EFFECTIVE PROPERTIES AND COLLECTIVE DYNAMICS IN
BACTERIAL SUSPENSIONS

A Dissertation in
Mathematics
by
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Abstract

This dissertation introduces novel computationally efficient PDE models, which are used to investigate the origin of self-organization in bacterial suspensions. The key feature of these models is the incorporation of interbacterial interactions motivated by recent experimental observations suggesting their importance in the emergence of collective swimming. Results on well-posedness, effective properties and the onset of the collective state are established through rigorous asymptotic and numerical analysis. Each problem considered is highly multiscale in that microscopic interactions result in changes in the macroscopic state. This work provides a better understanding of the physical mechanisms governing the transition to collective motion.

Throughout this dissertation, novel models are employed where a bacterium is represented as a point force dipole subject to two types of interactions: hydrodynamic interactions and excluded volume type interactions introduced through the use of a short-range Lennard-Jones type repelling potential. The point dipole model accounts for the particle size through this potential and shape via Jeffery’s equations modeling how an ellipsoid interacts with the surrounding fluid. Confirming experimental observation, the mathematical analysis reveals that the alignment of asymmetrical particles and the presence of self-propulsion change the effective rheological properties of the suspension such as a drastic reduction in the effective viscosity. By providing explicit formulas for the effective viscosity as well as the effective normal stress differences, the theory presented herein can describe the complete rheological behavior of an active suspension undergoing planar shear in terms of known physical parameters.

The first few chapters (1-4) of this dissertation are concerned with introducing the PDE/ODE model for the suspension allowing for the investigation of this decrease in the effective viscosity. The main challenge is added complexity due to the incorporation of interbacterial interactions, in contrast to previous models.
valid only in the dilute regime. Rigorous mathematical analysis is then performed on the associated nonlinear non-local kinetic equation governing the evolution of the particle distribution function for bacterial positions and orientations. Using this approach, an explicit asymptotic formula for the effective viscosity in terms of known physical parameters is derived. This formula reveals the physical mechanisms responsible for the striking decrease in the effective viscosity observed in experiment; namely, the combination of self-propulsion, a non-uniform spatial distribution of bacteria due to interactions, and a non-spherical shape of bacteria. The model developed in this dissertation also allows for computationally efficient GPU numerical simulations containing a large number of particles, which are in agreement with the analytical results and experiment. This work is the first to capture the qualitative behavior of the effective viscosity observed in active suspensions for all experimental concentrations. In addition to the effective viscosity, the effective normal stress coefficients are also computed. The main mathematical result, which is presented in Chapter 4, is that the model proposed is well-posed and provides the existence of unique particle trajectories for all time.

The later chapters (5-6) of this dissertation explore more recent work, which involves understanding the onset of collective motion by investigating the spatiotemporal correlations associated with bacterial velocities. Numerical analysis of a thin film PDE model provides novel understanding of which physical mechanisms govern the onset, size, and duration of the collective state. Using the proposed model, this work confirms the recent experimental observation that particle size and shape rather than the concentration of bacteria or swimming speed governs the size and duration of the collective state in bacterial suspensions. In addition to verifying experimental observation, this work studies the effects of system parameters that are difficult to control in experiment such as the particle aspect ratio as well as the decoupling of swimming speed and the tumbling rate of bacteria. The current state of experiments does not allow for such an investigation, but our theory provides testable predictions for future work. The results of the analysis in this dissertation exemplify the delicate balance between hydrodynamic interactions and collisions governing collective motion in bacterial suspensions and provide important insights into its mesoscopic nature.
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Dedication

To my loving wife and best friend Ashley

“Choose a job you love, and you will never have to work a day in your life.”

– Confucius
Introduction

Animal swarms such as flocks of birds, swimming bacteria, herds of mammals, and schools of fish have captivated recent scientific interest in the physics, biology, and mathematics communities. Bacteria, the most prevalent creatures on Earth, are self-locomoting microorganisms which can exhibit the physical phenomenon of self-organization. Self-organization arises in bacterial suspensions in the form of large scale structures such as vortices or channels of unidirectional flow in a fluid suspension [3, 4, 5, 6, 7, 8]. Such structures have been observed in other organisms such as algae, sperm cells, synthetic swimmers [9, 10], colloidal membranes [11], granular matter [12], and magnetic particles [13].

The main focus of this dissertation is to provide a better understanding of a specific type of self-organization exhibited by bacteria – collective motion. Collective motion occurs when bacteria act as a group to form global patterns and flows which arise from microscopic interbacterial interactions. Collective motion leads to interesting effective rheological properties such as enhanced diffusion and faster movement of particles [3, 4, 5, 7, 8] and has become a prime area of interest in the physics and mathematics communities [14, 15, 16, 17, 18, 19]. One of the most striking experimental results has been the observation of a seven-fold viscosity reduction in a suspension of swimming bacteria (Bacillus subtilis) [20]. In addition, a recent work has also shown the ability of a suspension containing interacting bacteria to produce useful work through the rotation of microscopic gears [17]. The authors argue that collective motion leads to a decrease in the effective viscosity of the fluid allowing the gears to turn more easily.
In this dissertation, simple mathematical models are proposed and analyzed, which capture the results of experiments; specifically, the change in the effective viscosity due to the presence of active particles in a suspension and the correlation properties of the collective state. Beyond verifying experimental results, the model is then used to predict new phenomenon that are too difficult to study experimentally. The underlying goal of this dissertation will be to discover the physical mechanisms which lead to the transition to collective motion in active particle suspensions as well as how each effects the properties of the collective state.

In Chapter 2, a coupled PDE/ODE model (fluid/equations of motion) is introduced where bacteria are represented as interacting point dipoles with excluded volume constraints. Numerical simulations are performed on this model to compute the effective viscosity, $\hat{\eta}$. The numerical simulations show that the model captures recent experimental results through a full range of concentrations [20]. In Chapter 3, a kinetic model for the bacterial suspension is introduced in order to study the effective viscosity analytically. This model is used to derive an explicit asymptotic formula for the effective viscosity using the shape (aspect ratio) of the particle as a small parameter. This analytical formula is then compared to the numerical results of Chapter 2 for a wide range of system parameters to pinpoint the physical mechanisms responsible for the drastic reduction in the effective viscosity.

In Chapter 4, the global solvability is proven for the particle trajectories described by discrete ODE particle equations of motion previously introduced in Chapter 3 and the fluid equations are shown to be well-posed. From these results it is then shown that the kinetic theory is well-defined as well as the effective viscosity for semidilute bacterial suspensions. The main difficulty is observing that the effective viscosity is a function of the stress which crucially depends on the particle configurations.

In Chapter 5, the intrinsic properties of the collective state such as its size and duration are studied. This will be investigated by considering the spatial and temporal correlations associated to a bacterial suspension as functions of the system parameters such as concentration, swimming speed, shape, and dipole strength. This work advances both the fields of physics and mathematical biology by providing new physical insight into the mechanisms governing collective motion in animal populations as well as providing rigorous mathematical analysis of the
models used to form these conclusions.

1.1 Bacteria and their significance

While bacteria represent the most abundant organisms on Earth, their movement and behavior are not fully understood. In particular, there is a lack of knowledge on how they coordinate their movement or respond to environmental stimuli. The key feature of each bacterium is the utilization of self-generated propulsion to perform a desired task such as moving along a surface, swimming in a group, or forming complex fluid structures. While their self-organization and complex movement remains a central object of study, the purpose of understanding it is clear: bacteria can influence carbon cycling and sequestration, contribute to the decomposition of biomass, and have the ability to transform contaminants in the environment into innocuous byproducts. Understanding the microbial action of collective swimming will also help in understanding cellular responses to chemical and physical perturbations as well as the interactions between cells. This dissertation will contribute to the current understanding by developing predictive PDE models for the analysis of the effective properties and bacterial self-organization.

The fundamental issue of study is how collective behavior can arise from the dynamics of microscopic discrete interacting components. The models developed herein for self-propelled objects will exhibit long-range order as well as show distinct changes in the properties of the medium such as the effective viscosity. In the absence of direct communication, these microorganisms develop techniques for how to move more efficiently as a collective unit. In experiment it can be difficult to track individual interbacterial interactions or bacterial-fluid interactions, thus illustrating the need for the development of new mathematical models to obtain predictions related to the complex bacterial interactions that are required for collective motion. The importance of collective swimming can be seen in a wide range of field such as medicine where swarming bacteria moving in collective groups have exhibited enhanced resistance to antibiotics [21]. The remainder of this section is devoted to particular applications where the work contained in this dissertation can be used in a practical manner.
1.1.1 Carbon cycling and sequestration

The carbon cycle is a biogeochemical process by which carbon is exchanged between the ground and the many layers of the atmosphere. This is one of the key processes by which Earth maintains the ability to sustain life. Specifically, carbon sequestration, the process of storing carbon in a reservoir, by microbe rich soil has become a recent focus of biological studies. The reason for its importance is that soil, which can store carbon for greater periods of time, has the ability to decrease the amount of greenhouse gases accumulating in the atmosphere. Therefore, it is important to understand this process and how society on the ground can affect it in either a positive or negative way.

In particular, a recent work has demonstrated that the composition of a bacterial community greatly affects the carbon cycling in soil [22]. The work contained in this dissertation on large structure formation and collective motion may also be useful in determining how these communities form and disburse throughout the environment. Understanding the structure formation of microbes in these communities will help answer the question of the long-term existence of carbon in soil and whether it will be sequestered. In addition, understanding microbial community dynamics could improve the ability to predict greenhouse gas fluxes in the future [23]. Another recent paper highlights the development of an ocean carbon sequestration pump containing bacterial communities in order to study how bacteria can influence environmental dynamics [24, 25]. The importance of the microorganisms is that they generate dissolved organic matter, which is resistant to biological decomposition and assimilation allowing it to persist in a water column. This bacterial pump would allow for a greater distribution of carbon to the reservoirs on Earth’s surface greatly influencing the possible effects of climate change [26]. These are just a few particular examples of the need to understand and model communities of bacteria, which have an influence on the ecosystem as well as the global climate system.
1.1.2 Decomposition of biomass and transformation of contaminants

Environmental contamination, especially related to the petroleum industry, has become a recent epidemic. From the oil leak in the Gulf of Mexico to the chemically contaminated water near Charleston, West Virginia, society is still looking for an efficient, cost-effective way to clean up these hazards. One such approach called bioremediation relies on bacteria to remove harmful hydrocarbons transforming them into innocuous byproducts such as carbon dioxide, water, or other simpler organic compounds [27]. While traditional mechanical and chemical methods can be quite expensive when spills are large, bioremediation has become a promising alternative. The effectiveness of bioremediation is determined by maintaining a controlled rate of oxygen and nutrient concentration for the greatest rate of decomposition by the bacteria [27]. This article explains that the full potential of bacteria has not been reached due to a lack of understanding in their remediation mechanisms.

In addition to purely bacterial bioremediation, recent work focuses on plant-bacterial partnerships whereby the plant stimulates the bacteria to breakdown harmful hydrocarbons while the bacteria helped the plant grow and develop by inhibiting contaminant-induced stress responses [28]. The ability to control and enhance the movement of bacteria, which would use the harmful contaminants as a source of energy, could help in both the aforementioned processes.

1.1.3 Modern technology: Microfluidic devices

The study of microfluidics is concerned with the behavior of fluids at the microscale (e.g., the size of a bacterium $\sim 5 - 10\mu m$), which can be fundamentally different than any macroscopic behavior observed [29]. A microfluidic device is any device containing one or more channels with at least one dimension less than 1 mm. These devices are obtained as the result of shrinking a fluid system to the micron or submicron level. In such devices, fluids are confined to sub-millimeter channels where the surface tension, fluid viscosity, and energy dissipation dominate the behavior of the fluid. Naturally as a fluid system gets smaller the fluid regime, characterized by a small Reynolds number, becomes extremely viscous. At low
Reynolds numbers, devices which rely on inertial effects for their operation will no longer work; in contrast, the advantage of this regime is that turbulence is non-existent [30].

![Image of a microfluidic device](image)

**Figure 1.1.** Example of microfluidic device consisting of a microchip with microchannels from [1]. This device was designed for the rapid exchange of fluids for use in pharmacological studies.

The purpose of creating microfluidic devices is to alter the behavior of the fluid at the microscale for new and interesting uses such as DNA chips, fuel cells, microorganism capturing, and in the study of microbial motility and chemotaxis [31, 32]. The most prominent use is the so-called “lab-on-a-chip”, which is a miniaturization of many chemical processes onto a single silicon chip [30] (e.g., see Figure 1.1). The specific application pertaining to this dissertation is the use of microfluidic devices to create mechanical motion from swimming bacteria [17].

Recent work has focused on designing new microfluidic devices seeking to drive fluid transport by harnessing flagellar motion [33]. By utilizing bacteria such as *E. coli*, these microfluidic devices drive currents capable of guiding micro-objects on predictable trajectories at much greater speeds [33]. Through the study of bacterial suspensions, particularly the results on the decrease in the effective viscosity as a result of collective swimming, one may be able to alter the fluid flow significantly. Additionally, a simple estimate for the time to mix by diffusion is $t_D = \frac{\ell^2}{D}$ from [30] where $\ell$ is the container size and $D$ is the strength of diffusion shows that microfluidic devices with bacteria is ideal. Namely, these devices have a small container size $\ell \ll 1$ and collective swimming of bacteria greatly enhances the strength of diffusion [3, 4, 5, 7, 8] therefore decreasing the mixing time significantly. This effect may also be used to transport molecules (e.g., through their wake) in various media while increasing the rate of mixing. How useful work can be
extracted from bacterial suspensions is discussed in detail in the next section.

### 1.1.4 Extraction of useful work from chaotic motion

A recent experimental work [17], showed the ability to harness bacterial motion for the generation of useful work. While the laws of thermodynamics prohibit the extraction of useful work from the Brownian motion of particles at equilibrium, such extraction may be rectified under non-equilibrium conditions [17]. One such example is the placement of asymmetric geometrical objects in a bacterial suspension. Here it was observed that aerobic bacteria in a fluid film could power tiny gears in the suspension [17]. As a result of seemingly random bacterial motion, the gears rotate in the direction determined by the orientation of the slanted edges of the gear teeth. The key ingredient for the observation of the gears turning is that a spatial inversion symmetry is broken when the object is rotated [34].

It has been demonstrated in [20], that the collective motion of *Bacillus subtilis* results in a drastic reduction in the effective viscosity. This in combination with asymmetrical gear teeth, where bacteria become trapped when swimming, could result in the gears turning much more easily. This work demonstrated that the ability to control and harness collective motion will be an important requirement for the further development of mechanical systems driven by microorganisms. The understanding of bacterial collective motion can lead to the creation of machines in which bacteria move objects much more massive than themselves [17].

### 1.1.5 Understanding collective motion in higher life forms

From herding mammals to schooling fish, the mystery of collective motion in biological systems remains a fascination. While mammals, birds, and fish have brains and can think for themselves, they, like bacteria, can be seen exhibiting collective behavior. The study of bacteria, as opposed to these higher life forms offers many advantages while still providing essential insight. Bacteria cannot think for themselves and must respond to environmental cues from the surrounding world. In that sense they are simpler to model as an object possessing certain physical mechanisms corresponding to motion while still having a simple cellular structure.

The study of bacteria reveals the physical mechanisms responsible for collective
motion and the mathematical models used may be a foundation for study of more complex biological systems. In addition, there exists a rich array of experimental data on bacteria, which can be used to refine and enhance existing mathematical models before attempting to use them in a different context. Bacteria in their own right possess many interesting applications as listed above, yet they still provide a building block for more advanced studies on collective motion.

1.1.6 Practical significance of collective motion

This dissertation develops and analyzes theoretical models for suspensions that will lead to a greater understanding of collective motion for use in practical applications. Suspensions of microswimmers as well as other forms of active matter display remarkable properties of self-organization including large regions of correlated motion, increased mixing/diffusivity as well as greatly enhanced swimming velocities [35, 36, 37]. The subsections prior outline many applications of the study of bacterial suspensions such as carbon sequestration, decomposition of contaminants and the extraction of useful work from chaotic motion. Each of these applications heavily relies on exploiting the key features of collective motion.

One of the most recent applications is the study of flagellar synchronization, which some put in the class of nonlinear oscillators with long-range coupling [38]. This synchronization occurs when two individual bacteria swimming independently start to interact with each other resulting in the flagella beating at a common frequency. Potential applications of the study of collective flagellar dynamics include pendulums or even pacemakers for hearts [39]. Another recent application is the study of bacteria immersed in a suspension of liquid crystals [40]. New patterns and dynamics are observed including the modification of the orientational order of the liquid crystal by the bacteria as well as the liquid crystal revealing details of bacterial behavior not previously observed.

However, the main motivation for the study of microsystems remains the demand for nanotechnological applications, which carry out specified functions at the nanoscale such as in drug delivery by nanoparticles to cellular targets or parallel assembly of micromachines by self-propelled agents [41]. By fully understanding the physically mechanisms behind collective swimming of bacteria one can then
design mechanical microswimmers, which are easier to control for a desired purpose and still capable of producing the same effects [9, 10]. Before proceeding to theoretical models for microswimmers in this dissertation one must fully understand the relevant physical features of bacterial suspensions.

1.2 Physical background

Recent experimental observations on *Bacillus subtilis* and *E. coli* provide the main motivation for this dissertation. Thus, the models herein are developed to study these types of motile swimmers. The defining characteristics of each are a body and several flagella, which bundle to form a helical structure, see Fig. 1.2 (left). Each is a single-celled rod-shaped microorganisms ranging from 5-10 µm in length, which is roughly six times its width. Each bacterium propels itself by bundling its flagella and exerting a force, $f_p$, on the fluid. In turn, this results in a drag force on the body of each bacterium. Naturally under these conditions a bacterium of this form is best represented by a force dipole where the two aforementioned forces are equal in magnitude and opposite in orientation. Bacteria spend the vast majority of time in the forward propelling state; however, at times when a bacterium’s environment (e.g., oxygen concentration in the surrounding fluid) displays unfavorable conditions they can be observed “tumbling”. This phenomenon is a random re-orientation occurring when a bacterium unbundles its flagella and each moves in an indeterminate way. In Chapters 2-4, the effect of tumbling is not considered, because the environment is assumed to be nutrient rich and tumbling is therefore a rare event. In Chapter 5, the effect of tumbling on the transition to the collective state is considered.

There are two standard classifications of swimmers by mode of propulsion. The first type referred to hereafter as a “pusher” propels itself from behind by bundling its flagella. Examples of pushers are *E. coli* and *B. Subtilis*, the primary strain of bacteria focused on in this dissertation. The other type uses its flagella in front to pull fluid towards its body like a breaststroke and referred to hereafter as a “puller”. This results in the forces present in the dipole to be inverted. Examples of pullers are algae such as *Chlamydomonas* and *Volvox* [2]. For a schematic of each type see Figure 1.2.
Figure 1.2. Left: Pushers such as *E. coli* bundle flagella to propel forward (outward force dipole). The bacterium’s body rotates in the opposite direction to conserve angular momentum. Right: Pullers such as *Chlamydomonas* swim via a breast stroke type motion using two large flagella to pull water towards its body (inward force dipole).

1.3 Review of mathematical notions

Throughout this dissertation the notation will be kept consistent and will follow the guidelines and procedures outlined in the following subsections unless otherwise indicated. The set of real numbers, integers, and natural numbers will be given by \( \mathbb{R}, \mathbb{Z}, \) and \( \mathbb{N} \) respectively. A point in \( n \) dimensional space is denoted by \( \mathbf{x} = (x_1, \ldots, x_n) \). The notion of a scalar product and the standard euclidean norm are also introduced as follows:

\[
(x, y) := x_1y_1 + \ldots + x_ny_n, \quad |\mathbf{x}| := \sqrt{(\mathbf{x}, \mathbf{x})} = (x_1^2 + \ldots + x_n^2)^{1/2}.
\] (1.1)

In addition, some notation for sets is employed. The closure of a set \( \Omega \) will be denoted by \( \overline{\Omega} \) and its boundary as \( \partial \Omega = \overline{\Omega} \setminus \Omega \). If a set \( \Omega' \) is bounded and its closure lies in \( \Omega \) then we indicate this by \( \Omega' \Subset \Omega \). In a few of the chapters a domain in the form of a cube of side length \( L, \mathbb{D} := \{ \mathbf{x} \in \mathbb{R}^3 \mid |x_i| \leq \frac{L}{2}\} \), is considered. Denote a ball centered at \( x_0 \) of radius \( r \) by \( B_r(x_0) \). The *characteristic function* of a set \( \Omega' \) is the function \( \chi_{\Omega'}(x) \) which is 1 for \( x \in \Omega' \) and 0 for \( x \notin \Omega' \).

A vector will be denoted with a bold letter, \( \mathbf{v} \), with components \( v_i \). A second rank tensor will have a capital bold letter, \( \mathbf{E} \), with components \( E_{ij} \). For tensor and vector operations Einstein summation convention will be adopted throughout this dissertation where repeated indices shall be summed, \( v_iw_i = \sum_i v_iw_i = \mathbf{v} \cdot \mathbf{w} \). In addition, a colon will indicate a contraction between two second rank tensors, \( \mathbf{E} : \mathbf{F} := E_{ij}F_{ij} \).
Differential operators will be denoted by $D = (D_1, \ldots, D_n)$ with $D_j = \frac{\partial}{\partial x_j}$ for $j = 1, \ldots, n$. Then

$$D^\alpha f(x) = \frac{\partial^{|\alpha|} f(x)}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}$$

for multi-index $\alpha = (\alpha_1, \ldots, \alpha_n)$ with $|\alpha| = \alpha_1 + \alpha_2 + \ldots + \alpha_n$. We will use $C^k(\Omega)$ to denote the set of all continuous functions $f(x)$ with continuous derivatives up to order $k$ and $C^\infty(\Omega)$ is the set of infinitely differentiable functions on $\Omega$.

The Lebesgue integral of a function $f(x)$ over an open set $\Omega$ is denoted by

$$\int_\Omega f(x) \, dx,$$

and over $\mathbb{R}^n$:

$$\int f(x) \, dx := \int_{\mathbb{R}^n} f(x) \, dx.$$

The space $L^p(\Omega)$ can now be defined as the collection of all measurable functions $f$ on $\Omega$ where the following quantity

$$\|f\|_{L^p(\Omega)} := \begin{cases} \left( \int_\Omega |f(x)|^p \, dx \right)^{1/p}, & 1 \leq p < \infty, \\ \text{ess sup}_{x \in \Omega} |f(x)|, & p = \infty, \end{cases}$$

defines a norm when it is finite. If the space $\Omega$ is not indicated then assume the norm is taken over $\mathbb{R}^n$. Extend this definition by defining the space of $p$–locally summable functions in $\Omega$, $L^p_{loc}(\Omega)$, as the collection of measurable functions $f$ such that $f \in L^p(\Omega')$ for all $\Omega' \subseteq \Omega$.

Next, a brief review of distributions is now provided. Any information on generalized functions (distributions) needed to understand the work carried out in this dissertation, specifically in Chapter 4, can be found within texts such as [42]. A summary of the basic notions is provided here. Consider first an important space of functions referred to as test functions, $\mathcal{D}(\Omega) = C^\infty_c(\Omega)$, composed of infinitely differentiable functions with compact support. A similar notation is used for functions in $n$ dimensions, $[\mathcal{D}(\Omega)]^n$. A notion of convergence can be defined on this space: A sequence of functions $\{\varphi_i\}_{i=1}^\infty \subset \mathcal{D}(\Omega)$ converges to a function $\varphi$ if there exists a set $\Omega' \subseteq \Omega$ such that $\text{supp}(\varphi_i) \subset \Omega'$ and for every $\alpha$

$$D^\alpha \varphi_i(x) \Rightarrow D^\alpha \varphi(x), \quad i \to \infty,$$

where $D^\alpha$ denotes derivatives of order $\alpha$ and $\Rightarrow$ denotes uniform convergence. In
other words, the function $\varphi_i$ and all its derivatives must converge uniformly to $\varphi$ on a compact subset of $\Omega$.

The space of distributions (also referred to as generalized functions), $\mathcal{D}'(\Omega)$, is the space of bounded linear functionals or the dual space of $\mathcal{D}(\Omega)$. The value of the functional $f \in \mathcal{D}'(\Omega)$ at $\varphi \in \mathcal{D}$ is denoted as a pairing $(f, \varphi)$. Generalized functions have three main properties:

(i) A generalized function $f$ is a functional on $\mathcal{D}(\Omega)$ in the sense that $f : \mathcal{D}(\Omega) \mapsto \mathbb{R}$.

(ii) A generalized function $f$ is linear on $\mathcal{D}(\Omega)$, for $\varphi_1, \varphi_2 \in \mathcal{D}(\Omega)$ and $a, b \in \mathbb{R}$ we have

$$ (f, a\varphi_1 + b\varphi_2) = a(f, \varphi_1) + b(f, \varphi_2). $$

(iii) A generalized function $f$ is continuous on $\mathcal{D}(\Omega)$, that is $\varphi_k \to \varphi$ as $k \to \infty$ in $\mathcal{D}(\Omega)$, then

$$ (f, \varphi_k) \to (f, \varphi), \quad \text{as } k \to \infty. $$

Two generalized functions are identified with one another, $f = g$, if $(f, \varphi) = (g, \varphi)$ for every $\varphi \in \mathcal{D}(\Omega)$. Examples of distributions are any function in $L^1_{\text{loc}}(\Omega)$ (regular distributions) or the delta function $\delta(x)$. A regular generalized function or distribution is a generalized function, which can be represented by a locally summable function in $\Omega$

$$ (f, \varphi) = \int_{\Omega} f(x)\varphi(x)dx, \quad \text{for all } \varphi \in \mathcal{D}(\Omega). $$

The natural notion of convergence on the space of generalized functions is called distributional convergence. A sequence of generalized functions $\{f_i\}_{i=1}^\infty \subset \mathcal{D}'(\Omega)$ converges to $f \in \mathcal{D}'(\Omega)$ if for any test function $\varphi \in \mathcal{D}(\Omega)$, $(f_k, \varphi) \to (f, \varphi)$ as $k \to \infty$. Distributional convergence is denoted by $f_k \to f \in \mathcal{D}'(\Omega)$. The space of generalized functions is complete with respect to the weak topology.

A generalized function $f(x) \in \mathcal{D}'(\mathbb{R}^n)$ is called periodic with period $T = (T_1, \ldots, T_n)$, $T_j > 0$, if it is periodic with respect to each argument $x_j$ with pe-
The collection of all periodic generalized functions of an \( n \)-period \( T \) are denoted by \( \mathcal{D}_T \). Let \( f \in \mathcal{D}_T \) and consider the formal series

\[
f(x) = \sum_{|k|>0} f_k e^{i(k\omega,x)}, \quad f_k := \frac{(f,e^{i(k\omega,x)})_T}{T_1...T_n},
\]

where \((f,\varphi)_T = \int_0^{T_1} ... \int_0^{T_n} f(x)\varphi(x)dx\). This quantity is the Fourier series and the numbers \( f_k \) are called the Fourier coefficients of \( f \). Note that a periodic generalized function is completely determined by its Fourier coefficients and if \( f \in L^1_{loc} \cap \mathcal{D}_T \), then its Fourier series coincides with the classical Fourier series [42].

### 1.4 Stokes equation

A bacterium such as \( B. \ subtilis \) has characteristic size \( \ell \sim 5\mu m \), characteristic swimming speed \( V_0 \sim 20\mu m/s \), and the kinematic viscosity for water \( \nu = \frac{\eta}{\rho} \sim 10^{-2} cm^2/s \) where \( \rho \) is the fluid density. Using these quantities one can compute the Reynolds number

\[
Re = \frac{V_0 \ell}{\nu} \sim 10^{-5} \ll 1.
\]

The Reynolds number gives the ratio of inertial to viscous forces. Since the Reynolds number for bacterial motion is so small, all inertial forces can effectively be neglected. Most fluids can be accurately modeled using the well-known nonlinear Navier-Stokes equations, but in this special case where the Reynolds number \( Re \ll 1 \) the fluid can instead be represented by Stokes equation. In addition, the time scale for bacterial motion is assumed to be much smaller than the characteristic time scale for the system. Therefore, one can reduce the model for the fluid to the steady Stokes equation

\[
\rho \left[ \frac{\partial}{\partial t} \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} \right] = -\nabla p + \eta \Delta \mathbf{u} + \mathbf{f} \quad \rightarrow \quad \eta \Delta \mathbf{u} = \nabla p - \mathbf{f}
\]
where \( \eta \) is the ambient viscosity, \( \mathbf{u} \) is the fluid velocity, \( p \) is the pressure, and \( \mathbf{f} \) are additional forces acting the fluid such as those due to particle self-propulsion. In addition, the fluid under consideration here is incompressible \( \nabla \cdot \mathbf{u} = 0 \). From henceforth when considering the fluid equations we will only consider the incompressible steady Stokes equations where \( \mathbf{f} \) is the force on the fluid due to bacterial self-propulsion defined explicitly in the following chapters.

### 1.5 Experimental results on collective motion

In this section, a few key experiments performed by Dr. Igor Aronson and his collaborators at Argonne National Laboratory are highlighted as well as recent results of other experimental groups from around the world. Collective motion, a drastic reduction in the effective viscosity, and enhanced diffusivity are just a small sample of the experimental observations any first principle model should seek to capture analytically. These experimental observations will serve as the primary motivation for the proceeding mathematical analysis carried out in this dissertation.

In [20], the first experimental comparison of the effective viscosity (as a function of concentration and swimming speed) of an active bacterial suspension to that of a passive suspension is performed. The viscosity was measured in two ways. First one can study the rate of decay of a vortex induced by a moving probe and second one can measure the viscous torque on a rotating magnetic particle immersed in the film. The authors found a few striking observations; namely, an up to 7-fold reduction in the effective viscosity as the concentration increases from 0 to 2% and a linear decrease in viscosity with increasing swimming speed. From two separate experiments it was observed that the viscosity of a bacterial suspension strongly depends on the concentration and the swimming speed. The mechanism for the reduction is the transformation of chemical energy from nutrients into kinetic energy in the form of fluid motion. The effective viscosity results from this work will be directly compared with the numerical results obtained in Chapter 2 through a full range of concentrations.

In [43], an experimental comparison of the effective viscosity for an active suspension of *Chlamydomonas Reinhardtii* (Pullers) to a suspension of dead cells
at the same volume fraction was performed. The authors discovered a suspension of living Pullers exhibits an increase in viscosity almost two times as great as that of a dead (passive) suspension. They conclude that there are two possible reasons for the greater increase in viscosity for active suspensions: Experimental observation suggested the torque due to gravity might be necessary or that the beating flagella give the particle a greater aspect ratio than its circular body leading to a preferential alignment consistent with the results shown in this dissertation. This provides evidence that shape is important in considering microscopic models in the study of effective properties. Brownian motion or thermal noise is negligible in their work since the radius of *Chlamydomonas* $R \sim 5 \mu m$ is large relative to the size of a fluid molecule. To obtain their result, the authors use an approximation similar to the Einstein formula to measure viscosity

$$\eta_{eff} \approx \eta_0 (1 + \alpha \varphi)$$

where experimentally the dead suspension was fit with $\alpha = 2.5$ consistent with Einstein’s work on passive suspensions [44, 45, 46] and $\alpha = 4.5$ for an active suspension explicitly showing the greater increase in viscosity. The work of Einstein has been rigorously justified in [47, 48].

In [35], experiments were performed to separate the effects of bioconvection (characterized by enhanced diffusion of oxygen and bacteria [35] and occurs even in dilute suspension based on the oxygen concentration) versus three-dimensional collective motion in bacterial suspensions both experimentally and theoretically. This work established the possible biological advantage of self-organization relative to random swimming motions and the relationship between collective motion and bioconvection. The authors found that beyond a certain film thickness ($z\text{-component open to oxygen}$) there exists a transition from quasi-2D to collective swimming characterized by enhanced diffusion of oxygen and bacteria (turbulent behavior). Recently, a theoretical study compared the instabilities associated to collective motion both due to chemotaxis and hydrodynamics [49]. The authors showed using a theoretical continuum model that these two forms of collective motion have a different nature. In this dissertation, bioconvection resulting from chemotaxis is not studied, but rather the complex motion observed by quasi-2D
collective swimming.

In [5], the authors investigate how spatiotemporal correlations depend on the concentration of microorganisms and how the concentration can be managed as a control parameter. They found for a thin film geometry, the correlation length varies smoothly and monotonically through the transition from individual to collective motion. This is explained as a noise-induced smearing of a dynamical phase transition where the source of noise can be due to 1. Spontaneous orientation fluctuations of individual bacteria due to tumbling, 2. Small-scale hydrodynamic fluctuations due to flagellum rotation, or 3. Size distribution of bacterium. The main result is the formation of collective swimming without chemotactic effects, which are also not accounted for in the models developed in this dissertation. Also, the oxygen gradient is kept uniform due to the thin film resulting in no bioconvection, which could disrupt the natural collective motion. In Chapter 5, this phase transition is captured through numerical simulations using the model presented in this dissertation by accounting for 1. and 2. but not 3. since all bacteria are taken to be uniform.

Chapter 5 of this dissertation is partially spent verifying the experimental observations in [50]. Namely, that hydrodynamic interactions and collisions lead to collective motion at high concentrations. The authors observed the following intriguing result: The correlation length and time remain constant beyond the critical threshold for collective motion even though the energy injection rate is proportional to the swimming speed and concentration. In addition, this study revealed that the radius for correlated motion is an intrinsic property of the bacteria suggesting that far beyond the concentration threshold the correlation length is entirely determined by properties of the swimmers: their size (including length of flagella) and shape.

In [2, 8, 51, 52, 53] the authors observe features of self-sustained active turbulence in bacterial suspensions. Chemotaxis is ignored since it is not relevant in closed chambers. The particles only move by their own propulsion and steric interactions (no hydrodynamic interactions). The authors suggest that future work should focus on more realistic models that account for hydrodynamic near-field interactions and intrinsic randomness in bacterial swimming. In [54], the authors carry out the first successful measurement of the three-dimensional velocity field in
a dense suspension of bacteria. They then study how energy is transported from the individual cell scale to the larger mesoscale in a suspension of bacteria and claim that the theories that model a bacterium as a force-dipole particle (as in this dissertation) predict mesoscale energy dissipation. These results all highlight the multiscale nature of this dissertation.

1.6 Previous work on suspensions

1.6.1 History

Particles such as bacteria in suspensions of fluid have been of interest since the early 20th century. Currently, given the advancements in nanotechnology and the power of modern day scientific equipment, studying bacteria is far easier than it had been. Physicists and mathematicians have been developing a model for particles in a suspension for around 90 years. This quest began with Jeffery (1922) when he studied the motion of small rigid spheroids in a Newtonian fluid undergoing a uniform shear flow [55]. Jeffery found that these particles will move with the velocity of the fluid at the particle’s center in the situation where no body forces or other interactions are present. He also found that the axis of rotation for such a particle is an infinite family of periodic orbits and a particle would remain in the same orbit for all time (see Appendix A). These so-called Jeffery orbits were observed in the absence of Brownian motion consistent with bacterial suspensions where thermal (Brownian) noise is negligible.

In 1962, Bretherton continued this work by showing that the analysis of any rigid body of revolution in a single shear flow is identical, one must just replace the aspect ratio, \( r \), with \( r_e \) which depends on the specific shape of the particle [56]. This work was mostly abandoned until 1971 when Leal and Hinch introduced a rigorous three-dimensional model for a dilute suspension of rigid spheroids [57, 58]. In their work a differential equation for the probability distribution of orientations is developed and solved using asymptotics, but is only good for limiting cases. Their results were used to determine the effective viscosity of a dilute suspension of passive ellipsoids.

In mathematics this problem was first considered in the dilute limit where
bacterium-bacterium interactions are not considered. The particle’s motion and orientation are determined only by its interaction with the fluid. As a suspension becomes more dilute the random reorientation by Brownian type motion becomes critical in determining how these particles will move and interact. The study of the orientation of a bacterium is crucial for understanding the evolution of a bacterial suspension. Effective properties of the suspension such as viscosity are dependent on the orientation of the particles [59]. Thus, it is important to develop a correct probability density function for orientations to ensure that experimental results can be captured by such a model.

1.6.2 Dilute active suspensions

Many past works of others have focused on studying models related to active suspensions, defined as suspensions where particles or inclusions inject energy into the system in this case through the force of self-propulsion on the surrounding fluid. These past works are now briefly reviewed. The first such model was proposed by Ramaswamy et al. in [14, 15]. This group of researchers pioneered the study of effective properties by introducing a continuum phenomenological model based on liquid crystals. In their model, evolution equations for liquid crystals are modified to resemble rod-like self-propelled particles coupled to the Navier-Stokes equations for the fluid. The authors performed the first stability analysis of a collection of low Reynolds number swimmers by studying an initially aligned swimmer suspension as an active nematic (particles align longitudinally resulting in the suspensions displaying long range order). Upon doing linear stability analysis, their model predicts that in the Stokes flow regime there is an instability of the uniform state providing the first theoretical signs of collective motion. While providing novel insights this model was not derived from first principles and cannot be used to pinpoint the exact physical mechanisms leading to the change in the rheological properties of the suspension unlike the model proposed in this dissertation. Graham et al. [60] also notes that the model in [14, 15] does not capture the first principles details of hydrodynamic interactions, is limited to very large length scales, and has too many free parameters for conclusive analysis beyond linear stability.

Next, slender-body theory based models with no near-field interactions were
extensively studied in [49, 61, 62, 63, 64]. Slender-body theory takes advantage of
the elongation of a body to obtain an approximation to the field surrounding it
and/or the net effect of the field on the body. Consider a rod with length \( \ell \) and
radius \( a \), then slender-body theory is concerned with \( a \ll \ell \), which modifies the
standard multipole expansion (see Appendix B.1.1) for the axissymetric rod case.
The authors introduce a first principles continuum kinetic model for dilute bacte-
rial suspensions and perform a linear stability analysis to investigate the stability
of the isotropic state. The kinetic theory was derived under the assumptions of
several separations of scale, no direct rod-rod interactions (dilute assumption), and
displayed finite domain effects (removed in future simulations [65]). Another key
feature of the model is the inclusion of randomness through a diffusion term in the
Fokker-Planck equation governing the evolution of the particle density. Slender-
body theory was also used in combination with regularized Stokeslets in [66] where
a singular fundamental solution is replaced by a radially symmetric smooth func-
tion defined over a small neighborhood in order to compute the flow around an
elongated body.

The authors find that the perturbation from isotropy grows without bound at
finite wavelengths for suspensions of pushers and decays to the uniform state for
suspensions composed of pullers extending the results of [14, 15]. Similar results
were derived concurrently by different authors in [67, 68]. The authors conclude
the reason for the growth of perturbations for pushers is not from fluctuations
in density, but due to oscillations in swimmer orientation. This model added
additional features not present in [60] such as an extended body, but still lacks
excluded volume constraints and the flow is different than a force dipole both shown
to be needed to capture experimental observations of real bacteria [2]. Similar
continuum kinetic models were also used by the same authors in [69, 70] where they
found that pairwise hydrodynamic interactions (within the Stokes approximation)
alone do not yield homogeneous orientational order in the suspension, but when
steric effects are incorporated in the model, the swimmers order in a nematic state
at high density. This shows the importance of adding excluded volume constraints
and incorporating the effects of collisions.

More recently, Haines et al. [59, 71, 72, 47] revisit and expand on the work
of Leal and Hinch and develop both a two and three-dimensional PDE model for
ellipsoids in a suspension as well as analyze the long-term dynamics of the particle
distribution density governed by a Fokker-Planck equation. The authors introduce
the presence of white noise so that they can ensure that the steady-state distribu-
tion of orientations of the bacteria is unique as well as considering the effect of
tumbling (random reorientation) equivalent to the Brownian motion present in [57]
and [58]. This white noise allows the evolution of the particle orientation distribu-
tion to be governed by a three-dimensional Fokker-Planck equation. This equation
could not be solved analytically and the authors used asymptotic techniques to
derive conclusions in limiting cases. An explicit asymptotic formula for the effec-
tive viscosity in dilute suspensions with tumbling was computed. In another recent
work [73], the authors consider a single dipole swimmer in a channel and study
the resulting stable trajectories in nonlinear Poiseuille flow. The conclusions from
all these works reaffirm recent experimental work outlined in Section 1.5.

The model presented in this dissertation will incorporate hydrodynamic inter-
actions and excluded volume constraints/collisions in the semidilute case with the
ability to derive similar results as Haines et al. as well as gain a better under-
standing of the role of interactions on the effective properties. The challenge is
the dramatic increase in complexity. For dilute suspensions one must solve essen-
tially a single bacterium problem in an infinite domain where the only quantity
of importance is the orientation of that single bacterium representing only 2 vari-
ables. In the semidilute case we must solve the complete system of $5N$ coupled
ordinary differential equations in order to analyze the effective properties of the
suspension. This requires introducing a more simplistic model that still captures
all the relevant physical features present in real bacteria.

1.7 Modeling semidilute active suspensions

The bacterial suspensions under consideration in this dissertation are a specific
example of an active suspension. The previous section reviewed the study of the
effective viscosity using models for dilute active suspensions in theoretical works
simulating very low concentrations [62, 71, 72, 74]. There the effective viscosity of
a bacterial suspension can be defined using the time average of the stress and then
ergodicity is used to replace the time average with an average over the phase space
of $N$ bacterial orientations of the suspension [59]. Similarly, the effective viscosity is considered in the semidilute regime where pairwise hydrodynamic interactions between particles are incorporated using the superposition principle such as in [75] where the flow acting on a given particle is the sum of flows from all other particles. There and in Chapters 2-3 it is shown that the reduction in the effective viscosity for low volume fractions in the absence of tumbling is due to these hydrodynamic interactions.

One of the first models for interacting particles was introduced by Vicsek et al. [76, 77] where each particle moves with a constant speed and a collision mechanism is replaced by the rule that a particle assumes the local average orientation of its neighbors. Also included is a random perturbation of the particle orientation, which accounts for any noise in the system. This is regarded as one of the first theoretical models to predict collective motion in interacting particle suspensions. There are key differences between this model and the model which is introduced in this dissertation. In the proposed model the orientation will evolve according to interaction with the background flow and hydrodynamic interactions with other particles in addition to explicit excluded volume constraints representing collisions as opposed to a rule based mechanism. Also, in the model proposed in this dissertation the mean particle velocity is not kept constant and in fact exhibits a dramatic increase once the suspension reaches the collective state consistent with experiment [5, 50].

Recently, another attempt was made to make a dilute model valid at higher concentrations by adding a torque from [78] due to steric effects in passive rodlike suspensions [64]. Through linear stability analysis the authors were able to show an instability in an isotropic suspension before the transition to nematic order in the rods. This shows that both hydrodynamic interactions and collisions are needed for collective motion. In this dissertation a first principles model is developed that directly incorporates both interbacterial hydrodynamic interactions as well as collisions due to excluded volume constraints.
1.7.1 Incorporating interactions

Mathematically, we define a semidilute suspension as one that satisfies the superposition principle: the flow at any point in the fluid is the sum of the flows induced by the individual moving particles (see, e.g., [75]). Since the fluid will be modeled throughout this dissertation with the linear incompressible Stokes equation, then all the contributions to the flow can be separated. In contrast to a dilute suspension where particles only interact with the ambient background flow, interparticle interactions will be the main contribution to the evolution of the particle trajectories. The model accounts for two forms: (i) interparticle hydrodynamic interactions which account for the fluid flow produced by one bacterium on another and (ii) collisions/excluded volume interactions which result from the fact that particles take up space and when near each particle’s body can effect another particle’s motion.

