Usage Report for Fiscal Year 2017

Project Title: Transport properties of self-propelled micro-swimmers

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I. Background And Purpose:

A type of specially designed synthetic micro-particles is capable of propelling itself by harvesting kinetic energy from an active environment. Unlike bacteria, self-propulsion of synthesized micro-swimmers is fueled by external non-equilibrium processes, like directional mechanical impulses from catalytic chemical reactions or self-phoresis by short-scale (electric, thermal, or chemical) gradients generated by the particles themselves through some built-in functional asymmetry. In a quiescent suspension fluid such "active" swimmers undergo time-correlated Brownian motion, also termed active Brownian motion.

Transport properties of artificial micro-swimmers, like, Janus particles, are very unusual as well as very interesting. They can exhibit autonomous motion when their interaction with substrate potential is asymmetric and periodic in nature. Even in asymmetric corrugated channels conspicuous ratcheting of Janus particles has been reported. In some special non-equilibrium situations JPs can move opposite to the driving force. All these features fascinate researchers to learn more precisely about the motion of particle so that they can be used in targeted drug delivery and other purposes in medical sciences.

Keeping mind all recent relevant advances of research on transport properties of self-propelled Janus particles, we studied their dynamics in a binary mixture of two active species. Adding a fraction of active micro-swimmers, such as self-propelled Janus particles, to a suspension of passive colloids, results in increasing mobility of the latter specie. However, in the case of active micro-swimmers, adding a fraction of other active particles, characterized by even higher motility, can result in a very non-trivial behavior when the hosted, i.e., "more active" specie transfers its motility to the host specie. This enhanced motility of the host specie can be controlled by tuning the parameters of the guest specie, e.g., the intensity of light in the case of light-induced Janus particles. Our findings can be potentially useful for various biological and medical applications. Thus, the fertilization rate can be improved in this way by enhancing the motility of "weak" sperm cells.

Effects of more active particles on the dynamics of less active particles can be characterized by computing velocity distribution, effusion, and diffusion for the both species in the mixture. Our study mainly based on numerical simulation of coupled Langevin equations. In the next section we formulate the Brownian dynamics of interacting Janus particles which we implement in our numerical simulation code.

II. Model

Consider a system comprised of two types of micro-swimmers with different propulsion velocities in a thermal bath. In this binary mixture, N_m self-propellers are moving with a modulus of self-propelled velocity, v_m and the rest have self-propelled velocity modulus, v_p. All the species are represented by interacting disks of radius r_0. They encounter repulsive force whenever they cross

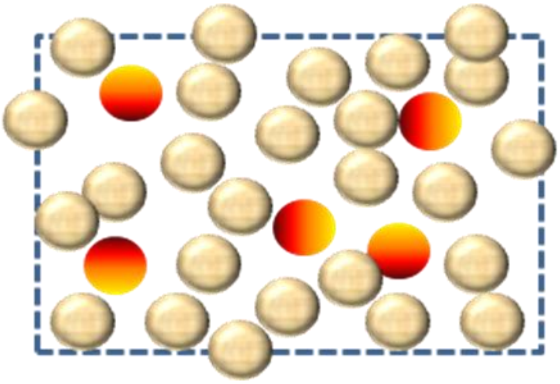

Fig1: Schematic of two types of active particles in the binary mixture.

a critical inter-particle distance. They encounter repulsive force whenever they overlap each other. The modulus of repulsive force has been represented as,

$$F_{ij} = k(2r_0 - r_{ij}) \qquad \text{if } r_{ij} \le 2r_0 \qquad ---(1)$$
$$= 0 \qquad\qquad \textit{otherwise}$$

Where, k is the interaction strength.

The dynamics of self-propelled particles in the xy-plane can be described by the following set of Langevin equations.

$$\ddot{x}_i = -\gamma\dot{x}_i + \gamma v_0 \cos\phi_i + \gamma\sum_j F_{ij}^{x} + \gamma\sqrt{2D_0}\,\xi_i^{x}(t) \text{-- } (2a)$$
$$\ddot{y}_i = -\gamma\dot{y}_i + \gamma v_0 \sin\phi_i + \gamma\sum_j F_{ij}^{y} + \gamma\sqrt{2D_0}\,\xi_i^{y}(t) \text{-- } (2b)$$
$$\dot{\phi} = \sqrt{2D_\phi}\,\xi_i^{\phi}(t). \qquad \text{--------------} \ (2c)$$

