Usage Report for Fiscal Year 2015

Project Title:

Transport properties of self-propelled micro-swimmers

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I.Background and purpose:

Self-propulsion is the ability of specially designed synthetic microparticles to propel themselves by harvesting kinetic energy from an active environment [1-5]. Contrary to bacteria, selfpropulsion of inorganic microswimmers is fueled by stationary *external* nonequilibrium processes, like directional “power-strokes" from catalytic chemical reactions or self-phoresis by short-scale (electric, thermal9 or chemical) gradients, generated by the paricles themselves, by virtue of some built-in functional asymmetry.

The simplest and, possibly, best established model of self-propulsion for artificial swimmers diffusing in an equilibrium suspension fluid at rest, is encoded by the two-dimensional (2D) Langevin equations [5]:

$$\dot{x} = v_0 \cos\phi + \sqrt{D_0}\xi_x(t)$$
$$\dot{y} = v_0 \sin\phi + \sqrt{D_0}\xi_y(t)$$
$$\dot{\phi} = \sqrt{D_\phi}\xi_\phi(t) \qquad (2)$$

where $r = (x,y)$ are the coordinates of spherically symmetric (or point like) swimmer in the plane, ϕ is the angle between the x-axis and its self-propulsion velocity vector of *constant* modulus v_0. The Gaussian noises $\xi_i(t)$, with i = $x;y;\phi$, are assumed to be zero mean valued and delta-correlated, that is $< \xi_i(t)\, \xi_j(0)> = 2\delta_{ij}\delta(t)$; $D\phi$ plays the role of an orientational diffusion constant, whose inverse, τ_ϕ, quantifies the temporal persistency of the ensuing *isotropic* Brownian motion. Indeed, for long observation times t, with $t >> \tau_\phi$, the asymptotic law limit $<r^2> = 4Dt$, defines an effective diffusion constant, $D = D_0 + D_s$. Here, D_0 is due to the environmental thermal fluctuations, while $Ds = v_0^2/2D_\phi$ is the (typically) much larger self-propulsion term, which depends on the activation properties of the swimmer in the suspension fluid.

The above model has a lot of successes in explaining experimental data and exploring non-equilibrium phenomena [1-5]. Example includes collective motion and clustering of artificial micro-swimmers [6], rectification of motion of the particles in ratchet potential [5], driving particle against applied force in symmetric channel [7] etc. Some of these works focus on controlling transport of microswimmers aiming application to nano-technology medical sciences.

Keeping in mind all these recent advancements in micro-swimmer technology, in the fiscal year 2015, we have explored the following two important aspects of diffusion of Janus particles

(i) *Diffusion of Janus particles in a fuel concentration gradient and pseudochemotactic drift*

We have studied diffusion of artificial micro-swimmers in presence of fuel concentration gradient. For this purpose, we consider a chemical reactor consisting of a narrow, straight channel of length *L* oriented along the *x* axis, and a free JP moving in it. A constant concentration gradient of the chemical that fuels the

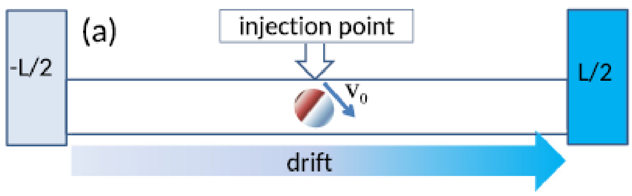

Figure-1: *Chemical reactor with a stationary fuel concentration gradient. A Janus particle injected in the middle with an arbitrary direction of self-propulsion velocity.*

particle’s self-propulsion is maintained by connecting the channel to two reservoirs in thermal equilibrium with concentrations $\rho_L < \rho_R$. The chemical concentration in the channel, $\rho(x)$, will then grow linearly from left to right. At the channel ends, x = $-L/2$ and $+L/2$ two porous membranes allow the chemical flow in and out but prevent the JP from escaping into the reservoirs.

