Path Integral Simulation of the Harmonic and Anharmonic Oscillators

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Abstract: In this work, the Path Integral Formulation of Quantum Mechanics is presented. Aside from providing an elegant and intuitive approach to Quantum Mechanics, this formalism has proven to be very useful in fields such as low-energy Quantum Chromodynamics, where the perturbative method cannot be used. Even though there is great difficulty in its analytic treatment, making the formalism not practical for situations where the analytical solution of Schrödinger's equation is known, the use of numerical methods through computer simulations has proven to be a powerful tool to solve complicated problems. The main focus of this project is the implementation of this method using importance sampling in Monte Carlo integration, through which several physical quantities of interest are computed for the quantum harmonic and anharmonic oscillators.

I. INTRODUCTION

An important aspect of Quantum Mechanics (QM) is the knowledge of the temporal evolution of a system. The rate at which a given system evolves with time is expressed in Schrödinger's equation, and one can get access to the evolution of the state from the computation of the energy spectrum for the relevant Hamiltonian. Even if this is the most common approach to Quantum Mechanics, Feynman took inspiration from Dirac's remarks [1] and looked for the classical equivalent between the Lagrangian and the Hamiltonian in Quantum Mechanics. In Classical Mechanics, motion is determined by the *principle of least action*. Such principle states that a particle of mass m moving from (x_a, t_a) to (x_b, t_b) will move along a path $x_{cl}(t)$, called the classical path, which minimizes a quantity S, the *action* of the system,

$$S[x(t)] = \int_{t_a}^{t_b} \mathcal{L}(\dot{x}, x, t)dt \ , \tag{1}$$

where

$$\mathcal{L}(\dot{x}, x, t) = \frac{m}{2}\dot{x}^2 - V(x) \tag{2}$$

is the corresponding Lagrangian.

Feynman looked for, and developed, an analogous approach in QM, known as the Path Integral Formulation of Quantum Mechanics, which ellucidates some important aspects of QM, such as the uncertainty in the position of a particle in time. However, even for simple systems such as the Harmonic Oscillator (H.O.), obtaining analytic solutions is rather involved, and computer simulations become a convenient way to obtain results. Despite this, the method has been proven useful in different research areas, such as Quantum Electrodynamics and Statistical Mechanics.

The goal of this work is first, to introduce the Path Integral formalism, and second, to illustrate the method by obtaining relevant physical quantities of interest for the quantum H.O., without and with a perturbative quartic anharmonic term.

II. THE PATH INTEGRAL FORMALISM

With two postulates [2], Feynman proposes that the *kernel* $K(b, a) = \langle x_a, t_a | x_b, t_b \rangle$, which is the probability amplitude of a particle moving through space-time from (x_a, t_a) to (x_b, t_b), is the sum over all paths which have those coordinates as starting and ending points, respectively. Furthermore, each path contributes the same, except for a complex phase proportional to the action of the system along the path, in units of $\hbar$. This can be expressed as the *path integral*

$$K(b, a) = \int_a^b e^{(i/\hbar)S[x(t)]}\mathcal{D}x(t) \ , \tag{3}$$

where

$$\mathcal{D}x(t) = \frac{1}{A}\int \frac{dx_1}{A} \cdots \int \frac{dx_{N-1}}{A} \ , \tag{4}$$

and A is a normalization constant. Here, a path $x(t) = (x_0 = x(t_0) = x_a, x_1 = x(t_1), \ldots, x_{N-1} = x(t_{N-1}), x_N = x(t_N) = x_b)$ is considered, where $T = t_b - t_a = N\Delta t$, $t_0 = t_a$, $t_i = t_0 + i\Delta t$ and $t_N = t_b$. This is to be understood in the limit $N \to \infty$, $\Delta t \to 0$, when the path becomes continuous, and the integration translates into the consideration of all paths between x_a and x_b. Generally, the limit does not exist. However, if the Lagrangian is independent of time, then

$$A = \left(\frac{2\pi i\hbar\Delta t}{m}\right)^{1/2} \tag{5}$$

and the integral converges.

