Effective aspect ratio of colloidal helices in shear flow

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We report the results of simulations of rigid helices suspended in a shear flow, using dissipative particle dynamics (DPD) for a coarse-grained representation of the suspending fluid. The shear flow produces non-uniform rotation of the helices, similar to other high-aspect ratio particles, such that longer helices spend more time aligned with the fluid velocity. We introduce a geometric effective aspect ratio calculated directly from the helix geometry and a dynamical effective aspect ratio derived from the trajectories of the particles and find that the two effective aspect ratios are approximately equal over the entire parameter range tested.

I. INTRODUCTION

The behavior of flowing suspensions of fibers and other high aspect ratio particles plays an important role in a wide range of commercially important processes and consequently has been intensively investigated [1, 2]. Fibers with intrinsic curvature, including those with helical shapes, appear in many contexts [2–4], and their behavior under flow represents an interesting and challenging fundamental problem [5].

A number of studies have specifically investigated the behavior of rigid helices in shear flow experimentally and computationally [5, 11]. Like other high aspect ratio particles such as rods or ellipsoids, shear flow will cause helical filaments to rotate about an axis perpendicular to the velocity gradient and the flow directions (the vorticity axis) with a non-uniform rotation rate, with the particles spending more time with their long axis parallel to the flow than parallel to the shear gradient. For rotationally symmetric ellipsoids at low Reynolds number and in the absence of Brownian motion, the trajectories represent closed orbits (Jeffery Orbits) with analytic solutions that depend only on the particle’s aspect ratio and its orientation with respect to the gradient axis, with no net motion along the vorticity direction [12]. More generally, any axisymmetric body with fore-aft symmetry will also follow Jeffery Orbits in shear flow, with an effective aspect ratio that is determined by the square root of the ratio of the torque exerted on the body when it is held at rest with its axis along the gradient direction to the torque with its axis along the flow direction [13].

Helical particles, by contrast, do not follow closed orbits, even in the absence of thermal fluctuations [5, 8]. Furthermore, the particles experience a net force in the vorticity direction with a sign dependent on the helicity, a phenomenon which has been exploited to use shear flows to separate chiral objects [5, 8, 10, 14, 15]. While considerable progress has been made understanding the average long time behavior of helices in shear flow in the presence of thermal fluctuations, we currently lack the ability to predict the short term dynamics of helical filaments, information that is critical for understanding the role of helical particles in suspension rheology or the behavior of particles in complex flows such as turbulence [14].

In this work, we report the results of Dissipative Particle Dynamics (DPD) computer simulations of rigid helices in the presence of a shear flow. The DPD technique produces stochastic forces similar to thermal fluctuations and we observe that the orbits of the helices are qualitatively similar to noisy Jeffery Orbits. We derive an analytic expression for a geometric effective aspect ratio calculated directly from the helix geometry and compare that to a dynamical effective aspect ratio calculated from the trajectories of the helices in the simulations. Over the entire parameter range tested, the geometric aspect ratio matches the measured dynamical aspect ratio, within the statistical uncertainty.

II. COMPUTATIONAL METHODS

There have been many simulations of fibers in fluid flow using various approximations of hydrodynamic and contact interactions, employing a variety of techniques available with varying degrees of complexity and accuracy [16]. For these studies, we have used Dissipative Particle Dynamics (DPD) [17, 18], an efficient coarse-grained fluid representation that can capture many aspects of the complex hydrodynamic interactions between the helical filament and the surrounding fluid and the effects of thermal fluctuations [19, 20] and is relatively simple to implement. The DPD implementation is similar to one we have used previously to study shear induced aggregation of straight rods [21] and is briefly summarized below.

