parameter determines the structure of the flow. Its value is positive, \( \kappa > 0 \), for pusher-type particles and negative, \( \kappa < 0 \), for puller-type particles [29]. The velocity field described by Eq. (2.1.6) has been found to match experimental results; The puller model has been observed to be a fair approximation for the flow generated by C. reinhardtii [43], while the pusher model was found to describe quite well the flow generated by E. coli [38] – see Fig. 2.2.

\[^\text{1}\]The incompressibility condition in the Fourier space yields \( k \cdot \mathbf{u}_d = 0 \), which means that the velocity field must be transversal to the wave-vector \( \mathbf{P} \cdot \mathbf{u}_d = \mathbf{u}_d \).

Figure 2.1: Self-propelling microorganism modeled as a hydrodynamic dipole.
2.1.3 Interacting microswimmers

Bacteria immersed in a fluid do not only create a hydrodynamic flow due to their self-propulsion mechanism, but their movement is also affected by the local dynamics of the fluid. In order to study the resulting movement of the bacterium equations for both positional $x$, as well as orientational $p$, degrees of freedom must be considered. The most straightforward way is to consider the following set of overdamped Langevin equations

$$\dot{x} = v_s p + \mathbf{U} + \sqrt{2D_t}\eta_x,$$

$$\dot{p} = (1 - pp) \cdot [(\nabla \mathbf{U} + B\mathbf{E}) \cdot p + \sqrt{2D_r}\eta_p].$$

(2.1.7)

(2.1.8)

The information stored in (2.1.7), and (2.1.8) is the following. Each microswimmer self-propels with the swimming speed $v_s$, and its centre of mass $x$ is advected by the local fluid velocity $\mathbf{U}(x; t)$. Microswimmer orientation $p$ changes due to the presence of velocity gradients at the position of the particle, and along its orientation [111, 112]. Mathematically, this is represented by terms such as $p \cdot \nabla \mathbf{U}$, which appear in the Jeffery’s equation (2.1.8). Here, $\mathbf{W} = \frac{1}{2}(\nabla \mathbf{U} - (\nabla \mathbf{U})^T)$ and $\mathbf{E} = \frac{1}{2}(\nabla \mathbf{U} + (\nabla \mathbf{U})^T)$ are the shear-rate and rate-of-strain tensors, and the parameter $B = (a^2 - 1)/(a^2 + 1)$ quantifies the swimmer’s ellipsoidal shape [111] based on the aspect ratio of it’s major and minor axes $a$ ($B = 0, 1$ for spherical/rod-like particles). Since any change in the orientation must be orthogonal to $p$, the right-hand-side of Eq. (2.1.8) must be contracted with the projection operator $(1 - pp)$. As mentioned earlier, the self-propulsion mechanism of bacteria generates long-ranged flows in the suspending fluid [35]. This flow, in turn, affects the surrounding swimmers in the suspension. In general, the flow at any point is given by the sum of all dipolar fields (2.1.6) generated by all microorganisms [1, 44],

$$\mathbf{U}(x; t) = \sum_{i=1}^{N} u_d(x - x_i(t), p_i(t)),$$

(2.1.9)

where $N$ is the total number of particles. Note that this linear sum of dipoles is possible only due to the linearity of the Stokes equations (2.1.4), which is an exclusive feature of low Re hydrodynamics.
Thermal fluctuations of the fluid also affect the movement of the microorganism [36], and result in diffusive behaviour of the bacterium’s position and orientation. In Eqs. (2.1.7)-(2.1.8), the translational, and rotational diffusions are represented by the noise terms $\eta_x, p$, that obey Gaussian statistics with two point correlators

$$\langle \eta_x(t) \eta_x(t') \rangle = \langle \eta_p(t) \eta_p(t') \rangle = 1 \delta(t - t'), \quad \langle \eta_x(t) \eta_p(t') \rangle = 0,$$

where $D_t$ and $D_r$ are the translational and rotational diffusions constants, respectively.

In order to study the $N$-particle system of microswimmers, a set of Langevin Eqs. (2.1.7)-(2.1.8) for every particle must be constructed [114,115]. The resulting macroscopic behaviour stemming from this stochastic model can be studied by the means of both analytical as well as numerical methods. In general, the former involves solving the Fokker-plank equation for $N$-particle probability density distribution. This approach leads to a model with too many independent variables, and certain approximations must be applied, as will be discussed below.

### 2.1.4 Run & tumble

The motion of bacteria, such as E. coli, does not only involve self-propulsion and transport by the local properties of the fluid, but is also affected by their intrinsically driven change of orientation. Each time period, $\lambda$, the motor driving individual filaments of the flagella reverses its spinning direction for a short period of time, resulting in unbundling and rebundling of the entire flagella. As a result, the bacteria undergo so-called run-and-tumble dynamics, where periods of swimming (‘runs’), are interspersed by random reorientation events (‘tumbles’) – see Fig. 2.3. This chaotic movement allows the bacteria to migrate towards places with higher nutrients [36].

The mathematical representation of the tumbling process is not as straightforward as in the rotational diffusion; Since the process requires discontinuous jump in the orientation of the particle $p$, the corresponding Langevin equation, such as (2.1.8), does not exist. An alternative approach based on the Master equation is required, which will be introduced in the following section.

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Figure 2.3: Run-and-tumble dynamics. The bacterium’s locomotion is interrupted by unbundling and rebundling of the flagella, leading to the change of the self-propulsion direction.

---

Note that the multiplicative noise in (2.1.8) must be interpreted in the Stratonovich sense in order to preserve the unit length of $p$ [113]

11
2.2 Continuum models of microswimmer suspensions

We now introduce continuum models for suspensions of many microswimmers. As it was mentioned in the previous section, modeling large number of particles as a stochastic process leads to a probabilistic model with a high number of independent variables. In order to simplify the system, but still preserve the crucial features of the model, the equation for a single particle experiencing hydrodynamic interaction generated by the ‘mean field’ of other particles is considered. The latter will now be discussed.

2.2.1 Kinetic theory

Microswimmer suspension represents a many-particle system with long-range hydrodynamic interactions. In order to study this problem, mean-field Kinetic theory was proposed by Saintillian and Shelley [45], and independently by Subramanian and Koch [73]. The system is considered to be composed of $N$ identical particles moving autonomously through a viscous fluid stored in a periodic box of linear size $H$. For any practical purposes, the suspension is considered to be dilute in order to avoid the effects of steric interaction and hydrodynamic screening (see below). The starting point is the one-particle phase space density $\Psi(x, p; t)$, that defines the instantaneous probability of finding a single particle at a spatial position $x$ with an orientation given by the unit vector $p$, fixed in the particle’s body frame. The distribution function satisfies the normalisation condition

$$\int \text{d}x \text{d}p \, \Psi(x, p; t) = 1.$$  \tag{2.2.1}

Furthermore, the correlations between individual swimmers are assumed to be negligible. Within this mean-field approximation the one-particle phase-space density obeys the following differential Master equation

$$\partial_t \Psi + \nabla \cdot (\dot{x} \Psi) + \partial \cdot (\dot{p} \Psi) = -\lambda \Psi + \lambda \int \frac{\text{d}p'}{\Omega_d} \Psi,$$  \tag{2.2.2}

where $\nabla \equiv \partial/\partial x$, $\partial \equiv (1 - pp)(\partial/\partial p)$ denotes the derivative on a unit sphere, and $\Omega_d$ is the surface of the $d$-dimensional unit sphere. Here, $\dot{x}$ and $\dot{p}$ are probability fluxes for the position and the orientation, which have the form

$$\dot{x} = v_s p + U - D_t \nabla \ln \Psi,$$  \tag{2.2.3}

$$\dot{p} = (1 - pp) \cdot (W + BE) \cdot p - D_r \partial \ln \Psi,$$  \tag{2.2.4}

and the sinks and sources of the probability distribution appearing on the right hand side of Eq. (2.2.2), responsible for discontinuous jumps in the phase space, mimics the run-and-tumble motion of the bacteria with the tumbling rate $\lambda$ [28, 73].

Excluding the tumbling effects, the formulation (2.2.2)-(2.2.4) has a similar form to the Fokker-Plank equation corresponding to the Langevin problem (2.1.7)-(2.1.8) for a charged particles is known as the Vlasov equation [115].

The kinetic theories with orientational degree of freedom $p$ are sometimes formulated using the rotational derivative $\mathcal{R} = p \times \partial/\partial p$, instead is of the orientational derivatives $\partial$ [108]. These descriptions are equivalent in two and three spatial dimensions (see Appendix A.2), but the advantage of $\partial$ over $\mathcal{R}$ is that the former can be generalized to arbitrary spatial dimension $d$.\footnote{\textsuperscript{3}From the mathematical point of view, an analogous equation describing the system of charged particles is known as the Vlasov equation [115].\textsuperscript{4}The kinetic theories with orientational degree of freedom $p$ are sometimes formulated using the rotational derivative $\mathcal{R} = p \times \partial/\partial p$, instead is of the orientational derivatives $\partial$ [108]. These descriptions are equivalent in two and three spatial dimensions (see Appendix A.2), but the advantage of $\partial$ over $\mathcal{R}$ is that the former can be generalized to arbitrary spatial dimension $d$.}
single particle [114]. The noise terms in (2.1.7)-(2.1.8) are present in (2.2.2) in the form of diffusive terms $D_t \nabla^2 \Phi$, and $D_r \partial^2 \Phi$, which were conveniently stored in the equations of motion for (2.2.3)-(2.2.4) in the form of chemical potentials $D_t \nabla \ln \Psi$, and $D_r \partial \ln \Psi$. Note, that the rotational diffusion in (2.1.8) has a form of multiplicative noise, where Stratonovich calculus must be used to obtain physically meaningful Fokker-Plank equation\(^6\).

The crucial difference between the one-particle Fokker-Plank equation corresponding to Eqs. 2.1.7, and (2.1.8) and the mean-field model (2.2.2) is the structure of the interaction, the velocity field $u_d$. A single particle in an otherwise empty environment represents a non-interacting system due to Eq. (2.1.9). In the mean-field approximation the many-particle system is modeled as an effective one-particle problem, where the velocity field is approximated by the ‘mean’ of the dipolar field (2.1.6), that is, its average over the one-particle distribution $U(x; t) = N \int dx' dp' u_d(x - x', p') \Psi(x', p'; t)$.

Note, that Eqs. (2.2.2)-(2.2.4) are similar to those of Doi’s Kinetic theory of rods, describing passive elongated objects in an external shear flow [108]. The only distinction from Doi is the activity appearing in the form of self-propulsion $v_s p$ in Eq. (2.2.3), and the dipole forces (2.1.4) that drive the velocity field $u_d$ in Eq. (2.2.5). As a result, a non-trivial chaotic motion can appear even in the absence of any shear flow which will be discussed below.

Let us now comment on the magnitude of the stochastic effects, which can be estimated on the basis of the available experimental data. For typical E. coli-like swimmer it is reasonable to assume that they self-propel as $v_s \sim 10 \mu m/s$, and tumble as $\lambda \sim 1 s^{-1}$ [36]. The corresponding effective translational and rotational diffusions then scale as $D_t \sim v_s^2 / \lambda \sim 10^2 \mu m^2/s$, and $D_r \sim (2 \pi \text{rad})^2 \lambda \sim 40 \text{rad}^2/s$. The thermal diffusive effects, can be estimated to be $D_t \sim 10^{-1} \mu m^2/s$, and $D_r \sim 10^{-1} \text{rad}^2/s$ [36], which shows that there are negligible compare to the quantities above. Hence, the self-propulsion, and tumbling are the main source of dynamics in realistic suspension, and we will not consider the effect of thermal diffusion in this thesis.

### 2.2.2 Mean-field moment equations

In general, the Kinetic description in the form (2.2.2) is inconvenient for practical calculations due to its large number of dependent variables. A number of approximate models have been derived that rely on equations for orientational moments of the phase space distribution $\Psi$ [29]. Due to the nematic nature of the microswimmer interaction (2.1.6), the most relevant moment must also possess nematic symmetry. Hence, it is common to consider all moments up to second order, namely the concentration, polar, and nematic order, defined as follows

$$c(x; t) = \bar{1}, \quad m(x; t) = \bar{p}, \quad Q(x; t) = \bar{pp} - \frac{1}{4} \bar{1},$$

\(^6\)Strictly speaking, the only meaningful description of a stochastic process is given by the Fokker-Plank equation for the probability conservation. In our case it must have the form (2.2.2), where any change in $\dot{p}$ must be perpendicular to $p$ due to the conservation of unit length $|p| = 1$. The latter constraint is actually not a necessary condition for the Langevin problem (2.1.8), which interpretation always depends on the time discretization [114].
where the orientational average is defined as
\[
\langle \ldots \rangle = \int \frac{dp}{\Omega_d} \langle \ldots \rangle \Psi(x, p; t).
\] (2.2.7)

Equations for \(c, m\) and \(Q\) are obtained from the Master equation (2.2.2) by taking the corresponding moments [29,116]
\[
D_t c = D_t \nabla^2 c - v_s \nabla \cdot m,
\] (2.2.8)
\[
\frac{1-e}{2} \Delta m + \frac{1+e}{2} \tilde{m} = D_t \nabla^2 m - (\lambda + (d - 1) D_r) m - v_s \nabla \cdot (Q + \frac{1}{d} 1 c)
- B \langle p p p \rangle : \epsilon,
\] (2.2.9)
\[
\frac{1-e}{2} \Delta Q + \frac{1+e}{2} \tilde{Q} = D_t \nabla^2 Q - (\lambda + 2 d D_r) Q - v_s (\nabla \cdot \langle p p p \rangle \Psi - \frac{1}{d} 1 \nabla \cdot m)
+ B e - 2 B \langle p p p p \rangle : \epsilon,
\] (2.2.10)

where \(D_t = \partial_t + \mathbf{U} \cdot \nabla\) is the usual material derivative, and
\[
\frac{\Delta}{2} m = D_t m \quad \text{and} \quad \frac{\Delta}{2} \tilde{m} = D_t \nabla^2 m - \lambda \nabla \cdot m,
\] (2.2.11)
\[
\frac{\Delta}{2} Q = D_t \nabla^2 Q - (\lambda + 2 d D_r) Q - v_s (\nabla \cdot \langle p p p \rangle \Psi - \frac{1}{d} 1 \nabla \cdot m),
\] (2.2.12)

are the lower and upper convective derivatives of individual tensorial fields [117]. The three moment equations (2.2.8)-(2.2.10) share similar features. First, translational diffusion enters the form of Laplace term in each equation. Second, the polar and nematic order contain damping terms due to the presence of tumbling and rotational diffusion. The latter two do not seem to have exactly the same effect, as once cannot introduce a single damping constant to replace \(\lambda\), and \(D_r\). At last, the main distinction of Eqs (2.2.8)-(2.2.10) from those that describe passive rods is the presence of activity – almost every moment is affected by the gradient term due to the self-propelling property of the microswimmers. Note that the only conserved field is the concentration field \(c\).

The mesoscopic equations for the velocity field are obtained by coarse-graining the microscopic equations for the fluid (2.1.4). Averaging the latter over the orientation with the phase space distribution \(\Psi(x_0, p; t)\), the Stokes equations become
\[
0 = \nabla^2 \mathbf{U} - \nabla P + \kappa \nabla \cdot Q,
\] (2.2.13)
\[
0 = \nabla \cdot \mathbf{U}.
\] (2.2.14)

where the pressure has been renormalized with the swimmer density. Eq. (2.2.13) shows that the presence of the hydrodynamic dipoles leads to an appearance of active stress \(\sigma_a = \kappa Q\). In other words, the hydrodynamic field in the microswimmer suspensions is a slow mode that immediately follows the nematic structure of the swimmers.

Dynamical equations for \(ppp\), and \(pppp\) in Eqs. (2.2.9), and (2.2.10) can be obtained similarly to the lower order moments, but they will contain higher order terms such as fifth, sixth, and so on. This is known as the closure problem, and certain approximations must be applied to obtain a close set of equations. Several closures have been proposed for the suspension of self-propelling rods [29], but perhaps the most popular one is to truncate the phase space density after the nematic tensor
\[
\Psi(x, p; t) = \frac{1}{\Omega_d} \left[ c(x, t) + d p \cdot m(x, t) + \frac{d(d+2)}{2} pp : Q(x, t) + \ldots \right],
\] (2.2.15)
with \( d \) being the dimensionality of the space, in which case all higher order moments can be expressed in terms of \( c, m \) and \( Q \),

\[
\begin{align*}
\frac{p_i p_j p_k}{p_i p_j p_k} = & \frac{m_i \delta_{jk} + m_j \delta_{ik} + m_k \delta_{ij}}{d+3}, \\
\frac{c (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})}{d(d+2)} + & \frac{\delta_{ij} Q_{kl} + \delta_{ik} Q_{jl} + \delta_{il} Q_{jk} + \delta_{jk} Q_{il} + \delta_{jl} Q_{ik} + \delta_{kl} Q_{ij}}{d+4}.
\end{align*}
\tag{2.2.16}
\tag{2.2.17}
\]

The above closure was used, for example, to study instabilities in confined two dimensional suspensions [118]. Note that the truncation (2.2.15) does not depend on the the field \( U \), and is therefore its a good approximation only if \( \Psi \) is nearly isotropic\(^7\).

The closure presented in Eq. (2.2.15) leaves open questions: Is neglecting higher order moments a reasonable approximation? Moreover, as the swimmer-swimmer interaction is nematic, can fluctuations of the density and polar order be neglected the same way? These questions will be addressed in Chap. 4.

2.3 Collective motion

In this section, we will review theoretical approaches used to study the collective motion; We start with discussing the linear stability analysis of the homogeneous and isotropic distribution of microswimmers, which leads to identification of critical density. No global order is expected in the system, as flucatutions about an aligned state are unstable at any circumstances. At last, as all the results are derived on the basis of the mean-field approximation, the validity of the latter is verified using the full form of the kinetic theory.

2.3.1 Transition to collective motion

Experimental observations show, that the suspension of microorganisms appears homogeneous and isotropic at low densities [2, 44, 65]. As the mean density of the swimmers increases, the aforementioned state becomes linearly unstable, and the collective motion appears. Within the presented theoretical frameworks, the appearance of this ‘transition’ can be understood by the means of the linear stability analysis of the Master Eq. (2.2.2), or, the moment Eqs. (2.2.8)-(2.2.14). As the derivation of the latter relies on certain approximations, the analysis of the former representation is certainly superior.

The one-particle formulation given by Master Eq. (2.2.2) describes the behaviour of a single particle in a fluid flow generated by the mean distribution of other particles (2.2.5). The linear stability of this system has been done in [44,45,72,73] in three dimensions by expanding the phase space density around the homogeneous and isotropic state

\[
\Psi(x, p; t) = \frac{1}{4\pi V} + \delta\Psi(k, p) e^{\chi t + i k \cdot x},
\tag{2.3.1}
\]

where \( k \) is the wave-vector, and the system becomes unstable whenever Re\[\chi]\) > 0. The largest eigenvalue \( \chi \) has been shown to be (neglecting rotational diffusion)

\(^7\)An alternative closure was proposed based on a quasiequilibrium approximation of the distribution function [119,120]. Although the latter closure might be accurate for very dense suspensions, where the phase space density might not be isotropic, close to the instability it is expected to provide the same result as the moment expansion (2.2.15)
Figure 2.4: a) Real, and b) imaginary part of the full dispersion obtained from linearising (2.2.2) using (2.3.1). The solution ceases to exist above $k^*$ [72].

$$\chi = -\lambda + \frac{B\kappa n_0}{5} - \left( \frac{15v_s^2}{7B\kappa n_0} + D_t \right) k^2 + O(k^4),$$  \hspace{1cm} (2.3.2)

where $n_0$ is the mean density, and the plot of the full dispersion law is shown in Fig. 2.4.

The results show, that the system becomes linearly unstable at vanishing wave-vectors $k \to 0$, and above the critical density

$$n_c = \frac{5\lambda}{B\kappa}.$$  \hspace{1cm} (2.3.3)

Eq. (2.3.3) indicates that the instability is due to microswimmer’s orientational degree of freedom, as spherical particles $B \to 0$ behave the same way as a non-interacting suspension $\kappa \to 0$. Moreover, the system is stabilised by the tumbling effects, as the critical density (2.3.3) increases with the tumbling rate $\lambda$.

The solution to the eigenvalue problem ceases to exist above certain wave-vector $k^*$. As it was pointed out by Landau [121], the linear stability of kinetic theories must be correctly assessed by treating the Master equation as an initial value problem, as the exponential ansatz (2.3.1) does not correctly capture the temporal behaviour in a certain region of the parameter space. Detailed numerical, as well as analytical analysis in the region of a ‘missing’ solution revealed that the homogeneous and isotropic state of the system is stable under any circumstances [74].

Unlike magnetic systems, or dry active matter models [122], the suspension of microswimmers does not show a stationary polar, nor nematic alignment. At the level of mean-field equations, the absence of polar state can be addressed by analysing the linear stability of the moment equations (2.2.8)-(2.2.9), and the velocity (2.2.13) as [45,72]

$$c(x; t) = n_0 + \delta c(k; t) e^{\chi t + i\mathbf{x} \cdot \mathbf{k}},$$  \hspace{1cm} (2.3.4)

$$m(x; t) = m_0 + \delta m(k; t) e^{\chi t + i\mathbf{x} \cdot \mathbf{k}},$$  \hspace{1cm} (2.3.5)

$$\mathcal{U}(x; t) = \delta \mathcal{U}(k; t) e^{\chi t + i\mathbf{x} \cdot \mathbf{k}},$$  \hspace{1cm} (2.3.6)

and similarly for the pressure. The largest eigenvalue has the following form

$$\chi = \frac{1}{2} \kappa \left[ (1 + B) \cos^2 \theta + (1 - B) \sin^2 \theta \right] \cos 2\theta + O(k)$$ \hspace{1cm} (2.3.7)

where $\theta$ is the angle between $\mathbf{m}_0$ and the wave vector $\mathbf{k}$, and higher order terms in $k$ lead to negative corrections. As $\chi$ has a maximum at $k \to 0$, the resulting dispersion law shows instability setting in again at largest spatial scales. These predictions were tested, and confirmed numerically in [45,72], where the snapshots of the simulations are shown.
in Fig. 2.5. The absence of the polar, as well as nematic, alignment due to hydrodynamic stresses caused by the activity of the particles was originally reported in [71], and its known as *Simha-Ramaswami instability*. At last, all of these theories predict exponential decay towards a flat distribution of all moments below any instability threshold.

While most of the instabilities have been analysed in bulk three-, and two-dimensional systems [118], a reasonable question arises: *How is the instability leading to the collective motion affected by the presence of boundaries, i.e. in an effectively two-dimensional systems?* Moreover, the instability in bulk suspension sets in at the scale of the system. *Does this feature persist even deeply in the collective motion regime, or does a finite length-scale appears?* We will address these questions in Chaps. 3, and 4.

### 2.3.2 The role of correlations

All analytical predictions derived from Eq. (2.2.2) rely on the mean-field approximation, where the correlations between the individual swimmers have are neglected. Such approximation, although appealing from a technical point of view, may not correctly capture all properties of the system. As the hydrodynamic interactions between swimmers are long-ranged in nature, it is reasonable to address a question whether the effect of correlations can actually be neglected.

To answer this question lattice Boltzmann simulations, as well as an extended kinetic theory for a system of $N$ interacting microswimmers were developed in [44]. Fig. 2.6 shows the fluid velocity variance measured in the simulations, for various values of the mean density $\rho_{\text{body}}$ (in their notation). As it is seen from the figure, the variance is non-zero even below the analytically predicted critical density $\rho_c$ leading to the collective motion, in contrast to the mean-field simulations where any perturbations below $\rho_c$ decay exponentially in time. The reason for this difference is in particular obvious from the snapshots of the particle-based simulations, also shown in Fig 2.6, where below the transition point the system reaches fluctuating stationary state in the long-time limit.

What is in particular interesting about these results, is that they do not appear to be showing any sharp transition as the density passes the ‘critical’ value predicted in (2.3.3). Deviations from central limit theorem $\langle U^2 \rangle \sim \rho_{\text{body}}$ were observed, followed by a continuous increase to larger values around the density $\rho_c$. Here, two important conclusions can be made: i) the mean-field approximation cannot provide accurate results, as it lacks the effect of correlations, ii) it is not clear whether the transition to collective motion is
actually a ‘phase transition’ in the statistical physics sense.

In order to provide theoretical explanation for the appearance of the correlations [44] constructed extension of the mean-field kinetic theory discussed previously. The starting point is the $N$-particle phase space density $F_N(\{x_i, p_i\}_{i=1}^N, t)$, which, similarly to Eq. (2.2.2), obeys conservation of the probability given by the Master equation

$$\partial_t F_N + \sum_{i=1}^N \left[ \nabla_i \cdot (\dot{x}_i F_N) + \partial_i \cdot (\dot{p}_i F_N) \right] = -N\lambda F_N + \frac{\lambda}{4\pi} \sum_{i=1}^N \int d\mathbf{p}_i F_N,$$  

(2.3.8)

where $x_i$, and $p_i$ are the position, and orientation of the $i$-th particle, and $\nabla_i$, and $\partial_i$ are derivatives w.r.t. these variables. Eq. (2.3.8) is form of the $N$-particle kinetic theory of interacting particles commonly used in non-equilibrium statistical physics [115]. The authors derived first two terms of the infinite hierarchy describing correlation functions of the system, also known as the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy. By expanding about the homogeneous and isotropic state, the behaviour of the variance below the transition to the collective motion was found to be

$$\langle U^2 \rangle \sim \kappa^2 \left( 1 \pm \frac{\Delta(2 \mp \Delta)}{2(1 \mp \Delta)} \right),$$  

(2.3.9)

where the upper and lower sign correspond to pushers $\kappa > 0$, and pullers $\kappa < 0$, and $\Delta$ the mean density, normalised with the critical density introduced in Eq. (2.3.3). The above result shows a power law divergence of the variance $\langle U^2 \rangle \sim (1 - \Delta)^{-1}$, as the system approaches the critical density $\Delta \rightarrow 1$. This result was tested against the lattice Boltzmann simulations, shown in Fig. 2.7, where a very good agreement with the analytical prediction was found. However, the analytical calculations, leading to the result (2.3.9), were done in the absence of the self-propulsion (in a so-called shaker limit), and it was not clear whether the swimming speed has an affect on the correlations, especially for fast microorganisms.

Naturally, a very important question arises at this stage: Are the correlations of the system affected by the swimming speed of the bacteria? If so, is there any limit where correlations can be actually neglected? We will address these questions in Chap. 5.
Figure 2.7: Variance of the fluid velocity normalised with the variance of non-interacting particles, measured in [44]. The particles were modeled as hydrodynamic dipoles with zero swimming speed (shakers, represented with rectangles), or non-zero swimming speed (swimmers, represented with circles). Analytical predictions are denoted with straight lines, and different colours correspond to different dipole amplitudes. Strong deviations from the non-interacting case were observed for both pushers, and pullers, with accordance to the theoretically predicted behaviour in Eq. (2.3.9)
Chapter 3

Linear stability in various geometries

The first step towards understanding collective behaviour is to identify under which condition it may appear. In the present chapter, we will perform a linear stability analysis of the mean-field kinetic theory. The results presented here serve as a starting point for further analysis carried out later in this thesis.

We will start with discussing different system geometries that can be used to model microswimmer suspensions. In particular, we will distinguish between bulk systems, where microswimmers can move through the entire fluid container, and confined systems, where movement of the microswimmers is limited. The latter results in effective compressibility, which modifies the functional form of the force dipole.

We then proceed to a general formulation of linear stability analysis for arbitrary spatial dimension, and velocity field. Our approach is rather different from procedures commonly found in the literature. Instead of assuming exponential solution to the linearised equations of motion, we directly solve the model using the Laplace transform. Solutions describing density and velocity fluctuations of the suspension are derived, which not only allow us to determine the instability condition, but also directly identify its origin.

Later, the linear stability of the bulk two- and three-dimensional suspensions is analysed. We show that density instability does not occur at the linear level, regardless of the system parameters. The orientational instability is found to set in at the largest possible spatial scales and only in for the pusher suspensions as was predicted in previous works. These results for the bulk suspensions appear to be qualitatively independent of the system’s dimensionality.

Finally, we turn our attention to microswimmer suspensions confined to a two-dimensional layer within a three-dimensional fluid. We show, that in contrast to bulk systems the pusher instability occurs at the smallest possible spatial scale. Our coarse-grained description does not allow to identify such scale, but a couple of possible candidates are suggested. A density instability for puller suspensions also appears with vanishing critical density in the thermodynamic limit. The finite size effects are discussed at last which result in a rich phase diagram.

The results of this chapter have been published in: [2,3].
3.1 The rôle of geometry

As it is often the case, the exact form of the instability may depend on the geometry of the system. Microswimmer experiments are in practice carried out in confined geometries, where the presence of boundaries influences the structure of the fluid flow [38]. In what follows, we will focus on two fundamentally different systems:

i) **Bulk suspensions** – microswimmers are free to swim in the entire space occupied by the fluid, either in two, or three dimensions

ii) **Confined suspensions** – microswimmers are confined to a two-dimensional layer embedded in a three dimensional fluid

The distinction between the above two scenarios is visualised in Fig. 3.1. While most of the time microswimmers occupy a bulk three-dimensional fluid, swimming close to the boundaries of surrounding container is effectively two-dimensional. Alternatively, one may consider confinement of the swimmers due to a thin membrane that only allows for passing of the fluid. An important physical effect, inherent to confined systems though rarely discussed explicitly, is the effective compressibility of the in-plane flow fields generated by a layer of microswimmers. To illustrate the point, we consider a dipolar particle oriented parallel to a solid wall at a distance \( h \) from it. The fluid velocity component \( \mathbf{u}_\parallel \) parallel to the wall can be deduced from the image system developed by [123] for a point force next to a solid boundary, and is given by

\[
\mathbf{u}_\parallel(\mathbf{r}) = \frac{\kappa}{8\pi} \left( \mathbf{r} \cdot \mathbf{p} \left[ 3 \frac{(|\mathbf{r}|^2)^2}{|\mathbf{r}|^4} - 1 \right] + \frac{\mathbf{r}}{R^3} \right.
\]

\[
- \frac{3r(r \cdot p)^2 + 6h^2 \{ r + 2p(r \cdot p) \}}{R^5} + \frac{30h^2(r \cdot p)^2r}{R^7}. \tag{3.1.1}
\]

Here, \( \mathbf{r} \) and \( \mathbf{p} \) are two-dimensional vectors that lie in the plane parallel to the wall and denote the point where the velocity is evaluated relative to the position of the swimmer and the dipole orientation, respectively; \( R = \sqrt{|\mathbf{r}|^2 + 4h^2} \), and \( \kappa \) is the strength of the dipole. Next, we calculate the total flux of the fluid through a circle of radius \( X \) centred on the microswimmer and parallel to the wall, as shown in Fig. 3.1, yielding

Figure 3.1: Left: Bulk suspension in three spatial dimensions. Swimmers are free to move within the entire fluid. Right: Suspension confined to a two-dimensional layer embedded in a three dimensional fluid (the wall is at infinity). The fluid in the layer is compressible due to its flux parallel to \( z \)-th direction (blue arrows). The net flow passing through the dashed circle is nonzero, and its sign is opposite for pushers and pullers.
\[
\int_{|r|=X} dr \cdot u_{||} = \frac{\kappa}{8X} \left[ 1 - \frac{X^4 - 10X^2h^2 + 64h^4}{(X^2 + 4h^2)^{7/2}}X^3 \right].
\]

(3.1.2)

Hence, the total flux through an arbitrary circle around a microswimmer is non-zero, indicating that if we only consider the velocity components parallel to the wall, they represent an effectively compressible velocity field. Moreover, one can show that the prefactor multiplying \( \kappa \) is strictly positive, and the sign of the flux is therefore determined by the sign of the dipolar strength: pushers with \( \kappa > 0 \) on average correspond to hydrodynamic sources in the plane parallel to the wall, while pullers with \( \kappa < 0 \) correspond to hydrodynamic sinks. Therefore, when averaged over all orientations, two pushers advect each other to maximise their mutual separation, while two pullers do the opposite. This argument suggests that hydrodynamic interactions between dipolar microswimmers moving next to a boundary have a very different nature than their bulk counterparts. We stress that this interaction does not correspond to extra forces or torques on the particles, as often assumed in the dry active matter literature [12], as the particles immersed in a fluid are strictly force and torque free, even when in contact with a solid boundary [5].

