MONTE CARLO SIMULATIONS FOR INSTANTONS

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Abstract

In this project, following the lectures by T. Schäfer [1], we use the Monte Carlo simulations to understand the role of tunneling events in quantum mechanics, instantons, using the double-well potential model. First we study the quantum mechanical problem on a Euclidean lattice using the path integral Monte Carlo techniques, in order to compute the partition function and the correlation functions. The results are compared with an "exact" solution of the same problem in the canonical quantization approach. Then we extract the instanton content using the cooling method and we show for completeness the opposite method, the heating, that allows to get correlation functions starting from a classical instanton ensemble perturbed with Gaussian fluctuations. All these interesting techniques have been used in QCD context. The data are obtained by programs written in C++ and analyzed with the framework ROOT.

1 Introduction

An *instanton* or *pseudoparticle* [2][3] is a classical solution to the *Euler-Lagrange equations of motion* with a finite, non zero action, either in quantum mechanics or in quantum field theory. More precisely is a solution to the equations of motion of a classical field theory on a *Euclidean spacetime*.

An instanton can be used to calculate the transition probability for a quantum mechanical particle tunneling through a potential barrier. A quantum toy model with an instanton effect is a particle in a *double-well potential*. In contrast to a classical particle, there is non-vanishing probability that it crosses a region of potential energy higher than its own energy. Thus we consider a non-relativistic particle moving in a potential $V(x)$ given by

$$V(x) = (x^2 - \eta^2)^2. \tag{1}$$

The potential energy takes its minimal value at $x = \pm\eta$, and these are called classical minima because the particle tends to lie in one of them in classical mechanics. There are two lowest energy states in the classical case. In quantum mechanics we solve the *Schroedinger equation*

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi = E\psi \tag{2}$$

to identify the energy eigenstates. If we do this we will find only the unique lowest-energy state instead of two states. The ground-state wave function localizes at both of the classical minima instead of only one of them because of the quantum interference or quantum tunneling.

Instantons are the tool to understand why this happens within the semi-classical approximation of the path-integral formulation in Euclidean time.

2 Exact Diagonalization

In order to compare the results obtained with the Monte Carlo methods, we want to solve the Schroedinger problem presented in the previous section. This can be achieved by choosing a basis and numerically diagonalizing the Hamilton operator in that basis. We have chosen a simple *harmonic oscillator* basis defined by the eigenstates of

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2, \tag{3}$$

that satisfy $H_0 |n\rangle = \omega_0 (n + \frac{1}{2}) |n\rangle$. The Hamiltonian H of the anharmonic oscillator with potential in (1) has a very simple structure in this basis. The only non-zero matrix elements are $\langle n| H |n\rangle$, $\langle n| H |n+2\rangle$, $\langle n| H |n+4\rangle$.

With the choice of $\omega_0 = 4\eta$ even modest basis sizes such $N = 40$ are sufficient in order to determine the first few eigenvectors very accurately.

In the following we will refer to this numerical solution as the "exact" one, to be compared with the Monte Carlo results. More specifically, the data are obtained with a diagonalization program which computes the spectrum $\{E_n\}$ and the ground state wave function $\psi(x)$ of the anharmonic oscillator, in order to compute euclidean correlation functions $\langle x(0)x(\tau)\rangle$ (also for x^2 and x^3) and the partition function $Z(\beta) = \sum_n \exp(-\beta E_n)$.

In Fig.(1) is presented the double well potential, choosing $\eta = 1.4$, with the ground state energy and the first three excited states, obtained with the diagonalization program.

