(Active) Brownian Transport in Narrow Channels

Fabio Marchesoni
Università di Camerino, Italy
Phononics Center, Tongji University, Shanghai

Gubbio, July 2017
Outline

self-propulsion

diffusion in a channel, autonomous rectification

experimental results

future developments
active diffusion
artificial active swimmers

**self-thermophoresis:** laser induced temp. gradient

**bubble propulsion:** from catalyzed \( \text{H}_2\text{O}_2 \) decomposition and moment transfer

**self-electrophoresis:** \( \text{H}^+ \) flow (from redox reactions catalyzed by the tips) induces a fluid flow and, thus, a swimmer backflow

---

Sano et al, PRL 105, 268301 (2010)

Gibbs&Zhao, APL 94, 163104 (2009)

A. Sen et al, PCCP 12 1423 (2010)
basic model

\[
\begin{align*}
\dot{x} &= v_0 \cos \phi + \xi_x (t) \\
\dot{y} &= v_0 \sin \phi + \xi_y (t) \\
\dot{\phi} &= \Omega + \xi_\phi (t), \quad \langle \xi_\phi (t) \xi_\phi (0) \rangle = 2D_\phi \delta(t)
\end{align*}
\]

thermal translational noise \( \langle \xi_i (t) \xi_j (0) \rangle = 2D_0 \delta_{ij} \delta(t) \)

white rotational noise mom. inertia \( I_0 = 1 \)

\[
\langle \cos \phi(t) \cos \phi(0) \rangle_{\text{asym}} = \left(\frac{1}{2}\right) e^{-\frac{D_\phi |t|}{\tau_\phi}}
\]

\[
\left\langle \Delta \hat{r}^2 (t) \right\rangle = 4(D_0 + D_s) t + 2D_s \tau_\phi \left( e^{-|t|/\tau_\phi} - 1 \right)
\]

\[
\overset{t \to \infty}{\Rightarrow} = 4(D_0 + D_s) t \quad \Rightarrow D_s = v_0^2 / 2D_\phi
\]

\( \Rightarrow \phi \) diffusion time \( \tau_\phi = 1/D_\phi \)

\( \Rightarrow \) persistence length \( l_\phi = v_0 / D_\phi \)

colored Brownian motion
chiral swimmers

asymmetric Janus particles: torque $\Omega$

\( D_s \rightarrow \frac{D_s}{1 + (\Omega / D_\phi)^2} \)

structured swimmers

(i) center of mass, O, and center of force, P, are a distance $\alpha$ apart on the JP axis;

(ii) $v_0$ fluctuates around the axis with constant $\kappa_\psi$ → additional instantaneous torque

\[
\begin{align*}
\dot{x} &= v_0 \cos(\phi + \psi) + \sqrt{D_0} \xi_x(t), \\
\dot{y} &= v_0 \sin(\phi + \psi) + \sqrt{D_0} \xi_y(t), \\
\dot{\phi} &= -(\alpha / I_\alpha) \sin \psi + \sqrt{D_\phi I_\phi} \xi_\phi(t), \\
\dot{\psi} &= -\kappa_\psi \psi + \sqrt{D_\psi} \xi_\psi(t),
\end{align*}
\]
**hydrodynamic effects**


**elastic dimer**: passive+active particles, constant $k$
finite radius $a \rightarrow$ hydrodynamic effects

laminar backflow by one particle affect the other:
**hydrodynamic coupling** (Oseen tensor)

as shown by dimer’s **diffusivity vs. radius**
active ratchets
swimmer rectifiers
asymmetric channels,

- **constant $v_0$, random $\phi$** with time constant $\tau_\phi$, overdamped, pointlike particle

- thermal noise and propulsion statistically **independent**

- **boundary conditions**: $\vec{r}$ elastically reflected, $\vec{v}_0$ unchanged (sliding b.c.);
  $\phi$ randomizing b.c. push particle away from walls, reduced efficiency

[Note: for both $\vec{r}$ and $\vec{v}_0$ elastically reflected $\Rightarrow$ inertial Brownian diffusion with $\gamma = 1/\tau_\phi$.]

Ghosh et al, PRL 110 268301 (2013)
autonomous pumps

binary mixture

- $N_m$ active (Janus) and $N_p$ passive with $N_m \ll N_p$ (low density)
- all soft repelling of the same geometry
- randomizing b.c. and no thermal noise (least favorable conditions)

a small fraction of Janus particles suffices to pump the entire mixture along the channel

elastic interaction $F = k(2a-r)$ for $r<2a = 0$ otherwise (soft repulsion)

$a=0.05$
chiral rectifiers
Li et al, PRE90 062301 (2014)

\[ R_{\Omega} = \frac{\Omega}{\nu_0} \]

\[ (x_0, \varepsilon) = (0, 1/4) \]

\[ w_+(x) = \frac{1}{2} \left[ \Delta + \varepsilon (y_L - \Delta) \sin^2 \left( \frac{\pi}{x_L} (x + x_0) \right) \right], \]

\[ w_-(x) = -\frac{1}{2} \left[ \Delta + (y_L - \Delta) \sin^2 \left( \frac{\pi}{x_L} x \right) \right], \]

boundary flow argument

\[ \hat{\nu} \]
experiments
unclogging (L. Balaban, Dresden)

active particles (low density) in a mixture of passive particles

transient effect due to “engagement” – no pumping in a symmetric channel
wall effects (HP Zhang, SJTU)

