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Hydrodynamic interactions in squirmer dumbbells: active stress-induced alignment and locomotion†

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Hydrodynamic interactions are fundamental for the dynamics of swimming self-propelled particles. Specifically, bonds between microswimmers enforce permanent spatial proximity and, thus, enhance emergent correlations by microswimmer-specific flow fields. We employ the squirmer model to study the swimming behavior of microswimmer dumbbells by mesoscale hydrodynamic simulations, where the squirmers' rotational motion is geometrically unrestricted. An important aspect of the applied particle-based simulation approach—the multiparticle collision dynamics method—is the intrinsic account for thermal fluctuations. We find a strong effect of active stress on the motility of dumbbells. In particular, pairs of strong pullers exhibit orders of magnitude smaller swimming efficiency than pairs of pushers. This is a consequence of the inherent thermal fluctuations in combination with the strong coupling of the squirmers' rotational motion, which implies non-exponentially decaying auto- and cross-correlation functions of the propulsion directions, and active stress-dependent characteristic decay times. As a consequence, specific stationary-state relative alignments of the squirmer propulsion directions emerge, where pullers are preferentially aligned in an antiparallel manner along the bond vector, whereas pushers are preferentially aligned normal to the bond vector with a relative angle of approximately 60° at weak active stress, and one of the propulsion directions is aligned with the bond at strong active stress. The distinct differences between dumbbells comprised of pusher or pullers suggest means to control microswimmer assemblies for future microbot applications.

1 Introduction

Active matter consists of autonomous agents which convert internal chemical energy or environmental energy into directed motion.[1–5] Characteristic features of active matter are broken time-reversal symmetry, broken detailed balance, and absence of a fluctuation–dissipation relation. This gives rise to phenomena, which are absent in passive counterparts, such as enhanced wall accumulation,[6–10] and cooperative[11] and large-scale collective motion.[12–19] Active matter-specific effects provide the basis for, and can be exploited in, the design of new functional soft materials.[20–23]

Theoretically, various models and approaches are applied to resolve the particular features of active matter systems. The paradigmatic model for dry active matter agents—in the absence of hydrodynamic interactions—are Active Brownian Particles (ABPs).[1–4,24–28] Ensembles of this generic model capture basic features of active systems, such as motility-induced phase separation (MIPS),[3,4,24–26,29–35] where the high density phase in two dimensions (2D) exhibits hexatic order,[32] whereas in 3D, ABPs are fluid-like and are highly mobile even in the high-density regime, and exhibit collective motion.[33]

Linear assemblies of freely rotating ABPs, where the orientational degrees of freedom are unconstrained, in form of dumbbells[36,37] and longer chains[22,23,38–44] have been studied. Here, the coupling of activity and internal degrees of freedom strongly affects their conformations and dynamics. Alternatively, active dumbbells propelled along the bond connecting the two monomers have been considered.[45,46] Here, dumbbell rotation is independent of activity and a consequence of thermal fluctuations only.[47] Moreover, fixation of the orientation between the propulsion directions of the two monomers with respect to each other and/or the bond vector, provides a wide spectrum of possible realizations. As an example, the phase behavior of dumbbells with fixed parallel propulsion directions undergoing Brownian motion has been studied.[37] Experiments show that dumbbells of Janus-particle monomers with a fixed non-parallel relative orientation exhibit a coupled translational and rotational motion. Hence, such structures provide means for the design of swimmers moving along specific trajectories[48,49] such as spirals.[49] Simulations reveal a strong influence of the propulsion mechanism on the activity-induced

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phase separation of dumbbells. For example, dumbbells propelled along the bond in 2D phase separate at smaller activities than ABPs.[50] In contrast, dumbbells of freely rotating ABPs phase separate at larger activities.[37] Hence, depending on the orientation of the propulsion directions and their correlations, the phase behavior can be controlled.

A generic model for wet active particles—in the presence of hydrodynamic interactions[28]—are squirmers,[11,51–57] originally intended to model ciliates and microalgae. Nowadays, squirmers are applied in studies of a broad range of both biological[58] and synthetic microswimmers,[59] because squirmers can be tuned to capture essential features of microswimmer flow fields—from pushers (*E. coli*) to ciliates (*Volvox*) and pullers (*Chlamydomonas reinhardtii*).[60] Studies on spherical squirmers in presence and absence of thermal fluctuations reveal attractive and repulsive interactions at distances larger than their diameter.[11,53,55,56,61] Remarkably, the hydrodynamic interactions between spherical squirmers,[60] and microswimmers in general,[62] suppresses MIPS and can lead to particular ordered structures in absence of thermal fluctuations.[63,64]

So far, very little is known about the effect of the microswimmer flow field on the properties of dumbbells composed of two squirmers, which are permanently linked by a bond. Theoretical studies on the athermal case show specific swimming behaviors different from those of dry active dumbbells.[65] In particular, no stable forward swimming can be achieved within a far-field consideration of freely rotating, torque-free squirmers. A restriction of the rotational motion of the individual squirmers by (rigid) bonds leads to torques and stable swimming motion for various dumbbell arrangements and pusher-puller combinations.[65] Thermal fluctuations can be expected to destabilize the predicted stationary states and to imply a yet unexplored swimming behavior, which is naturally absent in dry ABP-type systems.