### 3.2 Linearised kinetic theory

We will now proceed to studying the linearised version of the kinetic theory (2.2.2). The latter, together with the normalisation condition (2.2.1) admit a constant solution \( \Psi_{\text{HI}} = 1/(\Omega_d V_d) \), where \( \Omega_d \) is the surface of the unit sphere, and \( V_d \) is the \( d \)-dimensional volume of the suspension. The existence of this solution relies on the condition

\[
\int d\mathbf{x}' d\mathbf{p}' u^\alpha(x - x', p') = 0,
\]

(3.2.1)

which is true in all cases considered in this thesis. While integrals over \( \mathbf{x}' \) and \( \mathbf{p}' \) vanish independently in two- and three-dimensional bulk suspensions, only the positional integral vanishes for microswimmers confined to a two-dimensional plane in a three-dimensional fluid. The state with \( \Psi = \Psi_{\text{HI}} \) has equal probability for all positions and orientations of a particular microswimmer, and is thus referred to as the homogeneous and isotropic state.

The stability of this state is determined by time evolution of small perturbations around \( \Psi_{\text{HI}} \). Techniques to study such problems are well-established and have been extensively applied to linear stability of the homogeneous and isotropic state for dilute, three-dimensional suspensions of microswimmers [45, 72–74]. Here, we use a somewhat different methodology [2,44], which is better adapted for our problem.

First, we introduce a perturbation \( \delta \Psi(x, p, t) \) of the one-particle distribution function around the homogeneous and isotropic state, \( i.e., \)

\[
\Psi(x, p, t) = \frac{1}{\Omega_d V_d} + \delta \Psi(x, p, t),
\]

(3.2.2)

where \( \delta \Psi(x, p, t) \), is assumed to be small. The linearised Smoluchowski equation (2.2.2) in Fourier space (see Appendix A.1) reads

\[
\left[ \partial_t + \lambda + iv \cdot \mathbf{k} \right] \delta \hat{\Psi} = \frac{\lambda}{\Omega_d} \delta \hat{\rho} + \frac{n}{\Omega_d} \left[ dB p^\alpha p^\beta - (1 + B) \delta^{\alpha\beta} \right] ik^\alpha \delta \hat{U}^\beta,
\]

(3.2.3)
where \( n = N/V \) is the number density of particles, and we have defined the microswimmer density and the fluid velocity fluctuations as

\[
\delta \hat{\rho}(k, t) = \int d\mathbf{p} \, \delta \hat{\Psi}(k, \mathbf{p}, t), \quad (3.2.4)
\]

\[
\delta \hat{\mathbf{u}}^\alpha(k, t) = \int d\mathbf{p} \, \hat{u}^\alpha(k, \mathbf{p}) \delta \hat{\Psi}(k, \mathbf{p}, t). \quad (3.2.5)
\]

The linear stability analysis is often assessed by assuming an exponential solution of the linearised Eq. of motion (3.2.3). This procedure, however, is not always sufficient for determining the long-time behaviour of the kinetic theories; An analogous situation appears in the Vlasov equation describing the physics of plasma, where Landau pointed out that the long-time asymptotics must be determined by treating the linearised kinetic theory as an initial value problem [121]. Hence, we Laplace transform Eq. (3.2.3) (see Appendix A.1), which allows us to derive a closed set of equations for the density and velocity fluctuations

\[
\delta \hat{\rho}(s) = i n \delta \hat{\mathbf{u}}^\alpha \int \frac{d\mathbf{p}}{\Omega_d} \frac{Bdp^\alpha \mathbf{p} \cdot \mathbf{k} - (1 + B)k^\alpha}{s + \lambda + iv_\alpha \mathbf{p} \cdot \mathbf{k}}
+ \delta \hat{\rho} \int \frac{d\mathbf{p}}{\Omega_d} \frac{\lambda}{s + \lambda + iv_\alpha \mathbf{p} \cdot \mathbf{k}} + \int \frac{d\mathbf{p}}{\Omega_d} \frac{\lambda \delta \hat{\Psi}_0(k, \mathbf{p})}{s + \lambda + iv_\alpha \mathbf{p} \cdot \mathbf{k}}, \quad (3.2.6)
\]

\[
\delta \hat{\mathbf{u}}^\alpha(s) = i n \delta \hat{\mathbf{u}}^\alpha \int \frac{d\mathbf{p}}{\Omega_d} \frac{\hat{u}^\alpha(k, \mathbf{p})}{s + \lambda + iv_\alpha \mathbf{p} \cdot \mathbf{k}} \left[ Bdp^\beta \mathbf{p} \cdot \mathbf{k} - (1 + B)k^\beta \right]
+ \delta \hat{\mathbf{u}}^\alpha \int \frac{d\mathbf{p}}{\Omega_d} \frac{\lambda \hat{u}^\alpha(k, \mathbf{p})}{s + \lambda + iv_\alpha \mathbf{p} \cdot \mathbf{k}} + \int \frac{d\mathbf{p}}{\Omega_d} \frac{\lambda \hat{u}^\alpha(k, \mathbf{p}) \delta \hat{\Psi}_0(k, \mathbf{p})}{s + \lambda + iv_\alpha \mathbf{p} \cdot \mathbf{k}}, \quad (3.2.7)
\]

where \( \delta \hat{\Psi}_0 = \delta \hat{\Psi}(t = 0) \) represents the initial condition. The solution to the above equations depends on the precise form of the microscopic velocity field \( \hat{\mathbf{u}}(k, \mathbf{p}) \), which, in turn, depends on the dimensionality of space and the dimensionality of the vectors \( \mathbf{p} \) and \( \mathbf{k} \), as we show below. We now briefly recap the known results on linear stability of bulk three-dimensional suspensions before turning our attention to a two-dimensional layer of microswimmers embedded in a three-dimensional fluid. Note, that the poles coming from the initial conditions only appear if the problem is treated as an initial value problem. We will show below that these poles determine the behaviour in certain region of the parameter space, and that they cannot be found using an exponential Ansatz \( \delta \hat{\rho}(t) \sim e^{st} \).

### 3.3 Bulk suspensions

In this Section, we consider the case of microswimmers that move freely in the whole three-dimensional space filled with an incompressible fluid. An analogous calculation for the case of two-dimensional suspension, which shows no qualitative differences, can be found in Appendix B.1.2. The dipolar velocity field for \( d = 3 \) is given by [35]

\[
u^\alpha_{d=3}(x, \mathbf{p}) = \kappa \frac{x^\alpha}{8\pi |x|^3} \left[ \frac{3(x \cdot \mathbf{p})^2}{|x|^2} - 1 \right] , \quad (3.3.1)
\]

and its Fourier transform is given by (see Appendix A.3)

\[
\hat{u}^\alpha_{d=3}(k, \mathbf{p}) = -i \kappa \frac{k^\alpha}{k^2} p^\beta \mathbf{p}^\beta. \quad (3.3.2)
\]
Here, $\kappa$ is the dipolar strength (see Appendix A.3 for details), and $P^{\alpha\beta} = \delta^{\alpha\beta} - k^\alpha k^\beta/k^2$ is the transversal projection operator that ensures that equation (3.3.2) satisfies the incompressibility condition $k^\alpha \hat{u}_{\alpha = \beta} = 0$. Setting $d = 3$ in (3.2.6)-(3.2.7), and taking into account the incompressibility condition in the form $\hat{\delta U}^\alpha = P^{\alpha\beta} \delta \hat{U}^\beta$, we obtain the following set of equations

$$\delta \hat{\rho}(s) = \frac{1}{1 - \frac{v_s k}{v_s k} \arctan(b)} \int dp \frac{\lambda \delta \hat{\Psi}_0(k, p)}{(s + \lambda + iv_s p \cdot k)}, \quad (3.3.3)$$

$$\delta \hat{U}^\alpha(s) = \frac{\lambda}{1 - \frac{B_{nm} (3+2b^2)-3(b^2+1)\arctan(b)}{2v_s^2}} \int dp \frac{\lambda \hat{\delta U}^\alpha(k, p) \delta \hat{\Psi}_0(k, p)}{(s + \lambda + iv_s p \cdot k)}, \quad (3.3.4)$$

where we have introduced a dimensionless parameter

$$b = \frac{v_s k}{s + \lambda}. \quad (3.3.5)$$

We note that equations (3.3.3) and (3.3.4) are decoupled, and can be studied independently. The former equation only involves $\delta \hat{\rho}$, and so it describes evolution of the density fluctuations as a response to an initial perturbation given by $\delta \hat{\Psi}_0$. The latter equation has an analogous meaning for the velocity field fluctuations, and is known to lead to a long-wavelength instability associated with orientational degrees of freedom only [44,45,72–74]. These are now studied separately.

### 3.3.1 Density instability

Stability with respect to small density variations is determined by solving Eq. (3.3.3). In order to carry out the inverse Laplace transform (A.1.10), we first need to identify poles appearing in Eq. (3.3.3). There are two such poles

$$s_1 = -\lambda + \frac{v_s k}{\tan(\frac{v_s k}{\lambda})}, \quad s_2 = -\lambda - iv_s p \cdot k, \quad (3.3.6)$$

where $s_1$ exists only in the limited region of the parameter space $v_s k/\lambda < \pi/2$, due to inversion of the arctan in Eq. (3.3.3). The complex integral (A.1.10) of (3.3.3) can be evaluated by the means of Residue theorem, and the result is

$$\delta \hat{\rho}(t) = e^{-\left(\lambda - \frac{v_s k}{\tan(v_s k/\lambda)}\right)t} \int dp \left[ \frac{\frac{v_s k}{\lambda}}{1 + \tan^2(\frac{v_s k}{\lambda})} \frac{1}{1 + i \tan(\frac{v_s k}{\lambda}) p \cdot k} \delta \hat{\Psi}_0(k, p) \right] + e^{-\left(\lambda + iv_s k\right)t} \Omega\left(\frac{1}{v_s k t}\right). \quad (3.3.7)$$

where the first row corresponds to the pole $s_1$, and the higher order terms to the second pole $s_2$ (see Appendix B.1.1). Note, that the first row in (3.3.7) could have been obtained from the widely used Ansatz $\delta \hat{\rho}(t) \sim e^{st}$, while the higher order terms could not.

Looking at the exponential behaviour of the result (3.3.7), the system is stable w.r.t. small density variations provided that

$$\lambda - \frac{v_s k}{\tan(v_s k/\lambda)} > 0, \quad (3.3.8)$$

25
which is always true for $v_s k / \lambda < \pi / 2$. In the region $v_s k / \lambda > \pi / 2$ the system shows oscillatory behaviour with a decaying amplitude (second row in Eq. (3.3.7)). We would like to stress out that the stability analysis in the latter region would not be possible using the exponential Ansatz $\delta \rho(t) \sim e^{st}$. This highlights the importance of full treatment of the initial value problem. Our results show, that no density instability in the bulk three-dimensional system of microswimmers appears [2]. We note that the corresponding eigenstates represent spatial modulation of the microswimmer density, while the microswimmer orientations remain isotropically distributed regardless of their spatial positions.

Let us emphasize that in all problems discussed below the solution to the linearised equations of motion (3.2.6)-(3.2.7) will be analogous to what was presented here. Each solution will consist two parts, originating from two poles similar to (3.3.6). The pole $s_2 = -\lambda - iv_s k p$ will be always present, but as we have seen above it only leads to an oscillatory function in time which amplitude decays faster than exponential. This part of solution will not be explicitly derived below. The other pole, analogous to $s_1$ in Eq. (3.3.6), will lead to an exponential solution $\delta \rho(t) \sim e^{st}$, and the instability condition can be inferred from the vanishing real part of this pole $\text{Re}[s_1] = 0$. We will only focus on the latter type of solution from now on.

### 3.3.2 Orientational instability

The relevant pole determining the stability of the velocity field fluctuations in (3.3.4) is determined from

$$\alpha = \frac{5b(3 + 2b^2) - 3(b^2 + 1) \arctan(b)}{b^4}, \quad \alpha \equiv \frac{5v_s k}{B n},$$

(3.3.9)

Equation (3.3.9) can be inverted numerically, yielding $b(\alpha)$. Using the definition (3.3.5), we obtain for the eigenvalue $\chi$

$$s = -\lambda + \frac{1}{5} F(\alpha) B n, \quad F(\alpha) = \frac{\alpha}{b(\alpha)}.$$

(3.3.10)

It is important to note, that the only wave-vector dependence in (3.3.10) comes from the complex function $F(\alpha)$. The latter is only known numerically, although a semi-quantitative approximation to $F(\alpha)$ was developed by [1] and [2]. As can be seen in Fig. 3.2, the real part of $F(\alpha)$ decreases upon increasing $\alpha$, and since $\alpha \propto k$, this implies that
the instability sets in at the largest possible spatial scale. In the thermodynamic limit \( V \to \infty \), where the most unstable wavevector \( k_c \to 0 \), the system is unstable whenever

\[
1 \geq \frac{5\lambda}{B\kappa n} > 0.
\]

(3.3.11)

For pushers \((\kappa > 0)\) this condition defines the critical microswimmer number density in three dimensions,

\[
n_c = \frac{5\lambda}{B\kappa}.
\]

(3.3.12)

We note, however, that the threshold (3.3.11) can also be crossed by either increasing the dipolar strength or decreasing the tumble rate while keeping the microswimmer density constant. Moreover, the dipolar strength \( \kappa \) is always multiplied with the shape parameter \( B \). For spherical particles \( B = 0 \) and the instability disappears, which implies that its existence is related to mutual microswimmer alignment which is absent for spherical microswimmers [44, 45, 72–74]. Furthermore, the instability condition (3.3.11) does not involve the swimming speed \( v_s \), implying that the orientational instability persists even for shakers - microswimmers that do not self-propel, yet are capable of generating dipolar fields [44]. For pullers with \( \kappa < 0 \), the condition (3.3.11) can never be satisfied, showing that the orientational instability is always absent.

In real experiments, finite size of the system may cause quantitative shift of the critical density. The magnitude of this effect can derived selecting the minimal wave-vector to be \( k_{\min} = 2\pi/H \), where \( H \) is the system size, instead of vanishing wave-vector. The resulting critical density in the large \( H \) limit is then found to be [2]

\[
n_c(H) = \frac{5\lambda}{B\kappa} \left( 1 + \frac{3}{10} \frac{2\pi v_s}{\lambda H} + \frac{1}{5} \left( \frac{2\pi v_s}{\lambda H} \right)^2 + \ldots \right).
\]

(3.3.13)

For the purpose of comparing the finite size effects with the systems discussed below, we will quantify the above result for a wild-type \( E. \) coli bacterium. Assuming that the typical tumbling rate is \( \lambda \sim 1 s^{-1} \) [36], and using the reduced dipolar \( \kappa \sim 800 \mu m^3/s \) measured in [38], the critical density in the thermodynamic limit is \( n_c(H \to \infty) \sim 1/(10 \mu m)^3 \). Considering the typical swimming speed \( v_s \sim 15 \mu m/s \), and the system size \( H \sim 200 \mu m \) [2], the Eq. (3.3.13) gives about 11% increase of the critical density.

Finally, we note that the solution (3.3.10) ceases to exist for

\[
\alpha > \alpha^* \approx 2.8,
\]

(3.3.14)

Here, the temporal decay is determined from the pole \( s = -\lambda - iv_s p \cdot k \) in (3.3.4), in which case the solution is stable (see Sec. 3.3.1).

### 3.4 Confined suspensions

We now turn our attention to the main problem of this study – the case of a two-dimensional layer of microswimmers embedded in a three-dimensional bulk fluid. As discussed in Section 3.1, this spatial arrangement of microswimmers leads to the in-plane fluid velocity field being effectively compressible, with pushers acting on average as sources, while pullers act as sinks. Here, we study the consequences of this effective
compressibility on the onset and type of collective motion expected in this arrangement of microswimmers.

The Fourier representation of the in-plane velocity field created by a microswimmer is given by (see Appendix A.3 for details)

\[
\alpha_p \mathbf{u}^{(k,p)} = -i\kappa \frac{\mathbf{k} \cdot \mathbf{p}}{2k} \left[ \mathbb{P}\alpha\beta + \frac{1}{2} \mathbb{Q}\alpha\beta \right] p^\beta,
\]

where \(\kappa\) is the dipolar strength which has the same dimensions as in the three-dimensional case, \(\mathbf{k} = (k_x, k_y)\), and \(\mathbf{p} = (p_x, p_y)\) are now the in-plane wave and orientation vectors, respectively, not to be confused with the three-dimensional wave and orientation vectors in previous sections. Remarkably, the fact both \(\mathbf{p}\) and \(\mathbf{k}\) have lower dimensionality than the embedding space, combined with the two-dimensional nature of this problem, leads to \(\mathbf{u}_{\text{plane}}\) being dependent on the orientation of \(\mathbf{k}\), but independent of its length.

In writing Eq. (3.4.1), we explicitly separated the term proportional to the longitudinal projection operator \(\mathbb{Q}\alpha\beta = \frac{k^\alpha k^\beta}{k^2}\), to stress the compressible nature of \(\mathbf{u}_{\text{plane}}\). Since the fluid velocity perturbation \(\delta \hat{\mathbf{U}}\) does not satisfy the incompressibility condition, we define the transversal (incompressible) and longitudinal (compressible) velocity perturbations

\[
\delta \hat{U}_\alpha^\parallel = \mathbb{P}\alpha\beta \delta \hat{U}^\beta, \quad \delta \hat{U}_\alpha^\perp = \mathbb{Q}\alpha\beta \delta \hat{U}^\beta,
\]

Substituting (3.4.1) for \(\mathbf{u}_{\text{plane}}\) into (3.2.6)–(3.2.7), results in the following compact set of equations determining the linear stability of the system

\[
\begin{pmatrix}
1 - M_{11} & 0 & 0 \\
0 & 1 - M_{22} & -ik^\alpha M_{25} \\
0 & -ik^\alpha M_{32} & 1 - M_{33}
\end{pmatrix}
\begin{pmatrix}
\delta \hat{U}_\alpha^\perp \\
\delta \hat{U}_\alpha^\parallel \\
\delta \hat{\rho}
\end{pmatrix}
= \int d\mathbf{p} \begin{pmatrix}
\mathbb{P}\alpha\beta \hat{u}_\alpha^\parallel \\
\mathbb{Q}\alpha\beta \hat{u}_\alpha^\parallel \\
1
\end{pmatrix}
\begin{pmatrix}
\lambda \delta \hat{\Psi}_0 \\
\lambda^{\dagger} \delta \hat{\Psi}_0 \\
s + \lambda + iv_s \mathbf{p} \cdot \mathbf{k}
\end{pmatrix},
\]

where

\[
M_{11} = \frac{\kappa n B (b^2 - 2\sqrt{b^2 + 1} + 2)}{v_s}, \quad M_{22} = \frac{\kappa n B b^2 + (b^2 + 2B)(1 - \sqrt{b^2 + 1})}{4b^2\sqrt{b^2 + 1}},
\]

\[
M_{23} = \frac{\kappa \lambda}{v_s k^2 4b} \left( \frac{1}{\sqrt{b^2 + 1}} - 1 \right), \quad M_{32} = \frac{n}{v_s k} \frac{2B (\sqrt{b^2 + 1} - 1) - b^2 (B + 1)}{b\sqrt{b^2 + 1}},
\]

\[
M_{33} = \frac{\lambda}{kv_s} \frac{b}{\sqrt{1 + b^2}}.
\]

We see from Eq. (3.4.3) that the velocity field \(\delta \hat{U}_\alpha^\perp\), which is transversal to the wavevector \(k\), is decoupled from the velocity \(\delta \hat{U}_\alpha^\parallel\) parallel to it and the density fluctuation \(\delta \hat{\rho}\). This allows us to analyse the two subsets of equations independently, and, as will be shown below, they correspond to different types of instabilities.

### 3.4.1 Orientational instability

The first instability is related to the transversal mode \(\delta \hat{U}_\alpha^\perp\). As mentioned at the end of Sec. 3.3.1, the exact form of the instability condition can be obtained from (3.4.3) by looking at the poles that are different from \(s = -\lambda - iv_s \mathbf{k} \cdot \mathbf{p}\). In the case of transversal
mode \( \delta \mathcal{U}^a_x \) only a single such pole appears, that can be determined from \( M_{11} = 1 \), which can be re-written as

\[
\frac{b^2 - 2\sqrt{b^2 + 1} + 2 B\kappa n}{2v_s} = 1.
\]  

(3.4.7)

The solution procedure is analogous to that presented in Section 3.3, and yields the dispersion relation

\[
s = -\lambda + G \left( \frac{2v_s}{B\kappa n} \right) \frac{B\kappa n k}{2},
\]  

(3.4.8)

where the function \( G(x) \) is defined in (B.1.8), and its functional form is qualitatively very similar to the corresponding function \( F \) for the case of bulk suspensions shown in Fig. 3.2. We observe from Eq. (3.4.8) that the dipole amplitude \( \kappa \) is multiplied with the shape parameter \( B \), again implying that the instability is orientational in nature. Similar to in the bulk suspension, the solution (3.4.8) exists only for \( B\kappa n > 2\sqrt{2}v_s \), for which the second term on the RHS is positive. Below this threshold, the solution is given by oscillatory function in time with decaying amplitude, which can be obtained from the pole \( s = -\lambda - iv_s k_p \).

Since Eq. (3.4.8) is an increasing function of \( k \) the above result implies that the orientational instability in a two-dimensional layer of microswimmers embedded in a three-dimensional fluid sets in at the largest possible value of \( k \), in contrast to two- and three-dimensional bulk suspensions that become unstable at the smallest available wave vector. Since the orientational instability happens when the solution (3.4.8) exists, one may conclude that the critical density is

\[
n_c = \frac{2\sqrt{2}v_s}{B\kappa}.
\]  

(3.4.9)

This expression for \( n_c \) implies that pusher suspensions, where \( \kappa > 0 \), exhibit an orientational instability just as in a three-dimensional bulk suspension, but the instability criterion differs qualitatively from the corresponding one given in Eq. (3.3.12). For the confined suspension, \( n_c \) is a function of the swimming speed \( v_s \) rather than of the tumbling rate \( \lambda \), meaning that increasing the swimming speed will stabilize the suspension of confined pushers, which will become unstable for any density in the shaker limit \( v_s \to 0 \).

The above reasoning assumes that the most unstable wave vector \( k_c \to \infty \), which is clearly unphysical since it corresponds to microscopic length scales. In practice, the instability instead sets in at some finite length scale \( l_c \) set by the system parameters, corresponding to a finite value of \( k_c \). The choice of \( k_c \) will affect the instability threshold, although we cannot \textit{a priori} guess its exact value. In the following, we will however discuss two approximate such choices of instability length scale.

As was observed previously for three-dimensional bulk suspensions [28, 29, 45, 63, 72–74], the behaviour of the dispersion relation \( s(k) \) is regularised at large values of \( k \) by the spatial diffusivity of microswimmers. In this case the microscopic equation of motion for \( \dot{x} \) acquires an additional term, \(-D \nabla^2 \ln \Psi\), where \( D \) is the diffusion constant, as it was the case in Sec. 2.2.3. While spatial diffusion of an elongated microswimmer should be described by a diffusivity tensor that depends on its orientation [111], the one-constant diffusivity approximation suffices to assess the implications of microswimmer diffusivity on the lengthscale selection. Repeating the analysis above yields an additional
term, $-Dk^2$, on the RHS of (3.4.8). Minimising the real part of the eigenvalue with respect to $k$ leads to the lengthscale $l_c \sim \sqrt{D/\lambda}$ being selected at the instability. Using the approximate values $D \sim 0.2 - 0.4 \mu m/s$ [99] and $\lambda \sim 1 s^{-1}$, this lengthscale becomes comparable with the microswimmer size, $\sim 1 \mu m$, which is an unphysically small length scale for the instability to occur. It is therefore unlikely that spatial diffusivity is the relevant mechanism of the length scale selection in (3.4.8).

The second relevant microscopic length scale in the problem is the (density-dependent) average distance between microswimmers, below which the system can no longer be viewed as a continuum. Thus, we assume that the length scale selected at the instability is now $l_c \sim 2/\sqrt{\pi n}$, leading to a maximum wave vector

$$k_c = \frac{2\pi}{l_c} = \sqrt{\pi n}.$$

(3.4.10)

The calculation of the corresponding instability threshold is outlined in Appendix B.1.3, leading to the following approximate expression for $n_c$:

$$n_c \approx \frac{4}{\pi} \left( \frac{\lambda}{B\kappa} \right)^{2/3} + 2\sqrt{2} \frac{v_s}{B\kappa}.$$

(3.4.11)

We observe that the critical density (3.4.11) differs from its $k_c \to \infty$ counterpart Eq. (3.4.9) by the presence of a term that dominates at low swimming speeds $v_s \to 0$.

### 3.4.2 Density instability

The second subset of equations (3.4.3) couples $\delta \hat{U}_\parallel$ and $\delta \hat{\rho}$, and, thus, governs the appearance of density modulations along the microswimmer layer. After some algebra, the relevant poles are obtained from the following equation

$$\Phi \hat{k} \left[ B \left( b^2 + 2 - 2\sqrt{b^2 + 1} \right) y - b^2 \left( \sqrt{b^2 + 1} - 1 \right) (y + 1) \right] = 1,$$

(3.4.12)

where we have introduced the following dimensionless quantities

$$b = \frac{\hat{k}}{y + 1}, \quad y = \frac{\chi}{\lambda}, \quad \Phi = \frac{\kappa n}{v_s}, \quad \hat{k} = \frac{v_s}{\lambda} k.$$

(3.4.13)

Although Eq. (3.4.12) is exact, the solution to the eigenvalue problem can only be done numerically. The resulting dispersion relation for $B = 1$ and various values of the reduced density $\Phi$ is shown in Fig. 3.3. We observe that for small but negative $\Phi$, corresponding to a puller suspension, the dispersion law shows positive real part at the large spatial scales (small $\hat{k}$). In this regime, we can obtain an approximate expression for the eigenvalue $y$ valid for small $\hat{k}$: Series expanding the solution $y$ in terms of $\hat{k}$, we can identify the prefactors of the expansion from (3.4.13), which gives

$$y = -\frac{1}{8} \Phi \hat{k} - \left( \frac{1}{2} + \frac{B\Phi^2}{128} \right) \hat{k}^2 + O(\hat{k}^3).$$

(3.4.14)

Eq. (3.4.14) implies that confined suspensions of pushers, where $\Phi > 0$, are always stable, while puller suspensions with $\Phi < 0$ are always unstable with respect to large-scale density
Figure 3.3: The real (left) and imaginary (right) part of the eigenvalue \( y = \chi / \lambda \) corresponding to density perturbations, obtained by numerically solving Eq. (3.4.12). All plots correspond to infinitely thin particles \((B = 1)\), but look qualitatively similar for all values of \( B \). As the puller density increases from \( \Phi = 0 \), the real part of the eigenvalue becomes positive at small wave-vectors. For larger densities, the maximum value of \( \text{Re}[y] \) moves from small \( k \) (long wavelengths) to \( k \to \infty \) (short wavelengths). No solution exists in the region \( \text{Re}[y] < -1 \), where no instability should appear (see Appendix B.1.1).

fluctuations in the thermodynamic limit. This situation is qualitatively opposite to the orientational instability discussed in Section 3.4.1, where the instability occurs at smallest accessible spatial scale, and only for pusher particles. Moreover, the density instability for pullers occurs at any density in the thermodynamic limit, and finite values of \( n_c \) will only occur in finite systems.

As the eigenvalue \( y \) is real for small \( \tilde{k} \), the critical density for a finite system of size \( H \) can be obtained from (3.4.12) by setting \( y = 0 \), and \( k_c = 2\pi / H \), which gives

\[
n_c = -\frac{8\pi v_s^2}{H \lambda \kappa}.
\]  

This results demonstrates the significant finite size effects for the confined puller suspension, due to the long-wavelength nature of the density instability. We also note that this is qualitatively different from the finite-size corrections to the long-wavelength instability in three-dimensional pusher suspensions derived in [2], where the low-\( k \) cutoff merely leads to a minor shift of \( n_c \) in Eq. (3.3.12). Moreover, we note that the instability threshold (3.4.15) is independent of particle shape, as characterised by \( B \). This shows that the orientational degrees of freedom have no effect on the density instability, which is fully controlled by the mutual hydrodynamic advection of microswimmers.

The dispersion relation displayed in Fig. 3.3 shows further interesting features. As discussed above, for small values of \( \Phi \), the maximum real part of \( y \) occurs at small wave vectors. As the magnitude of \( \Phi \) increases sufficiently, this situation however changes. In the low density regime, the instability sets in at small, but non-vanishing spatial scales, determined by the local extrema of the semicircle at small \( \tilde{k} \). For larger densities the dispersion relation is an increasing function of \( \tilde{k} \) for large \( \tilde{k} \). Thus, similarly to the orientational instability discussed in Section 3.4.1, the density instability thus sets in at the smallest accessible spatial scale, corresponding to \( \tilde{k}_c \to \infty \).
Figure 3.4: Density instability in a 2d puller suspension embedded in a 3d fluid. The phase diagrams show regions of the two types of density instability obtained by numerical solution of Eq. (3.4.12). At high $\Phi$ (gray regions), the instability sets in at the smallest physically relevant spatial scale, which we assume to be the particle-particle separation, i.e., $\tilde{k}_c = \sqrt{\pi^3 \Phi}$. At moderate and low $\Phi$ (red heat map), the instability sets in at larger spatial scales set by the maximum of the semi-circle in the dispersion law; see Fig. 3.3. If the system size $H$ is too small, the latter maximum in the dispersion law cannot be accessed, and the instability instead sets in at the scale of the system. The two regimes are separated by the dotted line. Colours denote the value of $k$ at which the instability takes place.

To summarise the complex picture of the nature of the density instability, we numerically calculate the largest eigenvalue from Eq. (3.4.12). The resulting phase diagram is shown in Fig. 3.4, and confirms that the density instability in the two-dimensional suspension may set in at different spatial scales, depending on the values of the system parameters. Moreover, the structure of the phase diagram is weakly affected by the shape of the swimmers, $B$; For infinitely thin particles $B = 1$, the instability is sets in at large spatial scales at low densities, where the critical density is given by (3.4.15). At very large densities, however, the instability sets in at the smallest accessible spatial scales, which we assumed to be interparticle separation (i.e. $\tilde{k} = \sqrt{\pi^3 \Phi}$). This situation changes as $B$ decreases, because the dispersion law in Fig. 3.3 has much faster increase at large $k$ (not shown). As a result, for spherical particles the instability can set in at the smallest spatial scales at lesser densities. Similarly to the orientational instability discussed in Sec. 3.4.1, our approach does not allow us to determine the exact value of the smallest accessible wave-vector, but the key conclusion drawn from the presented result is that the system of pullers should show small-scale density fluctuations at these parameters.

We stress that the results presented above stem from the linear stability analysis. The non-linear fate of both the large-scale stationary mode and the small-scale density patterns in the form of travelling bands or rings can only be assessed by a non-linear method, usually involving numerical simulations. Finally, we note that, according to our analysis, suspensions of pushers, $\kappa > 0$, do not exhibit density instabilities.
3.5 Conclusion

In this chapter, we analysed linear stability of the homogeneous and isotropic distribution of microswimmers moving freely in the bulk three- and two-dimensional viscous fluid, and confined to a two-dimensional plane embedded in a three-dimensional viscous fluid. Our method, based on mean-field kinetic theory, is somewhat different from that used in the previous analysis of bulk suspensions \[45, 72–74\] and allows us to directly identify the origin of the instability as either an orientational mode, \(\text{i.e.}\), stemming from the mutual reorientation of microswimmers, or a density mode, \(\text{i.e.}\), stemming from local accumulation of microswimmers.

In the bulk two- or three-dimensional systems, linear stability analysis shows the presence of an orientational instability for pushers above the onset density given respectively by (B.1.10) and (3.3.11). This instability sets in at the largest scale available in the system, be it the smallest dimension of the experimental setup or the size of the simulation box. In the thermodynamic limit, the critical density is independent of the self-propulsion speed, although minor corrections do appear in finite systems. Furthermore, due to the incompressible nature of the embedding fluid, density perturbations are effectively suppressed, and no density instability due to hydrodynamic interactions are present. The linear stability analysis was carried out by solving the linearised Master equation using Laplace transform, instead of using the commonly applied exponential Ansatz for the expected solution. This procedure allows us to directly obtain the entire solution in the long-time limit, and hence avoid pathologies encountered in [74]. All of these results are consistent with previous works \[45, 72\].

