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Biased Brownian Motion

TFY 4235 - Computational Physics

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Abstract

Separation of particles of different sizes is an important technique in isolating and separating DNA-molecules. This short report explores the optimal parameters when separating particles by biased Brownian motion in an asymmetric flashing potential. The optimal flashing period, τ_{op}, is found to be $\approx 0.55\,\mathrm{s}$, for separating two particles of sizes $r_1 = 12\,\mathrm{nm}$ and $r_2 = 36\,\mathrm{nm}$. This parameter has been used to show that these two groups of particles can be almost totally separated after 100 seconds in the potential.

1 Introduction

The problem at hand is the separation of particles of different sizes by biased Brownian motion. This can, for instance, be applied to the separation of DNA molecules of different sizes. In this project, computer simulations, using the Langevin approach in 1D, will determine the optimal parameters for the separation and the results will be compared to literature.

2 Theory

The motion of a particle undergoing Brownian motion in a solvent can be described by the Langevin equation,

$$m\frac{d^2x}{dt^2} = -\frac{\partial U}{\partial x}(x,t) - \gamma\frac{dx}{dt} + \xi(t), \tag{1}$$

where m is the mass of the particle, U is the potential energy, $\gamma = 6\pi\eta r$ is the friction constant and ξ is a stochastic variable representing random collisions between the solvent molecules. $\xi(t)$ has a mean of zero and is uncorrelated. By assuming that the system is overdamped, the inertial term, $m\frac{d^2x}{dt^2}$ in 1, can be neglected and one obtains a first order stochastic differential equation,

$$\gamma\frac{dx}{dt} = -\frac{\partial U}{\partial x}(x,t) + \xi(t). \tag{2}$$

The Euler scheme for this equation, as presented in [2], is:

$$x_{n+1} = x_n - \frac{1}{\gamma}\frac{\partial U}{\partial x}(x_n, t_n)\delta t + \sqrt{\frac{2k_BT\delta t}{\gamma}}\hat{\xi}_n. \tag{3}$$

While there are more accurate methods for solving ODE's than using an Euler scheme, for instance Runge Kutta methods, the Euler scheme will suffice for this implementation. The potential, as defined later in 8, is linear, meaning that the force is constant. This means that there is nothing to gain from higher order methods, and being the computationally most efficient, it will be the main choice. Also, a main challenge for less accurate methods like Euler's is the accumulation of error after many time steps. Since Eq. 4 is stochastic, the next step will not be subject to a systematic error, due to the introduced random noise. By using reduced units, which is making sure that all variables are dimensionless, the Euler scheme Eq. 3 reads

$$\hat{x}_{n+1} = \hat{x}_n - \frac{\partial \hat{U}}{\partial \hat{x}}(\hat{x}_n, \hat{t}_n)\delta\hat{t} + \sqrt{2\hat{D}\delta\hat{t}}\hat{\xi}_n, \tag{4}$$

where

$$\hat{x} = \frac{x}{L}, \quad \hat{t} = \omega t, \quad \omega = \frac{\Delta U}{\gamma L^2}, \quad \hat{U}(\hat{x},\hat{t}) = \frac{U(x,t)}{\Delta U}, \quad \hat{D} = \frac{k_BT}{\Delta U}. \tag{5}$$

To show this is simply to substitute the variables in Eq. 5 into Eq. 3. By applying an asymmetric saw-tooth potential, modulated by an asymmetric square signal, it is possible to separate particles based on their sizes. This is due to the difference in mean diffusion length, which is governed by the equation

$$\langle x\rangle = \sqrt{2Dt}, \tag{6}$$

where $\langle x\rangle$ is the mean distance travelled from the origin during the time t and $D = \frac{k_BT}{\gamma}$ is the diffusion constant. A smaller particle will thus have a higher probability of diffusing past the steeper potential while the potential is turned off, thus being trapped in the next trench when the potential is turned on. In reduced units, the potential is defined as:

$$\hat{U}(\hat{x},\hat{t}) = \hat{U}_r(\hat{x},\hat{t})\hat{f}(\hat{t}), \tag{7}$$

where

$$\hat{U}_r(\hat{x}) = \begin{cases} \frac{\hat{x}}{\alpha} & \text{if } 0 \le \hat{x} < \alpha \\ \frac{1-\hat{x}}{1-\alpha} & \text{if } \alpha \le \hat{x} < 1 \end{cases}, \quad \hat{f}(\hat{t}) = \begin{cases} 0 & \text{if } 0 \le \hat{t} < \frac{3\tau\omega}{4} \\ 1 & \text{if } \frac{3\tau\omega}{4} \le \hat{t} < \tau\omega \end{cases}, \tag{8}$$

and $\alpha \in [0, 1]$ is the asymmetry factor and τ is the period. For the Euler scheme, the time step must be made sufficiently small, such that the particle cannot move through several variations of the potential in one step. Considering the random noise, $\hat{\xi}_n$, the criterion for $\delta\hat{t}$ is

$$max\left|\frac{\partial \hat{U}}{\partial \hat{x}}\right|\delta\hat{t} + 4\sqrt{2\hat{D}\delta\hat{t}} \ll \alpha \tag{9}$$

