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Problem set 3: Computational Molecular Physics

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1. Markov Chain Monte Carlo (25 points)
Implement in your favourite programming language a Markov Chain Monte Carlo algorithm. Generate a Markov chain of N=10000 points (x,y) as a "walk" in the following 2D-potentials

$$\mathrm{V(x,y)} = -(\frac{x^2}{2}+\frac{y^2}{2}) + 5$$

$$\mathrm{V(x,y)} = (\frac{x^2}{2}+\frac{y^2}{2}) - 5$$

The potentials has periodic boundary conditions such that V(x,5.0)=V(x,-5.0) and V(5.0,y)=V(-5.0,y). You can model this by setting e.g. (x,y)=(-6.0,1.0) to (x,y)=(4.0,1.0) or (x,y)=(3.0,7.5) to (x,y)=(3.0,-2.5) etc.

Choose a random initial point q_0=(x_0,y_0) from the distributions and propose a new point q_1=(x_1,y_1) by chosing it uniform randomly from an interval [-0.5,0.5] around q_0. Accept/Reject the newly proposed position q_i according to the Metropolis-Hastings acceptance criterion using a Boltzmann distribution with kT=0.5 .

Plot the sampled points as a 2D histogramm and explain the different distribution of points in each case.

2. Transition Matrix (25 points)
Consider the Markov chain with four states, that has the following transition matrix P

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

(i) Draw a diagram representing the states (e.g. as circles) and transitions (as arrows) for this chain.
(ii) Given the following vectors of probabilities of the four states w1=[1/6, 2/6, 2/6, 1/6], w2=[1/2, 1/2, 0, 0] and w3=[1/2, 1/4, 0, 1/4] check whether any of them represents a stationary distribution.
(iii) Apply the transition matrix to the distributions w1,w2, and w3 once, twice, n times. That is compute $\mathbf{w}^T\mathbf{P}^n$ with $n = 1, 2, ...7$. What do you observe?
(iv) Find the left and right eigenvalues and corresponding eigenvectors of the transition matrix. How can the eigenvalues and eigenvectors be understood in a more physical meaning?