Quantum Mechanics by Numerical Simulation of Path Integral

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Abstract: The Quantum Mechanics formulation of Feynman is based on the concept of path integrals, allowing to express the quantum transition between two space-time points without using the *bra* and *ket* formalism in the Hilbert space. A particular advantage of this approach is the ability to provide an intuitive representation of the classical limit of Quantum Mechanics. The practical importance of path integral formalism is being a powerful tool to solve quantum problems where the analytic solution of the Schrödinger equation is unknown. For this last type of physical systems, the path integrals can be calculated with the help of numerical integration methods suitable for implementation on a computer. Thus, they provide the development of arbitrarily accurate solutions. This is particularly important for the numerical simulation of strong interactions (QCD) which cannot be solved by a perturbative treatment. This thesis will focus on numerical techniques to calculate path integral on some physical systems of interest.

I. INTRODUCTION

Feynman's space-time approach based on path integrals is not too convenient for attacking practical problems in non-relativistic Quantum Mechanics. Even for the simple harmonic oscillator it is rather cumbersome to evaluate explicitly the relevant path integral. However, his approach is extremely gratifying from a conceptual point of view. By imposing a certain set of sensible requirements on a physical theory, we are inevitably led to a formalism equivalent to the usual formulation of Quantum Mechanics. Methods based on path integrals have been found to be very powerful in other branches of modern physics, such as Quantum Field Theory or Statistical Mechanics.

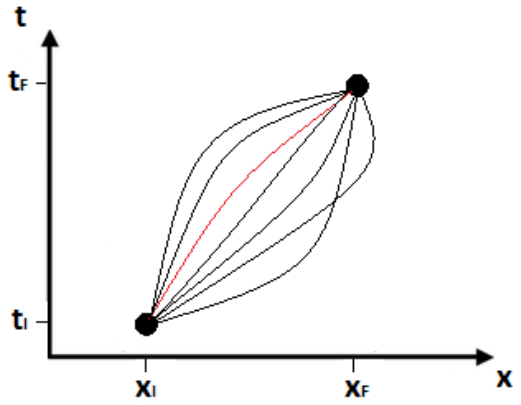

FIG. 1: Path integral qualitative representation for the connection between the initial state with the final state. The red line represents the classical trajectory, while the dark lines are paths corresponding to quantum particles.

Our study is based on the seminal paper of Feynman [1]. In the first section of our writeup, we introduce the basic concepts of path integral and numerical simulation. Next, we discuss some specific examples such as the harmonic oscillator.

II. QUANTUM MECHANICS BY PATH INTEGRAL

In this section, we recover the main ingredient of the path integral formalism for Quantum Mechanics introduced in [1]. Our purpose will be to show by concrete examples, such as the harmonic oscillator, that this formalism is equivalent to the Heisenberg and Shrödinger approach of Quantum Mechanics.

In the Feynman formalism, the matrix elements of the operator in the Heisenberg representation at position x_I and x_F respectively at times t_I and t_F is expressed in terms of multidimensional integrals in the x-space, namely

$$\langle x_F, t_F|\mathcal{O}(X(t))|x_I, t_I\rangle = \int_{t_I}^{t_F} \mathcal{D}[x] e^{-S_E(x)} \qquad (1)$$

where $|x,t\rangle = e^{iHt}|x\rangle_S$ is the position state at time t in the Heisenberg representation, $S_E(x)$ is the euclidean action and

$$\mathcal{D}[x] = \left(\frac{m}{2\pi\Delta t}\right)^{N/2} \int \prod_{k=1}^{N-1} dx_k \,. \qquad (2)$$

Here the time distance $T = t_F - t_I$ has been divided in N intervals of longitude $\Delta t = (t_F - t_I)/N$. For any time slice $t_k = t_0 + k\Delta t$ ($k = 0, \ldots, N$, $t_0 = t_I$ and $t_N = t_F$) we integrate over $x_k = x(t_k)$, which stands for the x-position of the path at time t_k with $x_0 = x_I$ and $x_N = x_F$. The above expression is understood in the limit $N \to \infty$ and $\Delta t \to 0$ with T kept constant. The action of the system in units of $\hbar$ is

$$S(x) = \int_{t_I}^{t_F} dt \mathcal{L} \,, \qquad (3)$$

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and the corresponding discretized Lagragian in the euclidean space is

$$\mathcal{L} = \frac{m}{2}\left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 + V\left(\frac{x_{k+1}-x_k}{2}\right). \quad (4)$$

