Dynamics and rectification of active Brownian particles

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Self-propelled (active) particles

Examples

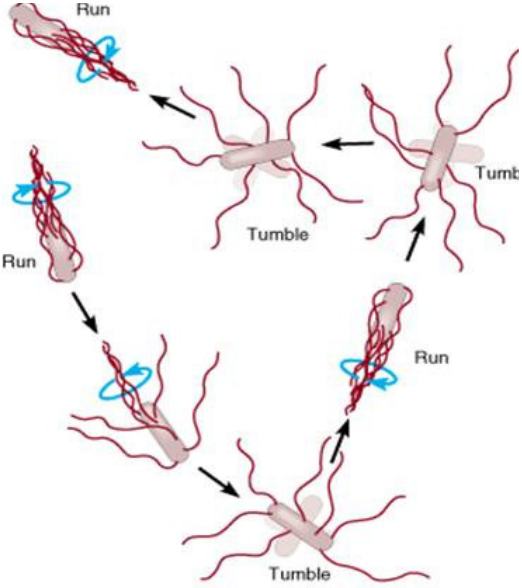
- Molecular motors (complex proteins inside a cell)
- Bacteria with flagellas, such as *E.coli*, *H.pylori* or sperm cells
- Insects, birds, fishes, humans, etc.
- Artificial active particles, such as *Janus* particles

Types of active motion

- Run-and-tumble, motion
- Active Brownian motion

Self-propelled (active) particles

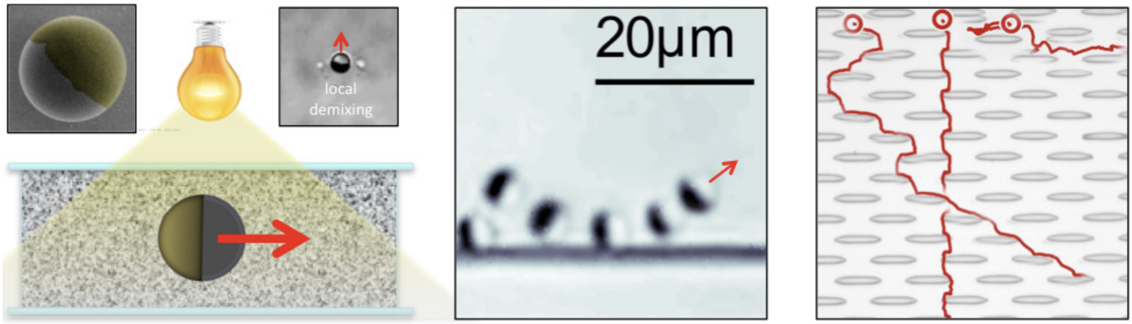
Run-and-tumble motion (picture by Dr. G. Kaiser)



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)]