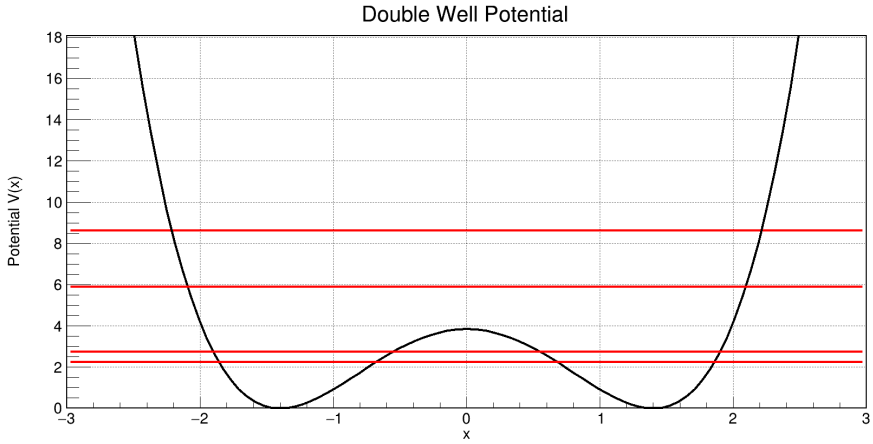

Figure 1: Double well potential $V(x) = (x^2 - \eta^2)^2$ with $\eta = 1.4$. We also indicated the position of the ground state and the first three excited levels.

3 Quantum Mechanics on a Euclidean Lattice

Alternatively to the canonical quantization approach, one can use the Feynman's *path integrals* formulation to compute the transition probability (we'll use natural units $c = \hbar = 1$ and also $2m = 1$ for simplicity)

$$\langle x_1| e^{-iHt_1} |x_0\rangle = \int_{x(0)=x_0}^{x(t_1)=x_1} \mathcal{D}x \; e^{iS[x]}, \qquad S[x] = \int_0^{t_1} dt \left(\frac{1}{4}\dot{x}^2 - (x^2 - \eta^2)^2 \right). \tag{4}$$

Following the process of *Wick rotation* (analytic continuation) to Euclidean spacetime ($it \to \tau$) and considering periodic boundary conditions, one gets the partition function

$$Z(T) = \int_{PBC} \mathcal{D}x \; e^{-S_E[x]}, \qquad\qquad S_E[x] = \int_0^\beta d\tau \left(\frac{1}{4} \left(\frac{dx}{d\tau} \right)^2 + (x^2 - \eta^2)^2 \right), \tag{5}$$

where $\beta = 1/T$ is the inverse temperature. To study numerical simulations we can consider the time slicing procedure $\tau_i = ia$, $i = 1, ..., n$, to get a discretized action

$$S = \sum_{i=1}^{n} \left(\frac{1}{4a} (x_i - x_{i-1})^2 + a(x_i^2 - \eta^2)^2 \right), \tag{6}$$

with $x_i = x(\tau_i)$ and periodic boundary conditions $x_0 = x_n$. Thus the discrete euclidean path integral is formally equivalent to the partition function of a statistical system of "spins" x_i on lattice with spacing a. We can study this system using standard Monte Carlo sampling methods, like the *Metropolis algorithm* [4]. This method generates an ensemble of configurations $\{x_i\}^{(k)}$ where $i = 1, ..., n$ labels the lattice points and $k = 1, ..., N_c$ labels the configurations. Quantum mechanical averages are computed by averaging observables over many configurations,

$$\langle O \rangle = \lim_{N_c \to \infty} \frac{1}{N_c} \sum_{k=1}^{N_c} O^{(k)}, \tag{7}$$

where O^k is the value of the classical observable O in the configuration $\{x_i\}^{(k)}$. The configurations are generated using Metropolis updates $\{x_i\}^{(k)} \to \{x_i\}^{(k+1)}$, and the update consists of a sweep through the lattice during which a trial update $x_i^{(k+1)} = x_i^{(k)} + \delta x$ is performed for every lattice site, with δx random number. The trial is accepted with probability

$$P\big(x_i^{(k)} \to x_i^{(k+1)}\big) = \min\{\exp(-\Delta S), 1\}, \tag{8}$$

where ΔS is the change in the action in (6). This ensure that the configuration are distributed according the *Boltzmann distribution* $\exp(-S)$. In order to study equilibration it is often useful to compare an ordered (cold) start with $\{x_i\}^{(0)} = \{\eta\}$ to a disordered (hot) start $\{x_i\}^{(0)} = \{r_i\}$, where r_i is a random variable.

The energy eigenvalues and wave functions of the quantum mechanical problem can be obtained from the euclidean correlation functions

$$\Pi(\tau) = \langle O(0) O(\tau) \rangle, \tag{9}$$

where $O(\tau)$ is an operator that can be constructed from the variables $x(\tau)$, e.g. some integer power $O(\tau) = x(\tau)^n$. The euclidean correlation functions are related to the quantum mechanical states via spectral representation with

$$\Pi(\tau) = \sum_n |\, \langle 0 |\, O(0)\, | n \rangle \,|^2 \exp(-(E_n - E_0)\tau), \tag{10}$$

where E_n is the energy of the state $|n\rangle$ and $|0\rangle$ is the ground state of the system. This relation was in fact used in order to calculate the correlation functions in the exact diagonalization program.

