Passive and active particles in a lattice of obstacles

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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)  
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:

\[
\begin{align*}
\text{d}X &= U \text{d}t + \sqrt{2D_X} \, \text{d}W_1 \\
\text{d}Y &= \sqrt{2D_Y} \, \text{d}W_2 \\
\text{d}\theta &= \sqrt{2D_r} \, \text{d}W_3
\end{align*}
\]

Diffusion tensor in body frame \((X, Y, \theta)\):

\[
\begin{pmatrix}
D_X & 0 & 0 \\
0 & D_Y & 0 \\
0 & 0 & D_r
\end{pmatrix}
\]

\((X, Y)\) in body frame, \((x, y)\) in lab frame.
Expressed in the fixed lab $(x, y)$ frame, the spatial diffusion tensor is

$$D(\theta) = \begin{pmatrix}
D_X \cos^2 \theta + D_Y \sin^2 \theta & \frac{1}{2}(D_X - D_Y) \sin 2\theta \\
\frac{1}{2}(D_X - D_Y) \sin 2\theta & D_X \sin^2 \theta + D_Y \cos^2 \theta
\end{pmatrix}.$$
Fokker–Planck equation for probability density $p(r, \theta, t)$:

$$\partial_t p + \nabla_r \cdot \mathbf{f} + \partial_{\theta} f_{\theta} = 0$$

Probability flux vector:

$$\mathbf{f} = \mathbf{U} p - \mathbb{D}(\theta) \cdot \nabla_r p - D_r \hat{\theta} p$$

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

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

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, $U = 0$), Rayleigh solved this by a reflection method.

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 \( \theta = \frac{m \pi}{2} \), can slide freely between pegs in narrow band of \((x, y)\).

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