Artificial Microswimmers in Narrow Channels : Autonomous Pumping

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1. Background and purpose of the project

Artificial self-propelled particles, or "microswimmers", which mimic the motion of living objects, are extensively studied both experimentally and theoretically during the last five years. The interest to these objects is first of all due to various promising applications in biology, medicine, physics and technology. For example, targeted delivery by self-propelled nano-robots is of high potential impact for cancer treatment and other medical applications. On the other hand, the dynamics of self-propelled motion (e.g., in various environments) offers new challenges for the fundamental knowledge.

An important property of the motion of self-propelled particles is their ability of carrying along a "cargo", i.e., some passive particles (or other objects). Examples include, e.g., transport of a cargo by self-organized magnetic particles [1], autonomous pumping of passive particles by self-rectified Janus particles in asymmetric channels [2].

In this project, we address the important case of artificial microswimmers self-propelling in a straight symmetric channel. Intuitively one would not expect any interesting dynamics in a symmetric channel. However, as we show below, the symmetry of the system at certain conditions can be broken (on a finite but large enough temporal and spatial scale). This occurs in form of a directional motion locking leading to much longer rotational diffusion times of a microswimmer in a channel with passive particles than that of a free self-propelled particle. As a result, just a few or even a single microswimmer can effectively clear up a channel of passive particles suggesting a number of potential useful applications, e.g., in medicine or technology.

2. The calculation method

To investigate the dynamics of the interacting Janus particles and the passive particles, we used the Langevin-type Molecular-Dynamics simulations. The initial state of the system was obtained using the Simulated Annealing Simulation (SAS) method. Then the temperature of the system was set to a constant, and the dynamics simulation was continued for varying system parameters such as the number of active microswimmers in the system, the total number of particles, the active particle velocity v_0, the time of the direct motion of the active particles between thy change the direction τ_θ, the system geometry, i.e., the size and the shape of the compartment.

The inter-particle interaction was modeled as "soft disks", i.e., the elastic repulsive force proportional to the overlap distance,

$$F_{ij} = -k\,(2r_0 - r_{ij}),$$

where k is the elastic constant, r_0 is the particle's radius, and r_{ij} is the distance between the centers of the particles.

The collisional dynamics of a Janus particle at the boundaries was modeled as follows. The translational velocity is elastically reflected, whereas for the coordinate we considered, in general case, two possibilities. (i) Frictionless collisions when the microswimmer slides along the walls for an average time of the order of τ_θ^{-1}, until the noise redirects it toward the center of the compartment. (ii) Rotation induced by a tangential friction, randomized.

3. Results

The motion of active Janus motors in a channel can be characterized by the velocity of the moving particles and the mean square displacement (MSD) extracted from the trajectories of the motors.

In Fig. 1, we show typical trajectories of the microswimmers moving in channels. Depending on the mean free path, l, a microswimmer either moves nearly as a free particle (when l is much smaller than the channel width, d) (a) or it experiences multiple collisions with the channel walls (when l is of the order of d) (b). The corresponding MSD curves rapidly decrease with decreasing the channel width indicating the transition from a free two-dimensional (2D) motion to quasi-1D regime (Fig. 2). Note that for long observation times the MSD slope for the microswimmers confined in channels of any width

