RICC Usage Report for Fiscal Year 2013

Project Title:

Using Artificial Microswimmers for Particle Rectification

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1. Background and purpose of the project

Diffusion in a narrow asymmetric channel can be rectified according to Curie's conjecture. The constituents of a mixture of repelling particles in a periodically modulated channel are pressed against the channel walls so that their dynamics becomes sensitive to any asymmetry of the channel compartments (collective geometric ratchet). Subjected to an ac drive oriented along the channel axis, the mixture drifts in the easy-flow direction, where the average compartment corrugation is the less steep, although with much lower efficiency than in ordinary ratchet potentials. Such a collective ratchet mechanism has been experimentally observed for ac drives and relatively high particle densities, whereas the net current apparently vanishes at low densities. A simple kinetic equation argument suggests that rectification of mixtures of repelling particles, or even single particles, in an asymmetric channel can also be induced by timecorrelated thermal fluctuations, like in thermal ratchets. However, being thermal ratchets weak in general and (low-density) 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 to use a special type of diffusive tracers, namely, active self-propelled Brownian particles. Self-propulsion is the ability of most living organisms to move, in the absence of external drives, thanks to an "engine" of their own. Self-propulsion of micro- and nanoparticles (artificial microswimmers) poses a challenge with respect to their unusual nonequilibrium diffusion properties as well as their applications to nanotechnology. Recently, a new type of microswimmers has been synthesized, where selfpropulsion 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, 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). Moreover, experiments demonstrated the ability of Janus microswimmers to perform guided motions through periodic arrays and separate colloidal mixtures, due to their selective interaction with the constituents of the mixture.

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 system temperature was set to a constant, and the dynamics simulation was analyzed 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 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

Autonomous Janus ratchets.

In Fig. 1 we report our results for the rectification current, of a pointlike Janus particle in a triangular channel with fixed compartment dimensions and varying τ_θ, panel (a), and pore size Δ, panel (b). In panel (a) the pore size was set to 0.1 and several curves were computed for different diffusion coefficients, at different temperatures, and sliding boundary conditions (bc, filled symbols). At large τ_θ, microswimmer diffusion is of the Knudsen type and rectification is dominated by self-propulsion; all curves $<v>(\tau_\theta)$ increase monotonically with τ_θ until they level off [see Fig. 1(b)]. Most importantly, we obtained ratios $<v>/v_0$ in excess of 20%, which means that here the rectification power is orders of magnitude larger than for single-particle thermal ratchets in an asymmetric potential. Moreover, the simulation parameter values adopted here, in rescaled units, are consistent with the corresponding values reported in the experimental literature, hence, the possibility of a direct demonstration of this striking effect. Moreover, we also enlarged the compartments by a scaling factor κ, so as to accommodate for a variety of experimental set-ups. One immediately sees that the rectification power decreases by only a factor 2 for x_0 up to 0.2 and is insensitive to κ. For much larger κ, the particle spends most of its time away from the (asymmetric) compartment walls and $<v>$ drops inversely proportional to κ.

