Instantons and Monte Carlo Methods in Quantum Mechanics

Francesco Cominelli
Pietro Falzoni

Department of Physics and Astronomy
University of Bologna

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Project objectives

Monte Carlo simulations to understand the role of (tunneling events) in a quantum mechanical toy model:

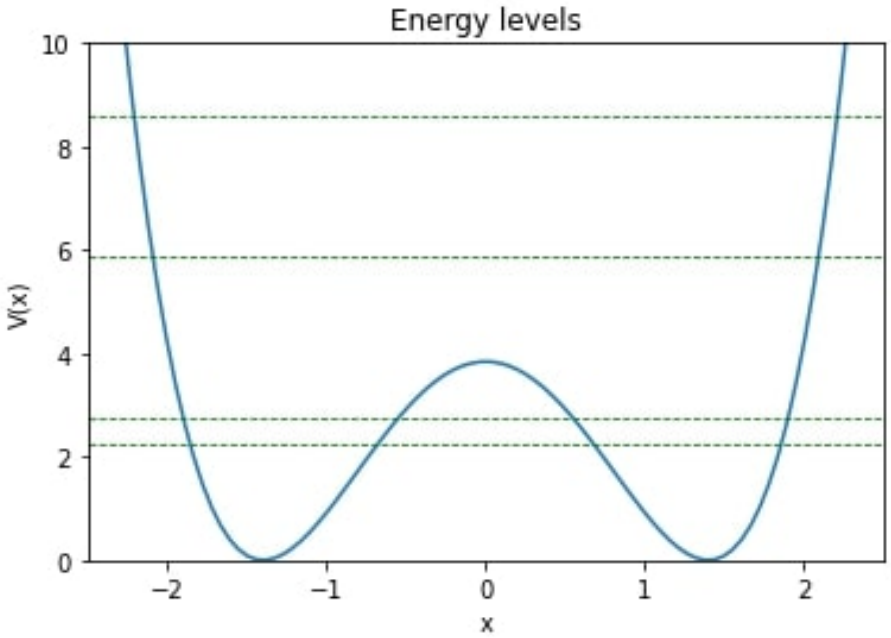
- Exact diagonalization of the Hamiltonian problem as reference for comparison
- Solution of the path integral formulation of the problem on a Euclidian lattice with Monte Carlo techniques
- Adiabatic switching technique to compute the free energy
- Extraction of instanton and anti-instanton content using cooling method
- Non-Gaussian corrections to the instanton density using adiabatic switching
- Analysis of a random instanton ensamble also with Gaussian fluctuations
- Solution of the path integral formulation on an interacting ensamble of instantons

Introduction

- Instanton $\longrightarrow$ Solution to the equations of motion (Euler-Lagrange) of the classical field theory on a Euclidean spacetime with a finite, non-zero action.

  $\hookrightarrow$ Used to calculate the transition probability for a quantum mechanical particle tunneling
- Double well potential $\longrightarrow$ two classical minima, one quantum ground state mixed.

$$H = \frac{p^2}{2m} + \lambda \left(x^2 - f^2\right)^2$$



Exact diagonalization

- Diagonalize the problem on harmonic oscillator basis to :

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2, \qquad H_0 |n\rangle = \omega_0 \left(n + \frac{1}{2}\right) |n\rangle$$

- The only non-zero matrix elements are:

$$\langle n| H |n\rangle = 3Ac^4 \left[(n+1)^2 + n^2\right] + Bc^2(2n+1) + \omega_0(n+1/2) + C$$
$$\langle n| H |n+2\rangle = Ac^4(4n+6)\sqrt{(n+1)(n+2)} + Bc^2\sqrt{(n+1)(n+2)}$$
$$\langle n| H |n+4\rangle = c^4\sqrt{(n+1)(n+2)(n+3)(n+4)}$$

with $A = 1, B = -2f^2 - \omega_0^2/4, C = f^4, c = 1/\sqrt{\omega_0}$.

