Active Brownian motion in confined geometries

Vyacheslav R. Misko[1,2]

[1]Departement Fysica, Universiteit Antwerpen, B-2020 Antwerpen, Belgium
e-mail address: Vyacheslav.Misko@uantwerpen.be
[2]CEMS, RIKEN, Saitama, 351-0198, Japan

I. INTRODUCTION

Rectification of Brownian motion has been the focus of a concerted effort, both conceptual[1] and technological[2], aimed at establishing net particle transport on a periodic substrate in the absence of external biases. According to the Pierre Curie's conjecture, two basic ingredients are required for this purpose: a spatial asymmetry of the substrate and a time correlation of the (non-equilibrium) fluctuations.

Brownian diffusion in a narrow, corrugated channel can also be rectified according to Curie's conjecture. Subjected to an a.c. drive, repelling particles drift in the easy-flow direction of such a collective geometric ratchet, where the average compartment corrugation is the less steep[3], although with much lower efficiency than in ordinary ratchet potentials. Such collective ratchets have been experimentally demosntrated for a.c. drives and relatively high particle densities[4], whereas the net current vanishes at low densities[3]. Rectification of repelling particles in an asymmetric channel can also be induced by time-correlated thermal fluctuations (thermal ratchets). However, being thermal ratchets weak in general and collective geometric ratchets less performing than potential ratchets, demonstration of such an effect seems beyond reach. On the other hand, rectification of Brownian diffusion by an internal energy source, like the nonequilibrium fluctuations invoked to power thermal ratchets, is very appealing: The diffusing particles would harvest kinetic energy directly from their environment, without requiring any externally applied field (though unbiased), and transport would ensue as an *autonomous* symmetry-directed particle flow.

To enhance rectification of time correlated-diffusion in a modulated channel with zero drives, we propose[6] to use active, or self-propelled, Brownian particles. Recently, a new type of microswimmers has been synthesized, where self-propulsion takes advantage of the local gradients that asymmetric particles can generate in the presence of an external energy source (self-phoretic effect). Such particles, called Janus particles[5], consist of two distinct "faces", only one of which is chemically or physically active. Such two-faced objects can induce either concentration gradients, by catalyzing some chemical reaction on their active surface, or thermal gradients, by inhomogeneous light absorption (self-thermophoresis) or magnetic excitation (magnetically induced self-thermophoresis. We also demonstrated the ability of Janus microswimmers to and separate colloidal mixtures, due to their selective interaction with the constituents of the mixture[7].

II. ACTIVE SWIMMER IN A CHANNEL

An active microswimmer acquires a continuous push from the environment, which in the overdamped regime corresponds to a self-propulsion velocity $\vec{v}_0$ with constant modulus v_0 and direction randomly varying in time with rate τ_θ^{-1}. In a two-dimensional (2D) boundless suspension, the position $\vec{r}(t) = (x(t), y(t))$ of the microswimmer diffuses according to Fürth's law $\langle \Delta\vec{r}(t)^2\rangle = 4(D_0 + v_0^2\tau_\theta/4)t + (v_0^2\tau_\theta^2/2)(e^{-2t/\tau_\theta} - 1)$, where $\Delta\vec{r}(t) = \vec{r}(t) - \vec{r}(0)$ and D_0 is the translational diffusion constant of a passive particle of the same geometry at a fixed temperature. The mechanisms responsible for translational and rotational diffusion are not necessarily the same and therefore D_0, v_0 and τ_θ can be treated as independent model parameters. The Fürth's diffusion law is due to the combined action of two statistically independent 2D Gaussian noise sources[8], a delta-correlated thermal noise, $\vec{\xi}_0(t)$ and a colored effective propulsion noise, $\vec{\xi}_c(t)$, with correlation functions $\langle\xi_{0,i}(t)\rangle = 0$, $\langle\xi_{c,i}(t)\rangle = 0$, $\langle\xi_{0,i}(t)\xi_{0,j}(0)\rangle = 2D_0\delta_{ij}\delta(t)$, and $\langle\xi_{c,i}(t)\xi_{c,j}(0)\rangle = 2(D_c/\tau_\theta)\delta_{ij}e^{-2|t|/\tau_\theta}$, with $i, j = x, y$ and $D_c = v_0^2\tau_\theta/4$. Correspondingly, the microswimmer mean self-propulsion path is $l_\theta = v_0\tau_\theta$.

In a channel, with compartment size smaller than l_θ, the microswimmer undergoes multiple collisions with the walls and the confining geometry comes into play (Knudsen diffusion). Contrary to standard thermal ratchets in asymmetric potentials[9], where the strength of the colored noise is kept constant, here D_c grows linearly with τ_θ (i.e., the variance of $\vec{\xi}_c(t)$ is set to v_0^2). As a consequence, increasing τ_θ not only makes geometric rectification effective even in the case of a single particle, but also enhances the power dissipated to fuel its self-propulsion. As a result, rectification in active Brownian ratchets can be so much stronger than in ordinary thermal ratchets that *direct observation* becomes possible.