If a particle diffuses in the absence of a potential, it can be shown that the probability density will be the following:

$$p(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp(-\frac{x^2}{4Dt}) \tag{10}$$

3 Implementation

The physics of the problem is implemented in the file `physics.py`. The code is suited for simulating an ensemble of particles, but it can also be called with only one. In this file, Eqs. 7 and 8 are implemented, as well as the analytical expression for the force in reduced units. A function, `gaussian(N)`, returning N random numbers modelling ξ is also implemented using NumPy's normal distribution. The code is thoroughly documented and only the outputs, which can also be run from the file, are shown here in figure 1 for validating the implementation.

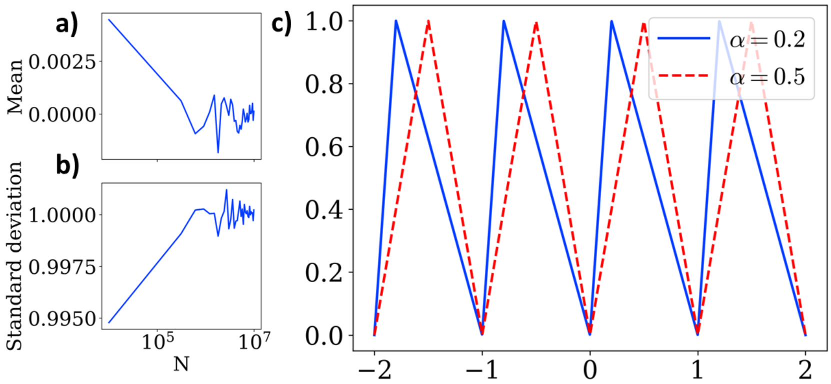

Figure 1: a) and b) show the mean and standard deviation of the random numbers generated using NumPy. c) shows an asymmetric (blue) and a symmetric (red) potential for reference.

The euler scheme as defined in Eq. 4 is implemented in the file `euler.py`. Again, the function `euler()` is suited for an ensemble of particles. The function `get_time_step()` returns a time step which satisfies Eq. 9, by testing decreasing values for δt. This code is only called once per simulation, so the time complexity is not a problem. In order to make sure that the LHS of Eq. 9 is much smaller than α, a factor 0.1 is multiplied by α.

The file `simulate.py` includes the functions needed for the simulation, including the conversion from real to reduced units and different functions to simulate different scenarios. All simulations follow the same structure:

1. For all timesteps, find the force on all particles by inserting their position into to `force()` function. It is vectorized and finds all forces at once.

2. Insert the current position and the force into the forward Euler scheme.

3. Store or update the positions depending on memory requirements.

4 Results

When the flashing is turned off, the particles will diffuse in the potential shown in figure 1c. As can be seen in figure 2a, when $\Delta U = 0.1k_BT$, the particles diffuse freely, while when $\Delta U = 10k_BT$, the particles are trapped within the wells of the potential. Since the potential is steeper towards the right, one might expect the average position of the particles to be shifted slightly left for intermediate values of ΔU, which can be seen in figure 2b. This verifies the code, but will not contribute to any major results when the flashing is turned on.

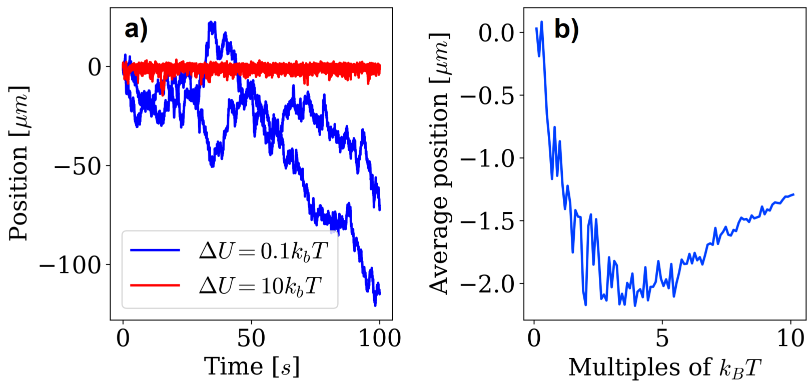

Figure 2: a) Shows the trajectories of particles in a potential with ΔU as labelled. There are two overlapping red particles and two blue. b) shows the average position of 10000 particles after 10 seconds of diffusion for different values of ΔU