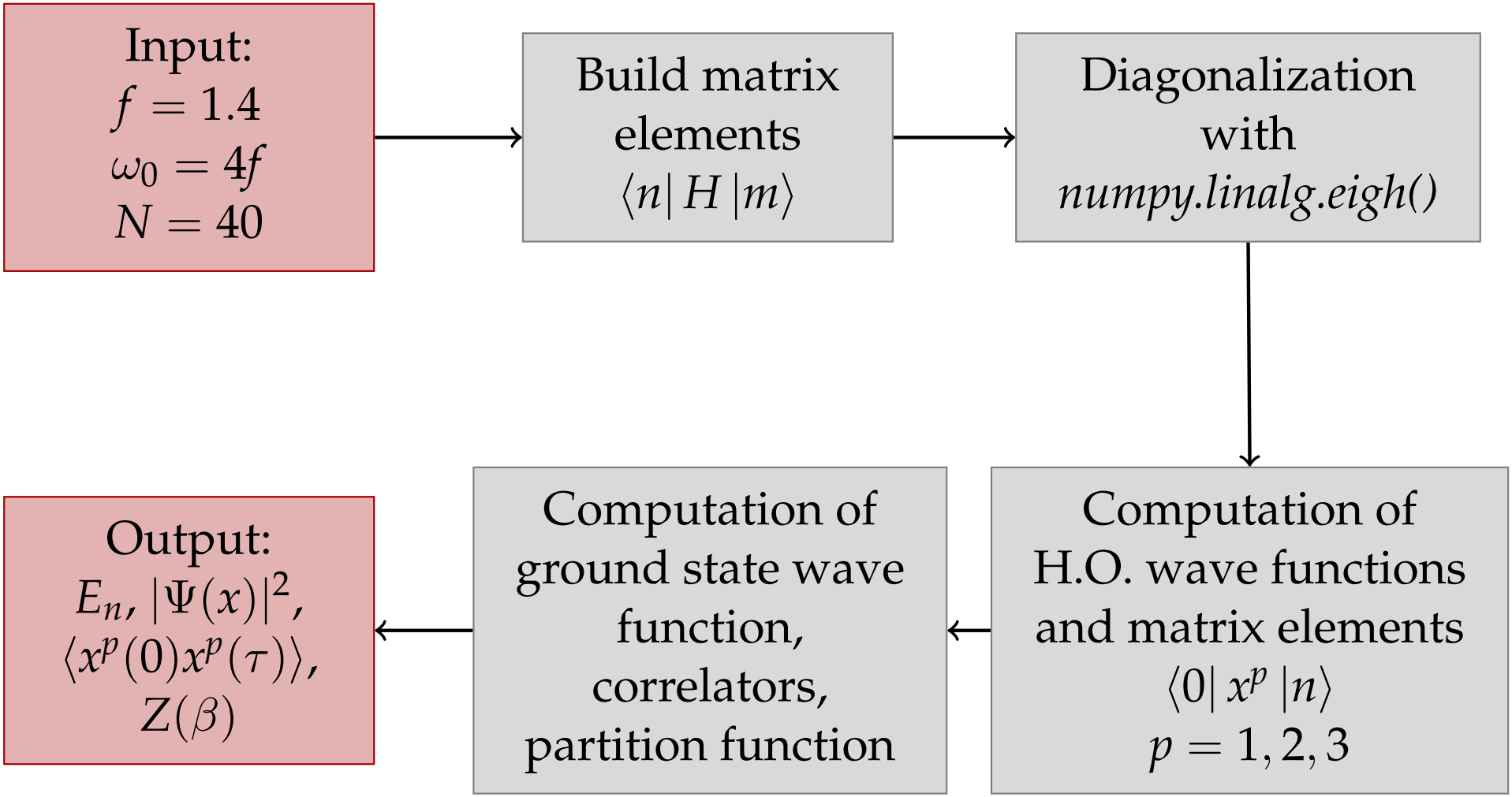
- H and H_0 conserve the parity, therefore we can write:

$$H = H_{even} + H_{odd}$$

  where the correspondent eigenvectors have positive (even) and negative (odd) parity.
- The program *qmdiag.py* computes:
  - Energy spectrum $\{E_n\}$
  - Ground state wave function $\psi(x)$
  - Partition function $Z(\beta) \quad \longrightarrow \quad Z(\beta) = \sum_n e^{(-\beta E_n)}$
  - Euclidean correlation functions $\langle x(0)x(\tau)\rangle$

$$\prod(\tau) = \langle O(0)O(\tau)\rangle, \qquad O(\tau) = x(\tau)^n,$$
$$\prod(\tau) = \sum_n |\langle 0|\, O(0)\, |n\rangle|^2 e^{-(E_n - E_0)\tau}$$

qmdiag.py


Input:
$f = 1.4$
$\omega_0 = 4f$
$N = 40$
Build matrix elements
$\langle n| H |m\rangle$
Diagonalization with
numpy.linalg.eigh()
Computation of H.O. wave functions and matrix elements
$\langle 0| x^p |n\rangle$
$p = 1, 2, 3$
Computation of ground state wave function, correlators, partition function
Output:
E_n, $|\Psi(x)|^2$,
$\langle x^p(0)x^p(\tau)\rangle$,
$Z(\beta)$

