Motion of a self-propelled rod with Brownian and hydrodynamics interactions

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Abstract. The dynamic behaviour of a self-propelled rod in a three-dimensional system with cut-and-shifted Lennard-Jones interaction is studied by stochastic Eulerian Lagrangian method which coupled the coarse-grained microstructure degrees of freedom to continuum stochastic field, and the relaxation and thermal fluctuation of the fluid dynamics mode are taken into account. The diffusion of the self-propelled rod is found to have four regimes. The distributions of the horizontal displacements tend to bimodal non-Gaussian at long time when the self-propelled forces are introduced. Furthermore, we study the distributions of the rod velocities in parallel and perpendicular to the rod axis in the body frame. They are all Gaussian, and their standard deviations increase when the self-propelled forces increase.

1. Introduction
Active matters are ubiquitous in nature. They can extract energy from either themselves or external environment to initiate the movement[1-7]. By applying force[14-17], such as magnetic field[18], light intensity[19-20], temperature[21], electric field[22], concentration and sound gradient[23-24], particles can generate self-propulsion. Meanwhile, with the movement of the particles, the hydrodynamic interaction between particles and the fluid cannot be ignored. The key factor of the self-propulsion is the asymmetry of the interaction with the environment.

A number of studies on activate matters can be found in the literature. Hagen et. al[14] analytically solve the Brownian dynamics problem of anisotropic self-propelled particles with different geometries. Cugliandolo et. al[15] studied the dynamical properties of a two-dimensional ensemble of self-propelled dumbbells. The motion of Janus particles at different concentrations of $H_2O_2$ solution shows that their diffusions have three stages: simple Brownian motion at short times, super-diffusion at intermediate times, and finally diffusive behavior again at long times[8]. Non-Gaussian displacement statistics are also observed in several further environments, such as particles in the glass state[25], self-propelled particles[22-24], or particles exposed to nonlinear friction[26].

However, most of numerical works use Langevin dynamics[14-16], which cannot accurately capture the hydrodynamic interactions mediated by the surrounding solvent and the particles. In this paper, a coarse-grained implicit-solvent model is introduced to capture both hydrodynamic and Brownian effects and is amenable to efficient computational simulations[28-29]. The mean square displacements (MSD) of a single rod without self-propelled force is compared with the theoretical results to verify the model. Secondly, the diffusion characteristics of a single self-propelled rod are calculated. The results show that the MSD of the rod can be divided into three stages: short-time simple Brownian motion, medium time super diffusion motion and long-time diffusion motion, which are similar to the results of[15]. The probability distributions of velocities parallel to and perpendicular to the rod are also studied. In addition,
we study the distribution of horizontal displacement of the center of mass, which appears non-Gaussian when the self-propelled forces are introduced.

2. Coarse-grained implicit-solvent Model

To study the diffusion of the active rod, both the dynamics momentum transfer at the level of hydrodynamics and thermal fluctuations should be considered. We do this by introducing the model of the Stochastic Eulerian Lagrangian Method.

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ \rho \frac{d\mathbf{u}}{dt} = \mu \nabla^2 \mathbf{u} + \Lambda[Y(v - \Gamma \mathbf{u})] - \nabla p + \mathbf{f}_{\text{thm}} \]

\[ m \frac{dv}{dt} = -Y(v - \Gamma \mathbf{u}) - \nabla \Phi(X) + \mathbf{F}_{\text{thm}} + \mathbf{F}_{\text{act}} \]

\[ \frac{dX}{dt} = \mathbf{v} \]

Here \( X \) and \( \mathbf{v} \) are the positions and velocities of the particles, then \( m \), \( \rho \), \( \mu \) and \( \Phi \) denote the mass of the particles, the density of the solvent, the shear viscosity, and the potential energy between the particles. \( \mathbf{F}_{\text{act}} \) represent the self-propelled force, and \( \mathbf{u} \) and \( p \) are the velocity and the pressure of the solvent. The thermal forces \( \mathbf{f}_{\text{thm}} \) and \( \mathbf{F}_{\text{thm}} \) are introduced by the \( \delta \)-correlation Gaussian random fields with mean zero and the covariances satisfies.

\[ \langle \mathbf{f}_{\text{thm}}(s) \mathbf{f}_{\text{thm}}(t)^T \rangle = -2K_B T(\mu \Delta - \Lambda Y T)\delta(t - s) \]

\[ \langle \mathbf{F}_{\text{thm}}(s) \mathbf{F}_{\text{thm}}(t)^T \rangle = -2K_B T \Lambda \delta(t - s) \]

where \( K_B \) and \( T \) denote Boltzmann constant and temperature, respectively.

The operator \( \Gamma \) and \( \Lambda \) describe the coupling structure and fluid dynamics, moreover, the coupling operator satisfies the adjoint condition \( \Gamma^T = \Lambda \). \( Y \) serves to calculate the drag force of microstructures from the solvent at different velocities. Here we use the specific coupling operators based on the immersed boundary method[27].

\[ \Gamma \mathbf{u} = \int_{\partial D} \eta(\mathbf{y} - X(t) \mathbf{u}(\mathbf{y}, t)) d\mathbf{y} \]

\[ \Lambda \mathbf{F} = \eta(\mathbf{x} - X(t)) \mathbf{F} \]

Where the kernel function \( \eta(x) \) is the Peskin \( \delta \)-Function.

The computational domain is set as \( L_x = L_y = L_z = 10 \mu m \) with periodic boundary conditions. We set the temperature \( T \) is 298.15 K with the Boltzmann constant \( K_B \) is 0.008314 \((amu \cdot \mu m^2)/(ns^2 \cdot K)\). The particle density is set to be the same as the fluid density so that the gravity can be ignored.

