

Project Title:

Transport properties of self-propelled micro-swimmers

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I. Introduction

Active Brownian particles, also known as microswimmers, are self-propelled micro- and nano-objects capable of directed random motion. Actually, self-propulsion [1] is the ability of most living organisms to move in the absence of external drives by means of an internal “engine” of their own. Recently, a new type of artificial microswimmer has been fabricated [2], where self-propulsion is powered by local gradients the particles themselves generate, when coupled to an external energy source (self-phoretic effects) [3]. Typically, such particles consist of two distinct “faces,” only one of which is chemically or physically active and for this reason are dubbed Janus particles (JPs) [4]. Such swimmers thus harvest energy from their environment through an external “engine,” which may involve concentration gradients (by catalyzing a chemical reaction on their active surface [5,6]) as well as thermal gradients (e.g., by inhomogeneous light absorption [7,8] or magnetic excitation [9]).

In the absence of any external force field, the motion of a self-propelled JP is directed parallel to the self-phoretic force. Gradient fluctuations or collisions with boundaries or the intrinsic rotational diffusion result in a random change of the direction of self-propulsion. Thus, self-propelled JPs exhibit time correlated active Brownian motions. Janus particles can be used as a special kind of diffusing tracer in experiments aimed at demonstrating non-equilibrium phenomena such as ratcheting autonomous pumps, absolute negative mobility, etc. A conspicuous feature reported in earlier experiments[10] and simulations[11] is that when the mean free path (λ) of a JP is much greater than the cavity size (L), the particle spends most of their time in the close vicinity of confining

walls. In many practical situations, the mean free path follows the condition $\lambda > L$. The self-propulsive forces press JPs against walls. As a result, the JPs keep diffusing in the tangential direction under the action of translational noises until an appropriate orientational change occurs by rotational diffusion. Taking advantage of this property, JPs can be captured by placing an obstruction of appropriate shape, driven against an applied force, and rectified in asymmetric channels with high efficiency.

Controlling transport of *artificial* microswimmers and JPs, in particular, through confined geometries is of utmost importance for the application of microswimmer technology to science and engineering [12, 13]. The rectification of *nonchiral* JPs through periodic arrays [8] and channels [11] surely is a suggestive option. Such devices do operate autonomously, that is, in the absence of external drives or gradients, but at the price of a strict fabrication requirement: Their geometry must be asymmetric under mirror reflection in the direction of the output current [13].

In the fiscal year 2014, we have explored the following two important aspects of diffusion of Janus particles in corrugated channels.

(i) *Giant negative mobility of Janus particles in a corrugated channel*

We proposed an affordable technique to direct the JP motion along a channel. Under appropriate conditions involving the geometry of both the particle and the channel, a tiny external drive (even in the absence of other biases) can orient the self-propulsion velocity of the microswimmers *against* the drive, a phenomenon known as absolute negative mobility. The roughness of the channel walls, mimicked here by randomly inserting small transverse wall protrusions, can drastically enhance this phenomenon, thus producing a *giant* absolute negative mobility. These features suggest most sensitive control techniques on JP transport with beneficial applications to nanotechnology and medical sciences.

(ii) *Rectification of chiral Janus particles in channels*

Symmetry breaking conditions play the central role in autonomous rectification of JPs in narrow channels. We explored more general symmetry breaking conditions than suggested by the one-dimensional reduction formalisms [13]. Based on numerical simulation we have shown that a sufficient condition for rectification of chiral JPs is that the cylindrical (in three dimensions, 3D) or mirror symmetry of the channel with respect to its axis (in two dimensions, 2D) be broken. This is the net effect of opposed boundary flows, which set on as the particle orients its self-propulsion velocity tangentially to the channel walls.

II. Methods

Our studies based on the numerical simulation of Langevin equation. Following is the details of model and methods.

Model: In order to avoid unessential complications, we restrict ourselves to the case of 2D channels and finite sized artificial micro-swimmers of the Janus particle type. In some cases, it is quite straightforward to extend conclusions of 2D problems to three-dimensional ones. A chiral Janus particle gets a continuous push from the suspension fluid, which amounts to a rotating self-propulsion force F with constant modulus F_0 and angular velocity $\dot{\theta}$. Additionally, the self-propulsion direction varies randomly with time due to the rotational diffusion. The bulk dynamics of a self-propelled Janus particles can be described by the following set of equations under the combined action of thermal noise and orientation fluctuations.

$$\ddot{x} = -\gamma\dot{x} + F_0 \cos\theta + \sqrt{\gamma kT} \xi_x(t)$$

$$\ddot{y} = -\gamma\dot{y} + F_0 \sin\theta + \sqrt{\gamma kT} \xi_y(t)$$

$$\dot{\theta} = \xi_\theta + \Omega$$

where (x, y) denote the position of the particle center of mass. $\xi_x(t)$, $\xi_y(t)$ and $\xi_\theta(t)$ are zero mean, delta-correlated Gaussian noises. γ is the damping

constant depends on the particle size and medium viscosity. k and T are Boltzmann constant and temperature, respectively. The effective dynamics of JPs becomes more complicated in the presence of hydrodynamics interactions and confinements.

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 numerically solve the Langevin equations using a Milstein algorithm [14] with appropriate boundary conditions 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 hydrodynamic interactions or due to intrinsic and externally applied forces have been incorporated into the Langevin description.