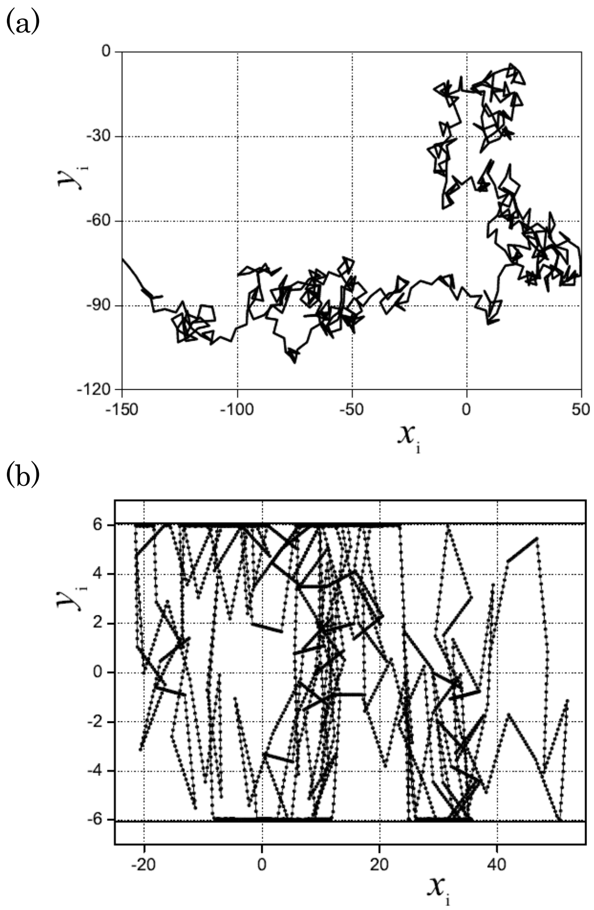

Figure 1. Calculated trajectories of microswimmers in a channel: for the case of the mean free path, l, smaller than the channel width, d, i.e., a wide channel (a), and for a narrow channel, when l is of the order of d (b).

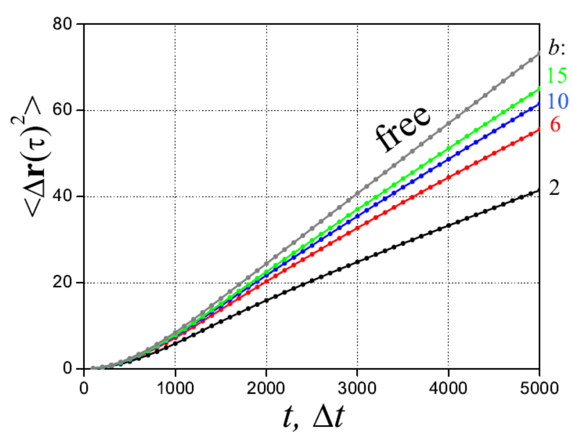

Figure 2. The mean square displacement of a microswimmer for channels of various widths: $d/(2r_0)$ = 2, 6, 10, 15 and for a free particle in 2D.

becomes the same and equal to the half of that for a free particle. This behavior is indicative for the transition from 2D to 1D diffusion (i.e., single-file diffusion).

After characterizing the motion of a single microswimmer in a channel, we consider a system of mocroswimmers (or a single microswimmer) in presence of passive particles. The question is, whether the microswimmers can be used as pumps of passive species in a straight symmetric channel? In our analysis, we distinguish two cases: (i) low density of passive particles, and (ii) high density case.

(i) Low density case.

In this case, a microswimmer can percolate between two sides of a channel, diffusing through dilute clouds of passive particles. This motion is similar to that of a microswimmer in absence of passive particles, although with re-normalized velocity of self-propelled motion and the mobility of passive particles. The passive species undergo thermal Brownian motion. In presence of microswimmers, the passive particles experience collisions with the active particles and thus effectively move faster which explains the observed re-normalization of their mobility. This effect has been discussed in the literature, although in absence of channel walls. Fig. 3 shows an example of a snapshot of a microswimmer moving through a dilute cloud of passive particles.

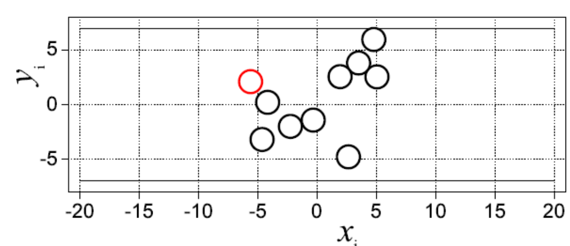

Figure 3. A snapshot showing a single microswimmer (red circle) propelling in a channel in presence of low-density passive particles. The motion of the microswimmer in this case is similar to that of a free microswimmer but with re-normalized self-propelled velocity and the mobility of passive particles.

(ii) High density case.

The most unusual behavior is observed in case of high density, which is the main point of interest of our project. In contrast to the above low-density case, the passive particles are able to form clusters bridging the channel's walls. The formation of these clusters can be either due to thermal fluctuations of the passive particles themselves or can be assisted by the active Janus motors. The motion of an active Janus motor in this crowded environment becomes rather complex. The free space is very limited, and a Janus swimmer spends most of the time either near the wall or being attached to the cluster of passive particles. When an active swimmer collides with a cluster, it becomes inserted in the cluster (i.e., becomes a part of the cluster). This considerably suppresses the ability of the microswimmer to rotate and thus increases the effective rotational diffusion time. This means that the microswimmer inserted in the cluster can perform much longer directed motion than a free microswimmer.

