ETH
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Computational Quantum Physics
Exercise 6

FS 16
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Problem 6.1 Path Integral Monte Carlo - Harmonic Oscillator

Solve the one-particle harmonic oscillator problem 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)
- Metropolis Monte-Carlo steps produce a series of correlated configurations. Implement binning analysis (described in Monte Carlo notes) to estimate the autocorrelation time for your observables and properly estimate the errors.

Hints for the implementation:

- Reasonable values for the simulation are:
  - $\beta = 10$
  - $M = 100$
  - thermalization sweeps: 20000
  - total sweeps: 300000
- 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.