The particle with instantaneous position $\{x_i, y_i\}$ diffuses in the force field under the combined action of self-propulsion and equilibrium thermal fluctuations. $\{\xi_{x_i}, \xi_{y_i}\}$ are components of random thermal fluctuation, responsible only for translational diffusion, is modeled by a Gaussian white noises with,

$$\left\langle \xi_i^q(t) \right\rangle = 0$$
$$\left\langle \xi_i^q(t)\xi_j^{q'}(0) \right\rangle = 2\delta_{ij}\delta_{qq'}\delta(t)$$

Where q or q' = $\{x, y\}$. The thermal noise strength, $D_0 = k_BT/\gamma$ can be estimated by measuring the translational diffusion of a free JP in the bulk in the absence of propulsion. In equations (2-3), γ plays the role of an effective viscous damping constant incorporating all additional effect that are not explicitly accounted for in Eq. (2), like hydrodynamic drag, particle-wall interactions, etc.

The propulsion velocity v_i, with modulus v_0, directed making an angle ϕ_i with respect to the laboratory x-axis. $v_0 = v_m$ or v_p depending upon the type of particle in the binary mixture. Due to rotational diffusion of the particle, $\square_i$ changes randomly, which can be described as a Wiener process, as described in eq.(2c), with following statistical properties

$$\left\langle \xi_\phi(t) \right\rangle = 0$$
$$\left\langle \xi_{\phi i}(t)\xi_{\phi j}(0) \right\rangle = 2\delta_{ij}\delta(t)$$

The rotational diffusion constant D_θ is related to the viscosity (η_v) of the medium, temperature (T) and size of the particle. For spherical particle with radius a, rotational diffusion constant can be expressed as $D_\phi = k_BT/8\pi\eta_v r_0^3$. However, rotational diffusion may contain contribution of gradient fluctuations that are very much related to mechanism of acquiring self-propulsion. The mechanisms and origins of the translational and rotational diffusion may not be the same. Thus, D_0, v_0, and $D_\square$ can be treated as independent model parameters.

The terms $\{F_{ij}^q\}$ in eq.(2) are the component of force described in the eq.(1).

III. Numerical simulations method

We numerically integrate Eq. (2) by a standard Milstein algorithm to obtain velocity distribution, diffusivity and effusion rate of the both kinds of species in the binary mixture. Numerical integration has been performed with very short time step, 10^{-4} -10^{-6}, to ensure numerical stability. For estimating velocity distribution and diffusivity no confinement is required. But to simulate the system with constant number density we set up a simulation box. Within the box total the number of particles is kept fixed using spatial periodic boundary condition. On the other hand, to simulate the effusion rate we assume the particles are confined in a box of dimension $x_L \times y_L$. This area is accessible for to center of the particles. The particles can exit the box through very small opening, $\Delta + 2r_0$ (effective size of the opening is Δ). The opening can be located at any position of the wall. Simulating a constrained JP requires defining its collisional dynamics at the boundaries. For the translational velocity we assumed elastic reflection. Regarding the coordinate ϕ, we assumed that it does not change upon collision (sliding boundary conditions (b.c.). As a consequence, the active particle slides along the walls until the orientational fluctuations, ξ_ϕ, redirect it toward the interior of the compartment. We compute the effusion rate, define as number of particles exit through pore per unit time, for different particle swimming properties and confinement geometries. At the initial time, t = 0, the particle are assumed to be uniformly distributed with random orientation in the box. To have constant number density, particles are re-injected to a randomly chosen position within the box with a random orientation whenever they escape from the confinement. The running time was set to $10^4 \times \tau_\phi$, or 10^4 whichever is greater, so as to neglect transient effects due to initial conditions. The data points reported in the figures (in the result and discussion section) obtained by ensemble averaging over no less than 1000 trajectories.

IV. Results and Discussion

Based on the above mentioned model and simulation scheme we produced some interesting simulation results for velocity distribution and effusion rate in the binary mixture.

Velocity distribution of active swimmers. — It is known that the velocity distribution is not defined for overdamped particles. In this case, particles perform motion only during the action of the external forces (e.g., a thermal Brownian motion and collisions to other particles) or due to self-foretic forces in the case of active particles moving with self-propulsion velocity v_0. Therefore, to be able to define the velocity distribution, one should introduce inertia effects. Our analysis shows that inertia effects are important when the inverse damping constant $1/\gamma$ is comparable or greater than the rotational relaxation time, $2/D_{\square}$. The corresponding velocity distribution for $\gamma = 1$ and varying rotational diffusion constant D_φ is shown in Fig. 2.