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

with

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

parameters and variables

$\boldsymbol{p} \ldots$ **the direction of swimming**

$\boldsymbol{r} \ldots$ **coordinate**

$v_0 \ldots$ **magnitude of the propulsion velocity**

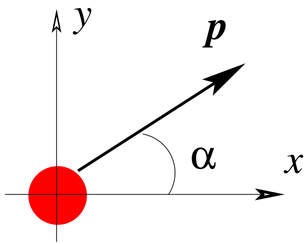
$T \ldots$ **temperature**

$\mu \ldots$ **mobility**

$D_r \ldots$ **rotational diffusivity**

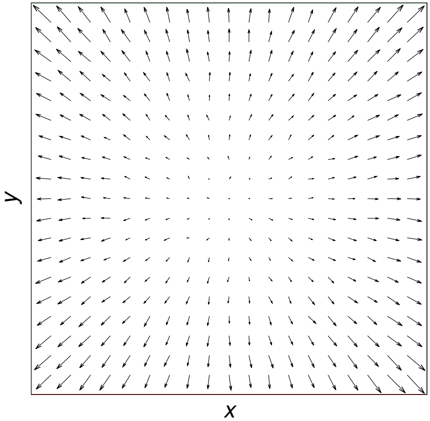
Motion in 2D

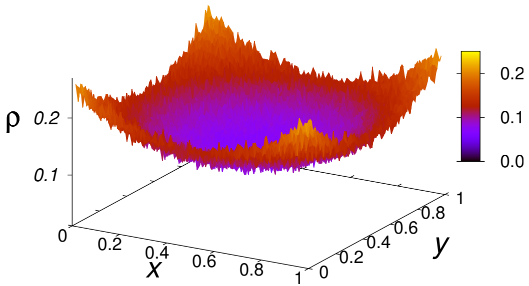
$$\begin{aligned}
\dot{x} &= -\mu \partial_x U(\boldsymbol{r}) + v_0 \cos\alpha + \xi_x(t), \\
\dot{y} &= -\mu \partial_y U(\boldsymbol{r}) + v_0 \sin\alpha + \xi_y(t), \\
\dot{\alpha} &= \eta(t)
\end{aligned}$$



Stationary velocity field and density in a square box

$$v_x = \langle \cos\alpha \rangle, \quad v_y = \langle \sin\alpha \rangle$$

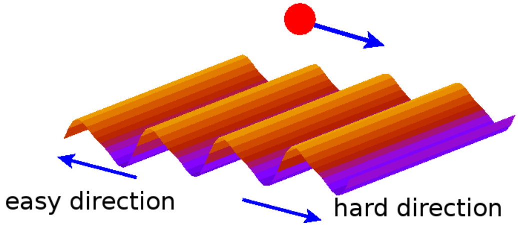




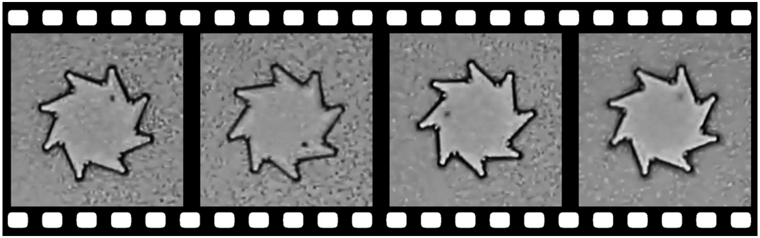
Rectification of self-propelled particles

Known fact:

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



Experiments by R. Di Leonardo *et al*, PNAS, 107 9541-9545 (2010)



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

L-periodic spatial modulation

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

Langevin equation in 3D

$$\dot{\boldsymbol{r}} = -\mu \partial_z U(z) \boldsymbol{e}_z + v(z)\boldsymbol{p} + \boldsymbol{\xi}(t), \;\; \dot{\boldsymbol{p}} \;=\; \boldsymbol{\eta}(t) \times \boldsymbol{p}.$$

projection of $\boldsymbol{p}$(t) onto z-axis

$$q(t) = \cos\theta = \boldsymbol{p}(t) \cdot \boldsymbol{e}_z$$

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)

$$(3D): \;\; \dot{q} \;=\; -D_r q + \sqrt{1-q^2}\,\eta(t), \quad (2D): \;\; \dot{q} = \sqrt{1-q^2}\,\eta(t)$$