A bacterium will be modeled as a point force dipole and is given excluded volume constraints via the use of a Lennard-Jones-type repelling potential. The point dipoles are considered as infinitesimal spheroids with shape incorporated through the particle equations of motion to be defined explicitly in Chapter 2. The main contributions to translational motion are self-propulsion, the flow induced by other particles, collisions, and the ambient background flow. Each of these will be incorporated into the proposed model governing particle motion.

1.7.2 Effective size of a bacterium

We impose an excluded volume constraint through the use of a truncated Lennard-Jones potential. The potential is truncated so that only the purely repulsive part is accounted for without incorporating additional attraction at long ranges. See Figure 4.3 for a depiction of the standard Lennard-Jones 6-12 potential and the truncated potential used throughout this dissertation. Consider the Lennard-Jones type potential, \( W(r) \), where \( r = |r| = |\mathbf{x}^i - \mathbf{x}^j| \) and \( \mathbf{F}(r) \) is the corresponding force due to Lennard-Jones interactions

\[
W(r) = \begin{cases} 
4\epsilon \left[ \left( \frac{\sigma_{LJ}}{r} \right)^{12} - \left( \frac{\sigma_{LJ}}{r} \right)^6 \right] + \epsilon, & r \leq 2^{1/6}\sigma_{LJ} \\
0, & r > 2^{1/6}\sigma_{LJ}
\end{cases}
\]
\[- \frac{\partial W(r)}{\partial r} = F(r) = \begin{cases} -24\epsilon \left[ 2 \left( \frac{\sigma_{LJ}^{12}}{r^{13}} \right) - \left( \frac{\sigma_{LJ}^6}{r^7} \right) \right] r, & r \leq 2^{1/6}\sigma_{LJ} \\ 0, & r > 2^{1/6}\sigma_{LJ} \end{cases}.\]

Here $\epsilon$ is a parameter controlling the strength of the potential and $\sigma_{LJ}$ is the distance where the inter-atomic Lennard-Jones 6-12 potential is zero. The cutoff is determined by finding the value of $r$ where the standard Lennard-Jones 6-12 potential achieves a balance between the attractive and repulsive portions:

\[0 = 2 \left( \frac{\sigma_{LJ}^{12}}{r^{13}} \right) - \left( \frac{\sigma_{LJ}^6}{r^7} \right) \Rightarrow r = 2^{1/6}\sigma_{LJ}.\]

So the radius $r = 2^{1/6}\sigma_{LJ}$ corresponds to a Lennard-Jones force of zero, which allows for a natural place to truncate $W(r)$.

**Figure 1.3.** Left: Plot of the standard Lennard-Jones 6-12 potential. Right: Plot of the truncated Lennard-Jones type potential where $r = |x|$ and $W(r)$ is radially symmetric.

The role of the repulsive potential is two-fold. First, short-range repulsion is needed for the regularization of the dipole forces, which diverge as $1/r^2$. The potential enforces that when bacteria approach a certain distance determined by the parameter $\sigma_{LJ}$, they are pushed away from each other. Thus, this parameter determines indirectly the “effective size” of a bacterium and therefore introduces excluded volume constraints to the point dipoles. Second, this potential introduces, on a very simplified level, additional dissipation due to inelastic collisions between bacteria and the associated deviations from the fluid velocity field of a point dipole. This represents the energy lost as macroscopic particles collide. The LJ force provides “soft” inelastic collisions due to the finite range of the potential (unlike hard-core repulsion). While the form of the potential is not crucial for the model, the Lennard-Jones type is convenient.
Now that an excluded volume has been introduced the following formula is used for the volume fraction in three dimensions

\[
\Phi = \frac{N}{L^3} \left( \frac{1}{6} \pi \sigma_{LJ}^3 \right) = \frac{N(\text{excl. vol.})}{\text{vol. of domain}} \tag{1.2}
\]

where \( N \) is the number of particles, \( L \) is the length of the side of the reference domain (\( \mathcal{D} \)), and \( \sigma_{LJ} \) is the size of a bacterium. This is the equivalent volume fraction for a sphere of radius \( \sigma_{LJ}/2 \). The adoption of Lennard-Jones interactions between particles into the model has allowed for better modeling of the effective viscosity through a full range of concentrations as compared with experiment, see [20] or Chapters 2.

### 1.8 Lees-Edwards boundary conditions

One of the main components of this dissertation is the implementation of numerical simulations to study active suspensions. Since numerically one cannot consider an infinite domain, boundary conditions must be chosen to provide similar effects. Also, this dissertation considers a model where the effect of the walls involved in producing a planar shear flow are not considered. This is due to the fact that they may create spatial inhomogenities close to the wall, which would not be present in the bulk. Instead, a clever choice of boundary conditions is implemented to reduce the finite size effect without introducing spurious results due to the presence of the walls.

In Chapters 2-4 a bacterial suspension undergoing planar shear flow (e.g., \( \mathbf{v}^{BG} = (0, \gamma x, 0) \) where \( \gamma = \frac{dv_y}{dx} \) is the shear rate) is considered. The basic setup of the problem consists of a reference cube \( \mathcal{D} \subset \mathbb{R}^3 \) containing \( N \) particles. Depending on time \( t \), a quasiperiodic tiling of the remainder of \( \mathbb{R}^3 \) is defined based on the reference cell, see Figure 1.4. This quasiperiodic tiling changes in time to account for the ambient flow. The basic notion behind Lees-Edwards boundary conditions is that in order to compute the correct flow acting on each particle the quasiperiodic images of each particle should be in the “correct location” to be described in Section 1.8.1.

Consider Figure 1.4. At time \( t = 0 \) the system is composed of a periodic
lattice of cells [79]. The bacteria in the central reference cell are initially placed at random positions within the cell and given a random orientation on the unit sphere. They are given the initial velocity of their non-dimensional swimming speed $V_0 = 1.0$ and velocities get updated based on each particle’s interactions with other bacteria. The flow acting on a given particle is composed of the ambient planar shear background flow in addition to the flow generated by other particles in the reference cell and their quasiperiodic images.

1.8.1 Comparison to periodic boundary conditions

To fully understand Lees-Edwards boundary conditions, consider the situation where a bacterium leaves the reference cell at a point $P = (\hat{x}, \hat{y}, \hat{z})$ with velocity $\mathbf{v} = (v_x, v_y, v_z)$. Under normal periodic boundary conditions the bacteria will cross the $x$-boundary and reenter the central cell at $P' = (\hat{x}', \hat{y}, \hat{z})$, where $\hat{x}' = \hat{x} \pm L$ is the identical position on the opposite boundary of the cell. This bacterium will reenter with the same three components of velocity unchanged; however, this is incorrect. Due to the ambient planar shear flow inducing a linear velocity profile the bacteria will in reality return to the box at $P'' = (\hat{x}'', \hat{y}'', \hat{z}'') = (\hat{x} \pm L, \hat{y} \pm \gamma L t, \hat{z})$ with modified velocity $\mathbf{v}' = (v'_x, v'_y, v'_z) = (v_x, v_y \pm \gamma L, v_z)$. The sign of $\gamma L$ is determined by the boundary crossed. The shear rate has units $\frac{1}{\text{sec}}$, and in order to get the change in velocity due to shear one must multiply by the length of the box, $\gamma L$, resulting in units of $\frac{m}{\text{sec}}$.

While periodic conditions work well on the $y$ and $z$ boundaries, a different set
of boundary conditions in $x$ are needed to reflect these observations. Due to the shear, the periodic cell on the other side of the $x$-boundary will be shifted by $\gamma L t$, where $L$ is the length of the unit cell and $t$ is the time elapsed, see Figure 1.4. Naively periodic conditions often allow one to represent a much larger system in a computationally efficient way. However, the implementation of periodic conditions, resulting in an image particle entering the reference cell at $P' = (\hat{x}', \hat{y}, \hat{z})$, does not produce stable velocity gradients over long periods of time resulting in a failure of the conservation of momentum [79]. This also results in incorrect flows acting on each particle (i.e., each bacterium will not feel the correct forces from other bacteria that have been advected by the shear flow). If implemented correctly, the quasiperiodic images of the bacteria should satisfy exactly the same equations of motion as the bacteria in the reference cell. This was proven to be true for Lees-Edwards boundary conditions in [80, 81]. The precise definition and further discussion will be addressed further in Section 4.3.

There are a couple of limitations to Lees-Edwards boundary conditions: 1) An external force field in the particle equations of motion cannot be enforced and thus linear response theory cannot be used to see how a system responds when driven from equilibrium. In this work when studying a suspension only non-equilibrium behavior is considered. 2) There exists some lag time in the response of system to the initiation of shear and therefore it cannot be used to examine time-dependent flows [79]. Throughout this work as mentioned in Section 1.4 we consider only the steady Stokes equation. So even though limitations exist for the research contained herein the advantages of Lees-Edwards conditions make them desirable for the study of suspensions consisting of a planar shear background flow.

### 1.9 Effective viscosity

In order to introduce the notion of effective viscosity, first recall the definition of the shear viscosity for a Newtonian fluid. This quantity represents the resistance of the fluid particles to the shear (Couette) flow. On the boundary of the fluid domain a tangential force per area $\sigma \cdot n = \frac{F}{A}$ is applied, which induces the movement of a plate (see Figure 1.5). Here $\sigma = \sigma_{ij}$ is the stress and $n$ is the outward unit normal. The bottom plate remains fixed and thus this movement introduces a
linear velocity gradient, \( \frac{\partial u_x}{\partial y} \), parallel to the plates. Thus, \( F_x = \eta A \frac{\partial u_x}{\partial y} \). The viscosity is the constant \( \eta := \frac{F_x}{A} \frac{\partial u_x}{\partial y} = \frac{1}{2} \sigma_{xy} \) where \( e_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \) is the rate of strain tensor. In addition, viscosity is directly proportional to the rate of energy dissipation per unit volume of fluid

\[
\eta \propto \frac{1}{|\Omega|} \int_{\Omega} \sigma : e \, dx. \tag{1.3}
\]

**Figure 1.5.** Depiction of how viscosity is computed for a Newtonian fluid in a channel between moving plates.

The effective viscosity for a bacterial suspension cannot be defined as easily due to the presence of the inclusions (particle bodies). The notion of effective viscosity for passive particle suspensions was developed in the 1980’s (e.g., [82]). This result of homogenization theory proved the existence of an equivalent Newtonian fluid with a scalar effective viscosity \( \hat{\eta} \). This viscosity is what will be referred to as the effective viscosity of the original suspension. Here the effective viscosity needs to be defined for an active particle suspension, which a priori may not satisfy the constitutive equation for a Newtonian fluid

\[
\sigma_{ij} = -(p - \eta e_{kk}) \delta_{ij} + 2\eta e_{ij}. 
\]

Instead, the definition of effective viscosity developed in works such as [59, 71] is used, where the energy dissipation of an isotropic homogeneous fluid of viscosity \( \hat{\eta} \) is equated to that of the suspension. By equating energy dissipation \( E := \int_{\Omega} \sigma : e \, dx \) one finds

\[
\int_{\partial \Omega} \sigma n \cdot (e x) dS = 2\eta \int_{\partial \Omega} e n \cdot (e x) dS. \tag{1.4}
\]

This uses the fact that in homogeneous fluid the constitutive law for the deviatoric
stress $\sigma = 2\eta e$ holds (see Figure 1.6). By transferring the computation to the boundary we avoid the difficulty presented by the solid inclusions in the interior of the suspension, which have an infinite viscosity.

The equation (1.4) can be rewritten as

$$\eta(t) = \frac{1}{2|\Omega|} \epsilon : \int_{\partial\Omega} \sigma(t) n \cdot (e x) dS$$

where $\sigma(t)$ is the instantaneous bulk deviatoric stress, which is a function of the microscopic configuration. Thus the instantaneous viscosity, $\eta(t)$, a macroscopic quantity has the information from the microstructure encoded in $\sigma(t)$.

![Figure 1.6](image)

**Figure 1.6.** To make the effective viscosity a well-defined quantity for an active suspension, homogenization techniques are applied to find an equivalent homogeneous suspension and take its viscosity as the effective viscosity.

This definition is not quite sufficient. The viscosity of a homogeneous Newtonian fluid is a constant independent of time and the microstructure. The quantity defined in (1.5) still depends on the initial positions and orientations of each particle. Thus, an averaging procedure is needed to identify the effective viscosity as a unique quantity. There are two equivalent ways of doing this. The first, as is done in experiment, is to take a long time average over many observation times. The second way to define the effective viscosity, which may be easier to compute mathematically, is to take the limit of the system as time $t \to \infty$ and compute the effective viscosity as an average over the phase space at the steady state, provided it exists.

One of the ultimate goals of this dissertation is to show that the effective viscosity is well-defined as a macroscopic quantity for semidilute suspensions. Thus, the
two definitions above must be shown to be equivalent. As in the study of passive suspensions [83], the effective viscosity of a bacterial suspension is assumed to be time-independent. Thus, it can be defined as the time average of the appropriate component of the volume–averaged stress divided by the same component of the volume–averaged rate of strain [84, 85]. By assuming the system is ergodic, the effective viscosity can then be rewritten as an ensemble average over phase space using the steady-state distribution. This procedure produces a well-defined viscosity in the dilute regime where a bacterium only interacts with the ambient background flow [59]. In the dilute case the steady state distribution depends only on the orientations of the particles, which are independent. However, due to the interactions present in the semidilute case, the steady state distribution must depend on both positions and orientations. This greatly increases the complexity, since present theories do not even guarantee the existence of particle trajectories beyond a finite time. These concerns are extensively studied in Chapter 4 where it is shown that there exists unique particle trajectories for all time and thus the equation governing the distribution of particles in phase space is well-defined.

For this dissertation, the effective viscosity will be defined as

\[ \hat{\eta} := \frac{\Sigma : E}{E : E}, \]  

(1.6)

where \( \Sigma \) is the bulk deviatoric stress and \( E \) is the constant rate of strain in the ambient fluid. This definition has been used by many authors studying such suspensions (e.g., G. K. Batchelor, H. Brenner, L. G. Leal and E. J. Hinch [57, 58, 59, 84, 85, 86]) and was shown to be an equivalent definition to (1.5) in [87].

Since the effective viscosity represents the ratio of the stress to the strain, heuristically, one may expect a decrease in viscosity when the point dipoles are aligned with the flow. There the propulsion force enhances the strain \( \gamma = \frac{\partial u_x}{\partial y} \) and effectively decreases the viscosity. However, the complex phenomenon of the decrease in the effective viscosity is not so straightforward. In [74] the authors show the presence of self-propulsion alone is insufficient to observe a decrease in the effective viscosity concluding that interactions or random tumbling are required to observe the decrease. In Chapters 2-3, the physical mechanisms responsible for the decrease in the effective viscosity are identified through mathematical analysis.
sheding new light on what causes this striking experimental observation.

1.10 Background on kinetic theory

The basic notion of passing from the discrete deterministic ordinary differential equations for particle motion to a continuum partial differential equation kinetic theory are presented here to prepare the reader for the subsequent chapters. In Chapter 2, the discrete system is numerically simulated and analyzed, but in the chapters that follow a kinetic theory approach is implemented to allow for rigorous mathematical analysis of the suspensions.

1.10.1 Derivation of the kinetic equation from a discrete ODE system

The main idea needed to pass from discrete ordinary differential equations to a partial differential equation is the introduction of a random distribution of initial conditions to the ordinary differential equations. The resulting continuum PDE model accounts for all realizations of the system at once removing the need for repeating numerous costly numerical simulations for different initial conditions.

Consider the basic example of a discrete ODE

\[
\begin{cases}
\dot{\xi}(t) = g(\xi(t)), & \xi : [0, T) \to \mathbb{R}, \ g : \mathbb{R} \to \mathbb{R} \\
\xi(0) = \xi_0
\end{cases}
\]

(1.7)

Let \( \Omega = \mathbb{R} \) and \( \mathcal{B} \) be the Borel \( \sigma \)-algebra on \( \mathbb{R} \). Given an initial distribution \( P(x, 0) \) for \( x \in \Omega \), then one can define a measure, \( \mu_0 \). For any \( A \in \mathcal{B} \)

\[
\mu_0(A) := \int_A P(x, 0) dx.
\]

(1.8)

Thus, \( \mu_0 \) is absolutely continuous with respect to Lebesgue measure. This defines a probability space \( (\Omega, \mathcal{B}, \mu_0) \). Define \( \xi^t(x) := \xi(t, x) : [0, T) \times \Omega \to \mathbb{R} \) as a random
process satisfying
\[
\begin{align*}
\dot{\xi}^t(x) &= g(\xi^t(x)) \\
\xi^0(x) &= \xi_0(x)
\end{align*}
\] (1.9)

with \(\xi^0(x)\) a random variable which induces the probability density \(P(x,0)\). Define the measure at time \(t\) for \(A_t \in \mathcal{B}_t\)
\[
\mu_t(A_t) := \mu_0(\xi^{-t}(A_t)) = \mu_0(A_0),
\] (1.10)

where \(\xi^t(A_0) = A_t\), which defines a probability space \((\Omega, \mathcal{B}_t, \mu_t)\).

For \(A_t \in \mathcal{B}_t\),
\[
\int_{\Omega} \chi_{A_t}(x) P(x,t) dx = \mu_t(A_t) = \mu_0(A_0) = \int_{\Omega} \chi_{A_0}(x) P(x,0) dx = \int_{\Omega} \chi_{A_t}(\xi^t(x)) P(x,0) dx.
\] (1.11)

Thus, by (1.11) and (1.12)
\[
\int_{\Omega} \chi_{A_t}(x) P(x,t) dx = \int_{\Omega} \chi_{A_t}(\xi^t(x)) P(x,0) dx.
\] (1.13)

holds for all characteristic functions. Therefore it holds for all simple functions and finally (using the Dominated Convergence Theorem) for all functions \(f \in C^\infty_c(\Omega)\), since they are the limit of a sequence of simple functions. From (1.13),
\[
\int_{\Omega} f(x) P(x,t) dx = \int_{\Omega} f(\xi^t(x)) P(x,0) dx.
\] (1.14)

Take the derivative of both sides and recall (1.9). Then, \(\frac{d}{dt}[f(\xi^t(x))] = \nabla f(\xi^t(x)) \cdot \dot{\xi}^t(x) = \nabla f(\xi^t(x)) \cdot \nabla f(\xi^t(x)) \cdot g(\xi^t(x))\) results in
\[
\int_{\Omega} f(x) \frac{\partial P}{\partial t} dx = \int_{\Omega} \nabla f(\xi^t(x)) \cdot g(\xi^t(x)) P(x,0) dx.
\]

By (1.14) and integration by parts
\[
\int_{\Omega} f(x) \frac{\partial P}{\partial t} (x,t) dx = -\int_{\Omega} f(x) \nabla \cdot (g(x) P(x,t)) dx.
\]
This holds for all \( f \in C_c^\infty(\Omega) \), so the differential (local) form is the Liouville equation
\[
\frac{\partial P}{\partial t} = -\nabla \cdot (gP).
\]

1.10.2 Advantages of the kinetic theory approach

The purpose for introducing the kinetic theory is to replace a large, possibly coupled, system of ordinary differential equations with a single continuum partial differential equation. Specifically, in this dissertation a kinetic model will be analyzed and comparisons will be made with simulations of over 100,000 coupled differential equations. The PDE can also be solved numerically with a fixed spatial or temporal grid, which will keep the computational cost manageable. Namely, the number of particles \( N \) does not increase the complexity [88].

Another advantage to introducing this probabilistic framework beyond being able to consider many different initial conditions at once is the ability to consider the limiting regime as \( N \to \infty \), the so-called mean field limit. Also, when studying probabilistic quantities and averaged effective properties one would like to consider the evolution of the probability distribution for the particles. As explained in Chapter 4, the effective properties of a suspension are derived from knowledge of microscopic configurations, which can be computed from the \( N \) particle distribution function.

Some of the seminal works on the derivation of kinetic equations were first published in the 1970’s [89, 90, 91]. Most recently studied are kinetic equations resulting from ODEs composed of a singular force derived from a potential, as in this dissertation where the main contribution to particle motion is the fluid velocity \( u \sim \frac{1}{|x|^2} \) [92, 93]. To define a time-independent effective viscosity one must find the steady state probability distribution. One such case where a steady state distribution was shown to exist was previously studied in [94, 95]. Here the ODEs, describing the motion of point force monopoles, consisted of singular terms of the form \( \frac{1}{|x|^{d-2}} \) where \( d \) is the dimension of the space. The global existence and longtime behavior of solutions to other kinetic equations derived from an ODE system have been investigated by Wollman (Vlasov-Poisson equations) [96] and Hamdache (Vlasov-Stokes equations) [97]. In addition, the existence and
uniqueness of solutions to the Liouville equation was proven for all interaction potentials of bounded variation outside the origin in [98]. Some recent kinetic models for the study of bacterial suspensions have been used (e.g., [49, 61, 63, 64, 99]) and for liquid crystals (e.g., [100]). Nevertheless, due to the singularity in our system (\( \sim \frac{1}{|x|^{d-1}} \) for \( d = 3 \)) as well as the nature of the boundary conditions in the PDE fluid equations, present theories are inadequate to guarantee the Liouville equation governing the semidilute suspension is well-defined.

Within this dissertation the existence of a steady state distribution is not proven to exist; however, this problem is addressed in Chapter 4 where it is shown that the Liouville equation governing the evolution of the probability distribution is well-defined for all time. This is shown to follow from the kinetic theory developed herein, which is used to convert the discrete particle motion equations, for which global existence is proven, into a Liouville equation describing the state of the system.

1.11 Simulation methods

The novel GPU numerical simulations used to study the effective properties of bacterial suspensions are presented in Chapters 2 and 5 in detail. In order to understand and interpret the results herein a brief summary of how the numerical simulations were implemented is provided. In particular, the algorithms used to evolve the system in time are presented. First, past numerical simulations studying active particle suspensions are reviewed below.

1.11.1 Previous numerical simulations

The common theme among all simulations of many particle systems is the implementation of direct particle simulations. The key challenge is how to implement these simulations in the most computationally efficient way while still capturing the essential physical features. In recent simulations [19, 65], direct particle numerical simulations are used to show the existence of a collective state (Pushers) or absence of one (Pullers) for bacterial suspensions. Various measures such as the correlation length and mean swimming speed are used to argue that a suspension
of pushers exhibit a collective state beyond a certain concentration (effective volume fraction) threshold of $\nu = .5$. The main theoretical model employed is the use of slender-body theory for rod-like particles and a fluid with periodic boundary conditions. The authors found that the correlation length and time increase up to 3 times the particle size as a function of the concentration. It is also shown that the mean velocity increases slightly for Pushers (less than two times) and for Pullers it remains the same as the isolated swimming speed. The authors conclude that the collective dynamics of a suspension of Pushers result in giant density fluctuations, local alignment of swimmers, and strongly mixing flows. In another work the effect of fluid viscoelasticity on swimming dynamics is investigated [101]. The main result is that viscoelastic fluid response can increase the speed and efficiency of a simple swimmer, which moves using a wave-lake motion.

This dissertation seeks to improve on their findings by introducing a different model developed herein. The previous authors do not consider the effect of excluded volume constraints, which have been shown to be necessary to capture experimental observation [51]. The model considered in this dissertation explicitly includes excluded volume constraints and uses the L-J radius, $\sigma_{LJ}$, to compute an effective, more realistic, volume fraction. Specifically, by replacing the generous use of the volume fraction from polymer models, as used in the previous work, with the true volume fraction for a spheroid. In addition, the relatively large error bars in the previous work’s findings suggest the possible need for larger simulations with a greater container volume and number of particles. It is also shown in Chapter 5 that our model is able to capture a 6-fold increase in the mean particle swimming speed in the collective state as well as showing the concentration threshold for collective motions is approximately at a volume fraction of .3, which both more closely match experimental observation.

In [7, 60, 102, 103], Graham et al. introduce a dumbbell model where two point forces are connected by a massless rigid rod. Similar to the model presented in this dissertation they impose an excluded volume constraint through an intermolecular potential. The authors then use this approximation for a bacterium to investigate correlated motion in confined suspensions. The major contribution of this work is showing that confinement can lead to false collective motion in the sense that small vortices and jets can form due to the presence of the walls, which
alter the flow patterns when compared to an unconfined geometry. The concentrations considered are in the dilute and semidilute regimes, but it is noted that the concentration is low enough that we do not expect steric interactions between organisms to be dominant (nematic-like ordering) [7]. These works have limitations in that they only considered confined 2D suspensions, while this dissertation considers the effect of geometry by comparing a confined quasi-2D and full 3D suspension. In addition, the authors here only account for shape indirectly using the Gay-Berne (ellipsoidal) repulsive potential. In contrast, shape is explicitly accounted for through the Bretherton constant in Jeffery’s equation throughout this work. Thus, particle orientations are directly altered due to interactions and collisions. Finally, the model presented herein is even more computationally efficient as described in Chapter 5.

Over the same time period, the work [104] considered particles modeled as spheres with prescribed velocities at the boundary. This model advanced the study of suspensions by resolving near and far-field interactions, but only for a discrete set of distances between particles. This was done by forming a database of pairwise hydrodynamic velocity fields. However, these simulations are so expensive that even though the authors resolve hydrodynamic interactions in 2D, it has only been done for 64 bacteria. In contrast, this dissertation seeks to develop a model which efficiently allows for more particles in order to study collective motion closer to that which has been observed in experiment. One additional result is the increase in the effective viscosity (as in the passive case) observed in a free suspension. This can be explained by the use of spherical bacteria and hence no particle alignment due to the absence of elongation. A decrease in the effective viscosity is only observed in the presence of an external gravitational field, which produces the necessary alignment, but should not be needed.

Other more computationally expensive simulations have been studied in recent years. Gyrya et al. [74, 105] fully resolved hydrodynamics in 2D (without the database of [104]) for 25 bacteria. However, to study collective motion and large scale structures, a large system of particles is needed. The authors, based on numerical observation, predicted that interactions have a similar effect to, and could possibly be modeled by, rotational noise. This is addressed in Chapter 3 where a direct comparison is made between the effects of random noise and
deterministic hydrodynamic interactions using mathematical analysis. In [106],
the authors show the emergence of clusters with a broad distribution of sizes at
critical volume fraction depends crucially on the particle aspect ratio (shape).

Recently, two-dimensional simulations of chemotactic self-propelled bacteria
swimming in a viscous fluid were performed [107, 108]. The fluid flow and the
motion of the bacteria are determined by solving a variational problem on the
whole domain including the fluid and particles through the use of a finite element
method. While their model reproduces complex collective dynamics observed in
concentrated bacterial suspensions such as bioconvection, it does not accurately
take into account hydrodynamic interactions and has not yet been used to study
three-dimensional suspensions. The major computational goal of this dissertation
is to develop an efficient model which allows for a much greater number of particles
in order to study collective effects and decrease the sources of error such as the
finite domain effect.

1.11.2 GPU computations

Numerical simulations presented in this dissertation were performed using Nvidia
graphics cards with GPU (graphics processing unit) computing. Before detailing
the simulation methods first one must understand what it means to program on
GPUs and what are potential limitations of this approach in contrast to direct
particle simulations on CPUs. The main advantage is that each graphics card has
far more computational cores than a CPU can handle at the present time making
computing much faster. The speed up seen is a result of splitting calculations
among all the cores and running them all simultaneously. For particle suspensions,
basically each core computes all the interactions for a given particle. Since all the
particles in the system have their evolution equations solved simultaneously the
process of evolving the system in time is very efficient.

One caveat to using GPUs for simulations is that the code must be paralleliz-
able. In other words, each time step cannot depend on other quantities calculated
simultaneously. Thus, the simulation can only use data from all the past time
steps to determine each particle’s next position and orientation. Numerically, this
means that implicit schemes cannot be implemented on GPUs (without signifi-
cant modification) and the simulations are restricted to primarily explicit schemes. Traditionally, implicit schemes are much more accurate and have greater stability. This potential problem is remedied by introducing an explicit iterative scheme to evolve the system outlined in Section 1.11.3. Due to the semidilute assumption, a particle’s next position and orientation are derived from the total flow acting on its given position, which is quantified by the flows from all other particles and their quasiperiodic images at the previous time step. Therefore, simulations on GPUs will be shown to work well for the needs of this dissertation, but future works should analyze the complexity of the desired system and determine if explicit numerical schemes offer sufficient stability.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Depiction of real time (sec) for the same code run on CPU vs. GPU. The code run corresponded to a simulation of interacting point dipoles in a planar shear (Couette) flow. This plot was generated using an Nvidia EVGA GeForce GTX-480 graphics card (GPU) and an Intel core i7 (CPU) at Argonne National Laboratory on the clusters operated by Dr. Igor Aronson.}
\end{figure}

For large systems of interacting particles, using GPUs to perform numerical simulations is much more efficient. However, see Figure 1.7, for small systems the computational cost of performing the simulations on a CPU is much less. This is due to the fact that most of the time for GPU computations is spent moving data from different locations in memory onto the GPU and back. For small systems this time is greater then the time required to perform the calculations directly. In addition, a more detailed comparison is made in Section 5.5 between the GPU method for solving large systems of interacting particles used throughout this dissertation and previous simulations of similar models.
1.11.3 Iterative trapezoid scheme

The numerical simulations use an (explicit) iterative trapezoid scheme when solving the ODE equations of motion to calculate the positions and orientations of each bacterium for the next time step. The naive approach using the Forward Euler method has error $O(h)$ and $h \sim \hat{\eta}$. Thus, there might be a problem with the error having the same magnitude as the quantity being computed. Instead of using Forward Euler,

$$y_{n+1} = y_n + hf(y_n) \quad (1.15)$$

where $h$ is the time step, an iterative scheme is implemented to reduce the error. This appears when calculating new positions given a particle’s current velocity, $f(y_n)$, and new orientations given the change in orientation $\frac{d\theta}{dt}$. The Iterative trapezoid scheme with error $O(h^2)$ is defined as

$$y_{n+1}^{i+1} = y_n^0 + \frac{h}{2}[f(y_n^0) + f(y_n^i)] \quad (1.16)$$

where the index $i$ corresponds to the iteration and the index $n$ corresponds to the time. In the case that the values for the next position and orientation start to diverge we set the maximum number of iterations to be five. The iteration procedure continues as long as the maximum distance in the $L^2$-norm between two iterates of the same particle is greater than $10^{-2}$. Through simulation one sees that implementing the iterative trapezoid scheme takes longer, but provides increased stability. One source of instability is the contribution to viscosity by the Lennard-Jones type interactions, which fluctuate a lot in time. However, the iterative trapezoid scheme controls these oscillations resulting in more stable numerical simulations.

1.12 Outline of the dissertation

The two main purposes of this dissertation are to use mathematical modeling and analysis to study the effective rheological properties of a suspension of interacting particles and to determine the physical mechanisms leading to collective motion of those particles. In Chapter 2, a first principles model is introduced in order to
study the striking decrease in the effective viscosity in suspensions of rod-shaped bacteria. The difficulty lies in solving a large coupled PDE/ODE system modeling bacterial motion in the suspension. Since this model incorporates both hydrodynamic interactions between the fluid and the particles as well as excluded volume interactions such as collisions each particle interacts with all others leading to greater computational complexity. Numerical simulations exploiting the efficiency of graphics processing units (GPU) are used to compute the effective viscosity, \( \hat{\eta} \), which matches qualitatively recent experimental results on active suspensions through all experimental concentrations [20].

In Chapter 3, mathematical analysis is carried out through the introduction of a kinetic model for the bacterial suspension. In contrast to past work on dilute suspensions with diffusion where a parabolic Fokker-Planck equation governs the probability density, here a hyperbolic Liouville equation must be studied where a priori well-posedness results are not present. Through asymptotic analysis of this equation, explicit formulas for the effective viscosity as well as the normal stress coefficients are derived using the shape of the particle as a small parameter. The analytical formula for viscosity is found to be in qualitative agreement when compared to experiment and the numerical results of Chapter 2 at low concentrations. In addition, the formula shows that hydrodynamic interactions, a moderate concentration, self-propulsion and an elongated particle shape are all necessary to recover the decrease in the effective viscosity.

In Chapter 4, the global existence and uniqueness of the discrete ODE equations of motion for the particle trajectories is proven and the fluid PDEs are shown to be well-posed. These results show that the kinetic theory used to derive the asymptotic formula in Chapter 3 is well-defined and thus the effective viscosity is a well-defined quantity for semidilute bacterial suspensions. The main difficulty is proving that the particle trajectories remain bounded away from each other for all time. This is mainly the result of an energy argument made possible by the excluded volume constraint imposed on the particles through a truncated repulsive potential.

In Chapter 5, the physical mechanisms that govern the intrinsic properties of the collective state are investigated. The main tool is the study of the spatial and temporal correlations associated to a bacteria suspension. How each change as
the concentration, swimming speed, tumbling rate, shape of bacteria, suspension film thickness, or the dipole moment are varied is carefully examined to identify the main features responsible for the collective effects. A striking result is observed; namely, the correlation length remains unchanged as the swimming speed and concentration are increased (injecting greater energy into the system). This is the first theoretical work to confirm this observation previously observed in experiment while providing testable predictions for the effect of shape a dipole moment, which may be studied in future experiments. The main achievement of the theory developed in this chapter is that the effective properties of the collective state such as size and duration are completely governed by the size and shape of each particle.

This work advances the fields of biology and physics, but mostly mathematics by applying rigorous mathematical analysis and numerical techniques in order to gain greater understanding of the physical mechanisms responsible for collective motion as well as the amazing decrease in viscosity for bacterial suspensions. The incorporation of interbacterial interactions into the model allowed provided a greater understanding of bacterial collective motion not realized in previous models valid in the dilute regime. Before this dissertation the physical mechanisms behind collective motion had not been verified completely. This work adds further evidence to theories of collective motion based on recent experiments, other theoretical models, and simulations. In addition, new phenomenon are investigated theoretically in Chapter 5 which at present are too difficult to study experimentally. Thus, this dissertation also provides predictions on the effects of system parameters, which may be verified experimentally in the future.
Effective viscosity in semidilute bacterial suspensions

In this chapter the viscosity of a suspension of swimming bacteria is investigated both analytically and numerically. A simple model that allows for efficient numerical computations for a large number of bacteria is proposed. The calculations herein show that long-range hydrodynamic interactions, intrinsic to self-locomoting objects in a viscous fluid, result in a dramatic reduction of the effective viscosity. In agreement with experimental observation on suspensions of Bacillus subtilis [20], it is shown that the viscosity reduction is related to the onset of large-scale collective motion due to interactions between the swimmers. The simulations reveal that the viscosity reduction occurs only for relatively low concentrations of swimmers: further increases of the concentration yield an increase of the viscosity due to excluded volume constraints/collisions. An explicit asymptotic formula for the effective viscosity in terms of known (measurable) physical parameters is formally derived. This explicit analytical formula is then compared to previous results on the dilute case with rotational noise and it is shown that hydrodynamic interactions could be manifested as self-induced noise in the absence of any external stochasticity imposed on the system. The main content of this Chapter has been published in [75].
2.1 Background: Experiment and recent theory

Collective dynamics of self-locomoting micro-organisms, such as bacteria, algae, and sperm cells [3, 4, 5, 6, 8, 60] as well as synthetic swimmers [9, 10] have attracted enormous attention, with a large number of experimental and theoretical works published in the last few years. A plethora of nontrivial properties have been predicted and consequently studied, including dynamic instabilities, anomalous density fluctuations, nontrivial stress-strain relations, and chaotic motion [14, 15, 16, 17, 18, 19, 103]. In particular, a seven-fold viscosity reduction in a suspension of swimming bacteria, Bacillus subtilis, has been observed recently [20]. This dramatic effect occurred above a certain critical concentration (about 1-2% of volume fraction) where large-scale collective bacterial motion is well-developed. For larger volume fractions (about 6-10%), the viscosity increases similar to that which would be expected for passive suspensions where increased friction due to the presence of the particles leads to a great dissipation of energy resulting in a larger viscosity (cf. Einstein’s work [44] or [47]).

The first work to consider the effects of self-propulsion on the viscosity of active suspensions was [15]. While very stimulating for its time, the authors in [15] assumed purely relaxational dynamics for particle alignment, whereas in a planar shear flow studied herein the individual swimmers perform periodic rotations (so-called Jeffery orbits). The viscosity reduction for dilute suspensions (i.e., for negligible interactions between the swimmers) has been previously addressed in a number of theoretical works [62, 71, 72, 74]. Their analysis led to rather counter-intuitive conclusions: for planar shear flow the viscosity reduction occurs only if swimmers undergo rotational diffusion (e.g., tumbling). Without tumbling, the net contribution to the viscosity of non-interacting swimmers is zero [71, 74]! In apparent contradiction to this, a viscosity reduction has been measured without noticeable tumbling (for most experimental conditions) in suspensions of Bacillus subtilis [5, 20].

In this Chapter, the influence of hydrodynamic interactions on the effective viscosity of a three-dimensional suspension of swimming bacteria is investigated numerically and analytically through formal asymptotics. It is demonstrated that hydrodynamic inter-bacterial interactions have a similar effect on the effective vis-
cosity as rotational diffusion or tumbling have in the dilute case (no interactions) [71]. Both simulations and rigorous asymptotic analysis (presented in Chapter 3) reveal that the viscosity reduction occurs due to hydrodynamic interactions between the swimmers, and no tumbling is needed. Simulations show that as the concentration increases, the viscosity initially decreases and then increases (Fig. 2.1) in qualitative agreement with recent experiments. The hydrodynamic interactions are further analyzed in the continuum limit (PDE) of the discrete ODE model and one can show that the viscosity reduction is associated with the breakdown of the uniform spatial distribution of particles. This breakdown is directly related to the concentration fluctuations through the course of collective motion.

2.2 Point dipole model for semidilute bacterial suspensions

At a fundamental level each bacteria can be viewed as a force dipole where the force of self-propulsion balances with the viscous drag on each bacterium’s body. Thus, each bacterium is represented by massless hydrodynamic point dipoles with dipole strength \( U_0 \sim V_0 l^2 \) swimming with speed \( V_0 \) along the orientation of its dipole moment \( d_i, i = 1, ..., N \). Here \( N \) is the number of bacteria and \( l \) is the characteristic size of a bacterium. To non-dimensionalize the system each velocity is scaled by the bacterium’s swimming speed \( V_0 \sim 20 \mu\text{m/sec} \), the positions by the characteristic size \( l = 1 \mu\text{m} \), and the dipole strength by \( l^2 \). The characteristic unit of time is taken to be 1/20 sec, which is the time it takes a bacterium to swim one body length. The position of the center of mass \( x_i \) and orientation \( d_i \) of the \( i \)th bacterium are governed by

\[
\begin{align*}
\frac{dx_i}{dt} &= V_0 d_i + \sum_{j\neq i} (v_{ij} + F_{ij}) + V_{BG}, \\
\frac{dd_i}{dt} &= -d_i \times \left( \omega_{BG} + \sum_{j\neq i} \omega_j + B d_i \times \left( E_{BG} + \sum_{j\neq i} E_j \right) \right) \cdot d_i \quad (2.1)
\end{align*}
\]

where \( BG \) denotes the contributions from the background flow and \( \frac{dd_i}{dt} \) obeys Jeffrey’s equation with added contributions due to interactions. Now each term contributing to the particle evolution equations will be explained. The fluid velocity
field produced by the \( j \)th bacterium on the \( i \)th is denoted \( v_{ij} \), which is obtained as the solution to Stokes equation at \( x_j - x_i \) for a point dipole at the origin with orientation \( \mathbf{d}_j \) defined via the derivative of the fundamental solution (Oseen tensor \( G \))

\[
v_i(x, \mathbf{d}) = \sum_{j=1}^{3} \sum_{k=1}^{3} \frac{D_{jk}(\mathbf{d})G_{i,j,k}(x)}{8\pi\eta_0} \nonumber \]

\[
= \frac{1}{8\pi\eta_0} \sum_{j=1}^{3} \sum_{k=1}^{3} U_0(d_j d_k - \delta_{jk}/3) \left[ \frac{-\delta_{ij}x + \delta_{ik}x_j + \delta_{jk}x_i}{|x|^3} - \frac{3x_i x_j x_k}{|x|^5} \right] \tag{2.2}
\]

where \( \eta_0 \) is the ambient fluid viscosity and \( D_{jk} = U_0 (d_j d_k - \delta_{jk}/3) \) is the dipole tensor. Impose a planar shear background flow in \( xy \)-plane through \( \mathbf{V}_{BG} = (0, \gamma x, 0) \) where \( \gamma \) is the strain rate. Here \( \omega_j = (\nabla \times v_{ij}) \) is the vorticity and \( \mathbf{E}_j = (1/2) (\nabla v_{ij} + \nabla v_{ij}^T) \) is the rate of strain tensor. Even though each particle is a point dipole, the shape is preserved through the Bretherton constant \( B \) \((B = 0/1 \) for spheres/needles) [109]. The hydrodynamic interactions are contained in the terms \( v_{ij}, \omega_j, E_j \) (see Chapter 3 for the explicit representations).

The repulsion force contribution to the evolution equations, \( \mathbf{F}_{ij} = -\partial L_{ij}/\partial x_{ij} \) in (2.1) is a short-range force modeled by a Lennard-Jones type (LJ) potential,

\[
L_{ij} := \begin{cases} 
4\varepsilon \left[ (\sigma_{LJ}/r_{ij})^{12} - (\sigma_{LJ}/r_{ij})^{6} \right] + \varepsilon, & r \leq 2^{1/6}\sigma_{LJ}, \\
0, & r > 2^{1/6}\sigma_{LJ}.
\end{cases} \tag{2.3}
\]

Here, \( r_{ij} = |x_i - x_j| \) is the distance between two particle centers of mass, \( \varepsilon \sim (\eta_0 l^2)^{-1} \) is the normalized strength of interaction, and \( \sigma_{LJ} \) determines the equilibrium distance where the potential is zero. Observe that the potential is defined in such a way so that it is purely repulsive while its gradient in \( x \) remains Lipschitz continuous outside a neighborhood of zero. This observation will be important in the proof of global existence of trajectories in Chapter 4.

The role of the repulsive potential is two-fold. First, short-range repulsion is needed for the regularization of the dipole forces; in particular, the flow \( v(r) \) diverges as \( 1/r^2 \). Thus, when bacteria approach a certain distance \( (2^{1/6}\sigma_{LJ}) \) between one another determined by the parameter \( \sigma_{LJ} \), they are pushed away. Therefore,
this parameter determines indirectly the size of a bacterium and introduces the excluded volume constraints. Second, this potential introduces on a very simplified level additional dissipation due to inelastic collisions between bacteria and the resulting deviations from the fluid velocity field of a point dipole. For this model, a spherically symmetric LJ potential is used. While the form of the potential is not crucial for the model, the Lennard-Jones type is convenient as a purely repelling short-range potential.

