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Collective Effects in Settling of Spheroids under Steady-State Sedimentation

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We study the settling dynamics of non-Brownian prolate spheroids under steady-state sedimentation. We consider the case of moderate particle Reynolds numbers properly taking into account the hydrodynamic effects. For small volume fractions, we find an orientational transition of the spheroids, characterized by enhanced density fluctuations. Around the transition, the average settling velocity has a maximum which may even exceed the terminal velocity of a single spheroid, in accordance with experiments.

The sedimentation of noncolloidal particles is a common phenomenon in nature on which many important technological processes are based, e.g., in the paper and pulp industry. It is also an interesting example of nonequilibrium dynamics, which is still poorly understood in the case of a finite volume fraction Φ of the particles. Under appropriate boundary conditions, such as in fluidized beds, a sedimenting system driven by gravity can reach a steady-state distribution, with a fixed average settling velocity $V(\Phi)$ [1]. The behavior of $V(\Phi)$ for spherical particles has been extensively studied in the limit where Brownian motion can be neglected. Because of backflow, $V(\Phi)$ in a suspension of monodisperse spheres is smaller than the single sphere settling velocity V_0. As Φ increases, $V(\Phi)$ decreases monotonically following the phenomenological Richardson-Zaki (RZ) law $V(\Phi)/V_0 = (1 - \Phi)^n$. The exponent n is around 4.5 in the low particle Reynolds number (Re) regime, decreasing with increasing Re to about 2.5 in a turbulent system [3]. The particle Re is defined by the ratio of inertia forces to viscous forces in the length scale of the particle dimensions [4]. Experiments, however, show a significantly faster decrease of $V(\Phi)$ in the dilute limit, and thus somewhat more complicated relations have been proposed for this case [5].

In striking contrast to the case of spheres, experiments with rodlike non-Brownian particles with Re $\ll$ 1 show that the mean settling velocity does not obey the RZ law even qualitatively. Kumar and Ramarao [6] studied the suspension of glass fibers (of length $\approx$250 and 50 μm, and diameter $\approx$10 μm) and found that the fibers had a tendency to flocculate, which significantly slowed down the average velocity. Even when a dispersion agent was added to the fluid to prevent cluster formation, $V(\Phi)$ decreased drastically when Φ increased beyond about 0.02. These results were corroborated by Turney *et al.* [7] who found by using magnetic resonance imaging that the functional form of $V(\Phi)$ in the suspension of rayon fibers (320 μm $\times$ 20 μm) was significantly different from the RZ picture in the nondilute limit. In particular, they found that $V(\Phi)$ decreased much more rapidly than the RZ law with $n = 4.5$, up to about $\Phi = 0.13$. The orientation of the fibers was, however, not measured in either of these experiments.

In the most recent set of experiments, Herzhaft *et al.* [8,9] studied the suspension of more macroscopic glass rods of dimensions 0.5–3 mm $\times$ 100 μm. They tracked the motion of single marked rods and measured the rod orientation in addition to the settling velocity. They found that in larger volume fractions $V(\Phi)$ was indeed hindered more drastically than for spheres. However, perhaps the most interesting result was that for small volume fractions $V(\Phi)$ *exceeded* that of an isolated rod. This result indicates that $V(\Phi)$ for fiberlike particles has *nonmonotonic* behavior for small Φ. They suggested that this phenomenon could be due to large inhomogeneities in the suspension, in the sense that there would be "fiber packets" which would settle faster than individual fibers [9]. They also observed that during sedimentation the majority of fibers were aligned parallel to gravity with no apparent dependence on either the fiber length or the volume fraction.

On the theoretical side, there exists some analytical results for single spheroidal sedimenting object in the limit Re = 0. In the case of an infinite system, the vertical component of the terminal settling velocity is [10]

$$V_0^{a_r}(\theta) = \frac{3V_0}{16e^3}\left[\cos^2\theta\left(-4e + (2 + 2e^2)\ln\frac{1 + e}{1 - e}\right)^{-1} \right.$$
$$\left. + \sin^2\theta\left(2e + (3e^2 - 1)\ln\frac{1 + e}{1 - e}\right)^{-1}\right]^{-1},$$
(1)

where $e = \sqrt{1 - a_r^{-2}}$ is the eccentricity, a_r is defined as half of the length of the axis of symmetry divided by the largest radius perpendicular to the axis, and $0 \leq \theta \leq \pi/2$ is the angle between the direction of gravity and the axis of symmetry of the spheroid. Here V_0 denotes the

terminal settling velocity of a sphere with unit radius. The maximum velocity is obtained when the particle is oriented parallel to the gravity, denoted here by $V_m^{a_r} \equiv V_0^{a_r}(\theta = 0)$, and the minimum when the spheroid is falling perpendicular to it. There is no torque on the spheroid, and thus any orientation is stable [10].

