1. **Quantum Wave Functions via Path Integrals: The Metropolis Algorithm**

In this exercise we consider ordinary quantum mechanics in the Path Integral formulation on a 1D lattice with N sites. The lattice action is given by

$$S_{\text{lattice}} = \sum_{i=0}^{N-1} \left(\frac{m}{2a} \left(x_{i+1} - x_i \right)^2 + a\, V(x_i) \right) , \tag{1}$$

The ground state to ground state propagator can be approximated by

$$\left\langle x \left| e^{-\tilde{H}T} \right| x \right\rangle = A \int_{-\infty}^{\infty} dx_1 ... dx_{N-1}\, e^{-S_{\text{lattice}}[x]} , \tag{2}$$

with the normalization factor $A = \left(\frac{m}{2\pi a}\right)^{\frac{N}{2}}$.

Your task is to calculate the ground state to ground state propagator for the potential of a harmonic oscillator given by

$$V(x) = k\frac{x^2}{2} , \tag{3}$$

using the *Metropolis* algorithm. For simplicity consider $k = m = 1$ and choose $a = 0.5$ and $N = 100$, with $x_N = x_0$.

The *Metropolis* algorithm performs a special kind of Monte Carlo integration. It works as follows:

(a) We choose values for the x_i first. Either choose a *cold* start (set all the x_i to zero) or a *warm* start (choose random values for all the x_i).

(b) The next step is to *thermalize* the configuration. The point of this step is to get rid of unphysical initial conditions. In order to thermalize the configuration we perform the following update step described in item (c) for 5 to 10 times the number of data samples that we assume to be correlated N_{cor}.

(c) Update the configuration:

1. Choose an uniform random number $r \in [-\varepsilon, \varepsilon]$.
2. Change a random x_i by r.
3. Calculate the difference in action between the old and the new configuration.
4. If the action is decreased, keep the new configuration.
5. If the action is not decreased, keep the new configuration with probability $\exp(-(S_{\text{new}} - S_{\text{old}}))$, otherwise restore the old configuration.

(d) Now we calculate a sample of N_{cf} configurations. There are two equivalent ways to do this:

- Perform steps (a) - (c) and take the last configuration for your sample, repeat this N_{cf} times
- Perform steps (a) - (c) only once and take N_{cf} configurations after the thermalization

The second method is obviously much faster. However, care has to be taken in order to obtain uncorrelated configurations. This can be done by performing N_{cor} update steps in between each obtained configuration.

Hint: Try $N_{\text{cf}} = 5000$*,* $N_{\text{cor}} = 50$ *and* $\varepsilon = 1.4$.

(e) We are interested in the transition matrix element, which translates to the calculation of the Green's function[1]

$$G(t) \equiv G_n = \frac{1}{N} \sum_{j=0}^{N-1} \langle x_{(j+n) \bmod N} x_j \rangle . \tag{4}$$

[1] Note that $\langle \ldots \rangle$ is the average over your configurations sample

All that is left to do is to calculate the energy difference ΔE, given by

$$\Delta E \approx a^{-1} \ln\left(\frac{G_n}{G_{n+1}}\right) . \tag{5}$$

Plot ΔE of the first few n and discuss the result.

(f) Determine the ground-state wave function $|\psi_0(x)|^2$

$$|\psi_0(x)|^2 = A \int_{-\infty}^{\infty} dx_0 ... dx_{N-1} \delta(x - x_0) e^{-S_{lattice}[x]} , \tag{6}$$

by filling a histogram with all N_{cf} samples of the first x coordinate x_0. Compare your result to the analytic solution

$$\left\langle x \left| e^{-\tilde{H}T} \right| x \right\rangle \approx \left| \frac{e^{-\frac{x^2}{2}}}{\pi^{\frac{1}{4}}} \right|^2 e^{-E_0 T} . \tag{7}$$

(g) Try changing the parameters for your simulation and investigate the behaviour of your simulation in dependence of these parameters. Especially, try to change N_{cor} and ε.