This model has been justified by experiments showing the flow created by a bacterium is accurately described by a point dipole [5]. The Lennard-Jones interactions introduce in a simplified way the net results of collisions between bacteria as compared to experiment [20]. While near-field interactions are important when considering two bacteria swimming close to one another, this Chapter considers only bulk properties where these individual interactions do not produce a noticeable difference in the macroscopic effective viscosity.

2.3 Numerical computation of the effective viscosity

The solution to the free space Stokes equation (2.2) is explicitly known. This expression is substituted into (2.1) and simulations are used to evolve the system in time. In the numerical simulations the effective instantaneous stress and strain are computed at each time step and the viscosity is defined via the longtime average of the instantaneous viscosity. The simulations were performed in a cubic domain (of size $L = 50$) with periodic boundary conditions in $y$ and $z$ and Lees-Edwards boundary conditions in the $x$-direction along the boundary being sheared [79]. Simulations of up to $N = 48^3 \approx 110,000$ particles were implemented on graphic processing units (GPUs), and performed for varying strain rates $\gamma$, swimming speeds $V_0$, and sizes of bacteria $l \sim \sigma_{LJ}$.

Remark 2.3.1. Note that the simulation results with non-spherical LJ potential show no qualitative difference with the spherically symmetric LJ potential. All results presented were obtained with the spherically symmetric potential, which greatly reduced the computational complexity.
Figure 2.1. Left: Effective viscosity $\eta$ vs. volume fraction $\Phi$ for pushers for three strain rates $\gamma$. The volume fraction $\Phi = \frac{4}{3}\pi\sigma_{LJ}^3\rho$, where $\rho$ is the concentration and isolated swimming speed $V_0 = 1$. Right: Dipolar stress $\Sigma_d$ vs LJ stress $\Sigma_{LJ}$ where the LJ parameter $\sigma_{LJ} = .35$, shape factor $B = .95$, and dipole moment $U_0 = -8\pi V_0$ (pushers).

Select results for the effective viscosity $\eta$ vs. volume fraction of bacteria $\Phi$ are shown in Fig. 2.1. The viscosity is defined using the ratio of stress to strain introduced in Chapter 1,

$$\eta = \eta_0 \left(1 + \frac{\Sigma_{xy}}{\gamma}\right), \quad (2.4)$$

where $\Sigma_{l,m}$ is the stress tensor,

$$\Sigma_{l,m} = \Sigma_d(d) + \Sigma_{LJ}(x) = \sum_{i=1}^{N} \left( \frac{U_0}{V_L} \left( d_i^{(m)} d_i^{(l)} - \frac{\delta_{lm}}{3} \right) + \frac{x_i^{(m)} F_i^{(l)}}{V_L} \right). \quad (2.5)$$

The first term is due to the dipolar contribution to the stress $\Sigma_d$ from [84] and the last term is the stress due to collisions $\Sigma_{LJ}$ [110]. The computational domain volume is taken to be $V_L = L^3$. For $U_0 < 0$ (pushers), the viscosity decreases with increasing volume fraction $\Phi$, see Fig. 2.1. Then, for high filling fractions, two simultaneous trends occur: (i) Stress due to collisions, $\Sigma_{LJ}$, leads to a viscosity increase; (ii) due to the increased concentration, collisions become increasingly frequent and alter the orientations of the bacteria resulting in a saturation of the contribution from dipolar interactions, $\Sigma_d$, in (2.5). The right side of Fig. 2.1 illustrates the relationship between stresses $\Sigma_d, \Sigma_{LJ}$ for varying swimming speeds, $V_0$, and fixed volume fraction $\Phi = 0.02$. When the collisional stress $\Sigma_{LJ}$ increases, the orientational order (characterized by $\Sigma_d$) decreases. Thus, the increase in viscosity in Fig 2.1 is not caused by only the increased concentration, but also by
the disruption of orientation caused by the collisions.

In Fig. 2.1, the increase in viscosity for a fixed swimming speed, \( V_0 = 1.0 \), begins where volume fractions are between 2 - 6\%, the so-called semidilute regime. For pullers (\( U_0 > 0 \)), an increase of the effective viscosity with concentration is always observed, see Fig. 2.2. The viscosity appears to increase with increasing strain rate \( \gamma \) (shear thickening). Fig. 2.1 shows that for small volume fraction \( \Phi \) with an increase of the strain rate \( \gamma \) the effect of interactions diminishes (resulting in a smaller viscosity reduction). Also, as \( \Phi \) becomes larger the LJ forces become the dominant contributor to the viscosity regardless of the shear rate resulting in the curves for differing shear rates being essentially the same. Finally, the effective viscosity decrease is inversely proportional to \( V_0 \) (see Fig. 2.2).

The fundamental change in the viscosity can be understood through viewing the change in the orientation distribution with concentration. The distribution of bacterial orientations \( P_d(\alpha, \beta) \) is shown in Fig. 2.3 with \( \alpha, \beta \) the spherical angles of the unit orientation vector: \( d_x = \cos \alpha \sin \beta, d_y = \sin \alpha \sin \beta, d_z = \cos \beta \). As seen from the figure, the maximum of the distribution shifts from \( (\alpha = \pi/2, \beta = \pi/2) \) to \( (\alpha = \pi/4, \beta = \pi/2) \) with increasing concentration. Note that a similar realignment occurs in a dilute suspension with tumbling [71]; however, for a different reason. There the transition is governed by the shear rate and the diffusion constant. In the next section, an analytical approach using kinetic theory is developed to provide further insight into the physical mechanisms behind the viscosity decrease.
Figure 2.3. The orientation distribution $P(\alpha, \beta)$ for volume fractions (a) $\Phi = .0003$ and (b) $\Phi = .005$. The vertical lines indicate angle $\alpha = \pi/4$ for $V_0 = 1, \sigma_{LJ} = .35, U_0 = -8\pi V_0, B = 0.95$. The maxima are shown in white and the minima in black.

2.4 Continuum kinetic model

In order to obtain further insights into the role of hydrodynamic interaction the continuum limit of (2.1) is considered. It is assumed that the suspension can be described by a probability density $P(t, x, d)$ of finding a bacterium at location $x$ with orientation $d$ at time $t$. This distribution satisfies the following kinetic equation

$$\partial_t P = -\nabla_x \cdot (VP) - \nabla_d \cdot (\Omega P)$$

(2.6)

where translational $V$ and rotational $\Omega$ fluxes are obtained by replacing sums by integrals in (2.1) as follows (similar to the Law of Large Numbers, see Appendix E):

$$\sum_{j \neq i} A_{ij} \to V_L^{-1} \int A(x - x', d, d') P(x', d') dx'dd' + \zeta,$$

where $A_{ij}$ is the velocity $v$ and $\omega$ or $E$ can be defined accordingly (e.g., $\omega = \nabla \times v$) and the primes denote integration variables. In the derivation of an analytical solution to (2.6) the term $\zeta$ describing deviations from the mean-field approximation
is neglected, but its specific role will be discussed later when the results for the two basic types of bacteria: pushers and pullers are distinguished in Section 2.4.1. The quantity of interest is the orientation distribution

$$P_d(d) = \frac{1}{\rho V_L} \int P(x, d) dx,$$

with the mean concentration

$$\rho = V_L^{-1} \int P(x, d) dx dd.$$ $\text{To obtain the equation governing the angular distribution, substitute } P(x, d) \text{ into (2.6) and formally integrate over } x.$$

The resulting equation cannot be solved analytically in the general case due to its non-linearity, non-locality, and large number of dimensions. Here the simpler, yet nontrivial, limit in small non-sphericity, $B \to 0$ is taken where $B = \frac{b^2 - a^2}{b^2 + a^2}$ for minor and major axes $a$ and $b$ of the particle. Assume for simplicity that a separation of variables $P(x, d) = P_x(x)P_d(d)$ can be considered, which is valid as $B \to 0$. Here

$$P_x(x) = \int P(x, d) dd = \int C_k \exp(2\pi i kx) dk$$

is the local concentration and $C_k$ its Fourier component. A steady-state solution of the form is sought

$$P_d(d) \approx (4\pi)^{-1} \left[ 1 + \sin^2 \beta (A \sin(2\alpha) + C \cos(2\alpha)) \right] + O(B^2) \quad (2.8)$$

where the coefficients $A, C \sim B$ are to be determined.

These calculations were performed in the regime where $U_0 B \sim O(1)$ in agreement with numerical simulations. Straightforward but very cumbersome formal calculations yield the following result for the coefficients $A, C$ (full details of these computations are in the Supplementary Information of [75]):

$$A = -\frac{48 B^2 \pi^2 U_0 \rho \epsilon}{50 \gamma R}, \quad C = -\frac{3B}{2R}. \quad (2.9)$$

Here $R = 1 + \xi^2$, constant $\xi = \frac{16\pi^2 \rho BU_0 \epsilon}{25\gamma}$, and $\epsilon = \nu / \rho^2$ is the time-averaged
normalized variance of concentration,

\[ \nu = \frac{1}{V_L^2} \int dk |C_k|^2 (1 - \delta(k)) = \frac{1}{V_L^2} \left[ \int dr P_x^2 - \left( \int dr P_x \right)^2 \right] \]

where \( \delta(k) \) is a Dirac point mass.

**Remark 2.4.1.** These calculations are modified and made rigorous with all details presented in Chapter 3. The purpose of performing the formal calculations here is to develop a physical intuition and provide a guide for what should be expected when each step is rigorously justified.

In the derivation of (2.9) isotropy of the positional fluctuations is assumed, i.e., \( |C_k|^2 \) only depends on the modulus \( |k| \). This assumption is justified by comparison with numerical simulations. In the interest of developing an intuition for the effect of dipolar hydrodynamic interactions, the contribution to stress due to LJ interactions \( \Sigma_{LJ} \) is neglected. This assumption is consistent with experimental observations at low concentrations. Finally, the following approximate expressions for the orientation distribution \( P_d \)

\[ P_d(\alpha, \beta) \approx \frac{1}{4\pi} - \frac{3B}{8\pi R} \sin^2 \beta \left( \cos(2\alpha) + \xi \sin(2\alpha) \right) \]  

(2.10)

and the viscosity \( \eta \) using (2.4)

\[ \frac{\eta}{\eta_0} - 1 = \frac{\rho U_0}{\gamma} \int dx dy P_d(d) dd = -\frac{16B^2 \pi^2 U_0^2 \rho^2 \epsilon}{125 \gamma^2 R} \]  

(2.11)

are obtained. In this proceeding section, the formula (2.11) is analyzed to provide physical insight into the decrease in the effective viscosity.

### 2.4.1 Analysis of the effective viscosity

**Effective Viscosity for Pushers**

Recall that pushers are bacteria which bundle their flagella and propel themselves forward from behind resulting in a dipole moment \( U_0 < 0 \). For low to moderate concentrations, the main contribution to the stress and hence the viscosity is essentially determined by the orientation distribution of the particles. Thus
by analyzing (2.10), one can identify the important physical mechanisms, which lead to a decrease in the viscosity.

First consider the effective viscosity as the strain rate $\gamma \to 0$. The observed effect on viscosity can be viewed as a competition between the background flow, dipolar hydrodynamic interactions and collisions. The limit $\gamma \to 0$ reduces the effect of the background flow, which can wash out the result of the remaining interactions when its magnitude is large. The behavior of the asymptotic solution is given by $P_d \sim (1/\gamma) \sin^2(\beta) \sin(2\alpha)$, which achieves a maximum at $\alpha = \pi/4$ and $\beta = \pi/2$ in agreement with the numerical simulations Fig. 2.3. This is also consistent with the large concentration limit where interactions also are the dominant contribution to the total flow.

To verify that our model is valid for a wide range of concentration we compare our results to those obtained in the dilute limit ($\rho \to 0$). The distribution function $P_d \sim - \sin^2(\beta) \cos(2\alpha)$ has a maximum at $\alpha = \pi/2$ and $\beta = \pi/2$ and no viscosity reduction is seen. This also occurs in the spatially-homogeneous case ($\epsilon = 0$), in contrast to a nonuniform particle distribution in space, $\epsilon \neq 0$, where there is a viscosity reduction in agreement with our simulations and experiments [20]. The results also hint at a relationship between collective motion and the viscosity reduction: local concentration fluctuations (leading to nonzero $\epsilon$) arise due to a large-scale organized motion of swimmers via an instability of the homogeneous state [19].

It is interesting to then compare the expression for the viscosity (2.11) with the relationship obtained in [71] for the non-interacting case in the presence of tumbling (i.e. rotational diffusion of strength $D$). The expressions for the effective viscosity become the same for $D := -(8\pi^2 \rho BU_0 \epsilon)/75 > 0$. This suggests that hydrodynamic interactions lead, via a breakdown of the spatially homogeneous state ($\epsilon \neq 0$), to an effective noise (diffusion/tumbling).

To check the predictions given by (2.11) numerical simulations were performed for small non-sphericity, $B = 0.2$. The results are summarized in Fig. 2.4. The concentration variance $\epsilon$ was extracted from the instantaneous particle positions averaged over long periods of time on a two-dimensional square mesh in the $xy$–plane. As one sees from Fig. 2.4 (left), the numerical results qualitatively agree with (2.11). Better agreement is obtained for lower concentrations due to the fact that
Figure 2.4. Left: Effective viscosity $\eta$ vs volume fraction $\Phi$ for shape parameter $B = 0.2$ and dipole moment $U_0 = -8\pi V_0$. Right: Effective viscosity $\eta$ vs. Bretherton constant $B$ for $\Phi = 0.01986$. The error bars in the analytical results are due to uncertainty in the numerical calculation of the concentration variance, $\epsilon$.

the analytical formula does not account for the LJ stress (a positive contribution to EV). Also, Fig. 2.4 (right) shows that the approximation breaks down for larger non-sphericity (elongation) $B$ and the theory overestimates the decrease in viscosity. This is expected for an asymptotic formula derived in the limit as $B \to 0$.

Effective Viscosity for Pullers

Pullers are bacteria which use their flagella in front of their bodies to pull themselves forward. This results in an inversion of the forces in the dipole and a dipole moment $U_0 > 0$. The discussion of pullers is very complicated and the mean field approximation is no longer valid due to the motion being dominated by the fluctuations $\zeta$. Experiments and simulations show an increase of viscosity for suspensions of pullers, whereas (2.11) predicts a reduction independent of the sign of $U_0$ [43] and Fig. 2.5. However, for pullers there is no instability towards collective motion [19] and thus the spatial distribution remains uniform, $\epsilon = 0$. Hence fluctuations (i.e., deviations from the mean-field approximation of (2.6)) cannot be neglected as in the case of pushers. For pushers in a well-developed collective state the fluctuations are small compared to the mean field and the mean-field approximation is justified. Thus, the formula derived herein should not be used to make predictions in the case of pullers; however, the goal of this dissertation is to provide insight into the physical mechanisms leading to collective motion and pullers do not exhibit collective motion.
2.4.2 Effective normal stress coefficients

Using the orientation distribution $P_d(d)$ from (2.10) one can also compute the effective first and second dipolar normal stress coefficients $N_{12} = \frac{\Sigma_{d11} - \Sigma_{d22}}{\gamma^2}$ and $N_{23} = \frac{\Sigma_{d22} - \Sigma_{d33}}{\gamma^2}$ to investigate the effect of hydrodynamic interactions. One advantage of the mathematical model is that the computation of the effective normal stress coefficients is straightforward, whereas its measurement in experiment can be quite complicated [111]. These coefficients can provide important information about the suspension. One example is the ratio of the first normal stress to the viscosity determines the effective relaxation time [111]. Also, phenomena such as extrudate swelling [112] and secondary flow [113] are important in many technological applications. A simple calculation shows that

$$N_{12} = \frac{\Sigma_{d11} - \Sigma_{d22}}{\gamma^2} = -\frac{6U_0B\rho}{15\gamma^2R} \quad (2.12)$$

$$N_{13} = \frac{\Sigma_{d22} - \Sigma_{d33}}{\gamma^2} = \frac{3U_0B\rho}{15\gamma^2R}. \quad (2.13)$$

For pushers ($U_0 < 0$) $N_{12} > 0$ and $N_{23} < 0$ where as for pullers ($U_0 > 0$) $N_{12} < 0$ and $N_{23} > 0$. Both results are consistent with the predictions in [59, 114] while providing the concentration dependence. Observe that for a Newtonian fluid experiencing simple shear flow the normal stress coefficients are zero, since they
are nonzero here it indicates the presence of non-Newtonian behavior in bacterial suspensions. The combination of the viscosity and the two normal stress coefficient provides important information about the rheological behavior of the fluid. In addition, one sees in (2.12)-(2.13) that as the shear rate $\gamma \to \infty$ the normal stresses approach zero indicating the dominance of the background flow on the suspension.

In conclusion, the viscosity reduction as a function of concentration observed for pushers occurs primarily due to hydrodynamic interactions between swimmers. The effect of interactions on the effective viscosity is analogous to that of rotational noise in the dilute case. This effect, arising due to density fluctuations and the breakdown of the uniform spatial distribution of the swimmers, can be interpreted as \textit{self-induced noise} in a system with no eternally imposed stochasticity. For pullers, in contrast, the uniform state is stable. Thus the mean-field approach presented here yields no contribution to the effective viscosity and the behavior can be roughly described by small-scale uncorrelated fluctuations [75]. The long term result of this Chapter is a testable prediction for the orientation distribution of interacting bacteria in suspensions undergoing planar shear. In the next Chapter, the analysis of the kinetic theory is re-derived rigorously and in greater detail to specifically pinpoint the physical mechanisms responsible for the decrease in the effective viscosity.
Chapter 3

Derivation of an explicit formula for the effective viscosity

In this Chapter, an extension of the work originally published in [75] is presented, in which an explicit formula for the contribution to the effective viscosity due to pairwise hydrodynamic interactions is formally derived. This Chapter lays the foundation and provides the motivation for [115], which seeks to show the kinetic theory used herein is well-defined. Here attention is focused on bacteria, such as *B. subtilis*, used to study collective motion and the interesting effective properties of bacterial suspensions observed in experiment such as enhanced diffusivity, the formation of sustained whorls and jets, and the ability to extract useful work [3, 5, 8, 17, 51]. This type of bacteria has been referred to as a “pusher” in previous chapters due to its rear-actuated propulsion mechanism, which propels each microorganism forward from behind.

A recent remarkable experimental result on the effective viscosity in a suspension of bacteria provides the motivation for studying its effective properties; namely, the observation of a seven-fold reduction in the effective viscosity of a suspension of swimming *Bacillus subtilis* [20]. This reduction is seen up to around 2% volume fraction. This concentration regime is typically referred to as the dilute regime where particles essentially only interact with the background fluid studied analytically in [62, 71, 72] to name a few. For example, in the model by Haines et al. [59], the observed reduction results from particles aligning along the principal axis of the rate of strain tensor in the presence of random rotational diffusion.
(tumbling). Here an explicit asymptotic analytical formula has been derived and analyzed using a kinetic theory approach where instead of studying the particle equations of motion one studies the evolution of the probability density of bacterial configurations. In the dilute regime, this amounts to studying the density associated to a single particle in an infinite medium. The results in [59] are used to explain the mechanisms contributing to the decrease in viscosity in the dilute regime. In this work bacterial tumbling was required in order for the formula to predict the decrease in the effective viscosity. However, in the absence of tumbling the decrease is still observed experimentally at these volume fractions [20]. Therefore, a formula needs to be developed, which still predicts a decrease in the effective viscosity even when bacteria do not tumble.

In contrast, when the concentration exceeds a volume fraction 2%, bacterial hydrodynamic interactions and collisions become the main contributions to bacteria alignment and increased friction resulting in both a decrease and an increase in the effective viscosity respectively. This was captured numerically through simulation in the prior work [75]. In this Chapter, a model for a suspension incorporating hydrodynamic interactions is studied in order to derive an analogous formula from which the mechanisms contributing to the drastic reduction in the viscosity even in the absence of tumbling can be analyzed. Here the analysis of the associated kinetic theory becomes more difficult. Due to the presence of interactions, the suspension of interacting particles is generally described analytically by the probability density of configurations of all bacteria. There are many challenges associated with implementing a kinetic approach. In addition to considering a suspension of \( N \) particles, the kinetic theory will include singular terms arising due to the presence of hydrodynamic interactions. These terms will diverge as each bacterium approaches one another. Such suspensions are referred to as semidilute, where hydrodynamic interactions are modeled as a sum of pairwise interactions. Due to the difficulties cited above, a rigorous formula for the effective viscosity incorporating interactions in a semidilute suspension has yet to be derived until now.

Section 3.1 of this Chapter introduces the model under consideration for a semidilute bacterial suspension. Here a bacterium is represented as a point dipole where the force of self-propulsion is balanced by the viscous drag on its body. We
will give each particle a size through the use of a short-range repulsion potential imposing an excluded volume constraint. In addition, each particle has a shape through the use of the Bretherton constant $B$ (0/1, spheres/needles) in the particle equations of motion derived from first principles. Using the equations of motion, the true object of study is considered: the kinetic theory for the probability density of bacterial positions and orientations. Then the definition of the effective (homogenized) viscosity for a suspension of point dipoles is introduced. In Section 3.3, we note that the stress, which is the main component of the effective viscosity, only depends on the particle orientations. Thus, an asymptotic expression in the small parameter $B$ is derived for the distribution of particle orientations up to order $O(B^3)$. In Section 3.4, the asymptotic expression for the orientation density is used to derive an explicit analytical formula for the effective viscosity.

The main assumptions that are used to derive this formula are that a steady state solution exists for the introduced kinetic theory and that solution as a distribution can be decorrelated into a spatial density multiplied by a density of bacterial orientations. This formula is then used to identify that the specific mechanisms required to achieve the dramatic decrease in viscosity are elongated particles ($B \neq 0$), self-propulsion, and a non-uniform distribution of particles in space (collective motion results in local clusters of particles). In addition, it is established that as the shear rate is increased the contribution due to hydrodynamic interactions is annihilated and the contribution to the effective viscosity approaches zero. From the expression for the effective viscosity a striking result emerges: when the formula derived for the present interacting system is compared to that for a dilute suspension with random noise (bacterial tumbling), the same effective viscosity is found for a specific value of the “effective noise” in terms of known (measurable) physical parameters. Thus, an effective randomness, referred to as self-induced noise emerges, in a completely deterministic system. The formula for the effective viscosity is then compared with the result of Chapter 2 and the previous work [75], which included far more simplifying assumptions such as the isotropy in Fourier space in the prior derivation.
3.1 Model

In order to derive the effective viscosity, begin by introducing a coupled PDE/ODE system modeling the bacterial suspension. The bacteria are represented as point force dipoles in a background fluid. This approximation has been experimentally verified by observing the flow due to a pusher-type bacterium (e.g., *Bacillus subtilis*) in a Stokesian fluid and comparing it to that of a force dipole [2], justifying this approximation. One force represents the bacterium’s propulsion mechanism (e.g., flagellar motion), and the other is the opposing viscous drag exerted by the bacterium’s body on the fluid due to the no-slip boundary condition. In this Chapter, the primary concern is studying bacteria known as “pushers”, which are swimming particles propelling themselves from behind. This type of bacteria exhibited the dramatic viscosity reduction in experimental observation [20]. One can also consider “pullers”, which propels itself from in front of its bodies by pulling the fluid toward itself. The distinction in classification is determined by the particle’s propulsion mechanism. Now that a point dipolar model for a particle is chosen, then one must consider how each bacterium will move through the fluid.

Each particle can be identified with two variables, the position of the center of mass \( \mathbf{x} = (x, y, z) \) and orientation \( \mathbf{d} = (d_x, d_y, d_z) \). Recall the equations of motion for particle positions \( \mathbf{x} \) and orientations \( \mathbf{d} \) introduced from first principles in Chapter 2 and [75].

\[
\dot{x}^i = V_0 d^i + \sum_{j \neq i} (u^j(x^i) + F^j(x^i)) + u^{BG}(x^i) \tag{3.1}
\]

\[
\dot{d}^i = -\frac{1}{2} d^i \times \left( \omega^{BG}(x^i) + \sum_{j \neq i} \omega^j(x^i) \right) - d^i \times \left[ B d^i \times \left( E^{BG}(x^i) + \sum_{j \neq i} E^j(x^i) \right) \right] \tag{3.2}
\]

where \( B \) is the Bretherton constant or shape factor and \( V_0 \) is an individual bacterium’s swimming speed. Given each particle’s eccentricity \( e \) (the ratio of the major and minor axes) \( B = \frac{e^2 - 1}{e^2 + 1} \), \( B = 0 \) for spheres, \( B = 1 \) for needles. For the main bacterium of interest, *B. subtilis*, \( B \approx .9 \). The externally-imposed background flow contributes to each particle’s motion through the velocity, \( u^{BG} = (0, \gamma x, 0)^T \), as well as the vorticity \( \omega^{BG} = \nabla \times u^{BG} \) and rate of strain \( E^{BG} = \frac{1}{2} (\nabla u^{BG} + (\nabla u^{BG})^T) \).

Semidilute suspensions are investigated herein meaning the contribution to the
equations of motion due to hydrodynamic interactions can be written as a sum of pairwise interactions represented by the velocity $\mathbf{u}^j$ appearing in (3.1). The additional contributions to Jeffery’s equation in (3.2) are due to hydrodynamic interactions. These contributions are due to the vorticity $\omega^j$ and rate of strain $\mathbf{E}^j$ generated by $j$-th dipole on location of the $i$-th dipole

$$
\omega^j = \nabla \times \mathbf{u}^j, \quad \mathbf{E}^j = \frac{1}{2} \left( \nabla \mathbf{u}^j + (\nabla \mathbf{u}^j)^T \right).
$$

Each of these terms depends on the fluid velocity $\mathbf{u}$, which solves Stokes equation and will be described in greater detail below. The dependence of these terms on the orientation $\mathbf{d}^j$ of the $j$-th dipole is suppressed for convenience in notation. Note also that the orientation is a unit vector $\|\mathbf{d}\| = 1$ and later its unique description in terms of its two angles ($\alpha$ azimuthal and $\beta$ polar) will be used.

**Remark 3.1.1.** In this work, lower concentrations of bacteria are considered where the primary contribution to the effective viscosity from interactions is the dipolar component of the stress, $\Sigma^d$, which only depends on the set of particle orientations. Thus, the $\dot{x}$ equation will not factor into the final formula; however, $\mathbf{F}$ is the force associated to a truncated Lennard-Jones type potential imposing excluded volume constraints. For more information on its definition and why it is needed for global solvability see Chapter 4 or [115].

**Remark 3.1.2.** The equations of motion are a $5N$ coupled system of ordinary differential equations in comparison to the dilute case studied in [59] where there were only two ODEs governing the evolution of a single particle in an infinite medium (only depends on a single particle’s orientation).

Now the appropriate equation to model the fluid in a semidilute bacterial suspension must be determined. Based on the typical size $l_0 \sim 1\mu m$ and swimming speed $V_0 \sim 20\mu m/s$ of a bacterium, in addition to the typical dynamic viscosity $\eta_0 \sim 10^{-3} Pa \cdot s$ and density $\rho \sim 10^3 kg/m^3$ of the suspending fluid, the flow has Reynolds number, $Re \sim 10^{-4} \ll 1$. Thus, inertial effects can be neglected. Also, it is assumed that a steady-state flow is established on a timescale much smaller than the characteristic timescale (the time for a bacterium to swim its length).

Given the Reynolds number $Re \ll 1$ and the timescale of bacterial motion, the use of Stokes equation to model the fluid present in the suspension is justified. The
fluid velocity acting on particle $i$ due to particle $j$ is given as $\mathbf{u}^j(\mathbf{x}^i) = \mathbf{u}(\mathbf{x}^j - \mathbf{x}^i)$ where $\mathbf{u}(\mathbf{x})$ is a solution of

$$
\begin{cases}
\eta_0 \Delta \mathbf{u}(\mathbf{x}) = \nabla p(\mathbf{x}) - \nabla \cdot \left[ \mathbf{D}(\delta)\delta(\mathbf{x}) \right] & \mathbf{x} \in \mathbb{R}^3 \\
\nabla \cdot \mathbf{u}(\mathbf{x}) = 0 & \mathbf{x} \in \mathbb{R}^3 \\
\mathbf{u}(\mathbf{x}) \to 0, & |\mathbf{x}| \to \infty
\end{cases}
$$

(3.3)

where $\eta_0$ is the ambient fluid viscosity, $\mathbf{u}$ is the fluid velocity and $p$ is the pressure. The fluid in a suspension of $N$ particles would be modeled the same way, but with a sum of $N$ dipoles on the right-hand side. The dipole tensor $\mathbf{D}$ is given by

$$D_{lm}(\delta) := U_0 \left( d_l d_m - \frac{1}{3} \delta_{lm} \right)$$

(3.4)

where $U_0 < 0$ (Pushers) is the stresslet force quantifying the strength of the dipole referred to as the dipole moment (for more details see Appendix B). The above equation (3.3) has an explicit solution using the gradient of the Oseen tensor,

$$G(\mathbf{x}) = \frac{1}{8\pi\eta_0} \left( \frac{1}{|\mathbf{x}|} + \frac{\mathbf{x}}{|\mathbf{x}|^3} \right),$$

where

$$u_k(\mathbf{x}, \delta) := \frac{1}{8\pi\eta_0} \sum_{l=1}^{3} \sum_{m=1}^{3} D_{lm}(\delta)G_{kl,m}(\mathbf{x}).$$

(3.5)

In order to analyze this system, the associated kinetic theory for the probability density of bacteria configurations–particle positions and orientations is studied. In general, to derive this equation one considers the equations of motion (3.1)-(3.2) with random initial conditions. Then each sum in the equations of motion is a sum of identically distributed random variables (due to the semidilute assumption). Replace all sums in the equations of motion by their expectations using the Generalized Law of Large Numbers (GLLN) first studied in [116] and given in Appendix E.1

$$\sum_{j \neq i} A(r^{(i,j)}, \delta) \to \frac{1}{|V_L|} \int_{S^2} \int_{V_L} A(\mathbf{x} - \mathbf{x'}, \delta')P(\mathbf{x'}, \delta')d\mathbf{x'}d\delta' + \zeta$$

(3.6)

where $r^{(i,j)} = \mathbf{x}^i - \mathbf{x}^j$, $S^2$ is the unit sphere, and $|V_L| = L^3$ is the volume of the support of $P$, supp($P$), where the $N$ particles reside. $\zeta$ is the error in the mean
field approximation due to fluctuations (deviations from the mean field). The main idea is that this allows one to replace all the sums representing interactions, \( \sum_{j \neq i} \), by integrals with respect to a probability density, \( P(x, d) \). \( P \) is the density associated to finding a particle at location \( x \) with orientation \( d \). In (3.6), \( A(r, d) \) can be either the fluid velocity \( u^j(r) \), the vorticity \( \omega^j(r) \), the rate of strain \( E^j(r) \), or the collisional term \( F^j \) (\( F^j \) will not contribute to the final calculations).

**Remark 3.1.3.** Note in equation (3.6), according to the Generalized Law of Large Numbers, a factor of \( N \) should appear in front. To simplify notation we build this factor of \( N \) into \( P \) and enforce that \( \int_{V_L} \int_{S^2} P dxdd = N \) instead of 1.

Introduce the following measure space \( (\mathbb{R}^3 \times S^2, \mathcal{B}(\mathbb{R}^3 \times S^2), \mu_P) \) where \( A : (\mathbb{R}^3 \times S^2) \rightarrow \mathbb{R}^3 \) is a random variable and \( \mu_p \) is the measure associated with the density \( P(x, d) \) and is defined as

\[
\mu_P(X) = \int_X P(x, d) dxdd, \quad X \in \mathcal{B}(\mathbb{R}^3 \times S^2).
\]

By replacing the sums with integrals in the system (3.1)-(3.2), an equation that describes the evolution of the density \( P \) must be found (derived in Section 1.10.1 where conservation of measure is enforced)

\[
\partial_t P + \nabla_x \cdot (VP) + \nabla_d \cdot (\Omega P) = 0,
\]

where the fluxes are defined below

\[
V(x, d) := V_0d + \frac{1}{|V_L|} \int_{S^2} \int_{V_L} [u(x - x', d')] P(x', d') dx'dd' + u^{BG},
\]

\[
\Omega(x, d) := \frac{1}{|V_L|} \int_{S^2} \langle \omega(x - x', d, d') + E(x - x', d, d'), P(x', d') \rangle_{x'}dd' + \omega^{BG} + E^{BG}
\]

Here \( \langle \cdot, \cdot \rangle \) denotes the duality with respect to the \( L^2 \)-norm (the exact definition can be found in Appendix C.1). Introducing this pairing is required to make sure the integral is well-defined in the principal value sense since neither \( \omega \) nor \( E \sim 1/|x - x'|^3 \) are integrable in three dimensions. In addition, the terms on the right-hand side are defined as follows

\[
u(x, d) = \frac{V_0}{8\pi \eta_0} \nabla_x \cdot [(dd - 1/3I)\mathcal{O}(x)], \quad \omega(x, d, d') = -\frac{d}{2} \times [\nabla_x \times u(x, d')], \quad E(x, d, d') = -Bd \times [d \times D_x(u(x, d'))]d,
\]
\[ \omega^{BG}(d) = -\frac{d}{2} \times [\nabla_x \times u^{BG}(x)], \quad E^{BG}(d) = -Bd \times [d \times D_x(u^{BG}(x))d] \] (3.12)

where \( D_x(u) := \frac{1}{2} \nabla_x u + [\nabla_x u]^T \) represents the symmetric gradient. Recall that the orientation vector \( d \) is a unit vector, \(|d| = 1\), and denote

\[
d := (\cos \alpha \sin \beta, \sin \alpha \sin \beta, \cos \beta) = (d_x, d_y, d_z),
\]

\[
\hat{\alpha} := (-\sin \alpha, \cos \alpha, 0) = 1/\sin \beta (-d_y, d_x, 0),
\]

\[
\hat{\beta} := (\cos \alpha \cos \beta, \sin \alpha \cos \beta, -\sin \beta)
\]

for \( \alpha \in [0, 2\pi), \beta \in [0, \pi) \) with unit vectors \( \hat{\alpha} \) and \( \hat{\beta} \) respectively.

Here one must be careful to note that the divergence in orientations in (3.7) is taken over the unit sphere. In other words, for any field \( A = A(d) \) we have the following definition

\[
\nabla_d \cdot A := \frac{1}{\sin \beta} \left[ \partial_\alpha (A_\alpha) + \partial_\beta (\sin \beta A_\beta) \right],
\]

(3.13)

where \( A_\alpha = A \cdot \hat{\alpha} \) and \( A_\beta = A \cdot \hat{\beta} \). For comparison, denote \( \tilde{\nabla}_d \) as the classical gradient with respect to \( d \), then one can easily check that

\[
\nabla_d \cdot A = \tilde{\nabla}_d \cdot A - \frac{\partial}{\partial |d|} \left\{|d|(A \cdot d)\right\}_{|d|=1}.
\]

(3.14)

Given this kinetic approach, one needs to introduce next the definition of the principal object of study: The effective viscosity.

### 3.1.1 Definition of the effective viscosity for a suspension of point force dipoles

In general, consider the two contributions to stress present in the model: the stress due to dipolar hydrodynamic interactions \( \Sigma^d_{lm}(d) := \sum_{i=1}^{N} \frac{U_0}{|V_L|} (d_l d_m - \delta_{lm}/3) \) [84] and the excluded volume stress due to soft collisions (LJ interactions \( \mathbf{F} \) in (4.4) or (3.8)) \( \Sigma^{LJ}_{lm}(\overline{x}) := \sum_{i=1}^{N} \sum_{j \neq i} \frac{F_l(x^i - x^j)(x^i_m - x^j_m)}{|V_L|} \) [110]. Here the bacterial configurations are denoted by \( \overline{x} := (x^1, ..., x^N) \) and \( \overline{d} := (d^1, ..., d^N) \). At small
concentrations, the contributions due to collisions can be neglected

\[ \Sigma(x, d) = \Sigma^d(d) + \Sigma^{LJ}(x) \approx \Sigma^d(d), \quad \text{for } \phi \text{ small.} \]  

(3.15)

The exact concentration interval where the formula (3.15) works well will be determined later by comparison with numerical simulations of the same suspension where the viscosity is extracted as a longtime average. Thus, for this Chapter, it is sufficient to restrict attention to just the density of orientations denoted \( P_d(d) \). In order to isolate this density, assume a “separation of variables”, (i.e., the positions and orientations are decorrelated at low concentrations)

\[ P(x, d) = P_x(x) P_d(d), \]

where \( \int_{V_L} \int_{S^2} P(x, d) dx dd = N \). This allows for the definition of the orientation density

\[ P_d(d) := \frac{1}{N} \int_{V_L} P(x, d) dx, \quad \text{where } \int_{S^2} P_d(d) = 1. \]  

(3.16)

The ultimate goal is to compute the effective viscosity due to hydrodynamic interactions at low concentrations and compare with experimental observation [20] and numerical results. Therefore, the effective viscosity can be defined as

\[ \frac{\hat{\eta} - \eta_0}{\eta_0} := \frac{1}{|V_L|} \int_{V_L} \int_{S^2} \frac{\Sigma_{xy}}{\gamma} P(x, d) dx dd = \int_{S^2} \frac{\Sigma_{xy}(d)}{\gamma} P_d(d) dd. \]  

(3.17)

as in [75, 115]. In order for the effective viscosity to be well-defined we assume throughout this Chapter that a steady-state solution to (3.7), \( P(x, d) \), exists. This definition is further explained in [115] and within this dissertation the explanation can be found in Chapter 4. In addition, define the mean concentration or number density

\[ \rho := \frac{N}{|V_L|} = \frac{1}{|V_L|} \int_{V_L} \int_{S^2} P(x, d) dx dd. \]  

(3.18)

By introducing this separation and searching only for an expression of \( P_d(d) \) the problem is simplified so that it is amenable to rigorous mathematical analysis.
3.2 Assumptions used to derive an explicit formula for the effective viscosity

Throughout the course of this work three assumptions are used:
1. Separation of variables on the density $P(x, d) = P_x(x)P_d(d)$.
2. The existence of a steady state.
3. The positional density (local concentration $P_x(x)$) is constant in the $z$-direction.

Below further details about each assumption are provided.

3.2.1 Separation of variables

Physically, note that in this Chapter only small concentrations are considered where collisions are not important, but the flow of each bacterium affects all others. However, the bacteria are at large distances apart. Thus, since the background flow provides the major contribution, then positions and orientations become mostly independent. This is justified from the experimental work of Aranson et al. (e.g., see [5, 18]). To make this work more amenable to mathematical analysis it is assumed that the positions and orientations are completely decoupled. The following assumption was used in the derivation of the explicit formula for the effective viscosity (3.17) above and is consistent with experiments at low concentration.

Assumption (A1): The density can be written as $P(x, d) = P_x(x)P_d(d)$ (separation of variables) where

$$P_d(d) := \frac{1}{N} \int_{V_L} P(x, d)dx$$

and $\int_{S^2} P_d(d)d\mathbf{d} = 1$. Here $N$ is the number of particles, $V_L := \text{supp}(P_x(x))$, and the spatial density $P_x(x) = \int_{S^2} P(x, d)d\mathbf{d}$.

This assumption was used for two reasons. First, the effective viscosity at low concentration only depends on the orientation distribution (see Remark 3.1.1). Thus, using this assumption an explicit equation for the evolution of the orientation distribution can be derived. Second, $V$ contains diverging integrals (e.g., $\int \int F dx d\mathbf{d}$ since $F \sim r^{-12}$), which will no longer be present in the equation for the orientation distribution $P_d(d)$ allowing for further mathematical analysis. It will
be observed at the end of this chapter that the asymptotic expansion for $P_d(d)$ depends on $P_x(x)$ through the coefficients, thus all the information about spatial patterns is preserved.

### 3.2.2 Existence of a steady state to the equation for $P_d(d)$

The following nonlinear, nonlocal integro-differential equation describes the evolution of the orientation density $P_d(d)$

$$\frac{\partial}{\partial t} P_d(d) = -\nabla_d \cdot (\langle \Omega \rangle_x P_d(d)) \quad (3.19)$$

where $\langle \Omega \rangle_x = \frac{1}{N} \int_{V_L} \Omega P_x(x) dx$, $\Omega$ contains BG flow and interaction terms

$$\Omega(x, d) = \omega^{BG} + E^{BG} + \frac{1}{N|V_L|} \int_{S^2} \int_{V_L} \langle [\omega(x - x', d', d) + E(x - x', d', d')]P(x', d') \rangle dx'd'd'. $$

Equation (3.19) is obtained by integrating (3.7) in $x$ and dividing by $N$. The notion of a steady state solution to (3.19) is defined as follows

**Definition 3.2.1.** $\hat{P}_d(d)$ is called a steady state solution to (3.19) if it solves

$$0 = -\nabla_d \cdot (\langle \Omega \rangle_x \hat{P}_d(d)).$$

In [35], a steady state distribution of particles is considered and shown to match experimental observation well in the study of large scale convective motion in bacterial suspensions.

**Assumption (A2): (Existence of a Steady State)** There exists a nontrivial steady state solution to (3.19).

First, note that there is no trivial steady state unless $B = 0$ in which case we find $\hat{P}_d(d) = \frac{1}{4\pi}$. This can be obtained both from the asymptotic results below for $P_d(d)$ and from observing that the trivial steady state would be a constant satisfying the constraint $\int_{S^2} P_d(d) d\mathbf{d} = 1$. One still needs to prove existence of any steady state in the general case $B \neq 0$. This assumption could be stated as a theorem and its proof is being studied currently and may be the topic of a future work. Two methods for approaching this are either to prove convergence of the asymptotic series or add a diffusion term $D\Delta P$ and let $D \sim B^2 \to 0$ as $B \to 0$. 
3.2.3 \( P_x(x) \) constant in the \( z \)-direction

The assumption that \( P_x(x) \) is constant in \( z \) is consistent with past numerical observations by Ryan et al. [75] and experimental observation in [35] since the suspension remains below any critical concentration for three-dimensional collective motion. Also, collective motion even in full 3D experiments and simulations in planar shear flow has been observed to be essentially 2D in the shearing plane. Thus, following these observations we can make our mathematical analysis tractable by also assuming the same thing.

**Assumption (A3):** The density \( P_x(x) \) is constant in \( z \).

This assumption essentially follows from the physical setup of the quasi-2D thin film suspension. The result of this assumption is that if motion is constant in the \( z \)-direction, then the Fourier transform of the spatial distribution behaves like a delta function, \( F[P_x]^2/\pi L \sim \delta(k_3) \) (see Appendix F.1 for the proof).

### 3.3 Derivation of the orientation density

In this section, an expression for the orientation density \( P_d(d) \) is derived. Since (3.7) is a nonlinear integro-differential equation it is challenging to find an analytical solution. Thus, look for the orientation distribution as an asymptotic expansion of in the limit of small non-sphericity (\( B \ll 1 \)). This will allow us to apply analytical techniques and derive an expression, which will provide physical insight into the mechanisms contributing to the decrease in the effective viscosity.