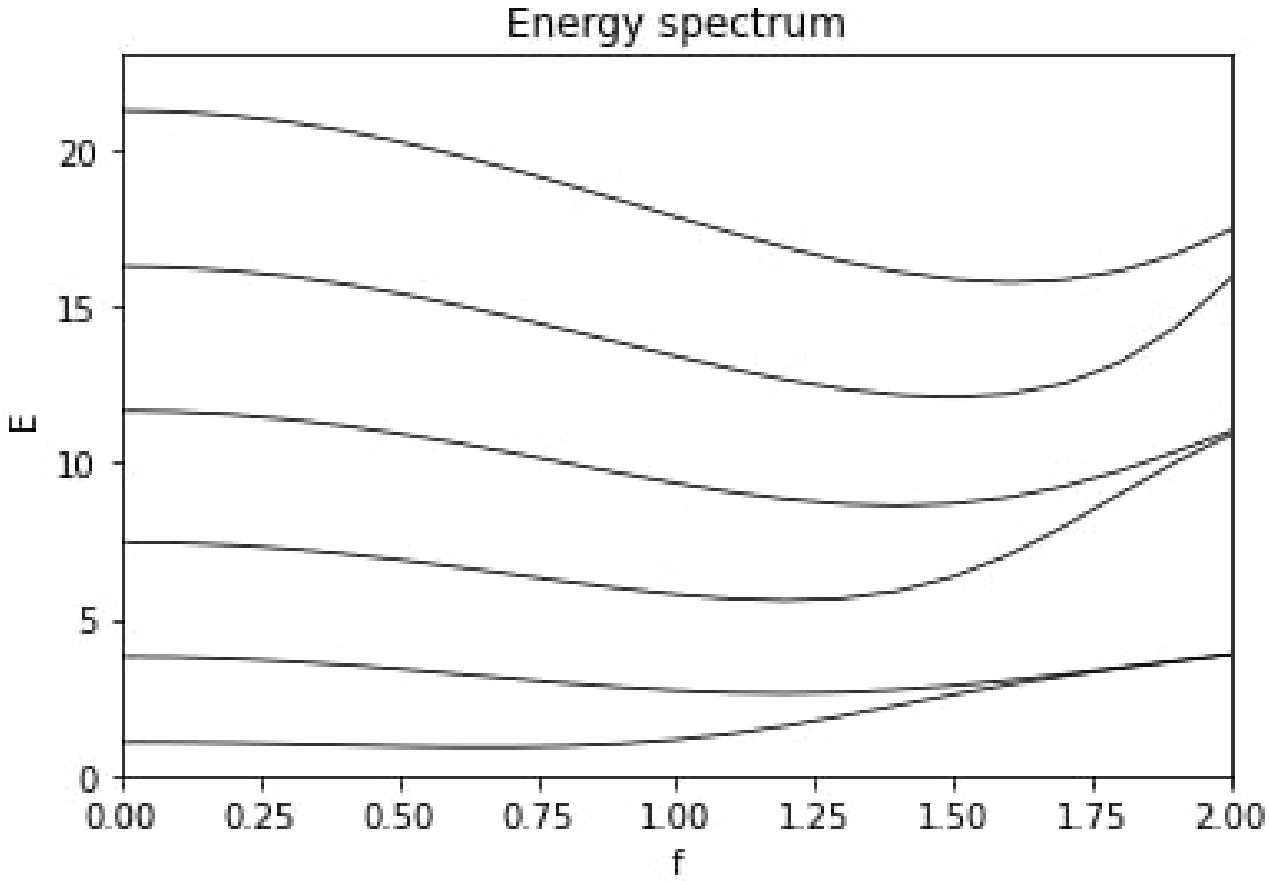


Figure 1: Spectrum of the double well potential as a function of the parameter f

Positive and negative parity states become degenerate when $f \to \infty$

Path Integral formulation

- Alternative formulation $\longrightarrow$ Path integral (Wick rotated: $it \to \tau$)

$$S_E = \int_0^\beta d\tau \left[\frac{1}{4}\dot{x}^4 + \left(x^2 - f^2\right)^2\right] \quad \Rightarrow \quad Z(T) = \int_{PBC} \mathcal{D}x \quad e^{-S_E}$$

- To study numerical simulations we need a discretized euclidean action: $\tau_i = ai,\ i = 1, \ldots n.$

$$S = \sum_{i=1}^{n} \left[\frac{1}{4a}(x_i - x_{i-1})^2 + a(x_i^2 - f^2)^2\right]$$

  hence the P.I. is equivalent to a statistical system of "spin" x_i arranged on a one-dimensional lattice.
- Monte Carlo sampling method Metropolis: configurations generated with trial updates with an acceptance probability.

