Correlations and fluctuations of stress and velocity in suspensions of swimming microorganisms

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Active systems, which are driven out of equilibrium, can produce long range correlations and large fluctuations that are not restricted by the fluctuation-dissipation theorem. We consider here the fluctuations and correlations in suspensions of swimming microorganisms that interact hydrodynamically. Modeling the organisms as force dipoles in Stokes flow and considering run-and-tumble and rotational diffusion models of their orientational dynamics allow derivation of closed form results for the stress fluctuations in the long-wave limit. Both of these models lead to Lorentzian distributions, in agreement with some experimental data. These fluctuations are not restricted by the fluctuation-dissipation theorem, as is explicitly verified by comparing the fluctuations with the viscosity of the suspension. In addition to the stress fluctuations in the suspension, we examine correlations between the organisms. Because of the hydrodynamic interactions, the velocities of two organisms are correlated even if the positions and orientations are uncorrelated. We develop a theory of the velocity correlations in this limit and compare with the results of computer simulations. We also formally include orientational correlations in the theory; and comparing with simulations, we are able to show that these are important even in the dilute limit and are responsible in large part for the velocity correlations. While the orientation correlations cannot as yet be predicted from this theory, by inserting the results from simulations into the theory it is possible to properly determine the form of the swimmer velocity correlations. These correlations of orientations are also the key to understanding the spatial correlations of the fluid velocity. Through simulations we show that the orientational correlations decay as $r^{-2}$ with distance—inserting this dependence into the theory leads to a logarithmic dependence of the velocity fluctuations on the size of the system. © 2011 American Institute of Physics.

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I. INTRODUCTION

Many biological systems exhibit fluctuations driven by active, nonequilibrium processes, and these fluctuations lead in turn to enhanced transport of chemical species within the system. Examples of such systems exist at many levels. For example, Spakowitz and coworkers have tracked the motion of chromosomal loci in E. coli.$^1$ The time-evolution of mean-squared displacement (MSD) follows the same (sub-diffusive) power law scaling in live and fixed cells, but the magnitude is a factor of ten or more larger in the live cells. A related phenomenon arises in solutions of DNA containing RNA polymerase. In the presence of ribonucleoside triphosphates (NTPs, which are RNA monomers), transcription occurs, as RNA polymerase moves along the DNA backbone catalyzing the formation of RNA. Schwartz and coworkers$^2$ have shown that the diffusivity of DNA is larger in the presence of NTPs than in their absence, implying that the motion of the RNA polymerase along the DNA during transcription (which cannot occur in the absence of NTPs) leads to enhanced fluctuations of the DNA. For the particular case studied, the DNA molecules were 310 bp long and the diffusivity was enhanced by about 25%. Finally, we describe the case that most directly motivates the present work: the enhanced diffusion of solutes in suspensions of swimming microorganisms. Wu and Libchaber$^3$ observed motions of 4 $\mu$m and 10 $\mu$m diameter fluorescent polystyrene spheres in a suspension of E. coli confined to a soap film. Note that in this case the tracer particles are substantially larger than the bacteria themselves. At short time, transport of these tracers is anomalous with the MSD scaling approximated as $t^{1.75}$, but at longer time it becomes diffusive, with an effective long-time diffusivity scaling linearly with bacterial concentration and reaching values two or more orders of magnitude larger than the Brownian diffusivity of the tracers. The authors suggested that this enhanced transport could be considered to be the result of an effective temperature associated with the fluctuations induced by the bacterial motions, and that this effective temperature could be much larger than the thermodynamic temperature in the system.

Since the work of Wu and Libchaber, many other studies have addressed the issue of enhanced transport in suspension of swimming microorganisms. Kim and Breuer$^4$ examined the diffusion of dye tracers (i.e., particles much smaller than the bacteria) in suspensions of E. coli in
microfluidic devices, finding an enhanced diffusion that scales linearly with concentration, and at high concentration a transition to slightly superdiffusive behavior. The linear scaling in the dilute regime agrees with theoretical predictions of Underhill et al.\textsuperscript{6} and Thiffeault and Childress.\textsuperscript{7} Arguments similar to those presented in these works lead to the prediction that the rotational diffusivity of the swimmers themselves should also scale linearly with concentration,\textsuperscript{6,8,9} leading to a prediction that translational diffusivity of smooth swimming organisms should scale inversely with swimmer concentration. This scaling has not yet been observed experimentally but is seen in the simulation results of a number of groups.\textsuperscript{6,8,9} (For organisms that execute a run-and-tumble motion, like wild-type \textit{E. coli}, the translational diffusivity of the swimmers is independent of concentration to leading order.) Dombrowski et al.\textsuperscript{10} performed experiments with suspensions of \textit{B. subtilis}, observing fluid motions on large scale compared to the bacteria themselves. Based on these results, they proposed that these large scale motions played a significant role in enhancing transport in bacterial suspension and that hydrodynamic interactions between the bacteria were responsible for these motions (we return to this point shortly). Related experimental observations are found in a more recent study by Sokolov et al.\textsuperscript{11} In very recent experiments, Leptos et al.\textsuperscript{12} studied tracer transport in suspensions of the algae Chlamydomonas, again finding that the diffusivity of tracers increases roughly linearly with swimmer concentration.

The issue of transport in suspensions of active particles is directly connected to spatial and temporal correlations in these systems. Lau et al.\textsuperscript{13} reported two-point micro rheology measurements from which they extracted the spectrum of stress fluctuations in mammalian cells. They found an $\omega^{-2}$ dependence of the spectrum on frequency $\omega$ and also found that the magnitude of the fluctuations was much larger than the thermal spectrum. This result for the stress spectrum is somewhat analogous to the result described above for intracellular diffusion reported by Spakowitz and coworkers,\textsuperscript{3} as enhanced fluctuations are the driving force for enhanced transport. Chen et al.\textsuperscript{14} applied a similar approach to the fluctuations in a dilute \textit{E. coli} suspension (volume fractions of 0.3\% or smaller). For a mutant bacterial strain that persistently tumbles, they found that one and two-point mean-squared displacements for tracer particles were both superdiffusive at short time and linear with time at longer time (as expected for diffusive behavior), and inferred from these results a stress spectrum that is nearly Lorentzian (though a high frequency power law is difficult to quantify). For wild-type \textit{E. coli}, which execute run-and-tumble swimming behavior, the results were quite different. Although the one-point results were the same as for tumbler, the two point mean-squared displacements displayed superdiffusive behavior over the entire time range, and the stress spectrum inferred from these displacements scales as $\omega^{-1/2}$. At low frequencies the stress fluctuations were substantially larger than purely thermal fluctuations, while the fluid viscosity was essentially unchanged from that in the absence of the bacteria, indicating that for this active system there is not a fluctuation-dissipation theorem that ties the fluctuations to the viscosity.

In passive systems, it has been shown that the comparison of one and two point micro rheology can be used to detect structural inhomogeneities at the scale of a probe particle. Therefore the results of Lau et al.\textsuperscript{13} suggest that any structures or inhomogeneities in the tumbler are at a scale smaller than the particle sizes (approximately 2 $\mu$m), while the structures for the wild type are between 2 $\mu$m and 10 $\mu$m. Motivated in part by this experimental result, Lau et al.\textsuperscript{15} present a phenomenological mean field model that assumes that the orientational correlations of the swimmers follow the same dynamics as that of molecules of a nematic liquid crystal, and that also predicts an $\omega^{-1/2}$ dependence of the stress fluctuation spectrum. If this phenomenological approach is correct, its correspondence with experiments implies that even very dilute suspensions of active particles can display long-range orientational order. Aranson et al.\textsuperscript{16} presented a different continuum model built around the idea that orientational correlations in suspensions of swimmers arise through inelastic collisions of the swimmers. This model, applied to thin films, predicts a transition with increasing concentration to a state where the correlation length for (fluid) velocity fluctuations is much larger than the swimmer size.

