Computational Physics

Hints for assignment 2

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NTNU, Trondheim, February 28, 2022

What you will find in these slides.

In these slides, we recall the basic idea behind the particle separation technique we are investigating in this assignment (briefing). Then, you will find a few graphs that should help you to check your results. How to check your random generator? Are trajectories for $\hat{D} \ll 1$ and $\hat{D} \gg 1$ reasonable? Do we get Boltzmann distribution for the probability density of visited potential? ... However **not all solutions** are given, so that you keep the thrill of the unknown!

Finally, for interested students who are done with all tasks and want to investigate deeper into the topic, we give a selection of investigation tasks of various difficulty. These are bonus just for the pleasure of it.

Briefing assignment 1

DNA molecules separation by using biased Brownian motion.

Simulation, comparison with a real experiment and separation optimization.

The problem

How can we separate micro-particles or macro-molecules of different sizes?

Recall on Brownian motion

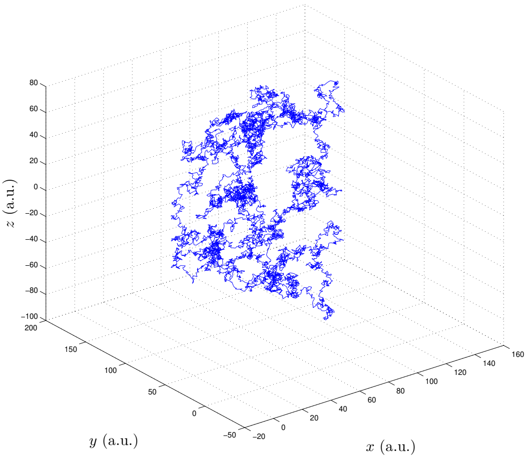
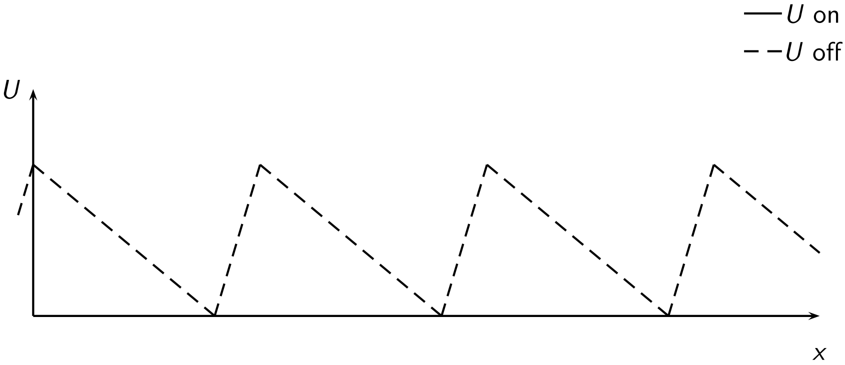
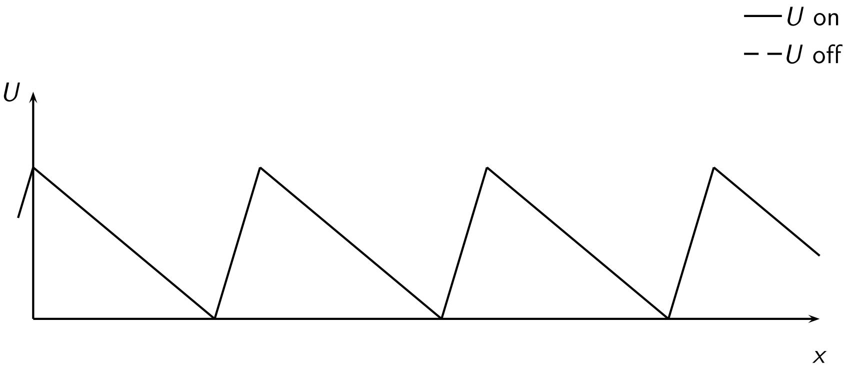


Figure: Trajectory of a Brownian particle.