The rod we use is made up of two spheres connected by harmonic bonds with the distance between the center of the sphere set to the diameter of the sphere. To ensure that the spheres in the same molecule do not overlap, the Weeks–Chandler–Anderson potential is introduced to prevent the spheres overlapping.

\[ \Phi(r) = \begin{cases} 4\varepsilon((\sigma/r)^{12} - (\sigma/r)^6) + \varepsilon, & r < r_c \\ 0, & r > r_c \end{cases} \]

where the energy \( \varepsilon = K_B T \), \( \sigma = 0.5 \mu m \) and \( r_c = 0.56 \mu m \).

The self-propelled force we apply acting on the principal rod axis \( \mathbf{n} \), the active force is the same for two spheres belonging to the same molecule, see Figure 1.

\[ \mathbf{F}_{\text{act}} = \mathbf{F}_{\text{act}} \mathbf{n} \]

Figure 1 the self-propelled rod.

The Péclet number, \( Pe \), which represents the strength of self-propulsion, is defined as
$Pe = \frac{\sigma f_{act}}{K_BT}.$  

(12)

3. Single rod dynamics
To validate our numerical model, we study the rod diffusion without self-propelled forces, i.e. $Pe=0$.

The dynamics of a rod is controlled by hydrodynamic interactions and thermal fluctuations, where friction between the rod and the solvent hinders the rod's motion. Kirkwood [30] gives the formulas for calculating the translational diffusion coefficients.

$$D = \frac{K_BT(nP)}{3\pi\mu L}$$  

(13)

where L is the length of the rod, and P is the aspect ratio of a rod.

From Figure 2, our results is consistent with the analytical curve which validates our model.

![Figure 2](image.png)

Figure 2 the mean square displacements of a single rod without self-propelled forces.

For different $Pe$, we plot the $MSD$, defined as $\Delta^2_{cm}$, of the center of the mass which are normalized with lag time in Figure 3. The rod diffusion has four regimes on different time scales: 2nd order ballistic regimes, 1st order diffusion regime, super-diffusion regime (2nd order) and then 1st order diffusion regime again at the long-time scale. In the ballistic regime, $\tau \ll \tau_n$ ($\tau_n = m/(6\pi\mu a)$), for all tested self-propelled systems, i.e. $Pe=0, 20, 40, 60$, their diffusions are similar, since the self-propelled forces have little effect at this time scale. When $\tau > \tau_n$ the self-propelled forces start to increase the diffusion of the rod. Its diffusion first becomes 1st order regular Brownian diffusion, and then immediately goes to super diffusion (2nd order). At large time scale, when $\tau \gg \tau_n$ ($\tau_n = 6\pi\mu a^3/(2K_BT)$), the rod diffusion goes back to a regular Brownian diffusion (1st order), since the rod loses its memory of the initial orientation due the rotation of the rod. These results are similar to Janus particle results[14].

![Figure 3](image.png)

Figure 3 For different self-propelled forces systems, ($Pe=0,20,40,60$) log-log plots of the center of the mass $MSDs$ are normalized with lag time. Figure (a) depicts the transition from regime 1 to regime 3. Figure (b) depicts the transition from regime 3 to regime 4.
Next, we study the distribution of center of mass displacement in the horizontal direction $\Delta X$, defined as

$$P(\Delta X) = \delta(\Delta X - \Delta X_{cm}(\Delta t))$$

(14)

For the rod without self-propelled force, its distribution exhibits a Gaussian distribution for all the times as shown in Figure 4. However, when the self-propelled force is introduced, its distributions are still Gaussian initially ($\tau = 0.07\tau_a, 0.35\tau_a$), and then tends to non-Gaussian bimodal shape ($\tau = 0.7\tau_a, 0.87\tau_a$) in Figure 5.

![Figure 4. The distribution of the horizontal displacement of the center of the mass without self-propelled forces (Pe=0)](image1)

![Figure 5. The distribution of the horizontal displacement of the center of the mass with self-propelled forces (Pe=20)](image2)
For rod diffusions, it would be more interest to report dynamical quantities in its body frame, relative to its unit vector \( \mathbf{n} \), which is defined as the rod axis direction. The distributions of the rod velocities in parallel, \( V_\parallel \), and perpendicular, \( V_\perp \), to the rod axis are shown in Figure 6. Figure 6(a) and 6(b) show the effect of the self-propelled force, where \( Pe = 0, 20, 40 \). With the increase of the self-propelled forces, both the parallel and the perpendicular velocities get large.

![Figure 6](image.png)

Figure 6 the distribution of velocities in parallel and perpendicular to the rod axis at different self-propelled forces.

4. Conclusion

In summary, we study the diffusion properties of a single self-propelled rod which takes into account both hydrodynamic and Brownian effects. Our numerical model is validated by comparing with theoretical results without self-propelled force i.e. \( Pe = 0 \). When the self-propelled forces are introduced, its diffusion can be divide into four regimes, 2\(^{nd}\) order ballistic regimes, 1\(^{st}\) order diffusion regime, super-diffusion regime (2\(^{nd}\) order) and then 1\(^{st}\) order diffusion regime again at the long-time scale. The distributions of the horizontal displacements of the center of the mass are also studied. Its distributions tend to non-Gaussian bimodal shape at large time scale for the self-propelled rod. Furthermore, the distributions of the rod velocities in parallel and perpendicular to the rod axis are presented, both velocities are increased when the self-propelled forces get larger. The model proposed in this work can also study the diffusion of self-propelled multi-rods in the bulk or in the confined geometry.

Acknowledgments

This work is financially supported by Tianjin postgraduate scientific research innovation project (2020YJSS143) and the National Natural Science Foundation of China (11601381).

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