

Solving path integrals using Monte-Carlo methods to study quantum anharmonic oscillator

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1 Introduction

The motivation of this project stems from trying to study the behaviour of qubits connected to thermal bath. Most widely used qubits now a days are the transmon qubits, which are superconducting qubits with small anharmonicity. Qubits inherently have to be anharmonic because we want to keep them in their lowest two-levels and also we want to control their states efficiently. This cannot be done with harmonic systems as the level spacing is equal, which means that the pulse which excites the system from the ground state to first excited state, also excites it from the first excited state to second excited state and so on. But anharmonic systems are difficult to study analytically as the Schrodinger's equation can be exactly solved only for harmonic potential. For any other potential we have to rely upon perturbative or numerical methods to calculate various properties of the system.

In this project we are trying to evaluate path integrals using Monte-Carlo methods. Evaluating path integrals exactly is also possible only for a system with a harmonic potential. Here, we are trying to use numerical methods of Markov Chain Monte Carlo (MCMC) method to calculate different properties of the system, like ground state energy, ground state wavefunction etc. We wish to calculate the partition function of a system of an anharmonic oscillator coupled to a thermal bath and thus study the thermodynamic properties.

In this project we use the imaginary time path integral formulation to calculate the ground

state energy and various expectation values. We first discretize the equations so that we can numerically compute them. We can vary the lattice spacing and find out the effect of this on the expectation values. We start with a harmonic oscillator and compute the ground state wave-function and the expectation values of different operators. We compare these results to [3]. Then we do similar analysis for the anharmonic oscillator case and compare the results to [2].

For this analysis I have written the codes both in Python and Julia programming languages. For producing the plots presented here with low errors, we need to sample a large number of paths, along with ignoring a $\mathcal{O}(10^2)$ paths in between to reduce correlations. Also, since producing these Monte-Carlo paths are independent of others, we can use multiple cores to do it quickly. Due to this, Julia has been preferred over Python as it is faster and provides easier ways for multi-threaded computing. All the codes can be found in github in - <https://github.com/Ashutosh-Mishra2/Path-Integral-Monte-Carlo>

2 The Path Integral

In this section we briefly follow the derivation given in [1–3] to introduce the ideas of imaginary time path integrals and discretizing it so that it can be evaluated on a lattice. Consider a general Hamiltonian given by (for the ease of writing I would be ignoring hats for the operators in the following derivation),

$$H = \frac{p^2}{2m} + V(x) \quad (1)$$

Then the propagator from (x_i, t_i) to $(x_f, t_i + \delta t)$ is given by,

$$\langle x_f, t_i + \delta t | x_i, t_i \rangle = \langle x_f | e^{-iH\delta t/\hbar} | x_i \rangle = \int \langle x_f | p \rangle \langle p | e^{-iH\delta t/\hbar} | x_i \rangle dp \quad (2)$$

And for small δt , we can write,

$$e^{-iH\delta t/\hbar} = 1 - \frac{iH\delta t}{\hbar} + \mathcal{O}(\delta t^2) \quad (3)$$

Using the identity,

$$\langle p | x \rangle = \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \quad (4)$$

The propagator is given by,

$$\langle x_f, t_i + \delta t | x_i, t_i \rangle = \sqrt{\frac{m}{2\pi i \hbar \delta t}} \exp\left\{\frac{i}{\hbar} \left[\frac{m(x_f - x_i)^2}{2\delta t} - V(x_i)\delta t \right]\right\} \quad (5)$$

$$= \sqrt{\frac{m}{2\pi i \hbar \delta t}} e^{iL\delta t/\hbar} \quad (6)$$

Now, any propagator from (x_i, t_i) to (x_f, t_f) can be broken down into N time slices of length δt , and then the total propagator would be the product of these.

$$\langle x_f, t_f | x_i, t_i \rangle = \int \prod_{n=1}^{N-1} dx_n \exp\left[\frac{i\delta t}{\hbar} \sum_{n=1}^{N-1} L(t_n)\right] \quad (7)$$

Which in the continuum limit $N \rightarrow \infty$ and $\delta t \rightarrow 0$, becomes,

$$\langle x_f, t_f | x_i, t_i \rangle = \int Dx(t) e^{-iS/\hbar} \quad (8)$$

where, $Dx(t) = \prod_{n=1}^{N-1} dx_n$ and the action

$$S = \int_{t_i}^{t_f} L(x(t)) dt = \int_{t_i}^{t_f} \left[\frac{m}{2} \left(\frac{dx}{dt} \right)^2 - V(x(t)) \right] dt \quad (9)$$

2.1 Imaginary Time Path Integrals

Here we replace the real time with an imaginary time ($t \rightarrow -i\tau$), where τ is real. In this formalism the imaginary time acts like temperature, i.e.

$$\tau = \frac{\hbar}{k_B T} \quad (10)$$

where T is the absolute temperature. Using this we can find the partition function,

$$Z = \int \langle x | e^{-H\tau/\hbar} | x \rangle dx = Tr(e^{-H\tau/\hbar}) \quad (11)$$

By inserting a complete set of basis in the above integral we can express the partition function in terms of propagators like as we saw in the last section, which again in the continuum limit $N \rightarrow \infty$, can be written as an integral over all the paths (for a detailed calculation refer to [3]). Thus the partition function can be written as,

$$Z = Tr(e^{-H(\tau_f - \tau_i)/\hbar}) = \int Dx(\tau) e^{-S/\hbar} \quad (12)$$

Now, to calculate these quantities numerically, we need to discretize all the above equations. We need a discrete version of action that can be evaluated on a lattice. Also, for the sake of easier computation, we work in the natural units, i.e. $\hbar = c = k_B = 1$, which makes that [time] = [length] = [mass⁻¹] = [energy⁻¹]. Thus converting the above integral of action Eq(9), we get,

$$S = \delta t \left(\sum_{i=1}^{N_\tau} \frac{1}{2} m \left(\frac{x_{i+1} - x_i}{\delta t} \right)^2 + V(x_i) \right) \quad (13)$$

where, $\tau = N_\tau \delta t$, and this defines the temperature of the simulation. For the case of a Harmonic oscillator, the action looks like,

$$S = \delta t \left(\sum_{i=1}^{N_\tau} \frac{1}{2} m \left(\frac{x_{i+1} - x_i}{\delta t} \right)^2 + \frac{1}{2} m \omega^2 x_i^2 \right) \quad (14)$$

