Homework 10. Due May 1

1. **(5 points)** Consider a system evolving according to

$$dX_t = b(X_t)dt + \sqrt{2\beta^{-1}}dw.$$

Let $U(x)$ be the quasipotential with respect to an attractor of $\dot{x} = b(x)$. Assume $U(x)$ is continuously differentiable everywhere. Decompose $b(x)$ into the potential component $-U(x)/2$ and a rotational component $l(x)$ which must be orthogonal to $U(x)$:

$$b(x) = -\tfrac{1}{2}\nabla U(x) + l(x), \quad \nabla U(x) \cdot l(x) = 0.$$

Prove that the equilibrium probability density is given by

$$m(x) = Z^{-1}\exp\{-\tfrac{\beta}{2}U(x)\},$$

whenever the rotational component $l(x)$ of the vector field $b(x)$ is divergence-free, i.e., $\nabla \cdot l(x) = 0$.

Remark If $l(x)$ is not divergence-free then $m(x) \asymp \exp\{-\beta U(x)/2\}$ in the basin of attraction of the attractor.

2. **(5 points)** The Freidlin-Wentzel action for the Langevin dynamics

$$\ddot{x} = -\dot{x} - \nabla V(x) + \sqrt{2\beta^{-1}}\eta_t, \quad \eta_i \text{ is the white noise,}$$

is given by

$$S_T(\phi) = \frac{1}{2}\int_0^T \|\ddot{\phi} + \dot{\phi} + \nabla V(\phi)\|^2 dt.$$

Let x_0 be a minimum of the potential $V(x)$ and x_f lies in the basin of attraction of the minimum x_0.

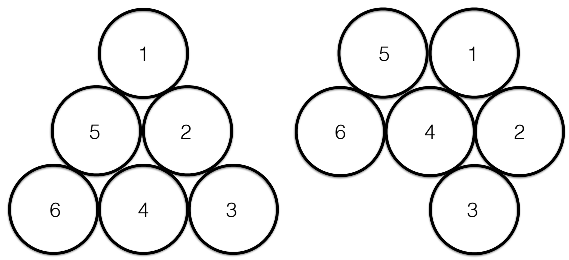
   (a) Show that the path ψ minimizing $S_T(\phi)$ over all paths starting at x_0 and ending at x_f and all times T satisfies $\ddot{\psi} = \dot{\psi} - \nabla V(\psi)$.

   (b) What is the value of the Freidlin-Wentzel action along the path ψ?

3. Consider 6 atoms in 2D interacting according to the Lennard-Jones pair potential. The potential energy of this system is given by

$$V = 4\sum_{i=1}^{5}\sum_{j=i+1}^{6}(r_{ij}^{-12} - r_{ij}^{-6}), \quad r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}.$$

(a) **(5 points)** Use the string method to find the Minimum Energy Path connecting the following two configurations:



Plot the energy along the found Minimum Energy Path.

(b) **(5 points)** Use the shrinking dimer method to find all of the saddle points encountered by the found Minimum Energy Path. Draw the found saddles. Indicate the value of the potential energy at them and indicate the norm of the gradient of the potential at them (it should be small, less than your tolerance, but it will no be exactly zero).

Hint: You might find helpful the code LJ7.m where a similar problem with 7 atoms in 2D interacting according to the Lennard-Jones potential is solved.