Now an equation for the orientation density \( P_d(d) \) is derived from (3.7). Begin by integrating (3.7) in \( x \) and divide by \( N \) to obtain

\[
\partial_t P_d(d) + \nabla_d \cdot \left[ (\omega^{BG}(d) + E^{BG}(d))P_d(d) \right] + \frac{1}{N|V_L|} \int \nabla_d \cdot (\hat{\Omega} P(x, d)) dx = 0. \tag{3.20}
\]

where

\[
\hat{\Omega}(x, d) = \frac{1}{|V_L|} \int_{S^2} \langle [\omega(x - x', d', d) + E(x - x', d', d), P_x(x')]_{x'} P_d(d') dd'. \tag{3.21}
\]

Herein \( \hat{\Omega} \) will denote the component of \( \Omega \) due to interactions. Notice that the difficulties contained in \( V \) such as the Lennard-Jones contribution \( F \) have been
removed by considering only the equation for the orientation distribution \( P_d(d) \).

In order to find the effective viscosity one needs to find the steady-state solution \( P_d(d) \) satisfying the following equation:

\[
0 = \nabla_d \cdot \left[ (\omega^{BG}(d) + \mathbf{E}^{BG}(d)) P_d(d) \right] + \frac{1}{N|V_L|} \int_{V_L} \nabla_d \cdot \left( \hat{\Omega}(x, d, d') P_x(x) P_d(d) dd'dx \right)
\]  

(3.22)

Before considering the non-local term, compute the contribution due to interaction with the background flow exactly

\[
\nabla_d \cdot \left[ (\omega^{BG}(d) + \mathbf{E}^{BG}(d)) P_d(d) \right] = 
\frac{\gamma}{2} \left[ -3B \sin^2 \beta \sin 2\alpha P_d(d) + (1 + B \cos 2\alpha) \partial_\alpha P_d(d) + \frac{B}{2} \sin 2\alpha \sin 2\beta \partial_\beta P_d(d) \right].
\]

The complete calculation can be found in Appendix D.1. Now rewrite the integral term in (3.20):

\[
\frac{1}{N|V_L|} \int_{V_L} \nabla_d \cdot (\hat{\Omega} P_x(x) P_d(d)) dd'dx = \frac{1}{N|V_L|} \left[ \int_{V_L} \nabla_d \cdot \hat{\Omega} P_x(x) P_d(d) dx 
\right. 
\left. + \int_{V_L} \hat{\Omega} \cdot \nabla_d P_x(x) P_d(d) dx \right].
\]  

(3.23)

Consider the first term and note also that the following equality holds (in the distributional sense):

\[
\nabla_d \cdot \hat{\Omega} = \nabla_d \cdot \int_{S^2} \langle \mathbf{E}(x - x', d', d), P_x(x') \rangle_d d'd'.
\]  

(3.24)

This is due to the equality \( \nabla_d \cdot \omega(x - x', d, d') = 0 \), which follows immediately from the definition of \( \omega \), \( \omega = d \times A \), where \( A = \nabla_x \mathbf{u} \) does not depend on \( d \). So, \( \nabla_d \cdot \omega(x - x', d, d') = \nabla_d \cdot (d \times A) = A \cdot (\nabla_d \times d) - d \cdot (\nabla_d \times A) = 0 \). The result is zero using (3.14) since the classical divergence with respect to \( d \) of \( \omega \) is zero and \( \omega \cdot d = 0 \). The second term of (3.23) will take the following form

\[
\frac{1}{N|V_L|} \int_{S^2} \langle \omega(x - x', d) - E(x - x', d, d'), P_x(x') \rangle_{d'} P_d(d') \cdot P_x(x)\nabla_d P_d(d) dd'.
\]

Notice the convolution form of the nonlocal terms. In the next section, the
Fourier transform will be utilized to compute quantities necessary to derive the formula for the effective viscosity. Specifically, using tools such as Parseval’s Theorem, one can take the spatial integrals and consider them in Fourier space where they will prove easier to analyze. After using the separation of variables assumption, the density will be expressed in terms of the frequencies $k$.

The main goal for the remainder of this section is to write the system in a convenient form for using Fourier Transforms. This idea follows naturally from the observation that all the interactions terms take the form of a convolution. Using this idea and the separation assumption, one can introduce the Fourier transform of $P_x(x)$ as follows

$$
P_x(x) = \frac{1}{(2\pi)^3} \int e^{ik \cdot x} C(k) dk. \quad (3.25)$$

Define $H(x - x', d, d') := \omega(x - x', d, d') + E(x - x', d, d')$, then the following equalities hold inside the integrals

$$
< H \star P, P >_x = < F[H \star P], F(P) >_k = < F[H](F[P])^2 >_k, \quad (3.26)
$$

where $\star$ and $F$ stand for convolution and Fourier transform, respectively. The first equality is Parseval’s identity and the second is the fact that the Fourier Transform of a convolution is the product of Fourier transforms. Thus, one can rewrite the equation (3.22) in the following form

$$
\nabla_d \cdot [(\omega^{BG} + E^{BG})P_d(d)] + \int_{S^2} \nabla_d \cdot \{P_d(d)P_d(d') < F[H](F[P])^2 >_k \} d'd' = 0. \quad (3.27)
$$

In order to compute $F[H]$ one must first understand how the Fourier transforms acts on the fluid velocity $u$ and its derivatives.

### 3.3.1 Evaluation of Fourier transforms

In order to analyze (3.27) an analytical expression for the Fourier transform $F[H] = F[\omega] + F[E]$ is needed. Both terms depend on the fluid velocity $u$. Thus, consider Stokes equation

$$
-\gamma_0 \Delta_x u + \nabla_x p = \nabla_x \cdot \Sigma(d), \quad \nabla_x \cdot u = 0 \quad (3.28)
$$
with $\Sigma(x, d) = U_0(dd - I/3)\delta(x)$, which is the stress due to hydrodynamic interactions. Denote the Fourier transform of a function as $\hat{f} = F[f] = \int e^{-i(k \cdot x)} f(x) dx$ and compute the Fourier transform of the fluid velocity.

**Proposition 3.3.1.** $\hat{u}(k) = \frac{i}{\eta_0 |k|} \left( I - \frac{kk^*}{|k|^2} \right) \hat{\Sigma}(k) \frac{k}{|k|}$.

**Proof.**

**Step 1: Evaluation of $F[p]$.** First take the divergence of (3.28) in $x$, which gives

$$\Delta_x p = \nabla_x \cdot (\nabla_x \cdot \Sigma). \quad (3.29)$$

Observe that

$$F[\Delta_x p] = -|k|^2 \tilde{p}(k), \quad F[\nabla_x \cdot (\nabla_x \cdot \Sigma)] = \int \Sigma : \nabla_x^2 e^{-i k \cdot x} dx = -\tilde{\Sigma}(k) : kk^*$$

where $*$ denotes the transpose. Here the stress $\Sigma(x, d') := (d'd'^* - I/3)\delta(x)$ when transformed becomes

$$\tilde{\Sigma}(d') = (d'd'^* - I/3), \quad (3.30)$$

since the Fourier transform of a $\delta$ function is 1. Thus, from (3.29) $-|k|^2 \tilde{p}(k) = -\tilde{\Sigma}(k) : kk^*$ one can find an expression for the transform of the pressure

$$\tilde{p}(k) = \frac{1}{|k|^2} \tilde{\Sigma}(k) : kk^*. \quad (3.31)$$

**Step 2: Evaluation of $F[u]$.** Return to Stokes equation (3.28) and observe that

$$\eta_0 F[\Delta_x u] = -\eta_0 |k|^2 \tilde{u}(k), \quad F[\nabla_x p] = i k \tilde{p}(k),$$

$$F[\nabla_x \cdot \Sigma] = -\int \Sigma \nabla_x e^{-i k \cdot x} dx = i \tilde{\Sigma}(k) k.$$

Using these relations one finds that $\eta_0 |k|^2 \tilde{u}(k) + i k \tilde{p}(k) = i \tilde{\Sigma}(k) k$. After rearranging the terms and using the expression for $\tilde{p}$ (3.31) the Fourier Transform of the fluid velocity is found

$$\tilde{u}(k) = \frac{i}{\eta_0 |k|} \left( I - \frac{kk^*}{|k|^2} \right) \tilde{\Sigma}(k) \frac{k}{|k|} \quad (3.32)$$

proving the proposition. \hfill \Box
In order to compute the term corresponding to the rate of strain, $F[E]$, we need the Fourier transform of the symmetric gradient $D_x(u) = \frac{1}{2} (\nabla_x u + [\nabla_x u]^T)$ using the following proposition.

**Proposition 3.3.2.** $F[D_x(u)] = -\frac{1}{2\eta_0|k|^2} \left( |k|^2 \tilde{\Sigma} kk^* - 2kk^* \tilde{\Sigma} kk^* + |k|^2 kk^* \tilde{\Sigma} \right)$.

**Proof.** First we observe that the Fourier transform of the symmetric gradient is $F[D_x(u)] = i \eta_0 (\tilde{u}k^* + k\tilde{u}^*)$. Plug the Fourier transform of $u$ (3.32) into this expression to find

$$F[D_x(u)] = i \eta_0 (\tilde{u}k^* + k\tilde{u}^*) = -\frac{1}{2\eta_0|k|^2} \left( (I - \frac{kk^*}{|k|^2}) \tilde{\Sigma}(k)kk^* + kk^* \tilde{\Sigma}(k)(I - \frac{kk^*}{|k|^2}) \right).$$

Using the fact that $\tilde{\Sigma}$ is symmetric ($\tilde{\Sigma} = \tilde{\Sigma}^*$)

$$F[D_x(u)] = -\frac{1}{2\eta_0|k|^4} \left( |k|^2 \tilde{\Sigma} kk^* - 2kk^* \tilde{\Sigma} kk^* + |k|^2 kk^* \tilde{\Sigma} \right).$$

completing the proof. \qed

**Remark 3.3.3.** It is easily seen that $F[D_x(u)]$ does not depend on $|k|$, since $F[D_x(u)]$ can be rewritten as

$$F[D_x(u)] = -\frac{1}{\eta_0} \frac{k k^*}{|k|^2} - \frac{2}{\eta_0} \frac{k k^*}{|k|^2} \tilde{\Sigma} \frac{k k^*}{|k|^2} + \frac{k k^*}{|k|^2} \tilde{\Sigma}.$$

Also, $\tilde{\Sigma} = \tilde{\Sigma}(d')$ still depends on the particle orientations.

This subsection is concluded by summarizing the analytical expressions for the two terms found in the integrand in (3.27)

$$F[E] = -B d \times (d \times F[D_x(u)] d) = B \{ F[D_x(u)] d - dd^* F[D_x(u)] d \} \quad (3.33)$$

$$F[\omega] = -\frac{1}{2} d \times F[\nabla_x u] = -\frac{1}{2} d \times [-ik \times F[u]]. \quad (3.34)$$

where $F[u]$ is given by Proposition 3.3.1 and $F[D_x(u)]$ is given by Proposition 3.3.2. In the next section, the asymptotics for the orientation density $P_d(d)$ will be introduced and its terms will be computed.
3.3.2 Asymptotic expansion in angles

Recall the steady-state Liouville equation (3.27) with the background terms substituted in
\[
\gamma \frac{1}{2} \left[ -3B \sin^2 \beta \sin 2\alpha P_\mathbf{d}(\mathbf{d}) + (1 + B \cos 2\alpha) \partial_\alpha P_\mathbf{d}(\mathbf{d}) + \frac{B}{2} \sin 2\alpha \sin 2\beta \partial_\beta P_\mathbf{d}(\mathbf{d}) \right]
+ \frac{1}{N|V_L|} \int_{S^2} \nabla_\mathbf{d} \cdot \{ P_\mathbf{d}(\mathbf{d}) P_\mathbf{d}(\mathbf{d}') < F[H], (F[P_x])^2 >_k \} \, d\mathbf{d}' = 0. \tag{3.35}
\]

This problem is very difficult to solve analytically, so consider the following asymptotic expansion in the Bretherton constant, \( B \), for the orientation distribution, \( P_\mathbf{d}(\mathbf{d}) \), up to second order
\[
P_\mathbf{d}(\alpha, \beta) = P_\mathbf{d}^{(0)}(\alpha, \beta) + P_\mathbf{d}^{(1)}(\alpha, \beta)B + P_\mathbf{d}^{(2)}(\alpha, \beta)B^2 + O(B^3). \tag{3.36}
\]

First address the terms at order \( O(1) \) by considering the uniform distribution on the surface of the unit sphere, which is \( P_\mathbf{d}^{(0)}(\alpha, \beta) = \frac{1}{4\pi} \) (surface area \( 4\pi \)). We want to considered our asymptotic expansion about the uniform distribution because it has been extensively documented in theory that as particles become spheres (\( B \to 0 \)), then the distribution in angles should become uniform [59, 75]. The uniform distribution in space would be the mean concentration or number density \( P^0_\mathbf{x}(\mathbf{x}) = \frac{N}{|V_L|} \). From \( \frac{1}{|V_L|} \int_{V_L} \int_{S^2} P^0_\mathbf{x}(\mathbf{x}, \mathbf{d}) d\mathbf{x} d\mathbf{d} = \frac{N}{|V_L|} \), one can verify that the uniform distribution in angles should be \( P_\mathbf{d}^{(0)}(\alpha, \beta) = \frac{1}{4\pi} = |S^2|^{-1} \) with the following computation
\[
\frac{1}{|V_L|} \int_{V_L} \int_{S^2} P^0_\mathbf{x}(\mathbf{x}, \mathbf{d}) d\mathbf{x} d\mathbf{d} = \frac{N}{|V_L|} \int_{V_L} \int_{S^2} \frac{1}{4\pi|V_L|} d\mathbf{x} d\mathbf{d}.
\]

Here \( \frac{1}{4\pi} \) comes from the constraint that \( \int_{S^2} P_\mathbf{d}(\mathbf{d}) d\mathbf{d} = 1 \). Thus, look for an expansion of the form
\[
P_\mathbf{d}(\alpha, \beta) = \frac{1}{4\pi} + P_\mathbf{d}^{(1)}(\alpha, \beta)B + P_\mathbf{d}^{(2)}(\alpha, \beta)B^2 + O(B^3) \tag{3.37}
\]
in the limit \( B \to 0 \). In the next two subsections, the linear order term \( P_\mathbf{d}^{(1)}(\alpha, \beta) \) and quadratic order term \( P_\mathbf{d}^{(2)}(\alpha, \beta) \) are computed.
3.3.3 Contribution at $O(B)$: Background flow

In order to analyze the linear terms of (3.35) consider its integral term and use the properties of divergence. The main observation will be the fact that $\nabla_d \cdot F[H] = \nabla_d \cdot F[E]$ by the argument proceeding (3.24). First expand the divergence to find

$$\frac{1}{N|V_L|} \int_{S^2} \nabla_d \cdot \{ P_d(d)P_d(d')\langle F[H](F[P_x])^2 \rangle_k \} \, dd' =$$

$$\frac{1}{N|V_L|} \int_{S^2} P_d(d')P_d(d)\langle \nabla_d \cdot (F[H](F[P_x]))^2 \rangle_k \, dd' 
+ \frac{1}{N|V_L|} \int_{S^2} \nabla_d [P_d(d)]P_d(d')\langle F[H](F[P_x])^2 \rangle_k \, dd'.$$

Thus the steady-state Liouville equation has the form

$$0 = \frac{\gamma}{2} [B \sin(2\alpha) \sin \beta (\cos \beta \partial_\beta P_d - 3 \sin \beta P_d) + [1 + B \cos(2\alpha)] \partial_\alpha P_d]$$

$$+ \frac{1}{N|V_L|} \int_{S^2} P_d(d')P_d(d)\langle \nabla_d \cdot (F[H](F[P_x]))^2 \rangle_k \, dd'$$

$$+ \frac{1}{N|V_L|} \int_{S^2} \nabla_d [P_d(d)]P_d(d')\langle F[H](F[P_x])^2 \rangle_k \, dd'.$$  \hspace{1cm} (3.38)

The first integral at $O(B)$ is zero since it can be written as (recall $E \sim O(B)$)

$$\frac{1}{16\pi^2 N|V_L|} \int_{S^2} \langle \nabla_d \cdot (F[E](d)](F[P_x])^2 \rangle_k \, dd'$$  \hspace{1cm} (3.39)

where the Fourier Transform $F[E] = B \{ F[D_x(u)]d - dd^* F[D_x(u)]d \}$ defined in (3.33) with $F[D_x(u(d'))] = \frac{1}{2|k|^2} \left[ |k|^2 \Sigma kk^* - 2kk^* \Sigma kk^* + |k|^2 kk^* \Sigma \right]$. The integral in (3.39) is seen to be zero by switching the order of integration and noting

$$\int_{S^2} \bar{\Sigma} dd' = \int_{S^2} U_0|d'(d')^* - I/3|dd' = 0.$$

In the second integral of (3.38) the term $\nabla_d P(x, d)$ contributes a term of $O(B)$. Thus $P_d(d')$ must contribute a constant, namely, $1/4\pi$. Similarly $H$ must only contribute terms of $O(1)$ and therefore $H = \omega$. This results in the second integral of (3.38) being zero due to the fact that $\int_{S^2} F[\omega]dd' \sim \int_{S^2} (d'd' - I/3)dd' = 0.$

Thus, the following steady state equation for $P_d(d)$ at order $B$ is found:

$$0 = \frac{\gamma}{2} \left[-3P_d^{(0)} \sin(2\alpha) \sin^2 \beta + \partial_\alpha P_d^{(1)} \right].$$ \hspace{1cm} (3.40)
After substituting \( P_d^{(0)} = \frac{1}{4\pi} \) and solving (3.40), one finds that \( P_d^{(1)}(\alpha, \beta) = -\frac{3}{8\pi} \sin^2 \beta \cos(2\alpha) \). Therefore, the contribution due to interactions will not appear until \( O(B^2) \) and thus this is only the contribution of the background flow. To this point

\[
P_d(\alpha, \beta) = \frac{1}{4\pi} - \frac{3}{8\pi} \sin^2 \beta \cos(2\alpha) B + P_d^{(2)}(\alpha, \beta) B^2 + O(B^3).
\]

It will be shown later that up to \( O(B) \) the contribution to the effective viscosity by the particles is zero. This will shed light on the fact that interactions are necessary to see the decrease in the effective viscosity. Note that even though this is the contribution due to the background flow the strain rate \( \gamma \) is not present. This is due to the fact that up to order \( O(B) \) only the background flow is present and interactions don’t contribute. Therefore, the magnitude of the flow will not have an effect on the longtime limit of the effective viscosity. However, once the terms at the next order are computed one observes a competition develop between the background flow and the flow due to interparticle interactions. In this case the magnitude of the shear \( \gamma \) will become important.

### 3.3.4 Contribution at \( O(B^2) \): Pairwise interactions

Now consider the terms in (3.38) of order \( O(B^2) \):

\[
0 = \frac{\gamma}{2} \sin(2\alpha) \sin \beta \cos \beta \partial_\beta P_d^{(1)}(\mathbf{d}) - \frac{3\gamma}{2} \sin(2\alpha) \sin^2(\beta) P_d^{(1)}(\mathbf{d}) + \frac{\gamma}{2} \partial_\alpha P_d^{(2)}(\mathbf{d}) + \frac{\gamma}{2} \cos(2\alpha) \partial_\alpha P_d^{(1)}(\mathbf{d}) + \frac{1}{4\pi N|V_L|} \nabla_d \cdot \int_{S^2} \langle F[\mathbf{E}]F[P_x]^2 \rangle_k P_d^{(1)}(\mathbf{d}')d'd' + \frac{1}{4\pi N|V_L|} \int_{S^2} \nabla_d[P_d^1(d)]\langle F[\omega](F[P_x])^2 \rangle_k d'd' + \frac{1}{N|V_L|} \int_{S^2} \nabla_d[P_d^1(d)]P_d^1(d')\langle F[\omega](F[P_x])^2 \rangle_k d'd'.
\]

By introducing spherical coordinates \((\theta, \phi)\) in Fourier space, the first integral in (3.42) at \( O(B^2) \) can be rewritten as:

\[
\frac{1}{4\pi N|V_L|} \nabla_d \cdot \int_{S^2} \langle F[\mathbf{E}]F[P_x]^2 \rangle_k P_d^{(1)}(\mathbf{d}')d'd' = \frac{1}{4\pi N|V_L|} \nabla_d \times \left\{ \int \left[ -\frac{1}{2\gamma_0|k|^4} \left( |k|^2Fkk^* - 2kk^*Fkk^* + |k|^2kk^*F \right) F[P_x]^2d\mathbf{k} \right] \cdot \nabla_d \right\}.
\]
\[
\frac{U_0}{40\pi \eta_0 |V_L|} \boldsymbol{\nabla} a \cdot \left( \mathbf{d} \times \mathbf{d} \times \int \left[ \begin{array}{ccc}
\sin^2(2\theta) & -\frac{1}{2} \sin(4\theta) & 0 \\
-\frac{1}{2} \sin(4\theta) & -\sin^2(2\theta) & 0 \\
0 & 0 & 0
\end{array} \right] \mathbf{d}_x \right)
P^2_{\mathbf{d}}(|k|, \theta, |k|^2 d|k| d\theta)
\]

where
\[
\mathcal{F} := \int_{S^2} \tilde{\Sigma} P_d^{(1)}(\mathbf{d'}) d\mathbf{d'} = -\frac{3U_0}{8\pi} \left[ \begin{array}{ccc}
\frac{8\pi}{15} & 0 & 0 \\
0 & -\frac{8\pi}{15} & 0 \\
0 & 0 & 0
\end{array} \right] = -\frac{U_0}{5} \left[ \begin{array}{ccc}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 0
\end{array} \right]
\]
(all the detailed calculations can be found in the Appendix D.3).

The second integral in (3.42) at \(O(B^2)\) can be written as:
\[
\frac{1}{4\pi N|V_L|} \int_{S^2} \nabla \mathbf{d} [P^2_d(\mathbf{d})] \langle F[\bar{\omega}](F[P_\omega])^2 \rangle_k d\mathbf{d'} = \\
\frac{\nabla \mathbf{d} [P^2_d(\mathbf{d})]}{4\pi N|V_L|} \int_{S^2} \int_{V_L} \langle \omega(\mathbf{x} - \mathbf{x'}, \mathbf{d}, \mathbf{d'}) P_\omega(\mathbf{x'}) P_\omega(\mathbf{x}) \rangle d\mathbf{x'} d\mathbf{d'} = 0
\]
since \(\int_{S^2} \omega d\mathbf{d'} = -\frac{1}{2} \mathbf{d} \times [\nabla \mathbf{x} \times \int_{S^2} \mathbf{u}(\mathbf{x}, \mathbf{d'}) d\mathbf{d'}] \) and
\[
\int_{S^2} \mathbf{u}(\mathbf{x}, \mathbf{d'}) d\mathbf{d'} = \int_{S^2} \nabla \mathbf{x} \cdot \left( \mathbf{d'} \left( \frac{I}{|\mathbf{x}|} + \frac{\mathbf{x}\mathbf{x}}{|\mathbf{x}|^3} \right) \right) d\mathbf{d'} = \left[ \int_{S^2} U_0(\mathbf{d'} - I/3) d\mathbf{d'} \right] : \nabla \mathbf{G} = 0.
\]

The third integral in (3.42) is zero since \(\int_{S^2} F[E] d\mathbf{d'} = 0\) (again using the fact that \(\int_{S^2} \tilde{\Sigma} d\mathbf{d'} = 0\)). Finally, the remaining integral has the following form (detailed calculations in Appendix D.4):
\[
\frac{\nabla \mathbf{d} [P^1_d(\mathbf{d})]}{N|V_L|} \int_{S^2} P^1_d(\mathbf{d'}) \langle F[\bar{\omega}](F[P_\omega])^2 \rangle_k d\mathbf{d'} = \frac{3U_0}{20\pi \eta_0} \int k_1 k_2 \sin(2\alpha) \sin^2 \beta |F[P_\omega]|^2 d\mathbf{k}.
\]

The following equation for \(P^2_d(\mathbf{d})\) at \(O(B^2)\) must be solved where all the expressions for the integral terms have been inserted:
\[
0 = \frac{\gamma}{2} \sin(2\alpha) \sin \beta \cos \beta \partial_\beta P^1_d(\mathbf{d}) - \frac{3\gamma}{2} \sin(2\alpha) \sin^2(\beta) P^1_d(\mathbf{d}) \\
+ \frac{\gamma}{2} \partial_\alpha P^2_d(\mathbf{d}) + \frac{\gamma}{2} \cos(2\alpha) \partial_\alpha P^1_d(\mathbf{d}) \\
+ \frac{U_0}{40\pi \eta_0 N|V_L|} (A \sin^2 \beta \cos(2\alpha) + C \sin^2 \beta \sin(2\alpha)) + \frac{3U_0}{10\pi \eta_0 N|V_L|} D \sin(2\alpha) \sin^2 \beta.
\]
where

\[
A := \frac{1}{2} \int \sin^2(2\theta) F[P_x]^2 |k|^2 d|k|d\theta
\]

\[
C := -\frac{1}{2} \int \sin(4\theta) F[P_x]^2 |k|^2 d|k|d\theta
\]

\[
D := \left( \int k_1 k_2 (F[P_x])^2 d\mathbf{k} \right).
\]

Now substitute in the expression for \( P_1^d(d) \) and use the following ansatz for \( P_2^d(d) \)

\[
P_2^d(d) = C_1 \sin^4 \beta \cos(4\alpha) + C_2 \sin^2 \beta \cos(2\alpha) + C_3 \sin^2 \beta \sin(2\alpha).
\]

Plugging both into the equation one finds

\[
0 = \left[ \frac{3\gamma}{4\pi} \sin(4\alpha) \sin^2 \beta \cos^2 \beta + \frac{9\gamma}{8\pi} \sin(4\alpha) \sin^4 \beta \right]
\]

\[
\frac{\gamma}{2} \left[ -4C_1 \sin^4 \beta \sin(4\alpha) - 2C_2 \sin^2 \beta \sin(2\alpha) + 2C_3 \sin^2 \beta \cos(2\alpha) \right] + \frac{3\gamma}{4\pi} \sin(4\alpha) \sin^2 \beta
\]

\[
+ \frac{U_0 A}{40\pi \eta_0 N|V_L|} \sin^2 \beta \cos(2\alpha) + \left[ \frac{U_0 C}{40\pi \eta_0 N|V_L|} + \frac{3U_0 D}{10\pi \eta_0 N|V_L|} \right] \sin^2 \beta \sin(2\alpha).
\]

Simplify and group like terms to see

\[
0 = \left[ \frac{-3\gamma}{4\pi} + \frac{9\gamma}{8\pi} - 2\gamma C_1 \right] \sin(4\alpha) \sin^4 \beta + \left[ \gamma C_3 + \frac{U_0 A}{40\pi \eta_0 N|V_L|} \right] \sin^2 \beta \cos(2\alpha)
\]

\[
+ \left[ -\gamma C_2 + \frac{U_0 C}{40\pi \eta_0 N|V_L|} + \frac{3U_0 D}{10\pi \eta_0 N|V_L|} \right] \sin^2 \beta \sin(2\alpha).
\]

Since the factors are linearly independent each coefficient should be zero, resulting in the following system of equations for the coefficients of \( P_2^d(d) \)

\[
\frac{3\gamma}{4\pi} + \frac{9\gamma}{8\pi} - 2\gamma C_1 = 0, \quad \Rightarrow C_1 = \frac{3}{16\pi}
\]

\[
-\gamma C_2 + \frac{U_0 C}{40\pi \eta_0 N|V_L|} + \frac{3U_0 D}{10\pi \eta_0 N|V_L|} = 0, \quad \Rightarrow C_2 = -U_0 \frac{C + 12D}{40\gamma \pi \eta_0 N|V_L|}
\]

\[
\gamma C_3 + \frac{U_0 A}{40\pi \eta_0 N|V_L|} = 0, \quad \Rightarrow C_3 = -\frac{U_0 A}{40\gamma \pi \eta_0 N|V_L|}.
\]
An explicit formula for the orientation distribution has been found

\[
P_d(\alpha, \beta) = \frac{1}{4\pi} - \frac{3}{8\pi} \sin^2 \beta \cos(2\alpha) B + \left[ \frac{3}{16\pi} \sin^4 \beta \cos(4\alpha) - U_0 C + \frac{12 D}{40\pi \eta_0 |V_L|} \sin^2 \beta \sin(2\alpha) \right] B^2 + O(B^3).
\]

In the following section, the contribution to the effective viscosity due to hydrodynamic interactions is computed.

### 3.4 Explicit formula for the effective viscosity

Using the orientation distribution derived in the previous section, compute the contribution to the effective viscosity due to interactions as a function of \(P_x(x)\) or \(F[P_x(x)]\) through the constants \(A > 0, C, \) and \(D\)

\[
\eta^{int} = \frac{1}{|V_L|} \int_{S^2} \int_{V_L} \frac{\Sigma_{xy}(d)}{\gamma} P(x, d) dx dd
\]

\[
= \frac{1}{\gamma |V_L|} \int_{S^2} \int_{V_L} U_0 d_x d_y P_x(x) \left[ \frac{1}{4\pi} + P_d^1(\alpha, \beta) B + P_d^2(\alpha, \beta) B^2 \right] dx dd
\]

\[
= \frac{U_0 N}{\gamma |V_L|} \int_{S^2} d_x d_y \left[ \frac{1}{4\pi} - \frac{3}{8\pi} \cos(2\alpha) \sin^2 \beta B
\]

\[
+ C_1 B^2 \sin^4 \beta \cos(4\alpha) + C_2 B^2 \sin^2 \beta \cos(2\alpha) + C_3 B^2 \sin^2 \beta \sin(2\alpha) \right] \sin \beta d_\alpha d_\beta
\]

\[
= -\frac{U_0^2 B^2 A}{40\gamma^2 \pi \eta_0 |V_L|^2} \int_{S^2} \cos(\alpha) \sin(\alpha) \sin^5 \beta \sin(2\alpha) d_\alpha d_\beta
\]

\[
= -\frac{U_0^2 B^2 A}{75\gamma^2 \pi \eta_0 |V_L|^2} = -\frac{U_0^2 B^2 \rho^2 \hat{A}}{75\gamma^2 \pi \eta_0} < 0.
\]

where \(\hat{A} \sim O(1)\), so this quantity behaves like \(\rho^2\) in concentration (cf. [117] where an expansion for the effective viscosity to order two in concentration corresponding to pairwise interactions is considered). Note that \(U_0^2/\eta_0 \sim \eta_0\) since \(U_0 \sim f_\rho \sim 6\pi \eta_0 V_0\).

As an additional check of consistency, consider the dimensions of the final quantity. The dipole moment \(U_0 = \frac{kg^2 m^2}{s^3}\), the Bretherton Constant and \(\hat{A}\) are dimensionless, the concentration/number density \(\rho = \frac{1}{m^3}\), the ambient viscosity \(\eta_0 = \frac{kg}{m \cdot s}\), and the strain rate \(\gamma = \frac{1}{s}\) resulting in \(\eta^{int}\) having units of viscosity \(\frac{kg}{m \cdot s}\).
In the next section, the specific mechanisms which need to be present in order to observe a decrease in the effective viscosity are examined.

As in Section 2.4.2, the orientation distribution $P_{d}(d)$ from (3.44) can be used to compute the effective first and second dipolar normal stress coefficients $N_{12} = \frac{\Sigma_{d}^{d}}{\gamma^{2} - \Sigma_{22}}$ and $N_{23} = \frac{\Sigma_{d}^{d}}{\gamma^{2} - \Sigma_{33}}$ to investigate the effect of hydrodynamic interactions. As before the main advantage of the mathematical model is that the computation of the effective normal stress coefficients is straightforward in contrast to experiment where its measurement can be quite complicated [111]. From the more rigorous derivation in this chapter one finds:

$$N_{12} = \frac{\Sigma_{11}^{d} - \Sigma_{22}^{d}}{\gamma^{2}} = \frac{U_{0}\rho}{\gamma^{2}} \left[ -\frac{2}{5} - \frac{2U_{0}\rho(C + 12D)}{75\gamma\pi\eta_{0}} B^{2} \right]$$

(3.45)

$$N_{13} = \frac{\Sigma_{22}^{d} - \Sigma_{33}^{d}}{\gamma^{2}} = \frac{U_{0}\rho}{\gamma^{2}} \left[ \frac{1}{5} + \frac{U_{0}\rho(C + 12D)}{75\gamma\pi\eta_{0}} B^{2} \right].$$

(3.46)

The approximations are valid as $B \ll 1$, so for pushers ($U_{0} < 0$) $N_{12} > 0$ and $N_{23} < 0$ where as for pullers ($U_{0} > 0$) $N_{12} < 0$ and $N_{23} > 0$. Both results are again consistent with the predictions in [59, 114] while providing the concentration dependence. One of the normal stress differences is negative, similar to what has been observed in the past for liquid crystals [118, 119]. As in Section 2.4.2, one sees in (3.45)-(3.46) that as the shear rate $\gamma \rightarrow \infty$ the normal stresses approach zero indicating the dominance of the background flow on the suspension.

### 3.4.1 Mechanisms required for the decrease in the effective viscosity

In this section, the mechanisms which lead to a decrease in the effective viscosity are investigated. These same mechanisms will be shown in Chapter 5 to be responsible for collective motion and large scale structure formation in suspensions of pushers. For spherical particles ($B = 0$) the net change in the effective viscosity is zero. Active particles are required, since $U_{0} \sim f_{p} = 0$ results in no change in the effective viscosity. If the positional distribution $P_{x}(x)$ is near uniform, then

$$\hat{A} = \frac{1}{2N^{2}} \int \sin^{2}(2\theta) F[P_{x}]^{2} d\mathbf{k} \approx 0,$$
resulting in no change in the effective viscosity. Also, in the limit $\gamma \to \infty$ the contribution to particle motion due to shear dominates the contribution due to interactions with $P_d(d)$ maximized at $\alpha = \pi/2$ and $\beta = \pi/2$ (alignment with $y$-axis). This is analogous to the passive case where particles in a planar shear flow tend to align with the direction where the fluid exerts the least amount of torque on the particle. To exhibit a decrease in the effective viscosity active, elongated particles whose interactions result in a non-uniform distribution in space are needed.

### 3.4.2 Effective noise conjecture

In this subsection, the results herein involving a semidilute suspension of point force dipoles are compared to the previous result for a suspension of prolate spheroids with propulsion modeled as a point force [59]. In this work by Haines et al., finite size particles are taken as spheroids with a point force ($\delta$ function) modeling self-propulsion and each particle experiences a random reorientation referred to as tumbling. Biologically tumbling corresponds to a reorientation of a particle in hopes of finding a more favorable environment. Typically in experiment this is observed when the concentration of oxygen is low and bacteria, such as $B. subtilis$, sense that the fluid around them does not contain the nutrients needed, so it enters a more dormant state resulting in a lower swimming speed and an increased tumbling rate [50].

Since only one term contributes to the effective viscosity, one can choose to match the coefficient of this term

$$P_d^{\text{int}} = \frac{1}{4\pi} - \frac{3}{8\pi} B \cos(2\alpha) \sin^2 \beta + \frac{3}{16\pi} B^2 \sin^4 \beta \cos(4\alpha)$$

$$- U_0 \rho \frac{C + 12D}{40\gamma \eta_0} B^2 \sin^2 \beta \cos(2\alpha) - \frac{U_0 \rho \hat{A}}{40\gamma \eta_0} B^2 \sin^2 \beta \sin(2\alpha) + O(B^3)$$

with the corresponding coefficient in the derivation by Haines et al. [59], which is quadratic in the diffusion strength $D$. To make the formulas for the effective viscosity identical, the strength of the effective noise/diffusion (tumbling) is chosen
to be
\[ \hat{D} := \frac{-15\eta_0 \gamma^2 + \sqrt{225\eta_0^2 \gamma^4 - \hat{A}^2 B^2 \gamma^2 \rho^2 U_0^2}}{12AB\rho U_0} > 0, \]
(since \( U_0 < 0 \) for pushers). Observe that if \( \hat{D} \) is chosen in this way, depending only on physical parameters present in the problem, then the same effective viscosity as the dilute case studied in [59] is found. The phenomenon where stochasticity arises from a completely deterministic system is called self-induced noise. A future challenge is to explain this phenomenon rigorously using mathematics. One heuristic idea is that the periodic (deterministic) Jeffrey orbits are destroyed by interactions resulting in stochastic behavior.

Some conclusions about this effective noise can be made that ensure its consistency with physical reality. As particles become spheres \( B \to 0 \), \( \hat{D} \to 0 \) resulting in no change in the effective viscosity consistent with [59]. Also as the strain/shear rate \( \gamma \to \infty \), \( \hat{D} \to 0 \). This is physically intuitive, because as the shear rate becomes large its contribution dominates that due to hydrodynamic interactions resulting in behavior that resembles that of a passive suspension. Thus, the contribution to the effective viscosity due to hydrodynamic interactions is zero.

3.4.3 Comparison to numerical simulations

In this section, the accuracy of the derived formula is tested by comparing it to recent numerical simulations. These simulations are highly efficient and parallel in nature allowing them to be carried out on GPUs. Details of the simulation methods can be found in Section 1.11. All simulations herein were run on computers at Argonne National Laboratory.

Figure 3.1 shows how both the formula and numerical computations of viscosity change with particle shape as all other system parameters remain fixed. Here shape is accounted for through the Bretherton constant \( B = \frac{b^2 - a^2}{\rho^2 + a^2} \) where \( b \) is the length of the major axis and \( a \) is the length of the minor axis. First notice that in both the formula and numerics the contribution to the effective viscosity due to hydrodynamic interactions decreases with \( B \). This is due to the fact that as particles become more asymmetrical \( B \to 1 \) the interparticle hydrodynamic interactions have a greater effect leading to alignment. This alignment increases
Figure 3.1. Comparison of the formula for the effective viscosity with numerical simulations as particle shape changes through the Bretherton constant $B$ for a fixed volume fraction $\Phi = 0.02$ and shear rate $\gamma = 0.1$. The vertical bars represent the error in the numerical approximation. Error in the analytical solutions comes from the numerical estimation of $\hat{A}$.

in magnitude the dipolar stress leading to an even bigger decrease in the effective viscosity. The agreement between the analytical formula and numerical simulations breaks down as $B$ becomes large, but this is expected due to the fact that the asymptotic formula is valid in the regime where $B \ll 1$ (small non-sphericity).

Figure 3.2 shows how both the formula and numerical computations of viscosity change with the concentration of the suspension as all other system parameters remain fixed. It is seen that as concentration increases the effective viscosity decreases. This can easily be explained by the fact that as particles move beyond the dilute regime ($\Phi < 0.02$) and into the semidilute regime particle motion begins to be dominated by interparticle hydrodynamic interactions. This leads to collective motion of the particles in the suspension, which subsequently decreases the viscosity. The two results begin to diverge near volume fraction $\Phi \approx 0.02$. The reason the numerical simulations do not decrease as much is that collisions are taken into account. It was shown in [75] that the stress due to collisions is a positive contribution to the effective viscosity which is not captured by the formula. This contribution begins to become important beyond the dilute regime ($\Phi > 0.02\%$).

Figure 3.3 shows how both the formula and numerical computations of vis-
Figure 3.2. Comparison of the formula for the effective viscosity with numerical simulations as the volume fraction $\Phi$ changes for a fixed shape $B = .2$ and shear rate $\gamma = .1$.

Figure 3.3. Comparison of the formula for the effective viscosity with numerical simulations as the shear rate $\gamma$ changes for a fixed volume fraction $\Phi = .02$ and shape $B = .2$.

cosity change with the shear rate of the background flow in the suspension as all other system parameters remain fixed. As expected when the shear rate is large in both the analytical formula and simulations, the decrease in viscosity due to hydrodynamic interactions is negligible. This is due to the fact that the background flow dominates particle motion wiping out the effects of interparticle interactions and stopping any collective structures from forming. When the shear rate is too
small the effective viscosity becomes unbounded. This makes sense given that at small shear rate the system becomes almost non-dissipative and thus the effective viscosity is not well-defined. This can easily be seen by noting that the viscosity is the ratio of the stress over the strain and when the strain is essentially zero the effective viscosity becomes unbounded. All three plots show good agreement with experimental observation and physical intuition.

Finally, we want to show the effect of shear thickening predicted by the model and simulations for the bacterial suspension. In Figure 3.4, the effective viscosity versus the shear rate is plotted for three different concentrations. One observes that as the concentration increases the effective viscosity predicted by formula derived in Section 3.4 decreases for some intermediate range of shear rates. As expected, if the shear rate is large, then the effect of interactions and concentration are overwhelmed by the background flow and the effective viscosity is just the ambient viscosity. Here $\tau$ is the relaxation time as estimated by the formula for EV from Chapter 2, which is easier to manipulate

$$\tau = \frac{\Sigma_{12}}{2\eta} = \frac{-U_0 B \rho}{5 \gamma^2 R \eta_0 \left[ 1 - \frac{16 \pi^2 B^2 U_0^2 \rho^2 \epsilon}{125 \gamma^2 R} \right]} \approx \frac{25}{16 \pi^2 B U_0 \rho \epsilon \eta_0} = 8.338, \tag{3.47}$$
where the Bretherton constant $B = .95$, concentration $2 \times 10^{16} m^{-3}$, dipole moment $U_0 = 10^{-12} Nm$, ambient viscosity $\eta_0 = 10^{-3} \frac{k_\theta}{m \cdot s}$, and $\varepsilon \approx .001$ (estimated from simulations). All of these values are taken from experimental data on B. subtilis. Note here that the stress due to collisions is not accounted for in this formula as well as the passive contribution to the effective viscosity from the particles taking up space. To understand the true effect of shear rate on the effective viscosity one must account for all these contributions, but the formula provides a testable prediction for future work.

### 3.4.4 Comparison to previous result

Recall the original formula for the contribution to the effective viscosity due to pairwise hydrodynamic interactions, which was formally derived in Chapter 2 and [75]

$$P_d^{\text{orig}} = \frac{1}{4\pi} \left[ 1 - \frac{3B\dot{\gamma}^2}{2(\dot{\gamma}^2 + (16\pi^2 \rho U_0 B \varepsilon / 25)^2)} \sin^2 \beta \left( \cos(2\alpha) + \frac{16\pi^2 \rho U_0 B \varepsilon}{25} \sin(2\alpha) \right) \right] + O(B^2).$$

The presence of an effective noise still holds if we choose $D = -\frac{8\pi^2 BU_0 \rho \varepsilon}{25}$, then $P_d(d) = P^{\infty}(d)$ from the dilute case (Haines et al. [59]). So also here hydrodynamic interactions have the same effect as random bacterial tumbling – self-induced noise. Since the orientation density $P_d(d)$ are the same, then both predict the same decrease in the effective viscosity.