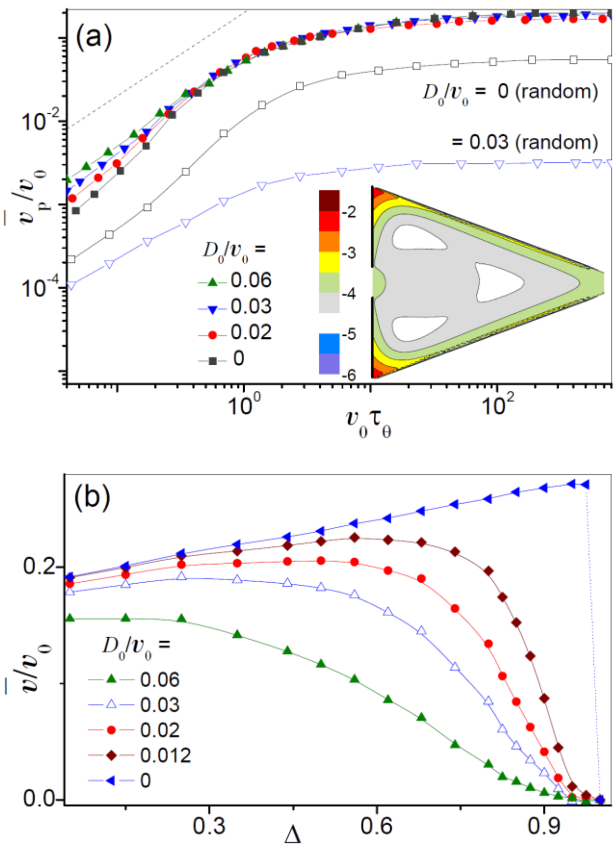

Figure 1. Rectification of a single point-like Janus particle with self-propulsion speed v_0 in a triangular channel with compartment size $x_L = y_L = 1$: (a) average velocity $<v>$ vs τ_θ for channel pore size D = 0.1, different diffusion constants D_0 and sliding (closed symbols), or randomized *bc* (open symbols). The dashed line has slope 1.

Inset: (logarithmic) contour plot of the stationary probability density $P(x,y)$ in a channel compartment; (b) average velocity $<v>$ vs D for different D_0, sliding bc, and $\tau_\theta = 300$.

In view of practical applications, we tested the robustness of Janus particle rectification in channels with variable degrees of asymmetry. In Fig. 2 we varied the channel geometry by symmetrically shifting the compartment corners by a fixed amount $0 < x_0 < 0.5$ (see inset).

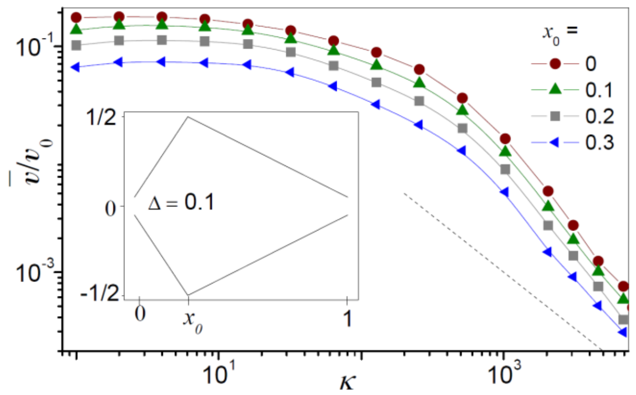

Figure 2. Rectification of a single Janus particle with self-propulsion speed v_0 in asymmetric channels with different geometries with compartment size $x_L = y_L = 1$, for channel pore size $\Delta = 0.1$, but the corners are shifted by x_0. A typical compartment is sketched in the inset. The compartment dimensions are rescaled by a magnification factor κ. Main panel: average velocity $<v>$ vs κ for $\tau_\theta = 300$, sliding *bc* and different x_0. The dashed line has slope -1.

Janus particles as autonomous pumps.

The remarkable robustness of the rectification mechanism investigated here lends itself to practical applications. Thus we investigated the effect of autonomous pumping in a binary mixture of N_m Janus microswimmers and N_p passive particles, when the microswimmers act on passive particles and induce their directed motion.