In figure 3 one can see that the probability of a particle occupying a certain potential follows the Boltzmann distribution closely. The distribution in a) is calculated from the average position of 10^6 particles after 10 seconds of diffusion. The distribution in b) is calculated from the average position of 10^4 particles after 10 seconds of diffusion. The numbers were chosen in order to get good statistics. When calculating the distribution in b) it became evident that it was essential that the time step calculated using `get_time_step` was sufficiently small. When the LHS of Eq. 9 was simply smaller than α, rather than much smaller, the maximum for p would be around $U = 0.1$, rather than $U = 0$, which is nonphysical, and the tolerance was adjusted in order to get good results.

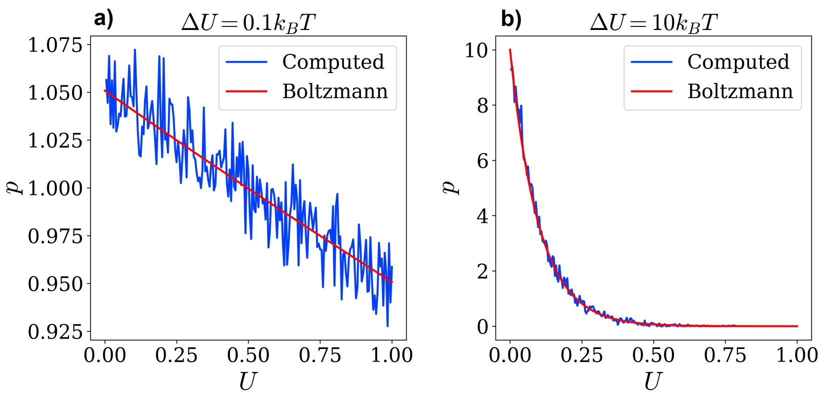

Figure 3: a) shows the probability distribution for the visited potential when $\Delta U = 0.1k_BT$. b) probability distribution for the visited potential when $\Delta U = 10k_BT$

The results presented in figure 2 and figure 3 shows that ΔU must be sufficiently high in order to make the particles drift to the right when the flashing is turned on. The first step to making the particles drift to the right would be to make sure that they do not drift anywhere when the potential is on. The potential would then have to be greater than $10k_BT$. This condition would be satisfied by setting $\Delta U = 80eV$. For high flashing frequencies, one can expect that the particles do not have time to diffuse across the potential maximum when the potential is turned off and will thus be stuck in place. For intermediate flashing frequencies, the particles might have time to diffuse across the maximum located to the right, since this distance is 4 times smaller than diffusion across the maximum to the left. One can thus expect effective transportation to the right. For very low flashing frequencies one can expect behaviour close to a random walk, since the potential will be off for prolonged times.

Some trajectories for different flashing frequencies ($\tau = 1/f$) are plotted in figure 4. These trajectories confirm the three assumed regions of drift. In a), the period is very short, leaving little time for diffusion, effectively keeping the particles in place. In b), the flashing frequency is intermediate and it is clear that the particle is transported right in jumps of 20 µm, as outlined by red circles. For the low frequency flashing regime, as shown in c), one can see that the particle diffuses freely for long amounts of time, except during the 10 seconds where the potential is on, as outlined by yellow circles.

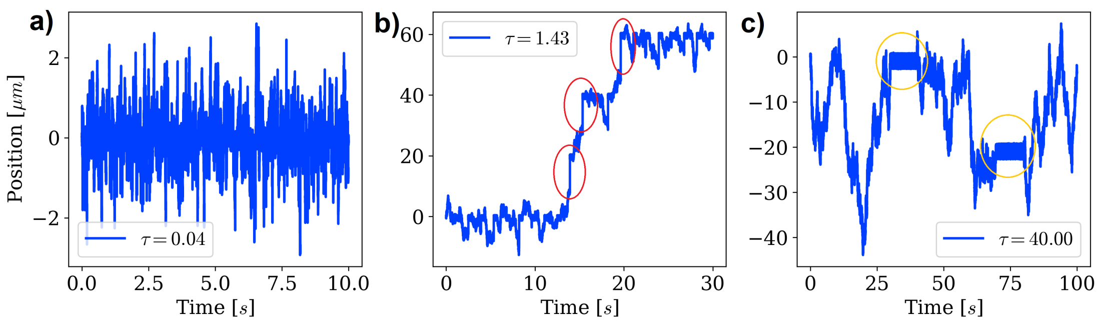

Figure 4: a) Shows the trajectory of a particle when the flashing frequency is 25 Hz. b) The frequency is 0.7 Hz. The red dots shows that the particle drift in steps of 20 µm when the potential is on. c) The frequency is 0.025 Hz. The yellow circles shows plateaus when the potential is turned on.