With the above setup we explored here to issues: (a) Upon injecting the JP at the center of the channel, $x = 0$, which containment membrane is the JP more likely to hit first? (b) On which side of the channel is it going to sojourn the most time? This might sound paradoxical, but we came to the conclusion that the injected JP is finally attracted toward the left (high fuel concentration end) exit, even if, immediately after injection, it may drift to either direction, depending on the x-dependence of the propulsion parameters v_0 and τ_φ. For the most common case when the x-dependence of τ_φ is much weaker than D_s, the injected particle points decidedly to the right (low fuel concentration end) exit. Reconciling these seemingly conflicting mechanisms is of paramount importance to control the chemotaxis of artificial microswimmers as opposed to bacterial chemotaxis.

(ii) Diffusion of Eccentric Microswimmers

We proposed a new model for dynamics, which can explain diffusion of all type of self-propelled Janus particles. In the standard model of equation (1) two main assumptions are implicit: (a) The self-propulsion velocity v_0 is constant and, most importantly, oriented along a certain symmetry axis of the particle, like the longitudinal axis in the case of an active nano-rod with one active tip , or the diameter perpendicular to the equatorial plane dividing the two faces of a spherical Janus particle, as sketched in Fig.2. The center of the force responsible for the swimmer's propulsion coincides with the swimmer's center of mass. Under these conditions, the only effect of the angular dynamics described by the process $\phi(t)$ is to make the swimmer change direction, so that its active motion, intrinsically ballistic according to the first two equations in (1), turns into a diffusive one with persistence time t_ϕ . Clearly, both assumptions,

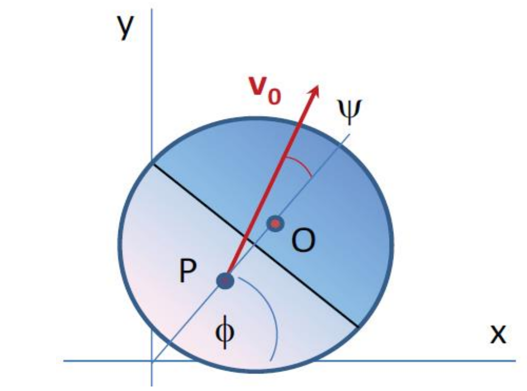

Figure-2: Swimmer's self-propulsion mechanism: O and P are respectively the center of mass and the center of force of a spherical Janus particle. $\mathbf{v_0}$ *represents the instantaneous self-propulsion velocity vector;* ϕ *and* ψ *denote the angle between the OP axis and, respectively, the x axis and* $\mathbf{v_0}$*. The average direction of* $\mathbf{v_0}$ *is oriented parallel to OP.*

although adequate to model a generic active Brownian particle, fail to reproduce specific features of the swimmer's propulsion mechanism that may well impact its diffusive properties. In particular, the finite spatiotemporal scales governing the propulsion mechanism suggest that changes in the orientation of the self-propulsion velocity do not necessarily imply body's rotations. As a consequence, the vector $\mathbf{v_0}$ ought to be allowed to fluctuate around its average direction (the body's axis of coordinate ϕ) with non-zero relaxation time and variance. On the other hand, the self-propulsion speed, $\mathbf{v_0}$, results from the "effective" force exerted by the suspension fluid on the active surface of the particle at low Reynolds numbers (overdamped regime). Contrary to the case of an externally applied driving force, the center of such a force does not necessarily coincide with the particle's center of mass. In general, the two centers are separated by a finite distance, which depends on the swimmer's composition, geometry and surface functionalization.

Based on the above analysis, we proposed following set of equation to describe motion of my micro-swimmer.

$$\dot{x} = v_0 \cos(\phi + \psi) + \sqrt{D_0}\xi_x(t)$$
$$\dot{y} = v_0 \cos(\phi + \psi) + \sqrt{D_0}\xi_y(t)$$
$$\dot{\phi} = \frac{-v_0\,\alpha}{\mathrm{I}_\alpha}\sin(\psi) + \sqrt{\frac{D_0}{\mathrm{I}_\alpha}}\xi_\phi(t)$$
$$\dot{\psi} = -\kappa\psi + \sqrt{D_\psi}\xi_\psi(t) \qquad (2)$$

We here assume that the center of force, P, and the center of mass, O, rest on a swimmer's symmetry axis. The instantaneous self-propulsion velocity is oriented at an angle ψ with respect to the axis OP and fluctuates around it, with constant modulus, $\mathbf{v}_0$, and finite relaxation rate, κ_ψ, and variance, $<\psi^2>$. For convenience, $\psi(t)$ is thus described by a stationary Ornstein-Uhlenbeck process. Due to the propulsion force applied in P, the overdamped swimmer tends to rotate around its center of mass, subject to a torque with ψ-dependent angular frequency, $\alpha\, v_0 \sin\psi$, and moment of inertia I_α. Other terms has same significance as equation (1). Based on the numerical solution of equation(2), we studied diffusion mechanism of micro-swimmer for various model parameter regimes.

