# 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.

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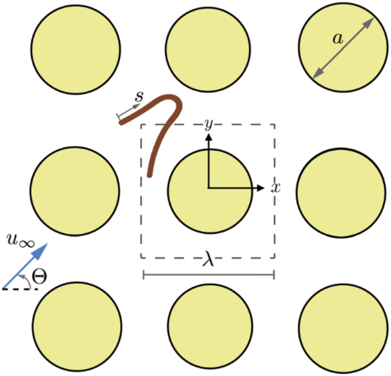
Brenner (1980)
Kamal & Keaveny (2018)
Alonso-Matilla *et al.* (2019)
Aceves-Sanchez *et al.* (2020)
Chakrabarti *et al.* (2020) $\Longrightarrow$
Amchin *et al.* (2022)
. . .




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

play movie

# Towards a mathematical theory

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

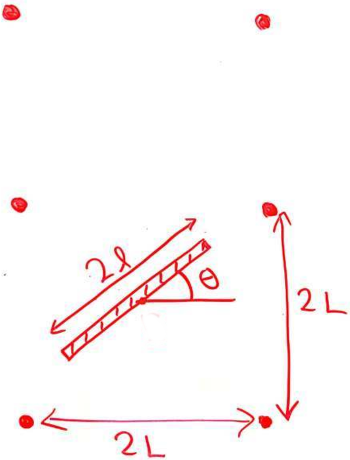
Today: take a few tentative steps towards a more analytical solution.

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.

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 $(X, Y, \theta)$:

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

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

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

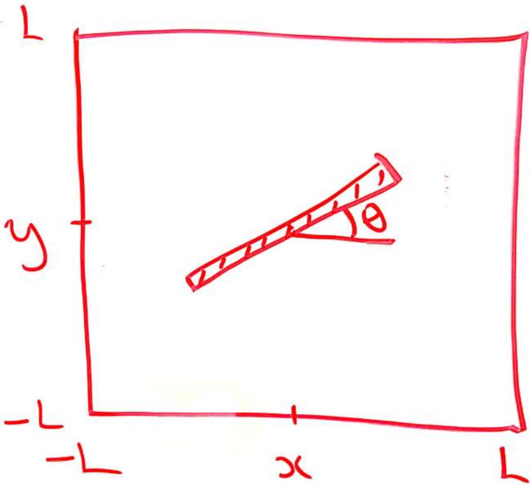
$$\boldsymbol{f} \cdot \hat{\boldsymbol{n}} = 0$$

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

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

# Configuration space: Fixed orientation

Configuration space gives allowable $(x, y)$ for fixed $\theta$.

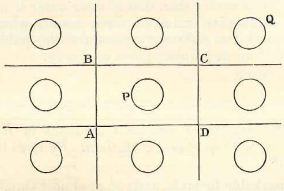



A point in this periodic cell is a realizable configuration of the rod.

# 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 ($\alpha$) of the rectangular structure. In this case lines parallel to $\alpha$,

Fig. 1.

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

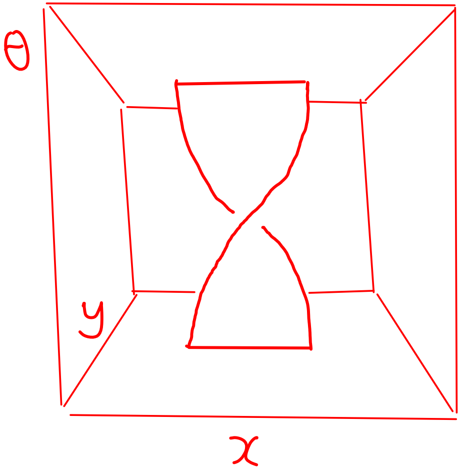
["On the influence of obstacles arranged in rectangular order upon the properties of a medium," Rayleigh, L. (1892). *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science,* **34** (211), 481–502]

# 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:

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

where the *effective diffusivity tensor* is

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

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

What is $\boldsymbol{\chi}$?

# The cell problem

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

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

Numerically this is not so bad, but analytically there is little hope.

# The transformed cell problem

The anisotropic diffusivity is a challenge. It would be better if the problem were harmonic.

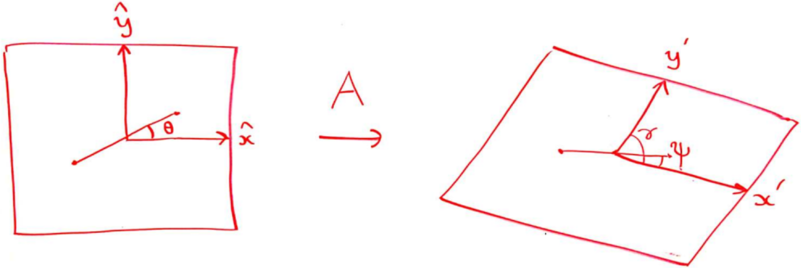
Choose $\mathbb{A}$ such that $\mathbb{A} \cdot \mathbb{D} \cdot \mathbb{A}^T = \mathbb{I}$:

$$\begin{aligned} \Delta_{\boldsymbol{r}'} \boldsymbol{\chi}' &= 0, & \boldsymbol{r}' &\in \mathbb{A} \cdot (\Omega \setminus \omega); \\ \hat{\boldsymbol{n}}' \cdot \nabla_{\boldsymbol{r}'} \boldsymbol{\chi}' &= -\hat{\boldsymbol{n}}', & \boldsymbol{r}' &\in \mathbb{A} \cdot (\partial \omega), \end{aligned}$$

where $\Delta_{\boldsymbol{r}}$ is the Laplacian, $\boldsymbol{n}' = \hat{\boldsymbol{n}} \cdot \mathbb{A}^{-1}$, and $\hat{\boldsymbol{n}}' = \boldsymbol{n}' / \|\boldsymbol{n}'\|$.