In contrast, we showed that a two-dimensional layer of microswimmers embedded in a three-dimensional fluid is unstable for both pushers and pullers. For the former swimmer class, an orientational instability similar to the pusher instability in a bulk fluid occurs for large enough densities. However, in contrast to the bulk case, the orientational instability in the two-dimensional layer sets in at the smallest spatial scale available to the system, in practice the average swimmer-swimmer separation. This qualitative difference is readily understood from dimensional analysis: In an infinite fluid, \(\lambda / \kappa n\) is the only nonredundant dimensionless quantity that can be constructed from the problem parameters (the length-scale \(v_s / \lambda\), which measures the persistence of microswimmer self-propulsion, is irrelevant for this instability in the thermodynamic limit due to its orientational nature \[44, 73, 74\]). This observation is corroborated by (3.3.11) and (B.1.10), which only differ by a numerical prefactor. In the case of a microswimmer layer confined in a three-dimensional fluid, the combination \(\lambda / \kappa n\) is no longer dimensionless, since \(n\) is now a two-dimensional microswimmer number density, and should be replaced by \(\lambda / \kappa n\), where \(\ell\) is some length scale. In the absence of any other length scale in the problem, \(\ell \sim k^{-1}\), where \(k\) is the wavelength of the unstable mode, leading to the instability setting in at the smallest possible spatial scale available in the system. Unlike the bulk case, there is no unique interpretation of this length scale as it corresponds to the smallest scale at which the coarse-grained, mean-field approach of (2.2.2) is still applicable. Normally, translational diffusion regularises the system at large wave vectors, leading to a cut-off at \(\ell \sim \sqrt{D / \lambda}\). For realistic suspensions this scale is however similar to microswimmer size, and therefore too small to be relevant. Instead, we choose to identify the relevant length scale as the average particle-particle separation, below which the continuum description of the suspension breaks down. The corresponding critical density was then found to be a linear
function of swimming speed (3.4.11), implying that swimming stabilises the suspension, again in qualitative contrast with bulk suspensions where \( n_c \) is independent of \( v_s \). While this choice of the maximal wave vector is not unique, as discussed in Section 3.4.1, it only influences the numerical value of the instability onset but not its phenomenology, and the onset of an orientational instability in a layer of pushers is therefore generically predicted to be marked by the appearance of small-scale vortices.

On the other hand, a layer of puller microswimmers is susceptible to a density instability, characterised by spatial aggregation of microswimmers independent of their orientations. This instability is caused by the mutual advection of the microswimmers and is the direct consequence of the sink-like nature of their in-plane velocity fields, as discussed in Section 3.1. In the thermodynamic limit, the puller suspension is shown to be unstable at any density, while a non-zero critical density emerges for finite systems (3.4.15). The scale at which this puller instability sets in depends on the microswimmer density: at small and moderate densities, the instability occurs at large length scales, while at high enough densities it is replaced by a small-scale, oscillatory instability. While the crossover between these two regimes depends on the particle shape through \( B \) 3.4.2, both instabilities are generically present regardless of particle shape.

We would like to stress once more that the behaviours discussed here are not the consequence of the spatial dimensionality, as two- and three-dimensional bulk suspensions exhibit qualitatively very similar behaviours. Instead, the qualitative differences to the corresponding bulk suspensions come from the fact that in our problem the dimensionality of the microswimmer position and orientation vectors is lower than that of the embedding space. While this statement is rather abstract, it has a direct physical consequence: the microswimmer velocity fields are effectively compressible in the plane of their motion. This effect is inherent to any motion confined to a subset of the embedding space, including microswimmer layers in the vicinity of solid and liquid boundaries.

The phenomenon of effective in-plane compressibility discussed here is not limited to the dipolar fields. As discussed by [37], all flow singularities relevant to self-propulsion of microorganisms can be obtained by repeatedly applying the \((p \cdot \nabla)\) operator to the Stokeslet and the point source singularity. Therefore, each flow singularity will have opposite parity with respect to the angle defined by \( r \cdot p \) compared to the previous singularity. In the context of the calculation presented in Section 3.1, this leads to a layer of force dipoles, force octupoles, etc., exhibiting effectively compressible in-plane velocity fields, while the remaining flow singularities remain incompressible even when confined to a lower-dimensional subset of the embedding space. The same reasoning holds for the source singularities, where sources, source quadrupoles, etc., exhibit effectively compressible in-plane velocity fields. This phenomenology is thus likely to be important for hydrodynamic interactions and collective motion of realistic microorganisms.

We conclude by observing that, while the linear stability analysis predicted here identifies the origin, the onset conditions, and the associated scales of the instabilities, their non-linear evolution can only be properly assessed in numerical simulations, which we will pursue in a separate study.
Chapter 4

Emergent length-scale

The linear stability analysis predicts that the instability leading to the collective motion sets in at the largest accessible spatial scale. The non-linear structures appearing at the transition point should then be the size of system. An important question is whether the latter remains true even for higher densities, or another spatial scale emerges deeply within the collective motion state. In this chapter, we will explore properties of the non-linear regime using numerical simulations of the mean-field moment equations.

We begin with revisiting the derivation of the moment equations. In contrast to previous works, where the moment expansion was truncated after the nematic tensor, we analyse the effect of higher order moments. Assuming behaviour at the vicinity of the transition point, we enslave higher order moments, and show that they lead to the appearance of an effective diffusion. Moreover, using scaling arguments we derive the system size dependence of the individual fields and show that the fluctuations of the concentration and polar order should be negligible close to the transition point.

We then turn our attention to the collective motion state. By performing large-scale pseudo-spectral simulations of the moment equations in two spatial dimensions, we reveal strong finite size effects close to the instability. As a result different non-linear regimes appear, such as stationary patterns, periodic orbits, and chaotic motion, where only the latter dominates for large systems. We measure the system size dependence of the kinetic energies, and confirm our previous predictions close to the instability point.

Finally, we simulate the system away from the transition point, that is, deep in the collective motion state. We observe emergence of a new finite length-scale, which sets the typical size of the strongly aligned clusters of swimmers. By measuring energy spectra and spatial correlations of both fluid velocity and nematic tensor, we identify the density dependence of the emergent length-scale. We then discuss the qualitative behaviour of the system below and above the length-scale, and reveal in intriguing connection to a ‘gas’ of non-interacting microswimmers.

At the end, we discuss the behaviour of the density fluctuations in the suspension. In contrast to theoretical predictions of strongly nematic systems, no giant number of fluctuations are observed, as we found density fluctuations typical for equilibrium systems.

The results of this chapter have been published in: [3].
4.1 Enslaved kinetic theory

Even at the mean-field level, the kinetic theory suffers from its complexity. At the level of phase space density the number of dependent variables is high, and at the level of moment expansion the number of moments is infinite. The common approximation used in the literature closes the set of equations by cutting the moment expansion after the second moment, the nematic tensor. This approach is questionable, however, as the higher order moments can influence the overall dynamics of the system. We will now explore the influence of higher order moments, and revisit the linear stability of the system.

4.1.1 Enslaving higher order moments

In Sec. (2.2.2) we discussed the moment expansion of the phase space density leading to the hierarchy (2.2.8)-(2.2.10). In order to obtain a closed set of equations, an approximation for the higher order terms \( \langle p^n \rangle \), and \( \langle p^n p^m \rangle \) is required. The simplest one is to assume weak fluctuations of the phase space density around a homogeneous and isotropic state, and expand the phase space density only up to the second moment (2.2.15).

However, higher order moments may behave as fast modes, which can lead to generation of new terms in the relevant equations of motion. In order to capture these effects we generalize the closure (2.2.15) with the full form of the phase space density expansion

\[
\Psi(x, p, t) = \frac{1}{\Omega} \left[ c(x, t) + dm^\alpha(x, t) + \frac{d(d + 2)}{2} p^\alpha p^\beta Q^{\alpha\beta}(x, t) + \ldots \right.
\]

\[
+ \left( \prod_{i=0}^{n} \frac{d + 2i}{1 + i} \right) p^{\alpha_1} p^{\alpha_2} \cdots p^{\alpha_n} Q_n^{\alpha_1 \alpha_2 \cdots \alpha_n}(x, t) + \ldots \right],
\]

(4.1.1)

where \( Q_n^{\alpha_1 \alpha_2 \cdots \alpha_n} \) is the \( n \)-th moment that is symmetric w.r.t. swap of any two indices, and the numerical prefactors ensure unit normalisation of the moments (see Eq. (2.2.6)). In order for the higher order moments not to affect the lower order moments, contractions of any two indices must vanish (\( Q_n^{\alpha_1 \alpha_2 \cdots \alpha_n} \) are the connected moments). For example, the third and fourth moments are defined as

\[
Q_3^{\alpha \beta \gamma} = p^\alpha p^\beta p^\gamma - \frac{1}{d+2} (p^\alpha \delta^\beta \gamma + 2\text{perm.}),
\]

(4.1.2)

\[
Q_4^{\beta \gamma \delta} = p^\alpha p^\beta p^\gamma p^\delta - \frac{1}{d(d+2)} (\delta^\alpha \delta^\beta \delta^\gamma \delta^\delta + 2\text{perm.}) - \frac{1}{d+4} ((p^\alpha p^\beta - \frac{1}{d} \delta^\alpha \delta^\beta) \delta^\gamma \delta^\delta + 5\text{perm.}),
\]

(4.1.3)

where perm. stands for permutations of indices leading to different tensorial structures. Higher order connected moments have an analogous form.

The procedure for incorporating the effects of higher order moments goes as follows. First, one must derive dynamical equations for these quantities by taking the moments of the mean-field model (2.2.2). As the activity is responsible for nematic interaction only, we may assume that \( Q_n \), with \( n \geq 3 \), behave as fast modes, that is, their temporal change occurs at much smaller time-scale as the temporal change of \( Q \). Hence, we may set \( \partial_t Q_n = 0 \), and solve the resulting set of equations for \( Q_n \). Upon inserting the result into Eqs. (2.2.9), and (2.2.10), and keeping only the leading order terms, we arrive at
(see Appendix C for detailed derivation)

\[ D_C = -v_s \nabla^\alpha m^\alpha, \]  
\[ b_1 \nabla^\mu + b_2 \Delta^\mu = -\lambda m^\mu - v_s \nabla^\alpha (Q^{\mu\alpha} + \frac{1}{2} \delta^{\mu\alpha} c), \]  
\[ a_1 Q^{\mu\nu} + a_2 \Delta^{\mu\nu} = \frac{\nu^2}{(d+2)(d+4)} \nabla^2 Q^{\mu\nu} + \frac{db^2}{(d+2)(d+4)} (\nabla^\mu \nabla^\gamma Q^{\gamma\nu} + \nabla^\nu \nabla^\gamma Q^{\gamma\mu} - \frac{2}{d} \delta^{\mu\nu} \nabla^\gamma \nabla^\delta Q^{\gamma\delta}) \]  
\[ - \lambda Q^{\mu\nu} - \frac{\nu}{d+2} \nabla^\alpha (m^\mu \delta^\nu^\alpha + m^\nu \delta^\mu^\alpha - \frac{2}{d} m^\alpha \delta^{\mu\nu}) \]  
\[ + \frac{B}{d+2} c (\nabla^\nu U^\mu + \nabla^\mu U^\nu) - \frac{2B}{d+4} \delta^{\mu\nu} Q^{\alpha\beta} \nabla^\alpha U^\beta. \]  

(4.1.4)

(4.1.5)

(4.1.6)

In the above, the lower, and upper convective derivatives are defined in Eqs. (2.2.11)-(2.2.11), the fluid obeys the usual Stokes equations

\[ 0 = \nabla^2 U^\mu - \nabla P + \kappa \nabla^\alpha Q^{\alpha\mu}, \]  
\[ 0 = \nabla^\nu U^\mu, \]  

and we have introduced amplitudes of the convective derivatives

\[ a_{1,2} = \frac{1}{2} (1 \pm \frac{dB}{d+2}), \quad b_{1,2} = \frac{1}{2} (1 \pm \frac{dB}{d+2}). \]  

(4.1.9)

In the above, the lower, and upper convective derivatives are defined in Eqs. (2.2.11)-(2.2.11), the fluid obeys the usual Stokes equations

\[ 0 = \nabla^2 U^\mu - \nabla P + \kappa \nabla^\alpha Q^{\alpha\mu}, \quad \nabla^\nu U^\mu, \]  

and we have introduced amplitudes of the convective derivatives

\[ a_{1,2} = \frac{1}{2} (1 \pm \frac{dB}{d+2}), \quad b_{1,2} = \frac{1}{2} (1 \pm \frac{dB}{d+2}). \]  

(4.1.9)

Note, that at the leading order enslaving higher order moments only leads to an effective diffusion at the level of nematic tensor in Eq. (4.1.6), and no further terms are generated. This presence of effective diffusion due to self-propulsion completely rules out the importance of thermal diffusion.

### 4.1.2 Transition to collective motion

In particle-based models, the smallest length-scale that appears in the system is the microswimmer size \( \epsilon \). However, the coarse-grained macroscopic description, given by Eqs. (4.1.4)-(4.1.8), has no knowledge of the swimmer size. An alternative reference length scale that appears in the system is the persistence length. In order to simplify our calculations we rescale all fields with the mean density \( n_0 \), and introduce the following dimensionless quantities

\[ \tilde{t} = \lambda t, \quad \tilde{x} = \lambda v_s x, \quad \tilde{k} = v_s k, \quad \Delta = \frac{B\kappa}{(d+2)\lambda} n_0. \]  

(4.1.10)

The definition of the reduced microswimmer density \( \Delta \) is chosen such that the instability sets in at \( \Delta = 1 \) in the thermodynamic limit (see below). Note, that the scale \( \tilde{k} = 2\pi \) represents the scale of the persistence length. The linear stability of the homogeneous and isotropic state is analysed by looking at the wave behaviour of the fields

\[ c = 1 + \delta c \ e^{\chi t + i k \cdot x}, \]  
\[ m = \delta m \ e^{\chi t + i k \cdot x}, \]  
\[ Q = \delta Q \ e^{\chi t + i k \cdot x}, \]  
\[ U = \delta U \ e^{\chi t + i k \cdot x}, \]  

(4.1.11)

(4.1.12)

(4.1.13)

(4.1.14)

and similarly for the pressure. The corresponding dispersion relation is obtained by linearising the moment Eqs. (4.1.4)-(4.1.6). This calculation is outlined in detail in Appendix C.2. As in the case of the closure (2.2.15), the instability sets in at vanishing
Figure 4.1: Real part of the linear stability eigenvalues obtained by neglecting third order moment, considering the full Kinetic theory Eq. (3.3.10), and enslaving the third order moment. The plots correspond to two spatial dimensions, and the mean density is $\Delta = 2$ in all cases. The third order moment is required for saturation of the dispersion law at higher wave-vectors. These situation is qualitatively identical in three spatial dimensions.

wave-vectors, where the actual unstable moment is the $Q$ tensor. The small $\tilde{k}$ expansion of the eigenvalue with the largest real part is

$$\chi_\lambda = -(1 - \Delta) - \frac{2(d + 1)\Delta + d + 4}{(d + 2)\Delta} \tilde{k}^2 + O(\tilde{k}^4) \quad (4.1.15)$$

The full dispersion law in $d = 2$ is compared with analogous law in the absence of enslaved higher order moments in Fig. 4.1. There are two important features here. First, neglecting higher order moments does not lead to saturation of the dispersion law at higher wave-vectors, as it was in the case of the original Kinetic theory. This problem is cured by enslaving higher order moments, as shown in Fig. 4.1. Second, enslaving of the higher order moments does not affect the critical scale, so that the instability still sets in at the largest spatial scale available to the system. The non-linear spatial structures appearing close to the transition point should therefore still be of system size. It remains to be seen whether a finite length-scale appears deep into the collective motion state, which we will explore later using numerical simulations.

As the instability sets in at the largest accessible spatial scale $k \rightarrow k_{\text{min}} = 2\pi/H$, where $H$ is the system size, we can write $H = \alpha v_s / \lambda$ so that the critical density is found to be

$$\Delta_c = 1 + \frac{3}{d + 4} \left( \frac{2\pi}{\alpha} \right)^2 + O \left( \frac{2\pi}{\alpha} \right)^4. \quad (4.1.16)$$

The expression (4.1.16) shows that finite size effects shift the critical density to larger values. This feature is in particular important for numerical simulations in a periodic box, which are done in the next Section.
4.1.3 Fully enslaved kinetic theory

The linear stability above shows that the unstable moment is the nematic tensor. This suggests that close to the collective motion transition all other moments behave as fast modes, and can be enslaved to a single slow mode \( Q \). The only exception is the density field, which cannot be a fast mode due to the absence of tumbling effects in the continuity equation \( \text{(4.1.4)} \).

Enslaving polar order is done by setting \( \partial_t m = 0 \), and solving the resulting equation for \( m \), which gives

\[
m^\alpha \approx -\frac{v_s}{\lambda} \nabla^\alpha \left( Q^{\mu\alpha} + \frac{1}{d} \delta^{\mu\alpha} c \right) - U^{\alpha} \nabla^\alpha m^\nu, \quad (4.1.17)
\]

\[
m^\alpha \approx -\frac{v_s}{\lambda} \left[ 1 + O(U) \right] \nabla^\beta \left( Q^{\mu\alpha} + \frac{1}{d} \delta^{\mu\alpha} c \right). \quad (4.1.18)
\]

Higher order terms in \( U \) can be neglected close to the instability point, and the final form of the minimal microswimmer model is

\[
\mathcal{D}_t c = \frac{v_s^2}{d+4} \nabla^2 c + \frac{v_s^2}{\lambda} \nabla^\alpha \nabla^\beta Q^{\alpha\beta}, \quad (4.1.19)
\]

\[
\mathcal{D}_t Q^{\mu\nu} = \frac{v_s^2}{(d+4)\lambda} \nabla^2 Q^{\mu\nu} + \frac{2v_s^2}{(d+4)\lambda} \left( \nabla^\mu \nabla^\gamma Q^{\gamma\nu} + \nabla^\nu \nabla^\gamma Q^{\mu\gamma} - \frac{2}{d} \delta^{\mu\nu} \nabla^\gamma \nabla^\delta Q^{\gamma\delta} \right) - \lambda Q^{\mu\nu} + \frac{B}{d+4} \left( \nabla^\mu U^\nu + \nabla^\nu U^\mu \right) - \frac{2B}{d+4} \delta^{\mu\nu} Q^{\alpha\beta} \nabla^\alpha U^\beta
\]

\[
+ \frac{d(B+1)+4}{2(d+4)} \left( Q^{\mu\alpha} \nabla^\alpha U^\nu + Q^{\nu\alpha} \nabla^\alpha U^\mu \right)
\]

\[
+ \frac{d(B-1)+4}{2(d+4)} \left( Q^{\mu\alpha} \nabla^\nu U^\alpha + Q^{\nu\alpha} \nabla^\mu U^\alpha \right). \quad (4.1.20)
\]

Besides linear stability, there is also a secondary procedure for justifying enslaving of the moments. By looking at how the fields scale with the system size, one can estimate which are the dominant moments in the thermodynamic limit.

Let us consider the full set of equations \( \text{(4.1.4)-(4.1.6)} \) being stored in the periodic box of a size \( H^d \), where \( d \) is the dimensionality of the space. By normalizing the spatial variable with the system size, every \( \nabla \) operator will be replaced with \( H^{-1} \tilde{\nabla} \), where the latter derivative is defined w.r.t \( \tilde{x} = x/H \). The Stokes Eq. \( \text{(2.2.13)} \) then implies \( Q \sim U/H \). Next, we note that Eq. \( \text{(4.1.6)} \) for \( Q \) is driven by quadratic terms of a form \( U \nabla Q \). From \( Q \sim U \nabla Q \), we have \( U \sim H \), which also gives \( Q \sim 1 \). Furthermore, Eq. \( \text{(4.1.5)} \) shows that \( m \) is driven as \( m \sim \nabla Q \), which gives \( m \sim 1/H \). At last, similar arguments applied to \( \text{(4.1.4)} \) give \( c \sim 1/H^2 \).

Based on the above arguments we conclude that not only the polar order field is a fast mode, but the density fluctuations should also vanish in the thermodynamic limit

\[
c \approx c_0. \quad (4.1.21)
\]

This drastic simplification has been previously observed in lattice Boltzmann simulations [44]. One should note that the velocity field fluctuations diverge in the thermodynamic limit, which may be interpreted as the following. The instability sets in at the system size, and as there is no other length-scale involved the resulting hydrodynamic vortices will be system size. The bigger the system size, the bigger the vortex and hence the resulting flow increases as well.
4.2 Finite size effects

We will proceed to numerically analyse of the mean-field moment equations (4.1.4)-(4.1.6). All simulations are done in two spatial dimensions using a pseudo-spectral algorithm. The explicit form of the equations, and further details can be found in Appendix C.3.

4.2.1 Non-linear regimes

We ran the pseudo-spectral simulations of the moment equations (C.3.1)-(C.3.5) and (C.3.10) for various values of system size $H$ and densities $\Delta$. The linear regime occurs for $\Delta$ lesser than $\Delta_c$ from (4.1.16), where any perturbation or initial inhomogenity decays to zero. As the density passes through the instability point $\Delta > \Delta_c$, three non-linear regimes may be observed, shown in Fig. 4.2. Their appearance is related to the number of temporal Fourier modes present in the kinetic energies of the fields (see below). These are the following:

i) **Stationary pattern.** For mean concentrations that are only slightly above $\Delta_c$ all fields reach non-vanishing stationary distributions. Note that this does not mean that the matter does not flow at all. Microscopically, the microorganisms still swim, it is only the macroscopic observables that are stationary.

ii) **Periodic orbit.** As the mean concentration increases, the system reaches a state that is characterized by a periodic evolution of observables. Here, all field distributions are oscillatory in time, where the number of temporal Fourier modes is related to the density.

iii) **Chaos.** A final state that emerges for large mean concentrations and its fully chaotic in time. The temporal spectrum of the observables are characterized by an infinite number of Fourier modes.

Fig. 4.3 shows kinetic energy (spatial average) of the fluid velocity in both real-time and Fourier representation, both for a fixed system size $H = 40v_s/\lambda$, and for various concentrations. As can be seen, the number of Fourier modes that appears in the system increases with the density until a fully chaotic regime is reached.

Figure 4.2: Snapshots from the pseudo-spectral simulations of the mean-field Kinetic theory; From the left: i) Stationary state, ii) Periodic orbit iii) Chaos. The color map represents the microswimmer concentration, while the arrows denote the fluid flow. All simulations are done in the periodic box with the size $H/(v_s/\lambda) = 250$. 

40
Figure 4.3: Kinetic energy of the fluid velocity in real-time (left column) and frequency (right column) domain, for various mean concentrations. Shortly after the instability (top row), the system relaxes to a stationary state with non-zero, but constant, kinetic energy. By increasing the density one observes a small number of Fourier modes which characterize periodic orbits. Further increase of $\Delta$ eventually results in appearance of infinite number of Fourier modes, which corresponds to the chaotic state (bottom row). The $y$ axis in all plots is in arbitrary units.

We have measured the range of densities in which individual regimes exist. The final

<table>
<thead>
<tr>
<th>$H\lambda/v_s$</th>
<th>SP$\leftrightarrow$PO</th>
<th>PO$\leftrightarrow$CM</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>0.024</td>
<td>0.090</td>
</tr>
<tr>
<td>50</td>
<td>0.013</td>
<td>0.050</td>
</tr>
<tr>
<td>60</td>
<td>0.008</td>
<td>0.031</td>
</tr>
<tr>
<td>70</td>
<td>0.005</td>
<td>0.021</td>
</tr>
<tr>
<td>80</td>
<td>0.004</td>
<td>0.016</td>
</tr>
</tbody>
</table>

Figure 4.4: Left: Phase diagram of the bacterial suspension above the instability point, Right: Table of transition densities between individual states: stationary pattern (SP), periodic orbit (PO), and collective motion (CM)
phase diagram is shown in Fig. 4.4, and the densities under which non-chaotic states appear decreases with the system size. The transition lines can be approximated as

\[
\Delta_{SS\leftrightarrow PO}(H) = 1.003(2) + 0.338(6) \exp\{-0.068(3)H\lambda/v_s\}, \tag{4.2.1}
\]

\[
\Delta_{PO\leftrightarrow CM}(H) = 1.011(1) + 0.934(8) \exp\{-0.063(0)H\lambda/v_s\}. \tag{4.2.2}
\]

These fits show that even in the infinite system size \( H \to \infty \), the boundaries of both states converge to a finite value. Hence, one may expect periodic orbits or stationary states in realistic experiments, where the system size can be as small as \( H = 15v_s/\lambda \). [2]

### 4.2.2 Thermodynamic limit

The scaling arguments discussed in Sec 2.2.1, led to the following relations between the fields and the system size

\[
U \sim H, \quad Q \sim 1, \quad m \sim H^{-1}, \quad c \sim H^{-2}. \tag{4.2.3}
\]

According to (4.2.3), amplitudes of the concentration and the polar order should be small in the thermodynamic limit. We have measured the average mean-square displacements of all fields for various system sizes. The final plot is shown in Fig. 4.5, which confirms our expectations. For densities close to the transition point the individual fields behave qualitatively as predicted in (4.2.3). Moreover, the numerical values of averages differ by several orders of magnitude, which shows that the important dynamics is driven by the fluid velocity and the nematic tensor. Away from the transition point, however, the properties of the system deviate from (4.2.3), and saturate above certain system size. Here, new physics emerges, which will be explored in the next section.

Figure 4.5: The mean values of individual fields for various system sizes. The solid lines denote measured values, where dashed lines are the analytical predictions.
4.3 Observables

We now proceed to calculating observables, that is, the energy spectra and spatial correlations of the suspension. All averages in this section are done by averaging the observables over many time steps, for very large system sizes. Let us start with a few snapshots of the fields for various mean concentrations above the threshold $\Delta > \Delta_c \approx 1$, displayed in Fig 4.6. Visual inspection reveals a clear sign of an emergent length-scale in the collective motion regime, which appears to be density dependent. In the proceeding sections, we will describe the behaviour of this length-scale and its implications on the suspension.

Figure 4.6: Snapshots of fields obtained from the pseudo-spectral simulations of the mean-field Kinetic theory for various mean concentrations; Fluctuations of the concentration $c$ (top row), eigenvalue of the $Q$ tensor (middle row), and the stream function $\psi$ (bottom row). Different columns represent different mean concentrations – from left: $\Delta = 1.1$, $\Delta = 1.3$, and $\Delta = 1.5$. All snapshots above have been produced from simulations in a periodic box with linear size $H\lambda/v_s = 1000$, and resolution $r = 2048^2$. 
4.3.1 Energy Spectra

We will start with the energy spectra of the velocity field \( E_U(k) \), and the nematic tensor \( E_Q(k) \). In our simulations the spectra are measured using an algorithm that directly incorporates the Jacobian into the definition of the spectra

\[
E_U(k) = 2\pi k \langle \hat{U}(k) \cdot \hat{U}(-k) \rangle, \quad E_Q(k) = 2\pi k \langle \hat{Q}(k) : \hat{Q}(-k) \rangle.
\] (4.3.1)

Let us repeat that the average in (4.3.1) is carried out over many time units, where we have used dimensionless variables (4.1.10).

As was mentioned in the previous sections, the suspension of microswimmers suffers heavily from finite-size effects. In order to correctly measure all statistical properties, we have carried out high resolution simulations with \( 4096^2 \) Fourier modes, and for various large system size. The size of the periodic box was chosen to be from the range \( H \lambda / v_s \in \langle 750, 3000 \rangle \), such that the absolute convergence of all observables was achieved for individual densities (see Appendix C.3.2 for further details).

The resulting energy spectra for densities \( \Delta = 1.3, ..., 2.0 \) are depicted in Fig. 4.7. Visual inspection reveals that the exact functional form changes with the mean concentration \( \Delta \). The spectra appear to have a two-phase behaviour, which is separated by an inflection point at \( k^* \), defining a new emergent length-scale \( l^* = 2\pi / k^* \). For small concentrations \( \Delta \to 1^+ \), this point moves towards the vanishing wave-vectors, and as the concentration increases, the \( k^* \) moves towards higher wave-vectors.

At our highest density \( \Delta = 2.0 \), convergence of the spectra is achieved with a power-law behaviour at large spatial scales \( k < k^* \). The velocity field behaves as \( E_U \sim k^{-1} \), which corresponds to the spectrum of a free swimmer – looking at the scaling of the hydrodynamic dipole in two spatial dimensions (A.3.5) we obtain the same functional form \( k |\hat{u}_{d=2}|^2 \sim k^{-1} \). The nematic tensor, on the other hand, scales as \( E_Q \sim k^{+1} \), which can be explained by looking at the Fourier transform of the Stokes equations (4.1.7), which gives \( Q \sim k \hat{U} \). At small spatial scales \( k > k^* \), no power-law behaviour is observed.

![Figure 4.7: Energy spectra for \( U \) and \( Q \) for various densities. In all simulations the resolution is \( r = 4096 \) Fourier modes, and the system sizes, have been chosen such that both short scale and large-scale behaviour are correctly resolved.](image)
4.3.2 Spatial correlations

In order to understand the behaviour of the emergent length-scale $l^*$, we measured spatial correlations for the velocity field, as well as the nematic tensor, defined as

$$C_U(R) = \int \frac{dr}{2V} \langle \mathbf{U}(r) \cdot \mathbf{U}(r + R) \rangle, \quad C_Q(R) = \int \frac{dr}{2V} \langle Q(r) : Q(r + R) \rangle,$$

(4.3.2)

where $R = |R|$, and $V$ is the volume of the periodic box. The results are shown in Fig. 4.8 in the log-linear plane, for various mean concentrations.

At small distances, the spatial correlations of the fluid velocity $C_U$ are flat, but eventually cross to a logarithmic decay at large distances. The crossover point is density dependent and decays with increasing density. The large-distance functional form is consistent with energy spectra measured above – the expected behaviour from the inverse Fourier transform should be

$$C_U(R) \sim \int_0^\infty dk \, E_U(k) e^{ikR} \sim -\log(R/R^*),$$

(4.3.3)

where we have found that the correlation function reaches zero at $R^* \approx H/3$. Above this point the fluid velocity becomes anticorrelated with the minimum being at the half of the system size $R = H/2$ independently of the concentration, which means that the fluid vortices always have the size of the system. The latter can be observed in the snapshots – see Fig. 4.6 – where the stream function splits into two regions at any density.

When it comes to spatial correlations of the nematic tensor $C_Q$, its qualitative form is somehow different. A plateau appears at small distances as well, but this time a crossover to a rapid decay occurs. The corresponding structure does not seem to obey an exponential, nor a power-law behaviour. At larger distances spatial correlations become weakly negative, and eventually vanish completely. The point at which the latter occurs defines correlation length of the microswimmer suspensions, which we identify to be the emergent length-scale $l^*$.

Figure 4.8: Spatial correlations for various mean concentrations. Left: correlations of the fluid velocity, with $x$-axis to be normalized with half of the system size. Right: correlations of the nematic tensor, normalized with their values at the origin.
Figure 4.9: Correlation length as a function of mean concentration measured from extrema of the $Q$ energy spectra (green), and by looking at the first minimum of the correlation function of $Q$ (blue). The errorbars denote averaging over several time-steps.

Measuring the correlation length from the point after which $C_Q$ remains zero is inconvenient due to the noise appearing in the simulations. Instead, we have measured $l^*$ by looking at the minimum of the weakly anticorrelated regime (see the subfigure of Fig 4.8). The resulting data is shown in Fig. 4.9, and compared against correlation length extracted from the inflection point of the nematic tensor spectra $E_Q(k)$ (Fig. 4.7). Although the exact values differ, the functional dependence of the emergent length-scale on concentration remains unchanged. Close to the transition $\Delta \to 1^+$, the length-scale diverges $l^* \to \infty$, but it decays with increasing mean concentration $\Delta$. The exact dependence of $l^*$ on $\Delta - 1$ does not follow any power-law, as one could expect for example from linear theory of Model A [124].

The physical interpretation of $l^*$ can be inferred from visual inspection of the scalar order parameter depicted in Fig. 4.6. As the system passes through the instability point, the suspension consists of a single strongly correlated region of swimmers with the typical length-scale $l^*$ being the size of the system (in our case half the size of the periodic box $H/2$). As the density increases the correlation length decreases, and the system splits into a set of strongly correlated regions of nematically aligned swimmers. These are mutually decorrelated due to the energy spectra $E_Q \sim k^{+1}$ at large spatial scales $k \to 0$. The number of clusters rapidly increases with density, leading to a gas of effectively non-interacting swimmers deeply in the collective motion regime.