III. AUTONOMOUS JANUS RATCHET

The rectification of a Janus particle in a 2D asymmetric channel was simulated[6] by numerically integrating the Langevin equations[8], $\dot{x} = v_0\cos\theta + \xi_{0,x}(t)$, $\dot{y} = v_0\sin\theta + \xi_{0,y}(t)$, $\dot{\theta} = \xi_\theta(t)$, where $\xi_{0,x}(t)$ and $\xi_{0,y}(t)$ have been defined above and $\xi_\theta(t)$ is an additional 1D Gaussian noise with $\langle\xi_\theta(t)\rangle = 0$ and $\langle\xi_\theta(t)\xi_\theta(0)\rangle = 2D_\theta\delta(t)$, modeling the fluctuations of the self-propulsion angle θ, measured, say, with respect to the *positive* channel easy-flow direction.

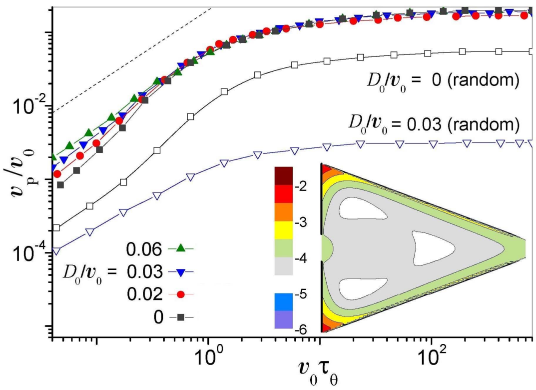

FIG. 1. Rectification of a single pointlike Janus particle with self-propulsion speed v_0 in a triangular channel with compartment size $x_L = y_L = 1$: the average velocity $\bar{v}$ vs. τ_θ for channel pore size $\Delta = 0.1$, different D_0 and sliding (filled symbols) or randomized b.c. (empty symbols). probability density $P(x, y)$ in a channel compartment. [*After* Ref. 6].

Fig. 1 shows the results[6] for the rectification current, $v_p \equiv \langle \dot{x} \rangle$ (in units of v_0), of a pointlike Janus particle in a triangular channel with fixed compartment dimensions and varying τ_θ. At large τ_θ, microswimmer diffusion is of the Knudsen type and rectification is dominated by self-propulsion; all curves $\bar{v}(\tau_\theta)$ increase monotonously with τ_θ until they level off. The curves $v_p(\tau_\theta)$ at low τ_θ shift upwards on raising the thermal noise level D_0, therefore, thermal noise *assists* the rectification process. At large τ_θ the rectification power is *suppressed* by the thermal fluctuations[6]: $\vec{\xi}_0(t)$ assists the Janus particle to bypass the compartment corners. Therefore, the diode-funneling effect exerted by the triangular compartments can be either enhanced or weakened by delta-correlated fluctuations.

IV. BINARY MIXTURES SEPARATION

We proposed[7] a new mechanism of binary mixtures separation, using self-propelled Janus microswimmers. The average velocity (along the channel) $\langle V_x \rangle$ of particles A and B versus the effective self-propulsion force $\vec{F}_{drx}$ is shown in Fig. 2. In general case, particles A (small) move *faster* than their counterpart. We distinguish four regimes. (1): *Rigid body motion.* (2): *Inverse velocity motion.* This unusual behavior is explained by the stronger interaction of the MS with particles B than with particles A. As a consequence, particles B are carried along by the MS while the dynamical friction due to the particle motion is very small in this case and can be neglected. (3): *Strong flow separation.* With increasing velocity, the dynamical friction becomes increasingly important, and type A particles (characterized by a larger self-diffusion coefficient) move faster. (4): *Fast MS motion.* At large F_{drx}, the system undergoes a transition to a "quasi-rigid body" regime when the MS moves too fast to produce any responce of the binary system.

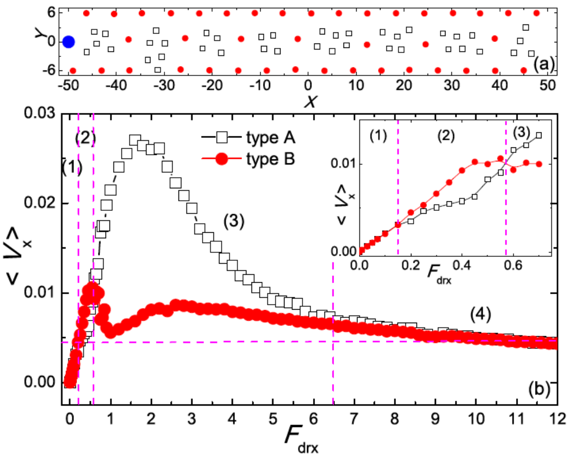

FIG. 2. (a) Equilibrium configuration of a system with equal number of particles of the two species $N_A = N_B = 40$. (b) The average velocity of particles of type A, $\langle V_x^A \rangle$ (open squares) and B, $\langle V_x^B \rangle$ (red dots), as a function of F_{drx}. The MS is shown by a blue filled circle. [*After* Ref. 7].

ACKNOWLEDGMENTS

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