The formula derived for the effective viscosity in this Chapter, $\eta^{\text{int}}$, is more general than that derived in [75]. First, we do not assume isotropy in Fourier $k$-space. In addition, here $U_0 B \sim O(B)$ whereas before it was assumed that $U_0 B \sim O(1)$ relying on justification using experimental values. What remains to be understood is how the two formulas compare with each other. Specifically, we need to analyze how $\hat{A} = \frac{1}{2\pi^2} \int \sin^2(2\theta) F[P_x]^2 dk$ differs from $\epsilon = \frac{1}{N^2} \left[ \int P_x(x)^2 dx - (\int P_x(x) dx)^2 \right]$. The main idea is to form a conclusion similar to Parseval’s theorem, namely that $\int F[P_x]^2 dk$ behaves similarly to $\int P_x^2 dx$. Also, if $P_x(x) \approx \text{const}$, then $F[P_x] \approx \delta(k)$. Therefore, for a uniform distribution $\epsilon = 0$ and $\hat{A} = 0$. 
3.4.5 Case of a uniform distribution in space

Consider the case where \( P_\mathbf{x}(\mathbf{x}) \) is uniform in \( V_L \) referred to as “cubic isotropy”

\[
F_{2D}[P_\mathbf{x}] = \int_{V_L} P^2_0 e^{-i(k_1 x + k_2 y)} dx dy = 4P_0^2 \frac{\sin(k_1 L)}{k_1} \cdot \frac{\sin(k_2 L)}{k_2}
\]

where \( P_0 = \frac{N^{1/3}}{L} \). Derive a bound for \( |A| \) noting that \( \left| \frac{4k_1^2 k_2^2}{|k|^4} \right| \leq 4 \):

\[
|A| = \left| \frac{1}{2} \int \sin^2(2\theta) F[P_\mathbf{x}]^2 |\mathbf{k}|^2 d|\mathbf{k}| d\theta \right|
\]

\[
= \left| \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{4k_1^2 k_2^2}{2|\mathbf{k}|^4} \cdot 16P_0^4 \left( \frac{\sin(k_1 L)}{k_1} \right)^2 \left( \frac{\sin(k_2 L)}{k_2} \right)^2 dk_1 dk_2 \right|
\]

\[
\leq \left( 32\pi^2 P_0^4 L^2 \right) \cdot \left\{ \frac{1}{\pi L} \int_{-\infty}^{\infty} \left( \frac{\sin(k_1 L)}{k_1} \right)^2 dk_1 \cdot \frac{1}{\pi L} \int_{-\infty}^{\infty} \left( \frac{\sin(k_2 L)}{k_2} \right)^2 dk_2 \right\}.
\]

where the terms inside \( \{ \cdots \} \) to converge to 1 (see Appendix F.1). Thus, \( \frac{1}{L^3} A \to 0 \) as \( L \to \infty \). Therefore, as \( N, L \to \infty \) in such a way that \( \rho = N/L^3 \) remains constant one finds that

\[
|\hat{A}| = \left| \frac{1}{2N^{5/3}} \int \sin^2(2\theta) F_{2D}[P_\mathbf{x}]^2 |\mathbf{k}|^2 d|\mathbf{k}| d\theta \right|
\]

\[
\leq \left| \frac{1}{N^{1/3} L^2} \left( 32\pi^2 \right) \cdot \left\{ \frac{1}{\pi L} \int_{-\infty}^{\infty} \left( \frac{\sin(k_1 L)}{k_1} \right)^2 dk_1 \cdot \frac{1}{\pi L} \int_{-\infty}^{\infty} \left( \frac{\sin(k_2 L)}{k_2} \right)^2 dk_2 \right\} \right| L^{-3} \to 0.
\]

Therefore, \( \hat{A} \) is quantified as a measure of the deviation of the positional distribution \( P_\mathbf{x}(\mathbf{x}) \) (local concentration) from uniform so that it behaves like \( \epsilon \) in the original formal derivation in Chapter 2 and [75]. As an additional note, for pullers (propulsion mechanism in front of body resulting in a change in direction of the forces composing the point dipole, \( U_0 > 0 \)), which are not covered here, the positional distribution is essentially uniform due to the absence of collective motion \( \hat{A} \approx \epsilon = 0 \) as was observed in [59, 75]. Thus, there is no decrease in viscosity due to hydrodynamic interactions consistent with the formula derived in this work.
3.5 Conclusions

In this chapter, the derivation of a formula for the effective viscosity formally derived in Chapter 2 was made rigorous and an additional term in the asymptotic expansion for the effective viscosity was derived (now up to $O(B^2)$). This formula revealed the physical mechanisms responsible for the decrease in the effective viscosity confirming the prior formal calculation. Namely, hydrodynamic interactions, an elongated body, and self-propulsion are required to observe a decrease. These features are all present in the bacteria *Bacillius subtillis* used in the experiments of Aronson et al. at Argonne National Laboratory, which motivated this study of the effective viscosity. In addition, an interesting phenomenon was uncovered: the emergence of self-induced noise where a completely deterministic system governed by interactions resembles a random system for certain regimes of the physical parameters. This chapter is also the foundation for studying the global solvability of solutions to the PDE kinetic equation as well as rigorously proving the convergence to a steady state distribution, which may be the subject of future work.
Suspending suspensions of self-propelled microscopic particles, such as swimming bacteria, exhibit collective motion leading to remarkable experimentally-observable macroscopic properties. Rigorous mathematical analysis of this emergent behavior can provide significant insight into the mechanisms behind these experimental observations; however, there are many theoretical questions remaining unanswered. In this Chapter, a coupled PDE/ODE system first introduced in the physics literature and used to investigate numerically the effective viscosity of a bacterial suspension is studied. Next, the kinetic theory associated to the coupled system, which is designed to capture the longtime behavior of a Stokesian suspension of point force dipoles (infinitesimal spheroids representing self-propelled particles) with Lennard-Jones-type repulsion is examined. A planar shear background flow is imposed on the suspension through the novel use of Lees-Edwards quasiperiodic boundary conditions applied to a representative volume. The existence and uniqueness of solutions for all time to the equations of motion for particle configurations – dipole orientations and relative positions – is established. This result follows from first establishing the regularity of the solution to the fluid equations. The existence and uniqueness result allows one to define the Liouville equation for the probability density of configurations. Then it is shown that this probability density defines the average bulk stress in the suspension underlying the definition of many macroscopic quantities of interest, in particular the effective viscosity. These effective
properties are determined by microscopic interactions highlighting the multiscale nature of this work. The main contents of this Chapter have been published in [115].

4.1 Introduction

Pattern formation, anomalous rheology, and increased diffusivity are just a few of the many interesting macroscopic phenomena which have been observed in bacterial suspensions [3, 4, 5, 8, 17, 18, 20, 43, 35, 60]. These properties result from the emergence of collective motion among the swimming bacteria and sharply distinguish suspensions of active particles from passive suspensions. Collective motion arises precisely because bacteria are self-locomoting microorganisms that move and interact through the fluid with each other and their environment.

One of the most striking experimental results in bacterial suspensions is the observation of a seven-fold reduction in the effective viscosity of a suspension of swimming *Bacillus subtilis* [20]. This reduction is seen as the volume fraction of bacteria increases to a critical value of about 2%. Below this concentration threshold, referred to as the dilute regime, interactions between bacteria are negligible. It is sufficient to accurately describe the statistical state of the suspension by the probability of configurations – positions and orientations – of a single bacterium swimming in an externally-imposed background flow. This simplifying assumption has been used theoretically in [62, 71, 72] and numerically in [74] to explain the observed viscosity reduction. The reduction was shown to be the result of a coherent injection of momentum by the bacteria spending significant time aligned to the principal extensional axes of the background flow. Here the equations governing the probability density of bacterial configurations can be explicitly derived and analyzed.

However, when the concentration exceeds 2%, interactions between the bacteria become significant drivers of both interbacterial alignment and increased friction, contributing both to the decrease and increase in the effective viscosity. This was captured numerically through simulation in Chapter 2 and prior work [75]. Analytically, the suspension of interacting particles is generally described by the probability density of configurations of *all* bacteria. The governing equations of the
probability density are sometimes known as the kinetic theory of the suspension. Due to the presence of hydrodynamic interactions the kinetic theory will typically include singular terms, which diverge as each bacterium approaches one another. Further, when approximating a bulk suspension by a periodic system, only the relative motion (relative positions between each particle) of the suspended bacteria is meaningful. Up until now it has not been rigorously shown that such a kinetic theory is well-defined and suitable to define an effective viscosity outside of the dilute limit.

In this Chapter, the gap starts to be closed by analyzing a particular kinetic theory aimed at defining the effective viscosity for a semidilute bacterial suspension under a planar shear flow. Mathematically, a semidilute suspension is defined as one that satisfies the superposition principle: the flow at any point in the fluid is the sum of the flows induced by the individual moving particles (see, e.g., [75]). This is also commonly known in the physics literature as mean field theory. Bacteria similar to *B. subtilis* used in the experimental work [20] are considered. These bacteria are rod-like and propel themselves through the cumulative pushing action of their rotating helical flagella.

The semidilute regime is defined by concentrations at which the interbacterial distances are typically much larger than the bacteria themselves, yet interactions between particles still play a prominent role. This allows the bacteria to be modeled as infinitesimal force dipoles acting on the fluid. This amounts to approximating the flow produced by each bacterium with its dipolar component [109], which captures the effect of its elongated shape and enforces the superposition principle. These assumptions are supported by experiment: recent work [60] shows that the flow from a swimming microorganism is well approximated by a dipolar flow at a distance, that the flow decays rather rapidly, and in the absence of significant alignment between the bacteria the flow is essentially negligible at distances comparable to the length of the bacterium. At shorter distances excluded volume interactions (collisions) dominate hydrodynamic interactions and are the main mechanism behind the initial alignment and the emergence of coherent motion. Therefore, we can expect that dipolar hydrodynamic interactions and Lennard-Jones-like excluded volume forces capture the main mechanisms of interbacterial interaction in the semidilute regime. In this Chapter it is established
that the addition of excluded volume forces to the model serves to regularize the theory making it well-defined and suitable for a definition of effective viscosity.

At a fixed time the instantaneous viscosity can be defined in terms of the volume-averaged stress [84, 85], a function of only the instantaneous configuration of the suspended particles. The effective viscosity, on the other hand, must be a measurable macroscopic quantity independent of the particular particle configuration and, hence, of time. It can be defined using the longtime average of the instantaneous viscosity, provided this limit exists and is independent of the initial configuration — the classical conditions for ergodicity — which can be challenging to establish in a rigorous mathematical framework. More basically, however, a necessary condition for the longtime limit to exist is that the kinetic theory must be well-defined for all times.

The kinetic theory used herein is defined as the Liouville equation for a suitable ODE governing the evolution of bacterial configurations. To ensure the Liouville equation is well-defined for all time, the ODE’s trajectories must exist for all time, for any initial condition in our phase space. The ODE is defined via a balance of forces and torques, which involves the hydrodynamic forces from the fluid governed by a PDE – the Stokes equation governing the flow generated by the force dipoles. The specific yet representative case of a planar shear is modeled by imposing time–dependent quasiperiodic boundary conditions first proposed by Lees and Edwards [79]. With these boundary conditions and a given configuration of finitely many dipoles at a fixed time, the Stokes equation is explicitly solvable, at least in the weak sense due to the fact that the right–hand side is a distribution. A weak solution is insufficient due to the hydrodynamic forces entering the ODE, which require a pointwise evaluation of the fluid velocity and its derivatives. Additionally, because of the quasiperiodic form of the shearing boundary conditions, the resulting fluid velocity is not unique, but is defined only up to an additive constant. As a result, only the relative motion of the bacteria is well defined. To address these issues the sufficient regularity of the PDE solution is established and it is shown that the ODE, the kinetic theory as well as the viscosity can be self-consistently defined in terms of relative particle positions. Finally, it is shown that for any separated initial state — where particles have distinct initial positions — the ODE solution is defined for all time and remains separated. This allows us
to conclude that the kinetic theory is also well-defined and the investigation of its longtime limit, including the question of effective viscosity, is meaningful.

The remainder of the Chapter is organized as follows. In Section 4.2 the definition of effective viscosity for bulk suspensions is discussed. Section 4.3 describes the model for the suspension as a coupled particle/fluid system as well as the modeling of shear. Section 4.4 establishes the main theoretical results: (i) the existence, uniqueness, and regularity of the solutions of the fluid equations, (ii) the global solvability of the particle equations of motion. Section 4.5 concludes the Chapter. Throughout this work, the Einstein summation convention is adopted. The following notation for derivatives \( u_{i,m} := \frac{\partial u_i}{\partial x_m} \) is used. To avoid confusion vectors in the standard basis are denoted with a superscript, \( \{e^1, e^2, e^3\} \).

### 4.2 Effective (homogenized) viscosity of suspensions

Viscosity quantifies the response of the bulk fluid flow to an applied stress. Conversely, viscosity is a measure of the bulk stress in the fluid necessary to maintain a prescribed bulk flow. Assuming this response is linear, the viscosity is represented as a 4th order tensor, \( \eta_{ijkl} \), quantifying the constitutive relationship between the deviatoric stress, \( \Sigma^d_{ij} = \Sigma_{ij} - \frac{1}{3} \delta_{ij} \Sigma_{mm} \), and the rate of strain, \( E_{kl} \), as follows:

\[ \Sigma^d_{ij} = \eta_{ijkl} E_{kl}. \]

In the case of an isotropic (same in all directions) fluid the tensor is uniquely characterized by a single scalar, also called the viscosity. In general, however, the relationship between the strain rate and the stress — the rheology of the fluid — is nonlinear and cannot be characterized by a constant scalar or tensor. Even in these situations, however, it is frequently possible to derive useful scalar constants quantifying some aspects of this constitutive relationship. Here the definition of the effective \textit{shear viscosity} is developed as a measure of the shear stress induced by a prescribed shear flow.

A rate of strain is imposed on the suspension by specifying a planar shear background flow or, equivalently, suitable velocity boundary conditions, and computing the resulting bulk stresses acting in the suspension. A \textit{configuration} of the suspension is defined as a set of bacterial positions \( \mathbf{x} = (x^1, ..., x^N) \in \mathbb{R}^{3N} \) and
orientations \( \mathbf{d} = (d^1, \ldots, d^N) \in \mathcal{S}^2 \), where \( \mathcal{S}^2 \) is the unit 2-sphere — the space of dipole orientations in \( \mathbb{R}^3 \). In contrast to the dilute regime where it was sufficient to consider two variables for a single bacterium’s orientation, the added difficulty of a semidilute suspension is that now \( 5N \) variables (three for each particle’s position and two for each orientation) must be considered. Assuming only dipolar and Lennard-Jones interactions as explained in Section 4.1, for a given configuration the instantaneous volume-averaged bulk stress is given by the symmetric trace-free tensor

\[
\Sigma_{lm}(\mathbf{x}, \mathbf{d}) := \sum_{i=1}^{N} \left( \frac{U_0}{|V_L|} \left( d^{(i)}_l d^{(i)}_m - \frac{\delta_{lm}}{3} \right) + \sum_{j \neq i} r_{i,j}^{(i,j)} F_l \left( \frac{r_{i,j}}{|V_L|} \right) \right) \quad (4.1)
\]

where \( l, m = 1, 2, 3 \), \( \mathbf{r}^{(i,j)} = \mathbf{x}^i - \mathbf{x}^j \), \( U_0 \) is the dipole moment, and \( |V_L| \) is the volume of the domain. The stress is broken into two components: the hydrodynamic dipolar stress [84] and the excluded volume stress due to the Lennard-Jones force \( F \) [110]. The key feature of the stress is that it only depends on the \( \frac{N(N-1)}{2} \) relative positions, \( \mathbf{r}^{(i,j)} \) for \( 1 \leq i < j \leq N \), and \( N \) orientations, \( \mathbf{d}^i \). This is because in the dipole limit the total hydrodynamic stress is independent of the particles’ positions, and the Lennard-Jones stress is defined in terms of relative positions. For a given background flow strength \( \gamma \) and a given bacterial configuration at time \( t \) one can calculate the instantaneous stress \( \Sigma(\mathbf{r}, \mathbf{d}) \) and define the instantaneous shear viscosity as follows:

\[
\hat{\eta}(\mathbf{r}(t), \mathbf{d}(t)) := \eta \left( 1 + \frac{\Sigma_{12}(\mathbf{r}, \mathbf{d})}{\gamma} \right),
\]

where \( \eta \) is the velocity of the ambient fluid.

The viscosity is an intrinsic bulk property of a fluid. Bulk properties are characterized by the average behavior of the fluid on sufficiently large scales, such as those larger than the suspended particles or interparticle distances, while the local variations on smaller scales are irrelevant. Thus, the effective viscosity, \( \hat{\eta} \), like the viscosity of a homogeneous fluid should be a property of the suspension independent of time and the microscopic configuration. Therefore, the effective viscosity
is defined using a longtime average of the instantaneous viscosity

\[ \eta((r_0, d_0)) := \eta \left( 1 + \lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{\Sigma_{12}(r(t), d(t))}{\gamma} dt \right) \]

similar to its computation in experiment. However, this quantity still depends on the initial configuration and in general is difficult to analyze. Instead, using the crucial assumption of ergodicity, replace the time average by an ensemble average with respect to the steady-state probability distribution \( P_N(r, d) \) representing a statistically stationary state of the suspension

\[ \hat{\eta} := \eta \left( 1 + \int_{V_L} \int_{S^2} \frac{\Sigma_{12}(r, d)}{\gamma} P_N(r, d) dr \cdot d \right). \quad (4.2) \]

Formally, the steady-state \( P_N(r, d) \) is the limit \( t \to \infty \) of \( P_N(r, d, t) \), which satisfies the Liouville equation

\[ \partial_t P^N = -\nabla \cdot (\dot{r} P^N) - \nabla \cdot (\dot{d} P^N) \quad (4.3) \]

where \( \dot{r} \) and \( \dot{d} \) are the relative equations of motion for the bacteria. To compute the effective viscosity it needs to be shown that the right–hand side of (4.2) is well-defined as a function of the relative positions and orientations of the particles. The existence of a steady-state for (4.3) is not known in general and is the subject of future work. Here the first step in that direction is taken by demonstrating that (4.3) is well-defined for all time. To this end, one needs to analyze the ODE equations of motion of the bacteria and establish the longtime existence of their solutions, which is the main focus of this Chapter.

### 4.3 Semidilute model

Based on the prior discussion, the coupled PDE/ODE system modeling the bacterial suspension is introduced. The bacteria are represented as point force dipoles in a fluid. Heuristically, a dipole is the limit of infinitesimal separation of a pair of oppositely directed forces, which are equal in magnitude (see Fig. 4.1). One force represents the bacterium’s propulsion force (the action of the flagella, for example),
and the other is the opposing drag exerted on the fluid by the bacterium’s body due to the no-slip boundary condition. This is a model of a “pusher”, a swimmer that propels itself by pushing the fluid back behind its body as if with a propeller, similar to \textit{B. subtilis}. “Pullers”, which propel themselves with a kind of “breast-stroke” by pulling the fluid in front of it (not considered here) can be modeled as contractile dipoles (Fig. 4.1 (right)). Based on the typical size \( l_0 \sim 1\mu m \) and swimming speed \( V_0 \sim 20\mu m/s \) of a bacterium, as well as the typical dynamic viscosity \( \sim 10^{-3} Pa\cdot s \) and density \( \sim 10^3 kg/m^3 \) of the suspending fluid, the typical forces the bacteria exert generate flows with Reynolds number, \( Re \sim 10^{-4} \ll 1 \). Similarly, inertial effects on the particle are negligible due to its small mass. Further it is assumed that a steady-state flow is established on a timescale much smaller than that associated with the time for a bacterium to swim its length (characteristic timescale). Thus, the fluid flow at any time is accurately modeled by the steady Stokes equation. It has been experimentally verified that the flow due to a force dipole in a Stokesian fluid is a good approximation to the flow around a swimming pusher [2], justifying our approximations.

To study the effective viscosity the influence of a prescribed bulk background flow must be modeled, as explained in Section 4.2. This problem is multiscale by nature: the effective properties such as the effective viscosity can only be defined on the macroscopic scale on the order of the size of the suspension, but are determined by the microscopic behavior on the scale of the particle size, \( l_0 \). On macroscopic length scales the flow in the suspension should be that of the background flow, but on the smaller length scales it will vary due the influence of the bacteria. Mathematically (see, e.g., [120]) the background flow is imposed on an unbounded system using suitable conditions at infinity, so that the result is free of finite boundary effects. This can be difficult to achieve numerically, however, as it would require very large computational domains. Instead, infinite bulk homogeneous systems are frequently modeled as periodic: the space is tiled with a lattice of periodic images of the fundamental cube \( \Box \), and the velocity and orientation of

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{dipoles.png}
\caption{Dipoles. Left: extensile dipole (pusher). Right: contractile dipole (puller).}
\end{figure}
the fluid and particles in each cube are equal to those of their periodic images. If
the size of the cube is much larger than the suspension’s correlation distance, as
in experiment [5], the statistics of the interparticle interactions will be similar to
those in the bulk.

This approach, however, is not suitable for modeling shear flows, since the
macroscopic fluid velocity obtained by averaging over the cubes, will be constant.
In order to ensure a linear variation in the velocity characteristic of shear an ap-
proach first proposed by Lees and Edwards [79] for molecular dynamics simulations
of fluids will be employed. Assume for concreteness that the size of \( \mathcal{C} \) is \( L \), it is
centered at the origin with the sides parallel to the coordinate axes. Initially there
are \( N \) periodically replicated particles in each cube. A shear of magnitude \( \gamma \) is
imposed in the \( xy \)-plane so that on large length scales the \( y \)-component of the flow
varies \( \sim \gamma x \). This is modeled as follows: (a) at time \( t \) each \( yz \)-layer of cubes is
shifted upwards in \( y \) by \( \gamma t \) relative to the proceeding adjacent layer in \( x \), and (b)
in each subsequent \( yz \)-layer the \( y \)-component of the bacterial velocity is larger by
\( \gamma \). This way the global characteristics of the flow are those of planar shear, while
the local interactions between the particles are as those in the bulk. In particular,
the Lees-Edwards boundary conditions guarantee (see [80]) that the suspended
particles in the image cells satisfy the same equations of motion as the particles in
the reference cube \( \mathcal{C} \), except with the velocity modified by the shear. This is not
the case for periodic boundary conditions where the conservation of momentum
may be violated [79]. For a two-dimensional illustration see Fig. 4.2.

A detailed mathematical description of this model is now developed. Observe
that in the quasiperiodic setting set out above only the relative positions and
velocities are meaningful. To simplify the presentation, however, the equations of
motion for the absolute positions and orientations of the bacteria based on those
of finite particles are derived first, and later are converted into the corresponding
relative equations.

4.3.1 Particle equations of motion

The equations of motion for a force dipole naturally follow from those for an
extended particle, which, given negligible inertial effects, are a consequence of the
balance of forces and torques (see e.g., [59] for a derivation). Essentially, the force of self-propulsion is balanced by the hydrodynamic force, resulting in the Stokes drag law (4.4). In addition, particles interact with the flow as infinitesimal spheroids resulting in Jeffery’s precessional equation (4.5) for an axisymmetric particle in a linear ambient flow. The semidilute assumption is increasingly more accurate as the size $l$ of the ellipsoidal bacterium shrinks, since the flow can be approximated by an increasingly more accurate linear Taylor expansion. The Stokes law determines the translation velocity $V_0$ of an isolated self-propelled spheroid for a given magnitude of the dipole moment $U_0 = f_0 \cdot l$ and eccentricity $e$ (see [59]; here $f_0$ is the magnitude of the self-propulsion force), and remains unchanged in the limit $l \to 0$ as long as $e$ and $U_0$ are kept fixed. The law given by Jeffery’s equation, first investigated for the case of passive ellipsoids [55] and derived in [109], depends only on the eccentricity and remains unchanged in the limit. This dependence of rotational motion on the bacterial asymmetry is crucial to the alignment dynamics.

Each particle in a given cube, $\mathcal{C}$, moves in the ambient flow generated by the other particles. Because of the infinitesimal size of the dipoles, this ambient flow is the sum of flows $u^j$ generated by each of the other $N - 1$ dipoles in $\mathcal{C}$ as well as
all of its quasiperiodic images. Additionally, the excluded volume interactions or “soft collisions” are modeled by implementing Lennard-Jones-like forces $F^j$ defined in Section 4.3.2, in contrast to pure hydrodynamic models [19, 61, 65, 67]. The specific choice of the potential is not crucial (e.g., the repulsive Yukawa-type potential is used in [53]), but it should dominate particle motion at short distances. A soft collision is a collision where kinetic energy is lost and takes into account excluded volume constraints in the sense that there is a radius of exclusion (see Section 4.4.4.1). These forces must balance self-propulsion and drag, so they enter into (4.4) but, being centrally-symmetric, contribute no torque and, therefore, are absent from (4.5). The Lennard-Jones terms have an artificial length scale characterizing the soft collision distance between the particles. Beyond this distance, chosen to be smaller than $L/2$, the LJ forces vanish, so each particle interacts with no more than $N - 1$ of the particles in the same $\mathbb{Z}$ or its nearest images. Thus, $F^j(x^i)$ will be interpreted as the force on the dipole $i$ in $\mathbb{Z}$ from dipole $j$ in the same $\mathbb{Z}$ or its closest quasiperiodic image. At most one of each particle’s quasiperiodic images exerts a nonzero LJ force on $i$ (see Fig. 4.2), resulting in no ambiguity.

With this convention for the sums $\sum_{j \neq i}$, the resulting equations of motion are

$$\dot{x}^i = V_0 d^i + \sum_{j \neq i} \left( u^j(x^i) + \frac{1}{6\pi\eta_0} F^j(x^i) \right) + u^{BG}(x^i) \quad (4.4)$$

$$\dot{d}^i = -d^i \times \left[ \omega^{BG} + \sum_{j \neq i} \omega^j(x^i) \right] - d^i \times \left[ B d^i \times \left( E^{BG} + \sum_{j \neq i} E^j(x^i) \right) \right] \cdot d^i. \quad (4.5)$$

Here, $B$ is the Bretherton constant quantifying the aspect ratio of the particles. For a spheroid with eccentricity $e$ (the ratio of the major and minor axes) it is given by $B = \frac{e^2 - 1}{e^2 + 1}$, ($B = 0$ for spheres, $B = 1$ for needles), and for $B. subtilis$ $B \approx .9$. The fluid velocity $u^j$ generated by the $j$-th dipole is determined from the fluid equations (Section 4.3.3), and defines the corresponding vorticity $\omega^j = \nabla \times u^j$ and the rate of strain $E^j = \frac{1}{2} \left( \nabla u^j + (\nabla u^j)^T \right)$. The background flow is represented by $u^{BG}(x) = (0, \gamma x, 0)$ in the case of planar shear flow with the corresponding vorticity, $\omega^{BG}$, and rate of strain, $E^{BG}$. The dependence of these terms on the orientation $d^j$ of the $j$-th particle is suppressed in the notation. The concentration, $\phi \sim N l_0^3 / |V_L|$, is implicitly present in the coupled system due to the fact that the sums depend on the number of particles in the suspension, $N$, and the volume of
the fluid domain $|V_L|$.

### 4.3.2 Lennard-Jones forces

As mentioned above, collisions between the bacteria are modeled as soft excluded volume interactions based on forces of the Lennard-Jones (LJ) type. Specifically, $F^j$ is the short-range repulsive force due to the $j$-th particle and derived from the potential given by

$$W(x) = \begin{cases} 
4\varepsilon_{LJ} \left( \left( \frac{\sigma_{LJ}}{|x|} \right)^{12} - \left( \frac{\sigma_{LJ}}{|x|} \right)^6 \right) + \varepsilon_{LJ}, & |x| \leq 2^{1/6} \sigma_{LJ} \\
0, & |x| > 2^{1/6} \sigma_{LJ},
\end{cases} \quad (4.6)$$

see Fig. 4.3. Define the associated force $F^j(x^i) := -\nabla_x W(x)|_{x=x^i-x^j}$, where $\varepsilon_{LJ} \sim (\eta l_0^2)^{-1}$ is a constant determining the normalized strength of repulsion defined in terms of the real particle size $l_0$. The parameter $\sigma_{LJ}$ determines the equilibrium distance $(2^{1/6} \sigma_{LJ})$ where the net force between two bacteria balances to zero, and is set to reflect the real particle size: $\sigma_{LJ} \sim l_0$. The truncation is imposed in order to ensure that this force is purely repulsive allowing soft collisions to be present. The truncated potential is only $C^1$-smooth (the constant shift $\varepsilon_{LJ}$, the minimum value of the Lennard-Jones 6-12 potential, is necessary to maintain continuity of the derivative). One can still easily show that the LJ force $F^j(x^i) = F(x^j - x^i) \in [C^{0,1}(\Omega \setminus \{0\})]^3$, where $C^{0,1}(\Omega)$ denotes the space of Lipschitz continuous functions on $\Omega$. This fact will be essential in Section 4.4.4 where the longtime existence and uniqueness of particle trajectories is established.

![Figure 4.3](image-url) **Figure 4.3.** Left: Plot of standard Lennard-Jones 6-12 potential. Right: Plot of truncated Lennard-Jones type potential where $r = |x|$ and $W(r)$ is radially symmetric.
4.3.3 PDE model for a force dipole in the fluid

To complete the definition of the equations of motion laid out in Section 4.3.1 one must define the flow $u^j(x)$ generated at point $x$ by the $j$-th dipole and its quasiperiodic images acting on the fluid. The total flow at any point is the sum of these individual dipolar flows in keeping with the semidilute assumption. Each dipole is subjected to an $xy$ planar shear flow of strength $\gamma$ used to define the effective viscosity (see Section 4.2). Shear flows are a representative linear flow frequently used in rheological experiments such as in [20]. The Lees-Edwards boundary conditions are adapted to the PDE setting to model the effects of the shear. Specifically, the $j$-th dipole is oriented along $d_j$ and located at $x_j$ in a representative cube of side length $L$ centered at the origin $\mathcal{B} := \{ x \in \mathbb{R}^3 \mid |x_i| < \frac{L}{2}, \text{ for } i = 1, 2, 3 \}$. The fluid around the dipole satisfies the following incompressible Stokes equation:

$$\begin{align*}
\eta \Delta u(x, t) &= \nabla p(x, t) - \nabla \cdot [D(d^j) \delta(x - x^j)] & x \in \mathcal{B} \\
\nabla \cdot u(x, t) &= 0 & x \in \mathcal{B} \\
u(x) &\in \mathcal{D}'(\mathbb{R}^3) \tag{4.7}
\end{align*}$$

where $u$ is the fluid velocity, $p$ is the pressure, and $\eta$ is the ambient fluid viscosity. The dipole tensor $D$ is given by

$$D_{jk}(d) := U_0 \left( d_j d_k - \frac{1}{3} \delta_{jk} \right) \tag{4.8}$$

where $U_0 < 0$ is the dipole moment. Look for quasiperiodic solutions by imposing that the distribution $u(x) \in \mathcal{D}'(\mathbb{R}^3)$ is invariant under shifts defined by the Lees-Edwards map: For $x \in \mathbb{R}^3$, $u(x, y, z, t) + (0, \gamma L, 0) = u(x + L, y + \gamma L t, z, t)$ and periodic in $y$ and $z$, see Figure 4.2. This subspace of $\mathcal{D}'(\mathbb{R}^3)$ will be denoted $\mathcal{D}_t'(\mathcal{B})$. More details on these spaces of distributions are presented in Section 4.4.1. Requiring that $u(x) \in \mathcal{D}_t'(\mathcal{B})$ mimics the more familiar pointwise definition of Lees-Edwards boundary conditions

$$\begin{align*}
u(-\frac{L}{2}, y - \frac{\gamma L t}{2}, z, t) &= u(\frac{L}{2}, y + \frac{\gamma L t}{2}, z, t) - (0, \gamma L, 0) & x \in \partial \mathcal{B} \\
u(x, -\frac{L}{2}, z, t) &= u(x, \frac{L}{2}, z, t), \quad u(x, y, -\frac{L}{2}, t) = u(x, y, \frac{L}{2}, t) & x \in \partial \mathcal{B}.
\end{align*}$$
To the best of our knowledge, the use of Lees-Edwards boundary conditions in the formulation of a PDE or in the study of bacterial suspensions is novel.

### 4.3.4 Relative equations of motion

The flow governed by (4.7) is defined only up to a constant. Therefore, the right-hand side of the equations of motion (4.4)-(4.5) is not well-defined. However, the main observable properties of the suspension, such as the stress (4.1) used to define viscosity, are only functions of the relative configuration of the particles. Therefore in place of (4.4)-(4.5), reformulate the equations of motion for the \( \frac{N(N-1)}{2} \) relative positions \( r^{(i,j)} := x^i - x^j \) for \( 1 \leq i < j \leq N \) and \( N \) orientations \( d^i \) for \( 1 \leq i \leq N \).

This leads to \( \frac{N(N-1)}{2} \) + \( N \) ordinary differential equations

\[
\begin{align*}
\dot{r}^{(i,j)} &= V_0(d^i - d^j) + \sum_{k \neq i} \left[ u(r^{(i,k)}) + \frac{F(r^{(i,k)})}{6\pi\eta l_0} \right] \\
&\quad - \sum_{k \neq j} \left[ u(r^{(j,k)}) + \frac{F(r^{(j,k)})}{6\pi\eta l_0} \right] + u^{BG}(r^{(i,j)}) \\
\dot{d}^i &= -d^i \times \left[ \omega^{BG} + \sum_{j \neq i} \omega(r^{(i,j)}) \right] - d^i \times \left[ Bd^i \times \left( E^{BG} + \sum_{j \neq i} E(r^{(i,j)}) \right) \right].
\end{align*}
\]

(4.9) (4.10)

with initial conditions \( r^{(i,j)}(0) = x^i_0 - x^j_0, \ d^i(0) = d^i_0 \). Here \( u(r^{(i,k)}) \) solves (4.7) with \( d = d^k \).

The time evolution of the relative positions and orientation associated with \( i \)th bacterium is completely determined by the relative positions and orientations of all other bacteria, and thus the system (4.9) – (4.10) is closed. As is clear from (4.7), \( u(x) \) is only defined up to an arbitrary constant, but this will cancel out in the reformulated equations. Recall from Section 4.2 that these equations were necessary to show the Liouville equation for the probability density is well-defined for all time. To calculate the effective viscosity, in addition to the probability distribution, one needs the bulk stress to be well-defined. To establish both results the longtime existence of unique trajectories for the relative particle equations of motion (4.9)-(4.10) must now be shown.
4.4 Global Solvability of the equations of motion

Now turn to the central question of this Chapter — the existence of a unique solution to the equations of motion (4.9)-(4.10) for all time. There are two essential difficulties here. First, the right-hand side of (4.9)-(4.10) features $u$ and its derivatives $\omega, E$. As a solution of the PDE (4.7) with a singular right-hand side and quasiperiodic boundary conditions, the velocity $u$ might not be unique or have enough a priori regularity to have well-defined pointwise values and derivatives. Second, under the best circumstances the regularity of $u$ cannot extend to the collision set, $x^i = x^j$, where the flow due to the $j$-th dipoles is expected to diverge. Thus, in order to show longtime existence, one must establish the dynamics result that particle trajectories remain separated for all times, so that (4.9)-(4.10) remain Lipschitz.

The fluid velocity is now examined in greater detail. To establish the existence, uniqueness, and regularity of solutions to (4.7), first, reduce it to a related periodic problem and later show how the general solution with Lees-Edwards boundary conditions can be obtained from a corresponding periodic problem by a linear coordinate transformation.

4.4.1 Incompressible Stokes with periodic boundary conditions

A few spaces must first be defined, which will be used throughout the remainder of this work. Denote the space of test functions, infinitely differentiable functions with compact support, as $D(\mathbb{R}^3)$. Denote its dual space, the space of distributions, as $D'(\mathbb{R}^3)$. A dual pairing between a distribution $f \in D'(\mathbb{R}^3)$ and a test function $\phi \in D(\mathbb{R})$ will be denoted by $(f, \phi)$. It is natural to consider solutions to (4.7) in the space of distributions due to the singularity on the right-hand side. Begin by considering the special case of a periodic flow. A periodic flow due a single dipole with orientation $d$ at the origin satisfies the following equation in the distributional
\begin{equation}
\begin{cases}
\eta \Delta u(x) = \nabla p(x) - \nabla \cdot [D(d) \delta(x)], & x \in \mathbb{R}^3, \\
\nabla \cdot u(x) = 0, & x \in \mathbb{R}^3, \\
u(x) \in \mathcal{D}'(\mathbb{R}^3)^3.
\end{cases}
\tag{4.11}
\end{equation}

in \( x \in \mathbb{R}^3 \). The space of periodic distributions on \( \mathbb{R}^3 \) is denoted by \( \mathcal{D}'(\mathbb{R}^3) \) where the subscript identifies the periodicity cell. Note here that divergence is to be understood in the distributional sense, \((u, \nabla \phi) = 0\) for all \( \phi \in \mathcal{D}(\mathbb{R}^3) \). First, establish the existence and regularity of the solutions to (4.11).

**Theorem 4.4.1. (Existence and Regularity of \( u(x) \))** Given \( d \in \mathcal{S}^2 \), there exists a solution \( u(x) \in \mathcal{D}'(\mathbb{R}^3) \) to (4.11) and furthermore, \( u(x) \in \mathcal{C}_\infty(\mathbb{R}^3 \setminus \{0\})^3 \).

**Proof.** A periodic distribution is completely determined by the set of its Fourier coefficients. Thus, expand \( u, p, \) and \( f := \nabla \cdot [D(d) \delta(x)] \) in Fourier series

\begin{equation}
\begin{aligned}
u & = \sum_{k \in \mathbb{Z}^3} u_k e^{2\pi i k \cdot x}, \\
p & = \sum_{k \in \mathbb{Z}^3} p_k e^{2\pi i k \cdot x}, \\
f & = \sum_{k \in \mathbb{Z}^3} f_k e^{2\pi i k \cdot x}
\end{aligned}
\tag{4.12}
\end{equation}

analogous to [121] understood as distributions. Using the incompressibility condition \( \mathbf{k} \cdot \mathbf{u}_k = 0 \) one finds

\begin{equation}
p_k = \frac{\mathbf{k} \cdot f_k}{2\pi i |\mathbf{k}|^2}, \\
u_k = -\frac{1}{4\pi^2 \eta |\mathbf{k}|^2} \left[ f_k - \frac{(\mathbf{k} \cdot f_k) \mathbf{k}}{|\mathbf{k}|^2} \right], \quad k \in \mathbb{Z}^3 \setminus \{0\}.
\tag{4.13}
\end{equation}

Since \( f \) is a periodic distribution, its Fourier series converges to \( f \) in \( \mathcal{S}'(\mathbb{R}^3) \subset \mathcal{D}'(\mathbb{R}^3) \), the space of tempered distributions on \( \mathbb{R}^3 \). In addition, for \( k \neq 0 \), \(|p_k| \leq |f_k|, |u_k| \leq |f_k| \). Thus, the Fourier series (4.12) converge to \( u \) and \( p \) in \( \mathcal{S}' \) and each is a periodic distribution (i.e., \((u, p) \in ([\mathcal{D}'(\mathbb{R}^3)^3, \mathcal{D}'(\mathbb{R}^3)]) \)). Therefore, a solution to (4.11) exists in the distributional sense.

Next, establish the regularity of the solution outside the origin. The intuitive idea is that the solution \((u, p)\) will only have singularities at the same points the right-hand side of (4.11) does. For this we appeal to a result for hypoelliptic equations [42]. Namely, a linear differential operator with constant coefficients \( \mathcal{L} \) is hypoelliptic if and only if for any open set \( \mathcal{O} \) every solution \( u(x) \) in \( \mathcal{D}'(\mathcal{O}) \) of the equation \( \mathcal{L}u = f \), where \( f \in C^\infty(\mathcal{O}) \) belongs to \( C^\infty(\mathcal{O}) \).
Apply the divergence free condition to Stokes equation in (4.11) to find

\[-\Delta p = \nabla \cdot f\]

in the distributional sense. Since all elliptic operators are hypoelliptic and \(\nabla \cdot f \in C^\infty(\mathbb{R} \setminus \{0\})\), one finds that \(p \in C^\infty(\mathbb{R} \setminus \{0\})\). Now consider Stokes equation for each component

\[-\eta \Delta u_i = -\frac{\partial}{\partial x_i}p + f_i, \quad i = 1, 2, 3.\]

Applying the same result for Laplace’s equation where the right-hand side belongs to \(C^\infty(\mathbb{R} \setminus \{0\})\), conclude that \(u \in [C^\infty(\mathbb{R}\setminus\{0\})]^3\) proving the regularity of solutions to (4.11) outside the origin.

An explicit construction of the solution \(u(x)\) to (4.11) can be found in Section 4.4.3. Now that the existence and regularity of a solution to equation (4.11) has been demonstrated, prove that \((u(x), p)\) is the unique solution pair up to a constant.

**Theorem 4.4.2.** \((u(x), p(x)) \in \left([\mathcal{D}'(\mathbb{R})]^3, \mathcal{D}'(\mathbb{R})\right)\) is the unique solution to (4.11) up to a constant.

**Proof.** Assume there exists two solutions to (4.11), denoted \((u(x), p(x))\) and \((v(x), q(x))\) in \(\left([\mathcal{D}'(\mathbb{R})]^3, \mathcal{D}'(\mathbb{R})\right)\). Define \(w(x) := u(x) - v(x)\) and the associated pressure \(\phi(x) := p(x) - q(x)\). Then \((w(x), \phi(x)) \in \left([\mathcal{D}'(\mathbb{R})]^3, \mathcal{D}'(\mathbb{R})\right)\) solves

\[
\begin{aligned}
\eta \Delta w(x) &= \nabla \phi(x) \quad \text{for } x \in \mathbb{R} \\
\nabla \cdot w(x) &= 0, \quad \text{for } x \in \mathbb{R} .
\end{aligned}
\]

(4.14)

Expand both \(w(x)\) and \(\phi(x)\) in a Fourier series analogous to the proof of Theorem 4.4.1 and [121]. Using equation (4.13) with \(f_k = 0\) and \(\{u_k, p_k\}\) replaced by \(\{w_k, \phi_k\}\) one immediately concludes that for \(k \neq 0\), \(\phi_k = 0\) and \(w_k = 0\). Therefore, \(w(x)\) and \(\phi(x)\) are constants. Since a periodic distribution is uniquely determined by its Fourier coefficients, \(u(x) = v(x)\) and \(p(x) = q(x)\) is the unique solution pair to (4.11) up to an additive constant.
4.4.2 Incompressible Stokes with Lees-Edwards boundary conditions

In this section, a linear coordinate transformation will be defined, which provides a relation between the solution to the L-E problem (4.7) and the solution to a related periodic problem for which one can establish an existence and uniqueness result in a similar way to the periodic case for Stokes equation in Section 4.4.1. The purpose of the time–dependent quasiperiodic boundary conditions is to account for the shear in the \(xy\)-plane. Thus, introduce the map

\[
\mathbf{f}_{LE}^t(\hat{x}) : \mathbb{R}^3 \to \mathbb{R}^3, \quad \hat{x} = (\hat{x}, \hat{y}, \hat{z}) \mapsto \begin{bmatrix} \hat{x} \\ \hat{y} + \gamma t \hat{x} \\ \hat{z} \end{bmatrix} =: \mathbf{x} = (x, y, z),
\]  

which transports a fluid particle located at \((\hat{x}, \hat{y}, \hat{z})\) to its location at time \(t\) if it were only advected by the background flow. This change of coordinates map is invertible with inverse

\[
(\mathbf{f}_{LE}^t)^{-1}(\mathbf{x}) : \mathbf{x} \mapsto \begin{bmatrix} x \\ y - \gamma tx \\ z \end{bmatrix} = \hat{x},
\]  

where the Jacobian and inverse Jacobian of the coordinate transformation are

\[
J_t = \begin{bmatrix} 1 & 0 & 0 \\ \gamma t & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad J_t^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ -\gamma t & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.
\]

**Remark 4.4.3.** If the inverse Lees-Edwards mapping is applied to \(u(x)\) solving (4.7), then the resulting distribution should be in \(D'\) the space of periodic distributions. This will be observed in the proof of Theorem 4.4.4.