Liao et al.\textsuperscript{17} also examined a dilute suspension of swimming \textit{E. coli}, measuring experimentally the pair velocity correlations of the swimming bacteria. They developed a theory based on two isolated bacteria interacting hydrodynamically and compared the predictions with the experiments. They found experimentally that the transverse and longitudinal correlations between organisms decayed approximately as $r^{-3}$ where $r$ is the separation of the organisms. Their theory predicted that quadrupole interactions led to the same rate of decay of correlations, $r^{-3}$. The pre-factor to the decay in the theory is related to the quadrupole moment of the swimmer, and depends on the swimming speed and forces exerted on the fluid due to the swimming. Predictions for \textit{E. coli} led to predictions for factor of 6 smaller than the experiments. This comparison was taken as evidence that the theory was correct (that quadrupole interactions were responsible for the correlations). It was speculated that the difference by a factor of 6 was due to the difficulty in estimating the quadrupole moment. We revisit this issue below with computer simulations and a theory that relaxes some of the assumptions of Liao et al. The quadrupole interactions are not the dominant effect in the simulations, suggesting that an incorrect quadrupole moment is not responsible for the factor of 6 difference. The simulated correlations are dominated by the orientational correlations between organisms, which were not measured experimentally or included in the theory of Liao et al.\textsuperscript{17}

A number of direct simulations of suspensions of swimmers in Stokes flow have also addressed the issue of fluctuations and correlations. Underhill et al.\textsuperscript{6} used a regularized dipole model for each swimmer that allowed for simulations of more than 70,000 swimmers in a triply periodic unbounded domain, finding dramatically enhanced transport and long-ranged tracer velocity correlations in suspensions of smooth-swimming “pushers”—organisms pushed from...
The present work describes analysis of the fluctuations and correlations in a suspension of active particles in a viscous Newtonian fluid. The active particles are modeled in most of the work as point force dipoles and inertia of the fluid will be ignored so the fluid phase will obey the Stokes equation, as driven by these dipoles. Beyond these modeling ansatzes, the focus will be on results that can be obtained from first principles rather than through phenomenological or mean-field approaches. Section II describes the stress field associated with the suspension of dipoles and shows that in the case of a dilute suspension of independently swimming run-and-tumble organisms, the stress autocorrelation function in the long-wave limit can be found exactly. Section III using the stress autocorrelation function to define one measure of an effective temperature of an active suspension. By comparing these fluctuations in stress with the suspension viscosity in Sec. IV, we can show explicitly that the fluctuation-dissipation theorem does not hold. In Sec. V, we examine the correlation of the velocities of swimming organisms that occur in dilute suspensions. We relax assumptions made in previous work and compare the theory with results from computer simulations. The results show the importance of orientational correlations of organisms even in the dilute limit. Finally, in Sec. VI, we examine how these orientational correlations of swimmers lead to enhanced fluid velocity spatial correlations.

II. STRESS FLUCTUATIONS AND CORRELATIONS IN A SUSPENSION OF POINT DIPOLE SWIMMERS

As an organism swims through the fluid, both the body and propulsion mechanism (e.g., flagella) exert forces on the fluid. These forces are equal in magnitude and opposite in direction because a neutrally buoyant and free-swimming organism exerts no net force on the fluid. The simplest model to capture this requirement is a suspension of point force dipoles: each organism is a dipole with a scalar dipole moment of \( d = -pf \ell \), where \( f \) is the magnitude of the forces, \( \ell \) is the separation of the forces, and \( p \) denotes the type of swimming mechanism. (The point dipole limit considers \( \ell \to 0 \) with \( d \) held constant.) An organism that is pushed from behind has \( p = 1 \), while one that is pulled from the front has \( p = -1 \). The extra stress due to swimming in a suspension of \( N \) swimmers in a three-dimensional periodic domain is

\[
\sigma(x, t) = \frac{N}{V} \sum_{x_1=1}^{N} d \left( n_x(t)n_x(t) - \frac{1}{3} \delta \right) \delta(x - x_2(t)), \tag{1}
\]

where \( n_x \) is the orientation vector of swimmer \( x \) and we have subtracted the isotropic part of the tensor. Note that we use a bold \( \delta \) as the identity tensor and a non-bold \( \delta \) as the Dirac delta function. Because the \( N \) swimmers are in a finite periodic system with volume \( V \), we perform a Fourier transform from the spatial coordinate into a discrete \( k \)-space giving

\[
\sigma(k, t) = \frac{1}{V} \sum_{x=1}^{N} d \left( n_x(t)n_x(t) - \frac{1}{3} \delta \right) \exp(-i\mathbf{k} \cdot \mathbf{x}_x(t)). \tag{2}
\]

Since two-point micro rheology measures the large-scale correlations in the system, we can then take the limit \( k \to 0 \)

\[
\sigma(k = 0, t) = \frac{1}{V} \sum_{x=1}^{N} d \left( n_x(t)n_x(t) - \frac{1}{3} \delta \right). \tag{3}
\]

Specifically we are interested in the temporal autocorrelation of this long-wave stress, which is

\[
S_{ijkl}(k = 0, t) = \lim_{V \to \infty} V \langle \sigma_{ij}(k = 0, t')\sigma_{kl}(k = 0, t' + t) \rangle, \tag{4}
\]

where the angle brackets denote an ensemble average. Inserting the expression for stress, this expression becomes

\[
S_{ijkl}(t) = \lim_{V \to \infty} \frac{d^2}{V} \left( N \langle \left( n_{i,1}(t')n_{j,1}(t') - \frac{1}{3} \delta_{ij} \right) \times \left( n_{k,1}(t' + t)n_{l,1}(t' + t) - \frac{1}{3} \delta_{kl} \right) \rangle + N(N-1)\langle \left( n_{i,1}(t')n_{j,1}(t') - \frac{1}{3} \delta_{ij} \right) \times \left( n_{k,2}(t' + t)n_{l,2}(t' + t) - \frac{1}{3} \delta_{kl} \right) \rangle \right), \tag{5}
\]

where \( n_{i,1} \) is the \( i \)th component of the orientation of swimmer 1. Note that we have taken advantage of the fact that all swimmers are equivalent. Therefore, we have written explicitly the first term for swimmer 1, while the second term for swimmers 1 and 2. We will only consider here the leading order behavior in concentration in which correlations between the same swimmer contribute. This contribution is

\[
S_{ijkl}(t) = \frac{Nd^2}{V} \left( \left( n_{i}(t')n_{j}(t') - \frac{1}{3} \delta_{ij} \right) \times \left( n_{k}(t' + t)n_{l}(t' + t) - \frac{1}{3} \delta_{kl} \right) \right), \tag{6}
\]

where we have dropped the label for which swimmer we are talking about because all swimmers have identical statistics. We see explicitly that the stress correlation is proportional to the concentration expressed as a number per unit volume. Note that this leading contribution depends on how the orientation of a swimmer is correlated to the orientation of the same swimmer at a later time, and therefore only depends implicitly on correlations between swimmers or any type of collective behavior. We can further simplify the correlations if we assume isotropy in the orientation distribution of the swimmers at any given time. In this case, the stress correlation is
\[ S_{ijkl}(t) = \frac{Nd^2}{15V} \left( \delta_i \delta_j + \delta_i \delta_k - \frac{2}{3} \delta_i \delta_l \right) \exp \left( -6D_r |t| \right). \] (7)

We consider two models here for how the orientation of a swimmer changes in time. The first assumes that the orientation vector undergoes Brownian diffusion with rotational diffusivity \( D_r \). The stress correlation for this model will be denoted by a superscript \( B \). In this case,

\[ \langle (n(t') \cdot n(t' + t))^2 \rangle = \frac{1}{3} + \frac{2}{3} \exp(-6D_r|t|). \] (9)

The stress autocorrelation is thus

\[ S^B_{ijkl}(t) = \frac{Nd^2}{15V} \left( \delta_i \delta_j + \delta_i \delta_k - \frac{2}{3} \delta_i \delta_l \right) \exp \left( -6D_r |t| \right). \] (10)

The other model assumes a run-and-tumble type behavior; the orientation remains unchanged during a run and changes instantaneously at a tumble to an uncorrelated direction. The length of time in a run is a random variable with distribution \( p(t) \) where \( p(t) \) is the probability that the swimmer is still in a run after time \( t \). The stress correlation for this model will be denoted by a superscript \( RT \). In this case,

\[ S^{RT}_{ijkl}(t) = \frac{Nd^2}{15V} \left( \delta_i \delta_j + \delta_i \delta_k - \frac{2}{3} \delta_i \delta_l \right) p(|t|). \] (11)

If we take this process to be a Poisson process, which is typically the first approximation,\(^{21}\) then \( p(|t|) = \exp(-|t|/\tau_{run}) \), where \( \tau_{run} \) is the mean run-time. It is interesting that even though the different models consider different mechanisms for the change of the orientation with time, the stress correlations have the same form. In real run-and-tumble dynamics, the dynamics we assume here are not exactly correct; the runs are not perfectly straight, the tumbling are not instantaneous, and the orientation after a tumble is not perfectly uncorrelated with the previous run direction. We expect these changes would mainly alter the short time behavior but the long time behavior would remain an exponential decay.