4.3.3 Density fluctuations

The last quantities of interest are the density fluctuations. In order to quantify their properties, we have first measured the probability density distribution for various system sizes, and mean densities, displayed in Fig 4.10.

At low densities finite size effects have a strong impact on the distribution of the fluctuations. As our result show, in order for the distribution to converge at $\Delta = 1.4$, the system size $H \approx 500$ is required. This number is much larger than the correlation length $l^* \approx 150$ extracted from the inflection point in Fig. 4.9, meaning that in order for the observables to converge, system sizes more than twice the correlation length are needed. In other words, one needs to resolve $l^*$. As the latter diverges at the transition point $\Delta \to 1^+$, the simulations close to the instability are computationally very expensive.
Once finite size effects are suppressed, we can study how the density fluctuations depend on the mean density $\Delta$. The measured distribution functions, as well as standard deviations are depicted in Fig. 4.10. As expected, close to the transition the standard deviation is negligibly small, but increases with $\Delta$. However, even for our highest density, $\Delta = 2.0$, the fluctuations are found to be about 25% only.

At last, we have measured the energy spectra of the density fluctuations, $E_c(k)$, defined analogously to 4.3.1. At large densities, they seem to converge to a linear power-law behaviour $E_c(k) \sim k$, which has the following implication. The number of fluctuations $(\delta N)^2$ can be determined from the following formula

$$\left( \frac{\delta N}{V} \right)^2 = \int \frac{dV}{V} \langle \delta c(r) \delta c(r) \rangle \quad (4.3.4)$$

Using $k^{-d} \sim V \sim N$, we obtain $(\delta N)^2 \sim E_c(k)/k^3 \sim N$ which is a result typical for equilibrium systems [125]. Hence, no giant number of fluctuations have been observed, in contrast to claims presented in [126] for fully developed nematic systems.

Let us emphasize that the emergent length-scale $l^*$ is not observed in the energy spectra of the density fluctuations in Fig. (4.10), although our earlier snapshots of the

Figure 4.10: Statistical properties of density fluctuations: a) probability distribution of density fluctuations at $\Delta = 1.4$, and for various system sizes, b) the same as before, but for various densities and system sizes such that the finite size effects are suppressed, c) standard deviation $\sigma(c)$ of distributions from b), and finally d) energy spectra.
concentration in Fig. (4.6) do display some quantitative change of spatial structures occurring with varying density. The latter spatial scale however, is not the sign of an emergent length-scale affecting the density fluctuations, but is just a result of the strongly aligned regions of swimmers driving the density fluctuations.

4.4 Conclusion

In this chapter, we have studied the properties of the collective motion of microswimmer suspensions by carrying out large-scale pseudo-spectral simulations of mean-field moment equations.

We started with questioning the validity of the commonly used moment equations for microswimmer suspensions. Their standard derivation involves expanding the one-particle phase space density distribution in terms of moments, and keeping only concentrations $c$, polar $m$, and nematic order $Q$. Neglecting higher order terms requires their effect to be negligible, which might not necessary be true. However, close to the transition point the dynamics is driven by the most unstable mode – the nematic tensor – and higher order terms may safely be enslaved to it. We have carried out this procedure which led to two important results. First, enslaving higher order terms results in the appearance of effective diffusion due to the self-propulsion mechanism $D_v \sim v_s^2/\lambda$. As a result the dispersion law saturates at high wave-vectors causing thermal diffusion to be absolutely irrelevant for microswimmer suspensions. Second, the critical scale remains unchanged so that the instability still sets in at the scale of the system. At the onset, one should expect the size of the non-linear structures to be of a similar size to the system, and whether this remains true deep in the collective motion regime was a key question of this project.

Later, we have briefly looked at the properties of the mean-field equations from an analytical point of view. Assuming that the system is stored in a periodic box of a size $H$, we derived the system size scaling of all fields relevant for the suspension: The fluid velocity scales linearly as $U \sim H$, the nematic tensor is of order of unity $Q \sim 1$, and polar order with the concentration represent decaying functions of the system size $m \sim 1/H$, and $c \sim 1/H^2$. Hence, one may expect that the fluctuations of $m$, and $c$ should have a negligible impact on the suspension in the thermodynamic limit.

We then turned our attention to the collective motion state by performing large-scale pseudo-spectral simulations in a periodic box. Close to the instability we confirmed our aforementioned analytical predictions for scaling of the observables with the system size, shown in Fig. 4.5. Strong finite size effects were observed, where the absolute convergence of the statistical quantities requires very large system sizes. This feature can be explained on the basis of linear stability, which says that the instability sets in at the size of the system – one may expect appearance of a diverging correlation length, which must be resolved for the absolute convergence of the observables. These expectations were confirmed with further simulations deeply in the collective motion state.

We have measured the energy spectra and spatial correlations for both fluid velocity, as well as nematic tensor, for various values of the mean density deep within the collective motion regime – Fig. 4.7. The energy spectra show a clear sign of an emergent length-scale $l^*$ defined through the inflection point at $k^* = 2\pi/l^*$. The exact value of the length-scale is density dependent – Fig. 4.9. It appears to diverge at the instability point, and
decays with increasing density. The functional form, however, does not appear to obey any power-law, nor an exponential decay. The inflection point $k^*$ separates the energy spectra into two ranges of scales with different behaviour. At large scales $k < k^*$ the energy spectra for the fluid velocity and the nematic tensor are $E_U \sim k^{-1}$ and $E_Q \sim k^{+1}$, respectively. As the former decay corresponds to a single hydrodynamic force dipole, we conclude that macroscopically the system behaves as a gas of non-interacting swimmers. These conclusions are supported with the measurements of the spatial correlations of the nematic tensor, $C_Q$, see Fig. 4.8. At small distances $C_Q = \text{constant}$ indicating strong correlations. The situation changes at large distances, where the correlations start rapidly decaying, become weakly anticorrelated, and eventually vanish entirely. The latter occurs at the distance of the correlation length $l^*$. For the spatial correlations of the fluid velocity a logarithmic decay was observed, with the minimum being at the half of the system size, independently of the mean concentration of the swimmers. This indicates that the vortices are always the system size, independently of the mean concentration of the swimmers, which can be seen in the snapshots Fig. 4.6.

Density fluctuations of the microswimmer suspension were measured as well. We have first extracted the distribution of the fluctuations at fixed density $\Delta = 1.4$, but for various system sizes. The results displayed in Fig. 4.10 show that fluctuations decay with increasing system size, with converging distribution at system sizes more than twice the size of the correlation length. This confirms that in order for the finite size effects to disappear the correlation length must be resolved. Once finite size effects were suppressed we looked at the variance of the density fluctuations as a function of the swimmer mean density. An increase was observed, but the even at our highest density, $\Delta = 2.0$, they were about 25% only.

Let us now discuss the relation of the presented results with previous works. Alert et al. [127] simulated collective motion in nematic systems; Assuming behaviour deeply in the nematic phase, they only considered equations of motion for the director field $n$, accompanied with the Stokes flow. Measurements of the energy spectra yielded power-law behaviour similar to the mean-field kinetic theory at large spatial scales for the fluid velocity $E_U \sim k^{-1}$. Interestingly, their measurement of the enstrophy spectra $E_\omega \sim k^{+1}$ is identical to our nematic tensor spectra at large wave-lengths. This might be due to the scaling relation $\omega \sim \nabla U \sim Q$ stemming from the Stokes equations (4.1.7). They also observed an emergent length-scale $k^*$ below which different behaviour appears. However, the small scale energy spectra show deviations, as they have measured $E_U \sim k^{-3}$, and $E_\omega \sim k^{-1}$ for $k > k^*$, whereas our kinetic theory does not predict any power-law decay at all. Finally, no giant number of fluctuations were observed, as predicted for strongly nematic active systems in [126].

We conclude that the kinetic theory for microswimmer suspension predicts emergence of a finite length-scale in the collective motion regime. The length-scale is infinite at the transition point, leading to strong finite-size effects, but decays fast as the density increases. It should be noted that these results are solely based on neglecting correlations arising from the tumbling of the bacteria. This effect of correlations on the suspension of microswimmers will be analysed in the following chapter.
Chapter 5

The role of correlations

The mean-field Kinetic theory discussed until now predicts appearance of no interesting physics below the transition point. However, recent lattice-boltzmann simulations show presence of strong correlations even within this regime. In this chapter, we analyse the role of correlations in the microswimmer suspension arising from tumbling effects, by explicitly calculating the fluid velocity-velocity correlation function below the onset to the collective motion $\Delta < 1$.

We being with discussing extension of the mean-field model to the $N$-particle Kinetic theory. In order to avoid technical difficulties originating from high number of dependent variables, the famous BBGKY hierarchy for reduced distribution functions is derived. The irrelevance of the higher order terms is discussed, which allows us to close the infinite hierarchy of equations.

To establish the connection between the two-point distribution function and spatio-temporal correlations we follow the approach pioneered by Klimontovich [128]. It is showed, that the fluctuations about the homogeneous and isotropic state are given by a linear integro-partial differential equation with noise. At first glance, obtaining any analytical solution appears to be technically quite challenging. However, we show that the treatment is greatly simplified due to the incompressibility of the fluid which allows for the calculation of relevant observables.

We then proceed with discussing the variance of fluid velocity. The relevant dimensionless parameters are found to be $i)$ the persistence length $L$, and $ii)$ the deviation from onset $\Delta$. We show, that deviations from the non-interacting system appear at any finite microswimmer density. Moreover, their magnitude grows rapidly and eventually diverges at the instability point $\Delta \to 1^-$. The spatial correlations of the fluid velocity are found to be already scale-free at large distances, hence a phenomenological correlation length is defined. Temporal correlations, on the other hand, have a well-defined correlation length. Furthermore, we use temporal correlations to determine the enhanced diffusivity of passive tracers.

Interestingly, it is showed that all correlations decay with persistence length $L$, implying that the self-propulsion reduces correlations in the suspension. However, correlations still diverge at the instability point $\Delta \to 1^-$ where the corresponding critical exponents are extracted.

The results of this chapter have been published in: [1].
5.1 $N$-particle Kinetic theory

We start by generalizing the one-particle kinetic theory described in Sec. 2.2.1 to the $N$-particle case. All quantities and parameters will have the same meaning, if not stated otherwise, and the number of spatial dimensions is considered to be three.

Let us recall that we consider a collection of $N$ microswimmers contained in a volume $V$ at a finite number density $n = N/V$, suspended in an incompressible fluid. In $N$-particle description, each microswimmer is described by its instantaneous position $\mathbf{x}_i$, and orientation $\mathbf{p}_i$, that we collectively denote by $\mathbf{z}_i = (\mathbf{x}_i, \mathbf{p}_i)$, where $i = 1\ldots N$ enumerates the particles – see Fig. 5.1. The entire information about the system is stored in the $N$-particle phase space density $F_N(\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N, t)$ that gives the geometric probability of the system occupying a particular point in the $5N$-dimensional phase space $\{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$ at time $t$. The $N$-particle phase space density is symmetric with respect to swapping particle labels, reflecting their indistinguishability, and is normalised

$$\int d\mathbf{z}_1 \ldots d\mathbf{z}_N F_N(\mathbf{z}_1, \ldots, \mathbf{z}_N, t) = 1. \quad (5.1.1)$$

Analogously to the one-particle case (2.2.2), its time dynamics is governed by the Master equation [115]

$$\partial_t F_N + \sum_{i=1}^{N} \left[ \nabla_i \cdot (\dot{\mathbf{x}}_i F_N) + \partial_i \cdot (\dot{\mathbf{p}}_i F_N) \right] = -N \lambda F_N + \frac{\lambda}{4\pi} \sum_{i=1}^{N} \int d\mathbf{p}_i F_N, \quad (5.1.2)$$

where $\nabla_i \equiv \partial/\partial \mathbf{x}_i$, and $\partial_i = (1-p_i p_i) \cdot \partial/\partial \mathbf{p}_i$ are positional and orientational derivatives w.r.t. the position and orientation of the $i$-th particle, respectively. The dynamics of each particle is set by the equations

$$\dot{\mathbf{x}}_i = v_s \mathbf{p}_i + \mathbf{U}(\mathbf{x}_i), \quad (5.1.3)$$
$$\dot{\mathbf{p}}_i = (1-p_i p_i) \cdot \left( \mathbf{W}(\mathbf{x}_i) + B \mathbf{E}(\mathbf{x}_i) \right) \cdot \mathbf{p}_i, \quad (5.1.4)$$

![Figure 5.1: Pictoral visualisation of $N$-particle kinetic theory. Each microswimmer has its position $\mathbf{x}_i$, orientation $\mathbf{p}_i$, and the self-propulsion mechanism generates the dipolar velocity field $\mathbf{u}_i$.](image)
where \( \mathbf{W}(\mathbf{x}_i) \) and \( \mathbf{E}(\mathbf{x}_i) \) are the vorticity and the rate-of-strain tensors at the position of the particle \( \mathbf{x}_i \) (see Sec. 2.1.3), \( v_s \) is the swimming speed, \( B \) is the shape-setting parameter \((B = 1 \text{ for rod-like particles, and } B = 0 \text{ for spheres})\), and \( \lambda \) is the tumbling rate. We note here that we have neglected the effects of rotational and translational diffusion in (5.1.3) and (5.1.4) on the particle’s dynamics, and random tumbling is thus the only source of stochasticity in our model. Justification of the latter approximation can be found in Sec. 2.2.1.

Besides the obvious difference in the number of degrees of freedom, the main distinction between the one-particle description (2.2.2)-(2.2.4), and the \( N \)-particle description (5.1.2)-(5.1.4), is that in the latter case the velocity field affecting particle’s positions and orientations is not set by its mean-field approximation (2.2.5). Instead, it consists of the sum of the dipolar contributions coming from all particles

\[
\mathbf{U}(\mathbf{x}_i) = \sum_{j \neq i}^N \mathbf{u}_d(\mathbf{x}_i; z_j),
\]

where we will use the regularised version of the hydrodynamic dipole \cite{129}

\[
\mathbf{u}_d(\mathbf{x}_i; z_j) = \frac{\kappa}{8\pi} \left[ 3 (\mathbf{p}_j \cdot \mathbf{x}')^2 \mathbf{x}' + \epsilon^2 (\mathbf{p}_j \cdot \mathbf{x}') \mathbf{p}_j \right] - \frac{\mathbf{x}'}{(x'^2 + \epsilon^2)^{3/2}}.
\]

Eq. (5.1.6) represents the velocity field generated at \( \mathbf{x}_i \) by a hydrodynamic dipole located at \( \mathbf{x}_j \) with the orientation \( \mathbf{p}_j \) (see Sec. 2.1.2). Here, we recall that \( \kappa = Fl/\mu \) is the dipolar strength, where \( F \) is the magnitude of the forces applied to the fluid, \( l \) is the dipolar length, and \( \mu \) is the viscosity of the fluid; \( \mathbf{x}' = \mathbf{x}_i - \mathbf{x}_j \), and \( x' \) denotes the length of \( \mathbf{x}' \). The dipole consists of two regularised Stokeslets, with \( \epsilon \) being the regularisation length of the order of swimmer size, that will serve as a UV cut-off in the wave-vector integrals (see below). In this section, we will only focus on the case of pushers, \( \kappa > 0 \), as the mean-field analysis carried out in the previous chapters did not predict transition to collective motion for the case of pullers, \( \kappa < 0 \). The generalisation to the latter case is, however, straightforward.

The main goal of this project is to calculate spatial and temporal correlations of the fluid velocity in microswimmer suspensions described by the model above. Both quantities can be succinctly expressed through a combined correlation function

\[
C(R,T) = \lim_{t \to \infty} \frac{1}{V} \int d\mathbf{x} \bar{U}^\alpha(\mathbf{x},t) U^\alpha(\mathbf{x} + \mathbf{R}, t + T),
\]

where \( U^\alpha(\mathbf{x},t) \) is the fluid velocity at the position \( \mathbf{x} \) at time \( t \), and the large-\( t \) limit guarantees independence of the initial conditions. The spatial and temporal correlation functions are trivially recovered by setting \( T = 0 \) and \( R = 0 \), respectively. The bar in Eq.(5.1.7) denotes the average over the history of tumble events, and reflect the stochastic nature of our model. To calculate this and similar averages, below we formulate a kinetic theory of microswimmer suspensions based on our macroscopic model. Here, we go beyond the mean-field approximation developed in the previous chapters, and explicitly take into account strong correlations between the swimmers caused by the long-range nature of their hydrodynamic fields, Eq.(5.1.6).
5.1.1 BBGKY hierarchy

The \(N\)-particle problem (5.1.2) depends on \(5N\) microscopic variables, plus time. In order to obtain measurable information, some approximations must be made. For experimental purposes, one is mostly interested only in correlations between a couple of microswimmers. The main idea is to integrate out redundant degree of freedom, and write down equations describing correlation functions between small number of particles \([115]\). The resulting set of equations will depend on higher order correlation functions, forming an infinite set of equations known as Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy. Certain physical arguments must be deployed in order close the hierarchy, which will be discussed below.

In order to integrate redundant degree of freedom, we introduce the \(s\)-particle correlation function

\[
F_s(z_1, \ldots, z_s, t) = \frac{N!}{(N-s)! N^s} \int dz_{s+1} \ldots dz_N F_N(z_1, \ldots, z_N, t), \tag{5.1.8}
\]

Below, we will only be interested in the first partial correlation functions \(F_1, F_2, \text{ and } F_3\), that we further express as

\[
\begin{align*}
F_2(z_1, z_2, t) &= F_1(z_1, t) F_1(z_2, t) + G(z_1, z_2, t), \tag{5.1.9} \\
F_3(z_1, z_2, z_3, t) &= F_1(z_1, t) F_1(z_2, t) F_1(z_3, t) + G(z_1, z_2, t) F_1(z_3, t) \\
&\quad + G(z_1, z_3, t) F_1(z_2, t) + G(z_2, z_3, t) F_1(z_1, t) \\
&\quad + H(z_1, z_2, z_3, t), \tag{5.1.10}
\end{align*}
\]

where \(G\) and \(H\) are the irreducible (connected) correlation functions \([115]\). The time evolution of \(F_s\) can be deduced from the Master equation (5.1.2) by integrating it over \(\{z_{s+1}, \ldots, z_N\}\).

Integrating by parts and using Eqs. (5.1.9) and (5.1.10), we obtain the following equations for the one- and two-particle irreducible correlation functions

\[
\begin{align*}
\partial_t F_1(z, t) + \mathcal{L}[F_1(z, t)](z) &= -N \nabla^\alpha \int dz' G(z, z', t) u_1^\alpha(x; z') \\
&\quad - NP_\alpha^\beta \frac{\partial}{\partial p^\beta} \int dz' G(z, z', t) \rho^\gamma X^{\alpha\mu\nu\gamma} \nabla^\mu u_1^\nu(x; z'), \tag{5.1.11}
\end{align*}
\]

\[
\begin{align*}
\partial_t G(z_1, z_2, t) + \mathcal{L}[G(z_1, z_2, t)](z_1) + \mathcal{L}[G(z_1, z_2, t)](z_2) \\
&+ N \nabla_1^\alpha \left[ F_1(z_1, t) \int dz' G(z_2, z', t) u_1^\alpha(x_1; z') \right] \\
&+ N \nabla_2^\alpha \left[ F_1(z_2, t) \int dz' G(z_1, z', t) u_1^\alpha(x_2; z') \right] \\
&+ N P_1^\alpha \frac{\partial}{\partial p_1^\beta} \left[ F_1(z_1, t) P_1^\gamma X_1^{\alpha\mu\nu\gamma} \int dz' G(z_2, z', t) \nabla_1^\mu u_1^\nu(x_1; z') \right] \\
&+ N P_2^\alpha \frac{\partial}{\partial p_2^\beta} \left[ F_1(z_2, t) P_2^\gamma X_2^{\alpha\mu\nu\gamma} \int dz' G(z_1, z', t) \nabla_2^\mu u_2^\nu(x_2; z') \right] \\
&= -S_{1,2}^F - S_{2,1}^F - S_{1,2}^G - S_{2,1}^G - S_{1,2}^H - S_{2,1}^H, \tag{5.1.12}
\end{align*}
\]

where the rank-4 tensor \(X_1^{\alpha\mu\nu\gamma} = P_1^{\alpha\beta} \left[ \frac{B+1}{2} \delta^\nu_\mu \delta^\beta_\gamma + \frac{B-1}{2} \delta^\mu_\beta \delta^\nu_\gamma \right] \), encodes the tensorial
structure of Jeffrey’s equation (5.1.4), we have introduced the operator

\[ \mathcal{L}[\Phi](z) = v_i p^\alpha \nabla^\alpha \Phi(z) + N \nabla^\alpha [\Phi(z) U_{\text{MF}}^\alpha(x)] \]

\[ + N \Phi^{\alpha\beta} \frac{\partial}{\partial p^\gamma} [\Phi(z) p^\gamma \mathcal{X}_i^{\alpha\mu\nu\gamma} \nabla^\mu u_\gamma(x_i; z_j)] + \lambda \Phi(z) - \frac{\lambda}{4\pi} \int dp \Phi(z), \]  

(5.1.13)

acting on the variable \( z \) of an arbitrary function \( \Phi = \Phi(z_1, \ldots, z_N) \), and defined the mean-field velocity field as

\[ U_{\text{MF}}^\alpha(x) = \int dz' F_1(z', t) u_\gamma^\alpha(x; z'). \]  

(5.1.14)

At last, the r.h.s. of Eq. (5.1.12) is given in terms of

\[ S_{i,j}^F = F_1(z_j, t)\left\{ \nabla_i^\alpha [F_1(z_i, t) u_\gamma^\alpha(x_i; z_j)] \right. \]

\[ + \Phi^{\alpha\beta} \frac{\partial}{\partial p_i^\gamma} [F_1(z_i, t) p_i^\gamma \mathcal{X}_i^{\alpha\mu\nu\gamma} \nabla^\mu u_\gamma^\beta(x_i; z_j)] \right\}, \]  

(5.1.15)

\[ S_{i,j}^G = \nabla_i^\alpha [G(z_i, z_j, t) u_\gamma^\alpha(x_i; z_j)] \]

\[ + \Phi^{\alpha\beta} \frac{\partial}{\partial p_i^\gamma} [G(z_i, z_j, t) p_i^\gamma \mathcal{X}_i^{\alpha\mu\nu\gamma} \nabla^\mu u_\gamma^\beta(x_i; z_j)], \]  

(5.1.16)

\[ S_{i,j}^H = N \int dz' \left\{ \nabla_i^\alpha [H(z_i, z_j, z', t) u_\gamma^\alpha(x_i; z')] \right. \]

\[ + \Phi^{\alpha\beta} \frac{\partial}{\partial p_i^\gamma} [H(z_i, z_j, z', t) p_i^\gamma \mathcal{X}_i^{\alpha\mu\nu\gamma} \nabla^\mu u_\gamma^\beta(x_i; z') \right\}. \]  

(5.1.17)

Eqs. (5.1.11) and (5.1.12) are the beginning of a BBGKY hierarchy of equations for partial distribution functions [115]. As such, they do not form a closed system as they also depend on the three-particle irreducible distribution function \( H \). The BBGKY equations have been extensively studied before [115, 130], and they form one of the main tools of analysing statistical properties of many-body systems. Here, we develop a similar technique for a collection of microswimmers with long-range hydrodynamic interactions. The assumptions we make below are based upon the previous literature on BBGKY equations in systems with long-range interactions [131–135], such as plasmas and self-gravitating matter.

Before discussing our choice of closure for this system of equations, let us briefly recall the predictions of the mean-field approximation to Eqs.(5.1.11) and (5.1.12), which consists of neglecting all correlation functions beyond \( s = 1 \). The remaining equation determines the mean-field approximation to the one-particle correlation function

\[ \partial_t F_1^{\text{MF}}(z, t) + \mathcal{L}[F_1^{\text{MF}}(z, t)](z) = 0, \]

(5.1.18)

which is exactly Eq. (2.2.2), analyzed in the previous chapters. One of the solutions of this equation is given by a constant, which is fixed to \( F_1^{\text{MF}}(z, t) = 1/(4\pi V) \) by the normalisation condition Eq.(5.1.1). This solution, which is valid at any number density, corresponds to a homogeneous and isotropic suspension of microswimmers. For pushers \((\kappa > 0)\), this state loses its stability [44, 45, 72–74] at the critical number density of microswimmers \( n_c = 5\lambda/(B\kappa) \), while for pullers \((\kappa < 0)\), the homogeneous and isotropic state is always linearly stable within the mean-field approximation.
The homogeneous and isotropic mean-field solution implies that \( NF_1^{MF} \sim n \sim \mathcal{O}(1) \) is finite in the thermodynamic limit. As it is shown in the Appendix D.1, rescaling the spatial and temporal scales leads to the observation that higher order correlations are of order, \( G \sim \mathcal{O}(N^{-2}) \), \( H \sim \mathcal{O}(N^{-3}) \), etc. Building upon these results, here we assume that upon approaching the thermodynamic limit, \( F_1^{MF} \) is well-approximated by \( F_1 \), since the r.h.s. of Eq.(5.1.11) is \( \mathcal{O}(1/N) \) compared to its l.h.s. In the homogeneous and isotropic state, the mean-field velocity vanishes \( U_\alpha^{MF}(x) = 0 \), since the integral in Eq.(5.1.14) is then proportional to the total flow rate through a surface surrounding the dipole, and the latter is zero due to incompressibility. Fluctuations around the homogeneous and isotropic state are then governed by Eq.(5.1.12) with \( F_1 = 1/(4\pi V) \). In the thermodynamic limit, \( S_{ij}^G \) and \( S_{ij}^H \) are small compared to \( S_{ij}^F \), and will thus be neglected. Effectively, this weak-coupling approximation \([132,133]\) ignores the three-point irreducible correlations \( H \) (and hence all higher order terms as well). The resulting equation reads

\[
\partial_t G(z_1, z_2, t) + \mathcal{L}_{12}[G] + \mathcal{L}_{21}[G] = \frac{3B}{(4\pi V)^2} \left\{ p_i^\mu p_j^\nu \nabla_\mu u_\nu^i(x_1; z_2) + p_i^\mu p_j^\nu \nabla_\mu u_\nu^j(x_2; z_1) \right\},
\]

(5.1.19)

where

\[
\mathcal{L}_{ij}[G] = v_s p_i^\mu \nabla_\mu G(z_1, z_2, t) - \frac{3nB}{4\pi} p_i^\mu p_j^\nu \int dz' G(z_j, z', t) \nabla_\mu u_\nu^i(x_i; z') + \lambda G(z_1, z_2, t) - \frac{\lambda}{4\pi} \int dp_i G(z_1, z_2, t).
\]

(5.1.20)

This equation has a transparent physical interpretation. First, correlations between two particles are generated by their mutual re-orientation, as encoded in the r.h.s of Eq.(5.1.19). Next, correlations are changed by each particle’s self-propulsion and tumbling, represented by the first, and third and fourth terms in Eq.(5.1.20), respectively. Finally, each particle in the pair is re-oriented by the velocity field created by all other particles that are correlated with the second particle in the pair. Effectively, this term renormalises the strength of the forcing on the r.h.s. of Eq.(5.1.19), and is reminiscent of the renormalisation techniques developed in sedimentation \([136,137]\). Remarkably, owing to the fact that \( U_\alpha^{MF}(x) = 0 \), Eq.(5.1.19) does not contain the effect of mutual advection by microswimmers underscoring the purely orientational origin of their correlations.

Eq.(5.1.19) has previously been derived and analysed for the case of shakers \( (v_s = 0) \) \([44]\). We will now proceed to solve it in the general case \( v_s > 0 \).

### 5.2 Phase space density fluctuations

While the two-point distribution function \( G \), given by Eq.(5.1.19), contains statistical information about fluctuations in the system, it is not straightforward to relate it to the spatial and temporal correlation function \( C(R, T) \), Eq.(5.1.7), that we seek to calculate. To establish this connection, we introduce a method based on the phase space density

\[
\varphi(z, t) = \sum_{i=1}^N \delta(z - z_i(t)),
\]

(5.2.1)
pioneered by Klimontovich [128]. Here, $\delta(z)$ is the three-dimensional Dirac delta function. The average of the phase space density is related to $F_1$ as can be seen from

$$\overline{\varphi}(z, t) = \int dz_1 \ldots dz_N \sum_{i=1}^{N} \delta(z - z_i) F_N(z_1, \ldots, z_N, t)$$

$$= NF_1(z, t), \quad (5.2.2)$$

where we used Eq.(5.1.8). Fluctuations of the phase space density can formally be defined as $\delta \varphi = \varphi - \overline{\varphi}$, and their second moment is given by

$$G_K(z', z'', t) \equiv \overline{\delta \varphi(z', t) \delta \varphi(z'', t)}$$

$$= N^2 G(z', z'', t) + NF_1(z', t) \delta(z' - z''). \quad (5.2.3)$$

Below, we refer to $G_K$ as the Klimontovich correlation function. Its utility is evident if one considers the spatial correlation function $C(R)$, defined in Eq.(5.1.7) as

$$C(R) = \lim_{t \to \infty} \frac{1}{V} \int dx U_\alpha(x, t) U_\alpha(x + R, t). \quad (5.2.4)$$

The velocity of the fluid at a position $x$ is given by the superposition of the velocity fields generated by all swimmers

$$U_\alpha(x, t) = \sum_{i=1}^{N} u_\alpha^i(x; z_i(t)) = \int dz' \varphi(z', t) u_\alpha^i(x; z'). \quad (5.2.5)$$

Separating the phase space density into its average and fluctuations, $\varphi = \overline{\varphi} + \delta \varphi$, the spatial correlation function (5.1.7) becomes

$$C(R) = \lim_{t \to \infty} \frac{1}{V} \int dx \int dz' dz'' u_\alpha^i(x; z') u_\alpha^j(x + R; z'') \times$$

$$\times \left[ F(z'; t) F(z''; t) + G_K(z', z'', t) \right]. \quad (5.2.6)$$

All derivations done up to this point are valid for any distributions $F_1$, and $G$. In this project, however, we are only interested in the fluctuations about the homogeneous and isotropic distribution. Hence, we set $F_1(z; t) = 1/(4\pi V)$, in which case the first integral in (5.2.6) vanishes, demonstrating that $G_K$ fully determines the spatial correlation function.