We can define a dimensionless variables,

$$\tilde{m} = m \delta t \quad (15)$$

$$\tilde{\omega} = \omega \delta t \quad (16)$$

$$\tilde{x}_i = \frac{x_i}{\delta t} \quad (17)$$

using these variables we can define a dimensionless action, given by,

$$S = \sum_{i=1}^{N_\tau} \frac{1}{2} \tilde{m} (\tilde{x}_{i+1} - \tilde{x}_i)^2 + \frac{1}{2} \tilde{m} \tilde{\omega}^2 \tilde{x}_i^2 \quad (18)$$

3 Numerical Methods

For this analysis, we use Markov Chain Monte Carlo (MCMC) method for solving path integrals to find different properties of the quantum system. We begin with a time lattice consisting of N_τ points with time increments δt . In this lattice, we sample paths, i.e. a set of points $\{\tilde{x}_i\}$, with $i = 1, 2, 3 \dots N_\tau$, with Boltzmann weights $\rho[\{\tilde{x}_i\}] \approx e^{-\tilde{S}\{\tilde{x}_i\}/\hbar}$ using the Metropolis-Hasting algorithm. We use periodic boundary conditions. One sweep of this algorithm visits N_τ sites randomly, where a site may be visited more than once or not at all. When a large number of sweeps are done every site is visited equally on an average. The Metropolis algorithm is as follows:

- Start with an initial path $P^{(0)}$, which can either be an array of zeros ("cold" start) else

an array of random numbers ("Hot" start).

- Generate a random number u from a uniform distribution in the interval $[-\frac{h}{2}, \frac{h}{2}]$. Here h is the step size.
- Propose a new path with $\tilde{x}_i \rightarrow \tilde{x}'_i = \tilde{x}_i + u$.
- Compute the change in action δS due to this new path.
- Accept the change with probability $\min\{1, e^{-\delta S}\}$. That is generate a random number r and accept the new path if $r < e^{-\delta S}$.

The sweeps produce paths that are dependent on the previous path, i.e. path $P(1)$ is obtained from $P(0)$ and so on. This means that the process forms a Markov chain, but the subsequent paths are correlated to each other. Thus we need to ignore N_{sep} number of paths between two paths such that this correlation can be reduced and would not bring artifacts to our analysis.

This whole process can be summarized by the following flow chart:

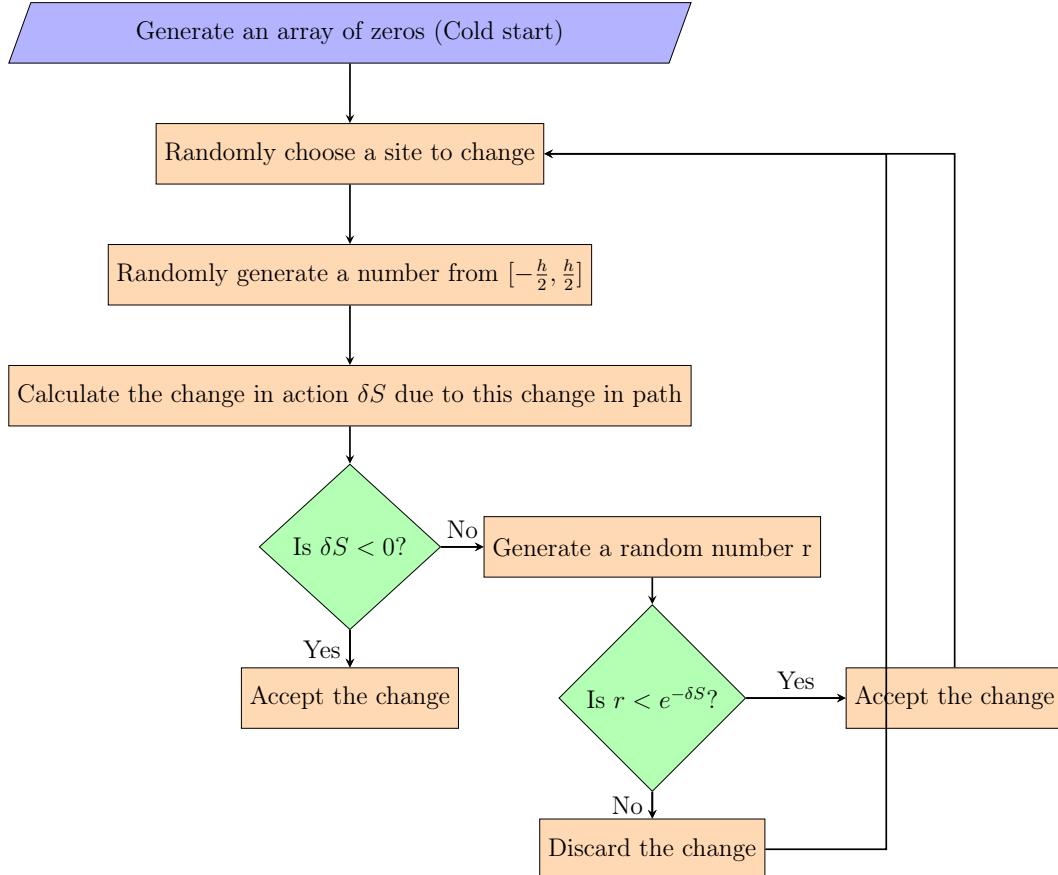


Figure 1: Flow Chart of the Metropolis-Hastings algorithm

The overall algorithm can be represented by the following flow chart:

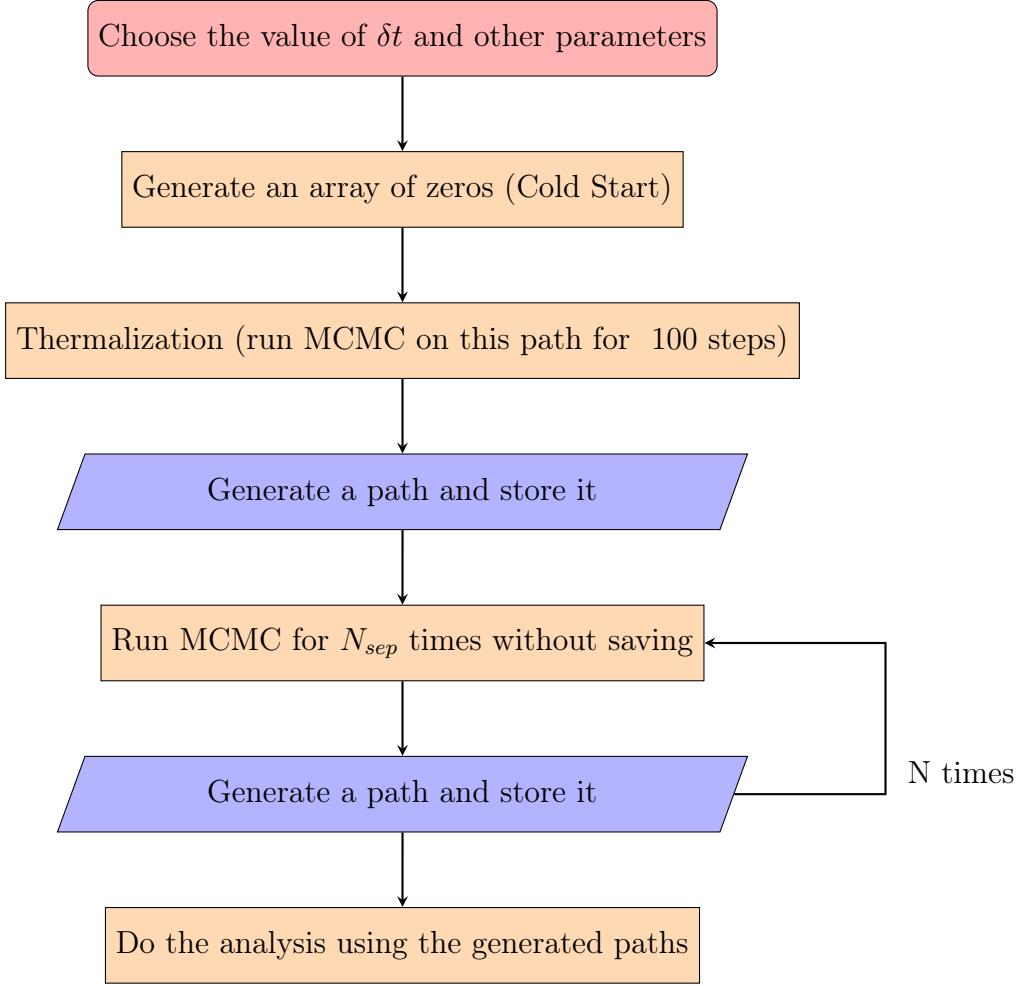


Figure 2: Flow Chart of the full algorithm

4 Simulation and Results

4.1 Harmonic Oscillator

We begin with the Harmonic oscillator as this is the most simple case and can be analytically solved. For the simulation, I have used Julia programming language to generate the final plots due to its higher speed of computation, in addition to easy of parallelization of code. For the Harmonic oscillator case, I have followed the paper by Westbroek et al. [3]. The Hamiltonian for this case is given by,

$$H = \frac{P^2}{2m} + \frac{m\omega^2 x^2}{2} \quad (19)$$

From this we can calculate the action for this case (formula is taken from [3] Eq(41)),

$$S = \sum_{i=1}^{N_\tau} \frac{1}{2} \tilde{m} (\tilde{x}_{i+1} - \tilde{x}_i)^2 + \frac{1}{2} \tilde{m} \tilde{\omega}^2 \tilde{x}_i^2 \quad (20)$$

Now if we look at a single trajectory after thermalization, we get something like the following,

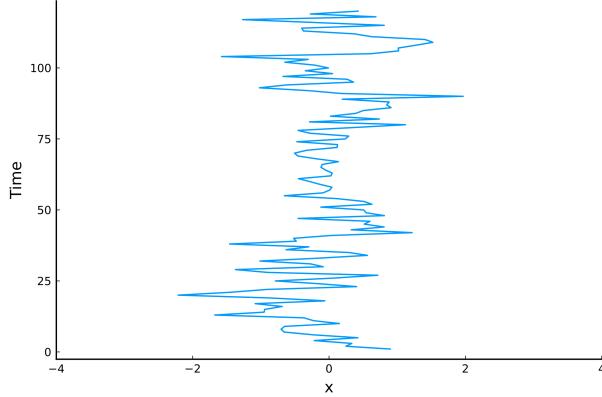


Figure 3: Single Monte-Carlo trajectory

Next, directly from an ensemble (N) of these trajectories we can calculate the ground state probability distribution of the Harmonic oscillator. This is done by "binning" the positions into bins of size Δx , and thus from [1] Eq(4.15), we get

$$|\psi_0(x)|^2 = \frac{\frac{1}{\Delta x} \sum_i^N \Theta(\Delta x - |x_i - x|)}{\sum_i^N 1} \quad (21)$$