To get the frequency dependence, we Fourier transform time into frequency and obtain

\[ S^B_{ijkl}(\omega) = \frac{Nd^2}{15V} \left( \delta_i \delta_j + \delta_i \delta_k - \frac{2}{3} \delta_i \delta_l \right) \left( \frac{12D_r}{36D_r^2 + \omega^2} \right). \] (12)

\[ S^{RT}_{ijkl}(\omega) = \frac{Nd^2}{15V} \left( \delta_i \delta_j + \delta_i \delta_k - \frac{2}{3} \delta_i \delta_l \right) \left( \frac{2\tau_{run}}{1 + 2\tau_{run}\omega^2} \right). \] (13)

The stress frequency spectrum \( \Delta(\omega) \), which is related to the two-point microrheology response,\(^{13,14}\) is the scalar part of the correlation, which for the two models are

\[ \Delta^B(\omega) = \frac{Nd^2}{15V} \left( \frac{12D_r}{36D_r^2 + \omega^2} \right). \] (14)

\[ \Delta^{RT}(\omega) = \frac{Nd^2}{15V} \left( \frac{2\tau_{run}}{1 + 3\tau_{run}\omega^2} \right). \] (15)

For both models, the stress frequency spectrum takes a Lorentzian form. At small frequencies, the spectrum becomes independent of frequency. At large frequencies, the spectrum decays as \( \omega^{-2} \). The frequency at the transition between the two regimes occurs at the characteristic frequency for a swimmer to change its orientation. The other key aspects to notice are the proportionality to concentration and the dependence on \( d^2 \), which means the stress spectrum in the dilute limit is the same for pushers and pullers.

The Lorentzian nature of the stress fluctuations found here is similar to that observed experimentally by Lau et al.\(^{13}\) as determined from the motion of endogenous refractive particles (presumed to be lipid granules and mitochondria) within cells. It is also at least qualitatively consistent with the results of Chen et al.\(^{14}\) for fluctuations in suspension of a persistently tumbling mutant of E. coli—they found a stress spectrum that looks Lorentzian with a crossover time of about 0.1 s. However, for wild-type bacteria which perform a run-and-tumble motion, they found a spectrum behaving as \( \omega^{-1/2} \), in disagreement with the results above. Nevertheless, the stress frequency spectrum is proportional to concentration, consistent with our results. This means that the bacteria act approximately independently of one another, and that the spectrum, and power-law exponent, is determined solely by the dynamics of how a single bacterium changes its orientation. We analyzed two examples of such dynamics here, the so-called Brownian and run-and-tumble cases. However, it is possible that wild-type bacteria do not follow these simplified dynamics. In particular, it has been shown that the wild-type run-and-tumble behavior may not be Poisson distributed\(^{22,23}\) but have a run-time distribution with truncated power law tails. If the cumulative distribution decays as \( p(t) \propto t^{-2} \) for large times before being cut off at even larger times, then \( \Delta(\omega) \) will behave as \( \omega^{\nu-1} \) for small frequencies.

Finally, let us mention how the two model cases described can be used to represent interacting organisms. Consider model organisms that, in absence of interactions, would swim in a straight line forever. This is represented by our Brownian model with \( D_r \rightarrow 0 \) or with our run-and-tumble model with \( \tau_{run} \rightarrow \infty \). In both cases, the Lorentzian becomes a delta-function,

\[ \Delta(\omega) \rightarrow \frac{Nd^2}{15V} (2\pi) \delta(\omega). \] (16)

However, at any finite concentration, the interactions between swimmers lead to a nonzero value of \( D_r \) or a non-infinite value of \( \tau_{run} \). The scaling arguments of Underhill and Graham\(^6\) indicate that \( \tau_{run} \sim (N_{sw} \bar{d}^2 / V)^{-1} \) or equivalently, \( D_r \sim N_{sw} \bar{d}^2 / V \). These scalings have been confirmed by simulations\(^{6,9,20}\) and can be inserted into the above results to provide a self-consistent mean field prediction for the dynamics of smooth-swimming organisms.
III. EFFECTIVE TEMPERATURE OF AN ACTIVE SUSPENSION

In a simple fluid, the fluctuation-dissipation theorem relates the thermal stress fluctuations $\sigma_{ij}^T$ in the fluid to the temperature and fluid viscosity. In Fourier space, this relation is given by

$$S_{ijkl}(k, \omega) = 2k_B T \eta \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right).$$  \tag{17}

A natural question for a suspension of active particles is whether a similar or at least analogous result holds. A related question is whether an “effective temperature” can be defined for an active suspension. We will consider this second question first.

From the above analysis, we have some information about the random stress associated with the motions of the active particles. In general, the active particles introduce a stress spectrum with a different frequency and wavevector dependence than the thermal spectrum. However, we attempt to match them in the long wave, low frequency limit, for which the active particle stress spectrum is

$$S_{ijkl}(0, 0) = \frac{2c d^2 \tau_{run}}{15} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right).$$  \tag{18}

Here $\tau_{run}$ is replaced by $6D^{-1} c$ if we are considering rotationally diffusing rather than run-and-tumble swimmers. The corresponding expression for the thermally driven stresses is

$$S_{ijkl}(0, 0) = 2k_B T \eta \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right).$$  \tag{19}

We can put the first of these expressions in the same form as the second by defining an effective temperature; in the long wave, low frequency limit this becomes

$$T_{eff}(k = 0, \omega = 0) = \frac{cd^2 \tau_{run}}{15k_B \eta}. $$  \tag{20}

The value of this expression can be estimated from, for example, the data of Wu and Libchaber.\textsuperscript{3} For their results, $c \approx 1 \cdot 10^{16} \text{m}^{-3}$, $1 \cdot 10^{-3} \text{Pa s}$. The dipole strength $d$ can be estimated as $6\pi \eta R$ times the swimming speed $v_s$. We will take $l = 6 \mu\text{m}$, $R = 1.5 \mu\text{m}$, and use the value $20 \mu\text{m/s}$ reported by Wu and Libchaber for $v_s$. They also reported a run time $\tau_{run} \approx 1 \text{s}$. With these numbers we estimate that $T_{eff} \approx 5.6 \cdot 10^5 K$, or $T_{eff}/T = 1850$.

Wu and Libchaber also report effective diffusivities of tracer particles that are large (10 $\mu\text{m}$) compared to the bacteria in their suspension. If we take the fluctuations that drive this effective diffusion to be the long-wave, low frequency fluctuations driven by the swimmers, then we can estimate the effective diffusivity as

$$D_{eff} \approx \frac{k_B T_{eff}(k = 0, \omega = 0)}{\zeta} = \frac{D_{eff}(k = 0, \omega = 0)}{T},$$  \tag{21}

where $D$ is the molecular diffusivity. Using the above estimate for $T_{eff}$ yields that $D_{eff} \approx 1850D$, in reasonable agreement with the experimental result $D_{eff} \approx 8 \cdot 10^2 D$ reported on Wu and Libchaber’s Fig. 2.

This development appears to become problematic when considering smooth-swimming organisms, for which $\tau_s$ is formally infinite, and by Eq. (20), so is $T_{eff}$. In reality, two phenomena will make $\tau_{run}$ finite. The first is conventional (Brownian) rotational diffusion and the second is the effective diffusion associated with hydrodynamic fluctuations generated by other swimmers at finite concentration. Even in the absence of thermal fluctuations, this effect leads to a finite rotational diffusivity (inverse run time) $D_{SS}^{-1} \sim \tau_{run}^{-1}$ that scales as $c^2 v_s$, as mentioned at the end of Sec. II.

