

# Computational Quantum Physics Exercise 5

---

## 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
  - potential term
  - 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 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.