$$x_i^{(k+1)} = x_i^{(k)} + \delta x \qquad P(x_i^{(k)} \to x_i^{(k+1)}) = min\{exp(-\Delta S), 1\}$$

- Avereges computed averaging observables over many configurations

$$\langle \mathcal{O} \rangle = \lim_{N_{conf} \to \infty} \frac{1}{N_{conf}} \sum_{k=1}^{N_{conf}} \mathcal{O}^{(k)}$$

- Fluctuation of $\mathcal{O}$ gives an estimate of the error on $\langle \mathcal{O} \rangle$

$$\Delta \langle \mathcal{O} \rangle = \sqrt{\frac{\langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2}{N_{conf}}}$$

- The program *qm.py* computes:
  - Normalized distribution of x
  - Average total action per configuration
  - Euclidean correlation functions for x, x^2, x^3

Time Scales

For a typical path that appears in Monte Carlo simulations there are two time scales:

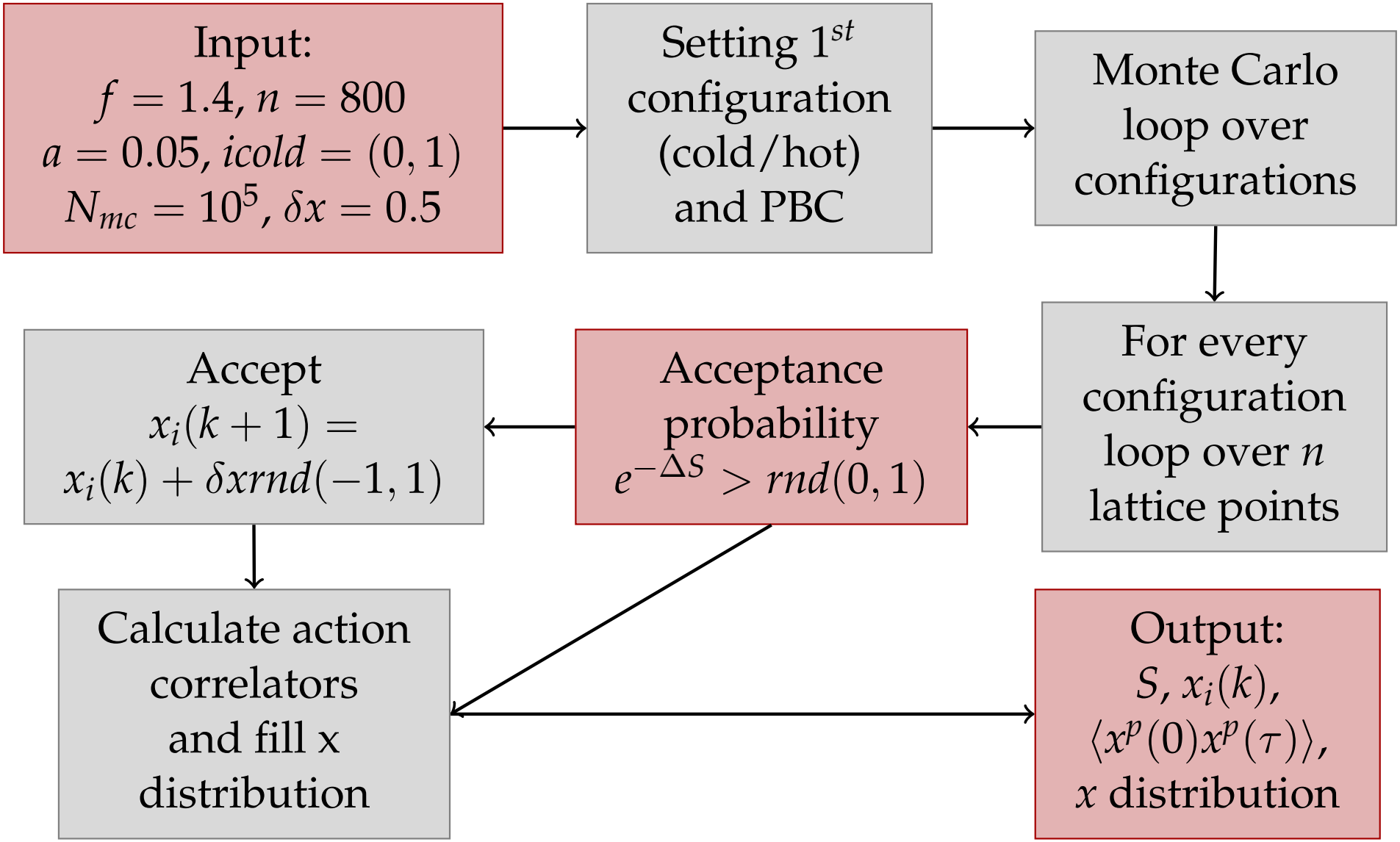
- **oscillation time**: $\tau_{osc} \sim \omega^{-1} \sim (4f)^{-1}$
- **tunnelling time**: $\tau_{tun} \sim e^{4f^3/3}$