III. Methods

Our studies are based on the numerical simulation of Langevin equations (1) and (2). Beside a few ideal cases, an exact analytical solution of the Langevin equation is impossible. One can overcome this difficulty by numerically solving the Langevin equations. We used Milstein algorithm [8] to numerically solve the equation (1) and (2). Appropriate boundary conditions have been used to account for the shape of the Janus particles and the structure of the confining walls. In addition to the thermal noise and self-propulsion, remaining physical force terms arise either due to intrinsic or externally applied forces have been incorporated into the Langevin description.

II. Results and conclusions

Diffusion of Janus particles in a fuel gradient and pseudochemotactic drift --

We numerically investigate the motion of active artificial microswimmers diffusing in a fuel concentration gradient. We assume self-propulsion velocity is proportional to fuel concentration in the channel. When one looks at the transient dynamics immediately following the particle injection, a surprising outcome appears. We injected the particle at $x = 0$ and clocked the time it takes to hit either the right or left containment membrane. We repeated this numerical experiment $N = 10^6$ times and determined the probability the particle first reached the right or left exit, and the corresponding mean-first-passage times (MFPT), from 0 to • $\pm L/2$.

Our simulation results show that, in the steady state, the probability density of JPs accumulates in the low-concentration regions, whereas a tagged swimmer drifts with velocity depending in modulus and orientation on how the concentration gradient affects the self-propulsion mechanism. Under most experimentally accessible conditions, the particle drifts toward the high-concentration regions (pseudochemotactic drift). A correct interpretation of experimental data must account for such an "anti-Fickian" behavior. For more details about this work we refer [9].

Diffusion of Eccentric Microswimmers --- Based on numerical simulations and analytical arguments we analyze diffusion of eccentric micro-swimmer for different regime of model parameters. Our results show the diffusion of eccentric swimmers exhibits a much richer phenomenology. Its most intriguing properties can be listed as follows:

(i) Model based on equation (1) show that diffusivity of JPs is proportion to the square of v_0. But eccentric micro-swimmers's diffusivity shows a transition from a quadratic to a linear dependence on v_0. The linear regime for high values of v_0 is peculiar of eccentric swimmers and disappears when centre of force coincide on the center of mass.

(ii) The square regime and linear regime in diffusivity versus v_0 plots are separated by a plateau at some intermediate v_0 values, which grows wider on increasing the eccentricity.

(iii) Decreasing the rotational diffusion tends to suppress the quadratic regime in diffusivity versus v_0 plots.

These interesting results are of practical use for a correct analysis of the experimental data. The current estimates of the dynamical parameters v_0 and D_ϕ of the standard model,

Eqs. (1), are generally extracted from the direct measurement of the active diffusion process. Our analysis show that the combination of angular fluctuations of the propulsion velocity in the body frame and swimmer's eccentricity, strongly modifies the dependence of the active diffusion constant on the swimmer's propulsion parameters. As a consequence, the current procedure employed to extract the key quantities v_0 and D_ϕ would still be tenable, but only at sufficiently low Ds values, where, however, the experimental accuracy worsens. An experimental evaluation of the eccentricity effects may thus become advisable. For more details about this work we refer [10].

IV. Future Plan

The following item is the main objectives for the next fiscal year which are the important and essential extension of our work done in 2015.

Effect of hydrodynamic interaction and flow field in diffusion of Janus particle in confined system.

Background and Purpose: In the diffusive dynamics of a system of self-propelled janus particles (whose mass and size are much larger than the surrounding solvent molecules) the host solvent mediated hydrodynamic interaction come into play in a significant way [2, 11]. Hydrodynamic effects on the Brownian dynamics in a confined geometry are quite different from the traditional bulk hydrodynamic interaction due to boundary effects [12]. One encounters such typical situations when studying diffusive behavior of colloidal particles in suspensions, protein dynamics in plasma membranes, and diffusion of large polymer molecules across a pore [12]. A detailed understanding of the underlying diffusive mechanisms of Janus particles in confined geometries is required to explain their dynamics in heterogeneous media for applications in biological sciences. Despite the potential demand, the problem of confined diffusion of self-propelled Janus particles in the presence of hydrodynamic interactions remains almost unexplored.

