Dynamics and rectification of active Brownian particles

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Self-propelled (active) particles

Examples

- Molecular motors (complex proteins inside a cell)
- Bacteria with flagellae, such as *E. coli*, *H. pylori* or sperm cells
- Insects, birds, fishes, humans, etc.
- Artificial active particles, such as *Janus* particles

Types of active motion

- Run-and-tumble, motion
- Active Brownian motion
Self-propelled (active) particles

Run-and-tumble motion (picture by Dr. G. Kaiser)
Self-propelled (active) particles

Active Brownian particles (Janus particle)
(picture by Prof. Clemens Bechinger)
Overdamped active particle

Equations of motion

[M. Enculescu and H. Stark, PRL 107, 058301 (2011)]

\[ \dot{r} = -\mu \nabla U + v_0 p + \xi(t) \quad \dot{p} = \eta(t) \times p, \]

with

\[ \langle \xi_i(t)\xi_k(t') \rangle = 2\mu k_B T \delta_{ik}\delta(t-t'), \quad \langle \eta_i(t)\eta_k(t') \rangle = 2D_r \delta_{ik}\delta(t-t'). \]

parameters and variables

\( p \) ... the direction of swimming
\( r \) ... coordinate
\( v_0 \) ... magnitude of the propulsion velocity
\( T \) ... temperature
\( \mu \) ... mobility
\( D_r \) ... rotational diffusivity
Motion in 2D

\[ \dot{x} = -\mu \partial_x U(r) + v_0 \cos \alpha + \xi_x(t), \]
\[ \dot{y} = -\mu \partial_y U(r) + v_0 \sin \alpha + \xi_y(t), \]
\[ \dot{\alpha} = \eta(t) \]

Stationary velocity field and density in a square box

\[ v_x = \langle \cos \alpha \rangle, \quad v_y = \langle \sin \alpha \rangle \]
Rectification of self-propelled particles

**Known fact:**
Static ratchet-like one-dimensional periodic potential produces a unidirectional drift of active particles (rectification)

Active Brownian particles with modulated propulsion velocity [A. Pototsky et al PRE (2013)]

$L$-periodic spatial modulation

\[ v(z) = v_0[1 + w(z)], \quad \int_0^L w(z) \, dz = 0, \quad \min[1 + w(z)] \geq 0. \]

Langevin equation in 3D

\[
\dot{r} = -\mu \partial_z U(z) e_z + v(z) p + \xi(t), \quad \dot{p} = \eta(t) \times p.
\]

projection of $p(t)$ onto $z$-axis

\[ q(t) = \cos \theta = p(t) \cdot e_z \]

Motion along $z$ axis is decoupled
Equivalence to randomly driven pulsating ratchets

Motion along the modulation direction
\[ \dot{z} = v_0 q(t) - \frac{\partial U_{\text{eff}}(z, q(t))}{\partial z} + \xi(t) \]

Effective potential
\[ U_{\text{eff}}(z, q(t)) = \mu U(z) - q(t)v_0 \int w(z) \, dz \]

Stochastic dynamics of \( q(t) \) (Stratonovich interpretation)
\[ (3D) : \quad \dot{q} = -D_r q + \sqrt{1 - q^2} \eta(t), \quad (2D) : \quad \dot{q} = \sqrt{1 - q^2} \eta(t) \]

with
\[ \langle \eta(t) \eta(t') \rangle = 2D_r \delta(t - t'). \]
Equivalence to randomly driven pulsating ratchets

Stationary distribution and correlation function of $q(t)$

\[(3D): \quad R(q) = \frac{1}{2}, \quad \langle q(t)q(t') \rangle = \frac{1}{3}e^{-2D_r|t-t'|},\]

\[(2D): \quad R(q) = \frac{1}{\pi \sqrt{1-q^2}}, \quad \langle q(t)q(t') \rangle = \frac{1}{2}e^{-D_r|t-t'|}\]

Different operating regimes

- Slow rotation $D_r^{-1} \gg L/v_0$ (analytics available)
- Fast rotation $D_r^{-1} \ll L/v_0$ (analytics available)
- Zero-temperature $T = 0$
- Finite-temperature $T \neq 0$
Rectification conditions

- Average drift vanishes if the potential is zero $U(z) = 0$

- Average drift can be induced by a combination of a \textit{symmetric} potential $U(z)$ and \textit{symmetric} velocity modulation $w(z)$.