From the simulation, using the parameters,

```
Ntau = 120
dt = 1
h = 0.1
m = 1
omega = 1
N = 10000
Nsep = 12
```

we obtain the following ground state probability density,

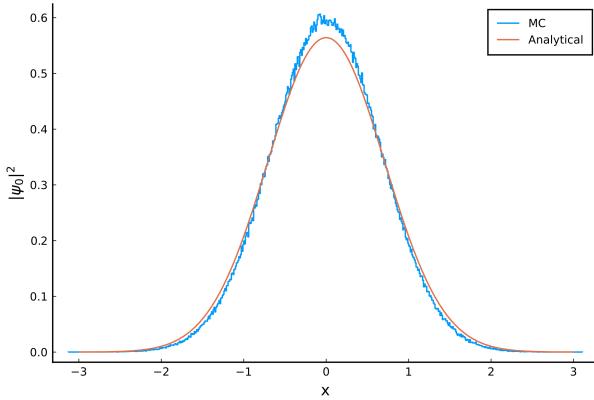


Figure 4: From simulation

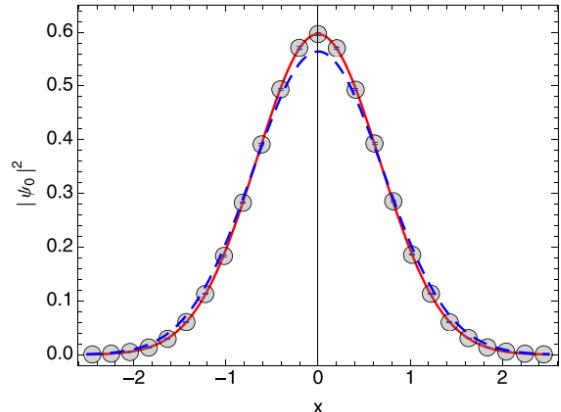


Figure 5: Reprinted from [3]

The analytical plot is made using the normalized ground state wavefunction of Harmonic oscillator,

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \exp\left(-\frac{m\omega x^2}{2\hbar} \right) \quad (22)$$

Next, we can also calculate the expectation value of operators. The expectation values of operator O can be calculated by taking the ensemble average of $\langle x|O|x\rangle$. For starters we can calculate the expectation values of \hat{x}^n , and this can give us the information about the ground state energy of the Harmonic oscillator. It is given by

$$E_0 = m\omega^2 \langle x^2 \rangle \quad (23)$$

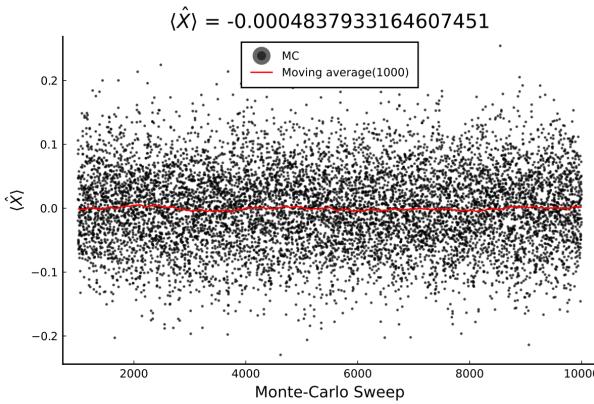


Figure 6: $\langle x \rangle$

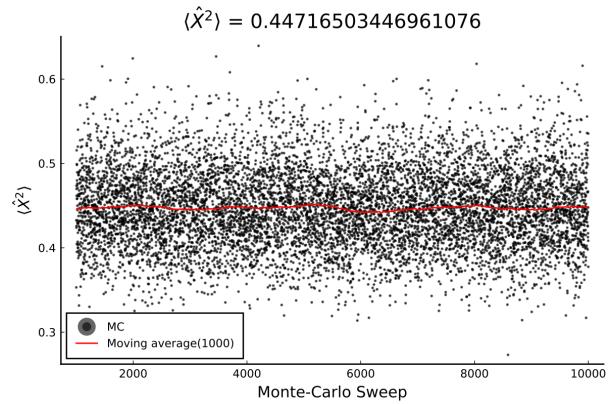


Figure 7: $\langle x^2 \rangle$

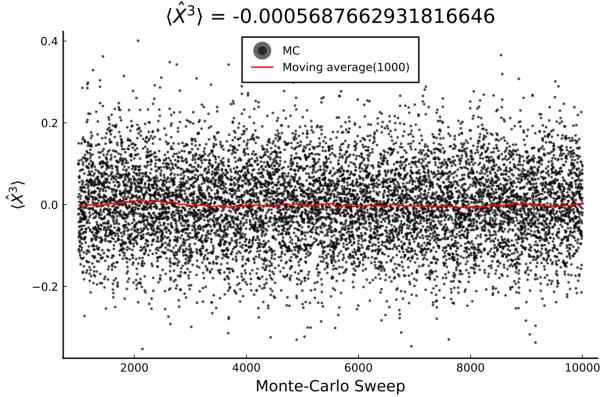


Figure 8: $\langle x^3 \rangle$

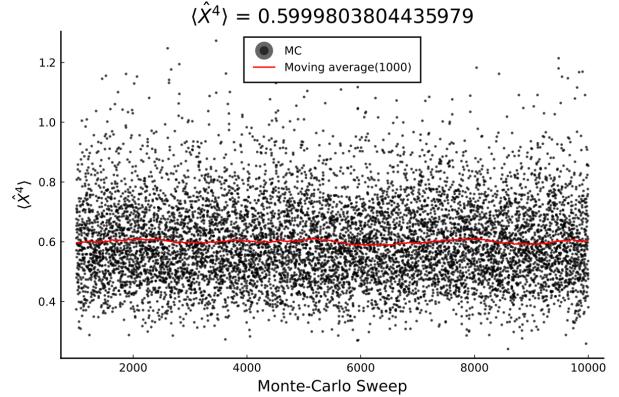


Figure 9: $\langle x^4 \rangle$

From this we can verify that expectation value of odd powers of x is zero. Also $\langle X^2 \rangle \approx \frac{1}{2}$, thus $E_0 \approx \frac{m\omega^2}{2}$, which matches with the analytical result.

4.2 Anharmonic Oscillator

For the anharmonic oscillator I have followed the paper by Mittal et al. [2].

