Active Particles in Confined Environments

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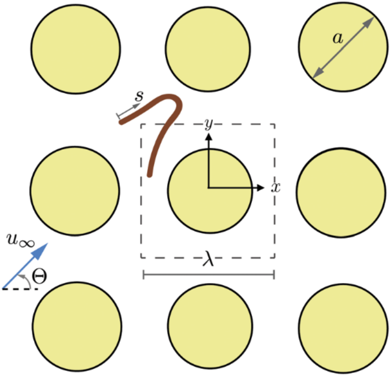
Active and passive particles in complex environments

Lots of interest, old and new, in passive and active particles scattering in periodic or random environments.

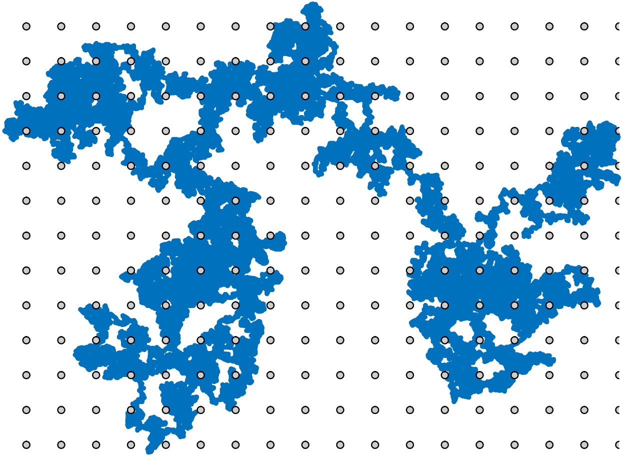
...
Brenner (1980)
Kamal & Keaveny (2018)
Alonso-Matilla *et al.* (2019)
Aceves-Sanchez *et al.* (2020)
Chakrabarti *et al.* (2020) $\Longrightarrow$
Amchin *et al.* (2022)
...



Many variations: different lattices, passive vs active, background flow, flexible vs rigid...

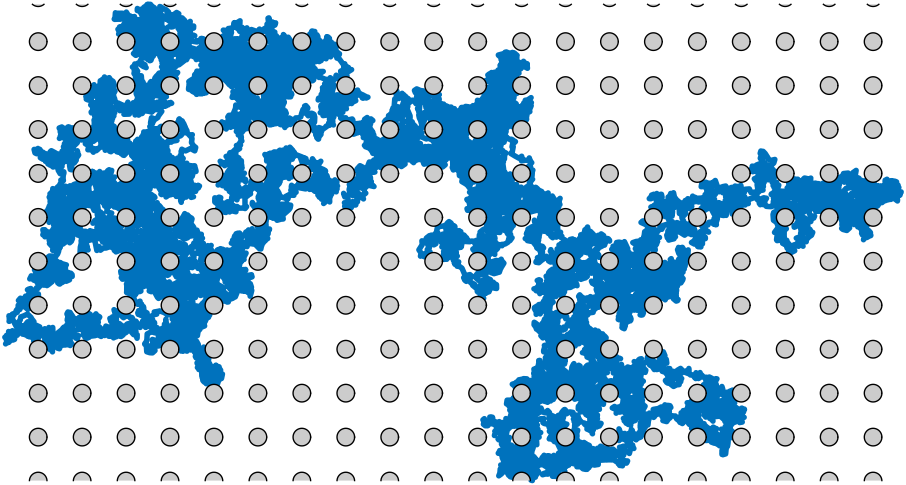
Passive disk in a lattice of point obstacles ($r = 0.1$)

A small disk doesn't feel the lattice much.

