Passive and active particles in a lattice of obstacles

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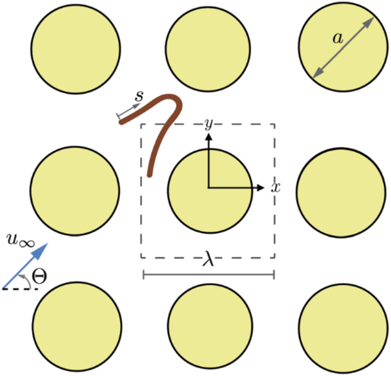
Active and passive particles in complex environments

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. . .

Towards a mathematical theory

Existing theoretical literature is mostly numerical, with some notable partial analytical results.

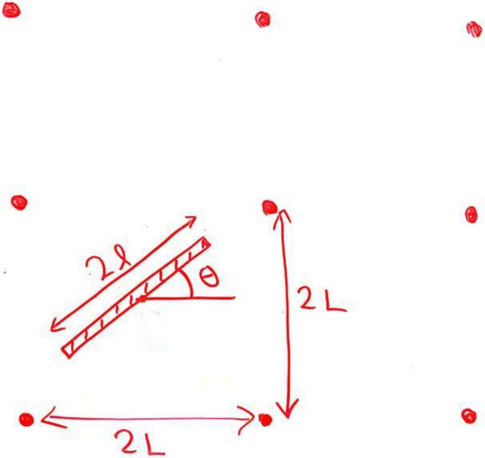
Today: take a few tentative steps towards a more analytical solution.

The difficulties and successes highlight promising directions for an asymptotic treatment.

In particular, thinking in terms of configuration space helps conceptually, and allows the reuse of 130-year-old results of Rayleigh in a different context.

A rod-shaped particle in a lattice of obstacles

2D periodic lattice of point obstacles.



Neglect hydrodynamic interactions.

Brownian dynamics

Particle undergoes Brownian motion in space and angle:

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

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:

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

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

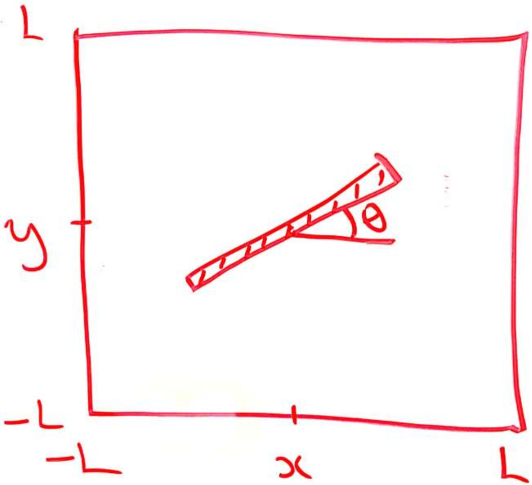
$$\boldsymbol{f} \cdot \hat{\boldsymbol{n}} = 0$$

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.

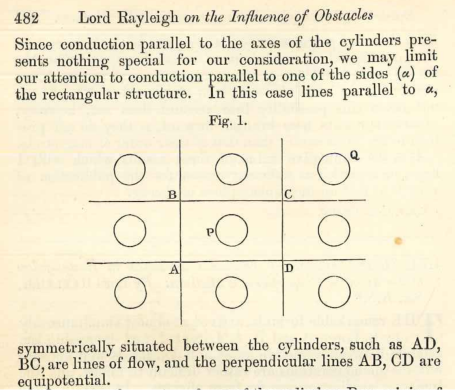


A point in this periodic cell is a realizable configuration of the rod.

Effective diffusivity: Rayleigh's problem

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

For a disk-shaped particle, in the absence of swimming (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.