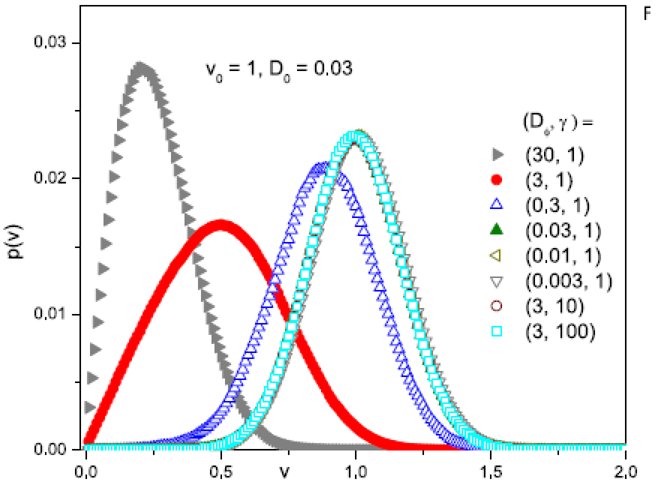

Fig.2: Velocity distribution of non-interacting active particles for different rotational diffusion and damping.

It is apparent from the Fig.2, when viscous relaxation time is much shorter than any other relevant time scale of the system, the distribution is centered at self-propelled velocity. As the broadening of the peak is due to thermal noise, one can expect a Gaussian type distribution center around v_0.

Next, we consider a mixture of active particles of two sorts. We call one of the species "passive" active particles, i.e., the ones with a fixed self-propulsion velocity. The other species, i.e., active particles with tunable self-propulsion velocity, is called "active" active particle. The results presented in Fig. 3 reveal the following behavior. The velocity distribution of "passive" particles hardly affected by slow "active" particles (i.e., small values of self-propulsion) and it is entered around their own propulsion speed. However for large self-propulsion of the active particles distribution peak is shifted to right. This signifies a substantial enhancement of the motility of “passive” particles. Our simulations show that, simultaneously, the corresponding velocity distributions of the “active” particles substantially decrease. This means that the velocity is effectively transferred from more active “active” particles to “less active” particles.

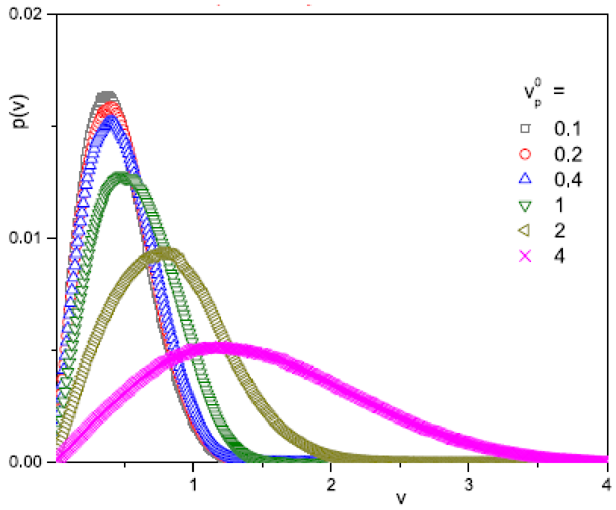

Fig.3: Velocity distribution of one active species for different propulsion velocity of active particles of another kind.

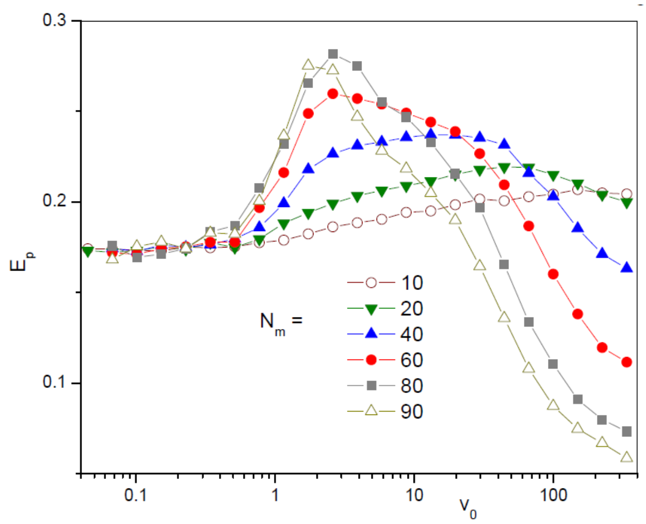

Fig.4: Effusion of passive (less active particles) as function of the self-propulsive velocity of more active particles for different composition of binary mixture comprise of 100 particles.

