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Autonomous motion of Janus particles in presence of space dependent propulsion strength

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Abstract
I have studied effect of fuel concentration gradient on autonomous rectification and mobility of Janus particles in confined geometries as well as in presence of interaction with substrates. For this purpose dynamics of an over damped Janus particle in presence of a space dependent self-propulsion have been considered. At first I have calculated the rectification average current and diffusivity of a point like Janus particle in corrugated channel with fixed compartment dimensions where the period of the self-propelled velocity is varying. Next I have calculated the rectification average current and diffusivity of a point like Janus particle in presence of interaction with substrates where each particle interacts with the substrate via a non-periodic potential. The present study provides a better understanding of the diffusion phenomenon in such a situation where fuel is distributed in homogeneously. Biological channel is an example of perfectly inhomogeneous medium. Thus, when, one attempts to transfer a Janus particle through such channel to a targeted place for drug delivery, particles diffuse in a medium where fuels are non-uniform. Thus, present study could motivate researcher to utilize Janus swimmers in medical sciences. It can help the experimentalists to fix the appropriate shape and size of the microwswimmers while guiding them through biological channel in the purpose of targeted drug delivery.

Keywords: Janus particles, fuel concentration gradient, rectification, confined geometries, targeted drug delivery

1. Introduction

Earlier investigations on ratcheting of Janus particles focus on transport in spatially periodic structures come into play due to interaction with substrate or confinement. In these studies space dependence of self-propulsion (which arises naturally due to gradient of fuel concentration) has been ignored. However, a type of chemical 'robots' have been designed that use artificial chemotaxis to navigate autonomously. Such systems are potentially important to design new and more efficient drug delivery applications. In view of this it is worthwhile to investigate ratcheting mechanisms of JPs in presence of fuel concentration gradient. I have studied effect of fuel concentration gradient on autonomous rectification and mobility of Janus particles in confined geometries as well as in presence of interaction with substrates. For this purpose dynamics of an over damped Janus particle in presence of a space dependent self-propulsion have been considered. Simulation results show a profound effect of space dependent self-propulsion (which may arise due to in homogenous distribution of fuel over space) on the diffusivity and ratcheting.

3. The Model

An artificial micro-swimmer enhances its diffusion by harvesting kinetic energy from its suspension fluid, as a result of some sort of functional asymmetry. The particle thus propels itself with constant speed v_0 but keeps changing direction due to both environmental fluctuations (and asymmetry, spatial disorder) and the intrinsic randomness of the propulsion mechanism itself. For sake of simplicity we restrict ourselves to the two-dimensional case of an over damped swimmer with coordinates x and y in a fixed Cartesian frame, then its spatial diffusion is described by the Langevin equations (LE).

$$\frac{dx}{dt} = v_0 \cos\theta + \sqrt{D_0}\,\xi_x(t) \ldots.(1), \quad \frac{dy}{dt} = v_0 \sin\theta + \sqrt{D_0}\,\xi_y(t) \ldots.(2)$$

$$\frac{dx}{dt} = v_0 \cos\theta + \sqrt{D_0}\,\xi_x(t) \ldots (1)$$

$$, \frac{dy}{dt} = v_0 \sin\theta + \sqrt{D_0}\,\xi_y(t) \ldots (2)$$

Where D_0 is the intensity of the thermal noise and θ (t) denotes the instantaneous direction of the propulsion velocity with respect to the x axis. Accordingly, the swimmer's angular dynamics modeled by a third LE,

$$\frac{d\theta}{dt} = \sqrt{D_\theta}\,\xi_\theta(t) \quad \ldots(3)$$

Where D_θ is the intensity of the rotational fluctuations. The noises appearing in all three Langevin equations are Gaussian, stationary, zero-mean valued and delta-correlated. The effective dynamics of Janus particles (JPs) becomes more complicated in the presence of hydrodynamics interactions, confinements and interaction with substrates. Therefore, we carry out research work based on Langevin description.

Numerical simulation of Langevin equation: Most often the exact analytical solution of the Langevin equation is very difficult. In such a situation one can bypass the difficulty by numerically solving the Langevin equation. The stochastic differentials equations (1-2) and (3) can be solved simultaneously by using standard Heun's method which is essentially an improved Euler method. The noise due to thermal fluctuation and rotational diffusion is generated by using a standard Box-Muller algorithm. A very small time step 10^{-3} to 10^{-2} for numerical integration is used depending on the requirements of the initial conditions are chosen. To calculate any average quantity the focus must be on the asymptotic regime where the effect due to the influence of initial conditions and transient processes are smoothed out. The time homogeneous statistical properties are obtained in the long time after the temporal and the ensemble averaging are performed. So in the calculation any time homogeneous statistical property double-averaging (temporal and ensemble) is performed.