\textbf{Mechanism}

- Phase shifted periodic $U(z)$ and $w(z)$ give rise to asymmetry.
- Similar to the \textit{Seebeck} ratchet: symmetric temperature modulation and symmetric potential

$$U_{\text{eff}}(+q,z) \quad v_0$$

$$U_{\text{eff}}(-q,z) \quad v_0$$
Similarity with the Seebeck ratchet

Classical *Seebeck* ratchet [M. Büttiker (1987)]

\[
\dot{z} = -\mu U'(z) + \sqrt{2\mu k_B T(z)} \xi(t), \quad \langle \xi(t) \xi(t') \rangle = \delta(t - t').
\]

Both functions \(U(z)\) and \(T(z)\) are \(L\)-periodic

**Rectification condition**

\[
\int_0^L \frac{U'(z)}{T(z)} \, dz \neq 0
\]

**Active particle at \(T = 0\) is equivalent to Seebeck ratchet**

\[
T(z) \rightarrow \frac{[v_0(1 + w(z))]^2}{2\mu k_B}, \quad \xi(t) \rightarrow q(t)
\]
Slow rotation limit

Average current $\langle J \rangle = \langle \dot{z} \rangle$ for

$$U(z) = U_0 \sin \left( \frac{2\pi z}{L} \right), \quad w(z) = a \sin \left( \frac{2\pi z}{L} + \delta \right)$$

Dimensionless units

$$\frac{v_0 L}{\mu U_0} \rightarrow v_0, \quad \tau D_r \rightarrow D_r, \quad \frac{k_B T}{U_0} \rightarrow T,$$

where $\tau = \frac{L^2}{\mu U_0}$
**Zero $T$ limit, large $v_0$, large $D_r$**

**Process $q(t)$**

$$v_0 q(t) = v_0 \cos \theta(t) \rightarrow \text{white Gaussian noise}$$

**Effective motion reduces to the Seebeck ratchet**

$$\dot{z} = -\mu U'(z) + [1 + w(z)] \eta(t), \quad \langle \eta(t)\eta(t') \rangle = 2T_{\text{eff}} \delta(t-t'), \quad T_{\text{eff}} = \frac{v_0^2}{6D_r}$$

**Average current for $T_{\text{eff}} \rightarrow \infty$**

$$\langle J \rangle = -L \int_0^L \frac{\mu \partial_z U(z)}{(1 + w(z))^2} \left[ \int_0^L \frac{dz}{1 + w(z)} \right]^{-2}$$
Slow vs fast rotation

Large $T_{\text{eff}}$ implies either slow or fast rotation

Slow rotation (S): $v_0 = \gamma D_r$, $\gamma \gg 1$, $T_{\text{eff}} = \frac{v_0^2}{6D_r} \to \infty$

Fast rotation (F): $v_0 = \gamma D_r$, $\gamma \ll 1$, $T_{\text{eff}} = \frac{v_0^2}{6D_r} \to \infty$
Asymmetric barriers and constant propulsion velocity

Similar results are known for the Drift Diffusion Model
[L. Angelani et al, EPL (2011)]
Asymmetric barriers and symmetric velocity modulation

Current enhancement and reversal

\[ U(z) = \sin 2\pi z + 0.25 \sin 4\pi z, \quad v(z) = v_0[1 + a \sin (2\pi z + \delta)] \]
Slow or fast rotation limit?