with

$$\langle \eta(t)\eta(t') \rangle \;=\; 2 D_r \delta(t - t').$$

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** $T \neq 0$

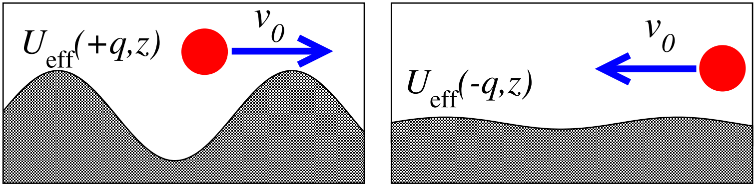
Rectification conditions

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

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

Mechanism

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



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

$$T(z) \to \frac{[v_0(1+w(z))]^2}{2\mu k_B}, \quad \xi(t) \to q(t)$$

Slow rotation limit

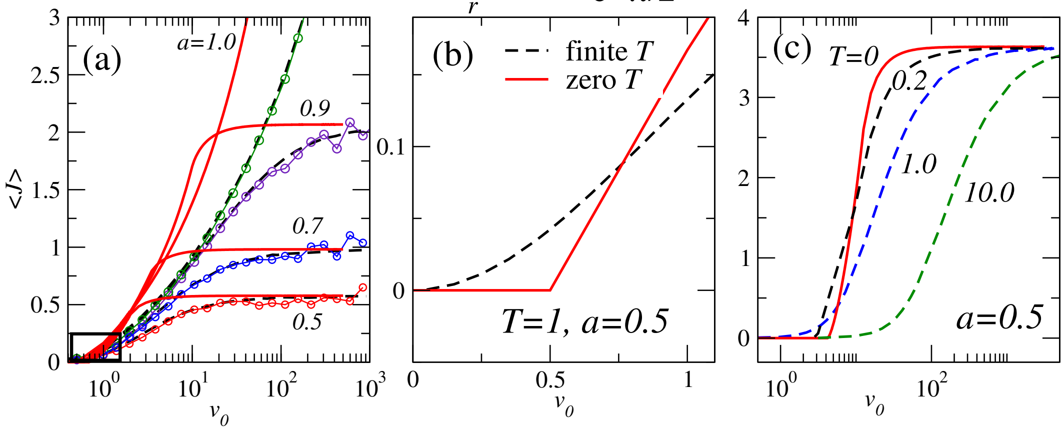
Average current $\langle J \rangle = \langle \dot{z} \rangle$ for

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

Dimensionless units

$$\frac{v_0 L}{\mu U_0} \to v_0, \quad \tau D_r \to D_r, \quad \frac{k_B T}{U_0} \to T, \quad \text{where } \tau = \frac{L^2}{\mu U_0}$$

$D_r = 20 \quad \delta = \pi/2$



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 $T_{\text{eff}} \to \infty$

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

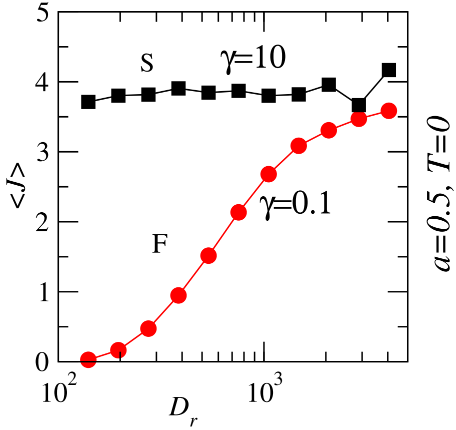
Slow *vs* fast rotation

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

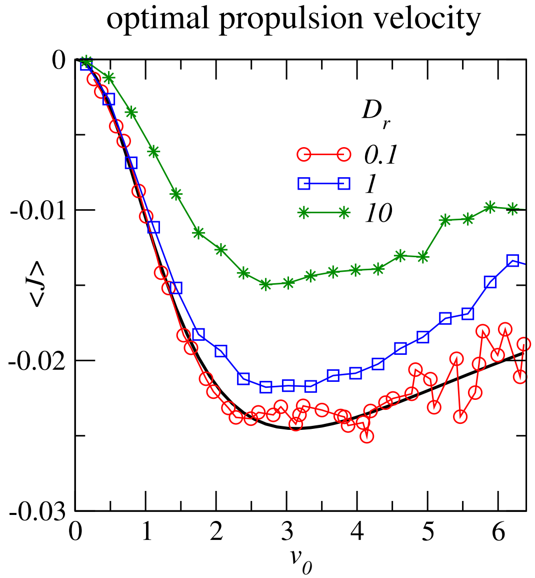
$$\text{Slow rotation (S)}: \; v_0 = \gamma D_r, \;\; \gamma \gg 1, \;\; T_{\rm eff} = \frac{v_0^2}{6D_r} \to \infty$$

$$\text{Fast rotation (F)}: \; v_0 = \gamma D_r, \;\; \gamma \ll 1, \;\; T_{\rm eff} = \frac{v_0^2}{6D_r} \to \infty$$