The Monte Carlo method is very useful in calculating expectation values in quantum or statistical mechanics. However, the Monte Carlo method does not directly give the partition function or the free energy. A very effective method for computing the free energy is the *adiabatic switching*

technique. The idea is to start from a reference system for which the free energy is known and calculate the free energy difference to the real system using Monte Carlo methods.

For this purpose we write the action as $S_\alpha = S_0 + \alpha \Delta S$ where S is the full action, S_0 is the action of the reference system, α is a coupling constant and $\Delta S = S - S_0$. The action S_α interpolates between the real and the reference system. Integrating the relation $\partial \log Z(\alpha)/\partial\alpha = -\langle \Delta S \rangle_\alpha$ we find

$$\log Z(\alpha = 1) = \log Z(\alpha = 0) + \int_0^1 d\alpha' \langle \Delta S \rangle_{\alpha'}, \tag{11}$$

where $\langle ... \rangle_\alpha$ is an expectation value over the action S_α. In this case is natural to use the harmonic oscillator with frequency ω_0 as reference system, so

$$\log Z(\alpha = 0) = \frac{\exp(-\beta\omega_0/2)}{1 - \exp(-\beta\omega_0)}. \tag{12}$$

The integral over the coupling constant α can easily be calculated in Monte Carlo simulations by slowly changing α from 0 to 1 during the simulation. In order to estimate systematic errors due to incomplete equilibration it is useful to repeat the calculation with α changing from 1 to 0 and study possible hysteresis effects.

3.1 Numerical Results

In the following are presented the numerical results from Monte Carlo simulations of the euclidean path integral. Typical paths that appear in Monte Carlo simulation are shown in Fig.(2). The figure clearly show that there are two characteristic time scales in the problem. On short time scales the motion is controlled by the oscillation time $\tau_{osc} \sim \omega^{-1}$, while for large τ the system is governed by the tunneling time $\tau_{tun} \sim \exp\left(-4\eta^3/3\right)$. In order to perform reliable simulations we have to make sure that the following conditions are satisfied:

$$\tau_{osc} \ll a, \qquad\qquad \tau_{tun} \ll na. \tag{13}$$

A typical choice of parameters for the case $\eta = 1.4$ is $n = 800$, $a = 0.05$ and a number of Metropolis sweeps $N_c = 10^5$.

Fig.(3) shows the distribution of x_i obtained in the Monte Carlo simulation compared to the square of the ground state wave function computed by the diagonalization method discussed previously.

Fig.(4) shows the correlation functions of the operators x, x^2 and x^3. The solid lines show the result obtained using the spectral representation in (10) together with the eigenvalues and eigenfunctions determined by numerical diagonalization of the Hamiltonian. The data points show the results from the Monte Carlo simulation and we see that the overall agreement is excellent.

In Fig.(5) we show Monte Carlo results for the partition function compared to "exact" results based on the spectrum of the anharmonic oscillator obtained previously. The Monte Carlo results agree with the direct calculations but the method is effectively limited to a small range of temperatures.

