

Computational Quantum Physics Exercise 4

Problem 4.1 Path Integral MonteCarlo - Harmonic Oscillator

Solve the harmonic oscillator problem with PIMC.

- Build a data structure that contains positions x_m for the M time slices between 0 and β for the harmonic oscillator.
- Write a function that computes the potential energy of such a configuration.
- Write a function that computes the kinetic energy of the corresponding classical system, using the proper boundary conditions.
- Implement the metropolis procedure for PIMC.
- Implement observables:
 - Kinetic Energy
 - Potential Energy
 - Wave function

Reasonable values for your simulation are:

- $\beta = 10$
- $M = 100$
- thermalization steps: 2000
- steps: 30000

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