For the anharmonic oscillator case, we add a higher order term to the Hamiltonian. Thus it is given by,

$$H = \frac{P^2}{2m} + \frac{m\omega^2 x^2}{2} + \lambda x^4 \quad (24)$$

For large values of λ it is difficult to solve this analytically and hence one has to use numerical methods to compute this.

The discretized and non-dimensional action for this case is given by,

$$S = \sum_{i=1}^{N_\tau} \frac{1}{2} \tilde{m} (\tilde{x}_{i+1} - \tilde{x}_i)^2 + \frac{1}{2} \tilde{m} \tilde{\omega}^2 \tilde{x}_i^2 + \tilde{\lambda} \tilde{m}^2 \tilde{\omega}^3 \tilde{x}_i^4 \quad (25)$$

The potential can be plotted for various values of λ to see how this differs from the Harmonic case,

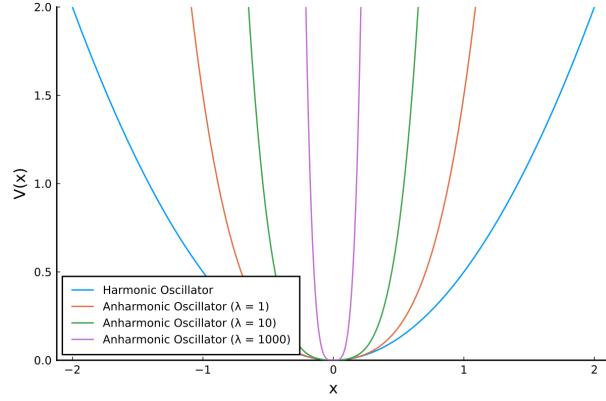


Figure 10: Plot of potential for different λ values

Next, we can find out how fast or how slow the equilibration process takes place for the anharmonic oscillator.

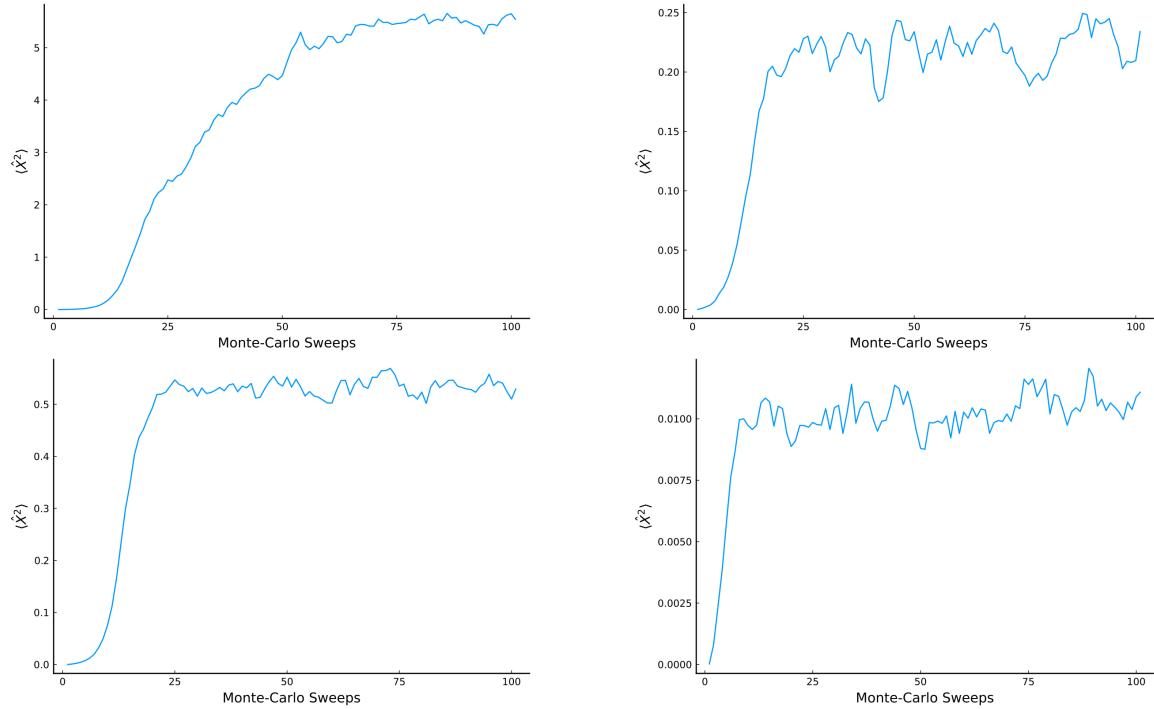


Figure 11: Simulated

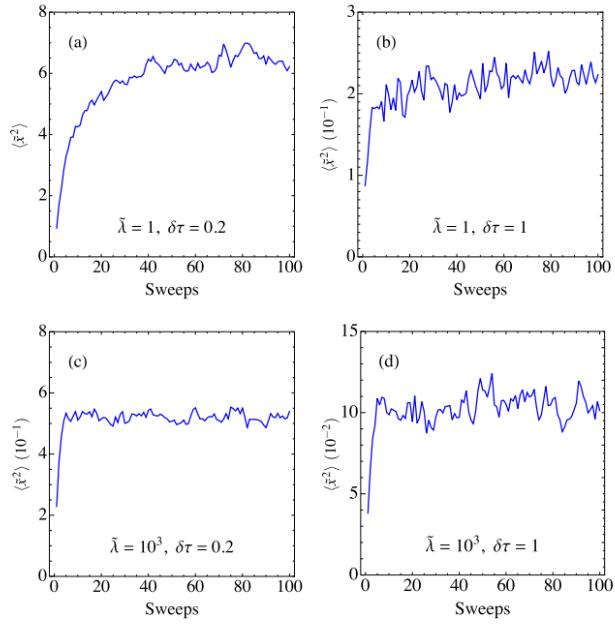


Figure 12: Reprinted from [2]

Next we calculate the ground state wave function, using the following parameters,

```
Ntau * dt = 250
N = 2000
Nsep = 100
m = omega = dt
```