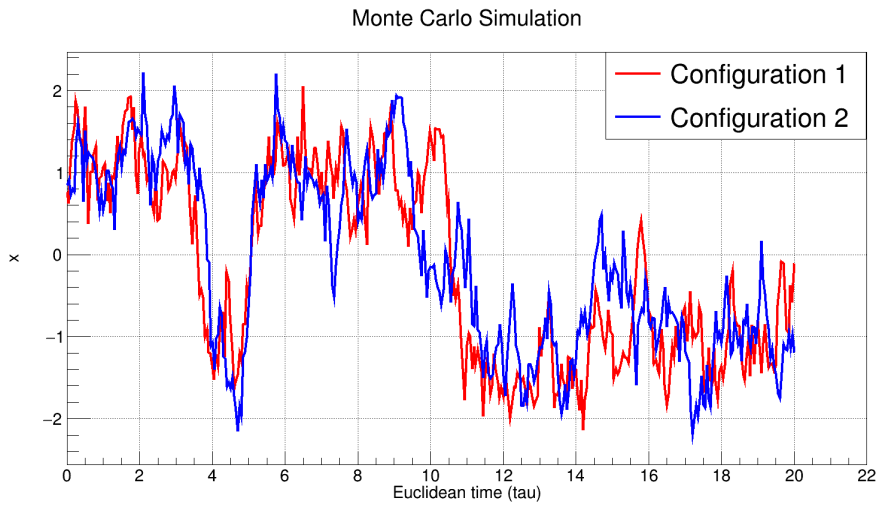

Figure 2: Typical euclidean paths, for two different configurations, obtained in a Monte Carlo simulation of the discretized euclidean action of the double well potential for $\eta = 1.4$. The lattice spacing in the euclidean time direction is $a = 0.05$ and the total number of lattice points is $n = 800$.

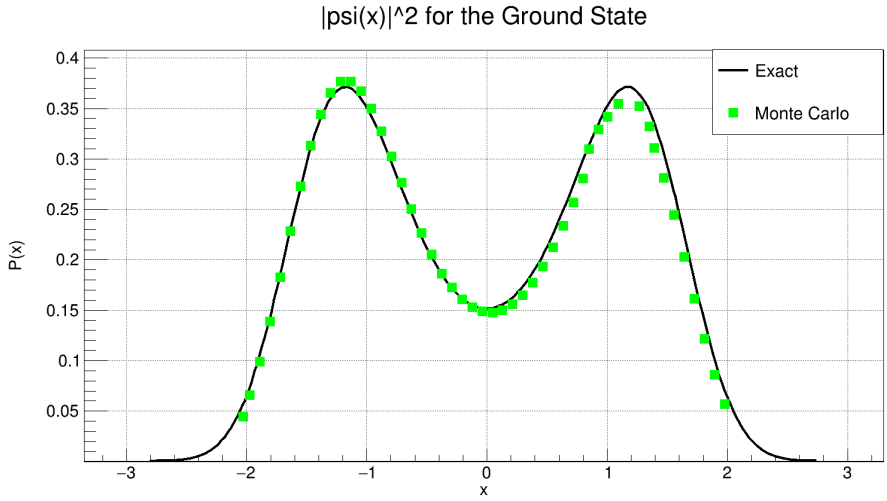

Figure 3: Probability distribution $|\psi(x)|^2$ in the double well potential for $\eta = 1.4$. The solid line shows the "exact" numerical result obtained by diagonalizing the Hamiltonian in an oscillator basis whereas the green points show the distribution of x for an ensemble of euclidean paths.

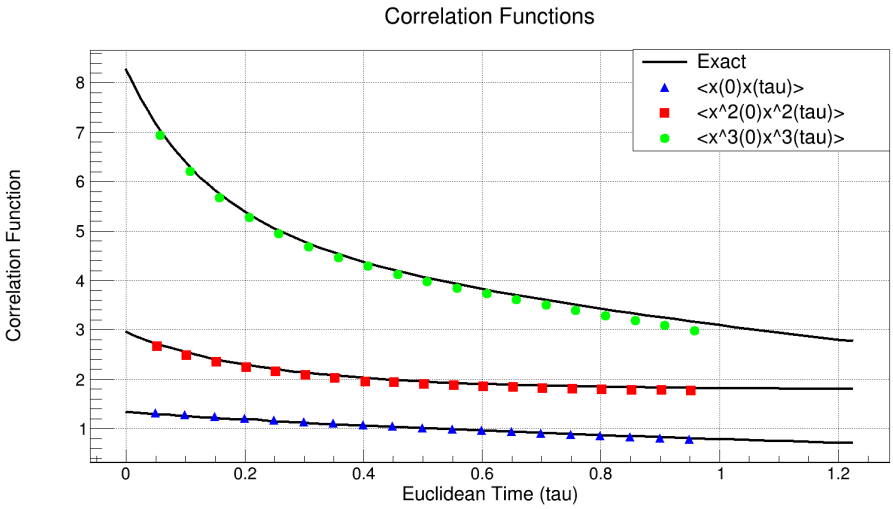

Figure 4: Correlation functions $\langle O(0)O(\tau)\rangle$ in the double well potential for $\eta = 1.4$ and $O = x, x^2, x^3$. The solid lines are "exact" numerical results obtained by diagonalizing the Hamiltonian in an oscillator basis whereas the data point were obtained from Monte Carlo simulations with $a = 0.05$ and $n = 800$.