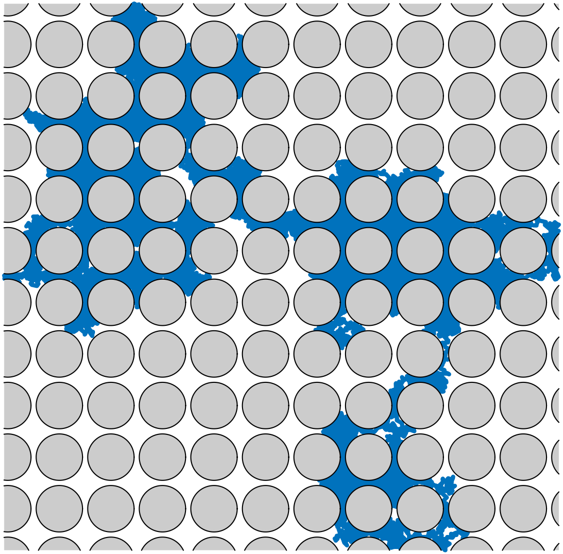


Passive disk ($r = 0.2$)

As the disk gets larger it is frustrated by the lattice.

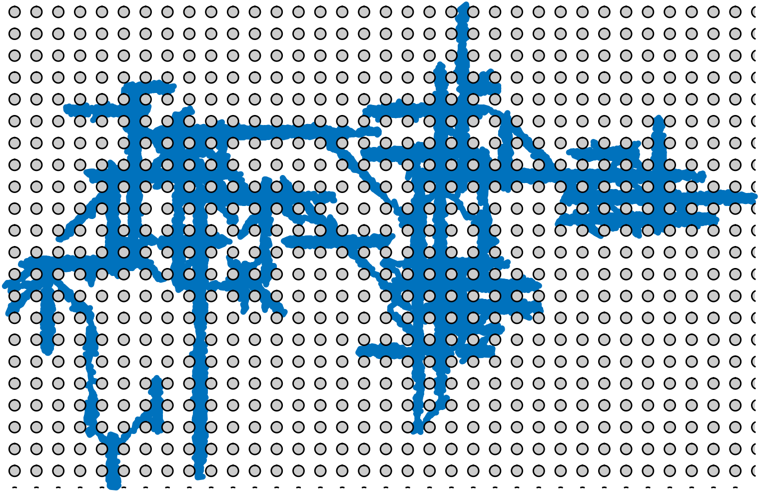


Passive disk ($r = 0.45$)



play movie

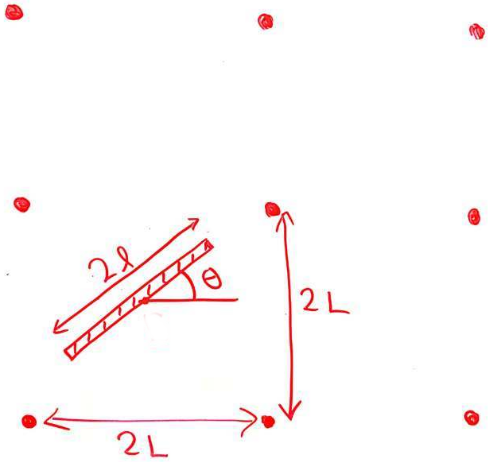
Passive ellipse ($a = 1,\ b = 0.25$)



For an ellipse the orientation angle is also Brownian.

A particle in a lattice of obstacles

2D periodic lattice of point obstacles, with rod-shaped particle as example.



Neglect hydrodynamic interactions.

Particle undergoes Brownian motion in space and angle:

$$\begin{aligned} \mathrm{d}X &= U\,\mathrm{d}t + \sqrt{2D_X}\,\mathrm{d}W_1 \\ \mathrm{d}Y &= \sqrt{2D_Y}\,\mathrm{d}W_2 \\ \mathrm{d}\theta &= \sqrt{2D_\mathsf{r}}\,\mathrm{d}W_3 \end{aligned}$$

Diffusion tensor in body frame (X, Y, θ):

$$\begin{pmatrix} D_X & 0 & 0 \\ 0 & D_Y & 0 \\ 0 & 0 & D_\mathsf{r} \end{pmatrix}$$

(X, Y) in body frame, (x, y) in lab frame.