In order to run consistent simulation we must satisfy:

$$a << \tau_{osc} \qquad \tau_{tun} << na$$

Then a typical choice for $f = 1.4$ is $nmc \sim 10^5$, $n = 800$ and $a = 0.05$.

qm.py


Input:
$f = 1.4, n = 800$
$a = 0.05, icold = (0,1)$
$N_{mc} = 10^5, \delta x = 0.5$
Setting 1^{st} configuration (cold/hot) and PBC
Monte Carlo loop over configurations
For every configuration loop over n lattice points
Acceptance probability
$e^{-\Delta S} > rnd(0,1)$
Accept
$x_i(k+1) = x_i(k) + \delta x rnd(-1,1)$
Calculate action correlators and fill x distribution
Output:
$S, x_i(k),$
$\langle x^p(0)x^p(\tau)\rangle,$
x distribution

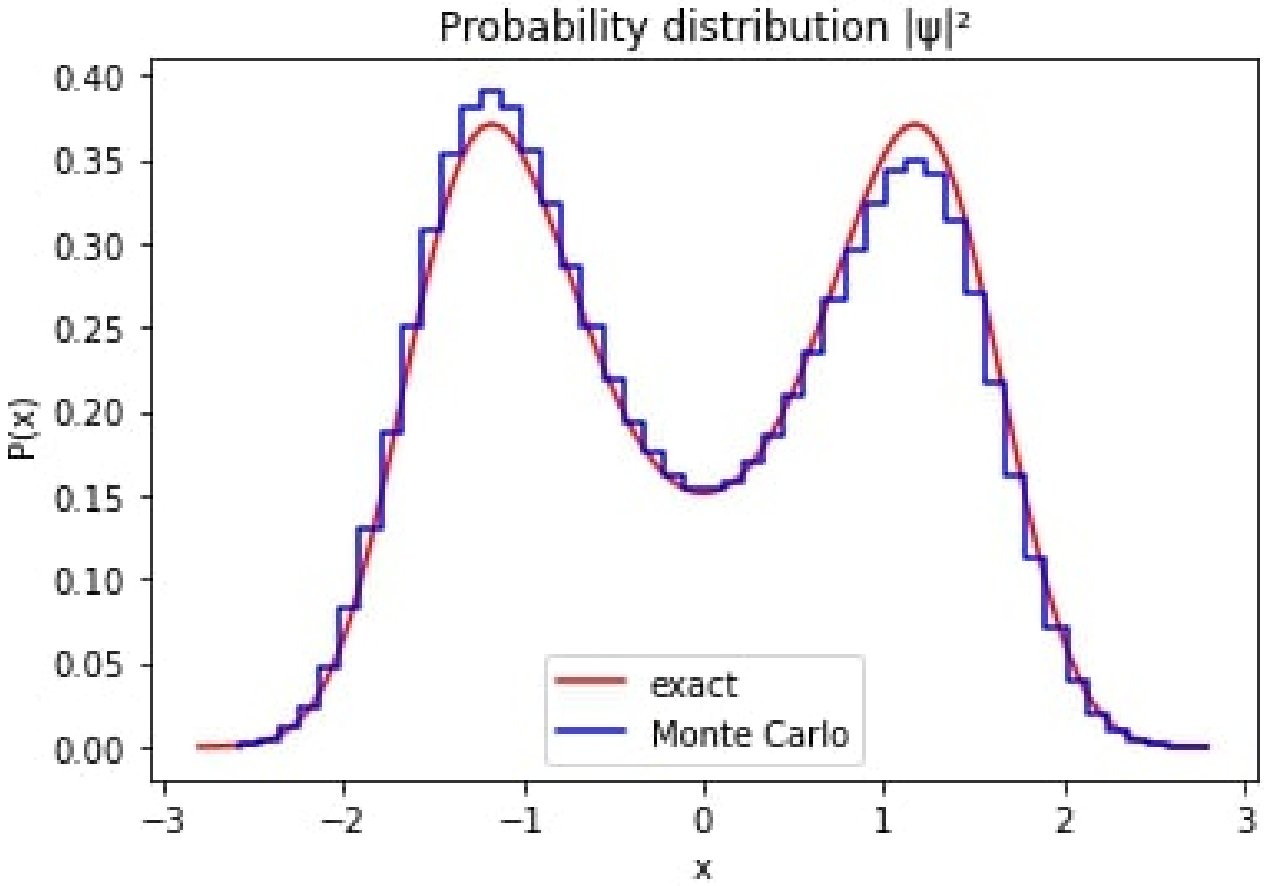


Figure 2: Probability distribution $|\psi(x)|^2$ in the double well potential for $f = 1.4$.solid line shows the "exact" numerical result whereas the histogram shows the distribution of x for an ensemble of euclidean paths.

