E3 Brownian motion and the power spectrum

Here you will consider Brownian motion in an external potential. You will apply the model to the motion of a small glass particle held in air by an optical tweezer. You are asked to determine both the power spectrum and the corresponding time correlation function and compare with the experimental data in Ref. [1].

This task is paired with code questions in Yata that are mandatory to pass before being allowed to present. The Yata questions will help you verify that your code is correct.

The Langevin's equation

Consider the motion of a heavy particle, a Brownian particle, immersed in a fluid, the solvent. Assume that the particle is hold in place by a trap, *e.g.* an optical trap created by laser beams. For simplicity consider motion in one dimension and assume that the trap can be described by a harmonic potential well

$$V(x) = \frac{k}{2}x^2 = \frac{m\omega_0^2}{2}x^2$$

The force on the particle can be split into the restoring force

$$F^{ext}(t) = -kx(t)$$

a smooth friction term $-m\eta v(t)$, which is assumed to be proportional to the velocity of the particle, and a rapidly fluctuating force $F^{st}(t) = m\xi(t)$, a stochastic force. The two latter forces both arise from the collisions with the individual solvent molecules. The equation of motion, the Langevin's equation, is then given by

$$\frac{d}{dt}x(t) = v(t) \tag{1}$$

$$\frac{d}{dt}v(t) = -\omega_0^2 x(t) - \eta v(t) + \xi(t) \tag{2}$$

where $\xi(t)$ is a Gaussian random process with

$$\langle \xi(t) \rangle = 0$$

and

$$\left\langle \xi(t)\xi(t') \right\rangle = 2\eta\frac{k_B T}{m}\delta(t-t')$$

The experimental measurements

The instantaneous velocity of a Brownian particle has been measured with a resolution such that both the ballistic and diffusive regime of the Brownian motion could be detected [1]. Li *et al.* [1] studied the motion of a silica particle with the size of about one μm in diameter. If it is dissolved in a liquid the motion becomes too overdamped and therefore they considered air as the solvent, which has a much lower viscosity. The authors managed to trap and monitor the motion of the silica particles using optical tweezers. Long-duration, ultra-high resolution measurements where performed over a wide range of air pressures and at room temperature (300K).

Consider the motion of the silica (SiO_2) particles studied by Li *et al* [1]. The particles have a diameter of 2.79 μm in average and their density is ρ=2.65 g/cm^3. The trap generates a harmonic potential well with a vibrational frequency of about $f_0 = \omega_0/2\pi = 3.1$ kHz for the silica particles. The measurements where performed at room temperature (297 K) and at two different pressures, 99.8 kPa and 2.75 kPa. They obtained the relaxation times τ=48.5 μs and τ=147.3 μs, respectively. The relaxation time is related to the friction coefficient η, introduced in the Langevin's equation, via $\tau = 1/\eta$.

Denote the two different cases as:

$$\begin{aligned} \text{case Low:} \quad & \tau = 147.3\ \mu\text{s} \\ \text{case High:} \quad & \tau = 48.5\ \mu\text{s} \end{aligned}$$

Task

1. Do E3 task 1 on Yata to convert the experimental parameters to reasonable simulation units

2. Do E3 task 2 on Yata to implement the BD3 algorithm in the lecture notes "Brownian dynamics" to to numerically solve the Langevin's equation with an external force.

3. Use your implementation of the BD3 algorithm to generate a single two-dimensional $(x(t), v(t))$ trajectory, one for case Low and one for case High. You should monitor a system in equilibrium. You can therefore start with some arbitrary initial condition $(x(0), v(0))$ and run for a time extension of several relaxation times. Throw away these initial data points, continue to run and use these subsequent data points for analysis. Perform the computation for two different time steps, $\Delta t = 0.005$ ms and $\Delta t = 0.001$ ms.

   Plot your results as in Fig 2 in Ref. [1]. Comment on your results! (1p)

4. Consider now the power spectrum of the velocity $\mathcal{P}_v(f)$, where f is the ordinary frequency, $f = \omega/2\pi$. Use the trajectories for $v(t)$ that you have obtained using $\Delta t = 0.001$ ms. Sample the signal $v(t)$ equidistant with time spacing $\Delta\tau = 50\Delta t = 0.05$ ms. This corresponds to the Nyqvist frequency $f_c = 10$ kHz. Determine the spectrum $\mathcal{P}_v(f)$ using

FFT for both case Low and case High. Plot your result as function of f, with $0< f <10$ kHz.

Repeat the calculation of $\mathcal{P}_v(f)$ but now with time spacing $\Delta\tau = 25\Delta t = 0.025$ ms. Plot the result in the same figure. Compare also with the analytical result for a damped harmonic oscillator, which you find in the lecture notes "Brownian dynamics". Comment on your result!

One would expect that if one runs longer trajectories and then make a fourier transformation, one would obtain a more accurate spectrum. However, if one then only performs a straightforward fourier transformation the corresponding spectrum is not more "accurate". You only get a more dense grid of frequency points. A way to increase the "accuracy" is to divide the long trajectory into say M segments, with equal number of time points, fourier transform each segment and then take an average over the M different power spectra. Perform such a test. Do you obtain a more "accurate" spectrum? (1p) Hint: You need good statistics, i.e., sufficiently many segments, M, to get a reasonable spectrum.

5. Consider now the motion in time domain. Determine the time correlation function for the velocity $v(t)$ using the direct approach defined in lecture notes "Molecular dynamics" section (8.1). Perform the evaluation for both case Low and case High. Compare your results with Fig 4B in Ref. [1]. Can you reproduce the experimental data? (1p) Hint: You need to average the time correlation for sufficiently many starting times, t, see (Eq. 71) in MD Lecture notes.

6. The power spectrum can be related to the time correlation function using the Wiener-Khintchin's theorem. Use this to derive the power spectrum from your computed time correlation function for the velocity. Do you obtain the same result as from the powerspectrum of the trajectory $v(t)$? (1p)

References

[1] T. Li, S. Kheifets, D. Medellin, M. G. Raizen, Science **328**, 1673 (2010).