In DPD, the coarse-grained fluid is represented by soft particles interacting via three pairwise forces: a repulsive force that determines the compressibility of the fluid, a dissipative force that models viscous dissipation, and a random force that determines the steady state temperature of the system. Thus the total force on particle $i$...
is:

$$\mathbf{F}_i = \sum_{j \neq i} \left( \mathbf{F}_C^{ij} + \mathbf{F}_R^{ij}/\sqrt{\Delta t} + \mathbf{F}_D^{ij} \right),$$

where:

$$\mathbf{F}_C^{ij} = \begin{cases} a_{ij}(1 - r_{ij})\mathbf{r}_{ij} & r_{ij} \leq 1 \\ 0 & r_{ij} > 1 \end{cases}$$

is the conservative, soft repulsion contribution to the force exerted by particle $j$ on particle $i$, where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and $r_{ij} = |\mathbf{r}_{ij}|$. The dissipative force is:

$$\mathbf{F}_D^{ij} = -\gamma w^D(r_{ij}) (\mathbf{r}_{ij} \cdot \mathbf{v}_{ij}) \mathbf{r}_{ij},$$

and the random force is:

$$\mathbf{F}_R^{ij} = \sigma w^R(r_{ij}) \mathbf{r}_{ij},$$

with the weighting functions:

$$w^D(r_{ij}) = (w^R(r_{ij}))^2 = \begin{cases} (1 - r/rc)^s & r \leq rc \\ 0 & r > rc \end{cases}$$

Following Groot & Warren [18], we set the repulsive parameter $a_{ij} = 18.75$, the density $\rho = 4$, the random force coefficient $\sigma = 3$, the dissipation coefficient $\gamma = 4.5$, and a timestep $\Delta t = 0.04$. Following Fan et al. [22], we use $s = 1/2$ and $rc = 1.5$ in the weighting functions for the random and dissipative forces in order to increase the Schmidt number, the ratio of the kinematic viscosity to the diffusion coefficient of the DPD particles. All numerical values are given in simulation units, with the relevant length scale being the particle size (unit diameter) and the time scale set by the applied shear. (In the absence of shear, the parameters used produce a temperature of $T = 2.5$ in simulation units). With parameters in this range, DPD has been shown to reproduce correct hydrodynamics at long length scales [23]. The helix length scales simulated in this work are not large compared to the DPD particle size, however, so quantitative agreement with Navier-Stokes hydrodynamics is not expected.

Shear flow is generated by directly simulating moving boundaries at the top and bottom of the simulated fluid. Specifically, referring to Fig. 1 fixed walls one particle diameter thick in the horizontal $(x, z)$ plane are moved at constant, opposite speeds in the $x$ direction, thus producing simple shear with $(x, y, z) = (\text{flow}, \text{gradient}, \text{vorticity})$ directions. Periodic boundaries are employed in the $x$ and $z$ directions.

Helices are simulated by rigid strands of spherical particles with centers separated by a fixed spacing of half-unit length in simulation units. The particles interact with the fluid particles by the same DPD interactions described above. The initial helix configuration was set to be

$$\begin{bmatrix} x(u) \\ y(u) \\ z(u) \end{bmatrix} = \begin{bmatrix} r \cos(u) \\ pu/(2\pi) \\ hr \sin(u) \end{bmatrix}$$

with $0 \leq u \leq 2\pi n$ and $h = \pm 1$ (1)

which gives a right(left)-handed helix when $h = 1(h = -1)$ with $n$ turns, pitch $p$, and radius $r$, initially oriented parallel to the gradient direction such that a perpendicular from the helical axis to the first bead on the $+y$ end of the helix was in the positive flow direction $(\phi, \theta, \psi) = (0, \pi/2, 0)$, see Fig. 2. All parameter sets were run for 50,000 timesteps, then extended until at least 2 “flips” were observed, representing at least one full orbit.

One hundred and five simulations of isolated helices with varying pitch ($p$), radius ($r$) and length ($\ell$) were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [24] environment, including the LAMMPS implementation of DPD and the LAMMPS rigid-body integrator for calculating net forces and torques on the helices. The resulting dynamical equations were solved using the velocity-Verlet integra-
the fixed helical filament, given by tangent to the filament [25]. We decompose the flow on the segments of the filament that compose the helix is anisotropic. From slender-body theory at low Reynolds number, the drag coefficient for flow normal to the filament is twice the drag coefficient for flow tangent to the filament [25]. We decompose the flow on the fixed helical filament, given by \( \dot{\gamma}(\mathbf{H} \cdot \hat{y}) \), into normal and tangent components

\[
\dot{\gamma}(\mathbf{H} \cdot \hat{y}) \approx w_1 \hat{t} + w_{n_1} \hat{n}_1 + w_{n_2} \hat{n}_2 \tag{2}
\]

