Monte Carlo approach to path integral: Quantum Harmonic Oscillator and 2-Point Correlations

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(Dated: March 24, 2024)

Monte Carlo methods are used for many stochastic processes, one of them is the generation of configurations from a physical system from a particulas lagrangian, in this project we explore the Metropolis-Hastings methdo to approach a path integral treatment of the quantum harmonic oscillator, the montecarlo estimate is calculated for the generated paths to perform a statistical average of the position observable and its powers, also the correlation 2-point function is estimated for the paths, showing the correlation between various times in the path. from it we can obtain the effective mass, the correlation time and even a lower bound for the number of times in the path suitable for accurate calculations.

Keywords: Monte Carlo, Metropolis-Hastings method, Path Integral, Two-Point Correlation Function, Quantum Harmonic Oscillator.

I. INTRODUCTION

The Monte Carlo method for path integrals is a numerical technique used to study quantum systems like the harmonic oscillator. It employs stochastic sampling to evaluate path integrals, which are otherwise complex to solve analytically. This method is particularly effective for calculating properties of the ground state and analyzing quantum fluctuations [1, 2].

In the context of the quantum harmonic oscillator, the Monte Carlo approach allows for the examination of the oscillator's behavior under various conditions, including different potentials and external forces [3].

The path integral formulation, integral to this approach, was developed as an alternative to the traditional Schrödinger equation, providing a more comprehensive understanding of quantum mechanics.

The two-point correlation function is another critical concept in quantum mechanics and statistical physics [2], measuring the probability of finding pairs of particles at a certain distance apart. It's a fundamental tool in fields ranging from particle physics to cosmology, helping to reveal the underlying structure and interactions within a system.

II. THEORETICAL BACKGROUND OF QUANTUM HARMONIC OSCILLATOR

The Hamiltonian for a particle of mass m bound by a harmonic potential with force constant k is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{mw^2\hat{x}^2}{2}, \tag{1}$$

The discretized Euclidean Lagrangian for this system is

$$L_i = \frac{m}{2}(\frac{x_{i+1} - x_i}{\delta\tau})^2 + \frac{mw^2(x_i)^2}{2}. \tag{2}$$

as the computer doesn't manage any units, we have to introduce our equations in dimensionless form, so we write all the parameters in terms of the lattice spacing $\delta\tau$

$$m\prime = m\delta\tau, \omega\prime = \omega\delta\tau, x_i\prime = \frac{x_i}{\delta\tau}, \tag{3}$$

so that the primed variables are the parameters of the computer and the unprimed variables are the physical ones. We allow $m = 1$ so that m' acts as the effective lattice spacing and we will need to account for it when calculating the real physica value of the position expected value. Thus, according to Westbroek and King [1], the discretized Euclidean action can be written as

$$S' = \sum_{i=1}^{N_\tau}[\frac{1}{2}m'(x'_{i+1} - x'_i)^2 + \frac{mw^2(x_i)^2}{2}]. \tag{4}$$

III. THEORETICAL EXPECTED VALUE OF THE POWERS OF $\hat{x}$

in Ref [2], Creutz and Freedman show that

$$\langle\hat{x}^2\rangle = \frac{1}{2m'\omega'\sqrt{1 + \frac{w'^2}{4}}}(\frac{1 + R^{N_\tau}}{1 - R^{N_\tau}}), \tag{5}$$

where

$$R = 1 + (\omega')^2 - \omega'\sqrt{1 + \frac{w'^2}{4}}. \tag{6}$$

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$$\langle \hat{x}^4 \rangle = \frac{3}{(2m'w')^2(1+\frac{w'^2}{4})}(\frac{1+R^{N_\tau}}{1-R^{N_\tau}})^2 = 3\langle \hat{x}^2 \rangle^2. \quad (7)$$

This expresions will help us to corroborate our computational results.

IV. COMPUTATIONAL METHODS

A. Metropolis-Hastings Method

For the configurations of the system to be simulated from its lagrangian we will implement the Metropolis-Hastings method, this methods randomly select a place of the path (a time) and propose a random change in x_i, if the action is reduced the change will be accepted, otherwise the probability (the exponential of the change in the action) is compared with a random uniform probability to decide to accept or reject the change. One application of N_t Metropolis-Hastings' updates produces a new path and is called one Metropolis sweep, using the path Monte Carlo estimate we can "measure" an observable for that path, so that after N_{sweeps} paths generated (we discard 200 paths between each measurement) we can average the "measure" of the observable for this stochastic process, according to Westbroek and King [1]. The steps for the Metropolis-Hastings algorithm are the following.

1. . Generate a random number u from a uniform distribution in the interval $[-h, h]$.
2. . Propose a change to the visited site, $x_i \to x_i' = x_i + u$.
3. . Compute the change in the action δS as a result of this trial modifcation.
4. . Accept the change with probability $min\{1, e^{-\delta S}\}$.

