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Exercise class in HCI J7.

This week's task is to implement the path-integral Monte Carlo algorithm and solve the harmonic and anharmonic 1D oscillator problems. We will consider two types of potentials:

$$V(x) = \frac{m\omega^2 x^2}{2} \tag{1}$$
$$V(x) = \lambda(x^2 - \eta^2)^2 \tag{2}$$

The former potential is just the 1D oscillator. The latter potential, known also as the "hat" potential, is often used to describe theories with spontaneous symmetry breaking such as the Higgs boson field. Define a class `Config` that will take also the external potential as an input. The class should have methods for the following operations:

- propose a new path x' out of current path x. There are different ways to propose a move: for instance, you may select random time slice and perform the shift `x += np.random.uniform(-maxshift, maxshift)`.
- based on the metropolis ratio
$$\min\left(1, \frac{\exp(-T(x') - V(x'))}{\exp(-T(x) - V(x))}\right) \tag{3}$$
decide whether the x' path will be accepted or rejected.
- plot the histogram of all positions that the particle occupied at all the paths accepted during the algorithm run. This histogram, if properly normalized, would give one $|\psi(x)|^2$ wave function density.

Exercise 1. *Harmonic potential*

Perform the simulation of the potential (1) using the path integral Monte Carlo algorithm for $\beta = 1, m = \omega = 1$. Use $\mathcal{O}(10^4)$ thermalisation steps and $\mathcal{O}(10^5)$ simulation steps.

- Plot the evolution of potential and kinetic energies as a function of the iteration. Estimate their converged values and error by performing the autocorrelation analysis.
- Plot the wave function $|\psi(x)|^2$ as a histogram of observed positions.

Exercise 2. *Higgs potential*

Perform the simulation of the potential (2) using the path integral Monte Carlo algorithm for $\beta = 1, m = \lambda = 1$ and $\eta = 1$ and 3. Use $\mathcal{O}(10^4)$ thermalisation steps and $\mathcal{O}(10^5)$ simulation steps.

- Plot the potential (2) for various values of η.

- Plot the evolution of potential and kinetic energies as a function of the iteration. Estimate their converged values and error by performing the autocorrelation analysis.
- Plot the wave function $|\psi(x)|^2$ as a histogram of observed positions.
- Consider $\eta = 1$ and a much longer $\mathcal{O}(10^6)$ simulation. Split this simulation into $\mathcal{O}(100)$ intervals and plot the wave function on each of them. Since the potential has two minima, the wave function will "tunnel" between them.
- Consider $\eta = 3$ and plot the wave function. Why do you observe such a picture? What does it tell us about the algorithm efficiency in case of this potential?