To conclude this discussion, we note that a different effective temperature can be defined, based directly on this scaling relation and the Stokes-Einstein expression for rotational diffusivity of a swimmer, $D_S^{-1} \approx k_B T/\eta g$. Equating $D_{SS}^{-1}$ to $D_S^{-1}$ and noting that $d \approx \eta v_s$, this yields that

$$T_{SS} \approx \frac{c d^2}{k_B \eta v_s}.$$  \tag{22}

This has the same form as Eq. (20), but with $\tau_{run}$ replaced by $l/v_s$, which is simply the time it takes for a swimmer to move its own length. This estimate of $T_{SS}$ is thus expected to be appropriate for phenomena on the scale of a swimmer—e.g., for the effective temperature felt by the swimmers themselves.

IV. VISCOSITY OF A DILUTE ACTIVE SUSPENSION

Having in hand an expression for effective temperature, a natural question is whether this temperature is related to the viscosity of the active suspension in a way that provides a generalized fluctuation-dissipation theorem. The simple model used here allows the issue to be addressed analytically. We will compute here the zero-shear viscosity $\eta_0$ of a suspension of independent point dipole swimmers. Related analyses have been made for viscosity, but not effective temperature, by other groups for different swimmer models.\textsuperscript{19,24,25}

The viscosity of a suspension is composed of the solvent contribution $\eta$ plus the contribution $\eta_s$ due to the suspended particles. In the dilute limit, the particles are noninteracting and their individual stresses are summed to yield the total stress in the fluid. In general, $\eta_s$ can be computed from the shear stress $\sigma_{yx}$ induced by an imposed shear flow $v_\infty = \dot{\gamma} e_x$, where $\dot{\gamma}$ is the imposed shear rate, as follows:

$$\eta_s = \sigma_{yx}/\dot{\gamma}. $$  \tag{23}

For rigid orientable particles, we can write a general expression for the shear stress as

$$\sigma_{yx} = c \int_0^{2\pi} \int_0^{\pi} D_{yx}(\phi) f(\theta, \phi) \sin \theta \, d\theta d\phi,$$  \tag{24}

where $D_{yx}$ is the $yx$ component of the force dipole tensor for the particle and $f(\theta, \phi)$ is the orientation distribution function for the orientation vector $\mathbf{n}$ of the particles.\textsuperscript{26} We further
note that the stress dipole, and accordingly the viscosity, has two components: one that is due to the self-propulsion of the particles and one that would be present even if the particle were not self-propelled (i.e., dead). To determine the latter, one must make an assumption about the structure of the particles. Here we will take the particles to be bead-rod dumbbells with center-to-center distance between the beads $l$ and bead friction coefficient $\zeta$. For this model, the rotational distribution function is known analytically for small shear rates,

$$f(\theta, \phi) = \frac{1}{4\pi} \left( 1 + D_r^{-1}\frac{1}{2}(1 - \cos^2 \theta) \sin 2\phi \right) + O\left((D_r^{-1}\frac{1}{2})^2\right),$$

(25)

In the classical case of a (passive) Brownian rigid dumbbell, $D_r = 2k_B T/\zeta^2$. The passive contribution $\eta_{SP}$ to the zero-shear viscosity is well-known $^{26}$ and is given by

$$\eta_{SP} = \frac{ck_BT}{6D_r}.$$  

(26)

The active contribution to the zero-shear viscosity, $\eta_{SA}$, is determined by noting that the active contribution to $D_r$, is simply $dn_n = d\sin^2\theta \sin \phi \cos \phi$. Inserting this expression along with Eq. (25) into Eq. (24) and evaluating the resulting integral gives

$$\eta_{SA} = \frac{cd}{30D_r},$$

(27)

yielding a total swimmer contribution to the viscosity as

$$\eta_S = \frac{c}{6D_r} \left( k_BT + \frac{d}{5} \right).$$

(28)

Note that the active contribution to the viscosity is negative when $d < 0$, a reflection of the fact that in this case a shear flow leads to a shear stress that enhances the original shear flow perturbation. This result is consistent with past theoretical expressions$^{19,24,25}$ as well as with experimental measurements of viscosity in active suspensions.$^{27,28}$ It is also the origin of the long-wave instability of a mean field model of a homogeneous isotropic suspension of pushers$^{6,18,19}$ that is thought to underlie, at least in part, the large scale fluid motions observed in these systems. Since the long-wave effective temperature is quadratic in $d$, and the active contribution to effective viscosity linear in it, we clearly see, consistent with Chen et al.$^{14}$ that there can be no general nonequilibrium fluctuation-dissipation relation for an active particle suspension.

V. VELOCITY CORRELATIONS BETWEEN SWIMMERS

The present section turns to the velocity correlations between a pair of swimmers in a suspension. In isolation, we consider that a swimmer moves at a constant speed $v_{is}$ in the direction of its axis $\mathbf{n}$. The swimming velocity vector would only change due to a change in the orientation, for example from Brownian motion or run-and-tumble like mechanisms. In a suspension containing other swimmers, however, each swimmer is affected by the motion generated by the other swimmers as they move through the fluid, as well as by direct collisions with other swimmers. We do not address here the effects of an externally imposed flow. These interactions lead to correlations between the velocities of two different swimmers, which we will address by considering the pair correlation function of swimmer velocities,

$$C_s(r) = \frac{\langle v_1 v_2 \delta(x_2 - x_1 - r) \rangle}{\delta(x_2 - x_1 - r)},$$

(29)

where $v_j$ is the velocity of swimmer $j$, $x_j$ is the position of swimmer $j$, the angle brackets represent an average over possible positions and orientations of all swimmers, and the delta function restricts the space to have two swimmers separated by a vector $r$. The denominator is the probability of having two swimmers at a separation $r$, making the correlation a conditional average. At large distances, we expect the velocities of the swimmers to be uncorrelated. If the system is isotropic, $\langle v_1 \rangle = 0$ and $\langle v_2 \rangle = 0$. Thus at large distances, the swimmer velocity correlation approaches zero. At short distances, we expect correlations between the velocities, and therefore a deviation of the velocity correlation from zero.

Neglecting collisions, as is appropriate for dilute solution, we approximate the velocity of a swimmer by the isolated velocity, directed along the axis of the swimmer, plus the fluid velocity $\mathbf{u}$ at the position of the swimmer,

$$v_j = v_{is} \mathbf{n}_j + u(x_j).$$

(30)

This fluid velocity is a sum of the disturbance velocities due to all other swimmers,

$$\mathbf{u}(x_j) \equiv \sum_{m=1, m \neq j}^{N} \mathbf{u}_m(x_j),$$

(31)

where we use the notation that $\mathbf{u}$ is the total fluid velocity at a point while $\mathbf{u}_m$ is the disturbance velocity due to a single organism. Writing out the product of two swimmer velocities yields four terms,

$$v_1 v_2 = v_{is}^2 \mathbf{n}_1 \mathbf{n}_2 + \mathbf{u}(x_1) \mathbf{u}(x_2) + v_{is} \mathbf{n}_1 \mathbf{u}(x_2) + v_{is} \mathbf{u}(x_1) \mathbf{n}_2.$$

(32)

The first term is the direct orientational correlation. The second term is the correlation between the fluid velocities. The third and fourth terms are the correlation between the orientation of one swimmer and the fluid velocity at the other swimmer. If there are spatial and orientational correlations between the swimmers, all of these terms remain. However, let us examine the simplified case for which the there are no spatial or orientational correlations between the swimmers. In this case, the first term, the direct orientational term, vanishes and the other terms simplify significantly.