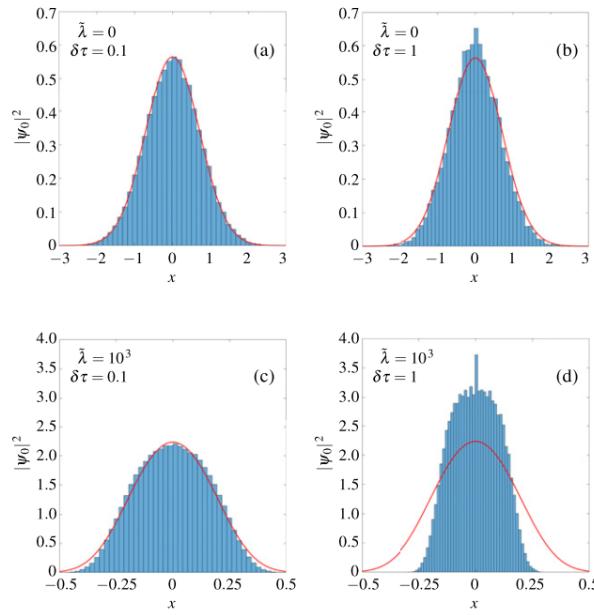


Figure 13: Reprinted from [2]

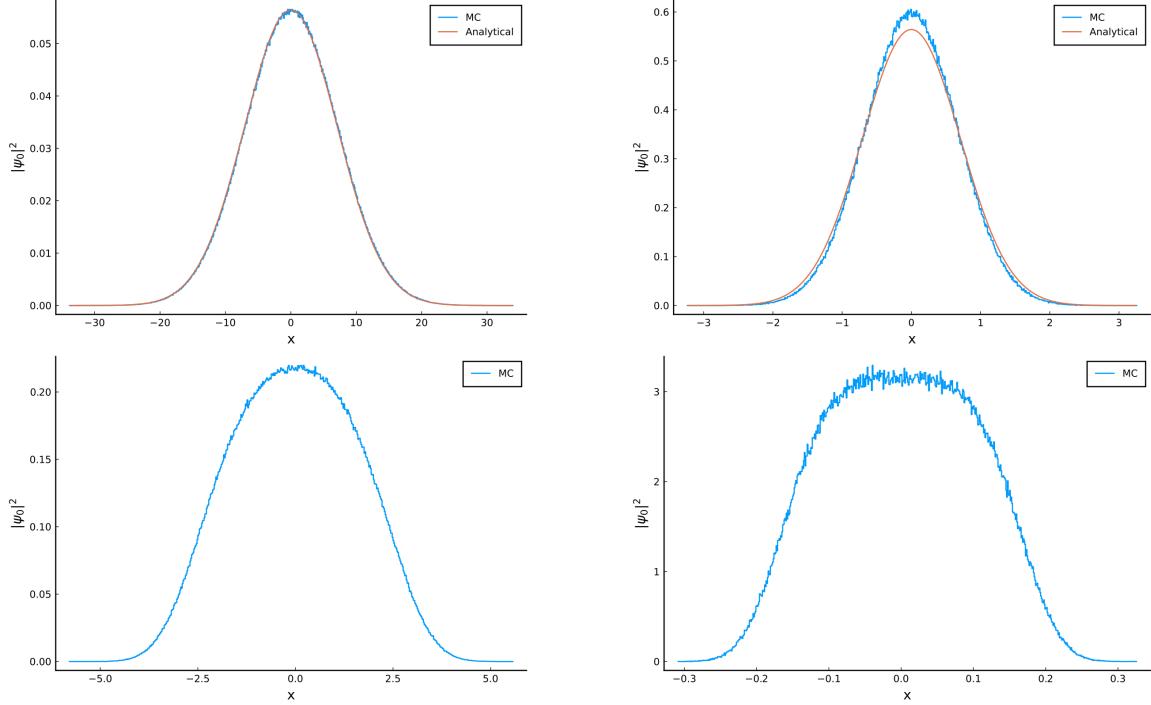


Figure 14: Simulated

Next we can calculate the expectation values of position operators, from which we can calculate the ground state energy. The following were calculated for $\lambda = 2$