4. Results and discussions

I have studied effect of fuel concentration gradient on autonomous rectification and mobility of Janus particles in confined geometries and in presence of interaction with substrates. For this purpose dynamics of an overdamped Janus particle in presence of a space dependent self-propulsion have been considered. Simulation results show a profound effect of space dependent self-propulsion (which may arise due to inhomogenous distribution of fuel over space) on the diffusivity and ratcheting. For confined structure, I have considered corrugated channel directed along x axis with sinusoidal form like, $w(x) = \sin(2\pi x / L_2) + 0.25\sin(4\pi x / L_2) + \Delta$, Where L_2 is the period of the channel and Δ determines the size of the opening. The particle transverse coordinate, y, is bounded between a lower and upper wall, $w_-(x) \le y \le w_+(x)$. Such a sinusoidal channel is periodic; its compartments have length L_2 and are mirror symmetric under both coordinate inversions, x→-x and y→-y, i.e. centro symmetric. Throughout analysis I have assumed that the width, Δ of the pores connecting the compartments are much narrower than the maximum channel cross-section. I have taken self-propulsion velocity by the following form: $v(x) = v_0(1 + a\sin(2.0\pi x / L_1 + \phi_1))$.

The effect of the heterogeneity in fuel distribution has been captured by the second term of the above equation, which varies in space periodically with a period L_1. With these form of the propulsion and confinement I have numerically simulated the Langevin equations to find average velocity and diffusivity. The dispersion of a Brownian particle along the channel axis is an important issue for experimentalists to address when trying to demonstrate rectification. Indeed drift currents, no matter how weak, can be detected over an affordable observation time only if the relevant dispersion is sufficiently small. This issue is of paramount importance when one handles with active Brownian particles, like JP, whose stochastic dynamics is characterized by strong persistency or long correlation times. Under such conditions the current literature on classical diffusion is of little help. To this purpose I have computed the transport diffusivity, D of a JP in the corrugated channel as the limit $D = \lim_{t\to\infty}[\langle x^2(t)\rangle - \langle x(t)\rangle^2]/(2t)$, which I have checked to exit for all simulation parameters(normal diffusion limit).

The most important simulation results are presented below

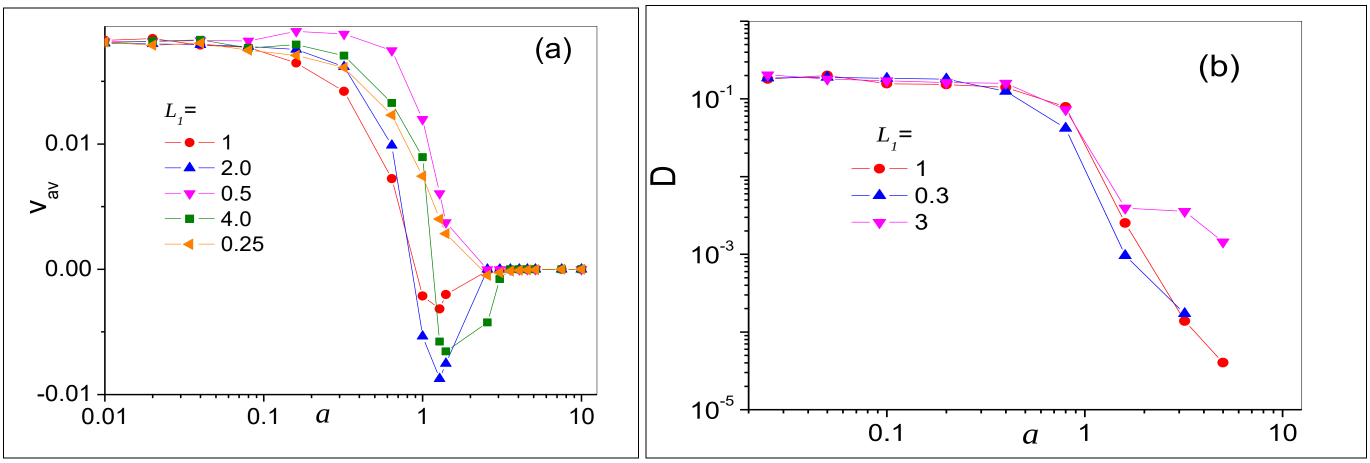

Fig.1 (a): Plot of the variation of average velocity of Janus particle with *a* for different L_1 where the choice of parameters are L_2=1.0, φ_1=0, v_0=2.0, D_0=0.03, D_θ=0.03. Fig.1 (b): Plot of the variation of diffusivity of Janus particle with *a* for different L_1 where the choice of parameters are L_2=1.0, φ_1=0, v_0=1.0, D_0=0.03, D_θ=0.03.

