Computational Quantum Physics
Exercise 11

PHYS-463
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Problem 11.1 Path Integral Monte Carlo - Harmonic Oscillator

In this exercise we want to use our knowledge about imaginary time evolution of quantum states from Exercise 10 to simulate the finite temperature properties of one particle confined by a harmonic oscillator. For this we will use the PIMC method introduced in Chapter 12.3.
For one particle the system configuration is given by the (ordered) set of positions $x = (x_0, ..., x_P)$ where we have a total of P time-slices between 0 and β ($x_0 \equiv x_P$).

a) To produce a new system configuration $\tilde{x} = (\tilde{x_0}, ..., \tilde{x_P})$ from an existing one (x) we use the single-bead Metropolis algorithm described in Chapter 12.3.1. Implement the Metropolis algorithm and compute the acceptance ratio of it.

b) To assess the quality of the configurations obtained with the above algorithm, we want to compare their energy to the exact one. For this you need to implement the potential and kinetic energy observable. The potential and kinetic energy estimators can be computed as described in Chapter 12.1.1. You obtain the observable by averaging over all your estimates. Implement the following observables:

   - Potential Energy
   - Kinetic Energy
   - Density operator in position space (optional)

   (*Hint*: You can estimate the density operator by producing a histogram of your system configuration for every sweep and averaging over all of them.)

c) Estimate the autocorrelation time and errors for the observables you computed in a).

Hints for the implementation:

- Reasonable values for the simulation are:
  - $\beta = 1$
  - $\Delta_\tau = 0.1$
  - thermalization sweeps: 20000
  - total sweeps: 250000
- The exact energy is given by $E = \frac{1}{2}\coth(\beta/2)$
- Choose the maximum displacement in each step such that your acceptance probability is neither close to one nor close to zero ($\approx 50\%$).
- In case your code takes a long time to complete, you might want to do the debugging with less sweeps.