Time evolution of the Klimontovich correlation function can readily be derived from Eqs. (5.1.19) and (5.2.3), yielding

$$\partial_t G_K(z_1, z_2, t) + \mathcal{L}_{12}[G_K] + \mathcal{L}_{21}[G_K] = 2\lambda \frac{n}{4\pi} \delta(x_1 - x_2) \left[ \delta(p_1 - p_2) - \frac{1}{4\pi} \right], \quad (5.2.7)$$

where $\mathcal{L}_{ij}$ is defined in Eq. (5.1.20). To solve Eq. (5.2.7), we introduce an auxiliary field $h(z_1, t)$, that satisfies the following equation

$$\partial_t h(z_1, t) + \mathcal{L}_{11}[h] = \chi(z_1, t), \quad (5.2.8)$$

where $\chi$ is a noise term with the following properties

$$\langle \chi(z_1, t) \rangle = 0, \quad (5.2.9)$$

$$\langle \chi(z_1, t) \chi(z_2, t') \rangle = 2\lambda \frac{n}{4\pi} \delta(t - t') \delta(x_1 - x_2) \left[ \delta(p_1 - p_2) - \frac{1}{4\pi} \right]. \quad (5.2.10)$$
Here, the angular brackets denote the average over the realisations of the noise $\chi$, and should not be confused with the ensemble averages that we denoted by bars in the equations above. Eq. (5.2.8) allows us to factorise the Klimontovich correlation function as

$$G_K(z_1, z_2, t) = \langle h(z_1, t) h(z_2, t) \rangle,$$

which replaces the deterministic Eq. (5.2.7) by a significantly simpler stochastic Eq. (5.2.8) with a fictitious noise $\chi$ with properly chosen spectral properties. Remarkably, the non-equal time correlations of the phase space density can be expressed through the same auxiliary field

$$\delta\varphi(z', t') \delta\varphi(z'', t'') = \langle h(z', t') h(z'', t'') \rangle,$$

as implied by a seminal work of Klimontovich and Silin [138]. This, finally, leads to a direct relationship between the field $h$, which encodes the statistical properties of fluctuations in the suspension, and the combined correlation function

$$C(R, T) = \lim_{t \to \infty} \frac{1}{V} \int dx \int dz' dz'' u^\alpha_d(x; z') u^\alpha_d(x + R; z'') \langle h(z', t) h(z'', t + T) \rangle.$$

### 5.2.1 Dynamics of the auxiliary field $h$

We first start by solving the Langevin equation (5.2.8), for the auxiliary field $h$. Performing the Fourier (A.1.1) and Laplace transforms (A.1.9), we obtain after re-arranging

$$\hat{h}(k, p, s) = \frac{1}{\sigma(k, p, s)} \left[ \hat{h}_0(k, p) + \hat{\chi}(k, p, s) + \frac{\lambda}{4\pi} I^{(0)}(k, s) \right],$$

$$+ \frac{15\lambda}{4\pi} \Delta A(k\epsilon) \left\{ (k \cdot p) I^{(1)}(k, p, s) - (k \cdot p)^2 I^{(2)}(k, s) \right\}. \quad (5.2.14)$$

Here, $\hat{\chi}(k, p, s)$ is the Fourier-Laplace transform of the noise, $\sigma(k, p, s) = s + \lambda + i v_s(k \cdot p)$, and we defined

$$I^{(0)}(k, s) = \int dp \hat{h}(k, p, s),$$

$$I^{(1)}(k, p, s) = \int dp' (k \cdot p') (p \cdot p') \hat{h}(k, p', s),$$

$$I^{(2)}(k, s) = \int dp (k \cdot p)^2 \hat{h}(k, p, s).$$

In Eq. (5.2.14), $\hat{h}(k, p, t = 0) = \hat{h}_0(k, p)$ denotes some arbitrary initial condition; below we demonstrate that the long-time statistical properties of the suspension are insensitive to $\hat{h}_0(k, p)$. In Eq. (5.2.14), we have also introduced an important dimensionless parameter $\Delta = n/n_{\text{crit}}$, where $n_{\text{crit}} = 5\lambda / (B\kappa)$ is the mean-field onset of collective motion in pusher suspensions, $\kappa > 0$. For pushers, $\Delta$ measures the dimensionless distance from the onset, with $\Delta = 1$ corresponding to the instability.
Eq. (5.2.14) is a linear integral equation for \( \hat{h}(k, p, s) \) and its solution is straightforward. Substituting Eq. (5.2.14) into Eqs. (5.2.15)-(5.2.17), gives

\[
I^{(0)}(k, s) = \frac{1}{1 - \frac{\lambda}{4\pi}} \int dp \frac{\hat{h}_0(k, p) + \hat{\chi}(k, p, s)}{\sigma(k, p, s)},
\]

\[
I^{(2)}(k, s) = \frac{\lambda}{4\pi} f_1 I^{(0)}(k, s) + \int dp (\hat{k} \cdot p)^2 \frac{\hat{h}_0(k, p) + \hat{\chi}(k, p, s)}{\sigma(k, p, s)},
\]

\[
I^{(1)}(k, p, s) = \frac{1}{1 + \frac{15\lambda}{8\pi} \Delta A(k\epsilon)(f_2 - f_1)} \left[ \int dp' (\hat{k} \cdot p')(p \cdot p') \frac{\hat{h}_0(k, p') + \hat{\chi}(k, p', s)}{\sigma(k, p', s)} + (\hat{k} \cdot p) \left\{ \frac{\lambda}{4\pi} f_1 I^{(0)}(k, s) + \frac{15\lambda}{8\pi} \Delta A(k\epsilon)(f_2 - f_1) I^{(2)}(k, s) \right\} \right],
\]

where

\[
f_n = 2\pi \int_{-1}^{1} dx \frac{x^{2n}}{s + \lambda + iv_kx}.
\]

Having found the explicit expression for \( \hat{h}(k, p, s) \), we proceed to calculate the combined correlation function, Eq. (5.2.13). Below, we show that only a small number of terms from Eqs. (5.2.14) and (5.2.18)-(5.2.20) contribute to \( C(R, T) \).

### 5.2.2 \( C(R, T) \) in terms of \( \hat{h}(k, p, s) \)

In what follows, it will be convenient to re-write \( C(R, T) \) in terms of the Fourier and Laplace transforms of all quantities. Using the Fourier representation of the regularised dipolar field (A.3.11), the correlation function becomes

\[
C(R, T) = \lim_{t \to \infty} \mathcal{L}_{s_1,1}^{-1} \mathcal{L}_{s_2,t+T}^{-1} \frac{k^2}{(2\pi)^3} \int dk e^{-ik \cdot R} A^2(k\epsilon) \frac{1}{k^2} \int dp_1 dp_2 (\hat{k} \cdot p_1)(\hat{k} \cdot p_2)
\times \langle (\hat{\chi}(k, p_1, s_1) \hat{\chi}(k, p_2, s_2) ) \rangle \hat{h}(k, p_1, s_1) \hat{h}(-k, p_2, s_2),
\]

where \( \mathcal{L}_{s,t}^{-1} \) formally denotes the inverse Laplace transform from \( s \) to \( t \), given by the Bromwich integral [139]. The angular brackets \( \langle \ldots \rangle \) denote the average with the Fourier-Laplace components of the noise \( \chi \), with the following spectral properties

\[
\langle \hat{\chi}(k, p, s) \rangle = 0,
\]

\[
\langle \hat{\chi}(k, p_1, s_1) \hat{\chi}(k, p_2, s_2) \rangle = 2\lambda V \frac{n}{4\pi} \frac{1}{s_1 + s_2} \left[ \delta(p_1 - p_2) - \frac{1}{4\pi} \right],
\]

obtained by applying the Fourier-Laplace transform to Eqs. (5.2.9) and (5.2.10). While the average in Eq. (5.2.22) can readily be formed using the solution for \( \hat{h} \) found in Section 5.2.2, the result is very cumbersome. Before proceeding, we make two observations that greatly reduce the number of terms contributing to Eq. (5.2.22).

First, we observe that

\[
(\delta^{\alpha\beta} - \hat{k}^\alpha \hat{k}^\beta) \int dp p^\beta f(\hat{k} \cdot p) = 0,
\]
where \( f \) is an arbitrary function of \( \mathbf{k} \cdot \mathbf{p} \). This statement is true as the latter integral must be proportional to \( \hat{k}^\beta \). This result has profound implications for the average \( \langle h(\mathbf{k}, \mathbf{p}_1, s_1) h(-\mathbf{k}, \mathbf{p}_2, s_2) \rangle \) in Eq.(5.2.22). Every term in \( \hat{h}(\mathbf{k}, \mathbf{p}_1, s_1) \), Eq.(5.2.14), that only depends on \( \mathbf{p}_1 \), through its dependence on \( (\mathbf{k} \cdot \mathbf{p}_1) \) does not contribute to \( C(R, T) \), as its integral over \( \mathbf{p}_1 \) with the corresponding dipolar field in Eq.(5.2.22) vanishes. The same applies to \( \hat{h}(-\mathbf{k}, \mathbf{p}_2, s_2) \).

The second observation is related to the initial condition. All terms that involve \( \hat{h}_0(\mathbf{k}, \mathbf{p}) \) only depend on the Laplace frequency \( s \) through \( 1/\sigma(\mathbf{k}, \mathbf{p}, s) \), and their inverse Laplace transform can be readily performed before any other integration. Since the inverse Laplace transform of \( 1/(s + a) \) is \( e^{-at} \), where \( a \) is a complex number, the dominant long-time behaviour of such terms is given by \( e^{-M} \), where we ignored the subdominant oscillatory dependencies. In Eq.(5.2.22), we are interested in the \( t \to \infty \), and these terms also do not contribute to \( C(R, T) \).

With these observations in mind, Eq.(5.2.14) can be significantly simplified to read

\[
\hat{h}(\mathbf{k}, \mathbf{p}, s) \cong \frac{\hat{\chi}(\mathbf{k}, \mathbf{p}, s)}{\sigma(\mathbf{k}, \mathbf{p}, s)} + \frac{(\mathbf{k} \cdot \mathbf{p})}{\sigma(\mathbf{k}, \mathbf{p}, s)} \frac{\frac{15\lambda}{2\pi}\Delta A(k\epsilon)}{1 + \frac{15\lambda}{2\pi}\Delta A(k\epsilon)(f_2 - f_1)} \times \int dp'(\mathbf{k} \cdot \mathbf{p}') (\mathbf{p} \cdot \mathbf{p}') \frac{\hat{\chi}(\mathbf{k}, \mathbf{p}', s)}{\sigma(\mathbf{k}, \mathbf{p}', s)},
\]

(5.2.26)

where \( \cong \) signifies that we only kept the terms that contribute to \( C(R, T) \). Now, the average \( \langle \hat{h}(\mathbf{k}, \mathbf{p}_1, s_1) h(-\mathbf{k}, \mathbf{p}_2, s_2) \rangle \) assumes a tractable form that can be used in Eq.(5.2.22). Separating the terms independent of \( \Delta \), we obtain

\[
C(R, T) = C_0(R, T) + C_1(R, T)
\]

(5.2.27)

Here,

\[
C_0(R, T) = \frac{\lambda n \kappa^2}{16\pi^4} \lim_{t \to \infty} L_{s_1}^{-1} L_{s_2}^{-1} \int d\mathbf{k} e^{-ik \cdot R} \int \frac{A^2(k\epsilon)}{k^2} \int dp(\mathbf{k} \cdot \mathbf{p})^2 \left[ 1 - (\mathbf{k} \cdot \mathbf{p})^2 \right]
\]

\[
\times \frac{1}{s_1 + s_2} \frac{1}{\lambda + s_1 + iv_s k(\mathbf{k} \cdot \mathbf{p})} \frac{1}{\lambda + s_2 - iv_s k(\mathbf{k} \cdot \mathbf{p})},
\]

(5.2.28)

represents correlations in the fluid created by non-interacting swimmers. All other terms in Eq.(5.2.22) correspond to additional correlations generated by the hydrodynamic interactions among the swimmers, and, as such, they are dependent on the dimensionless microswimmer density \( \Delta \). Performing the angular integration over \( \mathbf{p}_1 \) and \( \mathbf{p}_2 \), gives

\[
C_1(R, T) = \frac{2\lambda n \kappa^2}{15\pi^2} \lim_{t \to \infty} L_{s_1}^{-1} L_{s_2}^{-1} \int_0^\infty \frac{dk}{k R} \frac{A^2(k\epsilon)}{k^2} \frac{1}{\lambda + s_1} \frac{1}{\lambda + s_2} \frac{1}{s_1 + s_2} \times
\]

\[
\times \frac{z_1 \psi(z_1) + z_2 \psi(z_2)}{z_1 + z_2} \left[ \frac{z_1 \psi(z_1)}{\omega - z_1 \psi(z_1)} + \frac{z_2 \psi(z_2)}{\omega - z_2 \psi(z_2)} \right.
\]

\[
+ \frac{z_1 z_2 \psi(z_1) \psi(z_2)}{(\omega - z_1 \psi(z_1)) (\omega - z_2 \psi(z_2))} \right].
\]

(5.2.29)

Here, we introduced \( \omega = v_s k/((\lambda \Delta A(k\epsilon)) \), and the function \( \psi(z) \), defined as

\[
\psi(z) = \frac{5}{2} 3z + 2z^3 - 3(1 + z^2) \arctan z
\]

(5.2.30)
which is related to $f_2 - f_1$ used in the previous Section. The variable $z_i = v_s k / (\lambda + s_i)$ allows us to write Eq. (5.2.29) in a compact form but hides its complex dependence on the Laplace frequencies $s_1$ and $s_2$.

### 5.3 Observables

The explicit calculation of the correlation function (5.2.27) involving inverse Laplace transformations in (5.2.28), and (5.2.29) is rather lengthy, and can be found in the Appendix D.2. The final expression composes of two terms – the non-interacting part

$$C_0(\rho, \tau) = \frac{nk^2 e^{-\tau}}{\pi^2 \epsilon} \int_0^\infty d\xi \frac{\sin \xi \rho}{\xi \rho} A^2(\xi) \frac{y(12 - y^2) \cos y - (12 - 5y^2) \sin y}{y^5} \bigg|_{y=L\xi\tau}, \quad (5.3.1)$$

and the interacting part

$$C_1(\rho, \tau) = e^{-\tau} \frac{nk^2}{15\pi^2 \epsilon} \int_0^\infty d\xi \frac{\sin \xi \rho}{\xi \rho} A^2(\xi) \left[- \cos \left(\sqrt{\frac{3}{7}} L\xi\tau\right) + \frac{e^{\frac{1}{2} A(\xi) \Delta \tau}}{1 - A(\xi) \Delta + \frac{6}{7} L^2 \xi^2} \cosh \left(\frac{1}{2} A(\xi) \Delta \tau \sqrt{1 - \frac{12 L^2 \xi^2}{7 A^2(\xi) \Delta^2}}\right) \right] \right], \quad (5.3.2)$$

Here, $\rho = R/\epsilon$, where $\epsilon$ is a lengthscale comparable to the microswimmer size, and $\tau = \lambda T$, where $\lambda$ is the tumbling rate. The relative distance to the instability threshold is measured by $\Delta = n/n_c$, which is the dimensionless number density of the particles, where $n_c = 5\lambda/(B\kappa)$ is the microswimmer number density at the onset of collective motion for pusher-like microswimmers [44, 73, 74]; the parameter $B$ is defined after Eq. (5.1.4). Our theory is valid for $\Delta < 1$.

A central role in our theory is played by the dimensionless persistence length $L = v_s / (\lambda \epsilon)$ that compares the typical distance covered by a swimming microorganism between two tumble events to the dipolar regularisation lengthscale $\epsilon$. As we will see below, the observables we consider here depend strongly on $L$ and it is therefore important to estimate its realistic values. For wild-type $E. coli$ bacteria, the swimming speed is strain-dependent, and we use $v_s \sim 20 - 25 \mu\text{m/s}$ as a representative value [38, 140], while for the tumbling rate we use $\lambda \sim 1 \text{s}^{-1}$ [36]. The parameter $\epsilon$, which is introduced in Eq. (5.1.6), regularises our theory at the length-scale below which the dipolar velocity field does not approximate sufficiently well the full velocity field created by a single bacterium. Since the hydrodynamic dipole (2.1.4) consists of two point forces, one can naively identify $\epsilon$ with half the body length of $E. coli$, leading to $\epsilon \sim 1 \mu\text{m}$. A more hydrodynamically sound approach is to interpret $\epsilon$ as the length of the effective hydrodynamic dipole generated by a bacterium. Drescher et al. [38] have measured the velocity field of swimming $E. coli$ bacteria far away from boundaries and concluded that it is well-represented by a pair of equal and opposite forces applied to the fluid at a distance of 1.9 $\mu\text{m}$ apart. Identifying the cut-off distance with half of the dipolar length again gives $\epsilon \sim 1 \mu\text{m}$. In this work, we consider $L = 0 - 25$; we hypothesise that this range is relevant for the wild-type $E. coli$.  

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Furthermore, using the same hydrodynamic interpretation of $\epsilon$ as above, the $L = 5$ case approximately corresponds to the simulations of Stenhammar et al. [44], while the $L = 0$ case describes non-swimming bacteria (shakers). Ultimately, the values of $L$ suitable for a particular microorganism will have to be determined experimentally, as we discuss in the Conclusion 5.4. Finally, we observe that the typical values of $L$ are higher yet for non-tumbling bacteria, where the role of the main orientation decorrelation mechanism is played by the (effective) rotational diffusion.

The full expression, $C(\rho, \tau) = C_0(\rho, \tau) + C_1(\rho, \tau)$, given as a definite integral, constitutes the main technical result of our study. We now explicitly work out its predictions for the spatial and temporal correlation functions, and other experimentally accessible observables. When discussing their physical meaning, we are going to vary the dimensionless persistence length $L$, while keeping all the other parameters of the microswimmers fixed. We note that in reality the dipolar strength and shape of a microorganism uniquely determine its swimming speed, and hence $L$. We, however, see varying $L$ as a tool to disentangle the effects of self-propulsion (ability to change one’s position in space) from the strength of the hydrodynamic disturbances it causes. In particular, we will consider two limiting cases: shakers ($L = 0$) and fast swimmers ($L \to \infty$). The former case corresponds to microswimmers that exert dipolar forces on the fluid but do not self-propel, and only change their positions due to being advected by the velocity fields created by other microswimmers [44]. The latter case, while obviously non-physical, is a useful tool to assess the effect of fast swimming on various quantities of interest. When studying the behaviour of the observables listed above in the vicinity of the transition to collective motion, we will fix the value of $L$, so that fast swimming should be understood as large yet finite $L$, and consider the limit $\Delta \to 1$. We will not consider the opposite order of the limits, as the limit $L \to \infty$ corresponds to a rather unphysical scenario of infinitely fast swimmers. Finally, we note that the terms representing hydrodynamic interactions in Eq.(5.2.7) are proportional to the swimmer’s nonsphericity $B$ that enters Jeffrey equation, Eq.(5.1.4). The limit of non-interacting microswimmers therefore corresponds to setting $B$ to zero, which, in turn, can be achieved by setting $\Delta = 0$, while keeping $n$ finite.

### 5.3.1 Velocity variance

The first quantity of interest is the fluid velocity variance, $\langle U^2 \rangle \equiv C(\rho = 0, \tau = 0)$. In the absence of thermal noise, re-arrangements of the microswimmer positions and orientations is the sole source of fluid velocity fluctuations. For this reason, it was used in previous studies as an order parameter to identify the onset of collective motion [44,68]. Summing up Eqs.(5.3.1) and (D.2.11), and setting $\rho = 0$ and $\tau = 0$, we obtain

$$
\langle U^2 \rangle = \kappa^2 n \int_0^\infty d\xi A^2(\xi) \frac{2 - A(\xi)\Delta + 6 L^2 \xi^2}{(2 - A(\xi)\Delta)(1 - A(\xi)\Delta + \frac{3}{4} L^2 \xi^2)}. \tag{5.3.3}
$$

We evaluate this integral numerically and plot the fluid velocity variance normalised by its value in the non-interacting case, $\langle U^2 \rangle(\Delta = 0) \equiv \langle U^2 \rangle_0$, given by [68]

$$
\langle U^2 \rangle_0 = \frac{\kappa^2 n}{15\pi^2 \epsilon} \int_0^\infty d\xi A^2(\xi) = \frac{21\kappa^2 n}{2048\epsilon}. \tag{5.3.4}
$$

Note that $\langle U^2 \rangle_0$ corresponds to a superposition of uncorrelated fluctuations in the fluid velocity, which, by virtue of the central limit theorem, is proportional to $n$. Any deviations
of $\langle U^2 \rangle$ from that value signify the presence of correlations.

As can be seen in Fig. 5.2, the fluid velocity fluctuations exhibit significant correlations at any density of the microswimmers, as was recognised previously [44]. Starting from its non-interacting value at $\Delta = 0$, the variance increases with $\Delta$, until it diverges at the onset of collective motion. The strongest correlations are exhibited by suspensions of shakers, while swimming acts to reduce correlations. For large but finite values of $L$, the variance increases mildly from its non-interacting value, until it rises sharply in a small vicinity of $\Delta = 1$, with the size of this region shrinking with $L$. Interestingly, the rise of $\langle U^2 \rangle_0$ for $\Delta < 1$ remains finite even in the $L \to \infty$ limit. In other words, while swimming clearly reduces correlations, it does not remove them entirely, and the suspension is never described by the mean-field theory.

To determine the scaling of the fluid velocity variance as $\Delta \to 1^-$, we observe that in that limit the integrand in Eq. (5.3.3) is dominated by small values of $\xi$, where $A(\xi) \approx 1 - \xi^2/4$. Using this approximation in Eq. (5.3.3) and replacing the upper integration limit by unity, we obtain

$$\langle U^2 \rangle \sim \frac{\kappa^2 n}{15\pi \epsilon} \frac{1}{\sqrt{1 + \frac{12}{7} L^2 \sqrt{1 - \Delta}}}, \quad \Delta \to 1^-.$$  (5.3.5)

Therefore, our theory predicts that the fluid velocity variance diverges as $(1 - \Delta)^{-1/2}$ in the vicinity of the transition to collective motion, for any finite value of $L$.

### 5.3.2 Spatial correlations

Our next quantity of interest is the equal-time spatial correlation function, $C(\rho, T = 0)$, given by

$$C(\rho) = \frac{\kappa^2 n}{15\pi^2 \epsilon} \int_0^\infty d\xi \frac{\sin \xi \rho}{\xi \rho} A^2(\xi) \frac{2 - A(\xi) \Delta + \frac{6}{7} L^2 \xi^2}{(2 - A(\xi) \Delta)(1 - A(\xi) \Delta + \frac{3}{7} L^2 \xi^2)}. \quad (5.3.6)$$

Figure 5.2: The fluid velocity variance $\langle U^2 \rangle$ normalised by its non-interacting value $\langle U^2 \rangle_0$ for various values of $L$. The dotted line represents the non-interacting case $\langle U^2 \rangle = \langle U^2 \rangle_0$. Note that the $L \to \infty$ line turns sharply upwards and diverges in the vicinity of $\Delta = 1$ in a way that cannot be resolved on the scale of this graph.
Figure 5.3: The spatial correlation function $C(\rho)$ as a function of the distance $\rho$ for various values of $\Delta$. A: $L = 0$, B: $L = 5$, and C: $L = 25$. The solid lines are calculated by numerically evaluating Eq.(5.3.6), while the dashed lines are the analytic approximation, Eq.(5.3.7). The legend applies to all panels.

While this integral cannot be evaluated analytically, a good approximation can be obtained by setting $A(\xi) = 1$ in the integrand, yielding

$$C(\rho) \approx \frac{\kappa^2 n}{30\pi\epsilon (1 - \Delta)} \rho \left[ 1 - \frac{\Delta}{2 - \Delta} \exp \left\{ -\sqrt{\frac{7}{3}} \sqrt{1 - \Delta} \frac{\rho}{L} \right\} \right]. \quad (5.3.7)$$

For $\Delta = 0$, this equation reproduces the result obtained previously for non-interacting swimmers [68,85,141,142].

In Fig.5.3 we evaluate Eq.(5.3.6) numerically and compare it against the analytic approximation, Eq.(5.3.7); $\kappa^2 n_c/(15\pi^2\epsilon)$ is chosen as the normalisation factor. For all values of $L$ and $\Delta$, the approximation works well for all but small spatial separations $\rho$, where the spatial correlation function is, essentially, equal to the fluid velocity variance. As with the fluid velocity variance, the strongest correlations are exhibited by suspensions of shakers, $L = 0$. In this case, the spatial correlation function changes very slowly at short distances, and decays as $\rho^{-1}$ at large distances. Close to the onset of collective motion, the typical scale $\rho_0$ at which the crossover occurs can be estimated from Eqs.(5.3.5) and (5.3.7), by requiring that $C(\rho_0) = \langle U^2 \rangle$. For $L = 0$, this yields $\rho_0 \sim (1 - \Delta)^{-1/2}$. This is readily verified by the data in Fig.5.3A: As the system approaches the onset of collective motion, the overall strength of the correlations grows, with the region of strong correlations extending to progressively larger scales.

The effect of swimming on the behaviour of $C(\rho)$ is demonstrated in Figs.5.3B-5.3C. As $L$ increases, the strongly correlated core at moderate separations shrinks, indicating that the steady growth of orientational correlations is reduced by the mixing introduced by swimming. The overall strength of correlations inside the core also decreases with $L$, reflecting the reduction of the fluid velocity variance by swimming. At large distances, $C(\rho)$ recovers the behaviour seen in shakers, with the crossover distance given by $\rho_1 \sim L(1 - \Delta)^{-1/2}$, as can be deduced from the exponential in Eq.(5.3.7). This behaviour is further demonstrated in Fig.5.4, where we plot $C(\rho)$ for $\Delta = 0.9$ and various values of $L$. In the limit of fast swimming, $L \to \infty$, the correlation function deviates modestly
Figure 5.4: The spatial correlation function $C(\rho)$ as a function of the distance $\rho$ for $\Delta = 0.9$ and various values of $L$. At sufficiently large distances, $C(\rho)$ recovers the shaker behaviour, while at small distances correlations are suppressed by swimming. Note that the $L \to \infty$ line, serving as the limit beyond which correlations cannot be suppressed, joins the shaker line at $\rho \to \infty$.

from the non-interacting case for almost all values of $\Delta$, exhibiting a quick rise and the divergence associated with the onset of collective motion only in a very small vicinity of $\Delta = 1$.

The data in Fig.5.3 and Eq.(5.3.7) demonstrate that $C(\rho)$ exhibits an algebraic decay for large distances, and a true correlation length can thus not be defined. A phenomenological correlation length $\eta_{\text{corr}}$ can nevertheless be defined as a distance over which $C(\rho)$ decreases by certain amount, as has been employed in [48,68]. Setting $C(\eta_{\text{corr}}) = \alpha \langle U^2 \rangle$, with $\alpha < 1$, we obtain

$$\eta_{\text{corr}} \sim (1 - \Delta)^{-1/2}, \quad \Delta \to 1^-,$$

(5.3.8)

similar to any other typical distance discussed above.

5.3.3 Fluid velocity spectrum

Next, we discuss the fluid velocity energy spectrum $E(k)$ that is closely related to the spatial correlation function $C(\rho)$. Defined as

$$E(k) = 4\pi k^2 \hat{U}^\alpha(k) \hat{U}^{-\alpha}(-k),$$

(5.3.9)

this quantity is often used in turbulence research to study the cascade of the kinetic energy [110]. Although the kinetic energy is not a useful concept for Stokesian flows, $E(k)$ provides an insight into the relative strength of fluid motion at various scales. The energy spectrum is proportional to the Fourier transform of $C(\rho)$, and, up to a prefactor is given by the integrand of Eq.(5.3.6)

$$E(\xi) = \frac{8\pi}{15} \kappa^2 n A^2(\xi) \frac{2 - A(\xi) \Delta + \frac{6}{7} L^2 \xi^2}{(2 - A(\xi) \Delta) (1 - A(\xi) \Delta + \frac{6}{7} L^2 \xi^2)},$$

(5.3.10)

where, again, $\xi = k\epsilon$. This expression is plotted in Fig.5.5 for various values of $\Delta$ and $L$.

First, we observe that $E(\xi)$ has significant energy content at all large scales, $\xi < 1$, that quickly decays to zero at the organism-size scales, $\xi \sim 1$, due to the regularising
Figure 5.5: The fluid velocity energy spectra $E(\xi)$, Eq.(5.3.10), as a function of the dimensionless wavenumber $\xi$ for various values of $\Delta$. A: $L = 0$, B: $L = 5$, and C: $L = 25$. The legend applies to all panels.

factor $A(\xi)$. This is not caused by some form of energy cascade, but is due to the nature of the dipolar field created by the microswimmers. The dipolar velocity field decays in space as $r^{-2}$, while its Fourier transform scales as $k^{-1}$. Together with the definition of $E(k)$, Eq.(5.3.9), this implies that away from the instability point $E(k) \sim k^0$ even for a single microswimmer, i.e. the dipolar field has a constant energy content at every scale. In the presence of interactions, the energy spectrum for shakers ($L = 0$) preserves the overall structure described above, while its absolute value increases with $\Delta$ and, eventually, diverges at $\Delta = 1$. For swimmers, the increase in the energy content is mostly confined to large scales, while in the limit of fast swimming (not shown), the rise in the energy content on the approach to the onset of collective motion is confined to the largest scales available ($k \to 0$) and starts to be visible only in a very close vicinity of $\Delta = 1$.

At last, the large-scale structure of the energy spectra (5.3.10) can be easily seen from the vanishing wave-vector limit

$$E(\xi \to 0) = \frac{8\pi}{15} \kappa^2 n \frac{1}{1 - \Delta + \frac{7}{8} L^2 \xi^2}.$$  \hspace{1cm} (5.3.11)

which, as discussed above, behaves as $k^0$ for $\Delta < 1$, but as $k^{-2}$ close to the vicinity of the transition $\Delta \to 1^{-}$.

### 5.3.4 Temporal correlations

The temporal correlation function $C(\tau) = C_0(\rho = 0, \tau) + C_1(\rho = 0, \tau)$ is given by Eqs.(5.3.1) and (5.3.2). The corresponding expressions do not simplify significantly in the limit $\rho = 0$, and we do not repeat them here. In Fig.5.6 we plot $C(\tau)$ normalised by its value at $\tau = 0$, which is given by the fluid velocity variance $\langle U^2 \rangle$. As with the other quantities discussed above, the temporal correlation function exhibits a progressively slower decay as $\Delta$ approaches the onset of collective motion, eventually diverging at $\Delta = 1$. For swimmers, this is offset by a decay of $C(\tau)$ at short times that becomes more pronounced as $L$ increases. For very large swimming speeds, the temporal correlations differ only
Figure 5.6: The temporal correlation function $C(\tau)$ as a function of the dimensionless time $\tau$ for various values of $\Delta$. A: $L = 0$, B: $L = 5$, and C: $L = 25$. The solid lines are calculated by numerically evaluating Eqs.(5.3.1) and (D.2.11), while the dashed lines in B and C are the analytic approximation of the asymptotic behaviour for $\tau \to \infty$, Eq.(5.3.17). The legend applies to all panels.

marginally from the non-interacting case for most values of $\Delta$, eventually exhibiting a rapid increase and divergence in a very small vicinity of $\Delta = 1$.

To understand the behaviour of $C(\tau)$ at long times, we analyse its individual contributions. The integral in the non-interacting part, $C_0(T)$, can be explicitly evaluated giving

$$C_0(\tau) = \frac{n\kappa^2}{\pi\epsilon} \frac{e^{-\tau}}{8\alpha^4(4 + \alpha^2)^2} \left[ 4(24 + 8\alpha^2 + \alpha^4)E\left(-\frac{\alpha^2}{4}\right) 
- (4 + \alpha^2)(24 + 5\alpha^2)K\left(-\frac{\alpha^2}{4}\right) \right],$$

where $\alpha = L\tau$, and $K(x)$ and $E(x)$ are the complete elliptic integrals of the first and second order, respectively. In the limits of small and large $\alpha$ this equation predicts

$$C_0(\tau) \sim \frac{n\kappa^2}{\pi\epsilon} e^{-\tau} \times \begin{cases} \frac{21\pi}{2048}, & L\tau \to 0, \\ \frac{1}{4(L\tau)^2}, & L\tau \to \infty. \end{cases}$$

At short times, tumbling is the leading source of decorrelation, while at large $\tau$ the non-interacting temporal correlation function $C_0$ decays as $\tau^{-3}e^{-\tau}$, as reported previously [68,142]. The crossover time is set by $\alpha = L\tau = v_s t/\epsilon \sim 1$, and corresponds to the time interval needed for a microswimmer to swim its own size.

To understand the large-$\tau$ asymptotic behaviour of $C_1(\tau)$, we observe that

$$e^{-\tau} \int_0^{\infty} d\xi A(\xi)^2 \left\{ \frac{\sin \gamma \tau \xi}{\cos \gamma \tau \xi} \right\} \sim e^{-\tau} \left\{ \frac{\tau^{-1}}{\tau^{-5}} \right\},$$

where $\gamma$ is a real constant. This result implies that a trigonometric function in the integrand of Eq.(D.2.11) generates a contribution to $C_1(\tau)$ that decays on the same
timescale as the non-interacting part $C_0(\tau)$, and does not contribute to the slow decay in Fig. 5.6. In turn, this restricts the integration domain to $\xi \in [0, \xi^*]$, with

$$\xi^* = \sqrt{\frac{7}{12} \Delta L}, \quad (5.3.15)$$

which ensures that the arguments of the hyperbolic functions in Eq. (D.2.11) are real.

Introducing $\zeta = \frac{\xi}{\xi^*}$, $C_1(\tau)$ can be approximated as

$$C_1(\tau) \sim \frac{n\kappa^2}{15\pi^2 \epsilon} e^{-\tau(1 - \frac{1}{2} \Delta)} \xi^* \int_0^1 d\zeta \frac{1}{1 - \Delta + \frac{1}{2} \Delta^2 \zeta^2} \left\{ \frac{2 - \Delta + \frac{1}{2} \Delta^2 \zeta^2}{2 - \Delta} \cosh \left( \frac{1}{2} \Delta \tau \sqrt{1 - \zeta^2} \right) \right. + \left. \frac{1}{\sqrt{1 - \zeta^2}} \sinh \left( \frac{1}{2} \Delta \tau \sqrt{1 - \zeta^2} \right) \right\}, \quad (5.3.16)$$

where we used $A(\xi < \xi^*) \sim 1$ for not-too-small values of $L$. In the limit of large $\tau$, this can be further approximated by

$$C_1(\tau) \sim \frac{n\kappa^2}{15\pi^2 \epsilon} e^{-\tau(1 - \Delta)} \xi^* \int_0^1 d\zeta e^{-\frac{1}{2} \tau^2 \Delta \zeta^2} \sqrt{\tau \left( 1 - \Delta \right)} e^{-\tau(1 - \Delta)} \text{erf} \left( \frac{1}{2} \tau \Delta \right), \quad (5.3.17)$$

where $\text{erf}(x)$ denotes the error function. Predictions of Eq. (5.3.17) are plotted in Fig. 5.6B and C as dashed lines. We find a good agreement between its prediction and the true decay of $C(\tau)$ as $\tau \to \infty$.