The basic difference between Classical Mechanics and Quantum Mechanics should now be apparent. In Classical Mechanics, a definite path in the (x,t)-plane is associated with the particle's motion; in contrast, in Quantum Mechanics all possible paths must play a role, including those which do not bear any resemblance to the classical path. Yet we must somehow be able to reproduce Classical Mechanics in a smooth manner in the limit $h \to 0$.

A. Spectrum from a transition amplitude

Here we show that by knowing the transition amplitudes in eq. (1), all the physical properties of the system (namely eigenvalues and eigenstates) can be known. This approach is an alternative to that of Quantum Mechanics where we directly diagonalize the Hamiltonian. In the most familiar Shrödinger representation, the matrix element in eq. (1) reads as

$$\begin{aligned}&\langle x_F, t_F|\mathcal{O}(t)|x_I, t_I\rangle = \\ &= \langle x_F|e^{-iH(t_F-t)}\mathcal{O}(X)e^{-iH(t-t_I)}|x_I\rangle\,. \end{aligned} \quad (5)$$

Let's now insert in this expression a complete set of eigenstates $\sum_n |n\rangle\langle n| = 1$ and $H|n\rangle = E_n|n\rangle$, namely

$$\begin{aligned}&\langle x_F, t_F|\mathcal{O}(t)|x_I, t_I\rangle = \\ &= \sum_{n,n'}\langle x_F|e^{-iH(t_F-t)}|n\rangle\langle n|\mathcal{O}|n'\rangle\langle n'|e^{-iH(t-t_I)}|x_I\rangle \quad (6)\\ &= \sum_{n,n'} e^{-iE_n(t_F-t)}e^{-iE_{n'}(t-t_I)}\langle n|\mathcal{O}|n'\rangle\psi_n^*(x_F)\psi_{n'}(x_I)\end{aligned}$$

where $\langle x_F|n\rangle = \psi_n^*(x_F)$ is the eigenstates wave function. Now, by setting $x_F = x_I \equiv x_0$ and $t \to it$ and by integrating over x_0 we get in the euclidean space

$$\int dx_0\langle x_0, t_F|\mathcal{O}(t)|x_0, t_I\rangle = \sum_n e^{-E_n(t_F-t_I)}\langle n|\mathcal{O}|n\rangle\,, \quad (7)$$

where we have used the orthonormality of the wave functions $\int dx\,\psi_n^*(x)\psi_{n'}(x) = \delta_{nn'}$. With this change, the action of the system matches the hamiltonian, and is known as the euclidean action $S_E(x)$. At large time $T = t_F - t_I$ only the ground state will contribute to the above sum, namely

$$\int dx_0\langle x_0, t_F|\mathcal{O}(t)|x_0, t_I\rangle \overset{T\to\infty}{\to} e^{-E_0T}\langle 0|\mathcal{O}(X)|0\rangle. \quad (8)$$

By studying the special case $\mathcal{O}(X) = 1$, we can extract the energy-level of the ground state from the behaviour at large time of eq. (8),

$$\int dx_0\langle x_0, t_F|x_0, t_I\rangle = \sum_n e^{-E_nT} \overset{T\to\infty}{\to} e^{-E_0T}\,. \quad (9)$$

Moreover, in this case eq. (6) can be simplified and at large time can provide the ground state wave function

$$\langle x_0, t_F|x_0, t_I\rangle = \sum_n e^{-E_nT}|\psi_n(x_0)|^2 \quad (10)$$

$$\langle x_0, t_F|x_0, t_I\rangle \overset{T\to\infty}{\to} e^{-E_0T}|\psi_0(x_0)|^2\,. \quad (11)$$

So dividing the propagator over its integral over all the initial states we get the ground state wave function

$$\frac{\langle x, t_F|x, t_I\rangle}{\int dx\langle x, t_F|x, t_I\rangle} \overset{T\to\infty}{\to} |\psi_0(x)|^2\,. \quad (12)$$