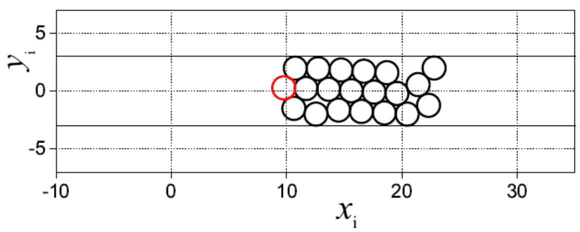

Figure 4 A snapshot of a single microswimmer (red circle) propelling in a crowded channel where passive particles form clusters. In the snapshot, the microswimmer moves from the left to the right carrying along a large cluster of passive particles.

Conclusions.

In this project, we investigated the motion of active artificial microswimmers, i.e., self-propelled Janus particles, in channels in presence of passive particles. When the density of passive particles is low, the microswimmer can percolate through the channel. In this case, its motion is similar to that of a free microswimmer although with re-normalized self-propulsion velocity and the mobility of passive particles which undergo thermal Brownian diffusion. In case of high density of passive particles, these particles can form clusters which extend from one wall of the channel to the other one. When colliding with such a cluster, an active microswimmer becomes inserted in the cluster which strongly suppresses its rotational diffusion. As a result, such a microswimmer acquires a much longer effective mean free path, as compared to a free self-propelled particle. Therefore, the microswimmer is capable of carrying along a large cluster of passive particles over long distance which can be useful for various applications in biology, medicine and physics, for example, for clearing channels of undesired particles by means of artificial microswimmers.

References.

[1] A. Snezhko, M. Belkin, I. S. Aranson, W.-K. Kwok: Self-assembled magnetic surface swimmers, Phys. Rev. Lett. 99, 158301 (2009).
[2] Pulak K. Ghosh, Vyacheslav R. Misko, Fabio Marchesoni, and Franco Nori: Self-Propelled Janus Particles in a Ratchet: Numerical Simulations, Phys. Rev. Lett. 110, 268301 (2013).

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

[Publication]

1. V. R. Misko, A. A. Vasylenko, L. Baraban, F. Marchesoni, and Franco Nori,
The Dynamics of Artificial Microswimmers in Narrow Channels, in preparation.

[Proceedings, etc.]

2. V. R. Misko,
Single-File Dynamics of Charged Particles in Finite-Sise Systems. Abstracts of the International Conference on Single File Dynamics in Biophysics,
Physics & Related Fields & Extensions in Higher Dimensions, Ettore Majorana Centre, Erice, Sicily, Italy, 4-9 July 2014, P. 5.

3. V. R. Misko,
Controlling active Brownian motion in confined geometries.
Abstracts of the International Soft Matter Conference "Jülich Soft Matter Days",
Bad Honnef, Germany, 11-14 November 2014, P. 16.

4. Vyacheslav R. Misko,
Using artificial microswimmers for controlling the motion of passive colloidal particles in straight and asymmetric channels, Abstracts of the 2015 March Meeting of the American Physical Society (APS), San Antonio, Texas, USA, March 2–6, 2015.
Bulletin of the American Physical Society (BAPS) 60, No. 2, J49.00002.

[Oral presentation at an international symposium]

1. Extended Invited Lecture:
V. R. Misko, Single-File Dynamics of Charged Particles in Finite-Sise Systems.
The International Conference on Single File Dynamics in Biophysics, Physics & Related Fields & Extensions in Higher Dimensions, Ettore Majorana Centre, Erice, Sicily, Italy, 4-9 July 2014.

2. Invited Talk:
V. R. Misko, Controlling active Brownian motion in confined geometries.
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Bad Honnef, Germany, 11-14 November 2014.

3. Talk:
Vyacheslav R. Misko, Using artificial microswimmers for controlling the motion of passive colloidal particles in straight and asymmetric channels, Abstracts of the 2015 March Meeting of the American Physical Society (APS), San Antonio, Texas, USA, March 2–6, 2015.