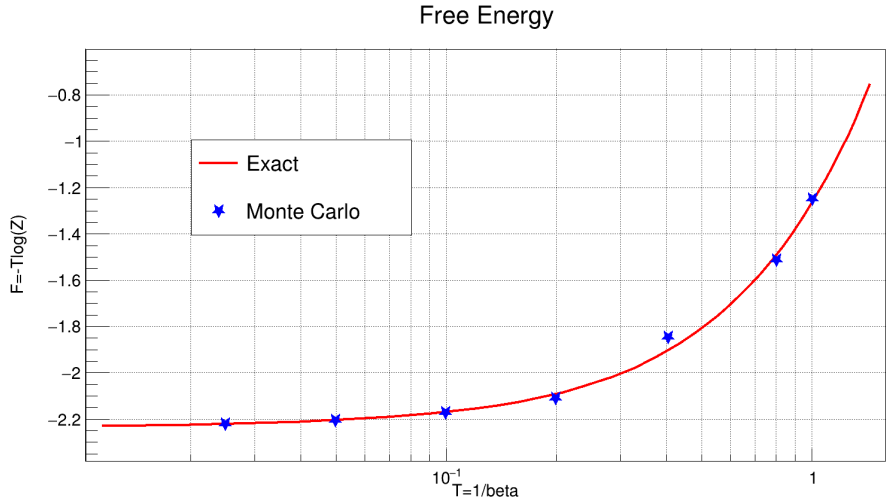

Figure 5: Free energy $F = -T\log(Z)$ of the anharmonic oscillator as a function of the temperature $T = 1/\beta$ with $\beta = na$. The solid line was calculated using the spectrum of the Hamiltonian. The data points were obtained using Monte Carlo calculations and the adiabatic switching method.

4 Instanton Density and Random Gas Model

From Fig.(2) we can clearly see that for this particular choice of the parameter η a typical path contains two components, one related to quantum fluctuations with frequency ω, and one related to tunneling events, instantons. Recall now the formula for the Euclidean action in (5): the potential energy changes sign $V(x) \to -V(x)$ under the Wick rotation and the minima transform into maxima, thereby $V(x)$ exhibits two "hills" of maximal energy. In the continuum limit the instanton solution can be found from the classical equation of motions

$$m\frac{d^2x}{d\tau^2} = \frac{dV(x)}{dx}, \tag{14}$$

varying the action according to the *least action principle* $\delta S_E/\delta x(\tau) = 0$.

Since we want to know how the two classically lowest energy states are connected, let us consider the boundary conditions $x(\tau \to \pm\infty) = \pm\eta$. In this case we get a solution to (14) given by

$$x_I(\tau) = \eta \tanh 2\eta(\tau - \tau_0), \tag{15}$$

with associated anti-instanton solution $x_A(\tau) = -x_I(\tau)$. Since this solution jumps from one classical vacuum $x = -\eta$ to another classical vacuum $x = \eta$ instantaneously around τ_0, creating a tunneling event, it is called instanton and τ_0 can be interpreted as its "location". The classical action of the instanton is

$$S_0 = \frac{4\eta^3}{3}. \tag{16}$$

The tunneling rate, or *instanton density*, $n_{I+A} = N_{I+A}/\beta$ is exponentially small, but to compute the exact expression one has to study small quantum fluctuations around the instanton solution. The calculation can be carried out to next-to-leading order in semi-classical approximation. The idea is to perturb around the classical solution $x(\tau) = x_I(\tau) + \sum_n c_n x_n(\tau)$ at first order in $\hbar$. This introduce "quantumness" to the equations of motion and integrating over all these perturbations is equivalent to integrate over all paths in order to obtain the transition probability $\langle\eta|\, e^{-H\tau}\, |-\eta\rangle$. The result is

$$n_{I+A} = 8\eta^{5/2}\sqrt{\frac{2}{\pi}}\exp\left(-S_0 - \frac{71}{72}\frac{1}{S_0}\right). \tag{17}$$

4.1 Cooling Method

The tunneling events can be studied in more detail after removing short distance fluctuations. A well known method for doing this is *cooling*. In the cooling method we only accept Metropolis updates that lower the action. This will drive the system towards the nearest classical solution. Since instantons are classical solutions, cooling can be used to study the instanton content of a quantum configurations. This is clearly seen in Fig.(6).

