# Computer simulations in physics

Plan for Project 2

## Path integral on the lattice

Dávid Pesznyák
Eötvös Loránd University
Physics MSc

# Contents

**1 Introduction** **2**

**2 Basic concepts and ideas** **2**

2.1 Path integral formalism . . . . . 2

2.2 Quantum mechanical potentials . . . . . 3

**3 Numerical methods** **4**

3.1 Markov chain Monte Carlo methods . . . . . 4

3.2 Autocorrelation times . . . . . 4

**4 Project layout** **4**

**References** **6**

# 1 Introduction

Apart from the well-known Schrödinger and Heisenberg pictures there exists a slightly different approach to treat and analyse quantum mechanical systems, which goes by the name of path integral formalism. In the '40s Richard Feynman reformulated quantum mechanics in a way that the probability amplitude for the transition between two distinct states of a given system is proportional to the sum of all, thus infinitely many, possible paths between the initial and final states – hence the name path integral – weighted by a factor of $\exp(iS/\hbar)$, in which $i$ is the imaginary unit, $S$ is the classical action and $\hbar$ is the reduced Planck constant.

The main purpose of my project is to familiarise with the path integral formalism and the evaluation of such integrals using Monte Carlo methods. I am going to numerically analyse rather simple one-dimensional systems with different, though physically relevant potentials. I will start with examples for which analytical solutions exist and afterwards continue to estimate certain properties of more complex cases. The bulk of my work will be based on [1, 2].

The origin of my personal motivation is related to my recent TDK research of evaluating and phenomenologically interpreting the results of lattice QCD simulations. The basics of such simulations are fundamentally connected to the path integral formalism and Markov chain Monte Carlo methods. Through this project I wish to learn the technical basics of the numerical experiments I analyse in my research.

# 2 Basic concepts and ideas

## 2.1 Path integral formalism

The aforementioned probability amplitude for the transition between states $|y\rangle$ and $|x\rangle$ over time $t$ can be written in the form of $A = \langle x|\mathcal{U}(t)|y\rangle$, in which $\mathcal{U}(t) = \exp(-i/\hbar\mathcal{H}t)$ is the time evolution operator with $\mathcal{H}$ Hamiltonian operator in the exponent corresponding to a mass $m$ particle moving in some potential. Naturally, the probability is $P(y \to x) = |A|^2$. For practical reasons one can perform an analytic continuation from real to imaginary time as $t = -i\tau$ ($\tau \in \mathbb{R}$), thus the probability amplitude in the path integral formalism in $\hbar = c = k_B = 1$ natural units

$$A = \int\limits_{y\to x} \mathcal{D}x\, e^{-S_\varepsilon^E} \,. \tag{2.1}$$

The $S_\varepsilon^E$ in the exponent denotes the Euclidean action discretised according to $\varepsilon = \tau/N$. The connection between the discretised Euclidean and classical action is $iS_\varepsilon^E = S_\varepsilon$, and as $N \to \infty$ one can get the continuous classical action. The formal integral measure can be expanded to

$$\mathcal{D}x = \lim_{N\to\infty} \left(\frac{m}{2\pi\varepsilon}\right)^{N/2} dx_1 dx_2 \dots dx_N \ , \tag{2.2}$$

which corresponds to the infinite number of possible paths.

With imaginary time the time evolution operator takes the form of a density operator from statistical mechanics: $\mathcal{U}(-i\tau) = e^{-\tau\mathcal{H}} = e^{-\beta\mathcal{H}}$, hence the temperature is

$$T = \frac{1}{\tau} = \frac{1}{N\varepsilon} \ . \tag{2.3}$$

This way the canonical partition function takes the form of

$$Z_N = \mathrm{Tr}(e^{-\beta\mathcal{H}}) = \int dx \, \langle x|e^{-\beta\mathcal{H}}|x\rangle = \int\limits_{x\to x} \mathcal{D}x \, e^{-S_\varepsilon^E} \ , \tag{2.4}$$

where Tr( ) denotes the trace of an operator and $x \to x$ means strictly periodic paths. Naturally, during the simulation $N$ will be some fixed finite value.

