Topology of configuration space for a particle in a lattice

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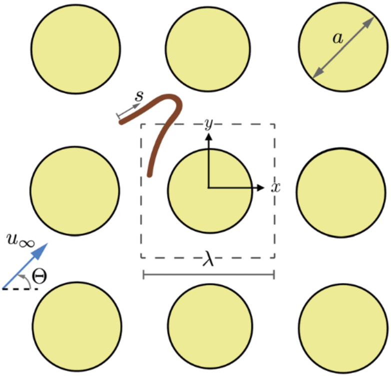
Equadiff 2024 Conference
Karlstad University, Sweden, 11 June 2024

Active and passive particles in complex environments

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

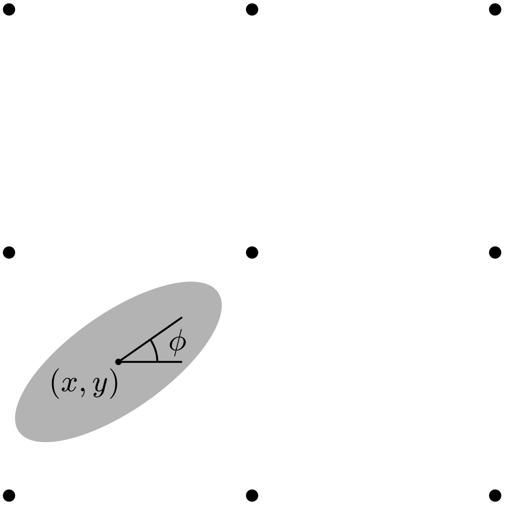
. . .
Brenner (1980)
Kamal & Keaveny (2018)
Alonso-Matilla *et al.* (2019)
Aceves-Sanchez *et al.* (2020)
Chakrabarti *et al.* (2020) $\Longrightarrow$
Amchin *et al.* (2022)
. . .



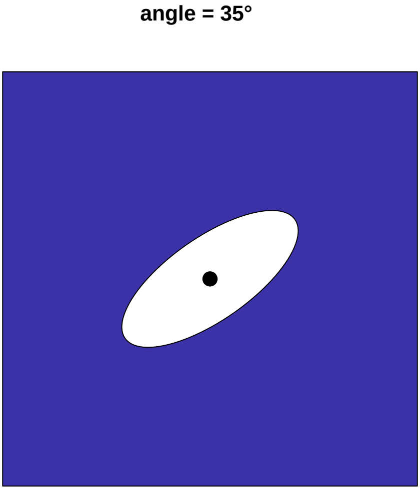
Many variations: different lattices, passive vs active, background flow, flexible vs rigid. . .

A particle in a lattice of obstacles

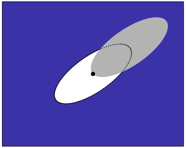
2D periodic lattice of point obstacles, with elliptical particle as example.



Configuration space of an ellipse in a lattice (cont'd)



Set of allowable coordinates (x, y, ϕ)



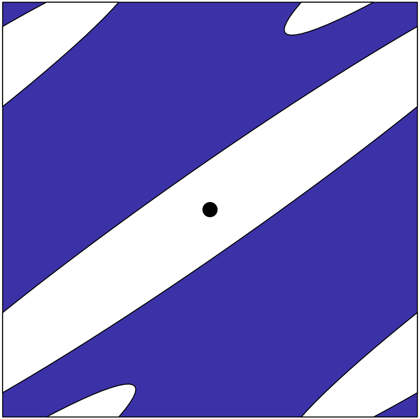
At fixed angle ϕ, the coordinates (x, y) must live in the blue periodic region.

The white region is an excluded region. We show the post at the center of the excluded region.

play movie play movie

What if the ellipse is longer than the period?

angle = 35°

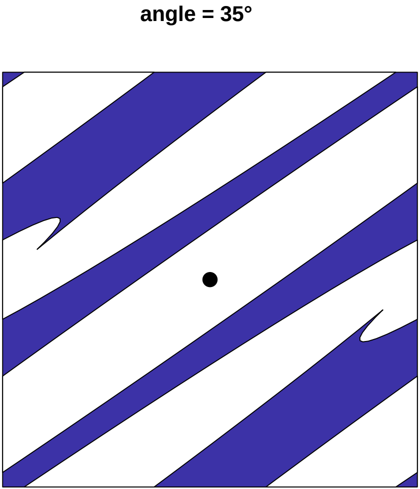


The excluded region overlaps the periodic cell and can self-intersect.

The periodicity comes from the excluded region around periodic images of the posts.

play movie

. . . or much longer than the period?



It gets real messy if the ellipse is much longer!