A. Ground state energy, wave function and expectation values

Since the Lagrangian does not depend on time, neither does the Hamiltonian $\mathcal{H}$. As a consequence, the latter has a spectrum of energy levels E_n with orthonormal wave functions $\psi_n(x) = \langle x|n\rangle$, which form a basis.

As such, any function $f(x)$ can be expressed as a linear combination of these, that is

$$f(x) = \sum_{n\geq 1} a_n \psi_n(x) \ , \tag{6}$$

$$a_n = \int_{-\infty}^{\infty} \psi_n^*(x) f(x) dx \ . \tag{7}$$

Furthermore, since any wave function of the system is a solution of the time-dependent Schrödinger's equation, it can be written as

$$\psi(x,t) = \sum_{n\geq 1} c_n e^{-(i/\hbar)E_n t} \psi_n(x) \ . \tag{8}$$

Thus, considering $f(x) = \psi(x, t_a)$, we can combine (6) and (8) to get

$$c_n = a_n e^{(i/h)E_n t_a} \ . \tag{9}$$

If instead we consider $\psi(x, t_b)$, where $t_b > t_a$, we can plug Eqs.(7) and (9) into Eq.(8) to obtain

$$\psi(x,t_b) = \int_{-\infty}^{\infty} \sum_{n\geq 1} \psi_n(x)\psi_n^*(y) e^{-i\frac{E_n T}{\hbar}} f(y) dy \ , \tag{10}$$

where $T = t_b - t_a$. Since the kernel is a probability amplitude, it obeys the rule of succession of events [3]

$$\psi(x_b,t_b) = \int_{-\infty}^{\infty} K(x_b,t_b;x_a,t_a)\psi(x_a,t_a)dx_a \tag{11}$$

which, after substituting $x_b \to x$, $x_a \to y$, $\psi(x_a, t_a) \to f(y)$, can be compared to Eq.(10), to conclude that

$$K(x_b,t_b;x_a,t_a) = \sum_{n\geq 1} \psi_n(x_b)\psi_n^*(x_a) e^{-i\frac{E_n T}{\hbar}} \ . \tag{12}$$

Consider the path presented before. Imposing the periodic boundary condition in the spatial direction, i.e. $x_0 = x_N$, and setting $t_N - t_0 = T \to -i\hbar T$ in order to turn the oscillating exponential into a decaying one, Eq.(12) now becomes

$$K(x_0,T) = \sum_{n=1}^{\infty} |\psi_n(x_0)|^2 e^{-E_n T} \ . \tag{13}$$

When taking the limit $T \to \infty$, the state with the lowest energy, and thus the state which makes the exponential the largest, will remain. Thus, integrating Eq.(13) over x_0 and taking the aforementioned limit,

$$\lim_{T\to\infty} \int_{-\infty}^{\infty} K(x_0,T)dx_0 = e^{-E_0 T} \ , \tag{14}$$

where we have taken into account the orthonormality of the eigenfunctions. Note that, if we just take the limit in Eq.(13), we get the expression for the ground state energy

$$\lim_{T\to\infty} K(x_0,T) = |\psi_0(x_0)|^2 e^{-E_0 T} \ . \tag{15}$$

Therefore, the ground state wave function can be extracted from

$$|\psi_0(x_0)|^2 = \lim_{T\to\infty} \frac{K(x_0,T)}{\int_{-\infty}^{\infty} K(x_0,T)dx_0} \ . \tag{16}$$

Let $\mathcal{A} = \mathcal{A}(X)$ be an observable depending only on the position operator X, which has eigenvalues $\mathcal{A}(x)$ on the eigenbasis $|x\rangle$. The expectation value for a state described by the wave function $\psi_n(x)$ is [4]

$$\langle \mathcal{A} \rangle_{\psi_n} = \int_{-\infty}^{\infty} |\psi_n(x)|^2 \mathcal{A}(x) dx \ . \tag{17}$$