direct observation of active ratchets still inconclusive

hydrodynamics effects in a confined geometry

Liu et al, PRL 117 (2016) 198001

rectification demonstrated

hydrodynamic and wall effects as additional control parameters

wall interactions

courtesy of HP Zhang, SJTU
more manipulation techniques
tactic effects

assume a spatio-temporal modulation of the self-propulsion mechanism (active wave)

\[ v_0 \rightarrow v(x, t) = v(x - ut) \]

e.g., \[ v(x - ut) = v_0 \sin^2(\pi(x - ut)/L) \]

positive/negative taxis

\[ u \leq v_0; \ L^2/2D_0 \leq L/v_0 \]
Tactic flows are robust vs ballistic

- hydrodynamic effects (polarization)
- propulsion chirality
- wall effects

\[
v(x, t) = v_0 \sin^2 \left( \frac{\pi (x - ut)}{L} \right)
\]

- Geiseler et al, PRE 94, 012613 (2016);
hydrodynamic chaos

two active swimmers in a harmonic trap (optical tweezer) and shear flow (Couette)

\[ \dot{x} = v_0 \cos \phi - kx + u_s(y) + \xi_x(t) \]
\[ \dot{y} = v_0 \sin \phi - ky + \xi_y(t) \]
\[ \dot{\phi} = \Omega(y) + \xi_\phi(t), \]
two identical trapped swimmers, hydrodynamically coupled (Oseen tensor)

$\alpha=0$, no HD effects
Conclusions

• artificial microswimmers have **biomimetic properties**

• eg, **geometry controlled autonomous** rectification

• are easy to **manipulate**

• ideal for **microfluidic devices** with applications to **nano-energetics**
tactic effects
Special cases:

✓ $\langle \psi^2 \rangle = D_\psi / \kappa_\psi \ll 1$ standard model
✓ $\alpha = -\alpha$ nothing changes

Diffusion constant of active Brownian motion undergoes a transition from a **quadratic** to a **linear dependence** on the self-propulsion speed

\[
\begin{align*}
(1) \quad D - D_0 &= D_\psi I_\alpha e^{-D_\psi / \kappa_\psi} \quad \kappa_\psi \gg D_\psi/l_\alpha, \\
(2) \quad D - D_0 &= \frac{D_\psi I_\alpha}{I_\alpha D_\psi / D_\phi + 1} \quad \kappa_\psi \ll D_\psi/l_\alpha
\end{align*}
\]

(3) \quad $D - D_0 = \frac{v_0}{2} \sqrt{\frac{\pi}{2} \frac{I_\alpha}{\alpha}} \sqrt{\frac{\kappa_\psi}{D_\psi}} \quad \kappa_\psi \gg D_\psi/l_\alpha$

(4) \quad $D - D_0 = \frac{v_0}{2} \sqrt{\frac{\pi}{2} \frac{I_\alpha}{\alpha}} \quad \kappa_\psi \ll D_\psi/l_\alpha$
Chiral swimmers \((\Omega > 0)\)

\[
\dot{\phi} = \Omega + \xi_\phi(t), \quad \langle \xi_\phi(t) \xi_\phi(0) \rangle = 2D_\phi \delta(t)
\]

**transverse** tactic current, \(v_y(-\Omega) = -v_y(\Omega)\)

**x-symmetry breaking** due to \(\Omega & u\)

B-q Ai et al, JSAT (2015);
Li Y. et al, PRE (2014)
entropic channels

\[ \vec{r} = F \vec{e}_x + \vec{\xi}(t) \]

\( \vec{\xi}(t) \): Gaussian, \( \langle \vec{\xi}(t) \rangle = 0 \)
\( \langle \xi_i(t)\xi_j(0) \rangle = D_0 \delta_{ij} \delta(t) \)

\( w(x) \): channel radius/profile

overdamped, infinite damping (or zero mass): in the bulk \( v_F = F, D = D_0 \)

no analytical methods for a generic profile \( w(x) \); approximate analytical techniques

\[ \partial_t P(x, y, z; t) = \left[ -F \partial_x + D_0 (\partial_x^2 + \partial_y^2 + \partial_z^2) \right] P(x, y, z; t) \]
• dimension reduction: from 3D, 2D to a 1D effective transport equation

\[ \partial_t P(x; t) = \partial_x D(x) \left[ \partial_x + U'_{\text{eff}}(x)/D_0 \right] P(x; t) \]

\[ U_{\text{eff}}(x) = -Fx - D_0 \ln \sigma(x) \quad \text{entropic term} \]

\[ \sigma(x) = 2w(x) \quad \text{in 2D} \]

\[ = \pi w(x)^2 \quad \text{in 3D} \quad \text{cross section} \]

• analytical difficulty: an uncontrolled expansion

\[ D(x) = D_0/[1 + w'(x)^2]^{\alpha}, \quad \alpha = 1/2 \ (\text{in 3D}) \]

\[ = 1/3 \ (\text{in 2D}) \]

Reguera & Rubi, PRE, 2001
entropic ratchets

\[ \vec{r} = F \vec{e}_x + \xi(t) \]

\( w(x) \): asymmetric channel profile

\[
\partial_t P(x; t) = \partial_x D(x) \left[ \partial_x + A'(x) / D_0 \right] P(x; t)
\]

\[
A(x) = -Fx - D_0 \ln \sigma(x) \quad \text{entropic term}
\]

\[
\sigma(x) = 2w(x) \quad \text{cross section, } D(x) \sim D_0
\]

\( \Rightarrow \) ratchet mechanism