It is useful to introduce the expectation value of a generic observable $\mathcal{O}$ as

$$\langle\mathcal{O}(t)\rangle = \frac{\int dx_0\langle x_0, t_F|\mathcal{O}(t)|x_0, t_I\rangle}{\int dx_0\langle x_0, t_F|x_0, t_I\rangle} = \int \mathcal{D}\mu(\vec{x})\mathcal{O}(x_t)\,, \quad (13)$$

where $\mathcal{D}\mu(\vec{x}) = \frac{1}{\mathcal{Z}}\prod_{k=0}^{N-1} dx_k\, e^{-S(\vec{x})}$ and the path variables are $\vec{x} = (x_0, \ldots, x_t, \ldots, x_N = x_0)$. Additionally, $\mathcal{Z} = \int \prod_{k=0}^{N-1} dx_k e^{-S(x)}$ has been set to have $\langle\mathcal{O}\rangle = 1$. According to eq. (9), at large time distance we have

$$\langle\mathcal{O}(t)\rangle \overset{T\to\infty}{\to} \langle 0|\mathcal{O}(x)|0\rangle\,. \quad (14)$$

Interestingly, the expectation value of $\mathcal{O}(t_0) = \delta(X(t_0) - x) \equiv \delta_0$ gives

$$\frac{\int dx_0\delta_0\langle x_0, t_F|x_0, t_I\rangle}{\int dx_0\langle x_0, t_F|x_0, t_I\rangle} = \frac{\langle x, t_F|x, t_I\rangle}{\int dx\langle x, t_F|x, t_I\rangle}\,, \quad (15)$$

which according to eq. (12) goes to $|\psi(x)|^2$ at large time distance, T.

III. HARMONIC OSCILLATOR VIA PATH INTEGRALS: ANALYTIC SOLUTION

Now we consider the case of the harmonic oscillator with potential $V(x) = \frac{1}{2}m\omega^2x^2$ and we estimate the wave function and the energy-level of the ground state by evaluating eq. (1) for the operator $\mathcal{O}(t) = 1 \equiv \mathcal{K}(t)$. The analytic solution for $\mathcal{K}(x_F, t_F; x_I, t_I) \equiv \langle x_F, t_F|x_I, t_I\rangle$ when $t_I = 0$ can be expressed as [2]:

$$\langle x_F, t_F | x_I, 0\rangle = \sqrt{\frac{a(t)}{\pi i}} e^{ia(t)((x_F^2+x_I^2)cos(\omega t)-2x_F x_I)} \,, \quad (16)$$

where $a(t) \equiv \dfrac{m\omega}{2sin(\omega t)}$. Therefore, by setting $x_F = x_I \equiv x$ and $t \to it$, we obtain

$$\langle x_F, t_F | x_I, 0\rangle = \sqrt{\frac{b(t)}{2\pi}} e^{ib(t)x^2(cosh(\omega t)-1)} \,, \quad (17)$$

where $b(t) \equiv \dfrac{m\omega}{sinh(\omega t)}$. Thus, by doing $t \to \infty$ we get

$$ln(\mathcal{K}(t\to\infty)) = \frac{1}{2}ln(\frac{m\omega}{\pi}) - \omega(mx^2+\frac{t}{2}) = \\ = ln(\sqrt{\frac{m\omega}{\pi}}e^{-\omega m x^2}) - \frac{\omega}{2}it \,, \quad (18)$$

and from eq. (11) we obtain the analytic solution of $|\psi_0(x)|^2$ for the harmonic oscillator.

IV. THE METROPOLIS ALGORITHM

From eq. (13), we can infer that the expectation value of an operator is a N-dimensional integral over a periodic path $\vec{x}$. Being $\mathcal{D}\mu(\vec{x})$ defined positive and normalized, it can be interpreted as a probability measure. Thus, we can estimate $\langle\mathcal{O}(t)\rangle$ as a statistical average over a sample of paths, $\vec{x}^{(k)}$ $(k = 1, \cdots, M)$, extracted randomly with weight $\mathcal{D}\mu(\vec{x})$:

$$\bar{\mathcal{O}} = \frac{1}{M}\sum_{k=1}^{M}\mathcal{O}(\vec{x}_t^{(k)}) \,. \quad (19)$$