Comparing (5.3.13), and (5.3.17), we observe that the interacting part certainly dominates over the non-interacting part, which again shows the importance of hydrodynamic interactions. To extract the typical timescale $\tau_{\text{corr}}$ of the fluid velocity fluctuations on the approach to collective motion, we combine Eqs. (5.3.5) and (5.3.17) to obtain

$$\frac{C(\tau)}{\langle U^2 \rangle} \sim \frac{e^{-\tau(1 - \Delta)}}{\sqrt{(1 - \Delta)}} \quad \Delta \to 1^-, \quad (5.3.18)$$

which implies

$$\tau_{\text{corr}} \sim (1 - \Delta)^{-1}. \quad (5.3.19)$$

### 5.3.5 Enhanced diffusivity

As the final observable, we consider here the enhanced diffusivity of a passive tracer particle embedded in a suspension of motile microorganisms. The tracer is assumed to be neutrally buoyant and move due to advection by the velocity fields created by the microswimmers. Brownian diffusion of the tracer is significantly weaker than its enhanced counterpart, and is neglected for simplicity. This problem has been extensively studied both experimentally [40, 41, 93, 96–99, 105] and theoretically [59, 94, 95, 100–104, 106, 143, 144] in the dilute regime, where $\Delta \ll 1$, and for arbitrary densities of shakers [44]. Here, we consider the case of arbitrary density $\Delta < 1$ and $L$. 

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The position of the tracer \( a(T) \) obeys the following equation of motion
\[
\dot{a}(T) = U(a(T), T), \tag{5.3.20}
\]
which implies that the tracer is point-like and follows the velocity of the fluid at its position. The long-time behaviour of such a tracer is diffusive \([40, 41, 104]\), and the associated diffusion coefficient can be extracted in the usual way
\[
D = \lim_{T \to \infty} \frac{1}{6T} \frac{\dot{a}(T) \cdot a(T)}{.} \tag{5.3.21}
\]
Here, the bar denotes the average over the history of tumble events, and has the same meaning as in Eq. (5.1.7). Solving formally Eq. (5.3.20),
\[
a(T) = a(0) + \int_0^T dt' U(a(t'), t'), \tag{5.3.22}
\]
the diffusion coefficient can be written as \([145]\)
\[
D = \frac{1}{3} \lim_{t \to \infty} \int_0^\infty dT U(a(t + T), t + T) \cdot U(a(t), t). \tag{5.3.23}
\]
Here, \( t \) is sufficiently large so that any influence of the initial conditions has died away. To proceed, we observe that \( U(a(t + T), t + T) \) can be iteratively calculated by substituting the formal solution for \( a(T) \) into its spatial argument, i.e.
\[
U(a(t + T), t + T) = U(a(t), t + T) + \nabla U(a(t), t + T) \cdot \int_t^{t+T} dt' U(a(t'), t') + \cdots. \tag{5.3.23}
\]
As was argued by Pushkin and Yeomans \([100]\), for very dilute suspensions velocity gradients over the typical distance travelled by the tracer particle during the microswimmer runtime are small compared to the velocity of the fluid at any of these positions, and can be neglected. Therefore, we can approximate the diffusion coefficient as
\[
D \approx \frac{1}{3} \int_0^\infty dT U(a(t), t + T) \cdot U(a(t), t) = \frac{1}{3} \int_0^\infty dT C(T). \tag{5.3.24}
\]
As we have seen in Section 5.3.4, as \( \Delta \) increases, the correlation time increases from \( \lambda^{-1} \) (corresponding to \( \tau_{corr} = 1 \)) in the very dilute regime to progressively larger values, eventually diverging as \( \Delta \to 1 \), implying that the second, etc. terms in Eq. (5.3.23) grow rapidly in this limit. However, the fluid velocity variance, which sets the magnitude of the leading term in Eq. (5.3.23) also diverges as \( \Delta \to 1 \). Further work is required to assess the validity of the approximation above for all values of \( \Delta \). Here, we proceed by using Eq. (5.3.24) with the potential caveat that it might not be accurate in the vicinity of \( \Delta = 1 \).

The integral in Eq. (5.3.24) can be evaluated explicitly, leading to \( D = D_0 + D_1 \), where the non-interacting and interacting contributions are given by
\[
D_0 = \frac{\kappa^2 n}{45\pi^2 \lambda c} \int_0^\infty d\xi A^2(\xi) \psi(\xi L), \tag{5.3.25}
\]
\[
D_1 = \frac{\kappa^2 n \Delta}{45\pi^2 \lambda c} \int_0^\infty d\xi A^3(\xi) \frac{2 - A(\xi) \Delta + \frac{6}{7} L^2 \xi^2}{(1 + \frac{3}{7} L^2 \xi^2)(1 - A(\xi) \Delta + \frac{3}{7} L^2 \xi^2)^2}, \tag{5.3.26}
\]
respectively, and \( \psi(x) \) is defined in Eq. (5.2.30). At this point, we would like to comment on the shaker limit of these expressions, when they should reduce to the ones obtained
by Stenhammar et al. [44]. Instead, we observe that the expression for $D_1$ reported there erroneously contained $A^2(\xi)$ instead of $A^3(\xi)$ under the integral. We note, however, that since $A(\xi)$ is a regularised representation of a step function, this has almost no bearing on the numerical evaluation of $D_1$ presented in [44].

The integral in the non-interacting part $D_0$ cannot be represented in terms of special functions, but its limiting behaviour can readily be obtained. Combining the asymptotic results for $L = 0$ and $L \to \infty$, results in the following approximation

$$D_0 \approx \frac{\kappa^2 n}{\lambda \epsilon} \frac{7}{2048 + 336\pi L}. \quad (5.3.27)$$

To derive an approximate expression for $D_1$, we set $A(\xi) \approx 1$ under the integral sign, to obtain

$$D_1 \approx \frac{\kappa^2 n}{90\pi \lambda \epsilon \sqrt{1 + \frac{12}{7} L^2}} \left\{ \frac{2 - \Delta}{(1 - \Delta)^{3/2}} - 2 \right\}. \quad (5.3.28)$$

In Fig.5.7 we compare the numerical evaluation of $D_0$ and $D_1$ against Eq.(5.3.27) and (5.3.28). We observe that while the uniform approximation Eq.(5.3.27) does not work well for small but finite values of $L \sim 1$, all other values of $L$ are well-represented by the approximation. The interacting part of the diffusivity is well-approximated by Eq.(5.3.28).

Finally, we remark that Eq.(5.3.28) predicts that

$$D_1 \sim (1 - \Delta)^{-3/2}, \quad \Delta \to 1^-, \quad (5.3.29)$$

even though this prediction should be treated with caution, as discussed above.

### 5.4 Conclusion

In this chapter, we have presented a kinetic theory for dilute suspensions of pusher-like microswimmers interacting via long-ranged dipolar fields. We have overcome a significant
technical difficulty in including particle self-propulsion into a theory that goes beyond the mean-field assumption and explicitly accounts for correlations between microswimmers. This difficulty has limited previous theoretical work on this problem to either the case of shaker microswimmers [44] or the case of swimming being subdominant compared to the translational thermal diffusion [146]. The only theory to date that has accounted for arbitrary swimming speeds was developed by Nambiar et al. [107], who analytically considered pair-wise correlations between microswimmers, i.e., their results are $O(\Delta^2)$ accurate. To deal with the problem posed by the self-propulsion term in their equations, Nambiar et al. [107] developed a perturbation theory in terms of the swimmer slenderness (aspect ratio), which is a reasonable approximation for long and slender bacteria. In contrast, the method developed in this work allows us to make explicit predictions for various experimentally relevant observables for any strength of self-propulsion and any density of microswimmers up to the onset of collective motion. All of its parameters can be independently measured or inferred from experiments, and its predictions can be directly compared against experimental data.

The results of our theory, presented in Section 5.3, reveal that all observables considered deviate from their mean-field values, which can be recovered from our results by setting $\Delta = 0$, indicating that the mean-field theory is incorrect at any density below the onset of collective motion. We have also uncovered the following interplay between the strength of correlations between microswimmers and their self-propulsion speed. For all observables considered, the strongest correlations are exhibited by suspensions of shakers, $L = 0$. This can be readily seen by observing that, in the absence of self-propulsion, the microswimmer positions only change due to their mutual advection. In dilute suspension, displacements thus accumulated over one correlation time are small compared to the interparticle distances, and, to first approximation, shaker suspensions perform orientational dynamics only. In turn, this implies that they spend maximum amount of time possible adjusting to the orientational fields created by other microswimmers. In contrast, motile microswimmers are aligning in a local velocity field that constantly changes due to their self-propulsion, implying weaker correlations in such suspensions. This effect becomes stronger as $L$ increases.

The degree to which correlations are suppressed by self-propulsion depends on the nature of the observable. Spatial-like observables (the fluid velocity variance, the energy spectrum, and the spatial correlation function) are significantly reduced as $L$ increases, but do not reach their mean-field values even in the limit $L \to \infty$. For instance, as can be seen from Fig.5.2, the fluid velocity variance is significantly larger than its mean-field value at any density $\Delta$, even in the limit of fast swimming. In a similar fashion, as $L \to \infty$, the spatial correlation function in Fig.5.4 does not reduce to its mean-field behaviour, which is given by the $\Delta \to 0$ limit in Fig.5.3. Instead, it recovers the strongly correlated shaker-like behaviour at sufficiently large distances. This can be understood by employing the same argument as above. For any value of $L$, there are such separations $\rho$ that the typical distance travelled by a microswimmer during one correlation time of the suspension is small compared to $\rho$. For such separations, the difference between swimmers and shakers vanishes and $C(\rho)$ recovers its shaker-like behaviour.

On the other hand, temporal-like observables (the temporal correlation function and the enhanced diffusivity of tracer particles) are almost completely suppressed as $L \to \infty$ for $\Delta < 1$, though they still diverge in the limit of $\Delta \to 1^-$. This behaviour mirrors the dependence of their mean-field values on $L$, which vanish in the limit of fast swimming.
below the onset of collective motion. An intuitive argument for this behaviour has been put forward by Dunkel et al. [94], who demonstrated that the total displacement of a tracer by a single motile particle vanishes as the length of a straight path covered by the swimmer diverges. This is fundamentally related to the time-reversibility of Stokesian flows. The presence of correlations between microswimmers breaks this time-reversibility: although the pathway between two states in phase space is still reversible, the probabilities of finding the suspension in those states are a priori different. Strong swimming introduces effective phase space mixing and recovers equal a priori probabilities for the phase space states. Again, this argument only holds for $\Delta < 1$ when $L$ is large, yet finite.

Previous studies have already reported measurements of the spatial [2,48] and temporal [46,50] correlation functions in dilute bacterial suspensions for a wide range of bacterial concentrations. While these observations qualitatively agree with our predictions and the results of previous simulations [63,65,68], quantitative comparison is problematic as the corresponding values of $\Delta$ in those experiments remain unknown. The enhanced diffusivity, on the other hand, has only been studied in the regime where $D$ scales linearly with the bacterial number density $n$ [93,97–99,103,105], with the highest density of Kasyap et al. [103] being the only exception. Those measurements are well-described by a non-interacting theory [99,100,102,144], i.e., $D_0$ in our analysis, and to test our theory they will need to be extended to higher concentrations. Therefore, to verify our predictions experimentally, it is necessary to measure any of these observables across a wide range of bacterial density while carefully controlling the distance to the threshold of collective motion $\Delta$. Although the latter can, in principle, be calculated from $\Delta = nB\kappa/5\lambda$, it requires the knowledge of the bacterial dipolar strength, tumble rate, and effective aspect ratio, and a precise control of the number density $n$. A significantly easier approach would be to determine $n_{crit}$ experimentally. This can be achieved, for instance, by measuring the apparent shear viscosity of bacterial suspensions at various densities, as was recently done by Martinez et al. [2]. In sufficiently wide geometries, the ratio of the apparent shear viscosity to the viscosity of the solvent decreases linearly with $\Delta$ [2,92], and vanishes precisely at the onset of collective motion [73]. Simultaneous measurement of one of the observables discussed above and the apparent shear viscosity would thus allow for a direct comparison with our theory. The remaining parameters, $\epsilon$ and $\lambda$ used to rescale space and time, respectively, and the dimensionless persistence length $L$, should be treated as fitting parameters. They can be fixed, for instance, by fitting the data for very low bacterial number densities, where the normalised correlation functions $C(\rho)/\langle U^2 \rangle$ and $C(\tau)/\langle U^2 \rangle$ are well-approximated by their non-interacting (i.e. $\Delta = 0$) components (see Eqs.(5.3.4), (5.3.6), and (5.3.13) and Refs. [68,142]). While the swimming speed $v_s$ and the tumbling rate $\lambda$ can be directly measured by either tracking individual bacteria or by differential dynamic microscopy [147], the hydrodynamic size of an $E. coli$ bacterium $\epsilon$ is somewhat open to interpretation, as discussed in Section 5.3. Therefore, $L$ should be seen as a fitting parameter.

Direct verification of our prediction that increasing $L$ suppresses correlations and brings the system closer to the mean-field predictions would require the ability to perform experiments at different values of $L$ at a fixed distance to the threshold $\Delta$. An obvious realisation of this protocol would involve the ability to control the tumbling rate $\lambda$, while keeping the swimming speed and the dipolar strength constant. We are currently not aware of a bacterial strain with such an ability. An interesting alternative would be to employ the recently created $E. coli$ mutants that only swim in the presence of
<table>
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<tr>
<th>Observable</th>
<th>Scaling law for $\Delta \to 1$</th>
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<tr>
<td>Fluid velocity variance</td>
<td>$(1 - \Delta)^{-1/2}$</td>
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<tr>
<td>(Pseudo-)correlation length</td>
<td>$(1 - \Delta)^{-1/2}$</td>
</tr>
<tr>
<td>Correlation time</td>
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<tr>
<td>Enhanced diffusivity</td>
<td>$(1 - \Delta)^{-3/2}$</td>
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Table 5.1: Critical exponents

light [148–150]. In such bacteria, the swimming speed can be increased by increasing the light intensity, while the tumbling rate seems to stay constant for upward sweeps in light intensity [150]. Performing light intensity sweeps at various bacterial densities would thus trace a set of straight lines in the $\Delta$-$L$ parameter space, since $v_s$ is expected to be proportional to the bacterial dipolar strength and, thus, to $\Delta$. Such data can then be used to of how the transition is approached at various values of $L$.

To gain further insight into the nature of the transition to collective motion exhibited by our model, we extracted the scaling behaviour of the observables considered in this work upon the approach to the onset, $\Delta = 1$. All of these quantities diverge at $\Delta = 1$ and the values of the critical exponents predicted by our theory are summarised in Table 5.1. We want to stress that these exponents rely on the approximation introduced in Section D.2.2, and while we are confident that it semi-quantitatively captures the spatial and temporal behaviour of the generalised correlation function $C(\rho, \tau)$ for $\Delta < 1$, its quality in the close vicinity of $\Delta = 1$ is untested. Moreover, the neglected non-linear fluctuations must be incorporated close to the onset using renormalization group methods. The values presented in Table 5.1 should thus be seen as result of a Gaussian approximation, which represents a first step in understanding the nature of this transition. Currently, neither the order of the mean-field transition, nor the influence of strong pre-transitional correlations on the transition are understood, and more work is needed to assess whether collective motion in dilute suspensions of hydrodynamically interacting microswimmers defines a new universality subclass of “wet” active matter models. The exponents from Table 5.1, however, could still be experimentally tested in dilute suspensions of E. coli bacteria, considered for example in [2].

In this work, we have only considered pusher-like microswimmers below the onset of collective motion. Recent simulations suggest [44,68] that suspensions of pullers also exhibit strong correlations, although their effect is opposite to what is observed for pushers. The results presented in this work cannot be used to study this effect, i.e. by replacing $\Delta$ with $-\Delta$ in the relevant expressions. Instead, to extend our theory to pullers, one would have to re-evaluate the long-term behaviour of the approximate double inverse Laplace transform in Section D.2.2 for negative values of $\Delta$.  

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Chapter 6

Summary

In this work we have developed mathematical and numerical tools to study collective motion of swimming microorganisms. Our approach is based on Kinetic theory, which treats swimmers as self-propelling ellipsoids moving through a viscous fluid, and interacting via long-range hydrodynamic interactions [45]. Due to the low Re of the system, the latter is described by Stokes equations within a sufficiently good accuracy.

Technical problems arising from the complexity of the $N$-particle system have been avoided by applying certain approximations. First, we have inspected properties at the mean-field level, where the effect of correlations stemming from the tumbling effects has been neglected. This approach allowed us to extract qualitative information about the system, such as instability conditions and general dependences of observables at the system parameters. Then, we looked at the effect of the aforementioned correlations, and show that accurate results cannot be obtained in their absence.

Behaviour at the linear level

We began our work in Chapter 3 by looking at the linear stability of the suspension within the mean-field kinetic theory. Different types of geometries were considered, as confinement is commonly present in realistic experiments [2]. Using linearised equations of motion, we derived formal solutions for density, and fluid velocity fluctuations in arbitrary geometry of the system. We then proceeded with the stability analysis in the bulk two- and three-spatial dimensions, and show that the instability conditions are qualitatively identical. In bulk systems, the orientational instability sets in only for pusher suspensions. Furthermore, the leading contribution to the critical density is independent of the swimming speed, and the instability sets in at the size of the system. Density fluctuations were analysed as well, which we found to be stable the linear level.

Then, we focused on the confined suspensions. Repeating the calculation analogous to the bulk suspensions, we show that the orientational instability in pushers sets in at the smallest possible scales. This difference is reflecting the fact that the dimensionality of the swimmer density in confined suspension is simply not the inverse of the system’s volume, hence another length-scale must be involved. Moreover, in contrast to bulk suspensions the density instability was observed as well, but in the case of puller suspensions, and with the critical scale being the system size. Interestingly, this critical density vanishes in the thermodynamic limit, and any finite value can therefore appear only as a result of finite size effects.
Collective motion state

Once the instability condition leading to the collective motion was determined, we have moved to the analysis of the collective motion itself. In our next project, Chapter 3, we carried out large-scale pseudo-spectral simulations of the mean-field moment equations in two spatial dimensions. We have confirmed the predictions of the linear stability analysis, that is, that the instability sets in at the size of the system. Moreover, scaling arguments allowed us to extract the dependence of the observables on the system size. Our simulations confirmed this scaling, but only close to the instability point, implying that new physics appears deep in the collective motion state. Finally, strong finite size effects and various non-linear regimes, such as stationary states and periodic orbits of the fields, were observed. These finite size effects were manifested at the transition point, but decay as the density increases.

For larger densities, where the system is considered to be deep in the collective motion state, we measured various observables by averaging over many time units. First, we looked at the energy spectra of the fluid velocity and the nematic tensor. We have found a clear sign of a finite length-scale $l^*$ emerging only at the non-linear level; The energy spectra consists two regions, which are separated by an inflection point $k^* = 2\pi/l^*$. Visual inspection of the snapshots shows, that this length-scale sets the typical size of nematicaly aligned regions. This length-scale appears to be the system size at the onset but decays as the density increases.

In order to further quantify the behaviour of the correlation length, we have measured the spatial correlations again for the velocity field, and the nematic tensor. The velocity field shows logarithmic decay with the minimum always being at half of the system size, implying that the vortices are always the size of the system regardless of the mean swimmer density. A different behaviour was observed for the nematic tensor. Here, spatial correlations are flat at small distances, but start decaying rapidly as the distance increases, then become weakly anticorrelated and eventually vanish entirely. The point where the latter occurs, defines the correlation length, which appears identical to the one extracted from the energy spectra. The correlation length was measured for various densities, and, in accordance to the inflection point of the energy spectra, is infinite at the transition to the collective motion, and decays as the density increases. However, no ‘nice’ functional form was found.

Finally, we have looked at the swimmer density fluctuations – they have been found vanishing at the onset, although the magnitude increases with the mean density. However, the statistics of these fluctuations resembles the behaviour of equilibrium systems and so giant number of fluctuations were observed.

The effect of correlations

In our last project, we questioned the validity of the mean-field approximation, by directly calculating the effect of correlations stemming from the tumbling effects. Our aim was to calculate spatial and temporal correlations of the fluid velocity, for various mean densities and persistance lengths. Our project is an extension of a previous work for the case of non-zero swimming speed [44]. We started with considering the general $N$-particle kinetic theory, and derived the leading two terms of the BBGKY hierarchy for the reduced phase space density distributions. Higher order terms were showed to be irrelevant in the thermodynamic limit.
In order to establish a connection between the fluid velocity correlation functions, and the distribution functions calculated above, we have used approach pioneered by Klimontovich. It was shown that the correlation function can be obtained by solving a linear integro-partial differential equation with noise. Solving to the latter appears technically demanding, but we have shown that it is possible in some asymptotic limits.

At first, we have focused on the fluid velocity variance. As was already derived in [44], the variance is non-zero at any finite density, and diverges at the onset to the collective motion. Our extension shows that the variance is maximal for the case of shakers, and that increasing self-propulsion speed leads to its reduction. However, even in the limit of infinite swimming speed variance does not vanish, yielding a mean-field approximation inaccurate at any circumstances.

Later, we focused on the energy spectra of the fluid velocity. The approximate form was derived with a fairly good accuracy close to the onset of the collective motion. We observed that most of the energy is stored at the largest spatial scales, while self-propulsion primarily affects small spatial scales. Within the very dilute regime the energy spectra was found to be flat \( E(k) \sim \text{const.} \), which is just the spectrum of non-interacting swimmers. Close to the transition, however, the spectra was found to be \( E(k) \sim k^{-2} \), a new prediction that can be tested experimentally.

Finally, we calculated approximate expressions for spatial and temporal correlations, and confirmed their accuracy numerically. Spatial correlations appear to be scale-free at large distances, and at any circumstances. Hence, we defined a phenomenological correlation length as a distance over which the correlations decrease by a finite amount. The short distance behaviour is suppressed by increasing swimming speed, as expected from the energy spectra. The temporal correlations on the other hand have a well defined correlation length. Moreover, temporal correlations allowed us to calculate the behaviour of enhanced diffusivity of passive tracers. In all cases we extracted the critical exponents, which are shown in Tab 5.1.

**Outlook**

All the above results represent significant theoretical advancement in the theory of collective motion of motile bacteria. The most important results are i) the instability conditions for various geometries ii) length-scale dependence on the mean concentration of the microswimmer density, and iii) effect of correlations, and their reduction with the swimming speed. All of these predictions should be measurable in an experiment, for example using *E. coli* suspensions [2], or particle-based models [44].

Understanding collective behaviour of microorganisms has several applications relevant for both industry and health care. For example, understanding the sperm motility is essential for both human, as well as livestock reproduction. Moreover, diffusivity of passive tracers discussed in Sec. 5.3.5 may help to develop better drug delivery technologies in health care.

Before any revolutionary technologies can be developed, however, further open questions must be answered. In this thesis, we only studied the effect of confinement on the instability, but the statistical properties of confined collective motion were not discussed. Moreover, the presence of correlations is expected to strongly influence the chaotic regime as well, hence the results of Chap. 5 need to be extended for larger densities. The latter extension is currently work in progress.
Appendix A

Formulas

Throughout this work, we utilise the Einstein summation convention for superscript indices, while no summation is assumed over repeated subscript indices. The domain of all integrals is \( \mathbb{R} \), unless stated otherwise.

A.1 Integral transforms

Fourier transform

For systems stored in a period box, and showing oscillatory behaviour in time, the spatio–temporal Fourier transform can be applied. This typically applies to long–time behaviour of systems in which the effect of initial conditions vanishes. The transformation, together with its inverse, are defined as

\[
\hat{f}(k, \omega) = \int \, dxd\omega \, f(x, t) e^{i(\omega t - k \cdot x)},
\]

(A.1.1)

\[
f(x, t) = \int_{|k|<1/\epsilon} \frac{dkd\omega}{(2\pi)^{d+1}} \hat{f}(k, \omega) e^{-i(\omega t - k \cdot x)},
\]

(A.1.2)

where \( \epsilon \) is a regularising parameter such that \( 1/\epsilon \) serves as a UV cut-off. Its interpretation, and hence its exact value, depends on the problem under consideration (e.g. it can be of order of microswimmer size, run-length, or particle-particle separation). Note, that for translationally invariant systems the above transformations reduce to

\[
\hat{f}(k, \omega) = \int \, d(x - x')d(t - t') \, f(x - x', t - t') e^{i(\omega(t-t') - k \cdot (x-x'))},
\]

(A.1.3)

\[
f(x - x', t - t') = \int_{|k|<1/\epsilon} \frac{dkd\omega}{(2\pi)^{d+1}} \hat{f}(k, \omega) e^{-i(\omega(t-t') - k \cdot (x-x'))},
\]

(A.1.4)

Using, within the above transformation, spatial and temporal derivatives are replaced as

\[
\nabla f(x, t) \to i k \hat{f}(k, \omega),
\]

(A.1.5)

\[
\partial_t f(x, t) \to -i \omega \hat{f}(k, \omega),
\]

(A.1.6)
and the Dirac’s delta distribution is defined as

\[(2\pi)^{d+1}\delta(k, \omega) = \int \! \! dx \! \! dt \, e^{i(\omega t - k \cdot x)}, \quad (A.1.7)\]

\[(2\pi)^{d+1}\delta(x, t) = \int \! \! dk \! \! d\omega \, e^{-i(\omega t - k \cdot x)}. \quad (A.1.8)\]

**Note.** The spatial Fourier transformation in the above form can be applied only to position vectors in the Cartesian coordinates. For orientational vector in spherical coordinates (such as the unit vector \( \mathbf{p} \)), transformation must be carried out using spherical harmonics [111]. As the latter is not used in this dissertation, we will not give the definition here.

### Laplace transform

Systems where the effect of initial conditions is of interests cannot be studied using Fourier transform. Instead, they must be treated as an initial value problem using Laplace transform, defined as

\[f(x, s) = \int_{0}^{\infty} \! \! dt \, f(x, t)e^{-st}, \quad (A.1.9)\]

\[f(x, t) = \int_{\gamma+i\infty}^{\gamma-i\infty} \! \! ds \, f(x, s)e^{st}, \quad (A.1.10)\]

where \( \gamma > 0 \) is chosen in a such way, that all the poles in \( s \) have lesser real part than \( \gamma \). In contrast to Fourier transform, the temporal derivative cannot be simply replaced with the new variable \( s \), as in (A.1.6). Instead, the Laplace transform of the temporal derivative becomes

\[\partial_t f(x, t) \to sf(x, s) - f(x, t = 0). \quad (A.1.11)\]

### A.2 Rotational derivative

The evolution of the microswimmer phase space density is often formulated in the mean-field approximation as

\[\partial_t \Psi + \nabla \cdot (\dot{x}\Psi) + \mathbf{R} \cdot (\dot{p}\Psi) + \lambda \Psi - \frac{\lambda}{\Omega} \int \! \! dp \, \Psi = 0, \quad (A.2.1)\]

where \( \nabla = \partial/\partial x \), \( \mathbf{R} = p \times \partial/\partial p \) are spatial and rotational del operators, and equations of motion are

\[\dot{x} = v_s p + \mathbf{U}, \quad (A.2.2)\]

\[\dot{p} = p \times (\nabla \mathbf{v} + B\mathbf{E}) \cdot \mathbf{p}. \quad (A.2.3)\]

The above set of equations is equivalent to the formulation (2.2.2)-(2.2.4) in \( d = 2 \), and 3, but it cannot be generalized to arbitrary dimension. In order to recast (A.2.1)-(A.2.3) into the form (2.2.2)-(2.2.4), the following identity must be used

\[\mathbf{R} \cdot [p \times T \cdot p\Psi] = (1 - d)p \cdot T \cdot p\Psi + \partial_p \cdot [T \cdot p\Psi] = \partial_p [\mathbf{P} \cdot T \cdot p\Psi], \quad (A.2.4)\]

where \( T \) is any tensor that does not depend on \( p \).
A.3 Hydodynamic force dipole

The far-field behaviour of the velocity field generated by a single swimming microorganism is within a sufficient accuracy described by the low Re hydrodynamic dipole, $u$ [35, 37]. The latter satisfies Stokes equation driven by two point-like forces $\pm f_p$ acting on the fluid at the positions $\pm \frac{1}{2}l_p$.

\[ \mu \partial^2 u^\alpha(x) - \partial^\alpha P(x) + f_p^\alpha [\delta(x - \frac{1}{2}l_p) - \delta(x + \frac{1}{2}l_p)] = 0, \]
\[ \frac{\partial}{\partial \alpha} u^\alpha(x) = 0, \]

(A.3.1) (A.3.2)

Here, $\mu$ is the viscosity of the fluid, $P$ is the pressure, and $\delta(x)$ denotes the Dirac delta-function. The solution to this system is readily found by performing the $d$-dimensional Fourier transform, (A.1.1), which gives

\[ -\mu k^2 \hat{u}^\alpha - ik^\alpha \hat{P} + f_p^\alpha [e^{-\frac{1}{2}ik \cdot p} - e^{\frac{1}{2}ik \cdot p}] = 0, \]
\[ k^\alpha \hat{u}^\alpha = 0. \]

(A.3.3) (A.3.4)

The point-dipole approximation, relevant at large scales where $kl \ll 1$, is obtained to linear order in the dipolar length $l$, yielding

\[ \hat{u}^\alpha(k, p) = -i\kappa \frac{k \cdot p}{k^2} \mathbb{P}^\alpha\beta p^\beta. \]

(A.3.5)

Here, $k = |k|$, $\kappa = fl/\mu$ is the dipolar strength, and

\[ \mathbb{P}^\alpha\beta = \delta^\alpha\beta - \frac{k^\alpha k^\beta}{k^2} \]

is the transversal projection operator ensuring the incompressibility of the fluid in the form $\mathbb{P}^\alpha\beta \hat{u}^\beta = \hat{u}^\alpha$.

**Bulk dipole**

The derivation presented above is independent of the space dimensionality $d$ and the Fourier transform of the dipolar field (A.3.5) has the same form for bulk systems of all dimensions. Its real space representation, however, strongly depends on $d$. In three dimensions, the inverse Fourier transform (A.1.2) yields

\[ u^\alpha_{d=3}(r, p) = \frac{\kappa}{8\pi |r|^3} \left[ \frac{3(r \cdot p)^2}{|r|^2} - 1 \right], \quad r = x - x_0, \]

(A.3.7)

where we have introduced an arbitrary position of the force dipole $x_0$. In two dimensions, the real-space representation is

\[ u^\alpha_{d=2}(r, p) = \frac{\kappa}{4\pi |r|^2} \left[ \frac{2(r \cdot p)^2}{|r|^2} - 1 \right], \quad r = x - x_0, \]

(A.3.8)

It is important to stress that the dipolar strength $\kappa = fl/\mu$ has different dimensions in two- and three-dimensional bulk systems.
In-plane dipole

The velocity field of a hydrodynamic dipole confined to a two-dimensional plane embedded in an infinite three-dimensional fluid can be obtained from (A.3.7). We select $z = 0$ to be the plane of the microswimmers, which implies that $r = (x, y, 0)$ and $p = (p_x, p_y, 0)$ become effectively two-dimensional vectors. Performing the corresponding two-dimensional Fourier transform of (A.3.7) with respect to $x$ and $y$, leads to

$$u_{i-p}^\alpha(k, p) = -\frac{i\kappa}{2} \frac{k \cdot p}{k} \left[ \mathbb{P}^{\alpha\beta} + \frac{1}{2} \mathbb{Q}^{\alpha\beta} \right] p^\beta,$$

where $k = (k_x, k_y)$ in (A.3.9) is a two-dimensional wave-vector, and we have introduced the longitudinal projection operator

$$\mathbb{Q}^{\alpha\beta} = \frac{k^\alpha k^\beta}{k^2},$$

representing the compressible component of the hydrodynamic flow.