The cooling method can be used in order to get an estimate of the total density of instantons and anti-instantons N_{I+A}/β. The numerical results for N_{I+A} in function of the cooling sweeps n_{cool} are shown in Fig.(7). We notice that after the quantum noise has disappeared the instanton density is close to the semi-classical result in (17).

In the case of the double well potential, the parameter η controls the instanton action $S_0 = 4\eta^3/3$. If $S_0 \gg 1$ (semiclassical limit) then instantons are easily identified but the tunneling rate is small. If $S_0 \sim 1$ then instantons are very abundant but it is hard to determine the instanton density precisely. This is why we focused on $S_0 \sim 3$ since with this choice the number of instantons extracted using the cooling method agrees very well with the semi-classical approximation.

However one have to take into account that correlation functions measured in cooled configurations are quite different since short distance fluctuations eliminated by cooling obviously play an important role. This result is shown in Fig.(8).

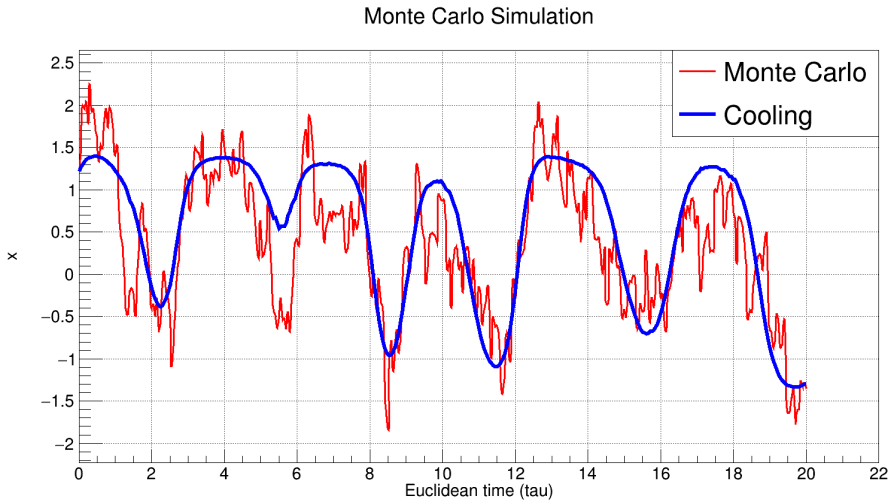

Figure 6: Cooled euclidean path (in blue) obtained by running 100 cooling sweeps on the original path (in red).

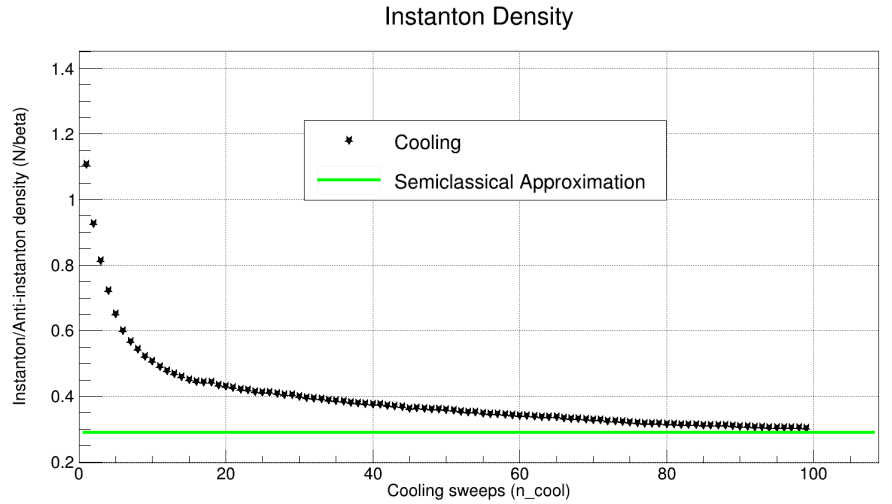

Figure 7: Instanton density as a function of the number of cooling sweeps for $\eta = 1.4$. The green line shows the semiclassical instanton density at one-loop order.