There exist some numerical simulations of sedimentation of many-particle fiber suspensions in the limit Re = 0. Mackaplow and Shaqfeh [11] studied particles with a large aspect ratio. They used the slender-body theory (see Ref. [12]) to calculate the average settling velocity for randomly formed static configurations of macroscopic elongated bodies with aspect ratio of 100. In these studies, they found monotonic decrease of $V(\Phi)$ in the dilute regime. However, in their case the spatial distribution and alignment of the fibers was random and not induced by the true sedimentation dynamics. Reference [11] and most recently Ref. [13] contain dynamical simulations for Re = 0 based on integrating the particle velocities obtained from the slender-body theory with some modifications. These approaches give a maximum for $V(\Phi)/V_0 > 1$ in accordance with the experiments [9], and support the cluster formation mechanism and parallel alignment of fibers in enhancing settling.

However, for Re > 0, the situation is very different. Both experiments [14] and theoretical arguments [15] show in the case of a single off-diagonally falling spheroid, there is a torque acting on it which changes its orientation perpendicular to gravity. For spheroids the magnitude of the torque is proportional to Re, but vanishes for spheres ($a_r \to 1$) and needles ($a_r \to \infty$). This means that it has a maximum around $a_r \approx 1.7$ [15]. However, the effect of Re > 0 for many-particle fiber suspension remains unexplored.

In this work our aim is to study sedimentation of fiberlike particles with realistic dynamics in the case of a finite Re = $\mathcal{O}(1)$. We will focus on the dependence of the average settling velocity $V(\Phi)$ on the volume fraction Φ and the particle orientation. Our results show that $V(\Phi)/V_0$ displays the experimentally observed maximum at small volume fractions. When properly scaled, this maximum does not depend on the value of a_r considered here. Furthermore, we find that the maximum is accompanied by an orientational transition not reported in the experiments, with enhanced collective density fluctuations.

We use an immersed boundary type of simulation method described in Ref. [16]. The fluid is treated as a continuum by using a finite-difference method on a regular grid to solve the Navier-Stokes equation. To properly include the hydrodynamic interactions, the boundary conditions between the fluid phase and the solid particles are taken into account by adding a fictitious force density to the equation of motion of the fluid so that in the interior of the particles the fluid moves like a rigid object. This force is derived by tracking explicitly the motion of the

solid particles, and whenever the motion of the fluid and the particle templates differ in certain predefined points, restoring force is added. The method is suitable for modeling non-Brownian suspensions and is valid for up to Re $\approx$ 10.

The fiberlike particles in our system are spheroids characterized by their aspect ratio a_r which is defined as half of the length of the axis of symmetry divided by the largest radius perpendicular to the axis. We have studied the cases $a_r = 1$ (reference spheres), 3, 5, and 7, keeping the smaller radius fixed. The density of the particles is 2.5 times the fluid density. In our system, the spheroids are noninteracting except for a soft collision potential [17]. This is to mimic the lubrication forces at distances closer than the grid size in the model. The technical details of the implementation of the method for spheroidal particles can be found in Ref. [18]. The system sizes used in this work are $32 \times 32 \times 64$ in units of the smaller radius of the particles, where the larger dimension is in the direction of gravity. Periodic boundary conditions in all directions were used to obtain the steady state which was checked from $V(\Phi)$ and its fluctuations. In our simulations, we have fixed the fluid viscosity so that the particle Reynolds number Re $\approx 0.5a_r$.

We have tested Eq. (1) by letting individual fibers settle with a fixed orientation θ. We find that the functional form of Eq. (1) is accurately satisfied but our velocities are about 20%–30% smaller, depending on a_r. This difference is due to finite system size and finite Re effects [19]. Thus, for normalization we have used our numerically obtained values of $V_0^{a_r}(\theta)$.