Brownian dynamics: Diffusion tensor

Expressed in the fixed lab (x, y) frame, the spatial diffusion tensor is

$$\mathbb{D}(\theta) = \begin{pmatrix} D_X \cos^2\theta + D_Y \sin^2\theta & \frac{1}{2}(D_X - D_Y)\sin 2\theta \\ \frac{1}{2}(D_X - D_Y)\sin 2\theta & D_X \sin^2\theta + D_Y \cos^2\theta \end{pmatrix}.$$

Brownian dynamics: Fokker–Planck equation

Fokker–Planck equation for probability density $p(\boldsymbol{r}, \theta, t)$:

$$\partial_t p + \nabla_{\boldsymbol{r}} \cdot \boldsymbol{f} + \partial_\theta f_\theta = 0$$

Probability flux vector:

$$\boldsymbol{f} = \boldsymbol{U} p - \mathbb{D}(\theta) \cdot \nabla_{\boldsymbol{r}} p - D_{\mathsf{r}} \, \hat{\boldsymbol{\theta}} \, \partial_\theta p$$

Key point: account for obstacles with no-flux boundary condition

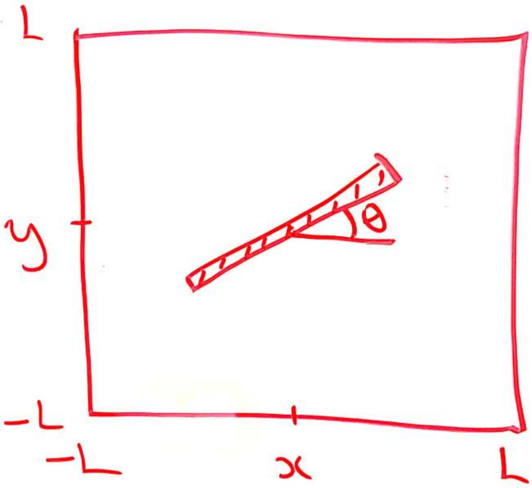
$$\boldsymbol{f} \cdot \hat{\boldsymbol{n}} = 0$$

on the surface of the obstacle, in the full 3D configuration space (x, y, θ).

[See Chen & Thiffeault (2021) for a similar approach in a channel.]

Configuration space: Fixed orientation

Configuration space gives allowable (x, y) for fixed θ.



A point in this periodic cell is a realizable configuration of the rod.

Effective diffusivity: Rayleigh's problem

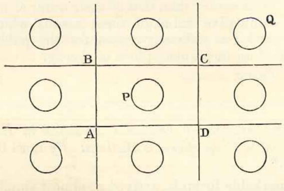
We've mapped the problem exactly onto heat conduction in a perforated medium.

For a disk-shaped passive particle (no drift, $\boldsymbol{U} = 0$), Rayleigh solved this by a reflection method.

482 Lord Rayleigh *on the Influence of Obstacles*

Since conduction parallel to the axes of the cylinders presents nothing special for our consideration, we may limit our attention to conduction parallel to one of the sides (α) of the rectangular structure. In this case lines parallel to α,

Fig. 1.



symmetrically situated between the cylinders, such as AD, BC, are lines of flow, and the perpendicular lines AB, CD are equipotential.

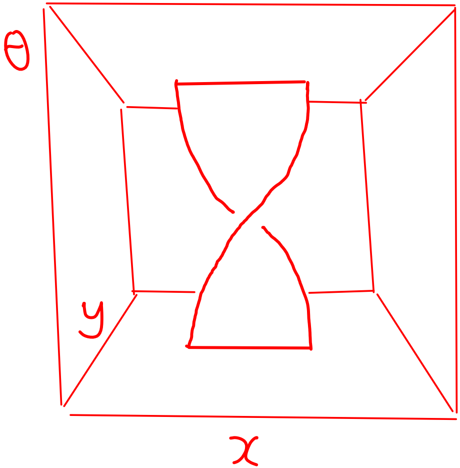
["On the influence of obstacles arranged in rectangular order upon the properties of a medium," Rayleigh, L. (1892). *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science,* **34** (211), 481–502]

Configuration space: Rotational diffusion

Now allowing $\theta \in [0, 2\pi]$ to vary, get 3D configuration space:

No-flux boundary condition at surface of 'obstacle,' so again we have a heat conduction problem, in a domain with obstacles in the shape of twisted ribbons.

As you might imagine, interesting things can happen when the 'ribbon' overflows the cell (long particle), but I won't talk about that today.