In Fig. 1(a) I report results for the rectification average current, v_{av} of a point like Janus particle in mentioned corrugated channel with fixed compartment dimensions where the period of the self-propelled velocity, L_1 is varying. Here pore size set to Δ=1.2. I have seen that the average current is almost unchanged upto a=1 for each curves. This is because for a<1 the self-propelled velocity of the Janus particle has the option to take such argument value of sine function that makes the modulus of self-propelled velocity quite same producing the average current almost unchanged. I have also seen that for greater value of 'a' average current falls quickly. This can be explained as for a>1, the argument of the sine function may take such value for which self-propelled velocity become zero making average current falls quickly. This is only possible when a>1. I have seen that for L_1=1 average current starts to increase producing minima. I have also noticed that this minima becomes more prominent for L_1=2 and 4. It can be explained in the way that for large values of L_1, the Janus particle traces the wall as it feels a potential energy surface as same as the profile of the confinement. So though the self-propelled velocity almost zero the Janus particle can fall as like a free particle under gravity. So the average velocity starts to increase which makes the minima.

In Fig.1 (b) I show results for the diffusivity of a point like Janus particle in mentioned corrugated channel with fixed compartment dimensions and varying L_1. I have seen that the diffusivity is almost unchanged up to a=1 for each curves. This is because for a<1 the self-propelled velocity of the Janus particle has the option to take such argument value of sine function that makes the modulus of self-propelled velocity quite same producing the diffusivity almost unchanged. I have also seen that for greater value of a diffusivity falls quickly. This can be explained as for a>1, the argument of the sine function may take such value for which self-propelled velocity becomes zero making diffusivity falls quickly. This is only possible when a>1. When a>1, the self-propelled velocity becomes nearly zero makes the active particle to simple Brownian particle.

I have also studied the effect of fuel concentration gradient on autonomous rectification and mobility of Janus particles in presence of interaction with substrates where each particle interacts with the substrate via a non-periodic potential of the form,

$$V(x,y) = -V_0 \sin(2\pi x/L) + 0.5c_0[1-\lambda\sin(2\pi x/L+\phi)]y^2,$$

Where L is the period of the potential, c_0 is the coupling constant, λ is the potential parameter and ϕ is the phase difference. The self-propulsion velocity is of earlier form. With these form of the propulsion and periodic substrate potential I have numerically simulated the Langevin equations to find average velocity and diffusivity. The most important simulation results are presented below:

