MSDM 5003 Homework 2 Solution

1. (a) See the program file `1D_random_walk_simulation.py`. The program is written in `Python` with the libraries `NumPy`, `SciPy` and `Matplotlib` and was executed using `Spyder`. After setting $\gamma = k_B T = 1$ and $U(x) = 0$, the differential equation whose solution is sought becomes

$$\frac{dx}{dt} = \zeta, \tag{1}$$

where the value of ζ at each time instance is to be sampled from the normally distributed random variable $Z \sim \mathcal{N}(0, 2/h)$ with h being the time resolution. By setting $x(0) = 0$, we have $\langle [x(t) - x(0)]^2 \rangle = \langle [x(t)]^2 \rangle$. The average was taken over an ensemble of 500 particles. Fig. 1 shows a plot of the mean square displacement ensemble average against time from the simulation together with a fitted straight line passing through the origin. The slope of the fitted line is 2.0168 with a standard deviation of 0.0014 therefore the diffusivity obtained from the simulation is 1.0084 with a standard deviation of 0.0007. This agrees with the theoretical value of the diffusivity at $D = k_B T/\gamma = 1$.

   (b) See the program file `1D_brownian_simulation.py`. The program is written in `Python` with the libraries `NumPy` and `Matplotlib` and was executed using `Spyder`. After setting $\gamma = k_B T = 1$ and $U(x) = x^2/2$, the differential equation whose solution is sought becomes

$$\frac{dx}{dt} = -x + \zeta, \tag{2}$$

where the value of ζ at each time instance is to be sampled from the normally distributed random variable $Z \sim \mathcal{N}(0, 2/h)$ with h being the time resolution. The trajectory of a single particle was followed in the simulation and after a certain time interval dedicated as the transient run, the position of the particle at every time step was recorded and the distribution was fitted to a normal distribution of $\mathcal{N}(-0.01731, 1.00869)$. On the other hand, the theoretical distribution is

$$f(x) = C \exp\left[-\frac{U(x)}{k_B T}\right] = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) = \mathcal{N}(0, 1). \tag{3}$$

Not only do the mean and variance of the simulated distribution agree with the theoretical values, we also see from Fig. 2 that indeed the simulated distribution looks like a normal distribution.

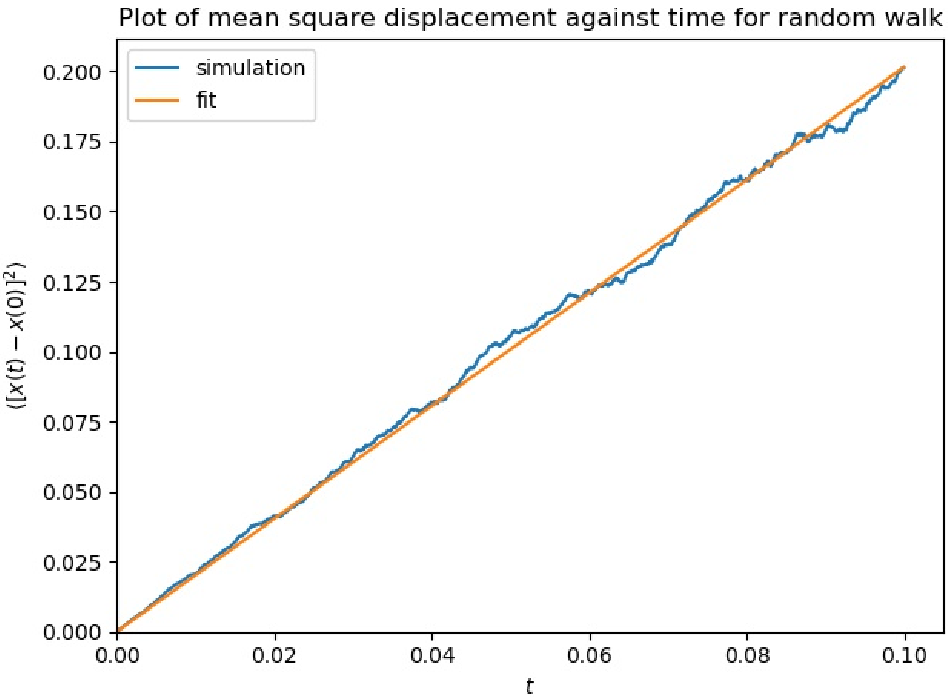

Figure 1: A plot of the mean square displacement ensemble average against time for particles under random walk. The fitted line gives a diffusivity of 1.0084, which agrees with the theoretical value of 1 for $\gamma = k_B T = 1$.

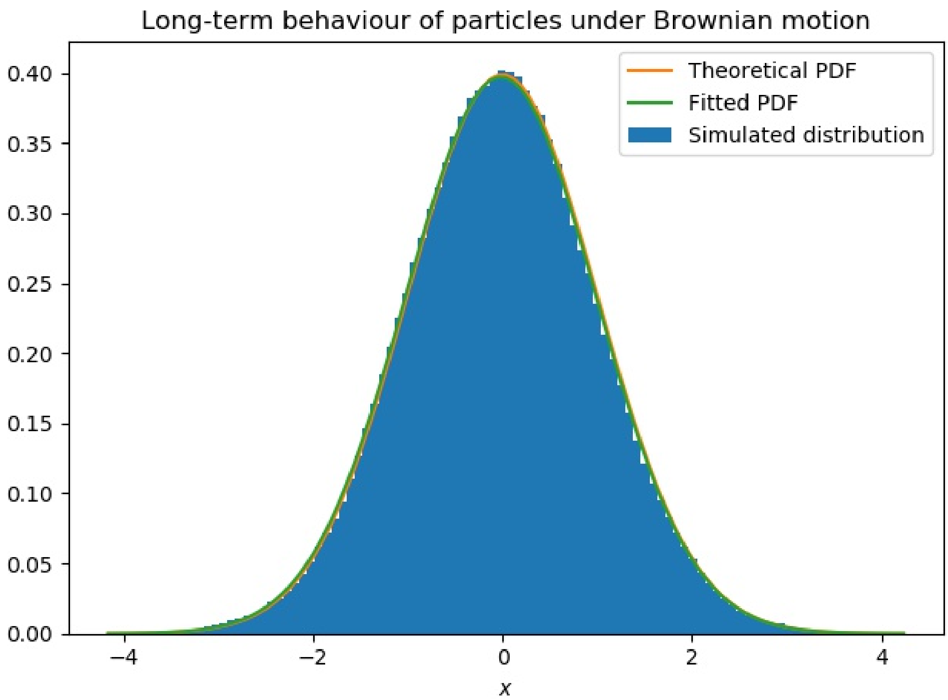

Figure 2: Normalised histogram of the samples for the long-term behaviour of a particle under Brownian motion with a confinement potential of $x^2/2$. The fitted normal distribution is $\mathcal{N}(-0.01731, 1.00869)$, which agrees with the theoretical distribution of $\mathcal{N}(0, 1)$ for $k_B T = 1$.