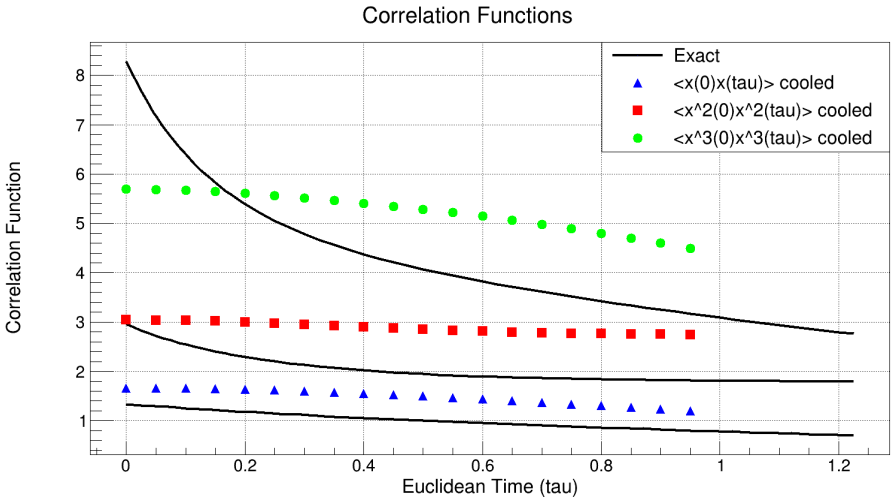

Figure 8: Correlation functions evaluated from cooled Monte Carlo configurations. The number of cooling sweeps $n_{cool} = 200$.

4.2 Heating Method

For completeness we present the "heating" method: as the name suggests, this is essentially the inverse of the cooling method. Using this technique one can determine the correlation functions numerically, starting from a classical ensemble of instantons.

The simplest approximation is to ignore the interactions between instantons, so $S = (N_I + N_A)S_0$ and to consider a random distribution of collective coordinates τ_i. This is known as the *instanton gas model*.

We begin by considering the contribution from the classical path only. In this case the simplest choice of a path for a multi-instanton configuration is a linear superposition of independent tunneling events. So we choose to the simple "sum ansatz"

$$x_{sum}(\tau) = \eta\left\{\sum_i Q_i \tanh\left[2\eta(\tau - \tau_i)\right] - 1\right\}, \tag{18}$$

where $Q_i = \pm 1$ is the topological charge of the instanton.

Like the the cooling calculation, the random instanton gas does not give a good description of the correlation functions. It is clear that the main feature that is missing from the ensemble of classical paths is quantum fluctuations. Quantum fluctuations appear at next order in the semi-classical approximation. We can write the path as $x(\tau) = x_{cl}(\tau) + \delta x(\tau)$ where $x_{cl}(\tau)$ is the classical path and $\delta x(\tau)$ is the fluctuating part.

To develop the heating method we start from a classical path and determine the Gaussian effective potential for small fluctuations $\delta x(\tau)$. For a single instanton, the action is given by

$$S = \int d\tau \left(\frac{1}{4}\delta\dot{x}^2(\tau) + 4\eta^2\left[1 - \frac{3}{2\cosh^2\left(2\eta(\tau - \tau_I)\right)}\right]\delta x^2(\tau)\right). \tag{19}$$

We can now perform Monte Carlo calculations using the Gaussian action for a multi-instanton configuration. The result is shown in Fig.(9). Clearly, this path looks very similar to the full quantum path already discussed and the correlation functions are in much better agreement than the correlators obtained from the cooling method. However we do not recover their exact value, as one can see in Fig.(10). This fact is due to a combination of instanton interactions and large

non-Gaussian effects. In fact, to get a better result, one has to consider a more exact model, called *instanton liquid model*, which we'll not discuss.

