

# Computational Quantum Physics Exercise 5

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## Problem 5.1 Path Integral Monte Carlo - Harmonic Oscillator

Solve the harmonic oscillator problem with PIMC.

- Build a data structure for a system configuration which contains positions  $x_m$  for the  $M$  time slices between 0 and  $\beta$  for the harmonic oscillator.
- Implement the metropolis procedure for PIMC. For this purpose write functions that evaluate the contributions of the
  1. potential term
  2. kinetic term

of the Hamiltonian to the energy of a configuration  $\{x_m\}$  using the proper boundary conditions. Then use these functions to implement the Metropolis algorithm to sample the path integrals.

- Implement observables:
  1. Potential Energy
  2. Kinetic Energy
  3. Wave function (bonus)

Reasonable values for your simulation are:

- $\beta = 10$
- $M = 100$
- thermalization sweeps: 20000
- sweeps: 300000

Choose the maximum displacement in each step such that your acceptance probability is neither close to one nor close to zero. **Hint:** In case your code takes a long time to complete, you might want to do the debugging with less sweeps.