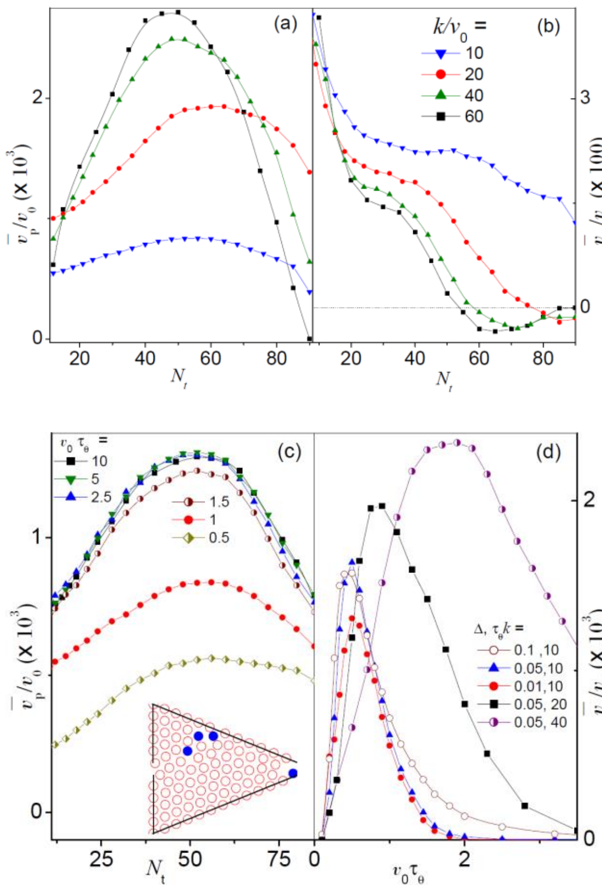

Figure 3. Rectification of a binary mixture made of $N_m = 4$ Janus particles with self-propulsion speed v_0, zero thermal fluctuations, $D_0 = 0$, and $N_p = N_t - N_m$ passive particles. All particles are modeled as elastically repelling soft disks of radius $r_0 = 0.05$; channel compartments are triangular with dimensions $x_L = y_L = 1$.

Inset: active particles are represented by (blue) closed circles, and passive particles by (red) open circles.

Panels (a) and (b): average rectification velocity of (a) passive, $<v_p>$ and (b) active particles, $<v_m>$, versus N_t for $\Delta = 0.1$ and different interaction constant, k [see legend in (b)].

Panels (c) and (d): (c) $<v_p>$ vs N_t for $\Delta = 0.1$ and different τ_θ; (d) $<v_p>$ vs τ_θ for $N_t = 72$ and different Δ and k. Note that $l_0 = v_0/k$ is a measure of the disk overlap, so that $\tau_\theta k = l/l_0$.

Conclusions

Using numerical simulations, Brownian transport of self-propelled overdamped microswimmers (i.e., Janus particles) in a 2D periodically compartmentalized asymmetric channel has been investigated for different compartment geometries, boundary collisional dynamics, and particle rotational diffusion. The resulting time-correlated active Brownian motion is subject to rectification in the presence of spatial asymmetry.

We demonstrated that ratcheting of Janus particles is much stronger than for ordinary thermal potential ratchets and thus experimentally accessible.

We showed that autonomous pumping of a large mixture of passive particles can be induced by just adding a small fraction of self-propelled Janus particles.

We stress that the autonomous rectification and pumping effects apply to biological and artificial swimmers regardless of their propulsion mechanism, and not only to especially fabricated Janus particles.

Examples:

- Autonomous laser-driven robots (with propulsion speed v_0 and 10mm across and thus negligible translational diffusion).
- Cellular systems where propulsion of macrobiomolecules can be fueled by the "power-stroke" associated with the hydrolysis of ATP in suspension. In that case, $v_0 \sim \delta r/\tau_\theta$, where δr is the net displacement produced by a single power-stroke and τ_θ-1 coincides with the ATP hydrolyzation rate in the vicinity of the biomolecule.

Fiscal Year 2013 List of Publications Resulting from the Use of RICC

[Publication]

1. 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). DOI: http://dx.doi.org/10.1103/PhysRevLett.110.268301

Featured as: PRL's Editors Suggestion

2. Pulak K. Ghosh, Vyacheslav R. Misko, Fabio Marchesoni, and Franco Nori, The Effects of Ratcheting and Autonomous Pumping of Self-Propelled Janus Particles, in preparation.

3. Fabio Marchesoni, Rectification of Janus particles in a narrow channel,
Abstracts of the 7th International Conference "Engineering of Chemical Complexity"
(Rostock-Warnemunde, Germany), June 10-13, 2013.

4. Vyacheslav R. Misko, Pulak K. Ghosh, Fabio Marchesoni, and Franco Nori, Self-propelled Janus particles in an asymmetric channel: Effects of rectification and autonomous pumping, Bulletin of the March Meeting 2014 of the American Physical Society (APS March Meeting 2014), Denver, Colorado, 3 – 7 March, 2014. S15.00002.