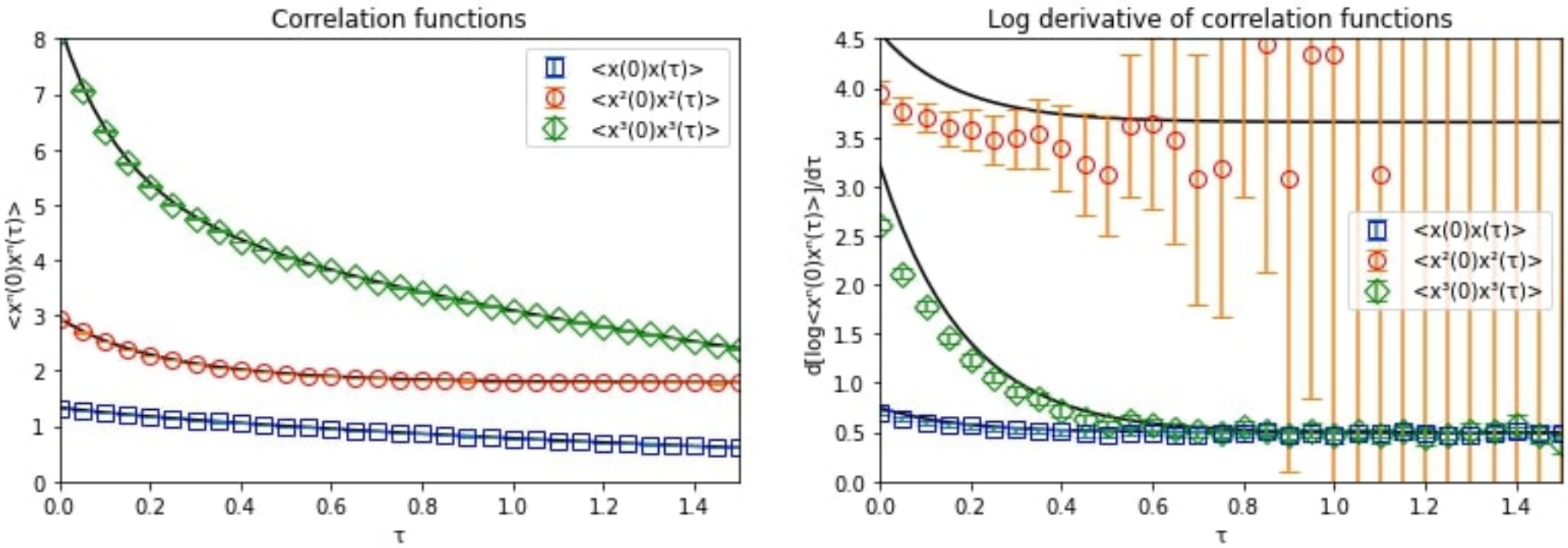


Figure 3: Correlation functions and logarithmic derivative correlation functions in the double well potential with $f = 1.4$. From Monte Carlo simulations with $a = 0.05$, $n = 800$.

- For even powers of x the correlator has a constant term $|\langle 0|\, x^{2n}\, |0\rangle|^2$.

Adiabatic switching

Monte Carlo method:

- advantages → expectation values calculations, in quantum or statistical mechanics
- disadvantages → does not give directly the partition function or the free energy, which have to be calculated from the energy eigenvalue (need to compute the full spectrum) ⇒ **Adiabatic switching technique**

Adiabatic switching: start from a known system and go to an unknown configuration by the use of Monte Carlo techniques, making a parameter vary. Let us write the action as:

$$S_\alpha = S_0 + \alpha \Delta S$$

where: $\Delta S = S - S_0$ and α is the coupling constant.