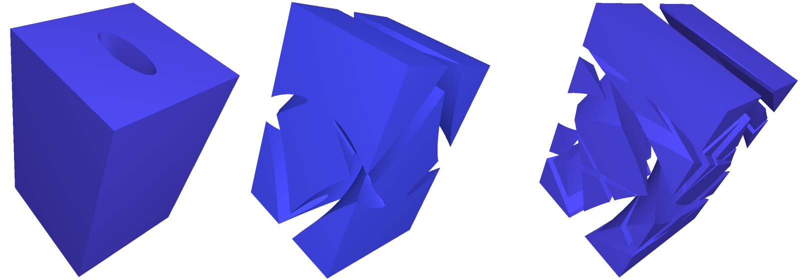
Turnaround problem: can the particle reverse direction in the lattice?

play movie

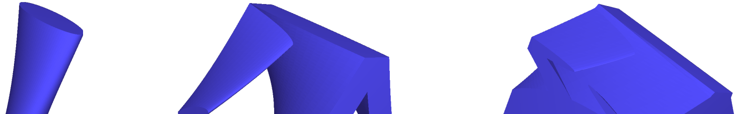
The full configuration space

The full configuration space is 3D, with coordinates (x, y, ϕ).

Many key questions, such as the turnaround problem, can only be answered by constructing the full 3D (x, y, ϕ) configuration space.



Complement:

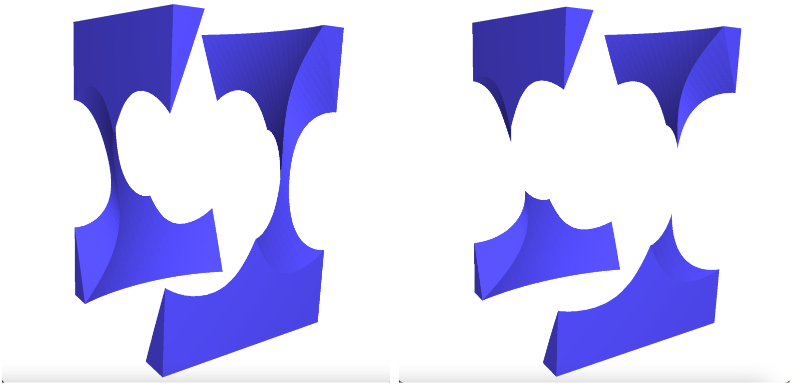


A note on programming: CGAL

- It becomes prohibitively hard to construct the configuration space manually as self-intersections become more intricate.
- Create 3D polyhedron consisting of periodic copies of (x, y, ϕ) configuration space for one post.
- Replicate this 3D polyhedron periodically for as many copies as needed.
- Intersect the union of these polyhedra with fundamental periodic box to obtain the configuration space periodic cell.
- This is computationally intensive! Intersection of 3D nonconvex polyhedra is hard.
- We use the C++ Computational Geometry Algorithms Library (`https://www.cgal.org/`), which uses objects called Nef polyhedra.

Critical ellipse size

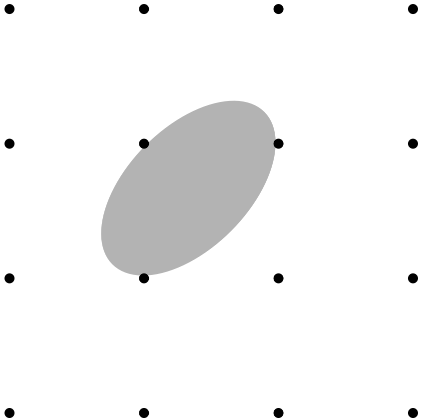
For a critical ellipse size, there are thin “bottlenecks” that connect the $\phi = 0$ configuration (bottom) to the $\phi = \pi/2$ configuration (top):



Move post location to corner:

The bottleneck

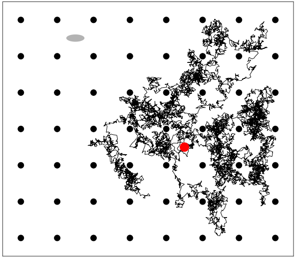
In order to turn by 90 degrees ($\pi/2$), the ellipse must go through this configuration at $\phi = \pi/4$:



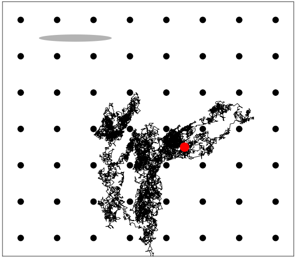
Can derive a polynomial condition for the critical ellipse size.