**Theorem 4.4.4.** Given \(t \in (0, \infty)\) and \(d \in S^2\), the PDE (4.7) has a unique solution; moreover, \(u(x) \in [C^\infty(\mathbb{T}^3 \setminus \{0\})]^3\).

**Proof.** The main idea for the proof is to introduce a natural transformation to a periodic problem based on the trajectories of fluid particles. Let \(u(x, t)\) be the
velocity of the fluid which occupies position \( x \) at time \( t \). By using the Lagrangian description, define a new function \( v(\hat{x}, t) := \frac{d}{dt}\hat{X}(t) \) such that at time \( t \), \( \hat{X}(t) = \hat{x} \). Now consider the relationship between \( u \) and \( v \). Define \( u \) in the following way

\[
u(x, t) := \frac{d}{dt} \left[ J_t \hat{X}(t) \right] = \left( \frac{d}{dt} J_t \right) \hat{X}(t) + J_t \frac{d}{dt} \hat{X}(t) = \left( \frac{d}{dt} J_t \right) \hat{x} + J_t v(\hat{x}, t)
\]

\[
\begin{bmatrix}
0 \\
\gamma x \\
0
\end{bmatrix} + J_t v(J_t^{-1} x, t).
\]

(4.17)

The corresponding problem for \( v(\hat{x}, t) \) must be derived. It will be shown that \( v(\hat{x}, t) \) satisfies a periodic problem possessing a unique solution up to a constant, which will allow one to prove that \( u \) defined as above satisfies (4.7). First, verify that if \( u \) satisfies (4.7), then \( v \) is a periodic distribution on \( \mathbb{R} \). Consider the boundary condition in the \( x \)-direction

\[
J_t v(x, y - \gamma t, z, t) = u(x, y, z, t) - \begin{bmatrix}
0 \\
\gamma x \\
0
\end{bmatrix}
\]

\[
= u(x + 1, y + \gamma t, z, t) - \begin{bmatrix}
0 \\
\gamma (x + 1) \\
0
\end{bmatrix} = J_t v(x + 1, y, z, t).
\]

Thus, if one multiplies through by \( J_t^{-1} \), then it is seen that \( v \) is periodic in \( x \) if \( u \) satisfies (4.7). Similarly, \( v(x, y, z, t) = v(x, y + 1, z, t) \) and \( v(x, y, z, t) = v(x, y, z + 1, t) \). Next, verify that \( v \) is incompressible when \( u \) is

\[
0 = \nabla_x \cdot u(x, t) = \nabla_x \cdot \{ J_t v(J_t^{-1} x, t) \} = \nabla_{\hat{x}} \cdot \{ J_t^{-1} J_t v(\hat{x}, t) \} = \nabla_{\hat{x}} \cdot v(\hat{x}, t).
\]

Finally, consider the equation for \( v(\hat{x}, t) \), but a proposition is needed to show how each linear operator present in (4.7) is effected by the coordinate transformation.

**Proposition 4.4.5.** For the given coordinate transformation \( x = J_t \hat{x} \) the following identities hold:

\[
(i) \ \nabla_x v(x, t) = (J_t^{-1})^T \nabla_{\hat{x}} v(\hat{x}).
\]
(ii) \( \Delta_x v(x, t) = \text{div}_x \left\{ J_t^{-1}(J_t^{-1})^T \nabla_x v(\hat{x}) \right\} \).

These identities are easy to check. Here \( (\nabla_x v)_{ij} := \frac{\partial v_j}{\partial x_i} \). In addition, note that from Proposition 4.4.5 (ii) if the Jacobian \( J_t \) were orthogonal then \( \Delta_x = \Delta_{\hat{x}} \). From Proposition 4.4.5 one finds

\[
0 = \eta \Delta u(x, t) - \nabla_x p(x, t) + \nabla_x \cdot [D(d)\delta(x)] \\
= \eta J_t \Delta v(\hat{x}, t) - (J_t^{-1})^T \nabla_x p(\hat{x}) + \nabla_x \cdot [J_t^{-1}D(d)\delta(x)] \\
= \eta \hat{\Delta} v(\hat{x}, t) - J_t^{-1}(J_t^{-1})^T \nabla_x p(\hat{x}) + \nabla_{\hat{x}} \cdot [\hat{J}_t^{-1}D(d)\delta(x)]
\]

where \( \hat{\Delta} := \left( \frac{\partial}{\partial \hat{x}} - \gamma t \frac{\partial}{\partial \hat{y}} \right)^2 + \left( \frac{\partial}{\partial \hat{y}} \right)^2 + \left( \frac{\partial}{\partial \hat{z}} \right)^2 \). A similar operator was also considered in the context of numerical simulations of fluids under deformation [122, 123]. Thus, \( u(x, t) \in \mathcal{D}'(\mathbb{R}^3) \) satisfies (4.7) in the distributional sense if and only if for fixed \( t \in (0, \infty) \), \( v(\hat{x}, t) \) satisfies

\[
\begin{cases}
\eta \hat{\Delta} v(\hat{x}, t) = J_t^{-1}(J_t^{-1})^T \nabla_x p(\hat{x}, t) - J_t^{-1} \nabla_{\hat{x}} \cdot [J_t^{-1}D(d)\delta(x)], & \hat{x} \in \mathcal{D} \\
\nabla_{\hat{x}} \cdot v(\hat{x}, t) = 0, & \hat{x} \in \mathcal{D} \\
v(\hat{x}, t) \in [\mathcal{D}'(\mathbb{R}^3)]^3.
\end{cases}
\]

The existence and uniqueness (up to a constant) of a solution to (4.18) can now be proven and its regularity will be established. This is completely analogous
to the Theorems 4.4.1-4.4.2. Begin by showing the existence of solutions through the use of Fourier series. Let \( f := J_t^{-1} \nabla_{\hat{x}} \cdot [J_t^{-1} D(d)\delta(x)] \) and expand \( v, p, \) and \( f \) in Fourier series

\[
v = \sum_{k \in \mathbb{Z}^3} v_k e^{2\pi i k \cdot x}, \quad p = \sum_{k \in \mathbb{Z}^3} p_k e^{2\pi i k \cdot x}, \quad f = \sum_{k \in \mathbb{Z}^3} f_k e^{2\pi i k \cdot x}
\]  

(4.19)

understood as distributions. Using the incompressibility condition \( k \cdot v_k = 0 \) one finds for \( k \in \mathbb{Z}^3 \setminus \{0\} \)

\[
p_k = \frac{k \cdot f_k}{2\pi i [(k_1 - \gamma tk_2)^2 + k_2^2 + k_3^2]}, \quad v_{k,j} = -\frac{f_{k,j} - p_k \psi_j}{4\pi^2 \eta [(k_1 - \gamma tk_2)^2 + k_2^2 + k_3^2]},
\]  

(4.20)

where \( \psi_i = 2\pi i [(k_1 - \gamma tk_2, -\gamma tk_1 + (1 + \gamma^2 t^2)k_2, k_3)] \). From the proof of ellipticity, for \( k \neq 0, [(k_1 - \gamma tk_2)^2 + k_2^2 + k_3^2] \geq \theta |k|^2 > 0 \). Since \( f \) is a periodic distribution, its Fourier series converges to \( f \) in \( \mathcal{S}'(\mathbb{R}^3) \subset \mathcal{D}'(\mathbb{R}^3) \), the space of tempered distributions on \( \mathbb{R}^3 \). In addition, for \( k \neq 0, |p_k| \leq |f_k|, |u_k| \leq |f_k| \). Thus, the Fourier series (4.19) converge to \( v \) and \( p \) in \( \mathcal{S}' \) and each is a periodic distribution (i.e., \( (v, p) \in ([\mathcal{D}'(\mathbb{R}^3)], \mathcal{D}'(\mathbb{R}^3)) \)). Thus a solution to (4.18) exists in the distributional sense.

Since \( \Delta \) is elliptic and if one takes the divergence of (4.18), then \( \hat{\Delta} p = \text{div}_{\hat{x}} f \). The proof of regularity is exactly the same as in the periodic case covered in Section 4.4.1. Therefore, conclude \( v(\hat{x}, t) \in [C^\infty(v \setminus \{0\})]^3 \). In addition, uniqueness follows in the same exact way as the proof of Theorem 4.4.2.

Due to the 1-1 correspondence between solutions to the fluid equations with Lees-Edwards boundary conditions (4.7) and solutions to the periodic problem (4.18) via the map (4.15), it has been proven that there exists a solution \( u \in [\mathcal{D}'(\mathbb{R}^3)]^3 \cap [C^\infty(\mathbb{R} \setminus \{0\})]^3 \) to (4.7) and it is unique up to a constant. Next, establish the main result of the paper, namely the global solvability of the ODE equations of motion. As mentioned earlier, these equations contain the solution \( u \) to (4.7). The fact that the solution is only unique up to a constant does not effect the global solvability of the relative equations of motion (4.9)-(4.10).
4.4.3 Construction of an explicit (series) solution

This section is devoted to an alternate proof of the above existence, uniqueness, and regularity results. Here an explicit solution is constructed, which may be used for further study of bacterial suspensions. Begin as in Section 4.4.1 by first constructing a solution to the periodic problem (4.11). Such a periodic flow to (4.11) is constructed from similar solutions in $\mathbb{R}^3$ by adapting the periodization technique as explained, for example, in [124, 125]. To that end, take the distributional solution of

$$\begin{align*}
\eta \Delta \hat{u}(x) &= \nabla \hat{p}(x) - \nabla \cdot \left[ D(d) \delta(x) \right], \\
\nabla \cdot \hat{u}(x) &= 0, \\
\hat{u}(x) &\to 0, \quad \text{as} \quad |x| \to \infty.
\end{align*}$$

(4.21)

in $\mathbb{R}^3$

$$\hat{u}_i(x) = \frac{1}{8\pi \eta} \sum_{j=1}^{3} \sum_{k=1}^{3} D_{jk}(d) G_{ij,k}(x)$$

and construct a formal sum of its translates

$$u_i(x) := \sum_{z \in \mathbb{Z}^3} \hat{u}_i(x + z).$$

The intuitive idea here is that one expects $u_i$ defined in this way to be periodic. Here $D_{jk}(d)$ is the dipole tensor as in (4.8) and $G(x)$ is the Oseen tensor (see [109])

with derivatives

$$G_{ij,k}(x) := -\frac{1}{|x|^2} \delta_{ij} x_k + \frac{1}{|x|^3} (\delta_{ik} x_j + \delta_{jk} x_i) - \frac{3}{|x|^5} x_i x_j x_k.$$

The decay inherited from $G_{ij,k}$ is too slow, $\hat{u}_i(x + z) \sim 1/|z|^2$, as the above series for $u_i$ does not converge. The essential idea, however, is sound: if a function decays sufficiently fast, the series of its translates will converge absolutely and uniformly to a periodic limit. To achieve the convergence of a series of translates, its terms can be modified by arbitrary elements of the kernel for the homogeneous Stokes operator (e.g., constants or suitable linear functions), namely

$$\bar{u}_i(x) := \hat{u}_i(x) + \sum_{z \in \mathbb{Z}^3 \setminus \{0\}} [\hat{u}_i(x + z) - \hat{u}_i(z) - \hat{u}_{i,p}(z)x_p],$$

(4.22)
which converges absolutely and uniformly due to each summand being $\sim O(|z|^4)$. Besides convergence, the sum must be periodic. To this end, periodicity can be ensured by enforcing that the derivatives of the constructed solution $u_{i,k}(x)$ integrate to zero over periodic contours $C^j$, which connect $x$ and $x + e^j$ avoiding any point in $Z^3$ for $j = 1, 2, 3$. Here $e^j$ denotes the unit vector in the $j$th direction. Thus we need to modify the sum by an additional linear term to ensure periodicity.

$$u_i(x) := \hat{u}_i(x) + \sum_{z \in Z^3 \setminus \{0\}} \left[ \hat{u}_i(x + z) - \hat{u}_i(z) - \hat{u}_{i,p}(z)x_p \right] - \Pi_{ij}x_j, \quad (4.23)$$

where

$$\Pi_{ij} = \int_{C^j} \left( \hat{u}_{i,k}(x) + \sum_{z \in Z^3 \setminus \{0\}} \left[ \hat{u}_{i,k}(x + z) - \hat{u}_{i,k}(z) \right] \right) dx_k = \bar{u}_i(x + e^j) - \bar{u}_i(x). \quad (4.24)$$

It will be shown that $\Pi_{ij}$ is a constant matrix independent of $x$ and that $\Pi_{ii} = 0$. Once proven, one can conclude that $\Pi_{ij}x_j$ is in the kernel of the homogeneous Stokes operator. Now proceed to the proof that this construction of $u$ indeed gives a solution to the periodic problem (4.11).

**Theorem 4.4.6.** Given $d \in S^2$, $u(x)$ defined in (4.23) solves (4.11) and furthermore $u(x) \in [D^{0}_{\mathbb{S}^2}]^3 \cap [C^\infty(\mathbb{Z}^3 \setminus \{0\})]^3$

**Proof.** Begin by showing that $u(x)$ in (4.23) is a well-defined periodic function for all $x \notin Z^3$. This requires further understanding of $\Pi_{ij}$, namely the proof that it is a constant matrix independent of $x$.

It can be easily shown, (e.g., see Appendix G.1) that $\bar{u}_{i,m}(x)$ defined in (4.22) is $k$-periodic for all $k \in Z^3$. Thus, in particular, $\bar{u}_{i,m}(x + e^j) - \bar{u}_{i,m}(x) = 0$. Since the gradient of $\Pi_{ij}$ is equal to zero, one finds that $\Pi_{ij} = C_{ij}$ a constant matrix independent of $x$. Now that each component is understood, $u(x)$ is a well-defined function as a uniform limit of partial sums for $x \notin Z^3$.

Next the regularity of $u(x)$ is established outside the origin. Since $u(x)$ is the uniform limit of functions in $[C^\infty(\mathbb{Z}^3 \setminus \{0\})]^3$, then one can conclude that $u(x) \in [C^\infty(\mathbb{Z}^3 \setminus \{0\})]^3$. Furthermore, by the uniform convergence of the partial sums of $k$th derivatives, $u(x) \in [C^k(\mathbb{Z}^3 \setminus \{0\})]^3$, $\forall k > 0$ and the regularity result follows.
It remains to show that the derivatives, $u_{i,k}$, integrate to zero over all periodic contours.

$$\int_{C_j} u_{i,k}(x)dx_k = \int_{C_j} \hat{u}_{i,k}(x) + \sum_{z \in \mathbb{Z}^3} [\hat{u}_{i,k}(x+z) - \hat{u}_{i,k}(z)]dx_k - \int_{C_j} \Pi_{ik} dx_k = \Pi_{ij} - \Pi_{ij} = 0$$

Thus, $\mathbf{u}(x)$ is periodic with periodicity cell $\mathcal{O}$, the unit cube.

To summarize, it has been shown above that $\mathbf{u}(x)$ is pointwise defined in $\mathbb{R}^3$ outside the origin. The distributional solution to (4.21), $\hat{\mathbf{u}} \in [L^1_{loc}(\mathbb{R}^3)]^3$. Since $\mathbf{u}(x)$ is the uniform limit of $[L^1_{loc}(\mathbb{R}^3)]^3$ functions over any compact set, then it is also in $[L^1_{loc}(\mathbb{R}^3)]^3$ and defines a regular distribution ($\mathbf{u}(x) \in [\mathcal{D}'(\mathbb{R}^3)]^3$). In addition, the periodicity of $\mathbf{u}(x)$ as an $[L^1_{loc}(\mathbb{R}^3)]^3$ function implies its periodicity as a distribution. Therefore, one concludes that $\mathbf{u}(x) \in [\mathcal{D}'(\mathbb{R}^3)]^3 \cap [C^\infty(\mathcal{O} \setminus \{0\})]^3$.

Now it must be shown that $\mathbf{u}(x)$ is divergence free in the distributional sense. Since $\hat{\mathbf{u}}(x)$ is a solution of the incompressible Stokes equation (4.21), it is divergence free, and thus

$$u_{i,i}(x) = \hat{u}_{i,i}(x) + \sum_{z \in \mathbb{Z}^3 \setminus \{0\}} [\hat{u}_{i,i}(x+z) - \hat{u}_{i,i}(z)] - \Pi_{ii} = -\Pi_{ii}.$$  

Therefore, it must be shown that $\Pi_{ii} = 0$. The following lemma will provide the result.

**Lemma 4.4.7.** For $\Pi_{ij}$, $\hat{\mathbf{u}}(x)$, and $\mathcal{O}$ defined above the following relation holds

$$\Pi_{ij}|_{\mathcal{O}} = \int_{\mathcal{O}} \hat{u}_i(x)\nu_j d^2x \quad (4.25)$$

where $\nu$ is the unit normal to the surface.

**Remark 4.4.8.** The proof is similar to the corresponding lemma in [124], where a solution is constructed to the periodic Laplace equation. This is a technical lemma proven in Appendix G.2.

Using this lemma, a short computation using the definition of $\hat{u}$ and $\hat{u}$ directly shows that in fact $\Pi_{ii}|_{\mathcal{O}} = \int_{\mathcal{O}} \hat{u}_i(x)\nu_j d^2x = 0$. Since $|\mathcal{O}| > 0$, we conclude that $\Pi_{ii} = 0$ and therefore $\mathbf{u}(x)$ is divergence free. Since the partial sums each solve the incompressible Stokes equations and the sum converges in distribution, then $\mathbf{u}(x)$...
also solves the incompressible Stokes equations in the distributional sense.

By the uniqueness result proven in Theorem 4.4.2, this is the unique solution to (4.11) up to a constant. This construction provides additional insight to the problem. Namely, we recover additional information that the solution found in Section 4.4.1 is not only a periodic distribution, but is also a regular distribution. In addition, this explicit construction could be used for further analysis of properties associated to solutions of (4.11) or numerical simulations in future work.

Remark 4.4.9. One can define an explicit solution $v(\mathbf{x},t)$ to (4.18) for a fixed time $t \in (0,\infty)$ from the constructed solution $u(x)$ by replacing $\hat{u}$ in (4.23) by $\hat{v}(\mathbf{x},t) = \hat{u}(J_t^{-1}x)$. In addition, to construct the solution to (4.7) we appeal to the relationship between $v$ and solutions to the Lees-Edwards problem

$$u^{LE}(x,t) := \begin{bmatrix} 0 \\ \gamma x \\ 0 \end{bmatrix} + J_t v(J_t^{-1}x,t)$$

defined in Section 4.4.2.

4.4.4 Global solvability for the relative equations of motion

In this section, the longtime existence of the solution to the relative equations of motion (4.9)-(4.10) will be shown. The first step to proving longtime existence is using the Picard-Lindelöf Theorem to establish the short time existence of a unique solution.

**Theorem 4.4.10.** Given a distinct set of initial relative positions $r^{(i,j)}(0) = x_0^i - x_0^j$ for $1 \leq i < j \leq N$ and orientations $d^i(0) = d_0^i$ for $i = 1,\ldots,N$, there exists a constant $T > 0$ such that the relative equations of motion (4.9)-(4.10) have a unique solution for times $t \in [0,T)$.

**Proof.** In order to invoke the Picard-Lindelöf Theorem one must establish that the right-hand side of (4.9)-(4.10) is Lipschitz continuous. This is an immediate consequence of the regularity result proven in Section 4.4.2 in Theorem 4.4.4. Namely, for all $\varepsilon > 0$, $u(x) \in [C^\infty (\mathbb{R}^3 \setminus B_\varepsilon(0))]^3$ and consequently $\omega(x), \mathbf{E}(x) \in \mathbb{R}^3$. 

\[ C^\infty(\mathbb{R}^3 \setminus B_\varepsilon(0)) \]. Also, by the definition of the short-range potential (4.6), \( \mathbf{F}(\mathbf{x}) \in C^0(\mathbb{R}^3 \setminus B_\varepsilon(0)) \). Thus, as long as the particle trajectories remain separated, \( |\mathbf{r}^{(i,j)}| = |\mathbf{x}^i - \mathbf{x}^j| > \varepsilon \), then the right-hand side of (4.9)-(4.10) is smooth. Therefore, outside the collision set, \( \{\mathbf{x}^i = \mathbf{x}^j\} \), (4.9)-(4.10) has a Lipschitz continuous right-hand side and is bounded on \( \mathbb{R}^3 \). Thus by the Picard-Lindelöf Theorem [126], there exists a \( T > 0 \) such that a unique solution to (4.9)-(4.10) exists for all \( t \in [0, T) \).

\[ \Box \]

4.4.4.1 Longtime existence – energy approach

To prove longtime existence one needs to show that the interval of time guaranteed by Theorem 4.4.10 can be extend to all time, (i.e., \( T = \infty \)). \( T \) can only be finite if the solution to (4.9)-(4.10) blows up in finite time. This occurs only if two particles collide, \( x^i(t) = x^j(t) \) for \( t = T \). However, heuristically, when \( |x^i - x^j| < 2^{1/6}\sigma_{LJ} \), the particles begin to strongly repel one another due to the short-range potential \( \mathbf{F}(x^i - x^j) \sim 1/|x^i - x^j|^13 \) and thus should remain apart for all time. If not the potential energy of the system will blow up. The following theorem will establish this intuitive idea rigorously and prove the main result of this work.

**Theorem 4.4.11.** Given a distinct set of initial relative positions \( \mathbf{r}^{(i,j)}(0) = \mathbf{x}^i_0 - \mathbf{x}^j_0 \) for \( 1 \leq i < j \leq N \) and orientations \( \mathbf{d}^i(0) = \mathbf{d}^i_0 \) for \( i = 1, ..., N \), there exists a unique solution to the relative equations of motion (4.9)-(4.10) for all time \( t \in [0, \infty) \).

**Proof.** The main idea of the proof is to show that the particle trajectories avoid the collision set

\[ \mathbf{C} := \{\mathbf{r} = (\mathbf{r}^{(1,2)}, ..., \mathbf{r}^{(N-1,N)}) \in \mathbb{R}^{3N(N-1)/2} \mid \mathbf{r}^{(i,j)} = 0 \text{ for some } 1 \leq i < j \leq N\}. \]

Consider the unique maximal trajectory of all relative positions \( \overrightarrow{\mathbf{r}}(t) \in \Gamma = \mathbb{R}^{3N(N-1)/2} \setminus \mathbf{C} \) starting at \( \overrightarrow{\mathbf{r}}_0 \in \Gamma \), which exists by Theorem 4.4.10 for \( t \in [0, T) \).

One needs to establish that \( T = \infty \) to prove the result.

Begin by defining a function representing the potential energy at time \( t \)

\[ E(t) := \sum_{i=1}^{N} \sum_{j>i} W(\mathbf{r}^{(i,j)}(t)), \quad (4.26) \]
where \( E : [0, T) \to \mathbb{R} \) and \( W(r) \) is the short-range potential \((4.6)\) defined in Section 4.3.2. As mentioned in Section 4.3.1, \( W(r^{(i,j)}(t)) \) is unambiguously defined as the interaction between the \( i \)th particle and the nearest image of the \( j \)th particle at time \( t \).

Assume, by contradiction, that \( T < \infty \). The time \( T \) can only be finite if the solution to \((4.9)-(4.10)\) blows up as \( t \to T \). This can only occur if as \( t \to T \), a collision occurs between a pair of particles in the following sense: dist\((\overrightarrow{r}(t), C) := \min_{i,j} |r^{(i,j)}(t)| \to 0\). As \( r^{(i,j)}(t) \to 0 \) for any \( 1 \leq i < j \leq N \), then \( W(r^{(i,j)}(t)) \to \infty \) and thus \( E(t) \to \infty \). In addition to \( E(t) \), compute its derivative

\[
\frac{dE}{dt} = \sum_{i=1}^{N} \sum_{j>i}^{N} \nabla W(r^{(i,j)}(t)) \cdot \dot{r}^{(i,j)}
\]

using the equations of motion for relative positions \((4.9)\). As dist\((\overrightarrow{r}(t), C) \to 0\), then \( \frac{dE}{dt} \sim -\frac{1}{(r^{(i,j)})^{26}} \to -\infty \) (since \( \dot{r}^{(i,j)} \sim F = -\nabla W \)). Recall that \( \nabla W = -F \) is Lipschitz continuous outside the origin.

Thus by the continuity of \( \frac{dE}{dt}(t) \) for \( t \in [0, T) \), there exists a \( \delta > 0 \) such that if \( \text{dist}(\overrightarrow{r}(t), C) < \delta \) for any \( t \in [0, T) \), then \( \frac{dE}{dt}(t) < 0 \). Since a collision occurs as time \( t \to T \), there exists a \( T_0 \in (0, T) \) such that for any \( t > T_0 \), \( \text{dist}(\overrightarrow{r}(t), C) < \delta \).

So for any \( t \in (T_0, T] \)

\[
E(t) = E(0) + \int_{T_0}^{t} \frac{dE}{dt}(\tau) d\tau < E(0) + \int_{T_0}^{T} \frac{dE}{dt}(\tau) d\tau = E(T_0) < \infty \quad (4.28)
\]

since \( \overrightarrow{r}(T_0) \notin C \). This is a contradiction since \( E(t) \to \infty \) as \( t \to T \).

The key observation is that as \( \text{dist}(\overrightarrow{r}(t), C) \to 0 \), \( E(t) \to \infty \), but \( \frac{dE}{dt} \to -\infty \). This leads to the contradiction by appealing to the continuity of \( E(t) \). Thus, \( T = \infty \) and there exists a unique maximal trajectory defined for \( t \in [0, \infty) \) given any initial relative configuration of positions \( \overrightarrow{r}_0 \in \Gamma \). As a result the relative positions of particles remain bounded away from the collision set by \( \delta > 0 \). Note that the right-hand side of the equations of motion consists of elements of \( C^\infty(\mathbb{R} \setminus B_\delta(0)) \). Since the arguments of each function remain in the compact set \( \mathbb{R} \setminus B_\delta(0) \), then the right-hand side remains Lipschitz continuous for all time. Thus by extending Theorem 4.4.10 one has a unique solution to \((4.9)-(4.10)\) for all time. \( \square \)
4.5 Conclusions

In this work the coupled PDE/ODE model for a semidilute suspension of self-propelled microscopic particles, first introduced in Chapter 2 and [75], was shown to possess a unique solution for all time given non-overlapping initial data. Using this result one can define a kinetic theory, in the form of the Liouville equation, which governs the time evolution of the system in phase space. This work was motivated by considering the macroscopic phenomenon, specifically the change in the effective viscosity, observed in experiments on bacterial suspensions. Previous works studying the effective viscosity have yet to establish that this quantity is a well-defined macroscopic quantity for a semidilute bacterial suspension. By proving the kinetic theory is well-defined, the explicit formula for the effective viscosity derived in our prior work [75] begins to be justified.

While it has been shown that the Liouville equation is well-defined, many important questions remain. One of the primary difficulties was the time–dependent quasiperiodic boundary conditions on the fluid equation imposed by the planar shear background flow. The results in this work may be extended to a larger class of background flows using methods outlined in [81]. Here the authors show that there are a wide class of flows referred to as viscometric that generalize Lees-Edwards boundary conditions beyond Couette (planar shear). Global viscometric flows (e.g., Poiseuille or Couette) are fluid motion, which is locally equivalent to simple steady shearing motion at every fluid particle. These flows possess the following properties:

(i) No spurious forces (e.g., due to thermal noise) at the molecular level

(ii) A time-dependent invariant manifold exists at the molecular level

(iii) The solution satisfies Stokes or its related equation exactly as in Theorem 4.4.4 and thus all particles obey the equations of motion

(iv) The solution is independent of the geometry of the problem and the boundary conditions of the experimental apparatus.

The “pullback” idea of mapping the PDE back to a periodic problem according to the linear map describing the ambient background flow can also be used to study
this wider class of flow. This is only briefly mentions and not covered within this dissertation. In addition, other flows beyond viscometric have yet to be considered.

In order to define the effective viscosity the two components necessary have been illustrated. The bulk stress needs to be well-defined for all time, which has been shown in this work, and there must exist a steady-state solution to the Liouville equation. Unlike the parabolic Fokker-Planck equation, where the existence of a steady-state probability distribution is known [127], one cannot appeal to such a result for the hyperbolic Liouville equation. Future work may establish this fact and allow the effective viscosity to be well-defined as a macroscopic quantity. Nevertheless, the development of the kinetic theory in this work could lead to the study of other effective properties, in addition to the effective viscosity, experimentally observed in semidilute suspensions.
Chapter 5

Collective dynamics in semidilute bacterial suspensions

The study of collective motion in bacterial suspensions has been of significant recent interest. While many experimental and theoretical studies have been performed, the overall picture lacks clarity, especially the identification of the specific physical mechanisms responsible for collective motion. To better understand the non-trivial spatio-temporal correlations emerging in the course of collective swimming in suspensions of motile bacteria, a simple model is employed: a bacterium is modeled as a force dipole with size, through the use of a short-range repelling potential, and shape. The model emphasizes two fundamental mechanisms: dipolar hydrodynamic interactions and short-range bacterial collisions. Using direct particle simulations validated by a dedicated experiment, it is shown that changing the swimming speed or concentration alters the time scale of sustained collective motion, consistent with experiment. Also, the correlation length in the collective state is almost constant as concentration and swimming speed change even though increasing each greatly increases the input of energy to the system. It is demonstrated that the particle shape is critical for the onset of collective effects. This work exemplifies the delicate balance between various physical mechanisms governing collective motion in bacterial suspensions and provides important insights into its mesoscopic nature.

This Chapter also illuminates the features leading to the collective behavior of simple microorganisms, such as the competition between collisions and hydrody-
dynamic forces and the critical role of the geometrical confinement and dimension. Most of the details in this Chapter were originally published in [36] and all experimental data reported on was obtained from experiments carried out at Argonne National Laboratory in Argonne, IL by Dr. Igor S. Aranson and Dr. Andrey Sokolov.

5.1 Introduction

The phenomenon of collective motion has been an active area in the last few years. Experiments have demonstrated that in the collective state a bacterial suspension can exhibit remarkable properties such as enhanced diffusivity, the formation of sustained whorls and jets, and the ability to extract useful work [3, 5, 8, 17, 51]. Specifically in suspensions of rear-actuated swimmers (so-called pushers) exemplified by bacteria, correlated mesoscopic collective motion is observed at length scales up to 10 times larger than that of a given particle while particle velocities exceed that of an isolated swimmer [4, 5].

While specific biological mechanisms such as chemotaxis and chemical signaling can be ruled out in most of the experiments on collective swimming in concentrated bacterial suspensions, the role of the physical mechanisms governing collective motion is still under discussion. A variety of theoretical models have been considered recently, with fundamentally different mechanisms attributed to the onset of collective motion, from flagella reversal dynamics [51], pure hydrodynamic [19, 61, 65, 67] to pure collisional [2, 7, 51, 53, 60, 103] interactions. While the existing models were able to reproduce some key experimental observations, such as the onset of collective motion above a certain critical concentration [4, 18, 67], but the agreement with experiment remains incomplete and mostly qualitative.

A variety of computational approaches were suggested to model individual swimmers, such as slender bodies [65], swimming dumbbells [7, 60, 103], hard self-propelled rods [53], self-propelled hydrodynamic point dipoles [75], squirmers [104], or more computationally-intensive “composite” swimmers [107, 108]. Each model, emphasizing different aspects of the balance between hydrodynamic forces and steric collisions, often yields to somewhat different conclusions on the critical concentration for the onset of collective motion, swimming speed in the collective...
state, or its correlation properties. In this Chapter, by introducing a minimal yet realistic model of a swimmer, the combined effect of hydrodynamic interactions and collisions on the collective dynamics of a bacterial suspension will be investigated numerically. A dedicated experimental study was conducted to determine the time required to establish the collective state from well-mixed initial conditions, and spectral and spatio-temporal velocity correlations in the corresponding collective state. The main goal of this study is to provide further understanding of the phenomena discovered in our recent experiments: the velocity correlation length and properly rescaled correlation time of the collective motion are essentially independent on the velocity and concentration of bacteria [50].

The structure of this Chapter is the following. First, an overview of experimental techniques are briefly presented. Then, the model for the suspension is introduced where a bacterium is represented as a point force dipole with size and shape, where the force of self-propulsion induced by the beating of flagella is balanced by the viscous drag force on the bacteria. The force dipole model for a bacterium has been experimentally verified by Drescher et al. [2]. Using this model the effects of the system parameters (swimming speed/propulsion force, concentration, and tumbling rate) on the collective dynamics of the suspension are investigated. It is shown that our model is justified by capturing earlier experimental results on the transition from individual to collective motion [4, 5]. Specifically, the effect of concentration on correlation length and mean particle velocity. Subsequently, the results of varying the system parameters in the simulation are presented and compared with similar experimental results. Moreover, the theoretical model allows for the separation of the contributions of tumbling and swimming speed as well as the effect of the particle shape on the correlation length, which at present has not been done experimentally.

5.2 Brief description of experiment

The experimental setup, based on a free-standing thin film, is similar to that described in [5, 50]. Collective motion is quantified by measuring the bacterial velocity field, then the associated correlation function is defined and the correlation length and time extracted (see Section 5.3.5 for the definition of the correlation
function). Specifically, collective motion is characterized by an increased correlation length (quantifying the size) and mean particle velocity [5]. In addition, recent experiments demonstrate the effects of system parameters such as concentration, tumbling rate, and swimming speed on the collective dynamics of the suspension [50]. These observations were made on both a three-dimensional thin film and quasi-two-dimensional film using a combination of both PTV (particle tracking velocimetry) imaging technique for low concentrations and the optical flow method or PIV (particle image velocimetry) for high concentrations. The experiments were performed on bacterial suspensions where the swimming and tumbling rate were both controlled by varying the ratio of oxygen and nitrogen in the chamber containing the suspension. The correlation between these two modes of motion results from the simple observation that when deprived of oxygen bacteria swim more slowly and sensing unfavorable conditions they begin to tumble more frequently. Experimental results, not reported earlier in [50], are shown in Figures 5.1, 5.2, 5.3, 5.6, and 5.10.

The main experimental observation made in [50] was that the correlation time of the bacterial flow field in the collective state scaled inversely with the swimming speed or concentration while the correlation length remained constant for negligible amounts of noise. Thus suggesting that changing the bacterial swimming speed or concentration is analogous to changing the overall time scale. This follows from the fact that the magnitude of a bacterium’s induced flow and the number of collisions between bacteria are proportional to their swimming speed and concentration. Each quantity is also proportional to the rate at which energy is injected into the system.

In a new experiment presented here the onset of collective swimming in a suspension of bacteria from an initially prepared isotropic disordered state is investigated. A small drop of bacterial suspension was placed on a microscope glass slide. An ultrasonic transducer was glued to the glass with epoxy, Fig 5.1(a). A square wave frequency modulated signal (sweep) in the range 35kHz-43kHz was applied to the transducer generating capillary waves on the open surface of the drop, with the typical wavelength of the order 60µm, Fig 5.1(b). The surface capillary waves effectively mix the suspension and completely destroy the collective motion. It was observed that after the signal is turned off the bacterial swimming pattern
Figure 5.1. (a) An experimental setup for “mixing bacteria” by the means of ultrasound (US) excitation. (b) A snapshot of capillary waves. (c)-(e) A sequence of snapshots illustrating the evolution of the velocity field of bacteria after the US transducer was switched off.

is different from the stationary collective state and bacteria swim much slower (see the movie in the supplementary information in [36]). However, the swimming speed increases in time during the first 5 seconds, Figure 5.6, and collective motion appears in $\approx 1$ sec, Figure 5.1(d).

For detailed analysis of the onset of collective behavior the evolution of the power spectrum distribution $P(k_n) = \langle |F(k_n)|^2 \rangle$ was monitored, where $F(k_n)$ are the coefficients of the Fourier transformation of the velocity field and $k_n$ is the dimensionless wavenumber defined as $k_n = \tilde{k}_n \cdot l$, assuming $l \approx 10^{-2} mm$ is an effective (bacterium body and flagella) bacterial length and $\tilde{k}_n$ is the dimensional wavenumber, both in experiment and simulations. Some results are presented in Figure 5.2. While in the steady state, after the transition, the power spectra in the experiment and simulations are qualitatively similar, the details of the time evolution are different due to the specifics of experiment. It was observed that the surface waves, excited by the ultrasound transducer, generate a rectified flow with a scale of a few millimeters. Thus, a large vortex with a big correlation length will be present initially, then slowly decrease to the stationary value. These large scale flows decay in time very slowly due to the reduction of the effective viscosity of
Figure 5.2. Experiment: (a) Time evolution of the power spectrum after the ultrasound transducer was switched off. The wavenumber is non-dimensionalized by an effective bacterial length $l \approx 10^{-2} \text{mm}$. The lightest regions correspond to a higher magnitude of the corresponding spectral component followed by a transition region as $k$ in terms increases to a dark region corresponding to zero. The dark line is an average wavenumber for each moment of time. (b) Power spectra $P(k)$ for several moments of time. Simulation: (c) Quasi-2D simulation, time evolution of the power spectrum from an initial vortex. (d) Quasi-2D simulation, power spectra for several moments of time from an initial vortex. (e) Quasi-2D simulation, time evolution of power spectrum from an initially random configuration. (f) Quasi-2D simulation, power spectra for several moments of time from an initially random configuration.

the bacterial suspension, [20]. To exclude the flow generated by the surface waves, the average velocity in the microscope field of view is subtracted from the velocity field. According to the experimental observation in Figures 5.2(a), (b), the average wavenumber is slightly increasing in time during the development of collective behavior. It can be evidence of the slow decay of a large scale flow generated by the surface waves to a flow with scales typical for collective swimming of the bacteria. In the simulations started from an initial vortex (vortex-like configuration of bacteria), Figure 5.2(c), (d), qualitatively the same behavior as in experiment is seen; however, in simulations started from a random configuration of bacteria with no external large-scale flow the average wavenumber is decreasing in time, Figures 5.2(c), (d).
In the steady state, both experiment and simulations yield power spectra with a well-pronounced peak at a “mesoscale” wavenumber $k \approx .3$, compare Figures 5.2(b), (d). Also, the energy spectra were investigated, $E(k) \sim kP(k)$, and qualitatively similar results as in [53] were obtained. However, it is not appropriate to interpret such energy spectra as evidence for the intermediate power-like behavior and, correspondingly, “mesoscale turbulence” – the interval in $k$-space for the power-like behavior is exceedingly small.

Figures 5.3(a), (b) illustrate the velocity field and vorticity observed in experiment at two different swimming speeds for a concentration in the collective state to show the onset of vortex-like structures in higher volume fraction suspensions. One sees that for a small oxygen concentration (i.e., small swimming speed) the flow pattern is rather disordered due to random tumbling, with the characteristic

**Figure 5.3.** Frames illustrating the velocity field (arrows) and vorticity with dark regions corresponding to larger vorticity (red positive and blue negative). (a) From experiment, low isolated swimming speed and large rotational diffusion $D_\theta$. (b) From experiment, large isolated swimming speed and low rotational diffusion. (c) Quasi-2D simulation, volume fraction $\Phi = .74$, rotational diffusion $D_\theta = 10^{-1}$ rad$^2$/sec, isolated swimming speed $V_0 \approx 1$. (d) Quasi-2D simulation, volume fraction $\Phi = .74$, rotational diffusion $D_\theta = 10^{-1}$rad$^2$/sec, isolated swimming speed $V_0 = 1.0$. 

In the steady state, both experiment and simulations yield power spectra with a well-pronounced peak at a “mesoscale” wavenumber $k \approx .3$, compare Figures 5.2(b), (d). Also, the energy spectra were investigated, $E(k) \sim kP(k)$, and qualitatively similar results as in [53] were obtained. However, it is not appropriate to interpret such energy spectra as evidence for the intermediate power-like behavior and, correspondingly, “mesoscale turbulence” – the interval in $k$-space for the power-like behavior is exceedingly small.

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size of the flow is on the order of the bacterial length. In contrast, for larger oxygen concentration (larger swimming speeds) the bacteria develop mesoscale patterns exhibiting collective motion manifested by self-organized vortices and jets with the characteristic size of about 6-10 bacterial lengths. Qualitatively similar behavior was also observed in the simulations, Figures 5.3(c), (d). Correspondingly, the movies 1-2 in the supplementary information of [36] taken from simulation illustrate the visual similarity between the simulations and experiment for the dynamics of a suspension for both low and high swimming speeds.

5.3 Semidilute model

Here a simple computationally effective model to investigate the role of collisions and hydrodynamic interactions on the collective behavior of bacterial suspensions is introduced for two and three dimensions. This model does not include buoyancy and oxygentaxis, and, therefore, cannot capture complex behavior such as bio-convection associated with collective motion in three-dimensional suspensions [68, 35]. Additional more computationally intensive simulations have also been performed which show some of the effects of collective motion [74, 104, 107, 108], but the purpose of this paper is to introduce a minimal yet realistic model capable of seeing the same effects as well as predicting new phenomenon. Since bacteria can come in diverse shapes and sizes, using the simulations one can determine if the effects of shape/aspect ratio change the collective motion. Additionally, bacteria do not swim in a straight line even in the absence of tumbling (the rotation of the flagella induces counter-rotation of the bacterial body), but this effect will be neglected for the purposes of the simulations.

In Chapter 2 and the previous theoretical work [75], a simple three-dimensional model for semidilute bacterial suspensions, which captured the qualitative effects of collective swimming on the effective viscosity observed in experiment was introduced. Simulations of this model performed on graphic processing units (GPUs) demonstrated, in agreement with experiment [20], an initial decrease and then subsequent increase in the effective viscosity with the increase in the concentration of bacteria over the full range of experimentally observed concentrations. In this Chapter an extension of this model in two and three dimensions will be used to
study the dependence of the correlation length of collective motion as function of swimming speed, concentration, dipolar strength, and geometrical confinement (2 vs. 3 dimensions).