Objectives: Our objectives here are twofold: Firstly, we want to explore diffusion dynamics of Janus dimer/trimer for different type of flow field (e.g., poiseuille flow and couette flow) and confining geometry. Secondly, we want explore noise-induced phelomena, like, ratcheting, absolute negative mobility, stochastic resonance considering hydrodynamic interaction and flow filed.

Method: To this purpose dynamics of a system of active Brownian particles will be considered. Here motion of one particle induces a flow which acts on the adjacent particles and thus the dynamics becomes considerably complicated. Such complicated interactions are taken into consideration through diffusion tensor in Langevin simulation scheme. The effective force balance equation in overdamped limit is given by,

$$dr = \left[u + \frac{1}{k_B T} D.f + \frac{\partial}{\partial r}.D\right] dt + \sqrt{2B}\,.dw \qquad (3)$$

Here k_B is Boltzmann's constant and T is the absolute temperature. The vector $\mathbf{r}$ contains all the spatial coordinates of the particles that constitute the system and f is the force acting on the constituent particles. u represent unperturbed velocity filed which can be determined by solving can the incompressible Stokes flow problem with appropriate boundary condition.

$$-\nabla P + \eta \nabla^2 u = 0 \qquad (4)$$

dw random number having Gaussian distribution with variance dt. The diffusion tensor D, is related to the coefficient of noise term by the following relation,

$$B.B^T = D \qquad (4)$$

The diffusion tensor D is a nonlinear function of the instantaneous position of the all particles in the system. For a system of spherical particles it is possible to express diffusion tensor as a power series of inter-particle distances. In lowest order approximation the diffusion tensor corresponds to an Oseen tensor [13] (and in the next to lowest order approximation is a Rone-Prager tensor [14]). In the confined geometry, the diffusion tensor is modified due to influence of the boundaries. Usually, boundary effects are important when the length scale of the confined system is the order of the size of the diffusing particle. To analyze boundary effects in the diffusion tensor we will follow the methods developed in ref [12], where authors considered the Green's function for Stokes flow as a sum of free-space Green's function and a correction which accounts no-slip constraint on the boundary surface. Thus, the velocity perturbation can be expressed as a function of the free-space Green's function and corrections, and the velocity correction terms are determined from the solution of the incompressible Stocks flow problem.

<u>Simulation technique</u>: To address the objectives presented in beginning of this section, we shall numerically solve the Langevin equations (3) using a Milstein algorithm with appropriate boundary conditions to account for the shape of the Janus particles and the structure of the confining walls. Velocity field and diffusion tensor will be calculated by numerically solving incompressible Stokes flow equation (4) by finite element method.

Currently, I have a "Quick Use" user account and I would like to get extension of computation facilities for next usage term (up to 31st March 2017) in the same user category.

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Usage Report for Fiscal Year 2015

Fiscal Year 2015 List of Publications Resulting from the Use of the supercomputer

[Publication]

1. Pseudochemotactic drifts of artificial microswimmers, P. K. Ghosh, Y. Li, F. Marchesoni, and F. Nori, Phys. Rev. E 92, 012114 (2015).

2. Diffusion of eccentric microswimmers, Debajyoti Debnath, P. K. Ghosh, Y. Li, F. Marchesoni and B. Li, Soft Matter, 12, 2017-2024 (2016).

[Proceedings, etc.]

None

[Oral presentation at an international symposium]

Our works have been presented in following international symposium:

(a) The 7th International Conference on Unsolved Problems on Noise (UPoN-2015), Casa Convalescència, Barcelona, Spain, July 13-17, 2015.

Title of talk: Active Brownian motion in confined geometries.

(b) Colloquium at Department of Physics, University of Palermo, Italy, May 20th, 2015.

Title: Active Brownian Motion

(c) Conference on "New Horizons in Nonequilibrium Thermodynamics",

Erice, Italy. October 26-30 2015.

Title: The Thermodynamics of Active Brownian Motion

[Others (Press release, Science lecture for the public)]

None