Consider the second term, which contains the product of the fluid velocities. Each velocity is a sum over disturbances so the product of velocities is a double sum. Assuming that different swimmers are not correlated, we obtain
\[
\langle u(x_1)u(x_2) \delta(x_2 - x_1 - r) \rangle = (N - 2) \langle u_2^2(x_1)u_2^2(x_2) \delta(x_2 - x_1 - r) \rangle.
\] (33)

When \( N \gg 2 \), this is just the correlation due to a single swimmer times the number of swimmers. Because we have assumed a uniform spatial and orientational distribution, this is exactly the same as the pair correlation of fluid velocities \( C_f(r) \), which is given by

\[
C_f(r) = \left\langle \frac{1}{V} \int u(x)u(x + r)dx \right\rangle.
\] (34)

In the dilute limit, this is given by \(^6\)

\[
C_f(r) = \frac{d^2N}{120\pi \eta^2 r} (\delta + \hat{r}r).
\] (35)

A more general expression for this correlation, valid at finite concentration, is given later in the article. Therefore, we find that the fluid-fluid part of the swimmer velocity correlation is

\[
\langle u(x_1)u(x_2) \delta(x_2 - x_1 - r) \rangle \quad \text{is} \quad \langle \delta(x_2 - x_1 - r) \rangle = C_f(r) = \frac{d^2c}{120\pi \eta^2 r} (\delta + \hat{r}r).
\] (36)

Important aspects of this term to note are that it is proportional to concentration and decays with distance, as \( r^{-1} \). The final two terms of the velocity correlation, which correlate a fluid velocity with an orientation vector, simplify in the case of independently distributed swimmers to become

\[
\langle u_nu_2 \delta(x_2 - x_1 - r) \rangle = \langle u_nu_2 \delta(x_2 - x_1 - r) \rangle,
\]

(37)

\[
\langle u_nu_2 \delta(x_2 - x_1 - r) \rangle = \langle u_nu_2 \delta(x_2 - x_1 - r) \rangle.
\] (38)

We will see that these two terms are independent of concentration and decay faster than \( r^{-1} \) and are equivalent to the terms considered in the analysis of Liao et al. \(^3\) who only addressed the problem of two swimmers in an infinite domain.

These terms can be simplified by a multipole expansion of the disturbance velocity. The forces exerted by an isolated swimmer on the fluid will be taken to be on the swimmer axis and parallel to it. This simplification will be true for a large class of self-propelled particles that are slender bodies. For this type of model, the multipole expansion becomes

\[
u_2^2(s) = d n_2 : V_r \Omega(s - r_2) \cdot n_2 + q n_2 n_2 : V_r V_r \Omega(s - r_2) \cdot n_2 + \cdots.
\] (39)

Here

\[
\Omega(r) = \frac{1}{8\pi \eta r} (\delta + \hat{r}r)
\] (40)

is the Oseen tensor (Green’s function for Stokes flow driven by a point force). This expression represents the fluid velocity disturbance produced by swimmer 2 evaluated at position \( s \) and depends on the moments of the force distribution including the dipole moment \( d \) and quadrupole moment \( q \). These are defined by

\[
d = -\int \xi f d\xi,
\] (41)

\[
q = \frac{1}{2} \int \xi^2 f d\xi,
\] (42)

where \( \xi \) denotes a position along the axis of the swimmer relative to the “center” of the swimmer and \( f \) is the force per unit length in the direction of the swimmer axis exerted by the swimmer on the fluid. The net force on the fluid is zero, which is equivalent to \( \int f d\xi = 0 \). A zero net force also leads to a dipole moment \( d \) that is independent of the choice for the swimmer center, which can be seen by translating \( \xi \) by a constant in the integral. However, because the \( d \) is nonzero, the quadrupole moment does depend on the definition of the swimmer center.

We can use the multipole expansion in Eq. (39) to perform the ensemble average in Eq. (38). After averaging over all orientations \( n_2 \), the dipole term will vanish, as in Liao et al., because of an odd number of \( n_2 \) terms integrated over all angles. However, the quadrupole term remains. Thus the cross terms in the swimmer velocity correlation become

\[
\langle v_nv_2 \delta(x_2 - x_1 - r) \rangle = \frac{v_nq}{15} \nabla^2 \Omega(r),
\] (43)

\[
\langle v_nv_2 \delta(x_2 - x_1 - r) \rangle = \frac{v_nq}{15} \nabla^2 \Omega(r).
\] (44)

Higher order terms in the multipole expansion do not contribute. They vanish either because there is an odd number of orientation vectors (as in the dipole term) or because \( \nabla \cdot \Omega = 0 \) and \( \nabla^4 \Omega = 0 \). Therefore the correlation function between swimmers if the swimmers are independently distributed in space and with isotropic uncorrelated orientations becomes

\[
C_f(r) = \frac{d^2c}{120\pi \eta^2 r} (\delta + \hat{r}r) + \frac{v_nq}{15} \nabla^2 \Omega(r).
\] (45)

Because

\[
\nabla^2 \Omega(r) = \frac{1}{4\pi \eta r} (\delta + \hat{r}r),
\] (46)

we obtain for the swimmer correlation

\[
C_f(r) = \frac{d^2c}{120\pi \eta^2 r} (\delta + \hat{r}r) + \frac{v_nq}{30\pi \eta^3} (\delta - 3\hat{r}r).
\] (47)

There are a number of aspects of this formula that are worth pointing out. The first concerns the limits of small volume fraction and large distances. The first term behaves as \( \phi \nu r^{-1} \) while the second term behaves as \( r^{-3} \) and is independent of concentration. Therefore, for any finite concentration, the correlation eventually behaves as \( r^{-1} \) at large enough distances.
However, at a given distance, as the concentration gets smaller and smaller, the correlation approaches $r^{-3}$.

Another important aspect of the correlation is the dependence on the quadrupole moment. While this was mentioned in Liao et al.,\textsuperscript{17} it was not mentioned that the quadrupole moment depends on the definition of the “center” of a swimmer, as discussed above. For the experiments of Liao et al., the center was chosen as the center of the body of the organism. This is reasonable because the body was the only part visible in the experiments. However, for the simulation model consisting of two beads (one for the body and one for the flagellum), a reasonable choice for the center is the center of mass of the two beads. For this choice the quadrupole moment is zero. This is not a special case of the two bead model. Any model, including the slender body model used by Liao et al., will have a certain point along the swimmer axis such that the quadrupole moment about that point is zero.

We also consider the scalar correlation, which is the trace of the tensorial correlation. Because the contribution containing the quadrupole moment has zero trace, it does not contribute to the scalar correlation. Therefore, the scalar swimmer correlation is equal to the scalar fluid correlation,

$$C_s(r) = C_f(r) = \frac{d^2 c}{50\pi \eta^2 r}. \quad (48)$$

It is common to express these formulas in terms of an effective volume fraction of swimmers instead of number density. The effective volume fraction is $\phi_e = \epsilon \ell^3 / 6$. In terms of $\phi_e$ the correlations are

$$C_s(r) = C_f(r) = \frac{d^2 \phi_e}{5\pi^2 \eta^2 \ell \epsilon r}. \quad (49)$$

Now that we have completed the derivation of the swimmer velocity correlations if the positions and orientations of the swimmers are uncorrelated, let us compare the predictions of the theory with computer simulations. The dumbbell model and simulation method of Ref. \textsuperscript{6} will be used. For simplicity, we will first focus on simulations that consist of 800 swimmers in a cubic, periodic domain at a volume fraction of $\phi_v = 10^{-2}$. This volume fraction is small enough that one might expect that correlations of the positions and orientations would be small. For \textit{E. coli}, this system would correspond to a periodic cube with side length approximately 400 $\mu m$ at a concentration of approximately $10^5$ cells/ml, almost two orders of magnitude smaller than the experiments of Liao et al.

Because of the structure of the tensor correlation, we can decompose the tensor correlation into two scalars representing the longitudinal $C_{s,LL}$ and transverse $C_{s,NN}$ contributions. These contributions are defined by

$$C_s(r) = C_{s,NN} \delta + (C_{s,LL} - C_{s,NN}) \hat{r} \hat{r}. \quad (50)$$

In Figure 1 we show the longitudinal and transverse correlation functions in which the “center” of the swimmer is chosen to be the head bead, i.e., the one that represents the body of the organism. Because the transverse correlation is negative, we plot it as $-C_{s,NN}$. This is analogous to the data from Liao et al. in which the quadrupole moment is negative. We also show in Figure 1 our theoretical prediction in which Eq. (47) is decomposed in the longitudinal and transverse components. Even at lower concentrations than the experiments, the correlations in our simulations have the same sign and order of magnitude as the experiments (approximately 0.1 when the organisms are separated by a distance equal to the total length of the body and flagella). Similar to the comparison in Liao et al. with experimental data, the theory underpredicts the correlations. The inclusion of the concentration-dependent term actually seems to have hurt the comparison because it changes the sign of the transverse correlations at large distances. Note that the theory curves in Figure 1 use the exact, known dipole and quadrupole moments for our simulation model, and therefore cannot be a reason for a difference between the simulations and theory.