An idea: Flashing ratchet potential



An idea: Flashing ratchet potential



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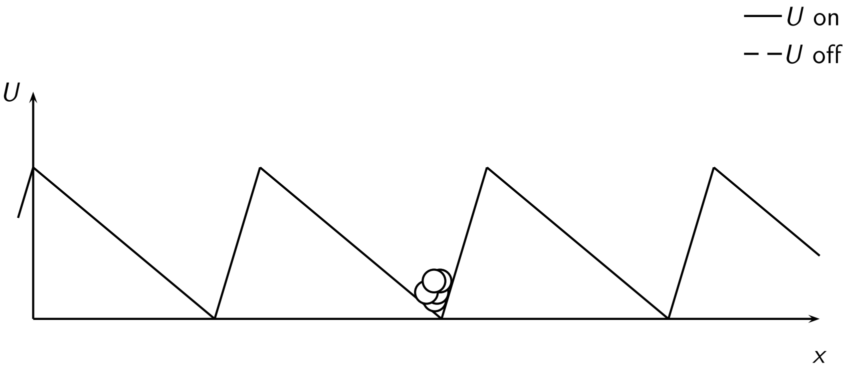
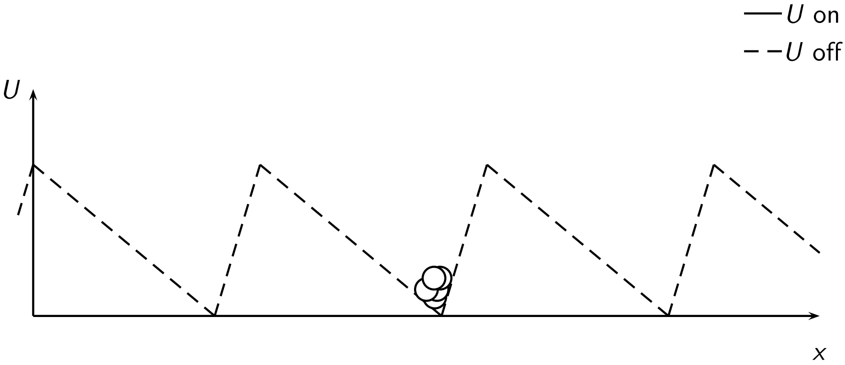
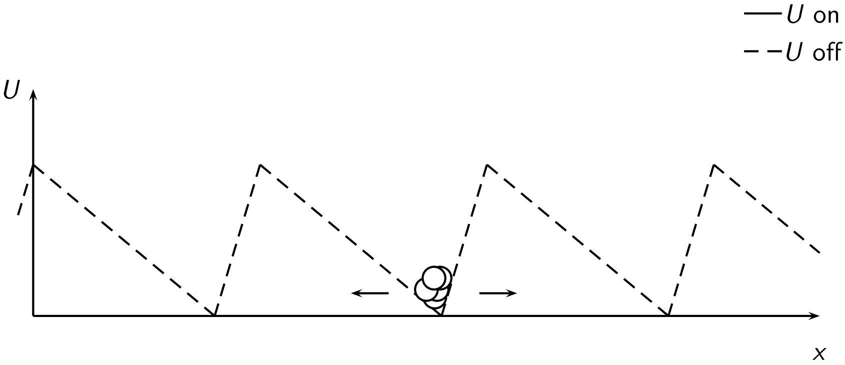


