

Consider a system of a one-dimensional particle under the action of a double-well potential and linearly coupled to a set of 30 harmonic oscillators. The system Hamiltonian is:  $H = H_S + H_B$ . Here,  $H_S = \frac{p_s^2}{2} + U_s(x)$  is the Hamiltonian of the one-dimensional particle, with the potential energy  $U_s(x) = U_0(x^2 - 1)^2$ , and  $x, p_s$  are the position and momentum of the one-dimensional particle;  $H_B = \sum_{j=1}^N \left( \frac{p_j^2}{2} + \frac{1}{2} \omega_j^2 q_j^2 - \gamma_j q_j x \right)$  is the Hamiltonian that accounts for the harmonic oscillators and their coupling with the one-dimensional particle, where  $N = 30$ ,  $q_j, p_j, \omega_j$  are the position, momentum and frequency of the  $j$ -th harmonic oscillator,  $\gamma_j$  is the coupling constant between the  $j$ -th harmonic oscillator and the one-dimensional particle. We choose  $\omega_j^2 = c \cdot j$ , for all  $1 \leq j \leq N$ , and  $c = \sum_{j=1}^N (\frac{1}{j}) / \sum_{j=1}^{10} (\frac{1}{j})$ ,  $\gamma_j = 1, 1 \leq j \leq N$ .

Do molecular simulation for two conditions: a)  $U_0 = 2, k_B T = 1$ , b)  $U_0 = 2.5, k_B T = 1$ , where  $k_B$  is the Boltzmann constant and  $T$  is the temperature. For each condition, the initial positions are:  $x = -1, q_j = 0, 1 \leq j \leq N$ , and the initial momenta should be drawn from the Maxwell

distribution:  $f(p) = \sqrt{\frac{1}{2k_B T}} e^{\frac{-p^2}{2k_B T}}$ . After you draw 31 random numbers,  $(p'_s, p'_1, \dots, p'_{31})$ , from

this distribution, normalize them with  $a = \left( \frac{0.5 \cdot (N+1) k_B T}{K'} \right)^{1/2}$ , where  $K' = \frac{p_s'^2}{2} + \sum_{j=1}^N \frac{p_j'^2}{2}$ . That is, use  $p_s = a \cdot p'_s, p_j = a \cdot p'_j$  as the initial momenta for the 1-D particle and the 30 harmonic oscillators.

For each simulation, 1) plot the potential, kinetic and total energy of the system as a function of the simulation time, 2) plot position of  $x_s$  as a function of time, which should stochastically transition between the two basins located at 1 and -1. 3) Run your MD simulation long enough so that you can compute a reliable distribution for the waiting time for the transitions. 4) Discuss what you learned from the distributions for the waiting time.