To motivate the cause for the error in the theory, in Figure 1 we compare the velocity correlations with the longitudinal and transverse parts of the direct orientational correlation, $C_n$, defined by

$$C_n(r) = \frac{\langle n_1 n_2 \delta(x_2 - x_1 - r) \rangle}{\langle \delta(x_2 - x_1 - r) \rangle}, \quad (51)$$

which are calculated directly from our simulations. Recall from Eq. (32) that these would directly lead to part of the velocity correlations, but were neglected in the theory. We see that the orientational correlations are quite close to the velocity correlations. In fact, using the orientation correlations alone would almost be a better approximation of the data than our entire theory. Therefore, the velocity correlations are not a result of the quadrupole moment, but are due to the fact that even at very low concentrations, the organisms have long-ranged orientational correlations. Unfortunately, we do not yet have a theory that quantitatively predicts these
orientation correlations at very small concentrations. Current phenomenological theories (e.g., Refs. 15 and 16) treat suspensions at an effective one-swimmer level and therefore cannot calculate correlations between two organisms. In principle, a theory using a two-swimmer (or effective two-swimmer) Fokker-Planck equation could calculate these correlations, but the equations are not easily solved for the steady state correlations.

In order to show quantitatively the exact role of the quadrupole moment and what leads to the small difference between the orientational and velocity correlations, it is best to start with the same simulations, but in which the vector \( \mathbf{r} \) connects the two centers of the swimmers. This is useful because the quadrupole moment is zero. Figure 2 shows the correlations in this case. Note that the correlations are almost exactly the same even though \( q \) has changed from a negative value to zero because the value of \( q \) has little effect on the measured correlations.

We again see that the direct orientational correlations are very close to the velocity correlations while the theory using Eq. (47) with \( q = 0 \) does not compare well. The theory now predicts the wrong sign of the transverse correlations over the entire range of \( r \). In order to find a better theory, consider our derivation from Eq. (32) to Eq. (47). If we consider the impact of direct orientation correlations but neglect the impact of those correlations on other aspects of the derivation, we would obtain a new theory which is simply the old theory plus the direct orientational part, which is given by

\[
C_s(r) \approx v_a^2 C_n(r) + \frac{v_a q}{30 \pi \eta r^5} (\delta - 3 \hat{r} \hat{r}).
\]

Equation (52) also accurately represents the simulations when the quadrupole moment changes sign. We can change the sign of \( q \) by choosing \( r \) to represent the separation of the flagella of the two organisms. Figure 5 shows the swimmer correlations for this case and the comparison with Eq. (52).

By using theory and computer simulations of hydrodynamically interacting swimming organisms, we have been able to better understand what leads to velocity correlations of the organisms in the dilute limit. These velocity correlations have been measured experimentally for swimming *E. coli* by Liao et al. They also developed a theory based on the quadrupole moment of the organisms to predict the correlations. This theory predicted the correct sign of the correlations and the rate of decay of the correlations with distance. However, the magnitude of the correlations was underpredicted by the
theory by a factor of 6. The authors speculated that the difference was due to a difference between the true quadrupole moment of the experimental bacteria and the theoretical estimate.

By relaxing some assumptions in the theory of Liao et al. \(^17\) and comparing with our simulations for which we know the quadrupole moment, we have found the dominant effect in our simulations causing velocity correlations is not the quadrupole moment, but that even at dilute concentrations the orientations of the organisms are correlated. Since our simulated swimmer velocity correlations are similar to those measured experimentally, it is possible that measurements of Liao et al. \(^17\) are also dominated by orientational correlations. This suggests that experiments which visualize the flagella and, therefore, can measure the orientation of the cell including flagellar bundle could reveal interesting orientational correlations even at low concentrations.

VI. FLUID DISTURBANCES

We have seen in Sec. V the importance of the fluid correlations because they play an important role in the correlations of the swimmers. The fluid correlations are also important because they are responsible for transport in the fluid. We also saw that even at low concentrations, the orientations of organisms can be correlated. In this section, we show how these correlations between swimmers lead to changes in the large scale fluid correlations.

As an organism swims through a fluid, it causes a fluid disturbance. At low Reynolds number, the disturbance fluid velocity is the solution to the Stokes equation including the forcing on the fluid due to the swimmers. We simplify the analysis by assuming the swimmers act as point dipoles.

Given a distribution of forces exerted on the fluid, \( q \), the fluid velocity is determined by the solution to Stokes equation and the continuity equation,

\[
- \nabla P + \eta \nabla^2 \mathbf{u} + \rho = 0,  \tag{53}
\]

\[
\nabla \cdot \mathbf{u} = 0.  \tag{54}
\]

Taking the Fourier transform and eliminating the pressure yields

\[
\mathbf{u}_k = \frac{1}{\eta k^2} \left( \delta - \hat{\mathbf{k}} \cdot \rho_k \right).  \tag{55}
\]

Because the swimmers are represented as force dipoles, the force distribution is the divergence of a dipole field, \( \rho = \nabla \cdot \mathbf{D} \), where the dipole field is

\[
\mathbf{D}(\mathbf{x}) = d \sum_{x=1}^{N} \mathbf{n}_x \delta(\mathbf{x} - \mathbf{x}_x).  \tag{56}
\]

This dipole field is closely related to the stress tensor introduced in Eq. (1)

\[
\mathbf{D} = \sigma + d \sum_{x=1}^{N} \frac{1}{3} \delta \delta(\mathbf{x} - \mathbf{x}_x).  \tag{57}
\]

Taking the Fourier transform of the force and dipole fields yields

\[
\rho_k = ik \cdot \mathbf{D}_k,  \tag{58}
\]

\[
\mathbf{D}_k = d \sum_{x=1}^{N} \mathbf{n}_x e^{-ik \cdot \mathbf{x}_x}.  \tag{59}
\]

Together, these formulas give the fluid velocity in Fourier space that results from being forced by point dipoles placed at positions \( \mathbf{x}_x \) with orientations \( \mathbf{n}_x \). This is a natural way to relate correlations between the swimmer positions and orientations into the resulting velocity correlations in the fluid.

The spatial structure in the fluid that is generated by the swimmers is quantified by the fluid velocity pair correlation function, which was defined earlier as

\[
C_f(\mathbf{r}) = \left\langle \frac{1}{V} \int \mathbf{u}(\mathbf{x}) \mathbf{u}(\mathbf{x} + \mathbf{r}) d\mathbf{x} \right\rangle,  \tag{60}
\]
where the angle brackets represent the average over swimmer positions and orientations. In Fourier space, this convolution is a product of the fluid velocity

\[ C_k = \langle u_k u_k^* \rangle, \]  

(61)

where the star signifies the complex conjugate. Using Eqs. (55) and (58) in Eq. (61) yields

\[ C_k = \frac{1}{n^2 k^2} \left( \hat{k} \cdot D_k \cdot (\delta - \hat{k}) \cdot (\delta - \hat{k}) \cdot D_k^* \cdot \hat{k} \right). \]  

(62)

Because the \( k \) vector is constant with respect to the average, the important average to compute is

\[ \langle D_k D_k^* \rangle = \frac{d^2 N}{15 V^2} \left( \delta \delta + I + I^* \right) \]

\[ + \frac{d^2 N (N-1)}{V^2} \left\langle n_i n_j n_\beta n_\alpha e^{-i k (s_i - s_j)} \right\rangle, \]  

(64)

where \( I \) and \( I^* \) are fourth-order isotropic tensors defined as\(^6\)

\[ I_{i j k m} = \delta_{i m} \delta_{j k}, \]  

(65)

\[ I^*_{i j k m} = \delta_{i k} \delta_{j m}. \]  

(66)

The first term will turn out proportional to the concentration and is the leading behavior in the dilute limit. The second term is explicitly proportional to the square of the concentration when \( N \gg 1 \) and depends on the correlations between the positions and orientations of the swimmers.