## 2.2 Quantum mechanical potentials

The $\mathcal{H}$ Hamiltonian for a mass $m$ particle moving in some $V$ one-dimensional potential can be generally written as

$$\mathcal{H} = \frac{p^2}{2m} + V(x) \ , \tag{2.5}$$

where $p$ is the momentum and $x$ is the position of the particle. The most popular and used potential is the simple harmonic potential $V(x) = m\omega^2 x^2/2$, the main benefit of which for us is that it has an analytical solution, hence it provides the perfect opportunity to check the obtained simulation results.

There are numerous possibilities to include and investigate further potentials; e.g. finite potential well, anharmonic potentials, Morse potential, Pöschl–Teller potential, Yukawa potential and its well-known special case, the Coulomb potential or the Lennard–Jones potential, etc [3].

# 3 Numerical methods

## 3.1 Markov chain Monte Carlo methods

Monte Carlo methods are widely used in all kinds of numerical simulations and calculations. Their main principle is the proper sampling of pseudorandom numbers from various probability distributions. The origins of the name of the method are linked to the famous casino of the city with the very same name.

The simulations will start from an initial path and will be iteratively updated by the proper Metropolis–Hastings algorithm. First of all, in order to measure the physically relevant quantities, one ought to wait for the system to reach – or to get close enough to – its stationary state (if it exists), in other words to thermalise. This possibly takes a more or less well-defined number of steps. The calculation of the $i$th state – or equivalently the $i$th path in this case – only depends on the $(i-1)$th, hence the trajectories will constitute a Markov chain. This dependence potentially leads to highly correlated paths, thus by considering all the realised trajectories, the chances for a feasible error estimation are short. To combat this effect one can discard a certain amount of paths discussed in the next subsection.

## 3.2 Autocorrelation times

To obtain the "right" data, one must discard a number of steps from the simulation. This number is strongly related to the so-called exponential and integrated autocorrelation times. For a random variable $X$ – which takes the value of $X_n$ in the $n$th step of the simulation – one can define the following autocorrelation function:

$$C_X(X_m, X_{m+t}) = \langle X_m X_{m+t} \rangle - \langle X_m \rangle \langle X_{m+t} \rangle \, , \tag{3.1}$$

where $\langle \, \rangle$ denotes averaging. One of the traits of such a function is its $\sim \exp(-t/\tau_{\text{exp}})$ decaying behaviour, in which $\tau_{\text{exp}}$ is the aforementioned exponential autocorrelation time. Using this quantity one can estimate the necessary number of simulation steps for thermalisation; from here on out the characteristic observables of the system can be measured; however, they will be still correlated.

In order to overcome the harmful correlations and obtain statistically well-behaving samples from the simulations, one must take into account the $\tau_{\text{int}}$ integrated autocorrelation time as well. Its definition is somewhat different from that of $\tau_{\text{exp}}$, although in most cases they can be considered approximately the same. Overall, one shall wait a multiple of $\tau_{\text{exp/int}}$ steps to get reliable data from Markov chain Monte Carlo simulations.

# 4 Project layout

During the project I shall create my own path integral evaluating simulation program and make sure that they produce the right data. To achieve this, I am going to start with the simple quantum harmonic

oscillator system. If the simulation of the analytically well-known scenario is successful, I shall move forward to incorporate more exotic potentials into the simulations and examine their characteristic properties and possible observables.

## References


[1] M. J. E. Westbroek, P. R. King, D. D. Vvedensky, S. Durr. *User's guide to Monte Carlo methods for evaluating path integrals.* American Journal of Physics, Vol. 86, Issue 4 (2018)

[2] R. H. Landau, M. J. Paez, C. Bordeianu. *A Survey of Computational Physics - introductory computational science.* Princeton University Press., 2008.

[3] `https://en.wikipedia.org/wiki/List_of_quantum-mechanical_potentials`