Unfortunately, the linear transformation $\mathbb{A}$ has deformed the domain.

# The transformed cell problem (cont'd)




$\mathbb{A}$ transforms our rod-shaped particle to a slightly different rod (no big deal), but the domain is now a parallelogram (which also depends on $\theta$).

# Fixed orientation $\theta$

Let's solve the problem for a fixed $\theta$, that is, neglecting rotational diffusion.

For a small particle, natural to use matched asymptotic expansion.

- The inner problem lives on an infinite domain and can be solved by conformal mapping, with unknown condition at $\infty$.
- The outer problem is essentially $\Delta \boldsymbol{\chi} = \nabla \delta$, the (modified) Green's function for Poisson's equation with periodic boundary conditions.

# The modified Green's function: Fourier

$$\Delta\phi = \delta(\boldsymbol{r}) - \frac{1}{|\Omega|}$$

For periodic boundary conditions, there is a Fourier series solution

$$\phi(\boldsymbol{r}) = -\frac{1}{|\Omega|}\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{k^2}$$

However, this is terrible! Converge is awful, and we don't know how to get the small-$r$ asymptotics for the purposes of matching.

# The modified Green's function: Ewald summation

Ewald summation (Poisson resummation) is a clever trick where the nasty $\boldsymbol{k}$ sum is broken up into two parts that are exponentially convergent:

$$\phi(\boldsymbol{r}) = -\frac{1}{4\pi}\sum_{\boldsymbol{n}} \Gamma\big(0, |\boldsymbol{r}-\boldsymbol{n}|^2/4\eta\big) - \frac{1}{|\Omega|}\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\mathrm{e}^{-k^2\eta}}{k^2}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$$

with $\eta$ a cutoff parameter and $\Gamma$ the incomplete Gamma function.

Possible to do the small-$r$ asymptotics, but $\eta$-dependent cancellation is annoying.

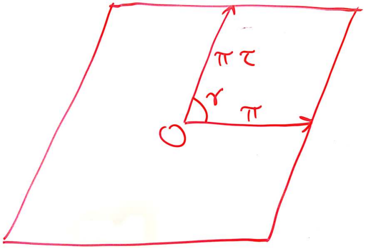
# The modified Green's function: Improvement

Instead, use the far less familiar complex form

$$\Phi(z, \bar{z}) = -\frac{1}{2|\Omega|}\, y^2 + \frac{1}{2\pi}\, \log \vartheta_1(z/2\,, q), \qquad q := \exp(\mathrm{i}\pi\tau),$$

where $z = x + \mathrm{i}y$, $\vartheta_1$ is a Jacobi elliptic theta function, and $q$ is the nome.

The complex parameter $\tau$ describes the shape of the lattice cell:



# The modified Green's function: Improvement

This can be rewritten as the (known?) explicit series

$$2\pi\Phi(z,\bar{z}) = \frac{1}{16\pi\tau_{\mathrm{i}}}\,(z-\bar{z})^2 + \log\sin(z/2) + 2\sum_{n=1}^{\infty}\frac{1}{n}\,\frac{\cos nz}{1-q^{-2n}}\,.$$

Note that the sum converges exponentially ($|q|<1$), and is a single sum, rather than the double-sums that appears in Ewald summation for a 2D lattice. The magic comes from the fact that the trig terms are already periodic in one direction.

The real part is doubly-periodic in the complex plane (but not the imaginary part).

Machine precision requires about 11 terms for any $z$.

I'm curious why this form is not used in 2D boundary integral simulations? Probably someone here can tell me.

# The modified Green's function: Expansion

Remember that our goal was to get a small-$|z|$ expansion of the Green's function, for matching to the inner solution. We can now find the small-$|z|$ analytic part

$$2\pi\Phi_{\mathrm{a}}(z) = -\frac{1}{8\pi\tau_{\mathrm{i}}}\,z^2 + \log z - \sum_{n=1}^{\infty}\mathcal{A}_n(\tau)\,\frac{z^{2n}}{(2n)!}\,.$$

The complex coefficients $\mathcal{A}_n$ are rather complicated, and involve combinatorial Bernoulli numbers.

This is a price we have to pay: the $\mathcal{A}_n$ are doing a lot of work for us. they are effectively carrying out Rayleigh's reflection method.

The matching to an inner conformal transformation solves our diffusivity problem in terms of the $\mathcal{A}_n$.

# Discussion

- I won't give the full expression for the effective diffusivity because it's fairly complicated and hasn't been properly validated against simulations yet.
- The goal of an asymptotic calculation is to get a better handle on parametric dependence.
- To allow for rotational diffusivity, can average over $\theta$ for small particles.
- We are in the process of doing this for active particles as well (restoring the drift).
- In the densely-packed case, there's some hope using the methods of Keller (1963). Potentially very powerful: exploit small gaps in configuration space.

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