Effusion — We also explore the effusion of the particles in the mixture to better understand velocity transfer between two kinds of particles. The effusion rate, is defined as a number of particles escaping the reservoir with particles through the opening, per unit time. Our simulation results show that effusion rate of the less active particles can be increased by adding more active particles in the mixture. It is apparent from the Fig.4, effusion rate of "passive" particles improved considerably even in the presence small fraction of "active" particles (large propulsion strength) in the mixture. All the curves display a maximum whose position depends on the density of the "active" particle.

In *summary*, we have analyzed the effect of active microswimmers characterized by tunable high motility on other active microswimmers which have a lower motility. that cannot be directly controlled. An example of such a system could be sperm cells (of insufficient motility for the fertilization) and active Janus microswimmers whose motility can be controlled in a broad range by, e.g., external light of tuned intensity. We showed that, by injecting a small fraction of more active" microswimmers (Janus particles, in the above example), we can substantially enhance the motility of the other, "less active", specie (slow sperm cells). This enhancement of the motility has been demonstrated by exploring velocity distributions and effusion rate.

V. Future plan

More simulations from last years' proposed research - In the last fiscal year, we have used Hokusai supercomputer mainly to explore velocity distribution and effusion rate. We have produced some interesting results to capture essential dynamical features of the interacting self-propelled particles in the binary mixture. However, to arrive at the concluding point on these issue we need some more simulation. Also we also need to simulate diffusivity for the both types of species in the mixture to have complete understanding about how dynamics of one kind of particles affected by another kind.

In the fiscal year 2018, in addition to the above item we intend to explore some important issues on entropic and hydrodynamic interaction of active particles.

Entropic and hydrodynamic effects - Two peculiar types of interactions – entropic and hydrodynamic – affect the motion of a Brownian particle, active and passive alike, diffusing in narrow channels (e.g., blood vessel system or artificial micro-tube systems). Brownian diffusion in a confined geometry is a difficult problem that attracted the interest of biologists as well as engineers. Recently published new exciting results, which go beyond the well-established phenomenology, reviewed in [5], and might be key to the success of the present project.

By measuring the diffusive dynamics of micrometric colloidal particles through tailored narrow channels, in collaboration with an experimental team from the Shanghai Jiao Tong University (China) [6], we discovered that, as the channel's width shrinks close to the particle diameter, hydrodynamic effects, largely ignored in previous studies, grow in strength and become comparable, or even larger than the known entropic effects.

By extending this kind of analysis to artificial micro-swimmers, we intend to numerically investigate the local diffusivity of active colloidal particles in confined structures with the purpose of separating the entropic and hydrodynamic contribution to active micro-fluidic transport.

In narrow channels, the hydrodynamic interactions between a micro-swimmer and the channel walls can influence the hydrodynamic near field associated with its self-propulsion mechanism. The resulting self-propulsion on the swimmer can be modulated in speed and persistence time, by the very geometry of the channel. This activity, prominently based on reduced ab intio calculation schemes, will greatly profit from the outstanding computing facility available at RIKEN. To addressed the above mentioned issues we will follow the similar numerical scheme as mentioned in the section III.

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 2019) under the same user category.

VI. References

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[4] D Debnath, P. K Ghosh, Y Li, F Marchesoni, B Li, Diffusion of eccentric microswimmers, Soft matter 12, 2017-2024 (2016).

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[6] X. Yang, C. Liu, Y. Li, F. Marchesoni, P. Hanggi, and H. P. Zhang, Colloidal diffusion in corrugated channels: Entropic versus hydrodynamic interactions, PNAS (2017), PNAS 114, 36 (2017)

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Fiscal Year 2017 List of Publications Resulting from the Use of the supercomputer

[Publication]

(1) Diffusion of active dimers in a Couette flow; T. Debnath, P. K Ghosh, F. Nori, Y. Li, F. Marchesoni, B. Li, Soft Matter, vol- 13, Issue-15, Pages 2793-2799, published on 16th March 2017.

(2) Two-dimensional dynamics of a trapped active Brownian particle in a shear flow
Yunyun Li, Fabio Marchesoni, Tanwi Debnath, and Pulak K. Ghosh, Physical Review E, vol. 96, Article no. 062138, published on 26 December 2017.

[Proceedings, etc.]

None

[Oral presentation at an international symposium]

Invited talk:
International Conference on Nanotechnology: Ideas, Innovations and Initiatives, held at IIT Roorkee, Roorkee, India
Title of the talk: Transport properties of Janus particles in corrugated channels
Date: 8th December 2017

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

None