In Fig. 1 we show the mean settling velocities for $a_r = 1, 3, 5$, and 7, where we have normalized by $V_m^{a_r}$. At higher volume fractions, all data follow the RZ law rather closely, while at smaller Φ the velocity for spheres decreases faster than predicted by the RZ law. However, the
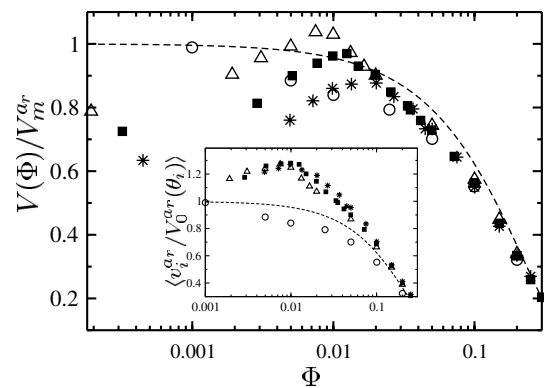

FIG. 1.   The normalized average settling velocity as a function of Φ for aspect ratios $a_r = 1$ ($\bigcirc$), 3 ($\triangle$), 5 ($\blacksquare$), and 7 (*). The dotted curve shows the RZ law $(1 - \Phi)^{4.5}$. The errors are about the size of the symbols. The first points in the spheroid data correspond to the case of single spheroids. In the inset the same data are scaled by $\langle v_i^{a_r}/V_0^{a_r}(\theta_i) \rangle$.

spheroidal particles show *nonmonotonic* dependence on Φ, with a clear maximum for each case where $a_r > 1$. Moreover, for the case $a_r = 3$, the maximum at $\Phi_m \approx 0.01$ is larger than V_m^3. The maximum seems to decrease with increasing a_r, and its position moves to slightly higher values of Φ. These results are in good agreement with the experiments of Refs. [8,9] on fibers with aspect ratios 5–30. There it was observed that the velocity maxima exceeded $V_m^{a_r}$, decreased somewhat with increasing fiber length, and there was also a slight shift to larger values of Φ.

The strikingly different behavior of $V(\Phi)$ between spheroids and fibers suggests that their orientation plays a role at low volume fractions. In the experiments of Refs. [8,9], it was observed that the majority of the fibers were oriented parallel to gravity for $\Phi = 0.001 - 0.155$. For the smallest volume fractions, however, there was some tendency towards perpendicular alignment. We have calculated the orientational distribution function $P(\cos\theta)$, which quantifies the proportion of spheroids that make an angle $0 \le \theta \le \pi/2$ with respect to the direction of gravity. In Fig. 2 we show this function for various volume fractions for the case $a_r = 5$. In the dilute limit, it can be seen that spheroids prefer the *perpendicular* alignment around $\cos\theta = 0$, in agreement with the theoretical and experimental results for a single prolate spheroid with $\text{Re} > 0$. However, when the volume fraction increases, the spheroids begin to orient themselves parallel to gravity [20].

It can be seen from the data that the maximum in $V^{a_r}(\Phi)$ roughly corresponds to the value of Φ where the distribution function $P(\cos\theta)$ flattens out. This indicates a change in the average orientation of the spheroids at Φ_m. To examine the influence of the change in the orientation of *single* spheroids on $V(\Phi)$, we have normalized the instantaneous velocity of each spheroid $v_i^{a_r}$ by the terminal velocity that the same spheroid with the same orien-

tation θ_i would have, denoted by $V_0^{a_r}(\theta_i)$. This should cancel out pure single-particle orientational effects. With this normalization the nonmonotonic behavior of the settling velocity still remains and the maximum is about 40% higher than for spheres. Also, the data for different a_r scale so that the locations and heights of the maxima at Φ_m are almost identical (see the inset of Fig. 1).

The change in the orientational distribution can be quantified through the "order parameter" $\psi = \langle 2\cos\theta - 1 \rangle$, which would have values -1, 0, and $+1$ if all the spheroids in the system were perpendicular to gravity, randomly oriented, or parallel to gravity, respectively. In Fig. 3 we show how ψ depends on Φ. In the dilute regime ψ increases strongly, while for approximately $\Phi > 0.01$–0.02, ψ changes more slowly. The values of Φ where $\psi \approx 0$ correspond roughly to where the settling velocity has a maximum. In the inset we also plot the "susceptibility" $\chi = [\langle \psi^2 \rangle - \langle \psi \rangle^2]$ which shows a broad maximum, which only weakly depends on the system sizes studied up to $64 \times 64 \times 128$. This indicates the existence of a *nonequilibrium orientational transition* not reported in the experiments [8,9]. The data of Ref. [9] indicate that there is a change in the average orientation as predicted here: there are fewer fibers along the gravity for small Φ and small a_r. It is worth noting that the torque forcing a single spheroid to the perpendicular alignment is proportional to the Reynolds number [15]. We have done a few simulations with Re reduced by a factor of 5 and seen the transition move to smaller volume fractions. This may explain why the transition was not clearly seen in the experiments where $\text{Re} \ll 1$ [9].