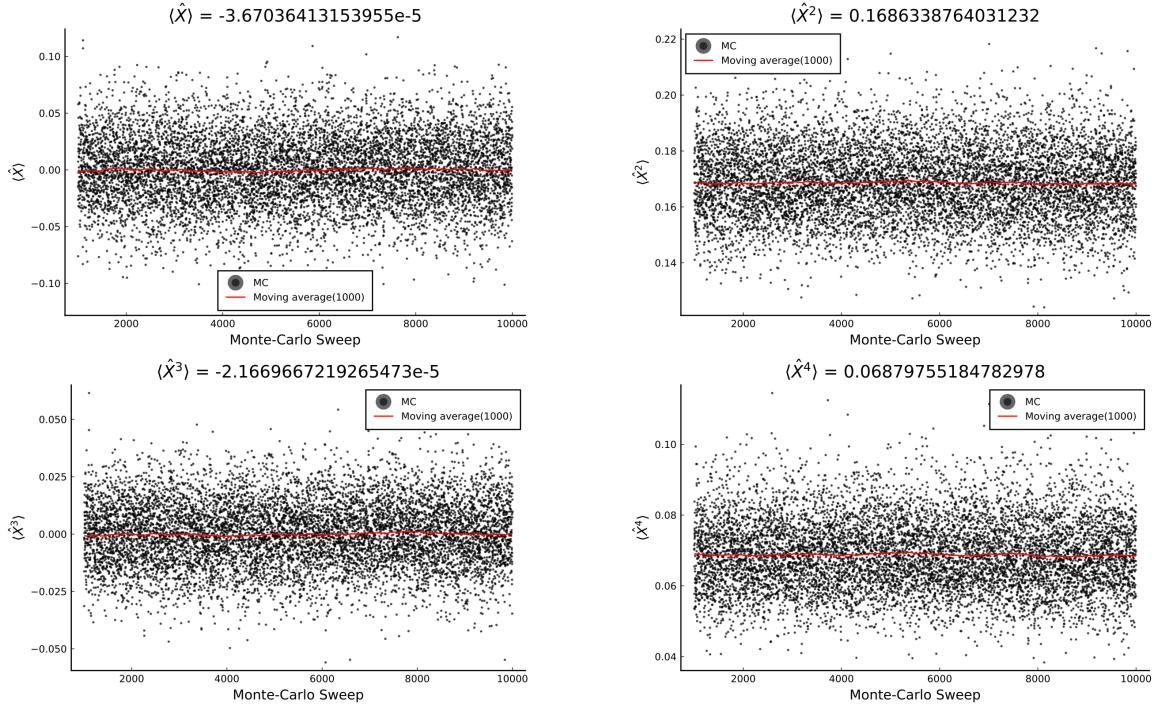


Figure 15: Simulated

Using Virial theorem, we can find the ground state energy of this system in terms of the expectation values of operators (which as we say in the previous case, can be calculated by MCMC). The ground state energy is given by,

$$E_0 = m\omega^2 \langle x^2 \rangle + 2\lambda \langle x^4 \rangle \quad (26)$$

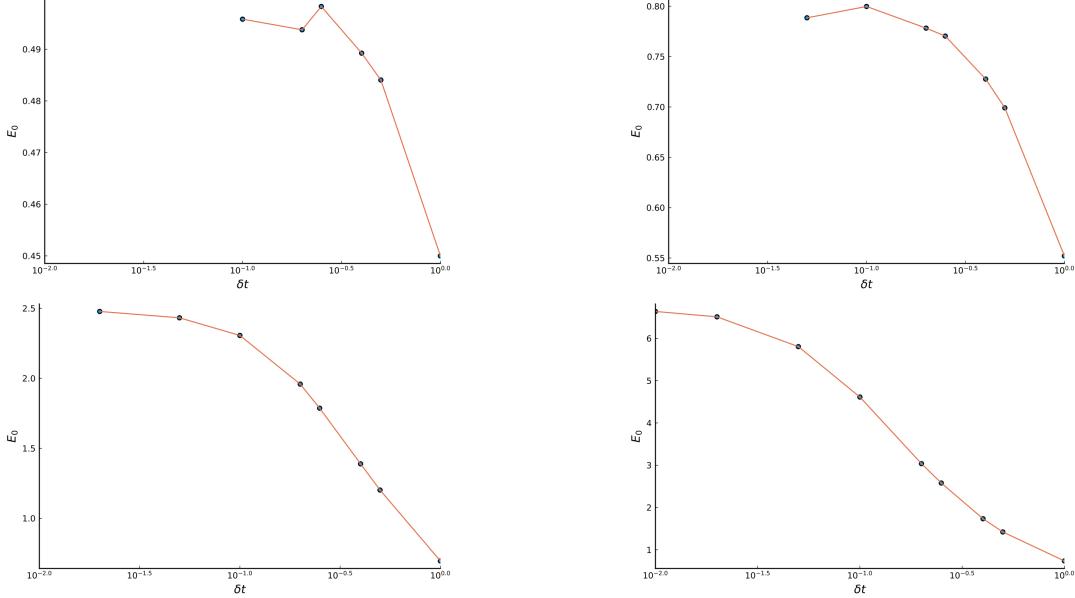


Figure 16: Simulated

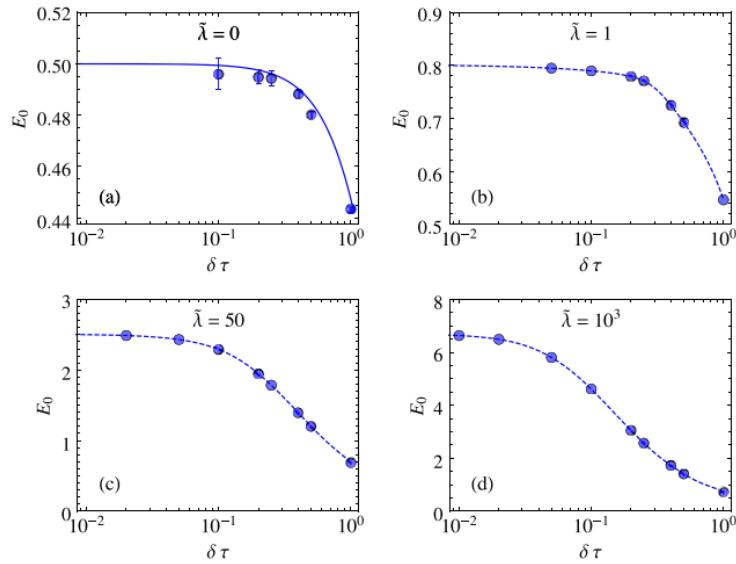


Figure 17: Reprinted from [2]

The following are the values of the ground state that is reported in the paper [2]

$\tilde{\lambda}$	MCMC	Spline	SE	Ref. [17]
0	0.496	0.501	$\frac{1}{2}$	—
1	0.795	0.801	0.8038	0.8038
50	2.488	2.511	2.4998	2.4997
10^3	6.634	6.702	6.6941	6.6942

The following are the calculated values,

λ	MCMC
0	0.49523
1	0.78929
50	2.47693
1000	6.63438

For calculating the energy of the first excited state, we have to evaluate the two point correlation function. Referring to Eq(19-21) of [2],

$$E_1 - E_0 = -\hbar \lim_{\tau \rightarrow \infty} \left[\frac{d \log G_2(\tau)}{d\tau} \right] \quad (27)$$

where,

$$G_2(\tau) = \lim_{\beta \rightarrow \infty} \langle x(\tau)x(0) \rangle_c \quad (28)$$

$$= \lim_{\beta \rightarrow \infty} (\langle x(\tau)x(0) \rangle - \langle x(\tau) \rangle \langle x(0) \rangle) \quad (29)$$