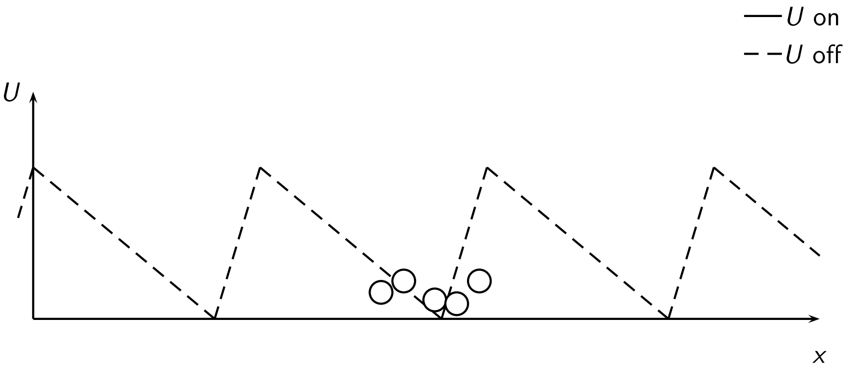
An idea: Flashing ratchet potential

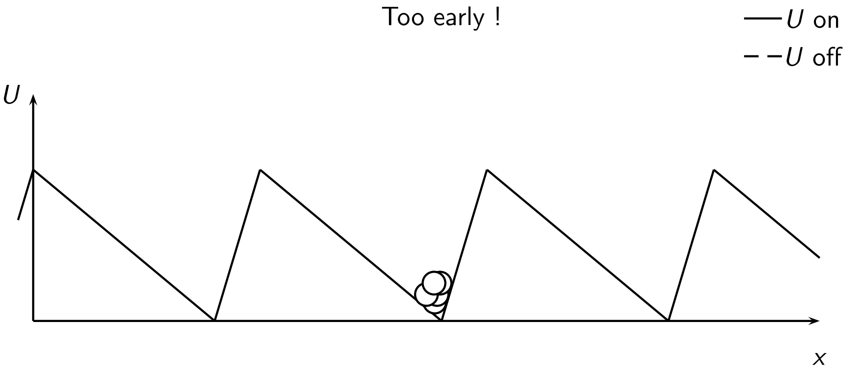


An idea: Flashing ratchet potential



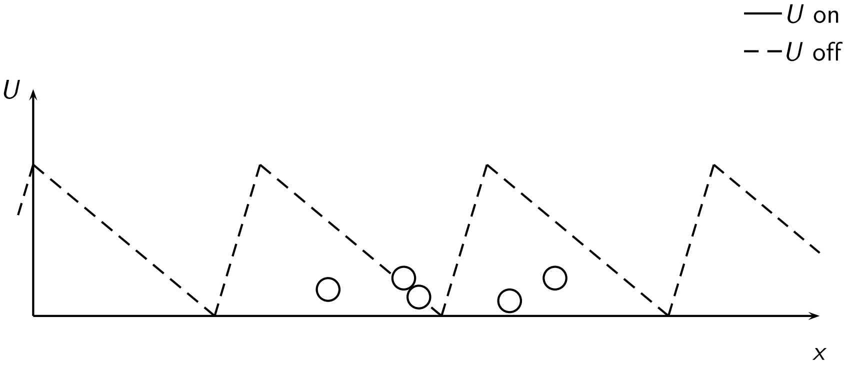
An idea: Flashing ratchet potential





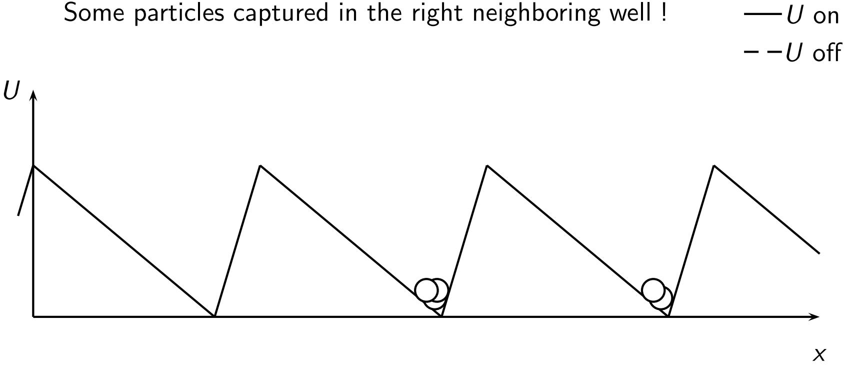
Too early !
U on
U off
U
x

An idea: Flashing ratchet potential



An idea: Flashing ratchet potential

Some particles captured in the right neighboring well !