Therefore, introducing $\mathcal{A}$ into Eq.(13) and integrating over x_0,

$$\int_{-\infty}^{\infty} \mathcal{A}K(x_0,T)dx_0 = \sum_{n=1}^{\infty} e^{-E_n T} \langle \mathcal{A} \rangle_{\psi_n} \ , \tag{18}$$

gives us the ground state expectation value of $\mathcal{A}$:

$$\langle \mathcal{A} \rangle_{\psi_0} = \lim_{T\to\infty} \frac{\int_{-\infty}^{\infty} \mathcal{A}K(x_0,T)dx_0}{\int_{-\infty}^{\infty} K(x_0,T)dx_0} \ . \tag{19}$$

III. DISCRETIZATION OF PATH INTEGRALS

The action of the system along the path $x(t) = (x_0, x_1, \ldots, x_N)$ can be written as

$$S[x(t)] = \sum_{n=0}^{N-1} S[x_{i+1}, x_i] \ , \tag{20}$$

with

$$S[x_{i+1}, x_i] = \int_{t_i}^{t_{i+1}} \left[\frac{m}{2}\dot{x}^2 - V(x) \right] dt \ . \tag{21}$$

Since this is done with the hopes of taking the limit $\Delta t \to 0$, we can approximate the values of $\dot{x}$ and x in every $S[x_{i+1}, x_i]$ by $\tilde{\dot{x}}_i = \frac{x_{i+1}-x_i}{\Delta t}$ (also known as Euler's rule) and $\tilde{x}_i = \frac{x_{i+1}+x_i}{2}$, respectively, giving:

$$S[x(t)] = \Delta t \sum_{n=0}^{N-1} \frac{m}{2}\tilde{\dot{x}}_i^2 - V(\tilde{x}_i) \ . \tag{22}$$

Now, consider a Wick rotation [5] $t \to -i\tau$,

$$S_E[x(\tau)] = i\Delta\tau \sum_{n=0}^{N-1} \frac{m}{2}\tilde{\dot{x}}_{i_\tau}^2 + V(\tilde{x}_i) \ , \tag{23}$$

where $\tilde{\dot{x}}_{i_\tau} = \frac{x_{i+1}-x_i}{\Delta\tau}$. We shall call this quantity *Euclidean Action*, which allows us to use importance sampling methods to numerically evaluate the path integral. Setting periodic boundary conditions $x_0 = x_N$ as well as $\hbar = 1$ and $T \to -iT$, Eq.(3) becomes

$$K(x_0,T) = \int_{x_0}^{x_0} e^{-S_E[x(t)]} \mathcal{D}x(t) \ , \tag{24}$$

which allows us to use the expressions derived above for the ground state wave function, energy and expectation values.

Monte Carlo integration and the Metropolis algorithm

The integrals we need to compute are of the form

$$I = \int_{-\infty}^{\infty} dx_0 \int_{x_0}^{x_0} f(x(t))g(x(t))\mathcal{D}x(t) \ , \qquad (25)$$

where $g(x(t)) = \frac{e^{-S_E[x(t)]}}{\int_{-\infty}^{\infty} K(x_0,T)dx_0}$ is a properly normalized probability density. To compute them, we use the Monte Carlo method of importance sampling, which consists of approximating the integral above by

$$I \approx \frac{1}{M}\sum_{k=1}^{M} f(x^k(t)) \ , \qquad (26)$$

where the paths $x^k(t); k = 1, \ldots, M$, have been sampled with probability density $g(x(t))$. The uncertainty in Eq.(26) is measured by the standard deviation [6], which goes as $1/\sqrt{M}$. Therefore, if we introduce $\delta(x_0' - x_0)$ into Eq.(16) and integrate over x_0' [6], the ground state wave function can be approximated by

$$|\psi_0(x_0)|^2 \approx \frac{1}{M}\sum_{k=1}^{M} \delta_{x_0^k,x_0} \ , \qquad (27)$$