Regularised dipole

The regularised dipole is defined in Eq. (5.1.6), its Fourier transform is found to be

$$\hat{u}^\alpha(k, p) = -i\kappa A(\epsilon k) \frac{k \cdot p}{k^2} \mathbb{P}^{\alpha\beta} p^\beta,$$

where $\epsilon > 0$ and the function $A$, defined as

$$A(x) = \frac{1}{2} x^2 K_2(x),$$

with $K_2(x)$ being the modified Bessel function of the second kind, is close to unity for $x < 1$, and quickly approaches zero for $x > 1$. It will serve as a regularisation of the integrals over $k$, suppressing contributions from lengthscales smaller than the size of individual microswimmers, set by $\epsilon$.

A.4 Stochastic calculus
Appendix B

Linear stability of kinetic theory

B.1 Analytics

B.1.1 Inverse Laplace transform

In this appendix, we will derive the solution to the density fluctuations corresponding to the pole \( s_2 \) in (3.3.6). The inverse Laplace transform (A.1.10) of (3.3.3), leads to the following residuum originating from \( s_2 \)

\[
\hat{\rho}(t) = \int dp \left[ \frac{\lambda}{1 - \frac{\lambda}{v_s k} \arctan \left( \frac{ik \cdot p}{kp} \right)} \exp^{-\left(\lambda + iv_s k \cdot p\right)t} \right] \hat{\Psi}_0(k, p). \tag{B.1.1}
\]

Assuming \( k = (0, 0, k) \), and transforming the system to spherical coordinates, we obtain

\[
\hat{\rho}(t) = e^{-\lambda t} \int_0^\pi d\theta \ F(\theta) e^{-iv_s kt \cos \theta}, \quad F(\theta) = \frac{\lambda}{1 - \frac{\lambda}{v_s k} \arctan \left( \frac{i}{\cos \theta} \right)} \tag{B.1.2}
\]

In the limit \( v_s kt \to \infty \), the integrand of Eq. (B.1.2) is a rapidly oscillating function of \( \theta \), so that the main contribution will come from the extrema of the phase \( \cos \theta \). Hence, we will apply the method of stationary phase approximation, i.e. we approximate the integral by its values at the local extrema. There are two extrema here, \( \theta_0 \in \{0, \pi\} \), hence after a series expansion of the phase \( \cos \theta \) at \( \theta_0 \) we arrive at

\[
\hat{\rho}(t) = \left( (1 + i) F(0) e^{-\left(\lambda - iv_s k\right)t} + (1 - i) F(\pi) e^{-\left(\lambda + iv_s k\right)t} \right) \sqrt{\frac{\pi}{4v_s kt}} + \cdots, \tag{B.1.3}
\]

where the ellipsis denote higher order terms in \( 1/(v_s kt) \). Interestingly, \( F(\theta_0 \in \{0, \pi\}) = 0 \), so that the leading order terms of the stationary phase approximation vanishes, and algebraic decay of the solution behaves as \( 1/(v_s kt) \) (or faster).

B.1.2 Bulk suspensions in two spatial dimensions

Here, we repeat the calculation presented in Section 3.3 for the case of microswimmers suspended in two-dimensional bulk fluid. We set \( d = 2 \) in (3.2.6)-(3.2.7), and employ (A.3.5), since the form of the dipolar Fourier transform is the same in all dimensions, as noted in Appendix A.3. Similar to the three-dimensional case, we obtain the following de-coupled eigenvalue problems
\[ \delta \rho = \lambda \frac{b}{v_s k \sqrt{1 + b^2}} \delta \hat{\rho}, \quad (B.1.4) \]

\[ \delta \hat{U}^\alpha = \frac{Bn\kappa b^2 - 2\sqrt{1 + b^2} + 2}{v_s k b^3} \delta \hat{U}^\alpha, \quad (B.1.5) \]

As in the three-dimensional case, the orientational eigenvalue problem can be re-written as

\[ \alpha_{2d} = \frac{b^2 - 2\sqrt{1 + b^2} + 2}{b^3}, \quad \alpha_{2d} = \frac{v_s k}{Bn\kappa}, \quad (B.1.6) \]

where, as before, \( b = v_s k/(\chi + \lambda) \). In contrast to (3.3.9), solution to (B.1.6) can be found analytically, yielding

\[ s = -\lambda + G(\alpha_{2d}) B\kappa n, \quad (B.1.7) \]

where

\[ G(x) = 6x^2 \left( 4 - \frac{(1 + i\sqrt{3})}{H(x)} \pm \left( 1 - i\sqrt{3} \right) H(x) \right)^{-1}, \quad (B.1.8) \]

\[ H(x) = 54x^2 - 1 + 6\sqrt{3}x\sqrt{27x^2 - 1}. \quad (B.1.9) \]

The function \( G(\alpha_{2d}) \) has the same qualitative form as \( F(\alpha) \) from Section 3.3, shown in Fig. 3.2. As in the three-dimensional case, the orientational instability only exists for pushers, \( \kappa > 0 \), and sets in at the largest possible scale, \( k \to 0 \). The corresponding instability condition is given by

\[ 1 \geq \frac{4\lambda}{B\kappa n} > 0. \quad (B.1.10) \]

where both the number density \( n \) and the dipolar strength \( \kappa \) have different dimensions than their three-dimensional counterparts. The solution (B.1.7) ceases to exist for \( \alpha_{2d} > 1/\sqrt{2} \).

It is interesting to see, that equations for the orientational instability of 2d suspension (B.1.5), differ from those that are confined into 2d plane (3.4.3) only by a \( k/2 \) factor. This is because the entire calculation of the transversal modes is the same, the only difference is \( k/2 \) factor in the dipolar fields (3.3.2) and (3.4.1).

At last, the density eigenvalue is given by

\[ s = -\lambda \pm \sqrt{\lambda^2 - k^2 v_s^2}, \quad (B.1.11) \]

which is stable for any \( k \).

**B.1.3 Approximative value of the critical density**

In this appendix, we will derive the approximative expression for the orientational instability setting at the scale of particle-particle separation (3.4.11). We set \( k_c = \sqrt{\pi^3 n_c} \) in (3.4.8), giving

\[ s = -\lambda + G \left( \frac{2v_s}{Bn_k} \right) \frac{B\kappa(\pi n_c)^{3/2}}{2}. \quad (B.1.12) \]
The calculation now consists of two steps: small and large $v_s$ approximation. First, we set the $v_s \to 0$ in (B.1.12), which gives

$$s = -\lambda + \frac{1}{8} B\kappa (\pi n_c)^{3/2},$$

(B.1.13)

The solution to Re[$s$] = 0 gives the vanishing speed approximation to the critical density $n_c = (4/\pi)(\lambda/B\kappa)^{2/3}$. For the fast microswimmers, $v_s \to \infty$, we use the result (3.4.9), i.e. we assume that the critical density is linearly proportional to the swimming speed $n_c = 2\sqrt{2}v_s/(B\kappa) + \mathcal{O}(1)$. Indeed, the large $v_s$ limit of eigenvalue (B.1.12) is then

$$s = \pm i 2^{5/4} \left(\frac{\pi v_s}{B\kappa}\right)^{3/2} + \mathcal{O}(1)$$

(B.1.14)

which is a purely imaginary number. Combining the slow and fast swimming approximations together gives the result (3.4.11). The latter shows very good quantitative agreement with the numerical solution of Eq. (B.1.12) as shown in Fig B.1.

**B.2 Numerics**

In this appendix, we verify some of our results of the linear stability analysis from Sec 3.4, by numerically solving Eq. (3.2.3) in $d = 2$. The latter can be written as

$$(\partial_\tau + 1 + i \tilde{k}\tilde{\alpha}^\alpha \rho^\alpha)\delta \hat{\Psi} = \frac{1}{2\pi} \delta \hat{\rho} + \frac{1}{2\pi} \Phi \tilde{k} [2Bp^\alpha p^\beta - (1 + B)\delta^{\alpha\beta}]i\tilde{k}\tilde{\alpha}^\delta \delta \hat{U}^\beta,$$

(B.2.1)

where $\tilde{k} = k/|k|$ is the unit wave-vector, and the dimensionless parameters are

$$\tau = \lambda t, \quad \tilde{k} = \frac{v_s}{\lambda}k, \quad \Phi = \frac{\kappa n}{v_s}.$$  

(B.2.2)

We now transform the system into polar coordinates $p = \{\cos \phi, \sin \phi\}$, which gives

$$\left(\partial_\tau + 1 + i \tilde{k}\cos \phi\right) \delta \hat{\Psi} = \int_0^{2\pi} \frac{d\phi'}{2\pi} \delta \hat{\Psi} + \Phi \tilde{k} \left[B \int_0^{2\pi} \frac{d\phi'}{2\pi} \cos \phi \cos \phi' \times \right.$$

$$\left. \times \left\{ \sin \phi \sin \phi' + \frac{1}{2} \cos \phi \cos \phi' \right\} \delta \hat{\Psi} - \frac{1}{4}(1 + B) \int_0^{2\pi} \frac{d\phi'}{2\pi} \cos^2 \phi' \delta \hat{\Psi} \right].$$

(B.2.3)
In order to solve the above equation numerically write first perform the change of variables to \( x = \phi/2\pi \), so that the linearised equation \((B.2.3)\) becomes

\[
[\partial_t + g(x)] \hat{\Psi}(x, t) = \int_{0}^{1} dx' \left[ h(x') + z(x, x') \right] \hat{\Psi}(x', t), \quad (B.2.4)
\]

with

\[
g(x) = 1 + i\tilde{k} \cos(2\pi x), \quad (B.2.5)
\]
\[
h(x) = 1 - \frac{1}{4}(1 + B)\Phi \tilde{k}^2 \cos(2\pi x), \quad (B.2.6)
\]
\[
z(x, x') = B\Phi \tilde{k} \sin(2\pi x) \cos(2\pi x') \cos(2\pi x') + \frac{1}{2} \cos^2(2\pi x) \cos^2(2\pi x'). \quad (B.2.7)
\]

In the Crank-Nicolson scheme, the Eq. \((B.2.4)\) can be discretised as

\[
\frac{1}{2\Delta t} (\hat{\Psi}_i^{t+1} - \hat{\Psi}_i^t) = \frac{1}{2} [-g_n(\hat{\Psi}_n^{t+1} + \hat{\Psi}_n^t) + \sum_m \Delta \theta (h_m + z_{n,m})(\hat{\Psi}_m^{t+1} + \hat{\Psi}_m^t)], \quad (B.2.8)
\]

where \( i \in \{0, \ldots, t\}, n \in \{0, \ldots, L - 2\} \) (since \( \hat{\Psi}_N-1 = \hat{\Psi}_0 \)), and discretized functions are defined as

\[
g_n \equiv g(x_n), \quad h_n \equiv h(x_n), \quad z_{n,m} \equiv z(x_n, x_m), \quad x_n = 2\pi n/(L - 1). \quad (B.2.9)
\]

Eq. \((B.2.8)\) can be further written in the matrix form as

\[
[1 - \frac{1}{2}\Delta t M] \hat{\Psi}_i^{t+1} = [1 + \frac{1}{2}\Delta t M] \hat{\Psi}_i^t, \quad (B.2.10)
\]

where \( 1 \) is the \((L-1) \times (L-1)\) unit matrix, and the matrix \( M \) has the same dimensionality with the following form

\[
M = -\begin{pmatrix}
g_1 & 0 & 0 & \cdots \\
0 & g_2 & 0 & \cdots \\
0 & 0 & g_3 & \cdots \\
\vdots & \vdots & \vdots & \ddots \\
\end{pmatrix} + \Delta \theta \begin{pmatrix}
h_1 + z_{1,1} & h_2 + z_{1,2} & h_3 + z_{1,3} & \cdots \\
h_1 + z_{2,1} & h_2 + z_{2,2} & h_3 + z_{2,3} & \cdots \\
h_1 + z_{3,1} & h_2 + z_{3,2} & h_3 + z_{3,3} & \cdots \\
\vdots & \vdots & \vdots & \ddots \\
\end{pmatrix}. \quad (B.2.11)
\]

We have numerically solved Eq. \((B.2.10)\) in Python for the following initial conditions

\[
\hat{\Psi}^0_n = \sum_{m=1}^{M} e^{-m\beta_m} \zeta_m \sin(mx_n) \quad (B.2.12)
\]

where \( \beta_m \) and \( \zeta_m \) are randomly chosen and \( M = 30 \). The resulting shape of \( \hat{\Phi}^t_n \) is shown in Fig. B.2 for various values of the reduced density \( B\Phi \). For densities \( B\Phi < 2\sqrt{2} \), i.e. within the region of the ‘missing’ solution, and in the absence of tumbling, the system shows oscillatory behaviour similar to what is observed in three-dimensional systems [74]. The amplitude of the oscillation decays in time due to the tumbling effects, and finally, the system is unstable for large densities. All these results are consistent with our analysis in the main text.
Figure B.2: Numerical solution of (B.2.10) with initial conditions (B.2.12), and for various parameters: a) In the absence of tumbling the system evolves towards an oscillatory structure with the envelope given by the initial conditions. The dimensionless quantities used in this case are $\tau = v_s \sqrt{nt}$, $\hat{k} = k/\sqrt{n}$. b)-d) The cases with non-zero tumbling for various densities and time steps - b), and c) both stable, and d) unstable solution. In all cases $\hat{k} = \pi/2$, and other parameters used are shown in every graph separately; Parameters in a)-c) are chosen such that the solution arising from the first pole in (3.3.6) does not exist, and the plots demonstrate oscillatory decaying behaviour.
Appendix C

Moment equations

This appendix contains all explicit calculations regarding the moment equation derivation, and their analysis.

C.1 Derivation of evolution equations

The moment equations are derived by multiplying the Master equation (2.2.2) with the corresponding number of $p$’s, and averaging over the orientation (2.2.7). First, we write the explicit form of the master equation

$$\partial_t \Psi + \nabla^\alpha ((v_s p^\alpha + U^\alpha) \Psi) + \partial^\alpha ((\delta^{\alpha\beta} - p^\alpha p^\beta) p^\gamma \Psi) (W^\beta\gamma + B E^\beta\gamma) = -\lambda \Psi + \lambda \Omega \int d\mathbf{p} \Psi. \quad (C.1.1)$$

The vector averages (with no density distribution in the integrand) are calculated using the following formulas

$$\int \frac{d\mathbf{p}}{\Omega_d} p^\alpha p^\beta p^\gamma \ldots p^\delta = \frac{\delta^{\alpha\beta} \ldots \delta^{\gamma\delta} + (A P)}{d(d+2)\ldots(d+2(n-1))}, \quad (C.1.2)$$

$$\int \frac{d\mathbf{p}}{\Omega_d} p^\alpha p^\beta p^\gamma \ldots p^\delta = 0, \quad (C.1.3)$$

where AP stands for all possible permutations of indexes, which total number is $(2n-1)!!$. Both of the above results are a direct consequence of the isotropy of the space. The averages (2.2.7) weighted with the probability distribution (4.1.1) are then

$$\bar{1} = c, \quad (C.1.4)$$

$$\bar{p} = m^\alpha, \quad (C.1.5)$$

$$\bar{p^\alpha p^\beta} = Q^{\alpha\beta}, \quad (C.1.6)$$

$$\bar{p^\alpha p^\beta p^\gamma} = Q^{\alpha\beta\gamma} + \frac{1}{d+2} (m^\alpha \delta^{\beta\gamma} + 2P), \quad (C.1.7)$$

$$\bar{p^\alpha p^\beta p^\gamma p^\delta} = Q^{\alpha\beta\gamma\delta} + \frac{1}{(d+2)(d+4)} (m^\alpha \delta^{\beta\gamma} \delta^{\omega} + 14P), \quad (C.1.8)$$

where $Q^{\alpha\beta\ldots\gamma}$ are connected correlation functions (whose summation over any two indexes must vanish), and $nP$ stands $n$ permutations of indexes within the brackets. First three
moments are found by multiplying Eq. (C.1.1) with corresponding number of $p^\mu$, and averaging over $p$

$$
\begin{align}
\partial_t \mathcal{T} + \nabla^\alpha (v_s p^\alpha \mathcal{T}) + \partial_\alpha (\mathcal{P}^\alpha_\beta p^\gamma ) (\mathcal{W}^{\beta \gamma} + \mathcal{B} \mathcal{E}^{\beta \gamma}) &= 0, \\
(\partial_t + \lambda)p^\alpha + \nabla^\alpha (v_s p^\mu p^\alpha \mathcal{U}^\alpha) + \partial_\alpha (\mathcal{P}^\alpha_\beta p^\gamma ) (\mathcal{W}^{\beta \gamma} + \mathcal{B} \mathcal{E}^{\beta \gamma}) &= 0,
\end{align}
$$

(C.1.10)

(C.1.11)

(C.1.12)

Note, that the distribution function $\Psi$ is implicitly assumed inside the brackets containing orientational derivatives $\partial_\alpha$. For example, the following terms can be simplified

$$
\begin{align}
\partial_\alpha (\ldots) &= 0, \\
p^\mu \partial_\alpha (\mathcal{P}^\alpha_\beta p^\gamma ) &= (p^\mu p^\beta p^\gamma - \delta^\mu_\beta p^\gamma), \\
p^\mu p^\nu \partial_\alpha (\mathcal{P}^\alpha_\beta p^\gamma ) &= (2p^\mu p^\nu p^\beta - p^\mu p^\gamma \delta^\nu_\beta - p^\nu p^\gamma \delta^\mu_\beta).
\end{align}
$$

The final form of the moment equations is then

$$
\begin{align}
\mathcal{D}_t c &= - v_s \nabla^\alpha m^\alpha, \\
\mathcal{D}_t m^\mu &= - \lambda m^\mu - v_s \nabla^\alpha (Q^{\mu \alpha} + \frac{1}{2} \delta^{\mu_\alpha} c) + (\mathcal{W}^{\mu \beta} + \mathcal{B} \mathcal{E}^{\mu \beta}) m^\beta \\
&- B \partial_\mu p^\gamma p^\alpha \Psi \mathcal{E}^{\beta \gamma}, \\
(Q^{\mu \nu} + \frac{1}{2} \delta^{\mu_\nu} c) &= - \lambda Q^{\mu \nu} - v_s \nabla^\alpha p^\mu p^\nu p^\alpha \Psi - 2B \partial_\mu p^\gamma p^\nu p^\gamma \Psi \mathcal{E}^{\beta \gamma},
\end{align}
$$

(C.1.13)

(C.1.14)

(C.1.15)

(C.1.16)

(C.1.17)

(C.1.18)

where the square above the LHS of the last equation denotes the Oldroid's derivative

$$
T^{\mu \nu} = \mathcal{D}_t T^{\mu \nu} - (\mathcal{W}^{\mu \alpha} T^{\alpha \nu} - T^{\mu \alpha} \mathcal{W}^{\alpha \nu}) - B(\mathcal{E}^{\mu \alpha} T^{\alpha \nu} + T^{\mu \alpha} \mathcal{E}^{\alpha \nu}).
$$

(C.1.19)

The only task is now to include higher order moments. Since the interaction is nematic, and we also assume that we are close to the transition, the higher order terms should be adiabatically enslaved into the first three moments $c$, $m^\mu$, and $Q^{\mu \nu}$. Within this approximation, it is sufficient to write down only linear equations for the third and fourth moment

$$
\begin{align}
(\partial_t + \lambda)p^\mu p^\nu p^\gamma p^\delta + v_s \nabla^\alpha p^\mu p^\nu p^\gamma p^\delta &= 0, \\
(\partial_t + \lambda)p^\mu p^\nu p^\gamma p^\delta - \lambda \frac{\delta^{\mu \nu} \delta^{\gamma \delta} + \delta^{\mu \gamma} \delta^{\nu \delta} + \delta^{\nu \gamma} \delta^{\mu \delta}}{d(d+2)} + v_s \nabla^\alpha p^\mu p^\nu p^\gamma p^\delta &= 0,
\end{align}
$$

(C.1.20)

(C.1.21)

\footnote{The calculation is greatly simplified using the following identities

$$
\mathcal{A}(p) \partial_{\gamma} B(p) = - B(p) \partial_{\gamma} \mathcal{A}(p), \\
\partial_{\alpha} p^\beta = \mathcal{P}^\alpha_\beta, \\
\partial_{\alpha} \mathcal{P}^{\beta \gamma} &= -(\mathcal{P}^\alpha_\beta \mathcal{P}^{\gamma} + \mathcal{P}^\alpha_\gamma \mathcal{P}^{\beta}).
$$
}
Using the relations (C.1.4)-(C.1.9), the first three moment equations become

\[ \mathcal{D}_t m^\mu = -\lambda m^\mu - v_s \nabla^\alpha (Q^{\mu\alpha} + \frac{1}{2} \delta^{\mu\alpha} c) \\
+ (\mathcal{W}^{\mu\alpha} + \frac{B d}{d+2} \mathcal{E}^{\mu\alpha}) m^\alpha, \tag{C.1.22} \]

\[ \mathcal{D}_t Q^{\mu\nu} = -\lambda Q^{\mu\nu} - \frac{v_s}{d+2} \nabla^\alpha (m^\mu \delta^{\nu\alpha} + m^\nu \delta^{\mu\alpha} - \frac{2}{d} m^\alpha \delta^{\mu\nu}) - v_s \nabla^\alpha Q^{\mu\nu} \\
+ \left( \mathcal{W}^{\mu\nu} - \frac{2}{d+2} \mathcal{E}^{\mu\nu} \right) + B \left( \mathcal{E}^{\mu\gamma} (Q^{\gamma\nu} + \frac{1}{2} \delta^{\gamma\nu}) + (Q^{\mu\gamma} + \frac{1}{2} \delta^{\mu\gamma}) \mathcal{E}^{\gamma\nu} \right) \\
- 2B \left( \frac{2}{(d+2)} \mathcal{E}^{\mu\nu} + \frac{2}{d+4} (Q^{\mu\gamma} \mathcal{E}^{\gamma\nu} + Q^{\nu\gamma} \mathcal{E}^{\gamma\nu} + \frac{1}{2} \delta^{\mu\nu} \mathcal{E}^{\gamma\delta} + Q^{\nu\gamma\delta} \mathcal{E}^{\gamma\delta}) \right). \tag{C.1.23} \]

At this stage we need equations for \( Q_3^{\mu
u\gamma} \) and \( Q_4^{\mu\nu\gamma\delta} \) and enslaved them into the above

\[ (\partial_t + \lambda) Q_3^{\mu\nu\gamma} + v_s \nabla^\delta \left[ Q_4^{\mu\nu\gamma\delta} + \frac{1}{d+4} \left( \delta^{\mu\rho} Q^{\rho\gamma} + \delta^{\nu\rho} Q^{\mu\rho\gamma} + \delta^{\delta\rho} Q^{\mu\nu\rho\gamma} \right) \\
- \frac{2}{(d+2)(d+4)} \left( Q^{\delta\mu\nu} Q^{\rho\gamma} + Q^{\delta\nu\mu} Q^{\rho\gamma} + Q^{\delta\gamma,\mu\nu} \right) \right] = 0, \tag{C.1.25} \]

In the process of enslaving, we note that equations for both \( Q_3^{\mu\nu\gamma} \) and \( Q_4^{\mu\nu\gamma\delta} \) contain terms that are gradients of \( m^\mu \) and \( Q^{\mu\nu} \), hence they represent higher order terms when contracted with \( \mathcal{E}^{\mu\nu} \) in (C.1.23), and (C.1.24). Therefore, these terms can be dropped. The only relevant contributions comes from the gradient of \( \nabla^\mu Q_3^{\mu\nu\gamma} \) in (C.1.24), which is

\[ \nabla^\gamma Q_3^{\mu\nu\gamma} = -\frac{v_s}{(d+4)\lambda} \left[ \nabla^2 Q^{\mu\nu} + \frac{d}{d+2} \left( \nabla^\mu \nabla^\gamma Q^{\nu\gamma} + \nabla^\nu \nabla^\gamma Q^{\mu\gamma} - \frac{2}{d} \delta^{\mu\nu} \nabla^\delta \nabla^\gamma Q^{\delta\gamma} \right) \right]. \tag{C.1.26} \]

The final form of the moment equations for polar and nematic order the becomes

\[ \mathcal{D}_t m^\mu = -\lambda m^\mu - v_s \nabla^\alpha (Q^{\mu\alpha} + \frac{1}{2} \delta^{\mu\alpha} c) \\
+ (\mathcal{W}^{\mu\alpha} + \frac{B d}{d+2} \mathcal{E}^{\mu\alpha}) m^\alpha, \tag{C.1.27} \]

\[ \mathcal{D}_t Q^{\mu\nu} = -\lambda Q^{\mu\nu} - \frac{v_s}{d+2} \nabla^\alpha (m^\mu \delta^{\nu\alpha} + m^\nu \delta^{\mu\alpha} - \frac{2}{d} m^\alpha \delta^{\mu\nu}) \\
+ \frac{v_s^2}{(d+4)\lambda} \left[ \nabla^2 Q^{\mu\nu} + \frac{d}{d+2} \left( \nabla^\mu \nabla^\gamma Q^{\nu\gamma} + \nabla^\nu \nabla^\gamma Q^{\mu\gamma} - \frac{2}{d} \delta^{\mu\nu} \nabla^\delta \nabla^\gamma Q^{\delta\gamma} \right) \right] \\
+ \mathcal{W}^{\mu\nu} - \mathcal{W}^{\nu\mu} + \frac{d}{d+4} B \left( \mathcal{E}^{\mu\gamma} Q^{\gamma\nu} + Q^{\mu\nu} \mathcal{E}^{\gamma\nu} \right) \\
+ \frac{2B}{d+4} \mathcal{E}^{\mu\nu} - \frac{2B}{d+4} \delta^{\mu\nu} \mathcal{E}^{\gamma\delta}, \tag{C.1.28} \]

where we have dropped the higher order terms.
C.2 Linear stability

Linearizing the equations, we obtain

\[ y_c = -\nabla^\alpha m^\alpha, \quad (C.2.1) \]
\[ y_m^\mu = -m^\mu - \nabla^\alpha (Q^{\mu\alpha} + \frac{1}{a} \delta^{\mu\alpha} c), \quad (C.2.2) \]
\[ yQ^{\mu\nu} = -Q^{\mu\nu} \left[ \frac{1}{d+1} P^{\mu\alpha} P^{\nu\beta} + \frac{2(d+1)}{(d+2)(d+4)} \left( P^{\mu\alpha} Q^{\nu\beta} + Q^{\mu\alpha} P^{\nu\beta} \right) \right] \\ + \frac{3d+2}{(d+2)(d+4)} Q^{\mu\alpha} Q^{\nu\beta} - \frac{2}{d(d+2)(d+4)} \delta^{\mu\nu} Q^{\alpha\beta} \nabla^2 Q^{\mu\nu} \\ - \frac{1}{d+2} \nabla^\alpha (m^\mu \delta^{\nu\alpha} + m^\nu \delta^{\mu\alpha} - \frac{2}{a} m^\alpha \delta^{\mu\nu}) + \frac{B}{a^2} \kappa (\nabla^\nu U^\mu + \nabla^\mu U^\nu), \quad (C.2.3) \]
\[ 0 = \nabla^2 U^\mu - \nabla^\mu (p + \frac{1}{a} c) - \kappa \nabla^\alpha Q^{\mu\alpha}, \quad (C.2.4) \]
\[ 0 = \nabla^\alpha U^\alpha. \quad (C.2.5) \]

Splitting the individual modes of the model

\[ m_\perp^{\mu} = \tilde{P}^{\mu\alpha} m^\alpha, \quad m_\parallel^{\mu} = Q^{\mu\alpha} m^\alpha, \quad (C.2.6) \]
\[ Q^{\mu\nu}_\perp = \tilde{P}^{\mu\alpha} Q^{\nu\beta} Q^{\alpha\beta}, \quad Q^{\mu\nu}_\parallel = Q^{\mu\alpha} Q^{\nu\beta} Q^{\alpha\beta}, \quad (C.2.7) \]
\[ Q^{\mu\nu} = (\tilde{P}^{\mu\alpha} Q^{\nu\beta} + Q^{\mu\alpha} \tilde{P}^{\nu\beta}) Q^{\alpha\beta}, \quad (C.2.8) \]

The corresponding equations into the set of two decoupled equations, which stability will be now analyzed independently

**Stable modes**

We proceed with studying the stability of the following modes\(^2\)

\[ y_c = -\nabla^\alpha m_\parallel^\alpha, \quad (C.2.9) \]
\[ y_m^\mu = -m_\parallel^\mu - \nabla^\alpha (Q^{\mu\alpha} Q^{\alpha\beta} + \frac{1}{a} \delta^{\mu\alpha} c), \quad (C.2.10) \]
\[ yQ^{\mu\nu}_\perp = -Q^{\mu\nu}_\perp + \frac{1}{(d+4)} \nabla^2 Q^{\mu\nu}_\perp - \frac{2}{d(d+2)(d+4)} \tilde{P}^{\mu\nu} \nabla^2 Q^{\alpha\alpha}_\parallel + \frac{2}{d(d+2)} \tilde{P}^{\mu\nu} \nabla^\alpha m_\parallel^\alpha, \quad (C.2.11) \]
\[ yQ^{\mu\nu}_\parallel = -Q^{\mu\nu}_\parallel + \frac{(3d+2)}{(d+2)(d+4)} \nabla^2 Q^{\mu\nu}_\parallel - \frac{2}{d(d+2)(d+4)} Q^{\mu\nu} \nabla^2 Q^{\alpha\alpha}_\parallel \\ - \frac{1}{d+2} (\nabla^\mu m_\parallel^\alpha + \nabla^\nu m_\parallel^\mu - \frac{2}{a} Q^{\mu\nu} \nabla^\alpha m_\parallel^\alpha), \quad (C.2.12) \]
\[ \nabla^\mu \nabla^\nu p = - (\frac{\kappa}{a})^2 Q^{\mu\nu}_\parallel. \quad (C.2.13) \]

As \(Q^{\mu\nu}_\perp\) is decoupled from all other modes, we set \(m_\perp^\mu, Q^{\mu\nu}_\perp = 0\) in (C.2.11), which gives

\[ y = -1 - \frac{1}{(d+3)^2}, \quad (C.2.14) \]

which means that \(Q^{\mu\nu}_\parallel\) is a stable mode. Stability of other modes is assessed by taking divergence of \(m_\parallel^\mu\), and the trace of \(Q^{\mu\nu}_\parallel\), which yields

\[ y_c = -\nabla^\alpha m_\parallel^\alpha, \quad (C.2.15) \]
\[ (y + 1) \nabla^\alpha m_\parallel^\alpha = -\nabla^2 (Q^{\alpha\alpha}_\parallel + \frac{1}{a} c), \quad (C.2.16) \]
\[ (y - \frac{d(3d+2)-2}{d(d+2)(d+4)} \nabla^2 + 1) Q^{\alpha\alpha}_\parallel = -\frac{2(d-1)}{d(d+2)} \nabla^\alpha m_\parallel^\alpha, \quad (C.2.17) \]

\(^2\)Note that \(Q^{\mu\nu}_\parallel\) mode is related to pressure
Performing the Fourier transform, we end up with the following equation determining the spectrum

\[
y + \frac{d(3d+2)}{d(d+2)(d+4)} \hat{k}^2 + 1 + \frac{2(d-1)}{d(d+2)} \frac{\hat{k}^2}{y + 1 + \frac{\hat{k}^2}{y}} = 0
\]  
(C.2.18)

Eq. (C.2.18) can be solved numerically, and it can be showed that the eigenvalues \( y \) have negative real part for any \( d \), and \( \hat{k} \). The above Note, that the mode \( Q_{||}^{\mu\nu} \) is related to pressure, where the latter is also stable.