Strategy

How can we model this?

The Langevin approach

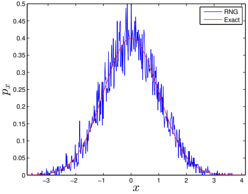
$$m \frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -\nabla U(\mathbf{x}, t) - \gamma \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} + \xi(t) \tag{1}$$

Theory

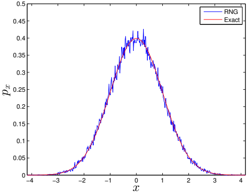
Read updated assignment with complements on the:

- overdamped approximation (i.e. when can we neglect the inertial term)
- fluctuation-dissipation theorem (i.e. where the $2\gamma k_B T$ is coming from)
- formal derivation of the Euler scheme for a stochastic differential equation

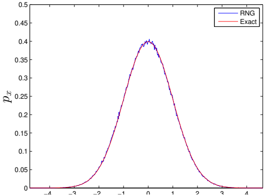
Example of results - Random number generator



(a) 10^4 realizations



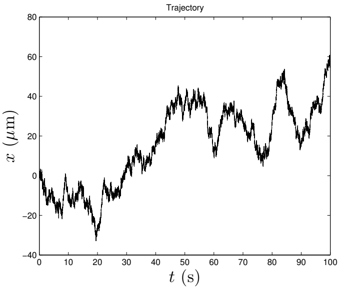
(b) 10^5 realizations



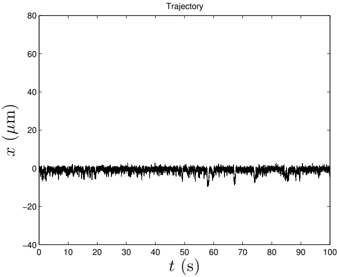
(c) 10^6 realizations

Figure: Probability density function of the random number generator.

Example of results - Typical trajectories in a non-flashing ratchet



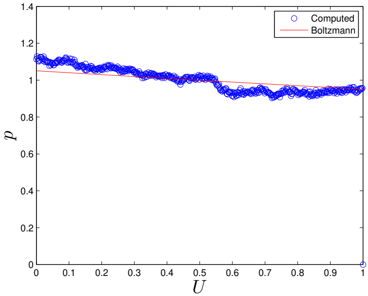
(a) $\Delta U = 0.1\ k_B T$



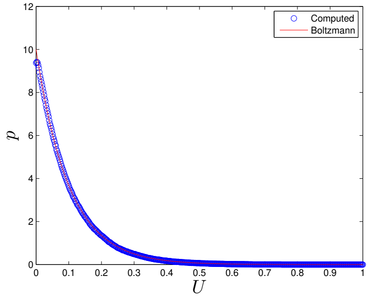
(b) $\Delta U = 10\ k_B T$

Figure: Typical trajectory in a non-flashing ratchet for different values of ΔU.

Boltzmann distribution



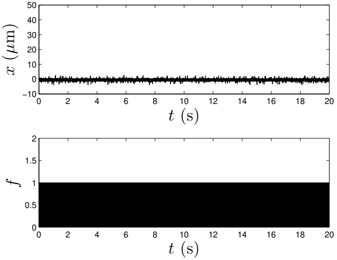
(a) $\Delta U = 0.1\ k_B T$



(b) $\Delta U = 10\ k_B T$

Figure: Probability density of 'visited' potential. Note: reduced units are used here.

Example of results - Typical trajectories in a flashing ratchet

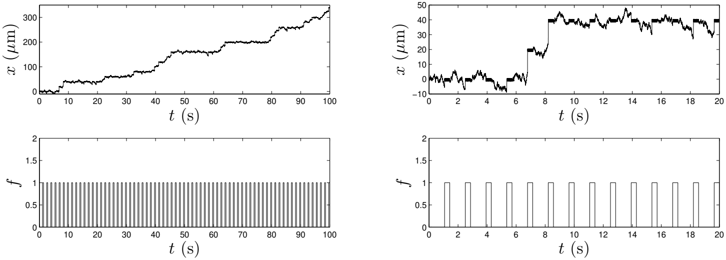


(a) Flashing frequency: 25 Hz

(b) Flashing frequency: 25 Hz

Figure: Typical trajectory in a high frequency flashing ratchet.