The kinetic energy of Eq. (4) for a certain time τ is calculated with the previous and next time i.e. for $\tau+\Delta\tau$ and $\tau-\Delta\tau$ imposing a dependence in the current time on the previous an next time, this correlation intrinsic of the system is studied in the last part of the results as a function of $\Delta\tau$.

B. 2-Point Correlation Function and Correlation time

$$\begin{aligned} G(\Delta\tau) &= \langle x(\tau)x(\tau+\Delta\tau)\rangle - \langle x(\tau)\rangle\langle x(\tau+\Delta\tau)\rangle \\ &= \langle x(\tau)x(\tau+\Delta\tau)\rangle, \end{aligned}$$

where the fact that $\langle x(\tau)\rangle = 0$ for the quantum harmonic oscillator was used. Then the 2-Point correlation function can be calculated from each of the paths as [1]

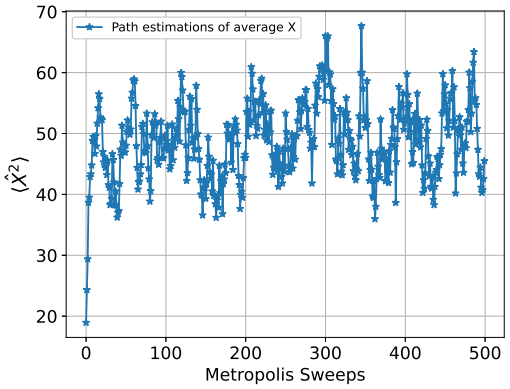

FIG. 1. Trial run to see when the behaviour of the paths thermilizes from the Lagrangian for 500 Metropolis sweeps, $N_\tau = 1200$ and $m = \omega = 0.1 = \delta\tau$.

$$G(\Delta\tau) = \frac{1}{N_\tau}\sum_{i=1}^{N_\tau} \sum_{\substack{j=1 \\ (j-i)modN_\tau=\Delta\tau}}^{N_\tau} x(i)x(j). \quad (8)$$

The effective mass is defined as

$$\frac{1}{\zeta'} = \frac{1}{2}\log[\frac{G(\Delta\tau-1)}{G(\Delta\tau+1)}] \quad (9)$$

where ζ is called the correlation time [1].

V. RESULTS AND DISCUSSION

A. Thermalization

The first paths generated by Metropolis-Hastings are not part of the real distribution as they do not capture the lagrangian yet, so we perform a simulation to see how many paths do we have to pass to get to the thermalized behaviour, in this case, from Fig. 1 it can be seen that between 50-100 is enough.

B. Expected value of position powers

the averaged value of the expected values was calculated from the multiple paths obtaining 0.5 for x^2 and 0.75 for x^4 as can be seen in Fig. 2

C. Time correlation through 2-point function

Fig. 3 shows that the measurements of correlations are not reliable from $\Delta\tau \approx 20$ for the $N_sweeps = 1000$ of our simulation, due to the error bars. We expect that