The focus will be on a semidilute suspension – the hydrodynamic interactions on each bacterium are represented as the sum of pairwise interactions. This approximation is exact for bacteria modeled as point dipoles. The model accounts for two basic forms of interactions: the bacterium with the fluid (hydrodynamic) and inter-bacterial short-range interactions (soft collisions). The combination of hydrodynamic interactions and collisions has been shown to be crucial for collective motion [18, 51]. The intuitive theoretical picture is that collisions align the particles and once aligned hydrodynamic interactions are enhanced. The main goal for the model is to capture properties of collective motion observed in suspensions of *Bacillus subtilis*, a pusher (a swimmer propelled from the rear). This point dipole model can be extended to study suspensions of “pullers” (swimmers propelled from the front) as well, such as the algae *Chlamydomonas*, by reversing the orientations of the point forces so that they point inward. The models introduced in the following sections capture the size, shape, hydrodynamic interactions between particles as well as collisions. Thus, leading to a simple yet realistic model accounting for the most relevant physical mechanisms.

Due to the typical size of a bacterium (*l* = 5 µm) and isolated swimming speed (*V*₀ = 20 µm/s), the Reynolds number *Re* = *lV*₀/ν ≪ 1 is exceedingly small, where ν is the kinematic viscosity. Since a steady state flow is established on a timescale much smaller than the characteristic time scale of bacterial motion, the fluid is modeled as an incompressible steady Stokes flow neglecting inertial effects.

### 5.3.1 Quasi two-dimensional model

Two models will be proposed to handle the cases of a thin film quasi-2D suspension and a full 3D model. The first is designed to capture the thin film geometry representative of the experimental setup of Sokolov et al. [5], see Figure 5.4. The domain is a thin film of length and width *L* ≫ *l* and thickness *w* ~ *l* approximately the characteristic length of a swimmer. While the experiments [5] were performed in a free-standing liquid film, the accumulation of bacteria metabolism products
results effectively in no-slip boundary conditions for the fluid on the top and bottom surfaces of the film. A suspension consists of \( N \) neutrally buoyant particles. Each particle will have two variables identifying it: the center of mass \( \mathbf{x} = (x, y, z) \) and the orientation \( \mathbf{d} = (d_x, d_y, d_z) \) directed along a given particle’s axis of symmetry.

Begin from a confined thin film model for the fluid studied in [128].

The flow at the middle 2D plane of the thin film \((z = 0)\) due to a point dipole bacterium with orientation \( \mathbf{d} \) at the origin \((|\mathbf{d}| = 1)\) is defined as

\[
  u(x, y) := -\frac{U_0 w}{3\pi} \nabla^3[\log(r)] \mathbf{d} \mathbf{d}^T, \tag{5.1}
\]

where \( r = |\mathbf{x}| \) is the distance from the origin to the dipole, \( U_0 = \zeta V_0 l^2 \) is the dipole strength where \( \zeta \) is a constant determined by the shape/aspect ratio. This formula for a point dipole is derived from that of two oppositely oriented force monopoles in the limit as the distance between them goes to zero (cf. [128]). Once obtained it is observed that the in-plane fluid velocity \( u_x(x), u_y(x) \sim r^{-3} \). Since the film has thickness approximately the size of a particle in the vertical dimension, consider the suspension in two dimensions \((x, y)\) for numerical simulations.

One can derive the explicit expression for the fluid velocity (5.2) by taking the flow produced by a monopole, \( u_{mon}(x) \), first derived in [128] and computing the associated point dipolar contribution:

\[
  u_{dip}(x) := \lim_{l \to \infty} \left[ u_{mon}(x + l\mathbf{d}/2) - u_{mon}(x - l\mathbf{d}/2) \right].
\]

as a function of interparticle distance \( \mathbf{x} = (x, y) \), which has the form

\[
  u_x(x, y) = \frac{4 \left[ (d_y^2 - d_z^2)x^3 - 6d_xd_yx^2y + 3(d_z^2 - d_y^2)xy^2 + 2d_xd_yy^3 \right]}{(x^2 + y^2)^3}, \tag{5.2}
\]

\[
  u_y(x, y) = \frac{4 \left[ 2d_xd_yx^3 + 3(d_y^2 - d_z^2)x^2y - 6d_xd_yxy^2 + (d_z^2 - d_y^2)y^3 \right]}{(x^2 + y^2)^3}.
\]
Figure 5.5. Left: Streamlines from fluid flow of a single bacterium measured in experiment [2], Right: Streamlines produced by (5.2) from the quasi-2D thin film model.

The flow in the z-direction (neglected in simulation) is exponentially small $u_z(x) \sim e^{-|x|/w}$ for $w \ll 1$. The flow due to a single bacterium in experiment is captured well by the point dipole model in quasi-2D as seen in Figure 5.5.

5.3.2 Full three-dimensional model

Also, a full 3D model for the suspension is considered where the fluid is again modeled using the incompressible Stokes equation. The flow induced by a single bacterium is taken to be

$$u(r) := \frac{U_0}{8\pi r^2} [3(\hat{r} \cdot d)^2 - 1] \hat{r}$$

(5.3)

where $\hat{r} = r/r$, $r = |r|$ is the distance vector relative to the center of dipole and $U_0 = \zeta V_0 l^2$. This scenario is representative of experiments done in the bulk of a suspension far from the boundary as in [50]. Particle motion is governed by the same equations of motion with (5.2) replaced by (5.3).

The fluid velocity for the suspension, $u(x)$, depends on the $N$ particle positions and orientations. The corresponding equations of motion, derived from the balance of forces and torques on each particle, are defined in 5.3.4. Due to the linearity of the Stokes equation, the flow due to $N$ particles will be the sum of flows due to a single particle (5.2) or (5.3).

A full range of concentrations is investigated where the area fraction is defined as $\Phi = \pi NL^2/4L^2$ in 2D and the volume fraction $\Phi = \pi NL^3/6L^3$ in 3D. These
are the associated area/volume fractions for a sphere of radius $l/2$. Since point dipoles are used, the particle size, $l$, and the excluded volume are defined via the radius of the short-range repulsive potential $\sigma_{LJ}$. In the simulations, for convenience the truncated Lennard-Jones potential $W \sim [(\sigma_{LJ}/r)^{12} - (\sigma_{LJ}/r)^{6}]$ is used. Spherical particles are formally used for computational efficiency, but the shape of the particle is implicitly defined by the strength of the hydrodynamic dipole in (5.2)-(5.3). While the specific choice of the repulsive potential is not important, (e.g., the exponential Yukawa potential instead of the Lennard-Jones potential was employed in [53]), the use of the truncated Lennard-Jones potential is computationally efficient\(^1\). In addition, a certain realigning torque was added to ensure that the particles swim off after a collision, see Section 5.3.5 and Fig. 5.7. This effect is also related to the shape of particle.

### 5.3.3 Numerical implementation

Simulations were run for $N$ identical particles, $N \sim 10^4 - 10^5$, where a typical simulation contains between 15,000 – 40,000 particles depending on the volume fraction. The typical domain has side length $L = 30 \sim 120l$ in 2D and $L = 10 \sim 30l$ in 3D, where $l = .25$ in 2D and $l = .35$ in 3D, reducing any finite size effects. $l$ is the non-dimensional length of a particle chosen so that the isolated swimming speed $V_0 = 1$. Due to the semidilute assumption, the flow acting on a particle is the sum of flows from all other particles including periodic images outside the computational domain. The periodic boundary conditions allowing for these flows are taken into account by generating virtual image particles and computing the flow due to each up to a distance from the reference cell beyond which the results do not change.

The present model captures the far-field hydrodynamic interactions while also introducing a mechanism for the displacement and realignment due to collisions. In addition, tumbling was introduced (see Section 5.3.4 for a more detailed comparison between experiment and simulations). Numerically, tumbling is accounted for in the two simulations depicted in Figures 5.9 and 5.10 by choosing a random portion $\chi$ of the total number of particles to tumble in a given time interval $\Delta t$.\(^1\)

\(^1\)Note also that the definition of volume fraction is different from that in [7, 60, 67, 103] where volume fraction is calculated according to the hydrodynamic radius of the particle.
Figure 5.6. (a) Rescaled correlation length ($L/l$) and mean particle velocity ($V/V_0$) vs. time for volume fraction $\Phi = .60$, $V_0 = 1.0$, in a quasi-2D suspension. (b) Mean velocity of bacteria vs. time in a drop of bacterial suspension on a microscope slide. Orientations of bacteria were randomized by ultrasound frequency-modulated signal before the measurements. Velocities of bacteria were measured using PIV.

In 2D, the rotational diffusion is then $D_\theta = \chi \pi^2/3\Delta t$ and in 3D $D_\theta = 2\chi \pi^2/3\Delta t$ (variance of the uniform distribution in the interval of $[-\pi, \pi]$ is $\pi^2/3$).

In all cases, the initial orientation of each particle is taken to be random and the initial positions are uniformly distributed throughout the domain, except the situation considered in Fig. 5.2 (a)-(d) where the bacteria were aligned along a large vortex. The simulations are then run until $t = 40\hat{t} = 10s$ before any physical quantities are computed to allow the particles sufficient time to interact. Here $\hat{t} = l/V_0$ is the characteristic time scale representing the time for a particle to swim its length. Figure 5.6 illustrates that beyond $t = 10s$ the system has settled and no major changes in the collective dynamics are observed.

5.3.4 Particle evolution equations

The particle equations of motion are determined by the balance of forces and torques on each particle

$$\dot{x}^i = V_0 d^i + \sum_{j\neq i} [u(x^i - x^j) + F(x^i - x^j)]$$ (5.4)

$$\dot{d}^i = -d^i \times \left[\sum_{j\neq i} \omega^j(x^i) + B d^i \times \sum_{j\neq i} E^j(x^i) \cdot d^i + \sum_{j\neq i} \omega^{L,j}(x^i - x^j)\right]$$ (5.5)
where \( \mathbf{u} \) is the flow defined in the Section 5.3 depending on whether a quasi-2D or full 3D model is considered. This term couples the fluid Stokes equations and particle equations of motion. The translational motion (5.4) is a generalization of Stokes drag law \( f = 6\pi \eta l \mathbf{u} \) from the balance of forces and (5.5) is Jeffery’s equation for the orientation of a passive ellipsoid [109] with additional contributions due to interactions and collisions. Modeling pure hydrodynamic interactions may cause the point dipole particles to overlap. This will result in an artificial divergence of velocities. Thus, introduce a truncated purely repulsive Lennard-Jones type potential, \( W = 4\varepsilon[(\sigma_{LJ}/r)^{12} - (\sigma_{LJ}/r)^{6}] + \varepsilon \) for \( r < 2^{1/6}\sigma_{LJ} \) and zero otherwise where \( \varepsilon = .01 \) in simulations. This enforces excluded volume constraints and soft collisions through a contribution to (5.4) by the repulsive force \( \mathbf{F} = -\nabla W \). \( \sigma_{LJ} \) is a parameter representing the characteristic length \( l \), \( r \) is the distance between two particles, and \( \varepsilon \) is a parameter which determines the strength of repulsion. In contrast to [7, 60, 103] where the evolution equations only govern the positions of the beads in their dumbbell model, the particle orientations here evolve according to explicit equations of motion due to the torques acting on a given particle (Jeffery’s equation, (5.5)). By enforcing Jeffery’s equation, it is ensured that the point dipoles interact with the fluid as ellipsoids. The shape/aspect ratio is accounted for explicitly through the Bretherton constant, \( B \) (0/1 corresponding to a sphere/needle). This results in each point dipole bacterium having a size and shape.

The vorticity and rate of strain induced by hydrodynamic interactions are \( \omega^i(x^i) = \nabla \mathbf{u}(x^i - x^j) \) and \( E^i(x^i) = (1/2)[\nabla \mathbf{u}(x^i - x^j) + (\nabla \mathbf{u}(x^i - x^j))^T] \) respectively. \( \omega^{LJ}(x^i - x^j) = \xi|\mathbf{F}(x^i - x^j)||\mathbf{d}^i \cdot \mathbf{d}^j|(\mathbf{d}^i \times \mathbf{d}^j) \) is a realignment term due to collisions between particles. This term reinforces the following interaction between the bacteria: if particles approach one another near parallel (\( \mathbf{d}^i \times \mathbf{d}^j \) small) or near perpendicular (\( \mathbf{d}^i \cdot \mathbf{d}^j \) small), then there is only a small torque. Also the coefficient \( |\mathbf{F}(x^i - x^j)| \) ensures that the torque after a short period of time will reorient the particles away from each other as seen in Figure 5.7. Here \( \xi \) controls the swim off rate and is taken to be 1 in the simulations presented in this work. This behavior is motivated by experimental observations of bacterial collisions [18] and the analysis of hydrodynamic interaction between two elongated self-propelled particles [105]. Simulations without this term yield the formation of densely-packed clusters of
bacteria separated by essentially empty domains. This behavior is in disagreement with experiment where a practically homogeneous distribution of bacteria is observed.

Since tumbling is present in the experimental data it must also be incorporated into the simulations. Numerically the strength and frequency of tumbling, which is a random reorientation on the unit sphere, is controlled by picking a random percentage of the particles to tumble in a given predefined interval of time (details presented in Section 5.3.3. From this $D_\theta$ can be calculated for comparison with experiment. Unless otherwise noted all simulations are run in the absence of tumbling.

5.3.5 Correlation functions

Consider the spatial and time autocorrelation functions in the suspension by computing the coarse-grained flow field, $V(x)$, generated by the fluid velocity, $u(x)$, on a discrete grid, see Figure 5.8. There are two basic sources of randomness in the system. One is the random initial configuration of the suspension both in positions and orientations. The second was first observed in Chapters 2-3 where interparticle interactions can introduce randomness in the form of self-induced noise, where the effect of interactions is similar to that of random diffusion. Once this field is computed the spatial correlation function can be defined as a function of distance $r = |r|$ between points in the fluid

$$C(r, t) := \frac{\langle V(x + r, t) \cdot V(x, t) \rangle_{x, \theta} - \langle V(x, t) \rangle_x^2}{\langle V^2(x, t) \rangle_x - \langle V(x, t) \rangle_x^2},$$

where $\langle \cdot \rangle_x$ is an average over spatial coordinates. This is consistent with its calculation in experiment [50]. The correlation length is then extracted by fitting the

Figure 5.7. Illustration of how the torque $\omega^{L-J}$ in (5.5) effects the orientations of two particles as they collide.
time-averaged correlation function to an exponential function of the form $e^{-r/L} + A$ where $A \ll 1$ and $L$ is the correlation length as in [5]. Similarly the time correlation can be extracted from

$$K(x, \tau) := \frac{\langle V(x, t + \tau) \cdot V(x, t) \rangle_t - \langle V(x, t) \rangle_t^2}{\langle V^2(x, t) \rangle_t - \langle V(x, t) \rangle_t^2},$$

which is then spatially-averaged. Non-dimensionalize the correlation length and time by the particle length $l \sim \sigma_{LJ}$ and the characteristic time scale $t_0 = l/V_0$ (time for a bacterium to swim its length). Specifically, the first set of results in Section 5.4 show the effect of the concentration and swimming speed on the correlation length and the latter results illustrate how the correlation time depends on these two parameters.

### 5.4 Effective properties of the collective state

#### 5.4.1 Correlation length

In this section, results for both the quasi-2D suspension and the 3D model are provided. First, the results of the quasi-2D simulations are compared to the experiments of Sokolov et al. performed on a thin film suspension of *Bacillus subtilis* [5]. Figure 5.9 depicts the results of simulations showing the relationship between the correlation length $L$ and the volume fraction $\Phi$. There are two clear regimes:
Figure 5.9. Rescaled mean particle velocity ($\bar{V}/V_0$) vs. volume fraction ($\Phi$), $V_0 = 1.0$, in a quasi-2D suspension with no tumbling (top). Effect of tumbling rate ($D_\theta$) and system size $L$ on the transition to collective motion in a quasi-2D suspension (bottom). Inset: Rescaled correlation time ($T/t_0$) vs. swimming speed ($V_0$), $\Phi = .60$, in quasi-2D and 3D suspensions.

Figure 5.9 illustrates the effects of tumbling. The first observation is that the larger the tumbling rate the higher the critical concentration is for the transition to collective motion. This is due to the fact that tumbling disrupts the alignment of particles (which is a characteristic of the collective state): more particles are needed to increase the contribution from collisions (that increase alignment) in order to dominate the effect of tumbling. Second, even in the absence of tumbling, there exists a critical concentration for the onset of collective motion. This behavior can
Figure 5.10. Rescaled correlation length \((L/l)\) vs. swimming speed \(V_0\), \(\Phi = .60\), in (a) quasi-2D, (b) 3D suspensions and (c) experiment for different tumbling rates. The experimental correlation length is normalized by the length of the bacterium (5 \(\mu\)m) and the velocity is normalized by (20 \(\mu\)m/sec), which is the velocity of an individual bacterium under a normal oxygen concentration. In experiment the tumbling rate is measured by tracking individual bacteria at low concentration for a fixed isolated swimming speed. (d) Rescaled correlation length \((L/l)\) vs. volume fraction \(\Phi\), \(V_0 = 1.0\), in a 3D suspension. Rescaled correlation time \((T/t_0)\) vs. volume fraction \(\Phi\), \(V_0 = 1.0\), in (e) quasi-2D and (f) 3D suspensions.

be interpreted as a manifestation of “intrinsic noise” generated due to interactions between multiple bacteria. This is consistent with the observation in Chapter 3 and the previous work, [75], that hydrodynamic interactions in a deterministic system of many interacting particles leads to the same effect as random tumbling. Also, it can be seen from Figure 5.9 that the correlation length, and, consequently, the scale of the collective motion is independent of the domain size for \(L > 30\).

In addition, the simulations show that in three dimensions the correlation length of collective motion is essentially constant as the volume fraction changes above a certain critical value \(\Phi_{crit} \approx .2 - .4\) in agreement with experiment, see Figure 5.10(d). This value is below the prediction of [67] that the transition to collective motion occurs when the volume fraction defined by the hydrodynamic radius of the particle becomes of the order one.

Figure 5.10(a) shows the effect of swimming speed \(V_0\) on the correlation length
for a quasi-2D suspension. In a suspension where particles do not tumble the
correlation length remains essentially constant as the swimming speed increases,
showing the correlation length is independent of \( V_0 \). If particles are allowed to
tumble, then at low swimming speeds the correlation length rapidly decreases to
the size of a particle (individual random motion). For higher swimming speeds the
effect of tumbling on the collective motion is less pronounced. This shows directly
that tumbling is the main cause of the decrease in the correlation length rather
than the slow-down of the particles due to tumbling\(^2\). The effect of tumbling was
also examined in full 3D simulations and the results are given in Figure 5.10(b).
When the tumbling rate is increased, the qualitative behavior observed in [50]
and in 2D simulations is recovered: a decrease in the correlation length at low
swimming speeds.

5.4.2 Correlation time

Consider the effect of the system parameters on the correlation time. In the simu-
lations, normalize the correlation time by the characteristic time scale \( t_0 = l/V_0 \) in
place of the mean free time \( \tilde{t}_0 = 1/V_0 cl \) in 2D and \( \tilde{t}_0 = 1/V_0 cl^2 \) in 3D) between
collisions used in experiment, where \( c \) is the concentration [50]. Figures 5.10(e),
(f) show the normalized correlation time is essentially constant when the volume
fraction increases, in 2D and 3D simulations respectively. The correlation time can
be thought of as the time scale on which coherent large-scale structures (vortices,
jets) in the collective motion are sustained. Thus for concentrations beyond the
threshold for collective motion this time scale remains essentially constant.

In addition to being independent of the concentration, the inset to Figure 5.9
demonstrates that the rescaled correlation time, \( T/t_0 \), is independent of the swim-
moving speed in the collective regime. This is consistent with experiment where the
correlation time is rescaled by the mean free time and was observed to be con-
stant as the swimming speed increased [50]. One limitation of the present model
is the introduction of a third time scale, collision time, in addition to the char-

---

\(^2\)In experiment, both tumbling and the swimming speed are controlled by the ratio of ni-
trogen to oxygen available to bacteria. When the oxygen concentration is small, the bacteria
tumble more frequently, and, more importantly, the swimming speed and tumbling rate are not
independent and their individual contributions to the correlation length cannot be isolated.
characteristic time scale and the time scale for collective motion: the collisions are soft and not instantaneous, and, therefore, time elapses as particles collide and reorient. The collision time, \( t_{\text{col}} \), is determined by the stiffness of the Lennard-Jones potential near the equilibrium distance \( r_0 = 2^{1/6} \sigma_{\text{LJ}} \) and is of the order \( t_{\text{col}} \approx \sigma_{\text{LJ}}^2/(36 \times 2^{2/3} \varepsilon) \). A simple calculation provides an estimate for the collision time in terms of the characteristic time scale and the mean free time \( t_0 \): \( t_{\text{col}} \approx 0.2t_0 - 0.4t_0 \). However, our study revealed that this effect does not change the qualitative behavior of the correlation time.

5.4.3 Beyond experiment

Now that it has been established that the model captures most experimental observations, the relationships which are difficult and have not yet been observed experimentally are investigated. One such example is the effect of the dipole moment, characterizing the strength of hydrodynamic interactions, which depends on the particle shape and aspect ratio. The relative dipole moment \( U_0 \) decreases for a slimmer particle with the decrease of its cross-section. Thus, for a given swimming speed and concentration the mean free time is fixed; therefore, by changing \( U_0 \) one can compare the relative contribution of hydrodynamic interactions compared to collisions as seen in (5.2)-(5.3). Figure 5.11 illustrates the dependence of the normalized correlation length \( (\mathcal{L}/l) \) on the dipole moment \( U_0 \) for a fixed swimming speed and volume fraction in the collective state. In quasi-2D simulations one sees a very minor increase in the correlation length and in 3D the correlation length

**Figure 5.11.** Rescaled correlation length \((\mathcal{L}/l)\) vs. dipole moment, \( \Phi = .60, V_0 = 1.0 \).
increases rapidly as the dipole strength decreases. These results indicate that the aspect ratio plays a critical role in the onset of collective motion in a suspension of microswimmers, consistent with the observations made in [53].

The aspect ratio or shape can also be quantified using the Bretherton constant $B = \frac{a^2 - 1}{a^2 + 1}$, where $a$ is the aspect ratio of the major and minor axes of an ellipsoid. Figure 5.12, provides the dependence of the correlation length on the $B$. Recall that in Jeffery’s equations (see Section 5.3.4) for particles in a shear flow: elongated particles ($B \to 1$) align along the stable axis of the rate of strain tensor [109] whereas spherical particles ($B = 0$) do not. This demonstrates the importance of the shape of a particle in determining the collective properties (e.g., alignment). As $B$ becomes small, particles effectively become spheres and no collective effects are observed.

Now briefly compare the simulation results with past works studying the collective state. First, Figure 5.2 shows that the power spectrum from the experiment and simulations is maximized below $k = .3$ consistent with the prediction of the instability of the isotropic state at low wave numbers [63, 67]. The transition to the collective state occurs at a volume fraction between $\Phi = .2 - .4$, which is consistent with the prior results of [60] whose analysis yields a critical concentration of $\Phi = .3$. In addition, [7, 103] show an increase in the mean particle velocity by an order of magnitude similar to the results in Figure 5.9, which predict a six-fold increase in the mean particle velocity matching more closely to experiment [5]. While these highlighted results are consistent with previous works, new results were introduced such as the consideration of the onset of collective motion as a function of time or the direct comparison of the effects of hydrodynamic interactions vs. collisions by
studying the effect of the dipole moment in Figure 5.11.

5.5 Conclusions

In this Chapter a simple model for studying correlation properties of mesoscopic collective motion in bacterial suspensions was introduced. Numerical simulations of this model demonstrate that both long-range hydrodynamic interactions and short-range collisions between bacteria are crucial to obtain agreement with experiment. Specifically, the simulations capture the qualitative effects on the correlation length and correlation time of a bacterial suspension as the main system parameters are varied: swimming speed, concentration, tumbling rate, and dipole moment. In addition, new results from simulations and experiments were presented on the time needed to establish collective motion.

Theoretical modeling also allows for results which are difficult to obtain experimentally. The model developed herein allows for the examination of the effect of particle shape/aspect ratio on the collective dynamics. The main result was that the collective state is independent on the concentration for $c > c_{cr}$ and the swimming speed. Therefore, the correlation length and time in the collective state are essentially controlled by the particle size and shape, as it was suggested by experiments [50, 53].

This work reveals the delicate balance between various physical mechanisms determining collective motion in the suspensions of bacteria, as well as a critical role of the geometrical confinement and dimension on its correlation properties. Our experiments and simulations suggest that the organization of collective motion in bacterial suspensions is governed by two competing mechanisms: short-range collisions and long-range hydrodynamic interactions. While collisions tend to increase the correlation length of collective motion, hydrodynamic interactions result in its decrease. This is demonstrated, for example, by Figure 5.11: the decrease of the hydrodynamic dipole strength in 3D results in a sharp increase of the correlation length. At the same time, in a quasi-2D suspension, the hydrodynamic interactions are screened due to effects of the confining walls and play a minor role on the correlation length. This observation is consistent with simulations in [53] where collective motion in two dimensions was studied essentially without long-range
hydrodynamic forces.

A pure hydrodynamic origin of the collective motion in bacterial suspension was suggested in a number of works [19, 61, 65, 67, 129]. These works demonstrated that the hydrodynamic interactions alone are sufficient to predict the instability of the isotropic state for suspensions of pushers and persistent turbulent-like behavior beyond the critical concentration. However, the resulting spatial scale of collective motion was determined essentially by the size of the integration domain. The model developed herein suggests that in suspensions studied in the experimental work [50] the main mechanism responsible for collective motion is in fact collisions, while the hydrodynamic interactions decrease the local order (e.g., correlation length). Also, in such suspensions the spatial scale of collective motion does not depend on the size of the domain. This implies that the collective states formed in systems described by pure hydrodynamic interactions, like in [19, 61, 65, 67, 129], may have a fundamentally different form of organization from that currently observed experimentally in [50].

While the model is computationally efficient and illuminates many interesting phenomena it does have some limitations. The simulations exhibit good qualitative agreement with experiment; however, the numerical value for the correlation length is 3-4 times smaller. The main reason for this discrepancy is the use of spherical particles (symmetric Lennard-Jones potential), with aspect ratio incorporated only in the parameter $B$. The use of true anisotropic particles is highly desirable, but ultimately leads to a drastic increase of the computation time. It was shown in experiment that hydrodynamic interactions and collisions are proportional to the swimming speed. In the model this remains mostly true, but some deviation is seen due to the third time scale that arises in relation to the collision time due to the use of a Lennard-Jones potential to model collisions. This time scale is only important at high swimming speeds, but did not inhibit the analysis of the qualitative effect of certain physical mechanisms on the properties of the collective dynamics of the system. By taking advantage of the minimal nature of the model and GPU architecture, computations can be done efficiently. For comparison in 2007, one could simulate a time step with 10,000 particles in 45 seconds [102]. Using the present full 3D model one time step can be simulated in .2 seconds and a time step with 100,000 bacteria takes 11.6 seconds.
Chapter 6

Conclusions and prospective

6.1 Overview

Throughout this dissertation the effect of interbacterial interactions (hydrodynamic and collisional) on the effective viscosity of the suspension as well as the properties of the collective state were investigated. A simple model was introduced, which led to computationally efficient numerical simulations using high-performance computing as well as being amenable to rigorous mathematical analysis. The analysis revealed the physical mechanisms responsible for both the striking decrease in viscosity as well as the size and duration of the collective state both previously observed numerically. In addition, the model allows for predictions of the effect of various system parameters which may be hard to control in experiment such as the strength of tumbling, the particle aspect ratio, and the dipole moment. In this Chapter a summary of the dissertation is provided as well as a prospective on the future of this direction of research.

6.1.1 Physical background

Self-organization in animal populations such as herding mammals, schooling fish, and flocking birds has been of significant recent interest. In particular, suspensions of self-propelled microscopic particles, such as swimming bacteria, exhibit collective motion leading to remarkable experimentally-observable macroscopic properties such as a dramatic decrease in viscosity or the formation of large scale structures.
The main idea behind all the work contained in this dissertation (consisting of three publications [75, 115, 36] and an ongoing project [130]) is introducing a mathematical model, which captures the experimental results on collective motion in bacterial suspensions while being amenable to mathematical analysis. Analysis of the model gives insight into the origins of collective motion. Specifically, this work provides a better understanding of what physical mechanisms or interactions at the microscopic level result in the aforementioned macroscopically observable properties of collective dynamics.

6.1.2 Semidilute model

To study the complex biological phenomenon of self-organization in active biological systems a first principles coupled differential equation (PDE/ODE) model is developed. The mathematical models throughout this work were motivated by experimental results concerning motile rod-like swimmers such as *Bacillus subtilis* or *E. coli*. The defining characteristics of each are a body and several flagella, which bundle to form a helical structure exerting a force, $f_p$, on the fluid. In turn this results in a drag force on the body of each bacterium. Hence, a bacterium is represented as a point force dipole where the propulsion force due to the flagella is balanced by the viscous drag force on the bacterium’s body. In addition, particle size is introduced through the use of a short-range repelling potential while the ellipsoidal shape of the body is preserved. The key feature of this model is that it accounts for two types of interactions: (i) pairwise hydrodynamic (bacterium with fluid) and (ii) excluded volume type (collisions).

The ability to harvest and control the power of bacterial motion is an important requirement for potential applications including the development of hybrid biomechanical energy conversion systems driven by microorganisms (bacteria turning gears) or the construction of bio-mimetic nano-swimmers harvesting the energy of solar light while swimming like bacteria. The work in this dissertation shows that the alignment of asymmetrical particles and the presence of self-propulsion change the effective rheological properties of the suspension and the theoretical model introduced provides a better understanding of the collective dynamics of a bacterial suspension.
6.1.3 Effective viscosity and self-induced noise

The portion of the work devoted to effective viscosity in Chapters 2-3 was motivated by the experiments performed by collaborators at Argonne National Laboratory [20], where a striking seven-fold decrease in viscosity was observed for suspensions of bacteria as compared to the ambient fluid. This is in contrast to passive suspensions where the viscosity greatly increases due to the dissipation caused by the presence of inclusions. In order to capture the experimental result, direct simulations of the model were performed first, which allowed for the computation of the effective viscosity as a longtime average of the instantaneous viscosity over many realizations. The simulations took advantage of novel GPU computer processors designed for computational efficiency through massive parallelization. The numerical results showed good qualitative agreement with experiment, while previous theoretical models were unable to capture the increasing portion beyond 2% volume fraction.

Next, the corresponding continuum (Liouville) equation governing the evolution of the particle distribution function, \( P(t, x, d) \), for bacterial positions and orientations is analyzed. Using this kinetic approach, an explicit asymptotic formula for the effective viscosity due to interactions in terms of known physical parameters is derived

\[
\eta_{\text{int}} \approx -\frac{16\pi^2 B^2 U_0^2 \rho^2 \varepsilon}{125\dot{\gamma}^2 R}, \quad \text{as } B \to 0
\]  

(6.1)

where \( B \) is the shape factor (0/1 corresponds to spheres/needles), \( U_0 \) is the dipole moment, \( \rho \) is the number density, \( \varepsilon \) is a parameter measuring the deviation from a uniform distribution, \( \dot{\gamma} \) is the strain rate, \( R := 1 + \left( \frac{16\pi^2 BU_0\rho\varepsilon}{25\dot{\gamma}} \right) \), and \( \eta_0 \) is the ambient fluid viscosity. This formula reveals the physical mechanisms responsible for the striking experimental observation on the effective viscosity. Namely, self-propulsion \( f_p \sim U_0 \neq 0 \), an elongated shape \( B \neq 0 \), and hydrodynamic interactions \( \varepsilon \neq 0 \) are required to observe the dramatic decrease. The process of making this derivation more rigorous as well as computing higher order terms is currently investigated in Chapter 3 and [130]. Finally, if one sets the strength of diffusion \( D := -\frac{8\pi^2 BU_0\rho\varepsilon}{75} > 0 \) in a dilute suspension (no interbacterial interactions) with tumbling (random reorientation), then the effective viscosity in the dilute case [59] is recovered. This phenomenon is referred to as self-induced noise and occurs when
randomness arises in a completely deterministic system (cf. Lorenz Attractor). The effective viscosity is determined by microscopic interactions highlighting the multiscale nature of this research.

6.1.4 Global solvability for particle trajectories

In the subsequent chapter, it was shown that the coupled PDE/ODE model introduced above in Chapters 2-3 and [75] admits unique solutions (particle trajectories) for all time given initially non-intersecting particles. A planar shear background flow is imposed on the suspension through the novel use of Lees-Edwards quasiperiodic boundary conditions applied to a representative volume [79]. These time-dependent quasiperiodic boundary conditions are one of the primary difficulties in establishing global solvability. The main result follows from first constructing the Green’s function for Stokes equation with Lees-Edwards boundary conditions and establishing the regularity of that solution. Then global solvability is proven using energy methods. As a consequence, the Liouville equation for the probability density used in Chapters 2-3 and [75] to derive the formula for the effective viscosity is well-defined.

6.1.5 Correlation properties of collective motion

The recent work in Chapter 5 involves understanding the nontrivial spatiotemporal correlations emerging in the course of collective swimming in suspensions of motile bacteria as the main system parameters are varied: swimming speed, concentration, tumbling rate, and dipole moment. Using direct particle simulations validated by a novel experiment, it is shown that the collective state is independent on the concentration for $c > c_{cr} \approx .3$ and the swimming speed even though increasing each increases the input of energy to the system, verifying [50]. Simulations of the theoretical model show qualitatively the same velocity and vorticity profile as experiment for different swim speeds. In addition to verifying the experimental observation of the collaborators at Argonne National Laboratory in [5, 50], this work moves beyond to study system parameters which may be difficult to control in experiment such as the particle aspect ratio as well as the decoupling of swimming speed and the tumbling rate of bacteria. The experiments and simu-
lations suggest that self-organization in bacterial suspensions is governed by two competing mechanisms: short-range collisions which tend to increase the correlation length of collective motion and long-range hydrodynamic interactions which decrease the local order. Thus, previous purely hydrodynamic models may exhibit fundamentally different collective structures than those observed in experiment [50] and simulation. This work exemplifies the delicate balance between various physical mechanisms governing collective motion in bacterial suspensions and provides important insights into its mesoscopic nature.

6.2 Prospective

This dissertation involved a lot of work on studying the effect of interactions on the effective properties and collective motion observed in bacterial suspensions, but some questions still remain. First, throughout this dissertation a simple model was employed where a bacterium was represented as a point force dipole. While this assumption led to great computational efficiency and easier mathematical analysis, the details of this unique swimming mechanism responsible for self-propulsion were lost. Currently, a study is underway investigating a model for a flagella as an elastic flexible rod. There is hope that even in the dilute case if a more detailed model for a flagellum is used then collective effects might be observed in the absence of tumbling (not possible in prior works on dilute suspensions [59, 71, 72, 74]). This is one promising direction which may provide even greater detail about the importance of the explicit swimming apparatus versus the current model that replaces this detail with a point force.

Next, in Chapters 2-3 the computation of the effective viscosity via a kinetic approach relied only on the orientation distribution $P_d(d)$. This was due to the fact that the concentrations was assumed to be small and the contribution due to stress from collisions was essentially zero. In reality this stress has an effect on the dynamics of the suspension as well as the effective viscosity and should be accounted for. This relies on proving rigorous results for the full kinetic model in both $x$ and $d$, which is a nonlinear, non-local PDE

$$\partial_t P(t, x, d) = -\nabla_x \cdot [\dot{x}(t)P(t, x, d)] - \nabla_d \cdot [\dot{d}(t)P(t, x, d)]$$

(6.2)
where the mean field approximation for the equations of motion is taken

\[
\dot{x}(t) = V_0 \mathbf{d} + \int_{V_L} \int_{S^2} [u(x - x', \mathbf{d}') + F(x - x')] P(t, x', \mathbf{d}') d\mathbf{d}' dx'
\]

\[
\dot{\mathbf{d}}(t) = -\mathbf{d} \times \int_{V_L} \int_{S^2} \omega(x - x', \mathbf{d}') P(t, x', \mathbf{d}') d\mathbf{d}' dx' - \mathbf{d} \times B \mathbf{d} \times \int_{V_L} \int_{S^2} \mathbf{E}(x - x', \mathbf{d}') dP(t, x', \mathbf{d}') d\mathbf{d}' dx'.
\]

The choice of the repulsion potential will be crucial. Currently, the truncated Lennard-Jones potential is insufficient since \( F \sim \frac{1}{|x - x'|^{12}} \) which produces a divergent integral in the mean field approximation. Therefore, before even moving further in this direction a refined model for collisions needs to be addressed. Possibly, one may consider a repulsive potential \( F \sim \frac{1}{r^{5/2}} \) so that it is integrable in the mean field approximation, yet still dominates hydrodynamic interactions \( (u \sim \frac{1}{r^2}) \) at short distances.

Finally, one of the most interesting outstanding questions are how these models can be used to study collective motion in higher life forms such as flocking birds, schooling fish, and herding mammals. Can the same principles be applied or are these models too simplistic for such complex animals? In any case, the models for bacteria introduced in this dissertation are building blocks for detailed studies of all active biosystems.
A

Appendix

Jeffery’s equation

A.1 Derivation of Jeffery’s equation

Jeffery’s equation is a classical model for the trajectory of the orientation vector for a prolate spheroid in a planar shear flow. In the absence of any interparticle interactions the trajectories of the orientation vectors on the unit sphere form so-called periodic Jeffery orbits. In order to derive the equations governing the evolution of the orientation vector, one first must consider the torque on a prolate spheroid with major axis $b$ and minor axis $a$ (this derivation is an expansion of that found in [109])

$$T_i = 8\pi \eta b^3 \left[ X^C d_i d_j + Y^C (\delta_{ij} - d_i d_j) \right] (\Omega_\infty^j - \omega_j) - 8\pi \eta b^3 Y^H \epsilon_{ijk} d_i d_k E_{jk}^\infty \quad (A.1)$$

where $\eta$ is the viscosity of suspending fluid, $d$ is the bacterium’s orientation unit vector, $\Omega_\infty$ and $E_\infty$ are respectively the vorticity and strain due to the background flow, $\omega$ is a bacterium’s angular velocity, $X^C, Y^C, Y^H$ are the following resistance functions

$$X^C = \frac{4e^3(1 - e^2)}{3 \left[ 2e - (1 - e^2)L \right]} \quad (A.2)$$

$$Y^C = \frac{4e^3(2 - e^2)}{3 \left[ -2e + (1 + e^2)L \right]} \quad (A.3)$$

$$Y^H = \frac{4e^5}{3 \left[ -2e + (1 + e^2)L \right]} \quad (A.4)$$
where \( e = \sqrt{\frac{b^2 - a^2}{b^2}} \) is the eccentricity and \( L = L(e) = \ln \left( \frac{1 + e}{1 - e} \right) \). Bacteria modeled as dipoles have no net force on them so they are also torque free \( T = \mathbf{r} \times F = \mathbf{r} \times 0 = 0 \). Thus,

\[
0 = T_i = 8\pi \eta b^3 \left[ X^C d_i d_j + Y^C (\delta_{ij} - d_i d_j) \right] (\Omega^\infty_j - \omega_j) - 8\pi \eta b^3 Y^H \epsilon_{ijkl} d_i d_k \mathbf{E}^\infty_{jk}. \quad (A.5)
\]

Take the dot product of \( (8\pi \eta b^3)^{-1} \left[ (X^C)^{-1} d_i d_j + (Y^C)^{-1} (\delta_{mi} - d_m d_i) \right] \) with both sides of \( (A.5) \) and note \( \mathbf{d} \cdot \mathbf{d} = \mathbf{d} \) (since \( \mathbf{d} \cdot \mathbf{d} = 1 \)) to find

\[
0 = \left\{ \mathbf{dd}^T + \frac{Y^C}{X^C} \mathbf{dd}^T - \frac{X^C}{Y^C} \mathbf{dd}^T + \frac{X^C}{Y^C} \mathbf{dd}^T + I_3 \right\} (\Omega^\infty_j - \omega_j) - \left[ (X^C)^{-1} d_i d_j + (Y^C)^{-1} (\delta_{mi} - d_m d_i) \right] Y^H \epsilon_{ijkl} d_i d_k \mathbf{E}^\infty_{jk} = (\Omega^\infty_m - \omega_m) - \left[ (X^C)^{-1} d_i d_j + (Y^C)^{-1} (\delta_{mi} - d_m d_i) \right] Y^H \epsilon_{ijkl} d_i d_k \mathbf{E}^\infty_{jk}.
\]

Next, solve for the angular velocity \( \omega \) (using tensor notation)

\[
\omega_m = \Omega^\infty_m - \left[ \frac{Y^H}{X^C} d_i d_j + \frac{Y^H}{Y^C} \delta_{mi} - \frac{Y^H}{Y^C} d_m d_i \right] \epsilon_{ijkl} d_i d_k \mathbf{E}^\infty_{jk}. \quad (A.6)
\]

Observe that the first and third terms vanish, since a symmetric tensor \( \mathbf{dd}^T \) is multiplied by an anti-symmetric tensor \( \epsilon_{ijkl} \). Thus,

\[
\omega_m = \Omega^\infty_m - \frac{Y^H}{Y^C} \delta_{mi} \epsilon_{ijkl} d_i d_k \mathbf{E}^\infty_{jk} = \Omega^\infty_m - \frac{Y^H}{Y^C} \epsilon_{mijkl} d_i d_k \mathbf{E}^\infty_{jk} \quad (A.7)
\]

and

\[
\frac{Y^H}{Y^C} = \frac{4}{3} e^5 \left( -2e + (1 + e^2) L \right)^{-1} = \frac{e^2}{2 - e^2} = \frac{b^2 - a^2}{b^2 + a^2} = B. \quad (A.8)
\]

Let \( A_j := d_k \mathbf{E}^\infty_{jk} \) and consider

\[
\epsilon_{mijkl} d_i A_j = (d_3 A_2 - d_2 A_3) \hat{i} + (-d_3 A_1 + d_1 A_3) \hat{j} + (d_2 A_1 - d_1 A_2) \hat{k} \quad (A.9)
\]
Therefore, the rotational motion of the particle is

\[
\omega \times x = \Omega^\infty \times x - B \left[ \begin{array}{c}
d_3 A_2 - d_2 A_3 \\
-d_3 A_1 + d_1 A_3 \\
d_2 A_1 - d_1 A_2 
\end{array} \right] \times x
\]

\[
= \Omega^\infty \times x - B \left[ \begin{array}{c}
d_1 A_3 x_3 + d_1 A_2 x_2 - d_3 A_1 x_3 - d_2 A_1 x_2 \\
d_2 A_1 x_1 + d_2 A_3 x_3 - d_1 A_1 x_1 - d_3 A_2 x_3 \\
d_3 A_2 x_2 + d_3 A_1 x_1 - d_2 A_3 x_2 - d_1 A_3 x_1 
\end{array} \right]
\]

\[
= \Omega^\infty \times x - B \left[ \begin{array}{c}
d_1 A_3 x_3 + d_1 A_2 x_2 + d_1 A_1 x_1 - d_3 A_1 x_3 - d_2 A_1 x_2 \\
d_2 A_1 x_1 + d_2 A_3 x_3 + d_2 A_2 x_2 - d_1 A_1 x_1 - d_3 A_2 x_3 \\
d_3 A_2 x_2 + d_3 A_1 x_1 + d_3 A_3 x_3 - d_2 A_3 x_2 - d_1 A_3 x_1 
\end{array} \right]
\]

Thus, the time evolution of a particle’s orientation, \(\dot{d}\), is obtained from (A.10) by replacing \(x\) with \(d\) and then the effect of background flow on a particle is given by Jeffery’s equation

\[
\dot{d} = \omega \times d = \Omega^\infty \times d + B \left[ E^\infty \cdot d - (E^\infty : dd^T) d \right].
\]
Appendix B

Dipolar stress

B.1 derivation of dipolar (deviatoric) stress $D_{jk}$

In the formula for stress, distinguish the contributions from particle self-propulsion and interparticle interactions. The stress tensor, $\Sigma_{l,m}$, is defined as

$$\Sigma_{l,m} := \sum_{i=1}^{N} \left( \frac{U_0}{V_L} \left( d_i^{(m)} d_i^{(l)} - \frac{\delta_{lm}}{3} \right) + \frac{r_i^{(m)} F_i^{(l)}}{V_L} \right)$$

where $U_0$ is the dipole moment, $V_L$ is the volume of the domain, $F$ is the Lennard-Jones force modeling collisions. The first term is due to the dipolar contribution [120], and the last term is due to the LJ forces between bacteria [110]. This formula captures the stress on the system due to point force dipoles. It is inaccurate to say the first term in the formula for stress is due to self-propulsion or interactions, it is purely stress due to the presence of dipoles. The interactions come into this formula indirectly, because they determine the bacterial orientations which then determine the stress due to the point force dipoles. The dipolar stress term comes from the first moment of the force density (second term in the multipole expansion) where $S_p$ is the surface of the particle. The information found in this appendix was expanded from the basic overview provided in [109].