For large M, $\langle\mathcal{O}(t)\rangle \simeq \bar{\mathcal{O}}$ and the error goes to zero as $1/\sqrt{M}$. The standard deviation of $\bar{\mathcal{O}}$ can be used to give an error on our estimation of $\langle\mathcal{O}(t)\rangle$ at finite M. Let's now discuss the technical part to generate a sample of paths $\vec{x}^{(k)}$ distributed according $\mathcal{D}\mu(\vec{x})$. This can be done by generating a Markov Chain of $\vec{x}^{(k)}$ paths through the Metropolis algorithm. The Metropolis algorithm starts setting randomly an initial path $\vec{x}^{(0)}$. In our simulation setup, we set $\vec{x}^{(0)} = 0$. Then, the following three steps come into play:

a. For each coordinate $x_i = x(t_i)$ we consider a new proposal x_i' randomly generated starting from the initial path. Specifically, we introduce a gaussian variable ξ distributed in such a way that $x_i' = x_i + \xi$.

b. The Metropolis algorithm consists of accepting or rejecting the new path $\vec{x}'$ in the following way. We calculate the change induced in the action $\Delta S = S(\vec{x}') - S(x)$ and if $\Delta S < 0$ (namely the action is diminished by the new path), we accept the new path $\vec{x}^{(1)} = \vec{x}'$ with probability $e^{-\Delta S}$. In practice, we generate a random number r uniformly distributed between 0 and 1. If $r < e^{-\Delta S}$ then the algorithm accepts the new path, otherwise it returns to the old value.

c. Then, the steps *a.* and *b.* are repeated even for the path $\vec{x}^{(1)}$, and it continues with $\vec{x}^{(2)}$ and so forth.

The algorithm stops when the $S(\vec{x}^{(k)})$ values on the updated $\vec{x}^{(k)}$ chain converge to a stable value, the so-called thermalization phase (FIG. 2). In the next section, we illustrate the algorithm with a concrete example.

V. HARMONIC OSCILLATOR VIA PATH INTEGRALS: NUMERICAL SIMULATION

In this section, we simulate the harmonic oscillator with the Metropolis algorithm [3]. This means that the euclidean action corresponding to a single path is

$$S_E(x_j) \equiv \sum_{j=1}^{N}[\frac{m}{2}(\frac{x_j - x_{j-1}}{\Delta t})^2 + \frac{m\omega^2}{2}\frac{(x_j + x_{j-1})}{2}] \,. \quad (20)$$

In order to get reliable numerical results, it is needed that our discrete simulation well approximates the continuum limit, $\Delta t \to 0$, and the infinite time extension, $T \to \infty$. Being ω related to the energy of our system, we require $\omega\Delta t \ll 1$ and $\omega T \gg 1$, which corresponds in our simulation to $m = 1/2$, $\omega = 1$, $T = 100$ and $\Delta t = 0.5$. Then the euclidean action reads as

$$S_E(x_j) \equiv \sum_{j=1}^{N}[\frac{(x_j - x_{j-1})^2}{16} + \frac{(x_j + x_{j-1})}{8}] \,. \quad (21)$$

A. Wave Function of the ground state

In order to obtain the wave function of the ground state, we can use a time saving trick [4]. This trick consists of introducing a delta function into the probability integral

$$|\psi_0(x)|^2 = \int dx_1 ... dx_N e^{-\varepsilon(x,x_1,...)} \,, \quad (22)$$

which allows us to calculate the wave function by only considering a concrete position of each path. For instance, using the trick for the first position of the paths, we have:

$$|\psi_0(x)|^2 = \int dx_0 ... dx_N \delta(x - x_0) e^{-\varepsilon(x,x_1,...)} \quad (23)$$

Hence, this value must be recovered by the expression:

$$|\psi_0(x)|^2 = \sqrt{\frac{m\omega}{\pi}}e^{-m\omega x^2} \to \sqrt{\frac{1}{2\pi}}e^{-\frac{x^2}{2}} \,, \quad (24)$$

when $m = \frac{1}{2}$ and $\omega = 1$. In this case, $E_n = n + \frac{1}{2}$ and $n = 0, 1, 2, ...$