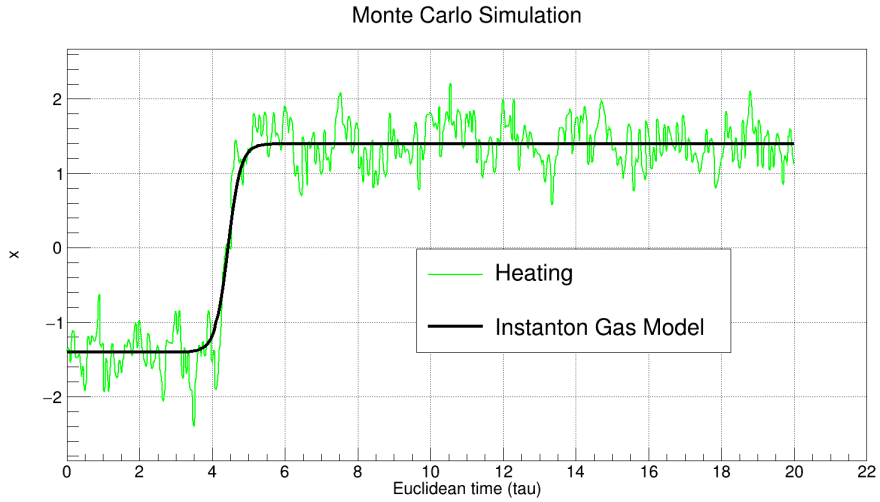

Figure 9: Typical random instanton configuration and the same configuration with Gaussian fluctuations. The noisy path was generated using 10 heating sweeps in the Gaussian potential around the classical path.

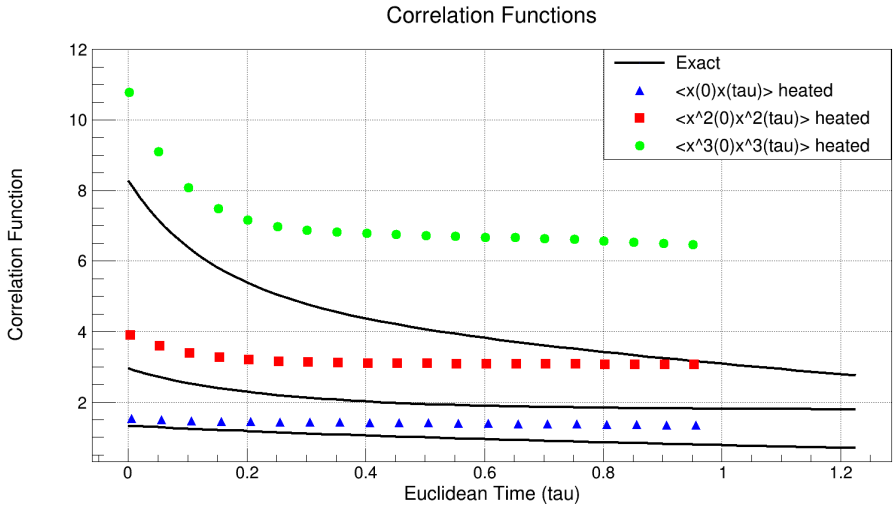

Figure 10: Correlation functions evaluated in a random instanton ensemble with Gaussian fluctuations. The number of heating sweeps is $n_{heat} = 10$.

5 Conclusion

In this work we presented Monte Carlo methods for studying the euclidean path integral in Quantum Mechanics. We should note that Monte Carlo calculations of the euclidean path integral are an extremely poor way to compute the spectrum or the correlation functions of the anharmonic oscillator. The code based on diagonalizing the Hamiltonian is both much faster and much more accurate than the Monte Carlo codes. However, if we proceed from quantum mechanics to sys-

tems involving many more degrees of freedom, such as four-dimensional field theories, Hamiltonian methods become more and more impractical and Monte Carlo calculations based on the euclidean path integral provide the most efficient method for computing the spectrum and the correlation functions known to date.

We also discussed Monte Carlo methods for studying the contribution of instantons to the euclidean path integral in the double well potential. In particular we used the cooling method in order to obtain the instanton content of the theory, i.e. tunneling rate.

Finally, for completeness, we presented the heating method to get the correlation functions, starting from a classical non-interacting instanton ensemble (instanton gas model) and perturbing with Gaussian fluctuations. However the results suggested that we should also consider non-Gaussian effects and interactions between instantons to obtain a better agreement (instanton liquid model).

References

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[4] R. Guardiola, *Monte Carlo Methods in Quantum Many Body Theory*, Springer, 2007.