**Unstable modes**

We obtain the following equations that describe the instability

\[
y m^\mu_\perp = -\lambda m^\mu_\perp - \nabla^\alpha \mathbb{P}^{\alpha\mu\beta} Q^{\alpha\beta}, \tag{C.2.19}
\]

\[
y Q^{\mu\nu} = \frac{2(d+1)}{(d+2)(d+4)} \nabla^2 Q^{\mu\nu} - (1 - \Delta) Q^{\mu\nu} - \frac{1}{d+2} (\nabla^\mu m^\nu_\perp + \nabla^\nu m^\mu_\perp), \tag{C.2.20}
\]

\[
0 = \nabla^\mu U^\alpha - \frac{\kappa}{\lambda} Q^{\mu\alpha\beta} Q^{\alpha\beta}, \tag{C.2.21}
\]

\[
0 = \nabla^\alpha U^\alpha. \tag{C.2.22}
\]

Fourier transforming (C.2.19)-(C.2.22), we obtain

\[
y (y + 1) m^\mu_\perp = -v_s i \hat{k}^\alpha \mathbb{P}^{\alpha\mu\beta} Q^{\alpha\beta}, \tag{C.2.23}
\]

\[
y + \frac{2(d-1)}{(d+2)(d+4)} \hat{k}^2 + 1 - \Delta) Q^{\mu\nu} = -\frac{1}{d+2} (i \hat{k}^\mu m^\nu_\perp + i \hat{k}^\nu m^\mu_\perp) \tag{C.2.24}
\]

where we have already contracted the stokes equation with \( \mathbb{P}^{\mu\nu} \), and introduced the reduced density \( \Delta = \frac{B_{c\alpha}}{(d+2)\lambda} \). We now need to combine equations for \( m^\mu_\perp \) and \( Q^{\mu\nu} \). This can be done in two different ways.

i) Enslaving \( m^\mu_\perp \). In such case we have \( m^\mu_\perp = -i \hat{k}^\alpha \mathbb{P}^{\alpha\mu\beta} Q^{\alpha\beta} \), which leads to

\[
y (y + \frac{3}{d+4} \hat{k}^2 + (1 - \Delta)) Q^{\mu\nu} = 0, \tag{C.2.25}
\]

The corresponding spectrum is

\[
y = -(1 - \Delta) - \frac{3}{d+4} \hat{k}^2, \tag{C.2.26}
\]

which is negative for all \( \hat{k} \) only for \( \Delta < 1 \).

ii) Not enslaving \( m^\mu_\perp \). Here, we obtain

\[
y + 1 - \Delta + C_1 \hat{k}^2 + \frac{C_2}{y+1} \hat{k}^2 \) Q^{\mu\nu} = 0, \tag{C.2.27}
\]

where \( C_1 = \frac{2(d+1)}{(d+2)(d+4)} \), \( C_2 = 1/(d+2) \). The final spectrum is found to be

\[
y \pm = -\frac{1}{2} \left( 2 - \Delta + C_1 \hat{k}^2 \pm \sqrt{(\Delta - C_1 \hat{k}^2)^2 - 4C_2 \hat{k}^2} \right). \tag{C.2.28}
\]

The small and large \( \hat{k} \) expansions can be done:

\[
y_\pm = \begin{cases} -1 + \frac{C_2}{\Delta} \hat{k}^2 + O(\hat{k}^4) \\
-(1 - \Delta) - \left( C_1 + \frac{C_2}{\Delta} \right) \hat{k}^2 + O(\hat{k}^4) \end{cases} \tag{C.2.29}
\]

\[
y_\pm = \begin{cases} -C_1 \hat{k}^2 - (1 - \Delta - \frac{C_2}{\Delta}) + O(1/\hat{k}^2) \\
-(1 + \frac{C_2}{C_1}) + O(1/\hat{k}^2) \end{cases} \tag{C.2.30}
\]
C.3 Numerics

This appendix contains all details on the numerical simulations of the moment equations.

C.3.1 Explicit form of equations

In order to simulate the mean-field kinetic theory (4.1.4)-(4.1.6), we will use standard dimension-less variables (4.1.10). Upon rescaling the moment field $c, m, Q$ with the mean concentration $c_0$, and the velocity field with the swimming speed $\mathbf{u} \rightarrow v_s \mathbf{u}$, we the explicit form of the moment equations in $2d$ becomes

\[
c : \quad \partial_t c + (\nabla^x m^x + \nabla^y m^y) + (U^x \nabla^x c + U^y \nabla^y c) = 0, \quad (C.3.1)
\]

\[
m^x : \quad (\partial_t + 1) m^x + (\nabla^x Q^{xx} + \nabla^y Q^{xy} + \frac{1}{2} \nabla^x c) + (U^x \nabla^x m^x + U^y \nabla^y m^x) - \frac{2sB}{4} (m^x \nabla^x U^x + m^y \nabla^y U^x) + \frac{2sB}{4} (m^y \nabla^y U^x + m^y \nabla^x U^y) = 0, \quad (C.3.2)
\]

\[
m^y : \quad (\partial_t + 1) m^y + (\nabla^x Q^{xy} + \nabla^y Q^{yy} + \frac{1}{2} \nabla^y c) + (U^x \nabla^x m^y + U^y \nabla^y m^y) - \frac{2sB}{4} (m^x \nabla^x U^x + m^y \nabla^y U^x) + \frac{2sB}{4} (m^y \nabla^y U^x + m^y \nabla^x U^y) = 0, \quad (C.3.3)
\]

\[
Q^{xx} : \quad (\partial_t - \frac{1}{4} \nabla^2 + 1) Q^{xx} + \frac{1}{2} (\nabla^x m^x - \nabla^y m^y) + (U^x \nabla^x Q^{xx} + U^y \nabla^y Q^{xx}) - \frac{B}{4} c \nabla^x U^x + Q^{xy} (\nabla^x U^y - \nabla^y U^x) = 0, \quad (C.3.4)
\]

\[
Q^{xy} : \quad (\partial_t - \frac{1}{4} \nabla^2 + 1) Q^{xy} + \frac{1}{2} (\nabla^x m^y + \nabla^y m^y) + (U^x \nabla^x Q^{xy} + U^y \nabla^y Q^{xy}) - \frac{B}{4} c (\nabla^x U^y + \nabla^y U^x) + Q^{xy} (\nabla^y U^x - \nabla^x U^y) = 0, \quad (C.3.5)
\]

together with the Stokes equations

\[
-\nabla^x p + \nabla^2 U^x - 4\Delta (\nabla^x Q^{xx} + \nabla^y Q^{xy}) = 0, \quad (C.3.6)
\]

\[
-\nabla^y p + \nabla^2 U^y - 4\Delta (\nabla^x Q^{xy} - \nabla^y Q^{xx}) = 0, \quad (C.3.7)
\]

\[
\nabla^x U^x + \nabla^y U^y = 0. \quad (C.3.8)
\]

In $2d$, a divergence-less velocity field can be expressed in terms of a single scalar field $\psi$

\[
\mathbf{u} = (\nabla^y \psi, -\nabla^x \psi), \quad (C.3.9)
\]

which can be used for simplifying the equations. Taking curl of Stokes Eq., and looking at the $z$-th component, we obtain

\[
-\nabla^x \nabla^2 \psi + 4\Delta (2\nabla^x \nabla^y Q^{xx} + \nabla^y \nabla^y Q^{xy} - \nabla^x \nabla^x Q^{xy}) = 0. \quad (C.3.10)
\]

C.3.2 Further details about the numerical simulations

The simulations have been carried out using a parallel pseudo-spectral solver with full $3/2$ dealiasing implemented in Dedalus [151] on a domain $[0, \tilde{H}] \times [0, \tilde{H}]$, where $\tilde{H} = H\lambda/v_s$ is the system size normalised with the persistence length. All fields were represented by the Fourier decompositions using resolution $r = N \times N$, with $N = 4096$ spectral modes in each dimension. The time stepping used 4th-order semi-implicit BDF scheme [152], with the step $\Delta t = \lambda\Delta t = 15 \times 10^{-5}$, that is normalised with the tumbling rate. Each simulation was performed on ARCHER2 supercomputer using 2048 CPU.

We have observed that the smallest length-scale to be resolved is the scale of the persistence length, so the number of Fourier modes must be

\[
N \gtrsim \tilde{H}. \quad (C.3.11)
\]
Table C.1: System sizes used for various densities.

<table>
<thead>
<tr>
<th>Δ</th>
<th>1.3</th>
<th>1.4</th>
<th>1.5</th>
<th>1.6</th>
<th>1.7</th>
<th>1.8</th>
<th>1.9</th>
<th>2.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tilde{H}$</td>
<td>3000</td>
<td>2000</td>
<td>1500</td>
<td>1000</td>
<td>1000</td>
<td>750</td>
<td>750</td>
<td>750</td>
</tr>
</tbody>
</table>

In order to avoid finite size effects, the largest length-scale to be resolved is the correlation length (see Sec. 4.3.2). As the latter diverges at the instability point, the simulations close to the transition point $\Delta \to 1^+$ are computationally very expensive. In practice, different system sizes were used for different densities, shown in Tab. (C.1). Using these values, the absolute convergence in all cases was achieved.
Appendix D

Correlations

D.1 System size scaling

In this subsection, we will discuss the scaling of the connected correlation functions w.r.t. the system size. All results are valid in the thermodynamic limit. Let us first introduce dimensionless spatial and temporal variables

\[ \tilde{x} = x/H, \quad \tilde{t} = t/\tau \]  

where the time-scale is \( \tau = 1/(|\kappa|n) \), where the time-scale is chosen in such way that the dipole amplitude of the velocity field is equal to unity (see below). Within these dimensionless variables, the equations of motion (5.1.3)-(5.1.4) become.

\[ \frac{d\tilde{x}_i}{dt} = \tilde{v}_s p_i + U(\tilde{x}_i), \]  

\[ \frac{dp_i}{dt} = (1 - p_i p_i) \cdot (W(\tilde{x}_i) + BE(\tilde{x}_i)) \cdot p_i, \]  

where \( \tilde{v}_s = v_s \tau/H \), and the local velocity field is

\[ U(\tilde{x}_i) = \sum_{j \neq i}^N u_d(\tilde{x}_i - \tilde{x}_j; p_j), \]

where the dipole filed is

\[ u_d(\tilde{x}; p) = \frac{\text{sign}(\kappa)}{8\pi} \frac{\tilde{x}}{|	ilde{x}|^3} \left[ 3 \left( p \cdot \frac{\tilde{x}}{|	ilde{x}|} \right)^2 - 1 \right]. \]

The above definitions allow us to rewrite the first two terms of the BBGKY hierarchy, Eqs. (5.1.11), and (5.1.12) in such a way that the number of particles will only be present on in the driving terms (on the right hand side). The first two terms of the hierarchy are

\[ \partial_t F_1(\tilde{z}, t) + \mathcal{L}[F_1(\tilde{z}, t)](\tilde{z}) = -\nabla^\alpha \int d\tilde{z}' G(\tilde{z}, \tilde{z}', t) u_d^\alpha(\tilde{x}; \tilde{z}') \]

\[ -\frac{\partial}{\partial p^\beta} \int d\tilde{z}' G(\tilde{z}, \tilde{z}', t) p^\gamma X^\alpha_{\mu\nu\gamma} \nabla^\mu u_d^\nu(\tilde{x}; \tilde{z}'), \]  

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\[
\partial_t G(\tilde{z}_1, \tilde{z}_2, t) + \mathcal{L}[G(\tilde{z}_1, \tilde{z}_2, t)](\tilde{z}_1) + \mathcal{L}[G(\tilde{z}_1, \tilde{z}_2, t)](\tilde{z}_2) \\
+ \nabla_1^a \left[ F_1(\tilde{z}_1, t) \int d\tilde{z}' G(\tilde{z}_1, \tilde{z}', t) u_2^a(\tilde{x}_1; \tilde{z}') \right] \\
+ \nabla_2^a \left[ F_1(\tilde{z}_2, t) \int d\tilde{z}' G(\tilde{z}_1, \tilde{z}', t) u_2^a(\tilde{x}_2; \tilde{z}') \right] \\
+ \mathbb{P}_1^{\alpha \beta} \frac{\partial}{\partial p_i} \left[ F_1(\tilde{z}_1, t) p_1^\gamma X_1^{\alpha \mu \nu \gamma} \int d\tilde{z}' G(\tilde{z}_1, \tilde{z}', t) \nabla_1^\mu u_\gamma^a(\tilde{x}_1; \tilde{z}') \right] \\
+ \mathbb{P}_2^{\alpha \beta} \frac{\partial}{\partial p_j} \left[ F_1(\tilde{z}_2, t) p_2^\gamma X_2^{\alpha \mu \nu \gamma} \int d\tilde{z}' G(\tilde{z}_1, \tilde{z}', t) \nabla_2^\mu u_\gamma^a(\tilde{x}_2; \tilde{z}') \right] \\
= -S_{i,2}^F - S_{1,2}^G - S_{2,1}^G - S_{1,2}^H - S_{2,1}^H,
\]

where we have denoted \( \tilde{z} = (\tilde{x}, \mathbf{p}) \), the linear operator (5.1.13) has the form

\[
\mathcal{L}[\Phi] (\tilde{z}) = v_x \partial^a \nabla^a \Phi(\tilde{z}) + \nabla^a [\Phi(\tilde{z}) \mathcal{U}^a_{\text{MF}}(\tilde{x})] \\
+ \mathbb{P}^{\alpha \beta} \frac{\partial}{\partial p_i} [\Phi(\tilde{z}) p_i^{\gamma} X_i^{\alpha \mu \nu \gamma} \nabla^\mu \mathcal{U}^\gamma_{\text{MF}}(\tilde{x})] + \tilde{\lambda} \Phi(\tilde{z}) - \frac{\tilde{\lambda}}{4\pi} \int d\mathbf{p} \Phi(\tilde{z}),
\]

acting on the variable \( \tilde{z} \) of an arbitrary function \( \Phi = \Phi(\tilde{z}_1, \ldots, \tilde{z}_N) \), and the driving terms have the form

\[
S_{i,j}^F = \frac{1}{N} F_1(\tilde{z}_j, t) \left\{ \nabla_1^a \left[ F_1(\tilde{z}_i, t) u_2^a(\tilde{x}_i; \tilde{z}_j) \right] \\
+ \mathbb{P}_1^{\alpha \beta} \frac{\partial}{\partial p_i} \left[ F_1(\tilde{z}_i, t) p_1^\gamma X_1^{\alpha \mu \nu \gamma} \nabla_1^\mu u_\gamma^a(\tilde{x}_i; \tilde{z}_j) \right] \right\},
\]

\[
S_{i,j}^G = \frac{1}{N} \nabla_1^a \left[ G(\tilde{z}_i, \tilde{z}_j, t) u_2^a(\tilde{x}_i; \tilde{z}_j) \right] \\
+ \frac{1}{N} \mathbb{P}_1^{\alpha \beta} \frac{\partial}{\partial p_i} \left[ G(\tilde{z}_i, \tilde{z}_j, t) p_1^\gamma X_1^{\alpha \mu \nu \gamma} \nabla_1^\mu u_\gamma^a(\tilde{x}_i; \tilde{z}_j) \right],
\]

\[
S_{i,j}^H = N \int d\tilde{z}' \left\{ \nabla_1^a \left[ H(\tilde{z}_i, \tilde{z}_j, \tilde{z}', t) u_2^a(\tilde{x}_i; \tilde{z}') \right] \\
+ \mathbb{P}_1^{\alpha \beta} \frac{\partial}{\partial p_i} \left[ H(\tilde{z}_i, \tilde{z}_j, \tilde{z}', t) p_1^\gamma X_1^{\alpha \mu \nu \gamma} \nabla_1^\mu u_\gamma^a(\tilde{x}_i; \tilde{z}') \right] \right\}.
\]

We can now discuss the scaling of the connected correlation functions. First, observe that the normalisation condition implies \( NF_1 \sim n \sim 1 \), which gives \( F_1 = \mathcal{O}(1/N) \). Following the standard arguments \([131, 135]\), if we now neglect \( H \) in Eq. (D.1.7), the two-point connected correlation \( G \) turns out to be \( \mathcal{O}(1/N^2) \), because this is the order of magnitude of the RHS that does not depend on \( G \). At the expense of considerably longer computation, one can show that the \( s \)-point connected correlation is of order \( \mathcal{O}(1/N^{s+1}) \).
D.2 Double inverse Laplace transform

D.2.1 Non-interacting part

The double inverse Laplace transform in Eqs. (5.2.28) is performed in the following way. We observe that the two Bromwich integrals [139], can be written as

\[
\lim_{t \to \infty} \int_{\Gamma_1} \frac{ds_1}{2\pi i \lambda + s_1 + iv_s k(\hat{k} \cdot \hat{p})} e^{s_1 t} J(s_1),
\]

where

\[
J(s_1) = \int_{\Gamma_2} \frac{ds_2}{2\pi i s_1 + s_2 + \lambda + s_2 - iv_s k(\hat{k} \cdot \hat{p})} e^{s_2(t+T)}.
\]

By the definition of the inverse Laplace transform [139], the contours defining the integrals above have to be chosen such that \(\Gamma_2\) passes on the right of \(-s_1\) and of \(-\lambda + iv_s k(\hat{k} \cdot \hat{p})\), while \(\Gamma_1\) should pass on the right of all the poles of \(J(s_1)\) and of \(-\lambda - iv_s k(\hat{k} \cdot \hat{p})\). Observe that the first condition implies that \(\Gamma_2\) should be chosen on the right of \(-\Gamma_1\).

Next, we observe that, again from the definition of the inverse Laplace transform, \(J(s_1)\) is only defined for \(\text{Re}(s_1) > 0\). To proceed, we follow the method often utilised in plasma physics to describe the Landau damping [115,121]. We perform the analytic continuation of \(J(s_1)\) to purely imaginary values of \(s_1\) (recall that the analytic continuation of a complex function defined on an open set is the only function \(\hat{J}(s_1)\) that is analytic, defined on a larger set, and equals \(J(s_1)\) on the original set), and replace \(J(s_1)\) with \(\hat{J}(s_1)\) in Eq. (D.2.1). Since \(\lambda > 0\), the difficulty in performing the analytic continuation of \(J(s_1)\) lies in the pole at \(s_2 = -s_1\) of the integrand from Eq.(D.2.2). We, therefore, define [131]

\[
\hat{J}(s_1) = \int^* \frac{ds_2}{2\pi i s_1 + s_2 + \lambda - iv_s k(\hat{k} \cdot \hat{p})} e^{s_2(t+T)} \left| \begin{array}{c}
\ell(s_1) = \begin{cases}
0, & \text{Re}(s_1) > 0, \\
1/2, & \text{Re}(s_1) = 0, \\
1, & \text{Re}(s_1) < 0.
\end{cases}
\end{array} \right.
\]

The meaning of the integral denoted by \(\int^* ds_2\) above depends on the sign of \(\text{Re}(s_1)\): If \(\text{Re}(s_1) > 0\), it is just a standard complex integral over a contour passing on the right of \(-s_1\) and of \(-\lambda + iv_s k(\hat{k} \cdot \hat{p})\); If \(\text{Re}(s_1) = 0\), \(\int^* ds_2\) stands for a principal value integral; Finally, if \(\text{Re}(s_1) < 0\), \(\int^* ds_2\) stands for a standard complex integral over a contour passing on the left of \(-s_1\) but on the right of \(-\lambda + iv_s k(\hat{k} \cdot \hat{p})\). Note, that the second term in (D.2.3) represents a residuum at the pole \(s_2 = -s_1\), that arises from exchanging the integration contours \(\Gamma_1\), and \(\Gamma_2\). With the definitions above, it is easy to show that \(\hat{J}(s_1)\) is holomorphic in an infinitesimal stripe around \(s_1 \in \mathbb{R}\). Hence, it is the analytic continuation of \(J(s_1)\).

Replacing \(J(s_1)\) by \(\hat{J}(s_1)\) in Eq.(D.2.1), we obtain two terms. The first term, containing \(\int^* ds_2\), vanishes for \(t \to \infty\), since we are now free to choose the integration contours...
Γ₁ and Γ₂ such that Re(s₁ + s₂) < 0. The other term reads
\[
\lim_{t \to \infty} \int_{\Gamma_1} \frac{ds_1}{2\pi i \ s_1 + \lambda + ivs\cdot k\cdot p} \frac{\ell(s_1) e^{-s_1T}}{s_1 + \lambda - ivs\cdot k\cdot p},
\]
(D.2.5)
Closing the contour at +∞, the only pole contributing to the integral is at \(s_1 = \lambda - ivs\cdot k\cdot p\), and we obtain
\[
\lim_{t \to \infty} \int_{\Gamma_1} \frac{ds_1}{2\pi i \ s_1 + \lambda + ivs\cdot k\cdot p} J(s_1) = e^{-\lambda T + ivs\cdot k\cdot p}.
\]
(D.2.6)
Performing the remaining angular integration in (5.2.28), we finally obtain
\[
C_0(R, T) = \frac{n\kappa e^{-\lambda T}}{\pi^2} \int_0^\infty dk \frac{\sin kR}{kR} A^2(k\epsilon) \frac{y(12 - y^2) \cos y - (12 - 5y^2) \sin y}{y^5} \bigg|_{y = vs\cdot kT}.
\]
(D.2.7)

D.2.2 Interacting part
The integrand of Eq.(5.2.29) is not a rational function of \(s_1\) and \(s_2\), and we were unable to calculate its double inverse Laplace transform exactly. Instead, here we develop a rational approximation to \(\psi(z)\) that will allow us to find \(C_1(R, T)\) analytically.

First, we observe that if the poles of an analytic function are known, its large-\(t\) behaviour is determined by the pole with the smallest negative real part [139]. Therefore, the presence of the pole at \(-\lambda\) in Eq.(5.2.29) makes all poles with real parts smaller than \(-\lambda\) irrelevant in the large-\(t\) limit. This reflects the fact that individual tumbling events are always a source of de-correlation between microswimmers.

Next, we introduce the dimensionless persistence length \(L = vs/(\lambda\epsilon)\), which compares the typical runlength of a swimmer to the dipolar regularisation size, see Eq.(5.1.6). Although our theory is correct for any value of \(L\), in this work we consider \(L = 0 - 25\), ranging from non-swimming (shaker) particles to wild-type E.coli bacteria (see Section 5.3 for discussion). Contributions to the integrand in Eq.(5.2.29) with \(k\epsilon > 1\) are strongly suppressed by the regularising factor \(A(k\epsilon)\), and therefore, when approximating \(\psi(z)\), the relevant domain is \(-\lambda < \text{Re}(s) < 0\), with \(vs\cdot k/\lambda\) not exceeding \(L\).

In Appendix D.2.3 we show that a surprisingly good approximation to \(\psi(z)\) on this domain is given by
\[
\psi_a(z) = \frac{7}{7 + 3z^2}.
\]
(D.2.8)
The simple structure of this expression allows us to deduce the pole structure of the integrand in Eq.(5.2.29). Indeed, with \(\psi(z)\) replaced by \(\psi_a(z)\), and factorising
\[
\frac{1}{\omega - z\psi(z)} = \frac{7 + 3z^2}{3\omega (z - z_+)(z - z_-)},
\]
(D.2.9)
where
\[
z_{\pm} = \frac{7}{6\omega} \left[ 1 \pm \sqrt{1 - \frac{12}{7} \omega^2} \right],
\]
(D.2.10)
the denominators in Eq.\((5.2.29)\) can now be written as products of linear polynomials in \(s_1\) and \(s_2\). It is now straightforward to perform the inverse Laplace transform of this expression using the method outlined in Appendix D.2.1. Taking the limit of \(t \to \infty\), finally gives

\[
C_1(\rho, \tau) = e^{-\tau} \frac{nk^2}{15\pi^2 \epsilon} \int_0^\infty d\xi \frac{\sin \xi \rho}{\xi \rho} A^2(\xi) \left[ -\cos \left( \sqrt{\frac{3}{7}} L \xi \tau \right) ight. \\
+ \left. \frac{e^{\frac{1}{2} A(\xi) \Delta \tau}}{1 - A(\xi) \Delta + \frac{3}{7} L^2 \xi^2} \left\{ \frac{2 - A(\xi) \Delta + \frac{3}{7} L^2 \xi^2}{2 - A(\xi) \Delta} \cosh \left( \frac{1}{2} A(\xi) \Delta \tau \sqrt{1 - \frac{12L^2\xi^2}{7A^2(\xi)\Delta^2}} \right) \right. \\
+ \left. \frac{\sinh \left( \frac{1}{2} A(\xi) \Delta \tau \sqrt{1 - \frac{12L^2\xi^2}{7A^2(\xi)\Delta^2}} \right)}{\sqrt{1 - \frac{12L^2\xi^2}{7A^2(\xi)\Delta^2}}} \right\} \right], \quad (D.2.11)
\]

where we changed the integration variable to \(\xi = k\epsilon\), and introduced the dimensionless parameters \(\rho = R/\epsilon\) and \(\tau = \lambda T\). In Appendix D.2.4, we verify that Eq.\((D.2.11)\) provides a good approximation to the long-time behaviour of Eq.\((5.2.29)\).

### D.2.3 Approximating \(\psi(z)\)

Here, we develop an approximation to \(\psi(z)\) from Eq.\((5.2.30)\). Our goal is to find a rational function with a pole structure that is similar to the original \(\psi(z)\). As discussed in Section D.2.2, the relevant domain is set by the values of \(z\) given by \(z = \beta/(1 + s/\lambda)\), with \(\beta = v_s k/\lambda\) varying from 0 to \(L = v_s/\lambda\epsilon = 0 - 25\), and by the real part of \(s\) ranging from \(-\lambda\) to 0.

Our starting point are the observations that as \(z \to 0\), \(\psi(z) \to 1 - 3z^2/7\), while for \(z \to \infty\), \(\psi(z) \to 0\). Both asymptotic behaviours can be combined into \(\psi_a(z) = 7/(7+3z^2)\). Now we show that this is a surprisingly good approximation to \(\psi(z)\), both reproducing its global shape and having a similar pole structure. In Fig.D.1 we compare \(\psi(z)\) and \(\psi_a(z)\) for real values of \(s\). We observe a good agreement between the two functions for various values of \(\beta\). Similar, semi-quantitative, degree of agreement is observed for larger values of \(\beta\) and also for complex values \(s\).

To demonstrate that \(\psi_a(z)\) also reproduces the pole structure of \(\psi(z)\), we consider a

![Figure D.1: Comparison between \(\psi(z)\) (solid lines) and \(\psi_a(z)\) (dotted lines) for \(z = \beta/(1 + s/\lambda)\) for real values of \(s\) and various values of \(\beta\).](image)
We compute its inverse Laplace transform numerically, using the original function $\psi(z)$, and compare the result with the analytic expression, which we obtain by replacing $\psi(z)$ with $\psi_a(z)$ in the expression above. The latter is straightforward: factorising $\omega(7 + 3z^2) - 7z = 3\omega(z - z_+)(z - z_-)$, where $z_\pm$ are given in Eq.(D.2.10), we obtain

$$\frac{1}{\lambda \Delta A(k\epsilon)} \frac{z}{\omega - z\psi_a(z)} = \frac{1}{7s + \lambda} \frac{7(s + \lambda)^2 + 3(v_s k)^2}{(s + \lambda - \frac{v_s k}{z_+})(s + \lambda - \frac{v_s k}{z_-})}.$$  (D.2.13)

Performing the inverse Laplace transform of this expression and introducing the dimensionless time $\tau = \lambda t$ yields

$$e^{-\tau} \left[ 1 + \frac{2}{\sqrt{1 - \frac{12\beta^2}{7\Delta^2}}} \exp \left( \frac{\tau \Delta}{2} \right) \sinh \left( \frac{\tau \Delta}{2} \sqrt{1 - \frac{12\beta^2}{7\Delta^2}} \right) \right].$$  (D.2.14)

Since both $A(k\epsilon)$ and $\Delta$ take values between 0 and 1, for the purpose of comparing to its numerical counterpart, we set $A(k\epsilon) = 1$ in the expression above, without loss of generality.

The inverse Laplace transform of the original function Eq.(D.2.12) written in terms of the same parameters is given by the Bromwich integral

$$\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{s\tau}}{s + 1 - \Delta \psi(\beta/(s + 1))},$$  (D.2.15)

where $\gamma$ is a real number, chosen to be greater than the real part of any singularity of the integrand [139]. We perform this integral numerically, using the Gaver–Wynn–Rho algorithm as presented by Valko and Abate [153]. A Mathematica notebook with the details of this calculation can be found in the supplementary material [154].

In Fig.D.2A we compare Eq.(D.2.14) against the numerical Laplace transform of Eq.(D.2.15) for $\Delta = 0.1$ and $\beta = 0.1, 1, 10$. We observe a very good agreement,
which is not surprising: At small microswimmer densities, the hydrodynamic interactions between particles affect their dynamics only weakly, and correlations decay as $e^{-\tau}$. This regime does not test the quality of our approximation. A more stringent test is provided, on the other hand, in Fig.D.2B, were we compare the two Laplace transforms for $\Delta = 0.9$. For $\beta < 1$, we observe a very good agreement even at such high values of $\Delta$ (close to the mean-field transition). This is the most interesting regime, corresponding to large-scale motion in the suspension, and it is encouraging that our approximation shows quantitative agreement with the numerical data. Note that the black line and the black circles, corresponding to $\beta = 0.1$, do not follow $e^{-\tau}$, i.e. our approximation is capable of capturing a non-trivial decay rate. At higher values of $\beta$, corresponding to scales comparable to individual microswimmers, the agreement is semi-quantitative, but the overall decay is again close to the tumbling-dominated decay $e^{-\tau}$.

In Appendix D.2.4, we assess the quality of our approximation, when used in Eq.(5.2.29), which is its ultimate purpose.

### D.2.4 Numerical verification

In Section D.2.2, we performed the double inverse Laplace transform in Eq.(5.2.29) analytically by replacing $\psi(z)$ with $\psi_a(z)$, which led to Eq.(D.2.11). Here, we assess the quality of that approximation by performing the double inverse Laplace transform in Eq.(5.2.29) numerically. The relevant part of Eq.(5.2.29) reads

$$
2\mathcal{L}^{-1}_{\hat{s}_1,t} \mathcal{L}^{-1}_{\hat{s}_2,\tilde{t}+\tau} \left[ \frac{1}{1 + \hat{s}_1} \frac{1}{1 + \hat{s}_2} \frac{\hat{z}_1 \psi(\hat{z}_1) + \hat{z}_2 \psi(\hat{z}_2)}{\hat{s}_1 + \hat{s}_2} \right] 
\times \left[ \frac{\hat{z}_1 \psi(\hat{z}_1)}{\hat{\omega} - \hat{z}_1 \psi(\hat{z}_1)} + \frac{\hat{z}_2 \psi(\hat{z}_2)}{\hat{\omega} - \hat{z}_2 \psi(\hat{z}_2)} + \frac{\hat{z}_1 \hat{z}_2 \psi(\hat{z}_1) \psi(\hat{z}_2)}{(\hat{\omega} - \hat{z}_1 \psi(\hat{z}_1))(\hat{\omega} - \hat{z}_2 \psi(\hat{z}_2))} \right],
$$

(D.2.16)

where, in anticipation of performing numerical calculations, we introduced the dimensionless times $\tau = \lambda \tau$ and $\tilde{t} = \lambda t$, Laplace frequencies $\hat{s}_{1,2} = s_{1,2}/\lambda$, $\hat{z}_{1,2} = \beta/(1 + \hat{s}_{1,2})$, and $\hat{\omega} = \beta/\Delta$, where we absorbed $A(ke)$ into $\Delta$, as in Appendix D.2.3. In what follows, we set $\tilde{t} = 20$ to imitate the limit $\tilde{t} \to \infty$. The calculations are performed in Mathematics using the combined Fixed-Talbot and Gaver–Wynn–Rho algorithm described by Valko and Abate [153]. A Mathematica notebook with the details of this calculation can be found here [154]. The results are compared to the relevant part of Eq.(D.2.11), recast in the same dimensionless variables

$$
e^{-\tau} \left[ -\cos \left( \sqrt{\frac{3}{7}} \beta \tau \right) + \frac{e^{\frac{1}{2} \Delta \tau}}{1 - \Delta + \frac{6}{7} \beta^2} \left\{ 2 - \Delta + \frac{6}{7} \beta^2 \right\} \cosh \left( \frac{1}{2} \Delta \tau \sqrt{1 - \frac{12 \beta^2}{7 \Delta^2}} \right) + \frac{\sinh \left( \frac{1}{2} \Delta \tau \sqrt{1 - \frac{12 \beta^2}{7 \Delta^2}} \right)}{\sqrt{1 - \frac{12 \beta^2}{7 \Delta^2}}} \right\} \right].
$$

(D.2.17)

The results of the numerical double inverse Laplace transform and its analytical counterpart are shown in Fig.D.3. As in Appendix D.2.3, we focus on high values of $\Delta$, which provide the most stringent test of our results. For $\beta \leq 1$, the analytic approximation agrees quite well with the numerical data, capturing not only the decay rate, but also the oscillatory behaviour, as can be seen from the $\beta = 1$ case. These calculations required a
very high number of terms, $O(100)$, in the combined Fixed-Talbot and Gaver–Wynn–Rho algorithm [153]. For $\beta > 1$, we were unable to obtain converged results for the numerical Laplace transform for any viable number of terms in the numerical algorithm. Nevertheless, the results of Appendix D.2.3, and the degree of agreement exhibited in Fig.D.3 for the physically most relevant case of $\beta < 1$ make us confident that Eq.(D.2.11) faithfully reproduces the long-time behaviour of Eq.(5.2.29).
Bibliography


Mathematica files can be found at: https://doi.org/10.7488/ds/2894.