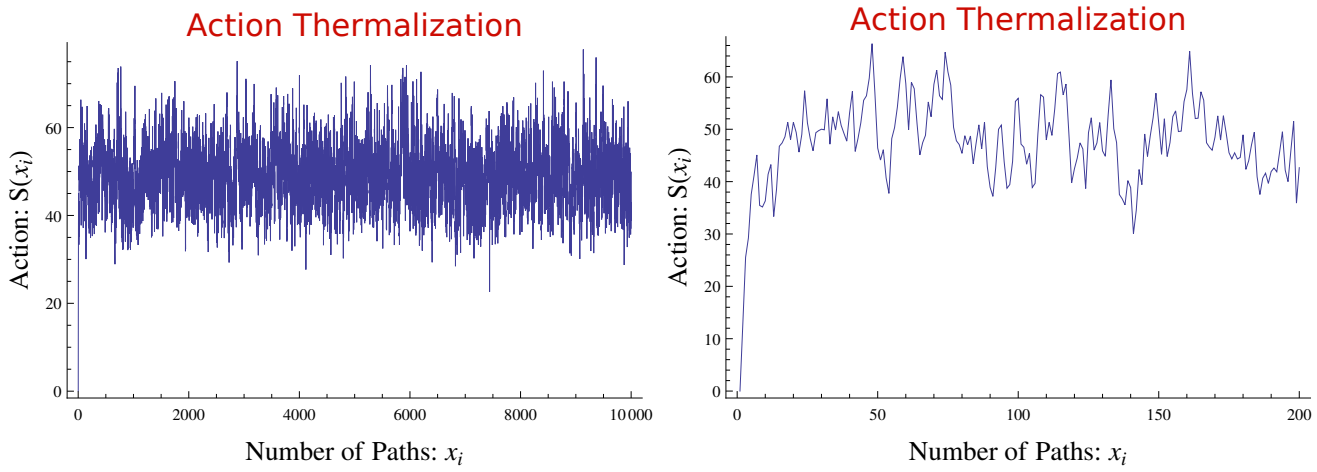

FIG. 2: Behaviour of the harmonic oscillator action as a function of sample of paths generated by the Metropolis algorithm. Left: We consider a large simulation of 10000 paths. Right: We focus on the first 200 paths of the same sample as the plot on the left. After 50 iterations, an asymptotic value is reached.

B. Expectation Values

From the numerical simulation we can calculate the following matrix elements of the position operator and their respective errors (σ) with the formulas introduced in the previous section. The values obtained are:

$$\langle\psi_0|X|\psi_0\rangle = 0.00 \pm 0.03 \quad (25)$$
$$\langle\psi_0|X^2|\psi_0\rangle = 1.01 \pm 0.02 \quad (26)$$
$$\langle\psi_0|X^3|\psi_0\rangle = 0.0 \pm 0.09 \quad (27)$$
$$\langle\psi_0|X^4|\psi_0\rangle = 3.12 \pm 0.09 \quad (28)$$

Whereas the analytic estimates from standard Quantum Mechanics are:

$$\langle\psi_0|X^2|\psi_0\rangle = 1 \quad (29)$$
$$\langle\psi_0|X^4|\psi_0\rangle = 3 \quad (30)$$

Notice that we can also estimate the previous matrix elements by knowing the wave function of the ground state, namely

$$\langle\psi_0|\mathcal{O}(x)|\psi_0\rangle = \int dx|\psi_0(x)|^2\mathcal{O}(x) \simeq \simeq \sum_k |\psi_0(x_k)|^2\mathcal{O}(x_k)\Delta x\,. \quad (31)$$

The estimated values in this way are:

$$\langle\psi_0|X^2|\psi_0\rangle = 0.98 \quad (32)$$
$$\langle\psi_0|X^4|\psi_0\rangle = 3.11 \quad (33)$$

where the difference is an estimate of the systematic error in the approach, produced due to the fact that in the right-hand side we have a discrete sum.