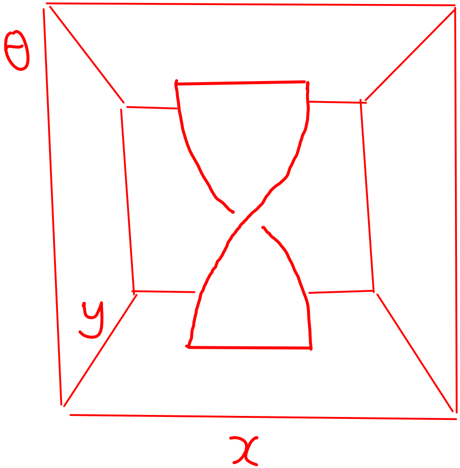
["On the influence of obstacles arranged in rectangular order upon the properties of a medium," Rayleigh, L. (1892). *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science,* **34** (211), 481–502]

Configuration space: Rotational diffusion

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

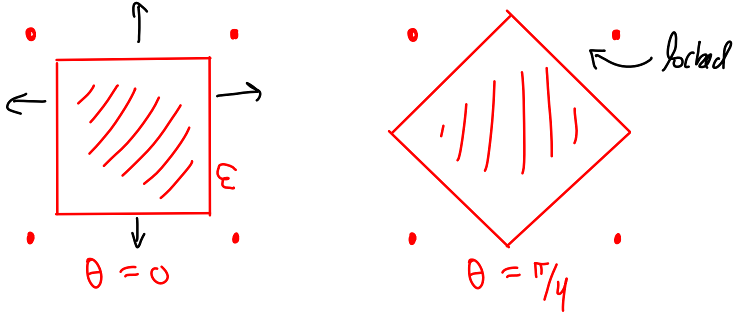
No-flux boundary condition at surface of 'obstacle,' so again we have a heat conduction problem, in a domain with obstacles in the shape of twisted ribbons.

As you might imagine, interesting things can happen when the 'ribbon' overflows the cell.



A better shape: Square in a square lattice!

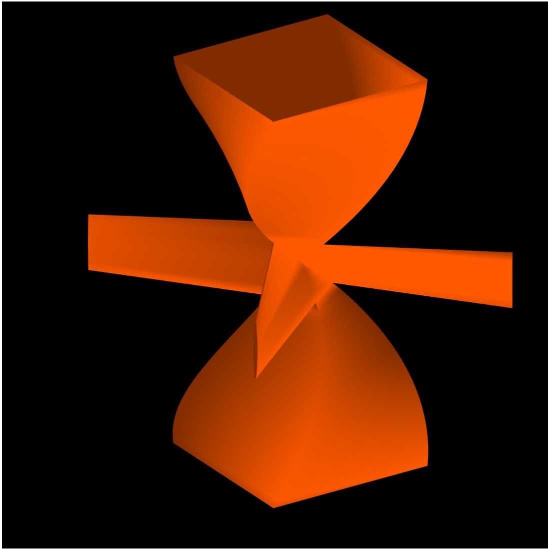
For analytical treatment, recently found that there is more promise in an extremely confined organism, like a square in a lattice.



For $\theta = m\pi/2$, can slide freely between pegs in narrow band of (x, y).

For $\theta = (2m+1)\pi/4$, locked in a cell for all (x, y).

Configuration space for a square in a lattice



- The funnels are where the particle is locked in one periodic cell.
- The $\theta = \pi/2$ arms lead to transition between cells.
- Can compute effective diffusivity as a first-passage problem from the large funnel to the narrow arms.
- Arm cross-section scales as $\varepsilon^{3/2}$ (target).

Discussion

- In summary, we can get a rather complicated formula for diffusion of a needle or ellipse in a lattice of obstacles. Related to Rayleigh's heat conduction problem.
- The square swimmer in a lattice offer much better prospects for a simple analytic result (ongoing).
- The goal of an asymptotic calculation is to get a better handle on parametric dependence, which should inform more complex situations.
- We are in the process of doing this for active particles as well (restoring the drift). Hard: boundary layers everywhere.

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