Lattice Monte-Carlo simulation of the quantum mechanical path integral

Instructions
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1 Introduction

• Study the introduction MC_introduction.pdf to the quantum mechanical path integral and to Monte-Carlo simulations.

• Study the provided C code MC_QM.C.

2 Simulation of the harmonic oscillator

2.1 First run

Check whether the following parameters in the code are defined as follows:

• m = 0.5
• omega = 0.75
• numSweepsOut = 10
• numSweepsThermalization = 1000
• numSweeps = 5000
• N = 64
• delta_t = 1.0
• delta_q = 3.0
• PathNumber = 0
• qMaxStart = 5.0

If not, define then accordingly. Compile and run the code, i.e. perform a first simulation.
2.2 The action $S$ and thermalization

Plot $\langle S \rangle$ (the action averaged over numSweepsOut) for a hot and a cold start for $\text{delta}_q = \{0.003, 0.03, 0.3, 3.0, 30.0, 300.0\}$.

- Are hot or cold starts preferable?
- Which is the best choice for $\text{delta}_q$?
- After approximately how many steps did the simulation thermalize in each of these twelve cases?

Crudely optimize $\text{delta}_q$ for the parameters defined in ???. A heuristic criterion is that around 50% of all Metropolis updates are accepted.

Now change $\omega$ to $\omega = 0.125$. Is the previously optimized $\text{delta}_q$ still optimal? If not, optimize again.

2.3 Investigation of paths generated during the simulation

Plot several arbitrary paths after thermalization taken from simulations at $\omega = \{0.75, 0.125, 5.0\}$. Explain and interpret your observation in particular the qualitative differences.

Plot the first ten paths of a simulation to study thermalization in more detail. To this end perform a simulation with a cold start and $\text{delta}_q = 5.0$.

2.4 Computation of correlation functions and extraction of energy differences

Return to $\omega = 0.75$ and the corresponding optimized $\text{delta}_q$.

- Use the code to compute the correlation function $C(t) = \langle x(t)x(0) \rangle$.
  - Study the details of the implementation. In particular explain how $\langle x(t)x(0) \rangle$ is implemented.

- Fit $A \exp(-\Delta Et)$ to the numerical results for $C(t)$ (fitting parameters $A, \Delta E$) to extract the energy difference of the first excited state and the ground state.
  - Why is it dangerous to include small $t$ in the fit in general?
  - Why is it not a problem here?
  - Why is it dangerous to include large $t$ in the fit?
  - Specify and use a reasonable fit window to extract $\Delta E$ and a corresponding statistical error.
  - Compare with your analytical expectation.
• Perform another two simulations with `numSweepsOut = 100, numSweeps = 50000` and `numSweepsOut = 400, numSweeps = 200000` (such that $C(t)$ is evaluated again on 500 paths).
  
  - Extract $\Delta E$ again for both cases.
  
  - Compare the three results for $\Delta E$, in particular the associated statistical errors. Interpret your observation.

• Vary `numSweeps` (keeping `numSweepsOut` fixed) at least by a factor of 10 and investigate the behavior of the error of the correlation function. How does the error behave as a function of `numSweeps`?

3 Simulation of the anharmonic oscillator

Now that you are an expert in lattice MC simulation, study another problem, which cannot be solved analytically. Change the potential $V(x)$ in `void S_E()` and `double DeltaS_E(int index, double q_new)` to $V(x) = \frac{m \omega^2}{2} x^2 + \lambda x^4$.

Of course the results you will obtain for $\Delta E$ do not only depend on $\omega$ but also on $\lambda$.

• Compute $\Delta E$ for $m = 0.5, \omega = 0.75$ and $\lambda = \{ 0.001, 0.002, 0.004, 0.006, 0.01, 0.02, 0.1 \}$.

• Use standard textbook perturbation theory to check your code modification and results for small $\lambda$. 