S_α interpolates between the real, and the reference system action.

$$Z(\alpha) = \int \mathcal{D}x e^{-S_\alpha} \quad \Rightarrow \quad \frac{\partial ln\left[Z(\alpha)\right]}{\partial \alpha} = -\left\langle \Delta S \right\rangle_\alpha$$

$$\Rightarrow \quad ln\left[Z(\alpha)\right] = ln\left[Z(0)\right] - \int_0^1 d\alpha' \left\langle \Delta S \right\rangle_{\alpha'}$$

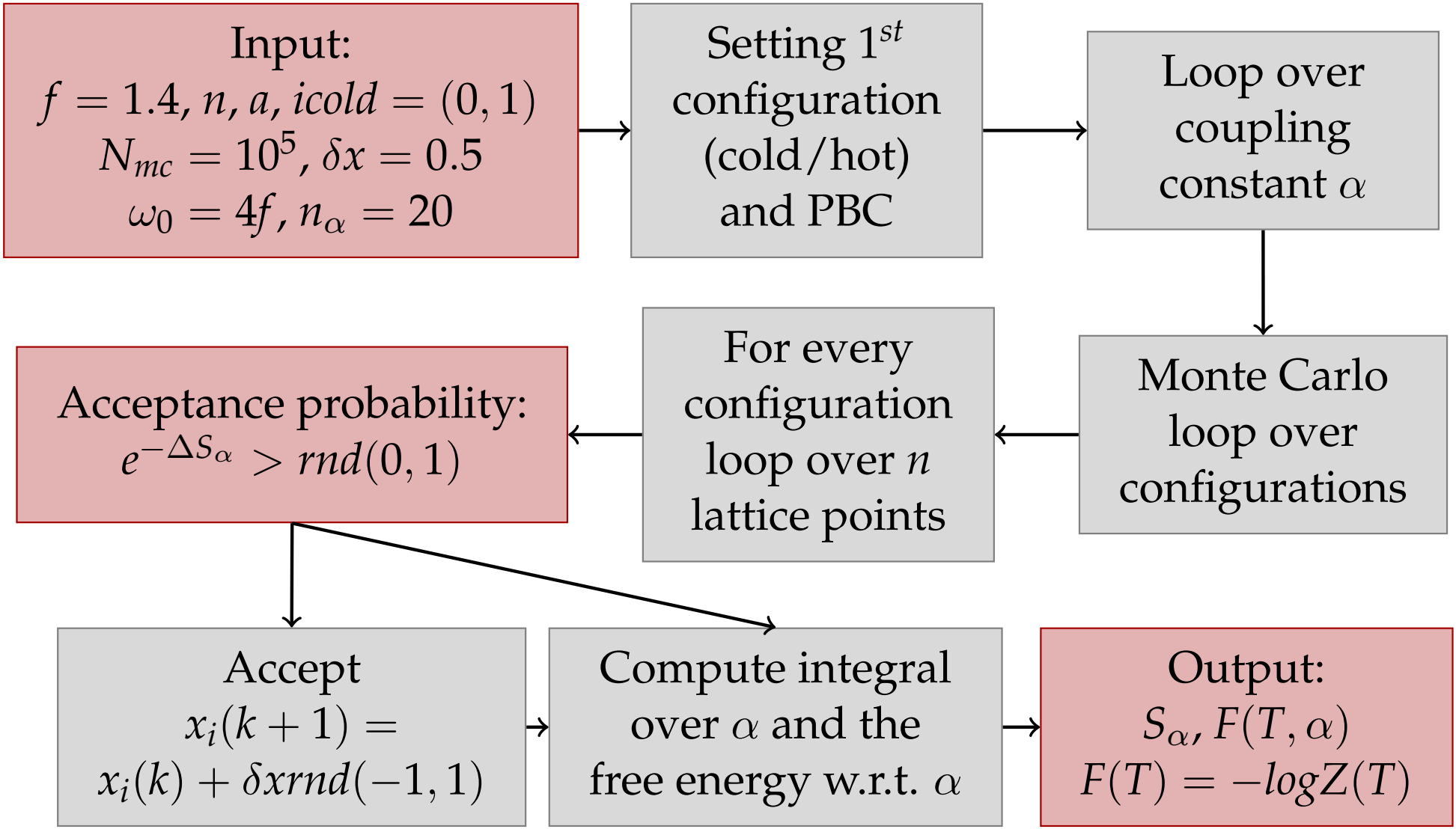
In our case:

$$Z(0) = \sum_n e^{-\beta E_n^0} = \frac{e^{-\beta\omega_0/2}}{1 - e^{-\beta\omega_0/2}}$$

The free energy of the anharmonic oscillator should be independent on ω_0.
The program *qmswitch.py* computes:

- the free energy $F = -TlogZ$.