Before discussing the more complicated interacting theory, let us start with this dilute limit result. Using the first term of Eq. (64) in Eq. (62) gives the fluid velocity correlation function for this case to be

\[ C_k = \frac{d^2 N}{15 V^2 n^2 k^2} (\delta - \hat{k}). \]  

(67)

The inverse Fourier transform back to real space is performed by

\[ C_f(r) = \sum_k C_k e^{i \hat{k} \cdot r}, \]  

(68)

where the sum over \( k \)-vectors is over all \( k \in \mathbb{Z} 2 \pi /L \) for integer vectors \( \mathbf{m} \), but excluding the zero vector. In the limit of large \( N \) and large \( L \) but at constant concentration, the sum can be converted to an integral, with a factor \((2\pi)^2 V\) becoming the volume element \( dk \). Thus in the infinite system size limit, the dilute, non-interacting swimmer result is

\[ C_f(r) = \frac{d^2 c}{120 \pi n^2 r^2} (\delta + \hat{r}). \]  

(69)

We have already seen this formula used in Sec. V. For the fluid correlations, it is more common to consider the scalar correlation function. The scalar correlation function is the trace of the tensor version, which corresponds to a dot product between the two velocities in Eq. (61) instead of a tensor product. Thus the scalar correlation function in this limit is

\[ C_f(r) = \frac{d^2 c}{30 \pi n^2 r}. \]  

(70)

This result was given previously.\(^6\) Important features to note are that it is proportional to the concentration, depends on the dipole moment as \( d^2 \) and so is the same for pushers and pullers, and decays as \( r^{-1} \) and so is a long range correlation in the fluid.

Having examined the dilute limit which does not depend on correlations between swimmers, let us consider the additional term which occurs at higher concentrations and depends on the correlations between organisms. For simplicity, we only consider the scalar version of this additional term. The details are not shown here, but the scalar fluid correlation can be simplified for \( N \gg 1 \) to

\[ C_f(r) = \frac{d^2 c}{30 \pi n^2 r} + \frac{d^2 c^2}{8 \pi n^2 r} f(r), \]  

(71)

\[ f(r) = \int dk \frac{1}{k^2} e^{i \hat{k} \cdot r} \left[ \int ds e^{-i s \cdot \hat{k}} g(s) h(s, \hat{k} \cdot \hat{s}) \right]. \]  

(72)

The equation takes the form of a Fourier transform, then an inverse Fourier transform. Two correlation functions of swimmer positions and orientations influence the fluid correlation, the radial distribution function, \( g \), and a new correlation function, \( h \), which depends on orientational correlations, and is defined as

\[ h(s, \hat{k} \cdot \hat{s}) = \int dn_1 dn_2 \left[ \hat{k} \cdot n_1 n_2 \cdot (\delta - \hat{k}) \cdot n_2 n_1 \cdot \hat{k} \right] \Psi(n_1, n_2 | s), \]  

(73)

where \( \Psi \) is the conditional probability of finding swimmer 1 with orientation \( n_1 \) and swimmer 2 with orientation \( n_2 \) given that they are separated by a vector \( s \). Figure 6 illustrates the key variables in determining how correlations between organisms lead to fluid correlations. The two organisms with orientations \( n_1 \) and \( n_2 \) are separated by a vector \( s \). The two fluid elements for which we are examining the velocity correlation are separated by a vector \( r \). A Fourier transform is used to convert...
from $\mathbf{r}$ to $\mathbf{k}$. In quantifying the correlations of swimmers, we consider two swimmers separated by a vector $\mathbf{s}$ and examine how their orientations are correlated.

A key feature of this function is that if the orientations of the two swimmers are uncorrelated and isotropic, then $h = 0$. Because the system is rotationally invariant, the function $h$ will only depend explicitly on the two scalars $s$ and $\mathbf{k} \cdot \mathbf{s}$. We can better understand this dependence by pulling the $\mathbf{k}$-dependence out of the integral average, focusing only on the fourth moment tensor of $\mathbf{n}$. Because the system is rotational invariant, this tensor must have a certain structure. This is similar to the decomposition into a transverse and longitudinal part used previously, but more complicated because it is a fourth order tensor. In particular, in index notation it must take the form,

$$
\int d\mathbf{n}_1 d\mathbf{n}_2 [\mathbf{n}_1, \mathbf{n}_2]_{ijkl} \Psi(\mathbf{n}_1, \mathbf{n}_2) \mathbf{s}
= A \delta_{ij} \delta_{jk} \delta_{ls} + B (\delta_{ij} \delta_{sl} \delta_{jk} + \delta_{ij} \delta_{sj} \delta_{lk})
+ C (\delta_{ki} \delta_{ls} \delta_{jk} + \delta_{ki} \delta_{sj} \delta_{lk} + \delta_{ik} \delta_{js} \delta_{lk})
+ H \delta_{ij} \delta_{kl} + I (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}),
$$

(74)

where the coefficients $A, B, C, H, \text{and } I$ are only functions of $s$. If the orientations are uncorrelated, then $A = B = C = I = 0$ while $H = 1/9$. Plugging Eq. (74) back into Eq. (73) and performing the dot products gives an expression for $h$ that shows explicitly the angle dependence. Defining $\zeta = \mathbf{k} \cdot \mathbf{s}$, we have that

$$
h(s, \zeta) = A \zeta^2 (1 - \zeta^2) + C (1 + \zeta^2) + 2I.
$$

(75)

The functions $A, C, \text{and } I$ can be expressed in terms of scalar moments of the conditional probability, which are particularly useful in computer simulations in order to minimize statistical errors. The four key moments are

$$
\alpha = \int d\mathbf{n}_1 d\mathbf{n}_2 (\mathbf{n}_1 \cdot \mathbf{n}_2)^2 \Psi(\mathbf{n}_1, \mathbf{n}_2) - \frac{1}{3},
$$

(76)

$$
\beta = \int d\mathbf{n}_1 d\mathbf{n}_2 (\mathbf{n}_1 \cdot \mathbf{s}) (\mathbf{n}_2 \cdot \mathbf{s}) \Psi(\mathbf{n}_1, \mathbf{n}_2) - \frac{1}{3},
$$

(77)

$$
\gamma = \int d\mathbf{n}_1 d\mathbf{n}_2 (\mathbf{n}_1 \cdot \mathbf{n}_2) (\mathbf{n}_1 \cdot \mathbf{s}) (\mathbf{n}_2 \cdot \mathbf{s}) \Psi(\mathbf{n}_1, \mathbf{n}_2) - \frac{1}{9},
$$

(78)

$$
\kappa = \int d\mathbf{n}_1 d\mathbf{n}_2 (\mathbf{n}_1 \cdot \mathbf{s})^2 (\mathbf{n}_2 \cdot \mathbf{s})^2 \Psi(\mathbf{n}_1, \mathbf{n}_2) - \frac{1}{9},
$$

(79)

where we have subtracted off the values of the moments if the swimmers are in the uniform and isotropic state. These four moments are only a function of the scalar separation of the swimmers. The scalar functions in our equation for $h$ are expressible as linear combinations of these moments. In particular, they are

$$
A = \frac{1}{8} (2\alpha - 10\beta - 20\gamma + 35\kappa),
$$

(80)

$$
C = \frac{1}{8} (-2\alpha - 2\beta + 8\gamma - 5\kappa),
$$

(81)

$$
I = \frac{1}{8} (2\alpha + 2\beta - 4\gamma + \kappa).
$$

(82)

Current work in progress includes trying to predict these functions for suspensions of interacting organisms. However, we can measure these functions directly in our computer simulations and use that to understand the impact they have on the fluid correlations. In particular, we can use these functions to help understand the differences seen between suspensions of pushers versus suspensions of pullers. At high concentrations, previous work has shown that, at high enough concentrations, an isotropic suspension of pushers is unstable to shear perturbations while an isotropic suspension of pullers is stable.

