Computational Quantum Physics – Exercise 4

Problem 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.