The combination of squirmers into dumbbells is particularly interesting, since it is a minimal model of linked microswimmers, and forms the basis for autonomous units, *e.g.*, linear polymers or more complex assemblies, as a possible prerequisite of autonomous microbots. Even more, the phase behavior of dumbbell ensembles is determined by interactions *via* the flow field of the microswimmers to an extent unexplored so far, but can be expected to be different from that of dry ABP dumbbell ensembles.

In this article, we study the properties of freely rotating squirmers linked by a bond of finite length embedded in a fluid. We apply the multiparticle collision dynamics approach (MPC) to model the fluid, a particle-based mesoscale simulation approach, which accounts for hydrodynamic interactions and thermal fluctuations.[58,66,67] MPC has successfully been utilized in studies of a broad range of nonequilibrium soft matter and active systems, in particular applying squirmers.[11,55,60,68–74] The presence of thermal fluctuations fundamentally alters the swimming properties of dumbbells compared to athermal ones. Most importantly, the fluctuations imply a rotational diffusive motion of the individual squirmers, and the dumbbells are able to swim in contrast to the athermal case.[65] Our detailed analysis of the squirmers' rotational motion reveals a pronounced dependence on their particular flow field, with the decay rate of autocorrelation function of the propulsion direction strongly depending on the active stress. This affects the dumbbells' swimming motion, with major differences in the dumbbell center-of-mass mean-square displacement, specifically between pusher and puller dumbbells. In particular, the squirmers' propulsion directions are no longer independent, but rather are correlated with preferred activity-dependent angles between them in the stationary state.

This article is structured as follows. In Section 2, the simulation approach is introduced with the squirmer dumbbell model and its coupling to the MPC fluid. Section 3 presents results on the orientational dynamics of the squirmers and the swimming behavior of dumbbells. In Section 4, the stationary-state orientational properties of the squirmer propulsion directions with respect to each other and the dumbbell bond vector are analyzed. Section 5 discusses the dynamics of the dumbbells, and, finally, Section 6 provides a summary of the results.

2 Simulation approach

2.1 Dumbbell model

The active dumbbell moving in three dimensions is composed of two freely rotating spherical squirmers as shown schematically in Fig. 1. An individual squirmer is modeled as a rigid sphere of diameter σ with the prescribed tangential slip velocity on its surface,

$$u_{sq} = B_1 \sin\theta(1 + \beta\cos\theta)\boldsymbol{e}_\theta, \tag{1}$$

which generates propulsion with a velocity $v_0 = 2B_1/3$ and an active stress characterized by β.[11,28,51–53,55,56,61,72,75] The sign of the active stress determines the squirmers' swimming mechanisms—for pullers (*C. reinhardtii*) $\beta > 0$ and the thrust mechanism is at the front, for pushers (*E. coli*) $\beta < 0$ and thrust is produced in the rear of the swimmer. The value $\beta = 0$, for neutral squirmers, corresponds to ciliates such as *Volvox* or *Paramecia*.[28,71] The corresponding flow fields of individual squirmers are discussed in ref. 27 and 71, and Fig. 2 provides examples of dumbbell flow fields for various active stresses β.[23]

The two squirmers at positions $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are connected by the harmonic potential

$$U_l = \frac{k}{2}(|\boldsymbol{R}| - l)^2, \tag{2}$$

with the bond vector $\boldsymbol{R} = \boldsymbol{r}_2 - \boldsymbol{r}_1$, the equilibrium bond length l, and the spring constant k. The squirmer orientations $\boldsymbol{e}_i$, $|\boldsymbol{e}_i| = 1$,

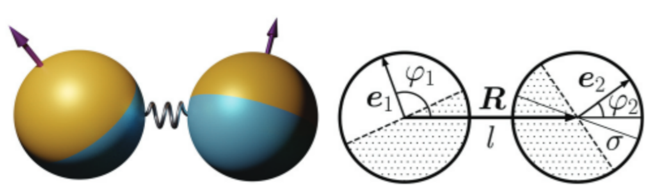

Fig. 1 Schematics of a squirmer dumbbell with squirmers of diameter σ, bond vector $\boldsymbol{R}$, and propulsion directions $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$. The colors of the semispheres indicate the propulsion asymmetry.