Brownian dynamics

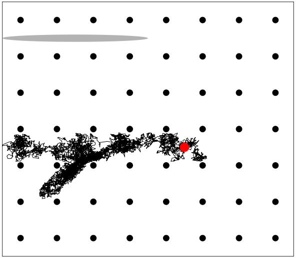
short ellipse



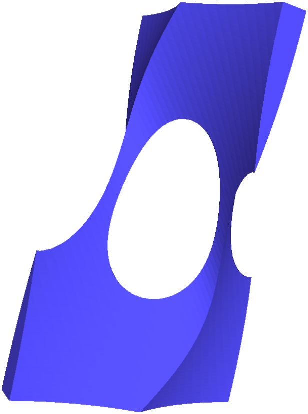
medium ellipse

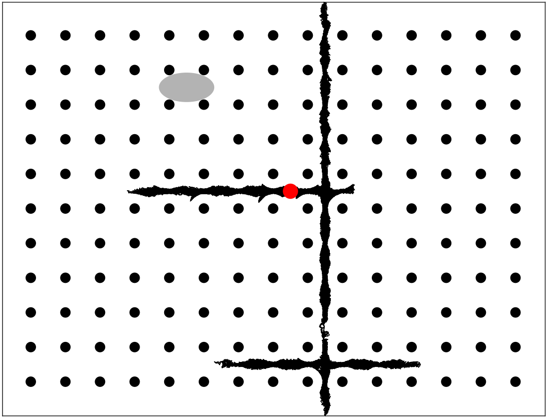


long ellipse



Brownian dynamics for critical ellipse

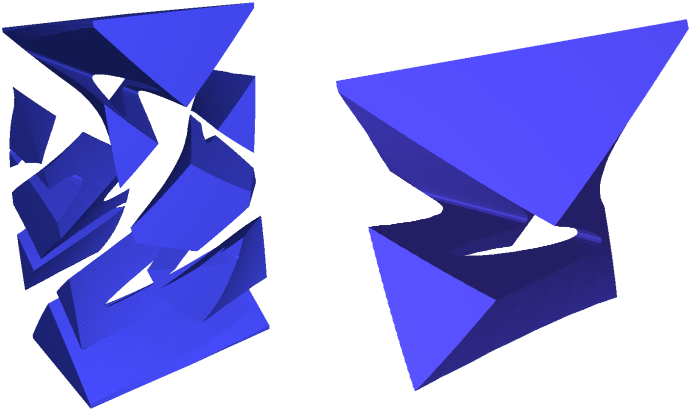




Ongoing work: estimate the 'turnaround' time by solving the first-passage time problem to cross the thin regions.

A long fat ellipse

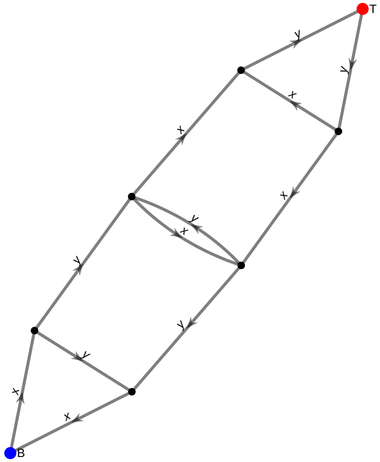
This ellipse is long and fat, so it has some trouble turning around:



The pieces of the configuration space are connected via the periodic directions.

A long fat ellipse

top-to-bottom graph $(2a = 4, 2b = 0.3)$



Make a graph of configuration space components, connected via periodic directions. A path from the blue to the red node represents a turn by $\pi/2$.

Sequence of 'parallel parking' moves.

Path lifts to $\mathbb{Z}^2$ to represent a path in lattice.

Conclusions

- Before even considering particle dynamics such as Brownian motion, ABP, or run-and-tumble, it is helpful to examine configuration space.
- Configuration space suggests 'bottlenecks' where the ellipse has to squeeze through to make progress.
- Bottlenecks open up Brownian motion to asymptotic analysis via PDEs – the Narrow Escape Problem [Holcman & Schuss (2014)].
- Longer objects potentially have to undergo complex motions to turn, and these are revealed by the configuration space.
- Computational geometry packages help — but higher dimensions will be a real challenge.
- Tools such as Topological Data Analysis may prove helpful.
- Choose ellipse as canonical case, but we also examined rectangle and will move on to nonconvex objects.

References I

Aceves-Sanchez, P., Degond, P., Keaveny, E. E., Manhart, A., & Sara Merino-Aceituno, D. P. (2020).

Alonso-Matilla, R., Chakrabarti, B., & Saintillan, D. (2019). *Phys. Rev. Fluids,* **4**, 043101.

Amchin, D. B., Ott, J. A., Bhattacharjee, T., & Datta, S. S. (2022). *PLOS Computational Biology,* **18** (5), e1010063.

Brenner, H. (1980). *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences,* **297** (1430), 81–133.

Chakrabarti, B., Gaillard, C., & Saintillan, D. (2020). *Soft Matter,* **16** (23), 5534–5544.

Holcman, D. & Schuss, Z. (2014). *SIAM Review,* **56** (2), 213–257.

Kamal, A. & Keaveny, E. E. (2018). *Journal of The Royal Society Interface,* **15** (148), 20180592.