B.1.1 Multipole expansion

Recall the Lorentz Reciprocal Theorem:
**Theorem B.1.1.** (Lorentz Reciprocal Theorem) Consider a closed region of fluid $V$ bounded by a surface $S$. Suppose that the velocity fields $v$ and $v'$ both satisfy Stokes equation. Denote the respective stress fields by $\sigma$ and $\sigma'$. Then

$$\oint_S v \cdot (\sigma' \cdot n) dS - \int_V v \cdot (\nabla \cdot \sigma') dV = \oint_S v' \cdot (\sigma \cdot n) dS - \int_V v' \cdot (\nabla \cdot \sigma) dV.$$  \hspace{1cm} (B.2)

Obtain the integral solution to Stokes equation for a particle undergoing rigid body motion (B.3) by setting $v' = G$ the Oseen tensor and $v$ to be a solution to the homogeneous Stokes equation. At distances $|x| \gg \xi$ (location of point force), the fluid cannot distinguish between a point force at location $\xi$ on the particle surface and a reference origin $0$ inside the particle, $G(x - \xi) \sim G(x)$, where $G$ is the velocity component of the fundamental solution to Stokes equation (Oseen tensor). Using the integral solution to Stokes equation for a particle undergoing rigid body motion one finds

$$v(x) = v^\infty(x) - \frac{1}{8\pi\eta} \int_{S_p} [\sigma(\xi) \cdot \hat{n}]G(x - \xi)dS(\xi) \approx v^\infty(x) - \frac{G(x)}{8\pi\eta} \int_{S_p} [\sigma(\xi) \cdot \hat{n}]dS(\xi)$$ \hspace{1cm} (B.3)

where $v^\infty(x)$ is the ambient fluid velocity, $\sigma(\xi) \cdot \hat{n}$ are the surface tractions or forces on the particle and $v(x) - v^\infty(x) = v^D(x)$ is the disturbance velocity due to a particle. With this approximation the disturbance velocity becomes

$$v^D(x) = -\frac{G(x)}{8\pi\eta} \int_{S_p} [\sigma(\xi) \cdot \hat{n}]dS(\xi) = -\frac{F}{8\pi\eta}$$  \hspace{1cm} (B.4)

which is the solution to Stokes equation for a point force at the origin in an infinite domain. One can make the approximation of the disturbance velocity due to a particle better by considering the Taylor expansion of $G(x - \xi)$ in $\xi$ about $\xi = 0$, which is the multipole expansion. For $|x| \gg |\xi|$ 

$$G_{ij}(x - \xi) = \sum_{n=0}^{\infty} \frac{1}{n!} (\xi \cdot \nabla \xi)^n G_{ij}(x - \xi)|_{\xi = 0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \xi_{k_1} \cdots \xi_{k_n} G_{ij,k_1 \cdots k_n}(x)$$ \hspace{1cm} (B.5)

Insert this into the integral representation for the velocity (B.3)

$$v_i(x) - v_i^\infty(x) = -\frac{1}{8\pi\eta} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{S_p} [(\sigma \cdot \hat{n})_j \xi_{k_1} \cdots \xi_{k_n}]dS(\xi) G_{ij,k_1 \cdots k_n}(x)$$ \hspace{1cm} (B.6)
\[ \frac{-F_j}{8\pi \eta} G_{ij}(x) + \frac{D_{jk}}{8\pi \eta} G_{ij,k}(x) + \ldots \]  

(B.7)

where \( F_j = \oint_{S_p} (\sigma \cdot \hat{n})_j dS(\xi) \) is the net force exerted by the fluid on the particle. This term is zero if the fluid and the particle exert a net force of zero on each other such as the case of the force dipole bacterium where the viscous drag force balances with the force of self-propulsion. \( D_{jk} = \oint_{S_p} (\sigma \cdot \hat{n})_j \xi_k dS(\xi) \) is the dipolar term in the multipole expansion.

### B.1.2 Dipolar stress

The dipolar stress comes from the dipolar term in the multipole expansion.

\[ D_{jk} = \oint_{S_p} (\sigma \cdot \hat{n})_j \xi_k dS(\xi). \]  

(B.8)

where \( \sigma \cdot \hat{n} \) are the tractions or surface forces. For a force dipole the two surface forces are \( \sigma(x) \cdot \hat{n} = F^p \delta(x^p - \xi) + F^d \delta(x^d - \xi) \). The dipolar term \( D_{jk} \) is a second-order tensor which can be decomposed into symmetric and anti-symmetric parts. By subtracting off the isotropic portion, the deviatoric stress is considered:

\[ D_{jk} - \frac{1}{3} D_{ii} \delta_{jk} = S_{jk} + R_{jk} \]  

(B.9)

The stresslet, symmetric dipole field \( S_{jk} \), is

\[ S_{jk} = \frac{1}{2} \oint_{S_p} (\sigma \cdot \hat{n})_j \xi_k + (\sigma \cdot \hat{n})_k \xi_j dS(\xi) - \oint_{S_p} \frac{1}{3} \sigma \cdot \hat{n} \cdot \xi dS(\delta_{jk}) \]  

(B.10)

\[ \sum_i \left[ \frac{1}{2} \left( F_j^{(i)} x_k^{(i)} + F_k^{(i)} x_j^{(i)} \right) - \frac{1}{3} F^{(i)} \cdot x^{(i)} \right] \]

where \( x^{(i)} \) is the location of the \( i \)th applied force and the sum over \( i = p, d \) for the force of self-propulsion \( F^p \) and the drag force \( F^d = -F_p \). The anti-symmetric term is the rotlet, \( R_{jk} \), or torque on the particle

\[ T_{jk} = \frac{1}{2} \oint_{S_p} (\sigma \cdot \hat{n})_j \xi_k - (\sigma \cdot \hat{n})_k \xi_j dS(\xi) = \frac{1}{2} \sum_i \left( F_j^{(i)} x_k^{(i)} - F_k^{(i)} x_j^{(i)} \right), \]  

(B.11)
which is zero for a dipole. This is due to the fact that the forces are directed along
the axis of symmetry there is no torque induced on the particle so $T_{jk} = 0$.

$$T_{jk} = \frac{1}{2}[F^p_j x^p_k - F^p_k x^p_j + F^d_j x^d_k - F^d_k x^d_j]$$ (B.12)

$$= \frac{1}{2}[F^p_j x^p_k - F^p_k x^p_j - F^p_j x^d_k + F^p_k x^d_j]$$ (B.13)

$$= \frac{1}{2}|F^p|d|d| - \frac{1}{2}|F^p|d|d| = 0$$ (B.14)

Note that $F^p = |F^p|d$ and $x^p - x^d = l|d|$. Keep the dipole moment fixed $U_0 = |F|l = \text{const}$, where $l$ is the distance between the locations of the dipole forces, as the particles are shrunk to a point where $|F|$ becomes large as $l \to 0$. Since $T_{jk} = 0$, consider only the stresslet, $S_{jk}$, with first term

$$\sum_i \frac{1}{2} \left( F^i_j x^i_k + F^i_k x^i_j \right) = \frac{1}{2} \left( |F^p|x^p + F^p x^p + F^d d^d + x^d F^d \right)$$

$$= \frac{1}{2} \left( |F^p|x^p + F^p x^p - F^p x^d - F^p x^d \right)$$

$$= \frac{1}{2} \left( |F^p|d + F^p |d| \right).$$

Note that $F^p = |F^p|d$. Thus

$$\sum_i \frac{1}{2} \left( F^i_j x^i_k + F^i_k x^i_j \right) = \frac{1}{2} \left( |F^p|d|dd + |F^p|d|dd \right) = U_0 d|d|.$$

Now consider the second term in (B.10)

$$\sum_i \frac{1}{3} (x^i \cdot F^i) = \frac{1}{3} (x^p \cdot F^p) - \frac{1}{3} (x^d \cdot F^d)$$

$$= \frac{1}{3} (l|d| \cdot |F^p|d) = -\frac{1}{3} l|F^p|d \cdot d = -\frac{1}{3} U_0 I.$$

Thus the dipolar contribution to the bulk deviotoric stress is

$$\Sigma^d (d) := D_{jk} - \frac{1}{3} D_{ii}\delta_{jk} = S_{jk} + T_{jk} = S_{jk} = U_0 \left( d_j d_k - \frac{1}{3} \delta_{jk} \right)$$ (B.15)
B.1.3 No change in flow: Deviatoric stress vs. total stress

Consider the following dipole $-F\delta(x - \frac{l}{2}d) - F\delta(x + \frac{l}{2}d)$, where $F = Fd$ and $Fl = -U_0$. This dipole produces the following flow:

$$u_t(x) = G\left(x - \frac{l}{2}d\right)F + G\left(x + \frac{l}{2}d\right)(-F),$$

(B.16)

where

$$G(y) = \frac{1}{8\pi\eta}\left(\frac{1}{|y|}I + \frac{1}{|y|^3}yy^T\right).$$

(B.17)

Recall $F = -\frac{U_0}{l}d$ and rewrite (B.16)

$$u_t(x) = \frac{U_0}{2} \left( G\left(x + \frac{l}{2}d\right) - G\left(x - \frac{l}{2}d\right) \right) d$$

(B.18)

$$= \frac{U_0}{2} \left( G\left(x + \frac{l}{2}d\right) - G(x) \right) d + \frac{U_0}{2} \left( G\left(x - \frac{l}{2}d\right) - G(x) \right) d. \quad \text{(B.19)}$$

Pass to the limit as $l \to 0$ to obtain

$$u_0(x) = U_0\nabla_d(G(x))d = U_0(d \cdot \nabla_x G(x))d = U_0dd^T \cdot G(x)$$

(B.20)

where $[dd^T\nabla G(x)]_i := d_j d_k G_{ij,k}(x)$.

From [109] using the deviatoric stress:

$$u_0^D(x) = \left[\frac{1}{2}(Fd^T + dF^T) - \frac{1}{3}(F \cdot d)I\right] \nabla G(x).$$

(B.21)

Here $F|d| = Fl = U_0$ and $Fd^T = Fldd^T = U_0dd^T$. Thus,

$$u_0^D(x) = U_0(dd^T \nabla G(x)) - \frac{1}{3}U_0(\nabla \cdot G(x)) = u_0(x)$$

(B.22)

since $\nabla \cdot G(x) = 0$. Thus the flows coincide whether considering deviatoric stress or total stress and the $\frac{1}{3}\delta_{jk}$ produces no contribution to the flow.
Appendix C

Principal value integral

C.1 Distributional derivatives and the principal value integral

The fluid velocity \( u \) can be rewritten in the following way

\[
 u(x, d) = U_0 d \cdot \nabla_x \left( \frac{d}{|x|} + \frac{(x, d)x}{|x|^3} \right) = U_0 \nabla_x \cdot \left( dd : \left( I \left| \frac{x}{|x|} \right| + \frac{x x}{|x|^3} \right) \right) \tag{C.1}
\]

where \( U_0 \) is a constant representing the dipole moment. Next, take an arbitrary test function \( \varphi \) such that \( \text{supp}(\varphi) \subset B_R(0) \).

\[
 < D_j u_i, \varphi > = - \int u_i \frac{\partial \varphi}{\partial x_j} \, dx = - \lim_{\varepsilon \to 0} \int_{\varepsilon < |x| < R} u_i \frac{\partial (\varphi(x) - \varphi(0))}{\partial x_j} \, dx
\]

\[
 = - \lim_{\varepsilon \to 0} \left\{ \int_{|x| = \varepsilon} u_i(\varphi(x) - \varphi(0)) n_j ds_x - \int_{|x| = R} u_i(\varphi(0)) n_j ds_x - \int_{\varepsilon < |x| < R} \frac{\partial u_i}{\partial x_j} (\varphi(x) - \varphi(0)) \, dx \right\} \tag{C.2}
\]

If \( |x| = \varepsilon \), then \( u_i \sim \varepsilon^{-2}, \varphi(x) - \varphi(0) \sim \varepsilon \) and \( |\{ |x| = \varepsilon \}| \sim \varepsilon^2 \). Thus, the first term in (C.2)

\[
 \lim_{\varepsilon \to 0} \int_{|x| = \varepsilon} u_i(\varphi(x) - \varphi(0)) n_j ds_x = 0. \tag{C.3}
\]

To investigate the second integral in (C.2) introduce the following notation

\[
 C_{ij} := \int_{|x| = R} u_i n_j ds_x = \begin{bmatrix} \xi := x/R, \\ R^2 ds_\xi = ds_x \\ R \nabla x = \nabla \xi \end{bmatrix} = \int_{|\xi| = 1} \nabla \xi \cdot \left( dd \left( \frac{I}{|\xi|} + \frac{\xi \xi}{|\xi|^3} \right) \right) n_j ds_\xi. \tag{C.4}
\]
Thus, from the change of variables we see that $C_{ij} = C_{ij}(d)$ does not depend on $R$ and one can write

$$\lim_{\varepsilon \to 0} \int_{|x|=R} u_i \varphi(0)n_j ds_x = C_{ij}(d)\varphi(0). \quad (C.5)$$

To analyze third term in (C.2), notice that if $|x| < R$, then $|\varphi(x) - \varphi(0)| < C|x|$ and therefore

$$\lim_{\varepsilon \to 0} \int_{\varepsilon < |x| < R} \frac{\partial u_i}{\partial x_j} (\varphi(x) - \varphi(0)) dx = \int_{|x| < R} \frac{\partial u_i}{\partial x_j} (\varphi(x) - \varphi(0)) dx. \quad (C.6)$$

Finally,

$$< D_j u_i, \varphi > = C_{ij}(d)\varphi(0) + \int \frac{\partial u_i}{\partial x_j} (\varphi(x) - \varphi(0)) dx, \quad (C.7)$$

which is integrable since the integrand in the second integral behaves as $\sim 1/|x|^2$. 
Appendix D

Contributions to the flow

D.1 Interaction with the background flow

In this appendix the terms due to interaction with the background flow in the kinetic theory are calculated

\[
\omega_{BG}(x, x', d) + E_{BG}(x, x', d) = \frac{\gamma}{2} (-d_y + Bd_x(1 - 2d_z^2), d_x + Bd_x(1 - 2d_z^2), -2Bd_xd_yd_z)
\]

where

\[
\omega_{BG}(x, x', d) := -\frac{1}{2} d \times [\nabla \times u^{BG}(x)]
\]

\[
E_{BG}(x, x', d) := -d \times [Bd \times D_x(u^{BG}(x))]
\]

with \(u^{BG}(x) = [0, \gamma x, 0]\) as defined in Chapter 3.1. Observe the following

\[
(\omega_{BG}(d) + E_{BG}(d)) \cdot d = 0,
\]

\[
(\omega_{BG}(d) + E_{BG}(d)) \cdot \hat{\alpha} = (1 + B \cos 2\alpha) \sin \beta,
\]

\[
(\omega_{BG}(d) + E_{BG}(d)) \cdot \hat{\beta} = \frac{1}{2} B \sin 2\alpha \sin 2\beta.
\]

Thus, using definition of the divergence on the unit sphere (3.13),

\[
\nabla_d \cdot [(\omega_{BG}(d) + E_{BG}(d))P_d(d)]
\]

\[
= \frac{\gamma}{2 \sin \beta} \left[ \partial_\alpha((1 + B \cos 2\alpha) \sin \beta P_d(d)) + \frac{B}{2} \partial_\beta(\sin \beta \sin 2\alpha \sin 2\beta P_d(d)) \right]
\]
\[
\frac{\gamma}{2} \left[ -2B \sin 2\alpha P_d(d) + (1 + B \cos 2\alpha) \partial_\alpha P_d(d) + B(\cos^2 \beta + \cos 2\beta) \sin 2\alpha P_d(d) \\
+ \frac{B}{2} \sin 2\alpha \sin 2\beta \partial_\beta P_d(d) \right]
= \frac{\gamma}{2} \left[ -3B \sin^2 \beta \sin 2\alpha P_d(d) + (1 + B \cos 2\alpha) \partial_\alpha P_d(d) + \frac{B}{2} \sin 2\alpha \sin 2\beta \partial_\beta P_d(d) \right].
\]

\section*{D.2 Form of kinetic terms involving the rate of strain}

Compute the general form of all integral terms involving the rate of strain where \(A\) is some function of \(E\)

\[
\nabla_d \cdot [d \times d \times A d] = \nabla_d \cdot [d(d, A d) - A d]
= \tilde{\nabla}_d \cdot [d(d, A d) - A d] - \frac{\partial}{\partial |d|} \left\{ |d| \left[ |d|^2 (d, A d) - (d, A d) \right] \right\} = I + J
\]

where

\[
I = 3(d, A d) + d \cdot \tilde{\nabla}(d, A d) - \text{Tr}(A)
J = -\frac{\partial}{\partial |d|} \left\{ |d|^5 (\hat{d}, \hat{A} d) - |d|^3 (\hat{d}, \hat{A} d) \right\}_{|d|=1} = (-5 + 3)(d, A d) = -2(d, A d).
\]

Here \(\hat{d} = d/|d|\). In addition,

\[
\tilde{\nabla}(d, A d) = \frac{\partial}{\partial d_k} \left( \sum_{i,j} A_{ij} d_i d_j \right) = \sum_{i,j} A_{ij} (\delta_{ik} d_j + \delta_{jk} d_i) = \sum_j A_{kj} d_j + \sum_i A_{ik} d_i = 2 A d
\]

\[
d \cdot \tilde{\nabla}(d, A d) = 2(d, A d), \quad \tilde{\nabla}_d \cdot A d = \sum_i \frac{\partial}{\partial d_i} \sum_j A_{ij} d_j = \sum_i A_{ii}.
\]

Therefore, conclude that

\[
\nabla_d \cdot [d \times d \times A d] = 3(d, A d) - \text{Tr}A.
\]
Furthermore, \((\mathbf{d}, \mathbf{A} \mathbf{d}) = A(d_x^2 - d_y^2) + 2Cd_xd_y\) for constants \(A, C\) if
\[
\mathbf{A} = \begin{bmatrix}
A & C & 0 \\
C & -A & 0 \\
0 & 0 & 0
\end{bmatrix}
\]
and it is seen that for the problem considered in Chapter 3,
\[
(\mathbf{d}, \mathbf{A} \mathbf{d}) = A \sin^2 \beta \cos(2\alpha) + C \sin^2 \beta \sin(2\alpha).
\]

### D.3 Explicit form of integral term involving the rate of strain at \(O(B^2)\)

The first integral in (3.42) at \(O(B^2)\) can be written as:
\[
\frac{1}{4\pi N|V_L|} \nabla \mathbf{d} \cdot \int_{S^2} \langle \mathbf{F}[\mathbf{E}]\mathbf{F}[\mathbf{P}]^2 \rangle_k \mathbf{P}_d^{(1)}(\mathbf{d}')d\mathbf{d}' = \\
\frac{1}{4\pi N|V_L|} \nabla \mathbf{d} \cdot \left[ \mathbf{d} \times \mathbf{d} \times \left\{ \int -\frac{1}{2\eta|\mathbf{k}|^4} (|\mathbf{k}|^2 \mathcal{F} \mathbf{k}^* - 2\mathbf{k}^* \mathcal{F} \mathbf{k}^* + |\mathbf{k}|^2 \mathbf{k}^* \mathcal{F}) \mathbf{F}[\mathbf{P}]^2 d\mathbf{k} \right\} \cdot \mathbf{d} \right].
\]

Let each term involving \(\mathbf{k}\) be defined as
\[
\mathcal{F} := \left[ \int_{S^2} \check{\Sigma} \mathbf{P}_d^{(1)}(\mathbf{d}')d\mathbf{d}' \right] = -\frac{3U_0}{8\pi} \begin{bmatrix}
\frac{8\pi}{15} & 0 & 0 \\
0 & -\frac{8\pi}{15} & 0 \\
0 & 0 & 0
\end{bmatrix} = -\frac{U_0}{5} \begin{bmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 0
\end{bmatrix}.
\]

Thus, (letting \(\mathbf{k}\) be a unit vector since this expression is independent of \(|\mathbf{k}|\)):
\[
\frac{U_0}{40\pi \eta N|V_L|} \nabla \mathbf{d} \cdot \left[ \mathbf{d} \times \mathbf{d} \times \left\{ \int \left( \begin{bmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 0
\end{bmatrix} \mathbf{k}^* \\
\mathbf{k}^* - 2\mathbf{k}^* \mathbf{k}^* + \mathbf{k}^* \mathbf{k}^* \mathcal{F} \mathbf{F}[\mathbf{P}]^2 d\mathbf{k} \right\} \cdot \mathbf{d} \right].
\]
where

\[
L := \begin{bmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 0
\end{bmatrix}
\quad \text{and} \quad
\mathbf{kk}' = \begin{bmatrix}
k_1^2 & k_1k_2 & k_1k_3 \\
-k_1k_2 & -k_2^2 & -k_2k_3 \\
0 & 0 & 0
\end{bmatrix}.
\]

\[
M := -2 \begin{bmatrix}
k_1^2 & k_1k_2 & k_1k_3 \\
k_1k_2 & k_2^2 & k_2k_3 \\
k_1k_3 & k_2k_3 & k_3^2
\end{bmatrix}
\quad \text{and} \quad
L = -2 \begin{bmatrix}
k_1^4 - k_1^2k_2^2 & k_1^2k_2 - k_1k_3^2 & k_1^2k_3 - k_1k_2k_3 \\
k_1^2k_2 - k_1k_3^2 & k_2^4 - k_2^2k_3^2 & k_2^2k_3 - k_2k_1k_3 \\
k_1^2k_3 - k_1k_2k_3 & k_2^2k_3 - k_2k_1k_3 & k_3^4 - k_3^2k_1^2
\end{bmatrix}.
\]

\[
N := \begin{bmatrix}
k_1^2 & k_1k_2 & k_1k_3 \\
k_1k_2 & k_2^2 & k_2k_3 \\
k_1k_3 & k_2k_3 & k_3^2
\end{bmatrix}
\quad \text{and} \quad
L = -2 \begin{bmatrix}
k_1^2 & -k_1k_2 & 0 \\
k_1k_2 & -k_2^2 & 0 \\
k_1k_3 & -k_2k_3 & 0
\end{bmatrix} = L^T.
\]

Thus,

\[
L + M + N = \begin{bmatrix}
2k_1^2 - 2k_1^2 + 2k_1k_2k_3 & -2k_1k_2 + 2k_1k_3^2 & k_1k_2 - 2k_1k_3k_3 + 2k_1k_2k_3 \\
-2k_1^2k_2 + 2k_1k_2^2 & -2k_1k_2^2 + 2k_1k_3^2 & -k_1k_2 - 2k_1k_2k_3 + 2k_1k_3k_3 \\
k_1k_3 - 2k_1k_3k_3 + 2k_1k_2k_3 & -k_2k_3 - 2k_1k_2k_3 + 2k_1k_3k_3 & -2k_1k_2k_3^2 + 2k_2k_3^2
\end{bmatrix}.
\]

Let \(k_3 = 0\) (in real coordinates motion is constant in \(z\)-direction). Then

\[
L + M + N = \begin{bmatrix}
2k_1^2[1 - k_1^2 + k_2^2] & -2k_1k_2[1 - k_2^2 - k_3^2] & 0 \\
-2k_1k_2[1 - k_2^2 - k_3^2] & -2k_2^2[1 + k_1^2 - k_3^2] & 0 \\
0 & 0 & 0
\end{bmatrix}
\]

\[
= \begin{bmatrix}
4k_1^2k_2^2 & -2k_1k_2[1 - k_2^2 - k_3^2] & 0 \\
-2k_1k_2[1 - k_2^2 - k_3^2] & -4k_2^2k_3^2 & 0 \\
0 & 0 & 0
\end{bmatrix}
\]

\[
= \begin{bmatrix}
sin^2(2\theta) & -\frac{1}{2}\sin(4\theta) & 0 \\
-\frac{1}{2}\sin(4\theta) & -\sin^2(2\theta) & 0 \\
0 & 0 & 0
\end{bmatrix}
\]

where the Fourier space variables are expressed in polar coordinates \(k_1 = \cos(\theta)\) and \(k_2 = \sin(\theta)\). Thus, the first integral in (3.42) becomes

\[
\frac{U_0}{40\pi\eta N|V_L|} \nabla d \cdot \left[ \mathbf{d} \times \mathbf{d} \times \int \begin{bmatrix}
\sin^2(2\theta) & -\frac{1}{2}\sin(4\theta) & 0 \\
-\frac{1}{2}\sin(4\theta) & -\sin^2(2\theta) & 0 \\
0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
d_x \\
d_y \\
d_z
\end{bmatrix} P_\mathbf{r}^2(|\mathbf{k}|, \theta)|\mathbf{k}|^2 d|\mathbf{k}|d\theta \right]. \quad (D.4)
\]
D.4 Explicit form of integral term involving the vorticity at $O(B^2)$

The last integral in (3.42) at $O(B^2)$ is investigated

$$\frac{\nabla_d [P_d^4(d)]}{N|V_L|} \int_{S^2} P_d^4(d') \langle F[\omega](F[P])^2 \rangle_k d'd',$$

which will be determined after finding $F[\omega]$. Compute

$$F[\omega] = -\frac{1}{2} \mathbf{d} \times [-i\mathbf{k} \times \hat{u}] = -\frac{1}{2} \mathbf{d} \times \left[ -i\mathbf{k} \times \frac{iU_0}{\eta|\mathbf{k}|} \left( I - \frac{\mathbf{k} \mathbf{k}^*}{|\mathbf{k}|^2} \right) \nabla \mathbf{k} \right]$$

$$= -\frac{\mathbf{d}}{2\eta} \times \left[ \hat{\mathbf{k}} \times U_0 \left( I - \hat{\mathbf{k}} \hat{\mathbf{k}}^* \right) (d'd' - I/3)\hat{\mathbf{k}} \right].$$

Here denote $\hat{\mathbf{k}} := \mathbf{k}/|\mathbf{k}|$ and since this quantity is independent of $|\mathbf{k}|$, then one can assume $\mathbf{k}$ is a unit vector. After integration with respect to $d'$ of $F[\omega]P_d^4(d)$:

$$\int_{S^2} F[\omega]P_d^4(d) d'd' = \frac{U_0}{10\eta} \mathbf{d} \times \left\{ \mathbf{k} \times \left[ \begin{array}{ccc} 1 - k_1^2 & -k_1 k_2 & -k_1 k_3 \\ -k_2 k_1 & 1 - k_2^2 & -k_2 k_3 \\ -k_3 k_1 & -k_2 k_3 & 1 - k_3^2 \end{array} \right] \begin{bmatrix} k_1 \\ k_2 \\ k_3 \end{bmatrix} \right\}$$

$$= \frac{U_0}{10\eta} \mathbf{d} \times \left\{ \mathbf{k} \times \left[ \begin{array}{ccc} 1 - k_1^2 & k_1 k_2 & 0 \\ -k_2 k_1 & k_2^2 - 1 & 0 \\ -k_3 k_1 & k_2 k_3 & 0 \end{array} \right] \begin{bmatrix} k_1 \\ k_2 \\ k_3 \end{bmatrix} \right\}$$

$$= \frac{U_0}{10\eta} \mathbf{d} \times \left\{ \mathbf{k} \times \left[ \begin{array}{c} k_1 - k_3^2 + k_3 k_2^2 \\ -k_2 k_1^2 + k_3^2 - k_2 \\ -k_3 k_1^2 + k_2^2 - k_3 \\ -2k_1 k_2 \end{array} \right] \right\}$$

$$= \frac{U_0}{10\eta} \mathbf{d} \times \left[ \begin{array}{c} k_2 k_3 \\ k_1 k_3 \\ k_1 k_2 \end{array} \right].$$

Now equate $k_3 = 0$

$$\int_{S^2} F[\omega]P_d^4(d) d'd' = \frac{U_0}{10\eta} \mathbf{d} \times \left[ \begin{array}{c} 0 \\ 0 \\ -2k_1 k_2 \end{array} \right] = \frac{2U_0}{10\eta} k_1 k_2 \begin{bmatrix} -d_y \\ d_x \\ 0 \end{bmatrix} = \frac{2U_0}{10\eta} k_1 k_2 \begin{bmatrix} -\sin \alpha \sin \beta \\ \cos \alpha \sin \beta \\ 0 \end{bmatrix}. $$
Recall $P^1(d) = -\frac{3}{8\pi} \sin^2 \beta \cos(2\alpha)$ and note that

$$\nabla_d P = \begin{bmatrix}
-\sin(\alpha) \partial_\alpha P + \cos(\alpha) \cos(\beta) \partial_\beta P \\
\cos(\alpha) \partial_\alpha + \sin(\alpha) \cos(\beta) \partial_\beta P \\
-\sin(\beta) \partial_\beta P
\end{bmatrix}.$$ 

Thus,

$$\nabla_d P^1(d) = -\frac{3}{8\pi} \begin{bmatrix}
-\sin(\alpha) \left(-2 \sin^2 \beta \sin(2\alpha)\right) + \cos \alpha \cos \beta (2 \sin \beta \cos \beta \cos(2\alpha)) \\
\cos(\alpha) \left(-2 \sin(2\alpha) \sin^2 \beta\right) + \sin \alpha \cos \beta (2 \sin \beta \cos \beta \cos(2\alpha)) \\
-\sin(\beta) (2 \sin \beta \cos \beta \cos(2\alpha))
\end{bmatrix}$$

$$= -\frac{3}{8\pi} \begin{bmatrix}
2 \sin \alpha \sin(2\alpha) \sin \beta + 2 \cos \alpha \cos(2\alpha) \sin \beta \cos^2 \beta \\
-2 \cos \alpha \sin(2\alpha) \sin \beta + 2 \sin \alpha \cos(2\alpha) \sin \beta \cos^2 \beta \\
-2 \sin^2 \beta \cos \beta \cos(2\alpha)
\end{bmatrix}.$$ 

and one concludes that

$$\nabla_d P^1(d) \int_{S^2} F[\omega] P^1(d)d'd = -\frac{3}{8\pi} \frac{2U_0}{10\eta} k_1 k_2 \left(-2 \sin^2 \alpha \sin(2\alpha) - 2 \cos^2 \alpha \sin(2\alpha)\right) \sin^2 \beta$$

$$= \frac{3U_0}{20\pi \eta} k_1 k_2 \sin(2\alpha) \sin^2 \beta.$$
Generalized law of large numbers

E.1 Generalized law of large numbers

The idea for a Law of Large numbers, which only requires random variables to be identically distributed and not independent, was first studied by Poznyak in [116]. Given the probability space \((\Omega, F, \mu)\) and a centered quadratic-integrable \(\mathbb{R}^n\)-valued random process \(\{\xi_i\}\), introduce the spatial characteristic “double-averaged” correlation function \(R_n\) defined by

\[
R_n := \frac{1}{n^2} \sum_{t=1}^{n} \sum_{s=1}^{n} \rho_{t,s} = \mathbb{E}[S_n^T S_n]
\]

where \(S_n = \sum_{i=1}^{n} \xi_i\) and \(\rho_{s,t}\) is the corresponding correlation function.

**Theorem E.1.1.** (GLLN) Let \(\xi_i\) be identically distributed random variables. If

\[
\sum_{n \in \mathbb{N}} \left[ \frac{\sigma_n}{n} \sqrt{R_{n-1}} + \frac{1}{n^2} \sigma_n^2 \right] < \infty
\]

then “the strong law of large numbers” holds, (i.e., \(\frac{1}{n} \sum_{i=1}^{n} \xi_i \to \mathbb{E}[\xi_i] \text{ a.s.}\)).

In other words

\[
\frac{1}{N} \sum_{i=1}^{N} \xi_i = \int_{V_L} \int_{S^2} \xi_i(x, d) P(x, d) dx dd + \tilde{\xi}(x, d, P)
\]
where $\tilde{\xi}$ is the error in the approximation referred to as the *fluctuations*. For this dissertation, the fluctuations were neglected and the integral portion is taken as the *mean-field approximation*. 
Quasi-2D flow

F.1 Mathematical consequences of $P_x(x)$ being independent of $z$

Consider the case of a spatial density, which is constant in $z$ (quasi-2D flow) so that $P_x(x, y, z) = \phi(z)P_{12}(x, y)$. From the total measure of the spatial density one finds that

$$N = \int P(x, y, z)dxdydz = \left(\int p_0dx\right)^3 = L^3P_0^3$$

where the constant $P_0 = \frac{N^{1/3}}{L}$. Next, consider

$$\varphi(k_3) = \int_{-L}^{L} P_0e^{-k_3x}dx = P_0\int_{-L}^{L} [\cos(k_3x) + i\sin(k_3x)]dx = -P_0\frac{2\sin(k_3L)}{k_3}.$$ 

This does not weakly converge to $\delta(k_3)$ as $L \to \infty$, but $\frac{\varphi(k_3)}{\pi L} \to \delta(k_3)$. Recall the term involving $A$ or $A_{new}$ in the final formula for the effective viscosity in Chapter 3

$$\frac{1}{4\pi N^2|V_L|} \mathcal{D} \int_{\mathbb{R}^3} P_0^2 \left(-\frac{2\sin(k_3L)}{k_3}\right)^2 \mathcal{C}\left(\frac{k}{|k|}\right) (F_{2D}[P_{12}(x, y)]) dk_1dk_2dk_3,$$
where $\mathcal{D}$ is an operator appearing at $O(B)$ and defined in Chapter 3. Using Maple one concludes that

$$
\int_{\mathbb{R}} \left( \frac{\sin(k_3L)}{k_3} \right)^2 dk_3 \sim \pi L
$$

$$
\lim_{L \to \infty} \frac{1}{\pi L} \int_{-\infty}^{\infty} f(k_3) \left( \frac{\sin(k_3L)}{k_3} \right)^2 dk_3 \to f(0).
$$

Now one must prove these observations.

**Proposition F.1.1.** For $f(k_3) \in L^1(\mathbb{R})$

$$
\lim_{L \to \infty} \frac{1}{\pi L} \int_{-\infty}^{\infty} f(k_3) \left( \frac{\sin(k_3L)}{k_3} \right)^2 dk_3 \to f(0).
$$

In addition,

$$
\lim_{L \to \infty} \frac{1}{\pi L} \int_{-\infty}^{\infty} \left[ \frac{\sin(k_3L)}{k_3} \right]^2 dk_3 \to 1.
$$

**Proof.** First without loss of generality let $f(k_3) \in C^1(\mathbb{R})$ and $f(0) = 0$. This implies that

$$
|f(k_3)| \leq C|k_3|, \quad \text{for } |k_3| \leq 1.
$$

Thus, noting that $\sin^2(k_3L) \leq 1$

$$
\left| \frac{1}{\pi L} \int_{-\infty}^{\infty} f(k_3) \left[ \frac{\sin(k_3L)}{k_3} \right]^2 dk_3 \right| \leq \left| \frac{1}{\pi L} \int_{|k_3| > \frac{1}{L^{1/3}}} f(k_3) \frac{1}{L^{1/3}} dk_3 \right| + C \int_{|k_3| < \frac{1}{L^{1/3}}} \frac{\sin^2(k_3L)}{Lk_3} dk_3
\leq \frac{L^{2/3}}{\pi L} \|f\|_{L^1} + C \frac{2}{\pi L^{1/3}} \overset{L \to \infty}{\longrightarrow} 0
$$

Now for the second part of the proposition

$$
\frac{1}{\pi L} \int_{-\infty}^{\infty} \left[ \frac{\sin(k_3L)}{k_3} \right]^2 dk_3 = \left[ \frac{t = k_3L}{dt} = dk_3 \right] = \frac{1}{\pi L} \int_{-\infty}^{\infty} \left[ \frac{\sin(t)}{t} \right]^2 \cdot L^2 dt \frac{L}{L}
= \frac{1}{\pi} \int_{-\infty}^{\infty} \left[ \frac{\sin(t)}{t} \right]^2 < \infty.
$$
It is easy to see that the integrand
\[
\left( \frac{\sin(t)}{t} \right)^2 \leq \begin{cases} 1, & |t| < 1 \\ \frac{1}{t^2}, & |t| \geq 1 \end{cases}.
\]

It was checked numerically that the integral is indeed 1. By the density of $C^1$ functions in $L^1$ the result follows.

So the term containing $A$ defined in (D.4) of the form
\[
\frac{1}{4\pi N|V_L|} (P_0)^2 \cdot \pi L \cdot \left( \frac{1}{\pi L} \mathcal{D} \int_{-\infty}^{\infty} \left( \frac{2\sin(k_3 L)}{k_3} \right)^2 \left\{ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} C \left( \frac{k}{|k|} \right) (F_{2D}[P_{12}])^2 dk_1 dk_2 \right\} dk_3 \right)
\]
\approx \frac{1}{N^{2/3}L^3} \mathcal{D} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} C \left( \frac{k}{|k|} \right) \bigg|_{k_3=0} \cdot (F_{2D}[P_{12}])^2 dk_1 dk_2.
\]

where $\mathcal{D}$ is a linear differential operator (e.g., $\mathcal{D} = \nabla_d [d \times d \times (\cdot) d]$) and $C$ is a function of the Fourier variable $k$. 
Periodicity of the constructed solution to Stokes equation

G.1 Periodicity of $\bar{u}_{i,k}(x)$

Periodicity for a series of translates, $\bar{u}_{i,k}$, can be established as follows. If a smooth function decays at infinity as $\phi(x) = O\left(\frac{1}{|x|^3}\right)$, then

$$\psi(x) = \sum_{z \in \mathbb{Z}} \left[ \phi(x + z) - \phi(z) \right]$$

converges absolutely and uniformly, since the terms in the series decay as $O\left(\frac{1}{|x|^4}\right)$. Then, for any $k \in \mathbb{Z}^3$ one can rearrange the two series in $\psi(x + k) - \psi(x)$ and resum over expanding balls $|z| < K$ of radius $K$ (cf. [125]):

$$\psi(x + k) - \psi(x) = \lim_{K \to \infty} \sum_{|z| < K} \left[ \phi(x + k + z) - \phi(x + z) \right].$$

For sufficiently large $K$ most terms within the above sum cancel, except those in the thin “boundary” shell defined by the symmetric difference

$$A_K := \{ z \in \mathbb{Z} : |z - k| < K \} \triangle \{ z \in \mathbb{Z} : |z| < K \}.$$

The sum of these, however, decays rapidly. Indeed, let $B_K := \{ z : K - \frac{|k|}{2} < |z - \frac{k}{2}| < K + \frac{|k|}{2} \}$ be an annular region covering $A_K$ as illustrated in Fig. G.1, and
thus the number of points in each of the sets satisfy $|A_k| \leq |B_k| \leq CK^2$, where $C > 0$ is a constant. Thus, the following estimate is established

$$|\psi(x + k) - \psi(x)| \leq \lim_{K \to \infty} \sum_{z \in B_k} \frac{C'}{|K - |k||^4} \leq \lim_{K \to \infty} \frac{C''}{|K - |k||^4} K^2 \to 0,$$

where $C'$ and $C''$ are some positive constants. Therefore, $\psi(x + k) - \psi(x) = 0$ and the periodicity of $\psi$ follows.

\textbf{Figure G.1.} Schematic illustration of the multicolored annular region $B_K$ (red) covering the symmetric difference $A_K$ (green).

\section*{G.2 Proof of technical lemma used in Theorem 4.4.6}

\textbf{Lemma G.2.1.} For $\Pi_{ij}$, $\bar{u}(x)$, and $\Box$ defined in Section 4.4.3 the following relation holds

$$\Pi_{ij}\Box = \int_{\partial\Box} \bar{u}_i(x)\nu_j d^2x. \quad (G.1)$$

\textbf{Proof.} Let $\Gamma^s_-, \Gamma^s_+$ denote the opposing faces of $\Box$ in the $s$ direction (normal to $e_s$) and let $\nu$ denote the unit normal. First, establish the following equality:

$$\int_{\partial\Box} \bar{u}_i(x)\nu_j d^2x = \sum_{s=1}^3 \int_{\Gamma^s_+} \Pi_{is}\nu_j d^2x. \quad (G.2)$$
Let \( y = x + e_s \), under this change of variables \( \Gamma_- \rightarrow \Gamma_+ \) and \( \nu \rightarrow -\nu \). Thus,

\[
\int_{\Gamma_+} \bar{u}_i(x) \nu_j d^2x + \int_{\Gamma_-} \bar{u}_i(x) \nu_j d^2x = \int_{\Gamma_+} \bar{u}_i(x) \nu_j d^2x - \int_{\Gamma_-} \bar{u}_i(y - e_s) \nu_j d^2y = \int_{\Gamma_+} \Pi_{is} \nu_j d^2x.
\]

By summing over all faces \( s = 1, 2, 3 \) (G.2) is established.

Rewrite the right-hand side of (G.2),

\[
\sum_{s=1}^{3} \int_{\Gamma_s} \Pi_{is} \nu_j d^2x = \sum_{k, s, p=1}^{3} \left[ \int_{\Gamma_p} \Pi_{is} e_k^s x_k \nu_j d^2x - \int_{\Gamma_p} \Pi_{is} e_k^s (x - e_p)_k \nu_j d^2x \right]. \quad \text{(G.3)}
\]

Using the above change of variables and the Divergence Theorem, (G.3) gives

\[
\sum_{s=1}^{3} \int_{\Gamma_s} \Pi_{is} \nu_j d^2x = \sum_{k, s=1}^{3} \int_{\partial \Box} \Pi_{is} e_k^s x_k \nu_j d^2x = \int \Box \Pi_{is} e_j^3 d^3x = \Pi_{ij} |\Box|.
\]

The result is proven. \( \square \)
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