C. Symmetries and improvement of the estimations

One could observe that the estimated values for X and X^3 have to be exactly zero, since they are odd and the action is symmetric for parity. However, in the last section we have seen that the estimated values are not exactly zero, with a small error. The reason why is because the sample of paths is not symmetrical under parity transformation. This happens since Metropolis algorithm takes paths randomly, thus it is not guaranteed that each path would have a symmetrical one in the sample because the algorithm breaks the parity symmetry. Nonetheless, since two symmetrical paths give the same value for the euclidean action $S_E(x) = S_E(-x)$, we can create an improved sample with symmetrical paths that implies having these values exactly zero, in addition to enhancing the statistics. Therefore, these new values are:

$$\langle\psi_0|X|\psi_0\rangle = (0.0 \pm 1)10^{-17} \quad (34)$$
$$\langle\psi_0|X^3|\psi_0\rangle = (0.0 \pm 1)10^{-17} \quad (35)$$

while the estimations of X^2 and X^4 are the same, beacuse of the symmetry of the problem. In fact, from eq. (23) we have made the calculations of (25)$\cdots$(28), (32) and (33) by considering the first position of each path, i.e. by fixing t at the initial time. However, time reversal invariance allows to calculate the same wave function at any time, since the fluctuations are the same.

D. Ground state energy Level

From Virial Theorem, we can estimate the ground state energy through the calculation of $\langle\psi_0|X^2|\psi_0\rangle$. In fact, in a stationary state in Quantum Mechanics the Virial Theorem is

$$2\langle T\rangle = \langle x\frac{dV}{dx}\rangle\,. \tag{36}$$

In the harmonic oscillator case, since the potential is $V = m\omega^2\frac{\langle x^2\rangle}{2}$, we obtain that

$$\langle x\frac{dV}{dx}\rangle = m\omega^2\langle x^2\rangle \tag{37}$$

$$\langle T\rangle = m\omega^2\frac{\langle x^2\rangle}{2}\,. \tag{38}$$

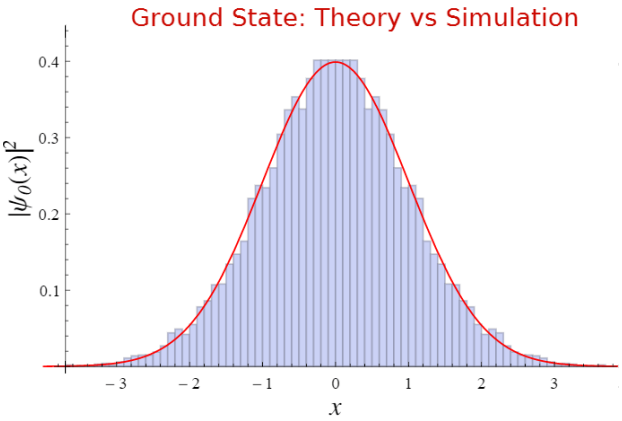

FIG. 3: Ground state wave function obtained through the time saving trick and with the symmetric sample. The red line represents the gaussian function of eq. (24).

Therefore, by setting $m = \frac{1}{2}$ and $\omega = 1$, we can estimate the ground state energy as

$$E_0 = \frac{\langle\psi_0|x^2|\psi_0\rangle}{2}\,. \tag{39}$$

That gives us a result of $E_0 = 0.51$, which compared to the analytic value $E_0 = 0.5$, we can infer that is a good estimation with a systematic error.

VI. CONCLUSIONS

In this thesis the goal has been studying one-dimensional quantum systems using the formulation of path integrals, both analytically and numerically. We have seen that Feynman's path integral formalism is equivalent to the Schrödinger and Heisenberg interpretations for Quantum Mechanics. In fact, by using path integral formalism some expected values in Quantum Mechanics can be obtained analytically in different ways. Furthermore, we have seen that Markov chains are useful for generating paths with the desired probability distribution and the Metropolis algorithm is suitable for the numerical simulations, which by using path integral formalism enables to solve systems where the analytic solution is unknown. With regards to the particular case of the harmonic oscillator, it can be solved analytically with the path integral formalism, which provides a semi-classical approach. However, it can also be easily solved by numerical simulations. For instance, it is useful to take advantage of the symmetries of the problem in order to obtain more accurate results. In general, the results presented in this thesis are well compared with the theoretical values or with other results presented in the literature.

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