III. Results and conclusions

Giant negative mobility of Janus particles in a corrugated channel -- We numerically simulated the transport of elongated Janus particles driven along a narrow channel. We have shown that key transport quantifiers, like mobility and diffusivity, strongly depend on the particle shape. Diffusion in smooth channels is characterized by exceedingly long transients, either ballistic or nondiffusive, respectively, for prolate and oblate active micro-swimmers. In compartmentalized channels with narrow pores, prolate Janus particles undergo absolute negative mobility, as an effect of the translational symmetry breaking due to the drive. More important, when the compartment dividers shrink to small side winglets, possibly randomly distributed along the channel walls, rod-like active particles greatly enhance their negative mobility, as the combined action of drive and channel roughness systematically reorients the particle self-propulsion velocity opposite to the drive itself. Since the geometric and dynamical parameters used in our simulations closely compare with those reported for actual experimental setups, we are confident that

giant negative mobility can soon be demonstrated, thus allowing a more effective transport control of active microswimmers. Such a control technique can be exploited, e.g., for medical applications, such as drug delivery via JPs to opposing physiological regions. Moreover, a dilute binary mixture of JPs of different shape can be driven along one such stylized rough channel so as to generate two-way traffic.

Rectification of chiral Janus particles in channels ---

Based on numerical simulations and analytical arguments we show that diffusion of chiral microswimmers can be rectified even in highly symmetric geometries as an effect of opposite oriented boundary flows. The “minimum spatial asymmetry” required to generate an autonomous current is that the channel walls have different corrugation. This type of rectification phenomenon allows one, in principle, to design a distinct class of active particle rectifiers, where, in contrast with the better known ratchet technology, spatial asymmetry in the direction of propagation would be unnecessary asymmetry control autonomous rectification. The investigated mechanism not only enhances transport of JPs in general, but also allows an accurate control of their flows; how the JP rectification power depends on the self-propulsion parameters and channel geometry. As a natural extension of our boundary flow approach, we notice that rectification of chiral microswimmers also occurs in different geometries, such as in annulus. Thus, specialized microfluidic circuits can be designed, for instance, to guide chiral microswimmers to a designated target. Taking advantage of the fact that the proposed mechanism is quite sensitive to the degree of chirality of the diffusing particles (engineered or accidental, alike), this effect can be utilized to fabricate monodisperse chiral microswimmers (presently a challenging technological task).

IV. Future Plan

The following items are the main objectives for the next fiscal year which are the important and essential extension of our work done in 2014.

A. Chemotactic motion of Janus particles:

Chemotaxis, defined the movement of motile cells or organisms in response to a chemical gradient, is a well-known phenomenon. Bacteria and other single-(multi-)cellular organisms direct their velocity in the direction of increasing or decreasing concentration gradient of a particular substance. By this type of movement, bacteria find food or avoid poisonous substance sources. Inspired by chemotaxis in biology, researchers synthesized artificial swimmers that can move in response to a chemical stimulus [15]. Recently, a type of chemical 'robots' have been designed that use artificial chemotaxis to navigate autonomously [16]. Such systems are potentially important to design new and more efficient drug delivery applications. Sen's group [15] showed that Janus particles with one Pt coated face (which can catalyze decomposition of hydrogen peroxide) are attracted by a hydrogen peroxide source. This study shows that such Janus particles act as a molecular 'robot' and can be used in many practical applications. To make this option viable the details of artificial chemotaxis must be investigated in more detail. To gain control over chemotaxis movement of Janus particles we intend to explore several important issues like, (i) The theoretical background of chemotaxis and how it relates to noise-induced drifts in non-equilibrium systems; (ii) How the chemotaxis efficiency depends on the concentration gradient (linear/nonlinear), the self-propulsion mechanism, and geometric confinement. All these issues will be explored by both analytical calculation and extensive numerical simulation of the relevant Langevin equations.

B. Effects of inertial dynamics on confined diffusion of Janus particles:

Earlier investigations on diffusion of Janus particles in confined space concern the limit of negligible inertia, as in the most practical situations the inertial forces are much smaller than the viscous drag, so that the particles motion is largely governed by the random impulses from surrounding medium

and the self-propulsion. However, when considering Brownian diffusion through a small orifice, whose size is less than the mean free path of the Janus particles, the effects of inertia become important even in a relatively high viscous medium. The combined effect of the deterministic inertial dynamics and diffusive motion of self-propelled Janus particles is important in separation of Janus particles of different masses in fluids of low viscosity [13]. In view of this it is worthwhile to investigate the diffusion mechanisms of Janus particles at intermediate Reynolds numbers in confined geometries.

To address the above issues we shall numerically integrate the Langevin dynamics of section II.

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Fiscal Year 2014 List of Publications Resulting from the Use of RICC

[Publication]

- Giant negative mobility of Janus particles in a corrugated channel, P. K. Ghosh, P. Hänggi, F. Marchesoni and F. Nori, *Phys. Rev. E* 89, 062115 (2014).
- Active Brownian motion in a narrow channel, X. Ao, P. K. Ghosh, Y. Li, G. Schmid, P. Hänggi and F. Marchesoni, *Eur. Phys. J. Special Topics* 223, 3227-3242 (2014).