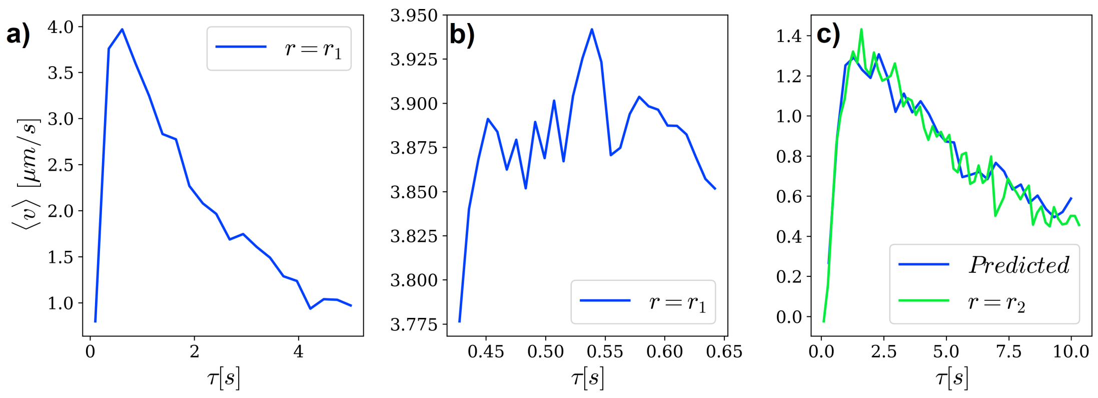

Figure 5: a) Shows the mean velocity of a particle with $r_1 = 12$ nm against the flashing period, τ. b) shows a zoomed in version of a), with more data points. c) is a plot of the predicted values for a particle with $r_2 = 36$ nm as well as actual simulated data for the particle.

The optimal flashing period, τ_{op}, was found by plotting the average drift velocity of a particle vs the period, τ. The average drift velocity was obtained for an ensemble of 10000 particles and calculated by dividing the final position by the elapsed time. In figure 5a,b, the results for a particle with radius $r_1 = 12$ nm are plotted. The optimal flashing period for this particle is around 0.55 s, corresponding to a mean velocity of $\approx 4\,\mu\text{m}\,\text{s}^{-1}$. In [1], an experiment is conducted with similar parameters. From figure 3 in the article, one can estimate the mean velocity to be $\approx 3.5\,\mu\text{m}\,\text{s}^{-1}$.

This shows that the simulated data is in compliance with experimental data.

The results in 5a,b can be used to predict the optimal flashing period and the mean velocity for a particle of a different size. Using 4, $\hat{t} = \omega t \propto \frac{1}{\gamma} \propto \frac{1}{r}$, one can see that an increase in size will lead to an increase in τ_{op} and a decrease in mean velocity. This is as expected from the physics of Brownian motion. For a particle with $r = 3r_1$, the optimal flashing period is expected to be $3\tau_{\text{op}}$ for the particle with $r = r_1$. As a consequence, the mean velocity is expected to be 3 times less than that of the smaller particle at its optimal flashing frequency. At $\tau_{\text{op}} = 0.55$, the speed of particle 2 can be found by $\frac{v_{\text{particle1}}(\tau = \tau_{\text{op}}/3)}{3} \approx \frac{2.1\,\mu\text{m}\,\text{s}^{-1}}{3}$. This is roughly $0.7\,\mu\text{m}\,\text{s}^{-1}$ which corresponds roughly to the simulated $0.8\,\mu\text{m}\,\text{s}^{-1}$ from Fig. 5c. The full prediction is plotted against simulated data in figure 5c, showing great overlap between the simulation and the prediction. It makes great physical sense that a larger particle would need a longer period in order to consistently reach the next trench compared to a smaller particle. In addition, it is slower, so it is "punished" twice.