where \( \hat{t} \) is a unit vector parallel to the filament (i.e. in the direction of \( \frac{dH}{dn} \)), \( \hat{n}_1 \) is parallel to \( \frac{dH}{dn} \) and \( \frac{dH}{dr} \), and \( \hat{n}_2 \) is perpendicular to \( \hat{t} \) and \( \hat{n}_1 \). Equation 2 can be solved to give \( w_1, w_{n_1} \) and \( w_{n_2} \) for all \( u \). The resulting expressions for \( w_1, w_{n_1} \) and \( w_{n_2} \) can be found in the Supplemental Material. The drag force is given by

\[
f_d \propto w_1 \hat{t} + 2(w_{n_1} \hat{n}_1 + w_{n_2} \hat{n}_2), \tag{3}
\]

and so the torque is simply

\[
\tau = \int_0^{2\pi n} du \mathbf{H} \times \mathbf{f}_d \tag{4}
\]

The resulting expression is very messy, but can be easily evaluated for any helix parameters and orientation, and is provided in the Supplemental Material.

Following Cox [13], we define a geometrical aspect ratio for the helix as

\[
r'_{G} = \sqrt{\frac{\tau_1}{\tau_2}} = \sqrt{\frac{2 \ell}{3 \pi n} \left( \frac{3\pi^2 n^2 \ell^2}{16\pi^2 n^2}, \frac{3\pi^2 n^2 \ell^2}{16\pi^2 n^2} \right) + (\ell^2 + \ell^2 \cos(2\psi))}, \tag{5}
\]

where \( \tau_1 = \tau \cdot \hat{z} \) when the helical axis is parallel to the gradient direction \( \hat{y} \) (\( \phi = 0, \theta = \pi/2 \)) and \( \tau_2 = \tau \cdot \hat{z} \) when the helical axis is parallel to the flow direction \( \hat{x} \) (\( \phi = \pi/2, \theta = \pi/2 \)) and \( l = np \) is the helix length.

Unlike the axisymmetric bodies studied by Cox, this definition does not uniquely specify \( r_G \) for a given geometry due to the dependence on the angle \( \psi \). Moreover, given that \( \psi \) will change during an orbit, the situation is clearly more complicated, and the simple ratio of torques at fixed position will not be sufficient to precisely determine the trajectory. Nonetheless, we can still use Eq. 5 to calculate an aspect ratio that depends only on the geometry and \( \psi \) and investigate the extent to which that quantity is a useful predictor of the approximate trajectories. We note that, for \( \theta = \pi/2 \), the torque along the helical axis is always minimized by \( \psi = \pm \pi/2 \), for which the torque is purely in the vorticity direction, as is the case for Jeffery Orbits. This suggests using \( \psi = \pi/2 \) in Eq. 5 in order to calculate a unique \( r_G \), yielding

\[
r_G = a \sqrt{\frac{2}{3} \left( \frac{a^2}{a^2 + 16\pi^2 n^2} \right)}, \tag{6}
\]

using \( a = \ell/r \), which is twice the aspect ratio of the helix’s bounding cylinder. An alternative approach is to integrate over all values of \( \psi \) to produce an average \( r_G \). Unfortunately this does not admit a clean analytic solution (that we could find), but it can be calculated numerically. Figure 3 shows a comparison of the two approaches, plotted as a function of the aspect ratio of the bounding cylinder. Over most of range, \( r_G \approx a/(2\sqrt{2}) = 0.35a \), with significant deviations only for small \( n \) (and therefore very large pitch). Below we show that \( r_G \) defined by Eq. 6 is an accurate predictor of the fraction of time helices spend aligned with the shear flow in our simulations.