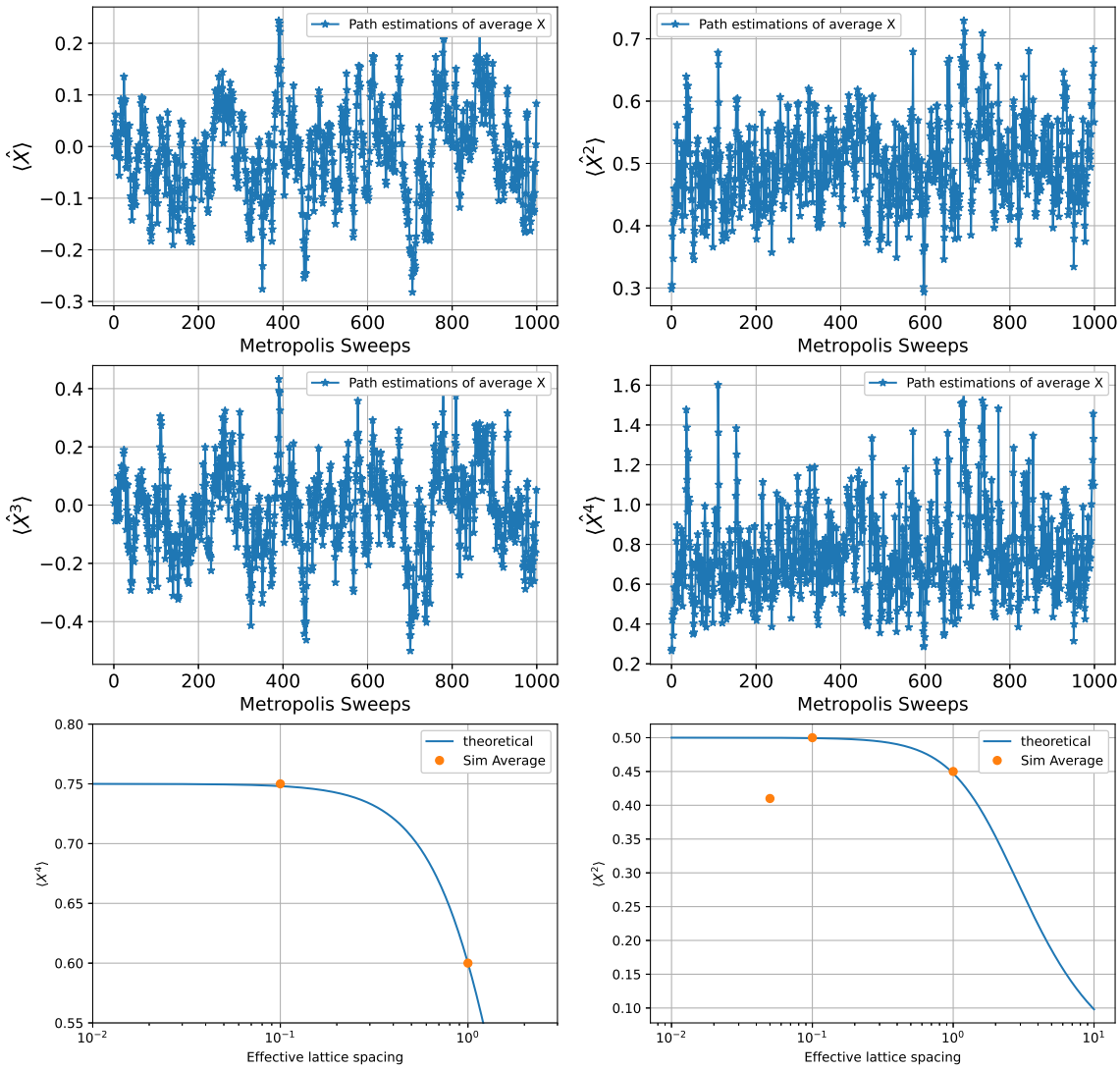

FIG. 2. various simulations of different paths and the Monte Carlo estimate of each of them for different powers of x, the estimates of each path are averaged for 1000 Metropolis sweeps, $N_\tau = 1200$ and $m = \omega = 0.1 = \delta\tau$.

for $N_sweeps = 10000$ the average of each point would be more reliable as it is shown in Ref [1]. The Figure also shows the exponentially decreasing behavior of the correlations depending on the distance of the times correlated.

VI. CONCLUSIONS

Monte Carlo Methods (Metropolis-Hastings) allow to simulate lagrangian configurations and also allow to calculate observables and 2-point correlation functions.

Throughout the process we found that it is very important to perform enough simulations (including the ones you discard) to accurately capture the statistical behaviour of the system, there are also more methods

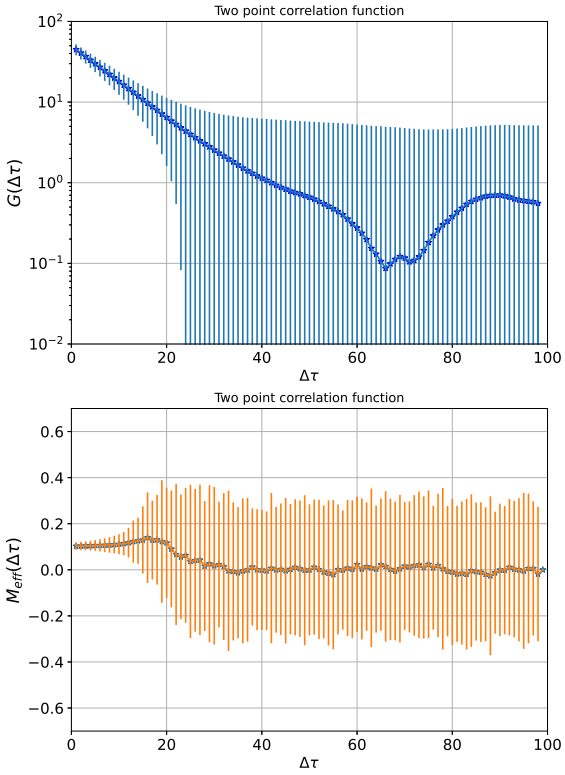

FIG. 3. 2-point correlation function as a function of $\Delta\tau$

to reduce autocorrelations capturing the randomness of the nature. From the simulatio it can also be seen that there are various type of correlations in this Monte Carlo process.

VII. FUTURE WORK

For considering the the real error with correlation, a Jackknife analysis must be implemented, this accounts for the other correlations (between paths, i.e. path generation correlation).

It is also important to parallelize the simulations to explore and graph more simulations with the parameter space of the harmonic oscillator

Finally we explect to implement this same computational methods to the Anharmonic Oscillator and then to field theory for a scalar field, considering the most simple interaction of fields ϕ^4.

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