To calculate on a lattice, we have to discretize it,

$$E_1 - E_0 = -\hbar \lim_{\tau \rightarrow \infty} \left\{ \frac{1}{\Delta\tau} \log \left[\frac{G_2(\tau + \Delta\tau)}{G_2(\tau)} \right] \right\} \quad (30)$$

where $\Delta\tau = n\delta t$

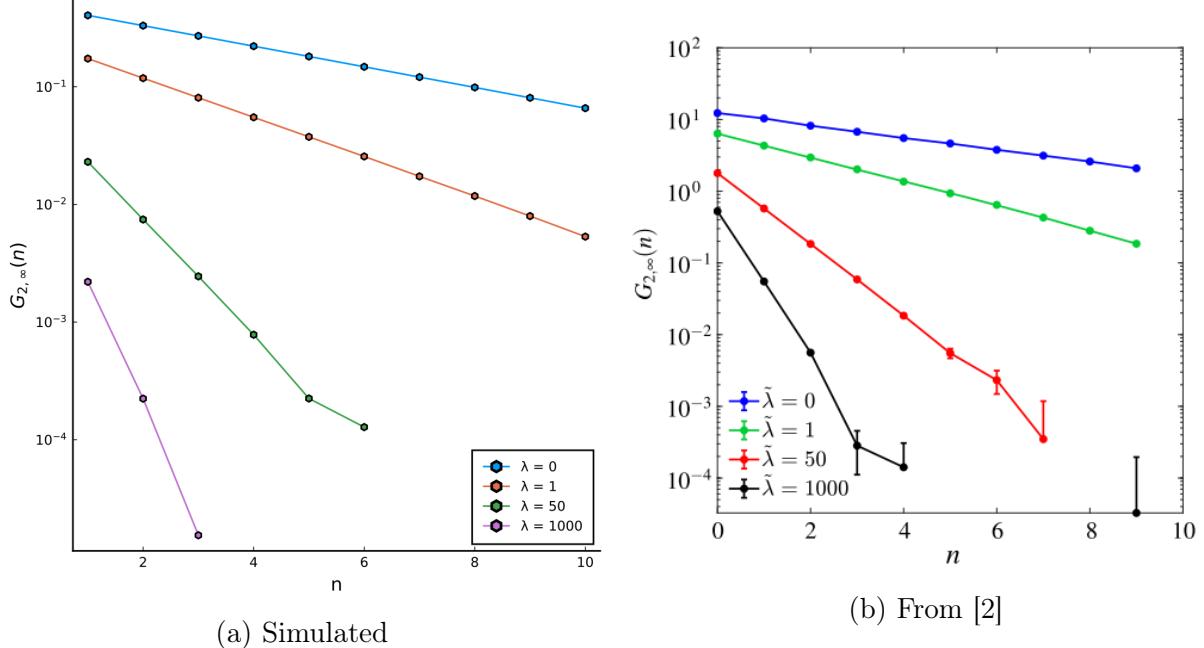


Figure 18: $G_2(n)$ vs n plot

Here we calculated $G_2(\tau)$ by calculating Eq(28). Since the $G_2(\tau)$ has to be calculated in the limit $\beta \rightarrow \infty$, we used the following parameters for this simulation.

```
dt = 0.2  
N = 500  
h = 0.1  
Nsep = 50  
Ntau * dt = 2000  
Ntau = 10000
```

This results in a big ensemble for calculating the results. Using these trajectories, we calculate auto-correlation function $\langle x(\tau)x(0) \rangle$. For this calculation we pick a point on the trajectory, say x_i and then choose another point $x_{i+\tau}$. For calculating the ensemble average we keep shifting x_i on the same trajectory, along with this we repeat this N times. Thus we calculate the auto-correlation function as,

$$\langle x(\tau)x(0) \rangle = \frac{1}{NN_\tau} \sum_i^N \sum_j^{N_\tau} x_{i,j}x_{i,j+\tau} \quad (31)$$

also, periodic boundary condition is used. Finally we subtract the product of $\langle x(\tau) \rangle$ and $\langle x(0) \rangle$ from this to calculate $G_2(\tau)$.

5 Conclusion and future work

Thus in the above work we saw how Markov Chain Monte Carlo can be used to study properties of quantum systems. We started with the Harmonic oscillator Hamiltonian and then obtained a discretized version of the action. Using this we generated Monte Carlo trajectories, at specific temperatures. Using this we calculated the ground state probability distribution, ground state energy and expectation of various powers of position operators. Then we moved on to a more difficult problem of anharmonic oscillator. Since there is no analytical solution for large values of λ , we did an analysis for equilibration/thermalization. Next we calculated the ground state wavefunction for various regimes of this potential. Then we calculated the expectation values of different powers of position operators. Using this we found out the value of ground state energy. We also showed how this depends on the lattice spacing δt . In the end we calculated the two point correlation function $G_2(\tau)$ to find the energy of the first excited state.

By now we are able to calculate the basic properties of a quantum system using the Path Integral Monte Carlo method. We plan to extend this to include calculations for operators other than the position operators. Also, for the calculation of E_1 , we have currently stopped at $G_2(\tau)$. Since the calculation of $G_2(\tau)$ has to be done at very high β values, this part of the code takes a long time to do. So we plan to optimise this calculation such that calculating higher energy levels becomes easier. In addition to this, this formalism can be used to calculate the partition function as a function of temperature ($Z(T)$). If we can calculate the partition function as a function of temperature we can calculate thermodynamic and statistical properties of this system without going to the master equation formalism.

References

- [1] M Creutz and B Freedman. A statistical approach to quantum mechanics. *Annals of Physics*, 132(2):427–462, 1981.
- [2] Shikhar Mittal, Marise JE Westbroek, Peter R King, and Dimitri D Vvedensky. Path integral monte carlo method for the quantum anharmonic oscillator. *European Journal of Physics*, 41(5):055401, 2020.
- [3] Marise JE Westbroek, Peter R King, Dimitri D Vvedensky, and Stephan Dürr. User’s guide to monte carlo methods for evaluating path integrals. *American Journal of Physics*, 86(4):293–304, 2018.