ETH
Eidgenössische Technische Hochschule Zürich
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Computational Quantum Physics
Exercise 4.

FS 2019
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Problem 1. *Path Integral Monte Carlo - Harmonic Oscillator*

Solve the one-particle harmonic oscillator problem at finite temperature with PIMC. The system configuration is comprised of positions x_i for the M time slices between 0 and β of a particle in harmonic potential.

- Implement functions that evaluate the potential and kinetic energy of a configuration $\{x_m\}$ using the proper boundary conditions.

- Implement the Metropolis algorithm of sampling the configurations as described in the section 7.1.4 of the script.

- Implement observables:

  1. Potential Energy

  2. Kinetic Energy

  3. Density operator in position space (optional)

- Estimate the autocorrelation time and errors for your observables.

Hints for the implementation:

- Reasonable values for the simulation are:

  - $\beta = 1$

  - $\tau = 0.1$

  - thermalization sweeps: 20000

  - total sweeps: 500000

- Choose the maximum displacement in each step such that your acceptance probability is neither close to one nor close to zero.

- In case your code takes long time to complete, you might want to do the debugging with less sweeps.