We are interested here in dilute systems which show orientational correlations between organisms but not necessarily large scale collective behavior, where how those correlations might give additional insight into the onset of collective behavior, and how those correlations differ between pushers and pullers. We find in our computer simulations that at large swimmer separations pushers have positive $C$ and $I$ and negative $A$, while for pullers $C$ and $I$ are negative while $A$ is positive. Figure 7 compares $C$ and $-A$ for pushers with $-C$ and $A$ for pullers for a suspension of 800 swimmers at an effective volume fraction of $10^{-2}$. Figure 8 compares $I$ for pushers with $-I$ for pullers under the same conditions. We find that at large $s$ the magnitude of the functions for pushers and pullers are quite similar. In general, $A$ is the largest in magnitude, $C$ is of intermediate magnitude, and $I$ is the smallest in magnitude. Both $A$ and $C$ seem to decay with distance as $s^{-2}$ while $I$ decays faster.

The decay with $s^{-2}$ turns out to be a very important feature, which will lead to a divergence of the fluid correlations as the size of the system increases at fixed concentration, which has been seen previously. Consider a simplified example in which $g(s) = 1$ provided $s > \ell$ and zero otherwise, while $h \propto s^{-2}$. Then from Eq. (72) the concentration-squared term is proportional to

![Figure 7](image-url)
where \( Si(x) \) is the Sine Integral function. Performing the \( s \) integral gives

\[
f(r) \propto \int dk \, \frac{1}{k^2} e^{ikr} \left[ \int_0^\infty ds \frac{\sin(ks)}{ks} \right].
\]  

(83)

Performing the \( s \) integral gives

\[
f(r) \propto \int dk \, \frac{1}{k^2} e^{ikr} \left[ \frac{\pi}{2} - Si(k\ell) \right],
\]  

(84)

where \( Si(x) \) is the Sine Integral function. Performing the angle integrals for \( k \) gives

\[
f(r) \propto \int_{2\pi/L}^{2\pi/\ell} dk \, \frac{\sin(kr)}{k^2} \left[ \frac{\pi}{2} - Si(k\ell) \right],
\]  

(85)

where the lower limit of integration approximately accounts for the finite periodic box while the upper limit approximately acts to regularize our point dipole theory. Since we are primarily focused on the key features of this expression, we can approximate \( Si(k\ell) \approx k\ell \) because for most of the range of integration, \( k\ell \) is small. The resulting integrals can be performed to obtain

\[
f(r) \propto \frac{\pi}{2} \left[ Ci(2\pi r/\ell) - \frac{\sin(2\pi r/\ell)}{2\pi r/\ell} - Ci(2\pi r/L) + \frac{\sin(2\pi r/L)}{2\pi r/L} \right]
\]  

\[= \frac{\ell}{r} [Si(2\pi r/\ell) - Si(2\pi r/L)],
\]  

(86)

where \( Ci(x) \) is the Cosine Integral function. Note the explicit dependence of this result on the size \( L \) of the domain—this dependence does not vanish in the limit of an infinite domain illustrating the inherent system-size dependence of correlations in systems of this type.

This expression simplifies nicely in two limits. In the limit \( r \ll \ell \ll L \) we obtain the constant value,

\[
f(r) \propto \frac{\pi}{2} \ln(L/\ell),
\]  

(87)

while in the limit that \( \ell \ll r \ll L \) we obtain

\[
f(r) \propto \frac{\pi}{2} \ln(L/r).
\]  

(88)

These limits match two key features of the computer simulations in terms of the system-size dependence of simulations. The value \( C_f(r = 0) \) equals the mean-squared velocity of fluid elements. Figure 9 shows \( C_f(r = 0) \) vs. \( L \) for pushers at an effective volume fraction of \( \phi_e = 10^{-1} \), showing an approximate logarithmic increase in agreement with Eq. (87) inserted into Eq. (71). The simulations also show \( L \)-dependence for \( r \gg \ell \) consistent with our approximate theory. Figure 10 shows the \( C_f(r) \) for pushers at \( \phi_e = 10^{-1} \) for different system sizes from \( N = 400 \) (\( L/\ell = 12.8 \)) to \( N = 6400 \) (\( L/\ell = 32.2 \)).

We compare the simulations to a theory which is not regularized (that uses point dipoles), and therefore Eq. (86) simplifies to

\[
f(r) \propto \frac{\pi}{2} \ln(L/(2\pi r)).
\]  

(89)

FIG. 8. (Color online) Measured correlation function \( I \) (triangles) as a function of \( s \) from Eq. (82) for pushers (dark (blue online)) and pullers (light (red online)) at \( \phi_e = 10^{-2} \). Because \( I \) for pullers is negative over most of the range, \(-I \) is plotted. The dashed line is a power law of \( s^{-2} \) for reference.

FIG. 9. Dependence of the mean-squared velocity of fluid elements on system size \( L \) for pushers at an effective volume fraction of \( \phi_e = 10^{-1} \).

FIG. 10. (Color online) Comparison of spatial fluid correlations for suspensions of pushers at \( \phi_e = 10^{-1} \) at different system sizes to the theory based on orientational correlations of the organisms. The symbols correspond to the simulations with number of organisms equal to \( N = 400 \) (circles), \( N = 800 \) (squares), \( N = 1600 \) (diamonds), \( N = 3200 \) (stars), and \( N = 6400 \) (\( \times \)). The corresponding theory from Eq. (90) is shown by the lines.
The first term in this expression results from the long tail of \( h(s) \) for large \( s \). The second term results from our assumption that the radial distribution function is zero if the organisms are separated from a distance smaller than \( \ell \). Since we do not know the proportionality factor for \( f(r) \), when inserting Eq. (89) into Eq. (71) to obtain the full prediction for the fluid correlation, we will have at least one fitting parameter.

The other alteration that must be made before fitting our data is to account for the finite periodic box. We have included the finite box by assuming spherical symmetry of the wavevectors \( k \) and integrating from a minimum wavevector of magnitude \( 2\pi/L \). For our cubic periodic domain, this is only an approximation. We will choose the minimum wavevector to be an order one factor times \( 2\pi/L \), where that factor is chosen to obtain a good fit with our data. Finally, the leading term in concentration shown in Eq. (71) does not account for a finite domain. Including this effect gives a result of the same form as the second term from Eq. (89). Including all of these effects gives the theoretical curve that matches the simulation curves well to be

\[
C_f(r) \approx \frac{0.12\ell}{r} \left[ \pi/2 - \text{Si}(2\pi r(0.8)/L) \right] \\
+ (0.2) \left[ -\text{Ci}(2\pi r(0.8)/L) + \frac{\sin(2\pi r(0.8)/L)}{2\pi r(0.8)/L} \right],
\]

where the numbers 0.12, 0.2, and 0.8 were chosen to match the simulation curves well.

**VII. CONCLUSION**

The present work has focused on development of a framework for understanding fluctuations and correlations in suspensions of swimming particles. The focus has been on point dipole swimmers and we have attempted to present a general formalism before deriving specific results in the dilute limit where analytical progress can be made. For a dilute solution of point dipole swimmers, the time-correlation of the stress fluctuations can be found in the long wave limit, and is closely associated with the time correlation of the swimmer orientation. This correlation can be used to extract a long-wave effective temperature for a suspension of swimmers. Taking this effective temperature to be that seen by a large tracer particle, estimates of diffusivity based on this temperature are in reasonable agreement with experimental observations of Wu and Libchaber.\(^5\) For the simple swimmer model used here, a closed form expression for the zero-shear viscosity can be found. This expression, in combination with the expression, for the stress fluctuations clearly indicates the absence of a fluctuation-dissipation theorem for suspensions of swimmers. A theory for the pair correlations of swimmer velocities was constructed. In the dilute limit, closed form expressions result. By comparing with simulations in which we know the dipole and quadrupole moments, we determined that the dominant part of swimmer velocity correlations in the dilute limit comes from orientational correlations between the organisms. This suggests that the correlations measured experimentally in Liao \textit{et al.}\(^17\) may also be dominated by orientational correlations. Experiments in which the flagella are visualized will help to better understand the role of orientational correlations even in very dilute suspensions. The formalism for the fluid velocity correlations in a suspension of point dipole swimmers was constructed. The key orientational moments were identified, which affect the fluid velocity correlations and they were measured from computer simulations. We again found that for both pushers and pullers orientations are correlated at low concentrations and that those correlations decay with separation distance \( s \) as approximately \( s^{-2} \). This rate of decay leads to a system-size dependence to the fluid correlations. This work will form the foundation for future theoretical research into the dynamics of active suspension and provide a framework for understanding experimental observations.

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