![Diagram](image_url)

**FIG. 2:** Coordinates used for measuring helix orientation relative to shear flow (Fig. 1) and parameters used for specifying helices.
IV. SIMULATION RESULTS

A. Jeffery-like Orbits

Isolated helices were simulated initially at rest, with their helical axis oriented in the gradient direction. In this configuration the shear flow exerts a torque on the helix parallel to the vorticity axis, resulting in a rapid rotation into the flow direction. The torque is reduced as the helix aligns with the flow, so the rotation rate decreases, reaching a minimum when the axis of the helix is perpendicular to the gradient (y) component of the orientation unit vector. This behavior is qualitatively similar to Jeffery Orbits of non-Brownian ellipsoids, which are deterministic, closed orbits with fixed angles relative to the vorticity direction (θ) axis. As an example, Fig. 4 displays an orbit for an ellipsoid with aspect ratio $r_e = \ell/2r = 4$ in a series of orientation snapshots and plots of $\phi$ and $\theta$ vs. time. An alternative way to visualize the trajectories is to track the evolution of components of the orientation vector, $\hat{u}$, a unit vector aligned with the axis of the helix, projected into the flow-gradient plane. The blue curve in Fig. 4 shows $u_y^2$ vs. time, where the relatively slow rotation rate when the particle is aligned in the flow direction produces an extended period of time when $u_y^2$ is small.

Figure 5 displays results from two representative trajectories from the DPD simulations, revealing both the non-uniform rotation rates and the stochastic variations that arise from the interactions with the individual DPD particles. As expected, we observe that squat helices, with length to radius ($a = \ell/r$) values closer to unity display relatively small variation is their rotation rates (top panel, $a = 5$), while helices with high values of $\ell/r$ show rotation rates that slow down dramatically when aligned in the flow direction (bottom panel, $a = 15$).

B. Effective Aspect Ratio

For ideal Jeffery Orbits, the angle $\phi$ of the particle relative to velocity direction is related to the aspect ratio $r_e$ according to

$$r_e = \frac{1}{\langle \cos^2 \phi \rangle} - 1,$$

where brackets represent a time average taken over a full orbit [12] [21]. A spherical particle $r_e = 1$ has a uniform rotation rate, producing $\langle \cos^2 \phi \rangle = 1/2$. As $r_e$ increases, the particle spends a longer fraction of its orbit aligned in the flow direction, so $\langle \cos^2 \phi \rangle$ (and $\langle u_y^2 \rangle$) decreases. Note that this result is independent of $\theta$, the angle with respect to the gradient-velocity plane (which is constant for a Jeffery Orbit and therefore determined uniquely by the initial conditions).

Equation 7 can be easily generalized to calculate an effective aspect ratio from our simulated trajectories (as in [21]), with a couple of caveats. One is that $\theta$ is not constant, varying due to both thermal fluctuations and torques with components in the flow-gradient plane. When $\theta$ approaches zero (helix aligned in the vorticity direction), thermal noise causes $\phi$ to fluctuate erratically. This issue does not create difficulties in this work, where we focus on relatively short trajectories with initial conditions of $\theta = \pi/2$. A second caveat is that the effective
 aspect ratio calculation requires an integral number of quarter orbits, which can create selection bias for finite length trajectories. In order to minimize this effect, we have included only parameter ranges where all simulated trajectories included at least one full rotation.

Here we seek to determine if the empirical effective aspect ratio \( r_e \) calculated from Eq. 6 can be simply related to geometric parameters of the helix. Figure 6 shows a scatter plot of \( r_e \) determined from the simulations versus \( r_G \) defined by Eq. 6 for a range of helix parameters. Although there is considerable scatter in the data, there is a strong correlation between the two quantities, with no evident dependence on either \( l \) or \( p \) (indicated by the size and color of the points, respectively). A least squares fit to \( \log r_e \) vs. \( \log r_G \) produces a result that is consistent with the two quantities being equivalent, \( r_e = Ar_G^\alpha \), with \( \alpha = 0.98, 1.12 \) and \( A = 0.89, 1.10 \) (95% CI).

While the geometric aspect ratio defined by Eq. 6 does a remarkably good job of predicting \( r_e \), it is worth noting that over much of the parameter range, \( r_G \) is close to \( a/(2\sqrt{2}) \) (see Fig. 5). A plot of \( r_e \) vs \( a \) looks qualitatively similar to Fig. 6 but shows systematic deviations for small \( n \). Excluding runs with \( n \leq 2 \), we find \( r_e = A_1a^{\alpha_1} \), with \( \alpha_1 = \{1.07, 1.24\} \) and \( A_1 = \{0.23, 0.34\} \).