slow vs fast rotation



Asymmetric barriers and constant propulsion velocity

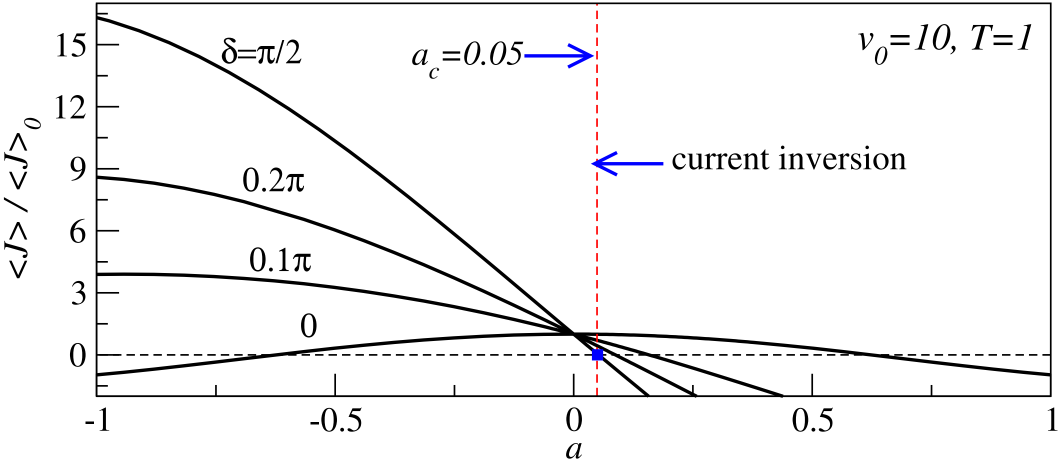


Similar results are known for the <u>Drift Diffusion Model</u>
[L. Angelani *et al*, EPL (2011)]

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*

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

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 fats rotation limit:** $D_r^{-1} \ll L/v_0$ **for** $D_r^{-1} \ll 30$

Left overs

The Fokker-Planck equation

$$\underline{(x(t), y(t), \alpha(t)) \Rightarrow \rho(x, y, \alpha, t)}$$

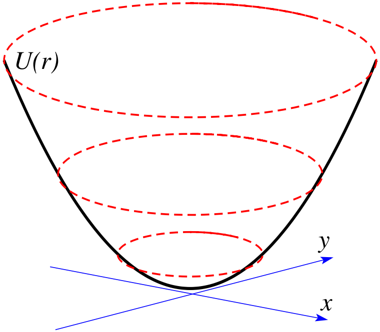
$$\partial_t \rho + \mathrm{div} \boldsymbol{J}_t - D_r \frac{\partial^2 \rho}{\partial \alpha^2} = 0,$$

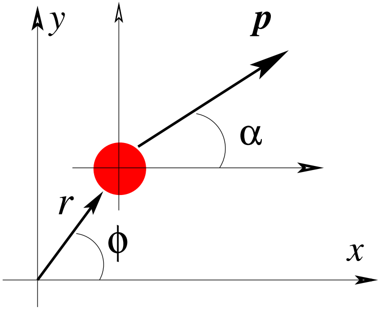
with the translational probability current $\boldsymbol{J}_t$

$$\boldsymbol{J}_t = -\mu \boldsymbol{\nabla} U(\boldsymbol{r}) + v_0 \boldsymbol{p} - \mu k_B T \boldsymbol{\nabla} \rho$$

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

$$\mathrm{div} \boldsymbol{J}_s^{\mathrm{eff}} = 0,$$

$\boldsymbol{J}_s^{\mathrm{eff}} \ldots$ **effective probability current**

$\psi = \alpha - \phi \ldots$ **new angle**

$\mu U^{\mathrm{eff}} = \mu U(\boldsymbol{r}) - v_0 r \cos(\psi) \ldots$ **effective potential**

Radial and angular effective current

$$\begin{aligned} (\boldsymbol{J}_s^{\mathrm{eff}})_r &= -\mu k_B T \partial_r \rho_s - (\mu \partial_r U^{\mathrm{eff}}) \rho_s, \\ r (\boldsymbol{J}_s^{\mathrm{eff}})_\psi &= -[D_r r^2 + \mu k_B T] \partial_\psi \rho_s - (\mu \partial_\psi U^{\mathrm{eff}}) \rho_s. \end{aligned}$$

