Exercise 1

Consider two particles in a 3-dimensional space, of coordinates r_1 and r_2, evolving at a temperature $T = 1$ under the action of a potential

$$V(r_1, r_2) = exp(-|r_1 - r_2|)\chi(R - |r_1|)$$

where $R > 0$ and $\chi(x) = 1$ if $x > 0$ and $\chi(x) = \infty$ otherwise

1. compute the free energy as a function of $S(r) = |r_1 - r_2|$

Exercise 2

Consider a system evolving under the action of a 2-dimensional potential

$$V(x, y) = -\log\left(6\exp\left(-2x^2 - \frac{1}{4}y^2\right) + 4\exp\left(-\left(x - \frac{3}{2}\right)^2 - \left(y - \frac{5}{2}\right)^2\right)\right)$$

at a temperature T=1

1. Compute the probabilities $P(x)$, $P(y)$ and the free energies $F(x)$ and $F(y)$.
2. By using the Arrhenius formula estimate the mean first passage time from the potential energy minimum in $(0, 0)$ and the potential energy minimum in $\left(\frac{3}{2}, \frac{5}{2}\right)$. Assume $\tau_{ex} = 1$ ps.

Exercise 3

Compute the average, the standard deviation and the estimated error on the average of the time series ts1.dat, ts2.dat and ts3.dat.