Homogenization approach

Rayleigh's approach is not very well suited to drift (swimmers) or to non-circular particles.

Homogenization theory allows us to find effective diffusivity by introducing a long time T and large scale $\boldsymbol{R}$ to get an effective heat equation:

$$\partial_T \Phi = \nabla_{\boldsymbol{R}} \cdot (\mathbb{D}_{\mathrm{eff}} \cdot \nabla_{\boldsymbol{R}} \Phi)$$

where the *effective diffusivity tensor* is

$$\mathbb{D}_{\mathrm{eff}} = \frac{1}{|\Omega \setminus \omega|} \left(\langle \mathbb{D} \rangle + \int_{\partial\omega} \hat{\boldsymbol{n}} \cdot \mathbb{D}\, \boldsymbol{\chi} \, \mathrm{d}A \right).$$

Notation: $\langle \cdot \rangle$ = integration over cell Ω, $|\cdot|$ = volume. The integral is over the 2D surface of the 3D perforation ω in (x, y, θ).

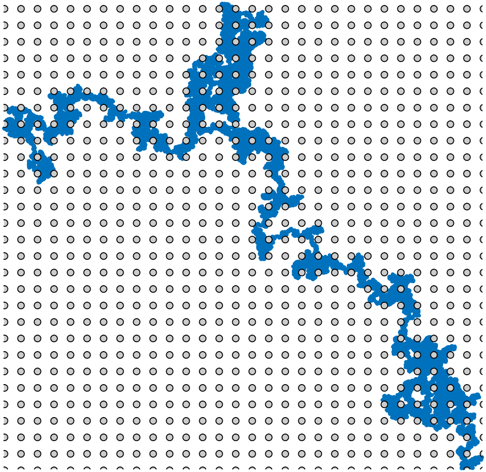
What is $\boldsymbol{\chi}$?

The cell problem

In the absence of drift, the cell problem for $\boldsymbol{\chi}$ is

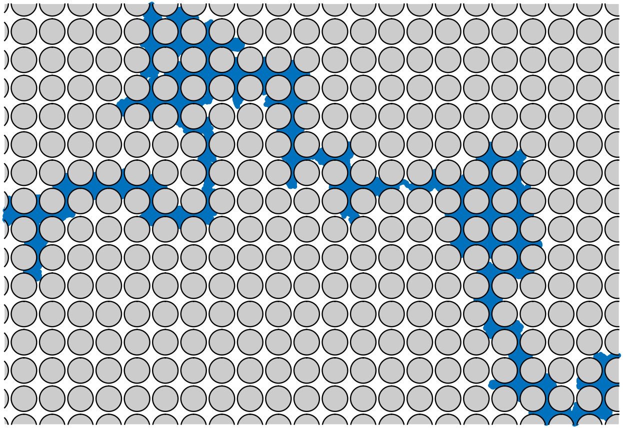
$$\begin{aligned} \mathbb{D} : \nabla_{\boldsymbol{r}} \nabla_{\boldsymbol{r}} \boldsymbol{\chi} &= 0, && \boldsymbol{r} \in \Omega \setminus \omega; \\ \hat{\boldsymbol{n}} \cdot \mathbb{D} \cdot \nabla_{\boldsymbol{r}} \boldsymbol{\chi} &= -\hat{\boldsymbol{n}} \cdot \mathbb{D}, && \boldsymbol{r} \in \partial\omega. \end{aligned}$$

Active disk ($r = 0.2$)



A "free" active particle has added diffusivity $U^2/2D_\mathsf{r}$.

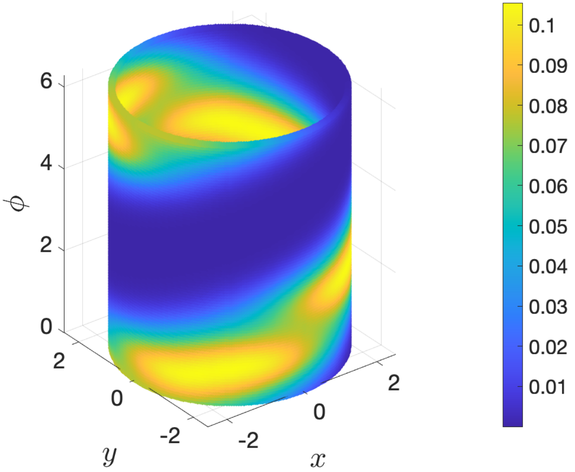
Active disk ($r = 0.45$)



An active disk progresses through the lattice much faster.