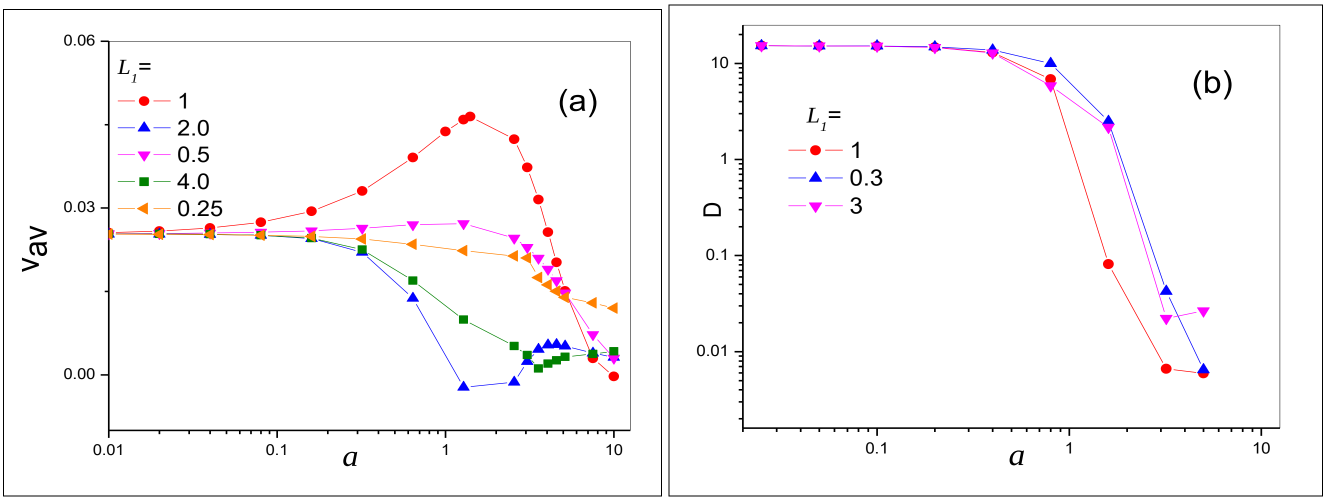

Fig.2 (a): Plot of the variation of v_{av} of Janus particle with a for different L_1 where the parameters are L=1.0, V_0=1.0, φ= π/2, φ_1= 0, λ=0.9, C_0=5.0, v_0=2.0, D_0=0.6, D_θ=0.03. Fig.2 (b): Plot of the variation of D of Janus particle with a for different L_1 where the parameters are φ_1 =0, v_0=1.0, D_0=0.03, D_θ=0.03.

In Fig.2 (a) I present results for the average current of a point like Janus particle in presence of interaction with substrates. Here different curves are taken where the period of the self-propelled velocity, L_1 is varying. I can categorize the observed results into three categories as follows. (i) For L_1<1(here L_1=0.25, 0.5): I have seen that average current is almost unchanged upto a=1. This is because for a<1 the self-propelled velocity of the Janus particle has the option to take such argument value of sine function that makes the modulus of self-propelled velocity quite same producing the average current almost unchanged. I have observed that average current falls gradually for a>1. This can be described as for a>1, the argument of the sine function may take such value for which self -propelled velocity becomes zero making average current falls.
(ii) For L_1=1: I have seen that when L_1=1 and L=1, average velocity increases upto a=1. This can be explained as for L_1=1 and L=1 the Janus particle gets a boost from substrates showing high value of self -propelled velocity. I have also observed that for greater value of a, average current falls due to already mentioned reason. So maxima is got due to interplay of propelled velocity and potential. (iii) For L_1>1 (here L_1=2, 4): I have seen that average current is almost unchanged upto a=1 due to already mentioned reason. I have also observed that for a>1, initially the average current falls quickly then increases producing minima. This can be explained as for L=1 and L_1>1, the Janus particle gets a late boost from substrates.

In Fig.2 (b) I depict results for the diffusivity of a point like Janus particle in the absence of both confinement and interaction with substrate. I have seen that the diffusivity is almost unchanged upto a=1 for every curves. This is because for a<1 the self-propelled velocity of the Janus particle has the option to take such argument value of sine function that makes the modulus of self-propelled velocity quite same producing the diffusivity almost unchanged. I have also seen that for greater value of a diffusivity falls quickly. This can be explained as for $a>1$, the argument of the sine function may take such value for which self-propelled velocity becomes zero making diffusivity falls quickly. This is only possible when $a>1$. When $a>1$, the self-propelled velocity becomes nearly zero makes the active particle to simple Brownian particle. So the nature of Fig.2 (b) is the same as Fig.1 (b) that means the diffusivity of a point like Janus particle with confinement behaves as neither confinement nor interaction with substrate.

5. Conclusions

In Fig.1 (a) I have got a new observation as for $L_1=1$ at $a>1$ average current produces minima. I have also noticed that this minima becomes more prominent for $L_1=2$ and 4.

In Fig.2 (a) I present results for the average current of a point like Janus particle in presence of interaction with substrates. Here different curves are taken where L_1 is varying. I have got several new observations which can be categorized into three categories as follows. (i) For $L_1<1$(here $L_1=0.25$, 0.5): I have observed that average current falls gradually for $a>1$. (ii) For $L_1=1$: I have seen that when $L_1=1$ and period of the potential, L=1, average velocity increases upto $a=1$ and for greater value of a average current falls. So maxima is got due to interplay of propelled velocity and potential. (iii) For $L_1>1$ (here $L_1=2$, 4): I have seen that average current is almost unchanged upto $a=1$. I have also observed that for $a>1$, initially the average current falls quickly then increases producing minima.

I have also got a significant observation that the nature of diffusivity of Janus particle with the variation of a in Fig.2 (b) is the same as in Fig.1(b). This means that the diffusivity of a point like Janus particle with confinement behaves same as for no confinement or for interaction with substrate.

The present study provides with us a better understanding of the diffusion phenomenon in such a situation where fuel is distributed inhomogeneously. Biological channel is an example of perfectly inhomogeneous medium. Thus, when, one attempts to transfer a Janus particle through such channel to a targeted place for drug delivery, particles diffuse in a medium where fuels are non-uniform. Thus, present study could motivate researcher to utilize Janus swimmers in medical sciences. It can help the experimentalists to fix the appropriate shape and size of the microwswimmers while guiding them through biological channel in the purpose of targeted drug delivery.

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