Typical parameter values used in experiments with Janus particles by C. Bechinger et al

\[ D_r^{-1} = 1 \ldots 100 \text{s}, \quad L \approx 30 \mu\text{m}, \quad v_0 = 1 \mu\text{m/s}. \]

\( D_r \) is controlled by \( R^3 \), where \( R \) is the particle radius

Implies

- slow rotation limit: \( D_r^{-1} \gg L/v_0 \) for \( D_r^{-1} > 30 \)

- Implies fast rotation limit: \( D_r^{-1} \ll L/v_0 \) for \( D_r^{-1} \ll 30 \)
Left overs
The Fokker-Planck equation

\[(x(t), y(t), \alpha(t)) \Rightarrow \rho(x, y, \alpha, t)\]

\[
\partial_t \rho + \text{div} J_t - D_r \frac{\partial^2 \rho}{\partial \alpha^2} = 0,
\]

with the translational probability current \(J_t\)

\[
J_t = -\mu \nabla U(r) + v_0 p - \mu k_B T \nabla \rho
\]

Radially symmetric trapping potential \(U(r)\)
cylindrical coordinates \(x = r \cos \phi, y = r \sin \phi\)
Stationary density $\rho_s(r, \phi, \alpha)$

Direction-averaged stationary density

$$\int_0^{2\pi} \rho_s(r, \phi, \alpha) \, d\alpha = f(r) \Rightarrow \rho_s(r, \phi, \alpha) = \rho_s(r, \phi - \alpha)$$

Stationary F-P equation

$$\text{div} J_s^{\text{eff}} = 0,$$

$J_s^{\text{eff}}$ . . . effective probability current

$\psi = \alpha - \phi$ . . . new angle

$\mu U^{\text{eff}} = \mu U(r) - v_0 r \cos (\psi)$ . . . effective potential

Radial and angular effective current

$$(J_s^{\text{eff}})_r = -\mu k_B T \partial_r \rho_s - (\mu \partial_r U^{\text{eff}}) \rho_s,$$

$$r(J_s^{\text{eff}})_\psi = -[D_r r^2 + \mu k_B T] \partial_\psi \rho_s - (\mu \partial_\psi U^{\text{eff}}) \rho_s.$$
Limit of small $D_r$

Asymptotic expansion for the stationary density

$$\rho_s(r, \psi) = \rho_s^{(0)} + D_r \rho_s^{(1)} + D_r^2 \rho_s^{(2)} + \ldots$$

Leading order solution (non-dimensional units)

$$\rho_s^{(0)}(r, \psi) = C \exp(-U(r) + Pe r \cos \psi)$$

$Pe = d\nu_0/\mu k_B T \ldots$ the Peclet number

Radial density

$$\tilde{\rho}_s^{(0)}(r) = \int_0^{2\pi} \rho_s^{(0)}(r, \psi) \, d\psi \sim e^{-U(r)}I_0(Pe \, r)$$

Non-Boltzmannian due to active component of motion
Limit of large $D_r$

Asymptotic expansion for the stationary density

$$\rho_s(r, \psi) = e^{-U(r)} \left( \rho_s^{(0)} + \frac{1}{D_r} \rho_s^{(1)} + \frac{1}{D_r^2} \rho_s^{(2)} + \ldots \right)$$

Solution up to the order $1/D_r$

$$\rho_s = C e^{-U(r)} \left( 1 + \frac{2\text{Pe} \partial_r U(r) \cos \psi + \text{Pe}^2 U(r)}{2D_r} + O(D_r^{-2}) \right)$$

Radial density

$$\tilde{\rho}_s \sim e^{-U(r)} \left( 1 + \frac{\text{Pe}^2 U(r)}{2D_r} + O(D_r^{-2}) \right)$$
Strong vs weak trapping

Harmonic trapping potential $U(r) = \gamma r^2$

Critical Peclet number $\text{Pe}_c = \sqrt{2U''(r = 0)}$. 
Active hard discs in a harmonic trap

Stationary radial density of 50 discs (small $D_r$)

(solid lines) ... Active hard discs in a radial trap $U(r)$

⇔

(dashed lines) ... passive hard discs in an effective potential

$W_{\text{eff}} = U(r) - \ln I_0(\text{Pe}r)$