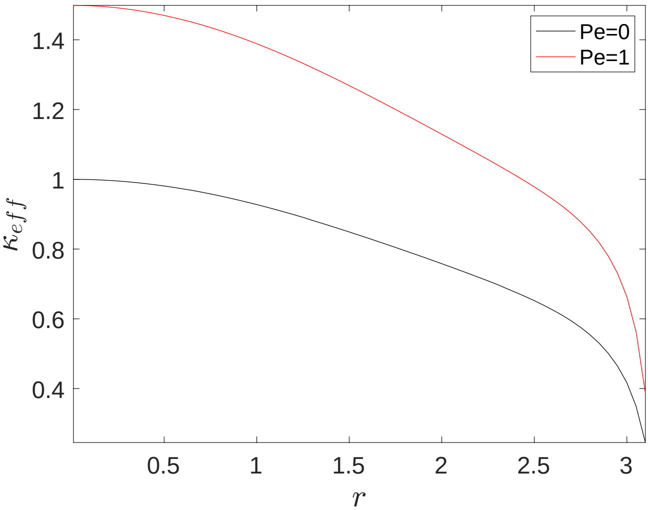
Invariant density for active disk

Concentration at the surface of the 'obstacle' shows barber pole pattern.



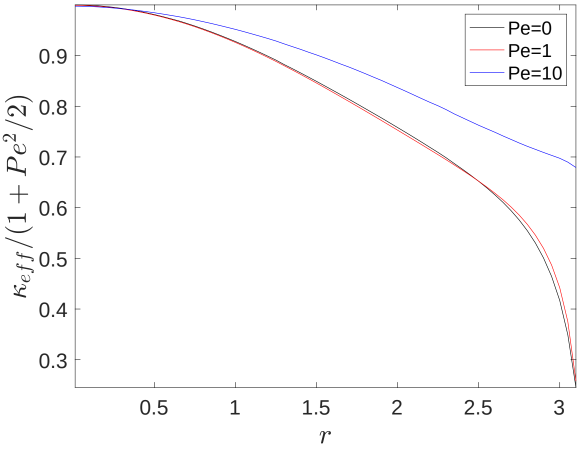
PDE solution by A. Tzella and D. Loghin. [Sorry, ϕ is θ here.]

Effective diffusivity for active disk



Effective diffusivity for active disk (large Pe)

Effective diff. normalized by free value.

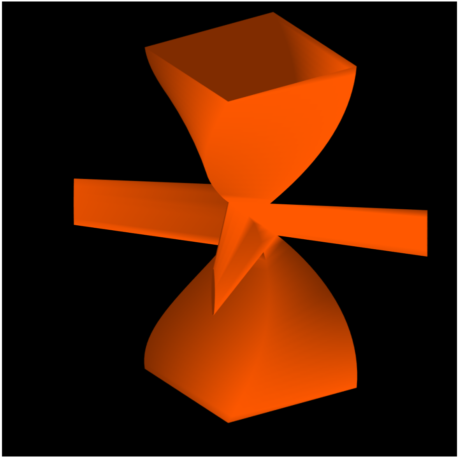


Discontinuous at $r = \pi$? Disk can always 'squeeze through.'

Discussion

- Configuration space viewpoint: think of a point in a funny domain rather than a shape in a lattice.
- Study with either stochastic particle simulations or Fokker–Planck equation.
- Homogenization theory is one approach in getting an effective diffusivity.
- Examples such as the ellipse in a lattice show that a lot is lost when considering only effective diffusivity.

Configuration space for a square particle



With Sanchita Chakraborti, we are looking at a tight-fitting square in a lattice. Can exploit 'small gaps' as in Keller (1963).

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