Example of results - Typical trajectories in a flashing ratchet



(a) Flashing frequency: 0.7 Hz

(b) Flashing frequency: 0.7 Hz

Figure: Typical trajectory in a medium frequency flashing ratchet.

Example of results - Typical trajectories in a flashing ratchet

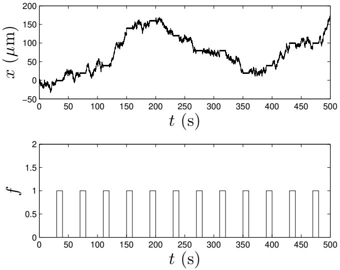


Figure: Typical trajectory in a low frequency flashing ratchet (flashing frequency: 0.025 Hz).

Average drift velocity

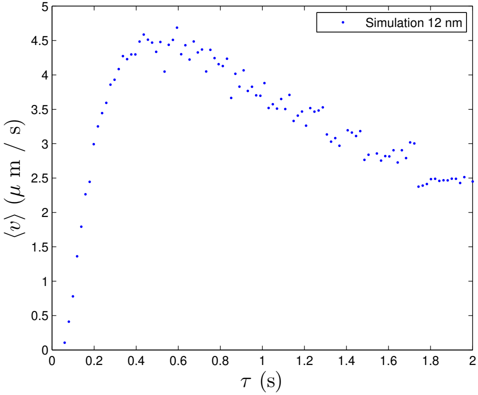


Figure: Average drift velocity as function of τ. $r = 12$ nm

Average drift velocity

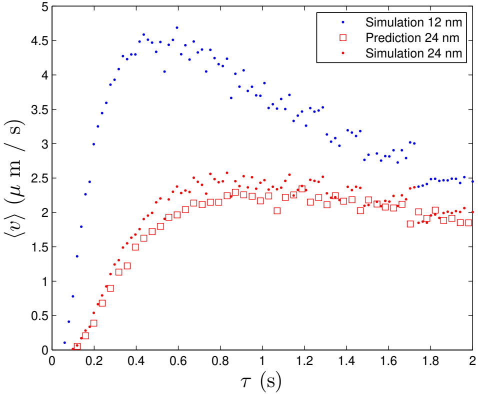
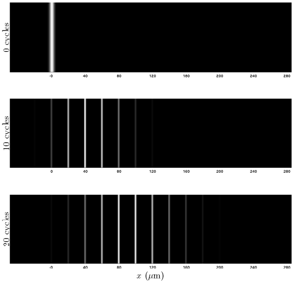
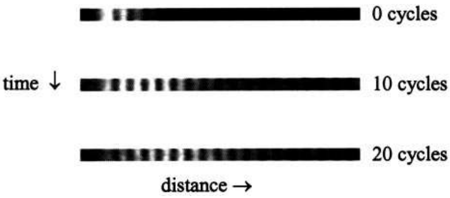


Figure: Average drift velocity as function of τ. $r = 12$ nm blue or $r = 24$ nm red.

Example of results - Simulation vs experiment



(a) Simulation



(b) Experiment

Figure: Comparison simulation vs experiment.

Investigation tasks - (Bonus)

If you are done with all the tasks in the assignment and want to, you can investigate on one of these suggestions. Note that some are more challenging than other.

- (easy) - Generalize to 2D.
- (be creative) - Which shape of the potential could be of interest? Can we make particles drift in different directions?
- (challenging) - Fokker-Planck approach: we have seen the Langevin approach which consists in solving the trajectory of a particle for several realizations and then compute the density of particles from their trajectories. Another approach consists in finding an equation for the evolution of the density directly (it will be a PDE) and solving this instead. This is known as the Fokker-Planck approach. Find and solve the relevant PDE for the same problem as the one in assignment 1.