where $\delta_{x_0^k,x_0} = 1$ if $x_0^k = x_0$ and $\delta_{x_0^k,x_0} = 0$ otherwise. Furthermore, expectation values can be computed using

$$\langle \mathcal{A} \rangle_{\psi_0} \approx \frac{1}{M}\sum_{k=1}^{M} \mathcal{A}[x^k(t)] \ , \qquad (28)$$

where $\mathcal{A}[x^k(t)] = \frac{1}{N+1}\sum_{i=0}^{i=N} \mathcal{A}(x_i^k)$. Eqs.(27) and (28) are to be understood in the limit $M \to \infty$, i.e. the sample has to be large enough in order to reduce the error made in the process of discretizing the integral into a finite sum over paths. To obtain a sample distributed with probability density $g(x(t))$, the Metropolis algorithm [7] is used, which consists of the following steps [1]:

1. Set an arbitrary initial path. In this case, $x^0(t) = (0, \ldots, 0)$ has been chosen.
2. For every coordinate x_i^k in a path $x^k(t)$, consider a deviation $x_i^{k'} = x_i^k + \gamma_i$, where γ_i is a random variable that follows a normal distribution $N(\mu, \sigma) = N(0, 1/6)$. The value of σ chosen guarantees that we do not exclude a large number of paths, while making the sample representative of its sampling distribution.
3. If the difference in actions ΔS is negative (that is, the new path has less action than the original), we accept the new path. Otherwise, we generate a random number r between 0 and 1. If $r < e^{-\Delta S}$, we accept the new path. If not, we reject it and repeat the process.
4. The process is repeated with the new path, if it was accepted, or the old one if the former was rejected.

The algorithm needs to thermalize. Its first iterations will not be distributed according to the target distribution, and therefore these first paths will be discarded from the final sample, since they are skewed.

IV. RESULTS: SIMULATION OF THE HARMONIC AND ANHARMONIC OSCILLATORS

In this section, the results of the simulation run on the harmonic and anharmonic oscillators will be exposed. The quantum H.O. has a potential energy

$$V_0(x) = \frac{1}{2}m\omega^2 x^2 \ . \qquad (29)$$

After introducing a quartic anharmonic term [8], the potential of the system, now called the Anharmonic Oscillator, is

$$V(x) = V_0(x) + \lambda\frac{m^2\omega^3}{\hbar}x^4 \ . \qquad (30)$$

where $\lambda << 1$ is a dimensionless quantity called *anharmonicity*, purposely made small in order to be able to treat the quartic term as a perturbation. The Euclidean action along the path $x(t) = (x_0, x_1, \ldots, x_N)$ is

$$S_E[x(t)] = \Delta t \sum_{n=0}^{N-1} \frac{m}{2}\tilde{x_i^2} + V_0(\tilde{x}_i) + \lambda\frac{m^2\omega^3}{\hbar}\tilde{x}_i^4 \ , \qquad (31)$$

where $\tilde{x}_i$ and $\tilde{\dot{x}}_i$ follow the same definition as before.
Results will be obtained for the Harmonic Oscillator by setting $\lambda = 0$, and for the Anharmonic Oscillator by setting $\lambda = 0,01$. These will be compared with literature values [3, 4] in the case of the Harmonic Oscillator, and computed using perturbation theory [4] to first order in λ for the Anharmonic Oscillator. For simplicity, we have set $\hbar = \omega = m = 1$.
After executing the code, we have obtained a sample consisting of $M = 10000$ paths of $N+1 = 201$ positions each for both the harmonic and the anharmonic oscillators. In Figure 2, one can observe the action behaviour for the paths in the sample for both systems. For the Harmonic Oscillator, after focusing on the first 400 paths, we can see that, even though the action does not stop fluctuating, the algorithm thermalizes around the 60th path. For the Anharmonic Oscillator, this thermalization takes longer and, after focusing on the first 1000 paths of the sample, is determined to be around the 200th path.