In figure 6, the analytical expression for the probability density, as given by Eq. 10, is plotted against the simulated probability density for two types of particles. It can be seen that the bigger particle has a more narrow distribution compared to the smaller one. This is consistent with the previous discussion, showing that increasing the radius is equivalent to a change in the time scale. This effect is highlighted in Fig. 6c, which shows that the probability distribution for the bigger particle at t = 3 s overlaps with the probability distribution for the smaller one at t = 1 s.

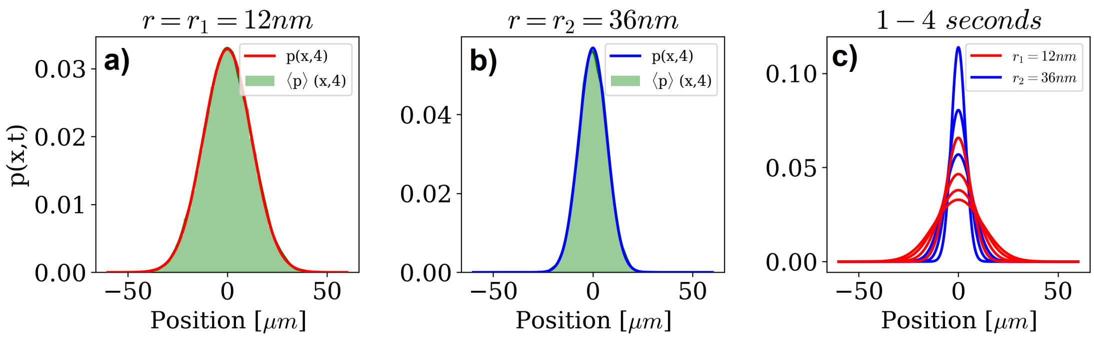

Figure 6: a) Shows the analytical probability distribution plotted against the simulated probability distribution for a particle with $r_1 = 12$ nm. b) shows the same for a particle with $r_2 = 36$ nm. The simulated data in a) and b) are for an ensemble of 50000 particles. c) shows the time evolution of the analytical probability distribution. Each line corresponds to one second. It can be observed that the distributions broadens over time and at t = 3 s, the analytical expressions overlap.

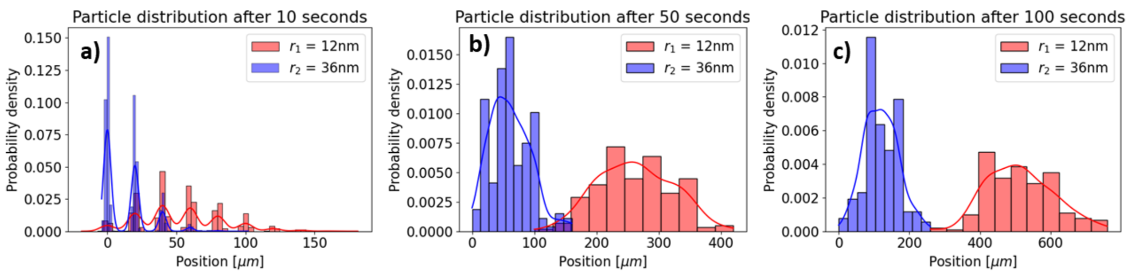

Figure 7: The figure shows the time evolution of the probability density for particles with $r_1 = 12$ nm and $r_2 = 36$ nm. The simulation is for an ensemble of 200 particles.

Putting these elements together, it is possible to separate particles moving in an asymmetric flashing potential. Plotted in Fig. 7 is the time evolution of an ensemble of 200 particles of radius $r_1 = 12$ nm and $r_2 = 36$ nm in such a potential. In a), one can that the particles settles at $x = 20, 40, 60nm$ etc., as expected. After 100 seconds, the distributions have almost no overlap, meaning that they are almost totally separated. As time progresses one can in b) and c) see two separate travelling gaussian wave packets, gradually delocalizing. The dispersive nature of the solution suggests that the probability density could be described by the Schrödinger equation. This would be consistent with the constant group velocity and a width that increases approximately linearly with time.

5 Conclusion

In this short report, it has been shown that it is possible to separate two particles of different sizes in an asymmetric flashing potential. It is shown that the optimal flashing period for separation of particles of sizes $r_1 = 12\,\mathrm{nm}$ and $r_2 = 36\,\mathrm{nm}$ is $\tau_{\mathrm{op}} \approx 0.55$. Comparing the average drift velocity of particles at this frequency yields results on the same order of magnitude as is found experimentally.

Bibliography

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[2] I. Simonsen J. Banon. *Assignment 2: Biased Brownian motion: An application to particle separation.* 2022. URL: http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Assignments/TFY4235_Assignment_02.pdf.