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)

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

$\mathrm{Pe} = dv_0/\mu k_B T \ldots$ **the Peclet number**

Radial density

$$\tilde{\rho}_s^{(0)}(r) \;=\; \int_0^{2\pi} \rho_s^{(0)}(r,\psi)\, d\psi \sim e^{-U(r)} \mathrm{I}_0\left(\mathrm{Pe}\, r\right)$$

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 $1/D_r$

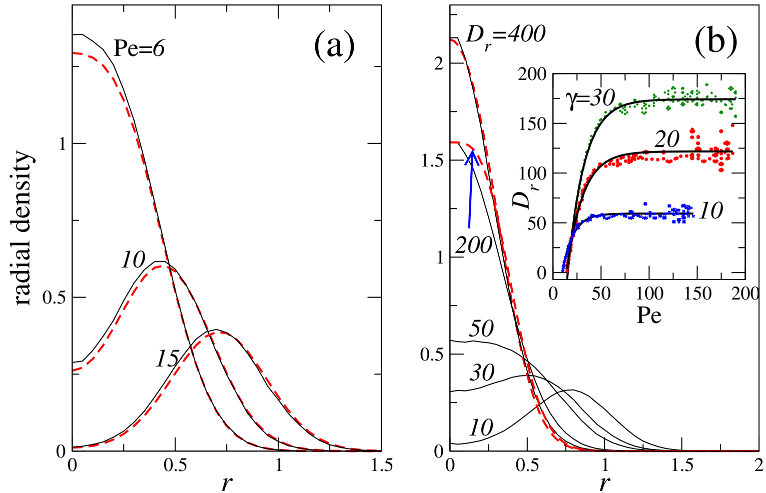
$$\rho_s = Ce^{-U(r)}\left(1 + \frac{2\mathrm{Pe}\,\partial_r U(r)\cos\psi + \mathrm{Pe}^{\,2}U(r)}{2D_r} + O(D_r^{-2})\right)$$

Radial density

$$\tilde{\rho}_s \sim e^{-U(r)}\left(1 + \frac{\mathrm{Pe}^{\,2}U(r)}{2D_r} + O(D_r^{-2})\right)$$

Strong *vs* weak trapping

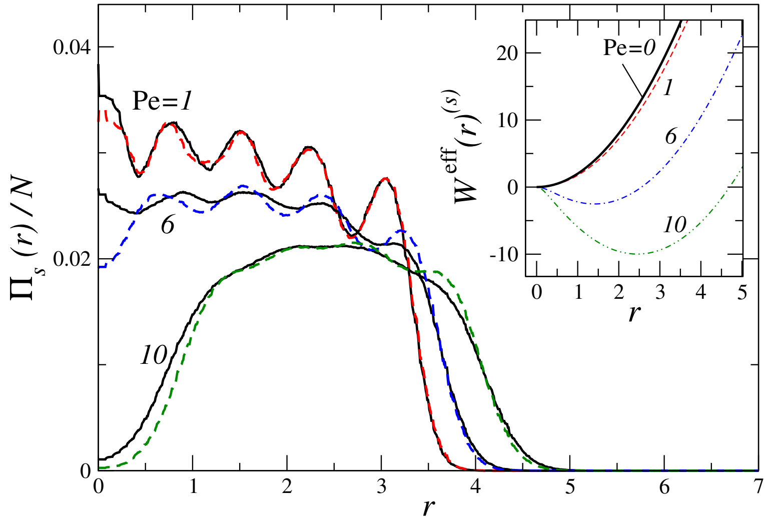
Harmonic trapping potential $U(r) = \gamma r^2$



Critical Peclet number $\mathrm{Pe}_c = \sqrt{2U''(r=0)}$.

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** $U(r)$

$\Updownarrow$

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

$$W_{\text{eff}} = U(r) - \ln \mathrm{I}_0(\mathrm{Pe}\, r)$$