[1] All the codes have been written in C++ by the author of this work.

Expectation value	**Harmonic Oscillator**			**Anharmonic Oscillator**		
	Path integral	*Wave function*	*Theory*	*Path integral*	*Wave function*	*Theory*
$\langle X \rangle$	0.006 ± 0.002	0	0	0.035 ± 0.001	0	0
$\langle X^2 \rangle$	0.503 ± 0.001	0.504	0.500	0.494 ± 0.001	0.495	0.485
$\langle X^3 \rangle$	-0.001 ± 0.002	0	0	0.051 ± 0.002	0	0
$\langle X^4 \rangle$	0.756 ± 0.002	0.759	0.750	0.714 ± 0.002	0.716	0.698

TABLE I: Ground state expectation values of X, X^2, X^3 and X^4 for both the harmonic and anharmonic oscillators.

A. Expectation values

The simulation results for the expectation values of different powers of the position operator can be found in Table I. Whereas the values in the first column for each oscillator have been computed by the numerical evaluation of Eq.(19), the ones in the second column are computed, after finding the ground state wave function, by evaluating Eq.(17).
While for the H.O. the estimations recover the analytical values within 1σ for X^3 and X^4 and within 3σ for X and X^2, the Anharmonic Oscillator calculation lies slightly away from the analytic (perturbative) value.
For the expectation values computed using the wave function, the numerical calculation gives us a 1% and a 2% deviation from the corresponding theoretical values for the H.O and the Anharmonic Oscillator, respectively. These differences can be attributed to the error associated with the numerical evaluation of the integrals. Furthermore, one can observe that we do not obtain the expected zero values for $\langle X \rangle$ and $\langle X^3 \rangle$. This is due to an inherent asymmetry in the algorithm, and will be properly dealt with in the next section.

B. Sample symmetrization

At first glance, one can see that Eq.(31) is an even function, that is, it has the same value for a path $x(t)$ than for its symmetrical $-x(t)$. This allows to improve the estimations by including $-x(t)$ for every $x(t)$ sampled, since the difference in actions is zero, and therefore the algorithm would have accepted it. Otherwise, the algorithm breaks parity, leading to non-zero expectation values for the odd powers of X. After including the aforementioned paths, the improved expectation values are

$$\langle X \rangle = 2 \cdot 10^{-18} \ , \ \langle X^3 \rangle = -6 \cdot 10^{-18} \tag{32}$$

for the H.O. and

$$\langle X \rangle = -6 \cdot 10^{-19} \ , \ \langle X^3 \rangle = 1 \cdot 10^{-18} \tag{33}$$

for the Anharmonic Oscillator. Clearly, these are only expectation values improved by this symmetrization, since for the ones corresponding to the even powers of X, the results will be exactly the same.
Moreover, this improvement of the sample allows for a more precise computation of the ground state wave function, since the number of paths in the sample is now doubled, and therefore the histogram will more closely resemble the theoretical wave function.
This can be seen in Figure 1, where the wave function histogram has been plotted against the theoretical wave function for both harmonic and anharmonic oscillators. Since the quartic term is a perturbation, the change in the wave function is barely noticeable, and therefore both histograms look very similar.

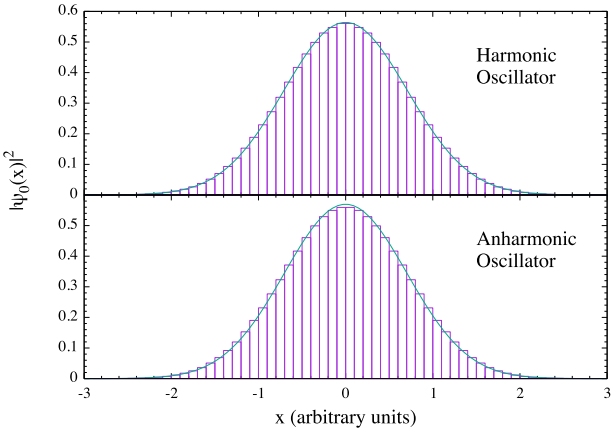

FIG. 1: Wave function histogram superposed with the theoretical wave function (blue line)[3]. **Top:** Harmonic Oscillator. **Bottom:** Anharmonic Oscillator.