An interesting question at the transition concerns the role of density fluctuations and cluster formation. We have examined this by computing the pair correlation function $g(x) = \frac{1}{2\Omega}\langle \sum_{i \ne j} \delta(x - |\vec{x}_i + \vec{x}_j|) \rangle$, where $\vec{x}_i$ is the position of the ith particle and the summation is carried out over all the particle pairs within the system volume Ω. When
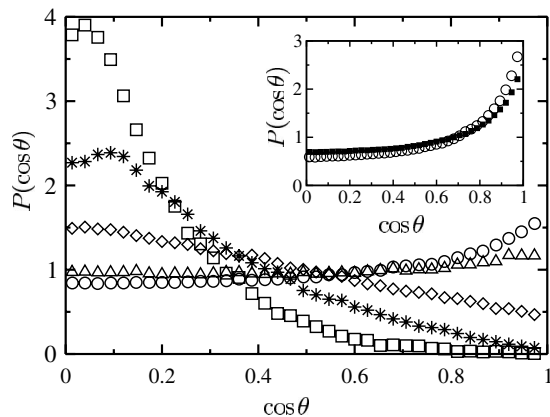
FIG. 2. The distribution function $P(\cos\theta)$ for spheroids with $a_r = 5$. In the main figure we show data for volume fractions 0.0029 ($\square$), 0.005 (*), 0.0099 ($\diamond$), 0.019 ($\triangle$), and 0.034 ($\bigcirc$), and in the inset for 0.10 ($\blacksquare$) and 0.20 ($\bigcirc$).
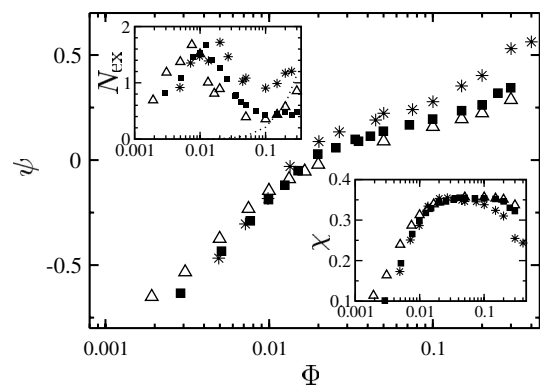
FIG. 3. The order parameter $\psi = \langle 2\cos\theta - 1 \rangle$ as a function of the volume fraction Φ with aspect ratios 3 ($\triangle$), 5 ($\blacksquare$), and 7 (*). Lower inset shows the susceptibility χ from the same data. Upper inset shows the excess particle number N_ex (see text for details).

the average particle number density n is subtracted and an integration is performed over the area where $g(x) - n$ is positive, we get a measure on the average number of excess additional particles, N_{ex}, around the reference particle. This integral also measures subsystem density fluctuations through the sum rule [21]. For spheres we find that N_{ex} is almost zero for $\Phi \lesssim 0.1$ and slowly increases with Φ as included by the dotted line in the inset of Fig. 3. In contrast, for spheroids the density fluctuations have a clear *maximum* which coincides with the maximum of $V(\Phi)$ (see Fig. 3). This supports the observation [9] that around Φ_m there are enhanced density inhomogeneities that appear as ''clusters'' of fibers exchanging particles with the surrounding fluid.

In conclusion, we have shown that the steady-state settling velocity of spheroidal objects has a maximum at small volume fractions. This maximum, which may even exceed the maximal velocity of a single particle, has been experimentally seen and attributed to cluster formation. However, our results reveal that it is accompanied by a change in the average orientation, from perpendicular to approximately parallel to gravity with increasing Φ. During the change, the average orientational order parameter shows a rapid change, and its fluctuations are strongly enhanced. Moreover, there are also enhanced density fluctuations for spheroids. It would be of great interest to experimentally study this nonequilibrium transition for moderate Reynolds numbers.

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[1] The hydrodynamic interactions induce velocity fluctuations which lead to *diffusive* behavior even in the non-Brownian limit for $\Phi > 0$. However, at present there is some amount of controversy in theoretical explanations for experimentally observed system size dependence of these fluctuations, see, e.g., Refs. [2].

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[20] We have examined the motion of a single particle in the denser systems and find it similar to that described in Ref. [9]. While a single spheroid is aligned most of the time parallel to gravity, it occasionally flips around. Thus, while in the dilute limit there are virtually no particles oriented parallel to gravity, even the densest systems studied here have a considerable fraction of spheroids oriented close to $\theta = \pi/2$, as can be seen in Fig. 2.

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