To our knowledge, this is the first test of an effective aspect ratio of helices in shear flow. Marcos et al. calculated an effective aspect ratio for helical bacteria based on the calculated ratio of rotation rates for \( \theta = 0 \) and \( \pi/2 \), which appears to be consistent with \( r_G \) defined here, but cannot be easily calculated from our trajectories due to the thermal noise.

C. Deflections in Vorticity Direction

Although the primary focus of this study is the rotation about the vorticity axis, we close by noting an interesting behavior that we observed in many, but not all, of our simulated trajectories. Figure 7 shows the evolution of \( u_y^2 \) for two simulated trajectories, along with \( u_y^2 \). We find a transient deflection in the vorticity direction that peaks when \( u_y^2 \) is maximum, i.e when \( \phi = n\pi \) and the rotation rate of the Jeffery-like Orbit is at its maximum. The trajectory suggests that there is a contribution to the torque that has a component in the flow direction that changes sign at \( \phi = n\pi \). As can be seen in the example trajectories, the deflection is somewhat variable.
in magnitude, and is sometimes absent altogether. The direction of deflection (i.e. increasing or decreasing $\theta$) varies from run to run and even within the same run. We have yet to be able to determine the pattern governing this behavior.

![Plot of $u_y^2$ and $u_z^2$ vs. time for two trajectories demonstrating the deflection into the vorticity direction, and subsequent recovery, as the helix axis rotates past the gradient direction. Top: $l/2r = 9.8$, $n = 4$. Bottom $l/2r = 8.5$, $n = 25$.](image)

**V. DISCUSSION**

As described in the Introduction, rigid helical filaments initially oriented parallel to a shear gradient will rotate about the vorticity axis, with a rotation rate that decreases as the helix aligns in the flow direction. Our simulations show, as expected, that the reduction of the rotation rate increases with the aspect ratio of the bounding cylinder ($\ell/r$, Fig. 2). We find that $\ell/r$ is the primary determinant of the degree of alignment and therefore that it is relatively insensitive to the other dimensionless ratios that describe a particular helix (such as the number of turns, $n = \ell/p$, and the pitch angle (related to $r/p$)), at least in the range simulated here ($2 < \ell/2r < 10$, $1 < n < 29$, $0.07 < r/p < 2$). (The thickness of helical filament itself (one particle diameter) was not varied.)

Qualitatively, this behavior can be understood as follows: When the helix is aligned in the gradient direction, the effect of the fluid drag will cause the particle to rotate about the vorticity axis with a rotation rate that is comparable to the shear rate. When the helix is aligned in the velocity direction, the torque due to the shear flow, and therefore the rotation rate, is reduced, as with other high aspect ratio particles. The ratio of the torques in those two orientations is mostly determined by $\ell/r$. Decreasing the pitch $p$ (or, equivalently, increasing $n$) for a given $\ell$ will increase the torque overall, but not the asymmetry.

We do find, however, that there are significant deviations from the degree of alignment that would be predicted by only considering $\ell/r$, particularly for small values of $n$. The geometric aspect ratio defined by Eq. 6, based on the ratio of the torque exerted on the helix held at rest with its axis along the shear to the torque with its axis in the flow direction using slender body theory appropriate for low Reynolds number flow, accurately accounts for those deviations. In fact the data displayed in Fig. 6 shows that $r_G$ is equal to $r_e$ to within statistical uncertainty, over the entire parameter range simulated. However, there is considerable scatter in the data for large aspect ratio helices, because of the relatively small number of complete orbits observed, leaving the possibility that the behavior in some regimes is more complex.

While the extent of the flow alignment of the helices appears to be insensitive to the pitch, it would likely impact other important physical quantities. As the pitch gets very small, the tightly wound helix will approach a rigid cylindrical shell, which we expect would rotate like a solid cylinder but with nearly complete fluid entrainment. By contrast, if $p$ is large (compared to $r$), the amount of fluid displaced by the helix will be determined by filament length, with a logarithmic dependence on the filament thickness, and will be relatively insensitive to the helix radius. Finally, in this study we have only considered isolated helices, but interactions between helices, such as the nature of entanglements, will likely depend on $p/r$.

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