C. Ground state energy

The ground state energy can be computed using the Quantum Virial Theorem [9], which in this case allows us to express this quantity in terms of the expectation values of the powers of the position operator

$$E_0 = \langle \mathcal{H} \rangle_{\psi_0} = m\omega^2 \langle X^2 \rangle_{\psi_0} + 3\frac{m^2\omega^3}{\hbar}\lambda \langle X^4 \rangle_{\psi_0} \ . \tag{34}$$

Using the values obtained through the simulation, we get $E_0 = 0.503$ for the H.O., which differs less than 1% from its theoretical value of $E_0 = 0.500$, and $E_0 = 0.516$ for the Anharmonic Oscillator, which differs less than 2% from the value computed with perturbation theory, $E_0 = 0.508$.

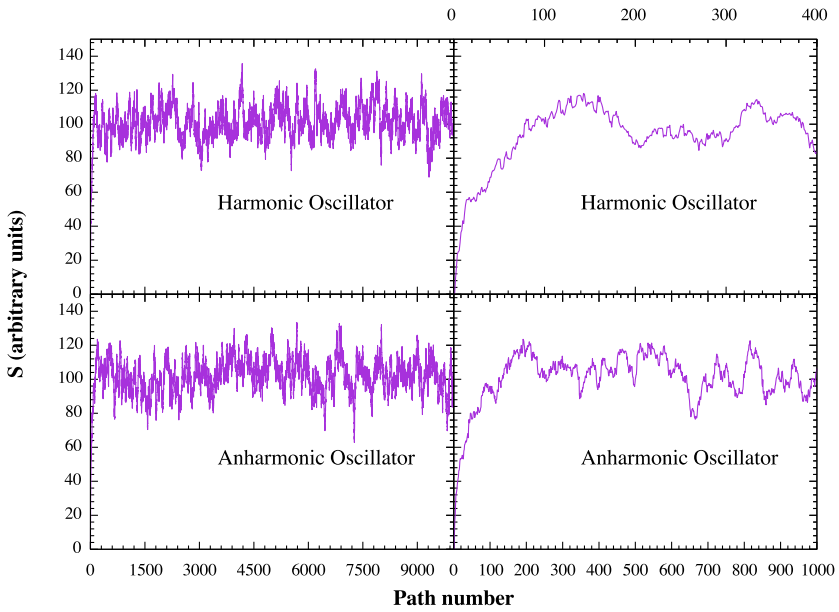

FIG. 2: **Left:** Behaviour of the action of the H.O. (top) and Anharmonic Oscillator (bottom) for the whole sample. **Right:** Behaviour of the action for the first 400 in the H.O. sample (top) and for the first 1000 paths in the Anharmonic Oscillator (bottom).

V. CONCLUSIONS

In this work, the path integral formalism of Quantum Mechanics has been introduced, as well as its ability to obtain quantities available to other formulations of QM. Furthermore, a numerical simulation using Monte Carlo integration and the Metropolis algorithm has been performed, through which results for the quantum Harmonic Oscillator have been obtained, with the inclusion of a perturbative anharmonic term.

The simulation has provided good estimations of the expectation values of different powers of the position operator X, which have been computed by numerical evaluation of both a path integral and Eq.(17), as well as values for the ground state energy that closely resemble those found in literature.

Moreover, there has been an improvement in the sample arising from an inherent asymmetry of the algorithm used to sample paths which has allowed a more precise estimation for the expectation values of X^2 and X^4. Furthermore, it allowed for a better computation of the ground state wave function, leading to a histogram that reproduces the theoretical result more accurately.

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