qmswitch.py


Input:
$f = 1.4, n, a, icold = (0, 1)$
$N_{mc} = 10^5, \delta x = 0.5$
$\omega_0 = 4f, n_\alpha = 20$
Setting 1^{st} configuration (cold/hot) and PBC
Loop over coupling constant α
Monte Carlo loop over configurations
For every configuration loop over n lattice points
Acceptance probability:
$e^{-\Delta S_\alpha} > rnd(0, 1)$
Accept
$x_i(k+1) = x_i(k) + \delta x rnd(-1, 1)$
Compute integral over α and the free energy w.r.t. α
Output:
$S_\alpha, F(T, \alpha)$
$F(T) = -logZ(T)$

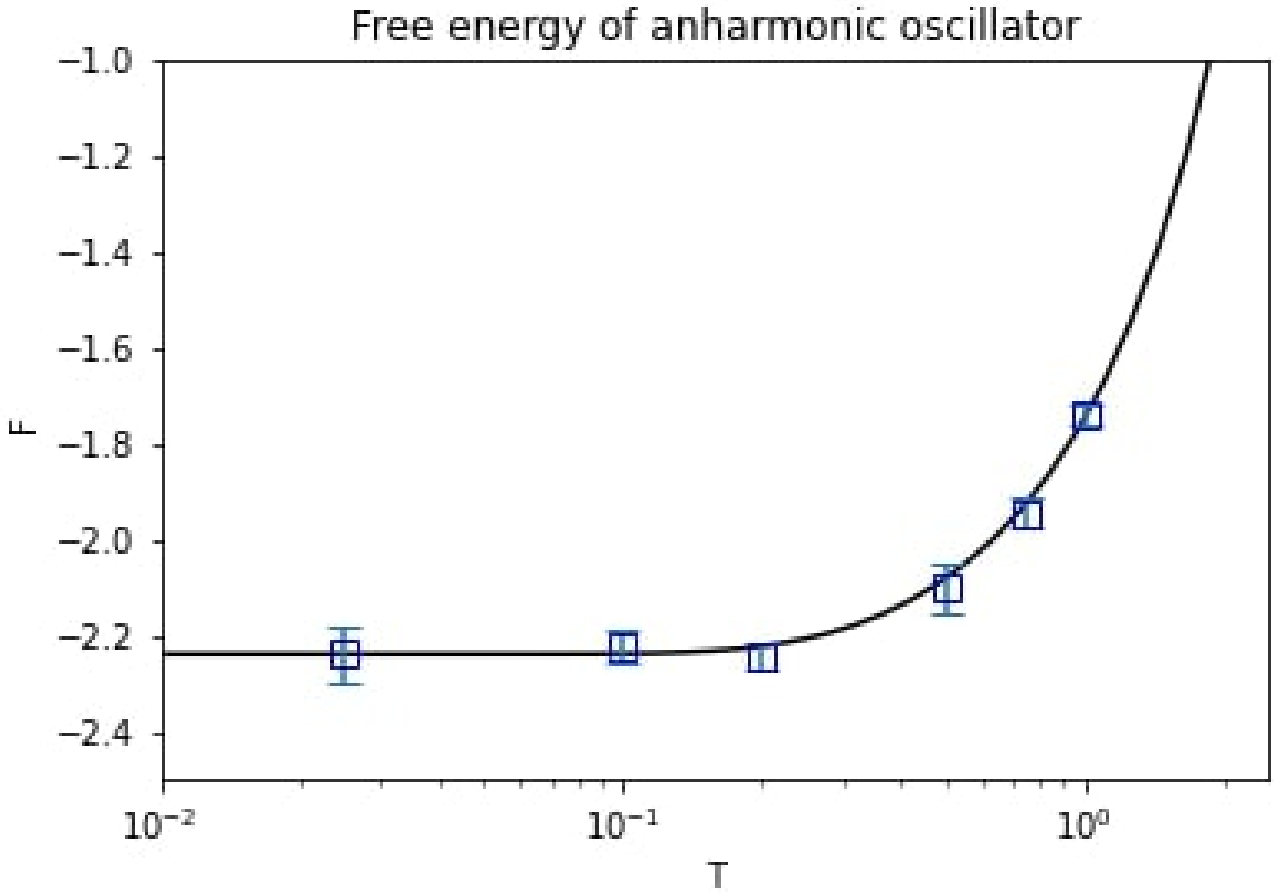


Figure 4: Free energy of the anharmonic oscillator as a function of the temperature T. The solid line is calculated using the spectrum of the Hamiltonian.

$$F = Tln(Z), \qquad T = 1/\beta, \qquad \beta = na$$

Instantons

Instanton solution can be found from the classical equation of motion:

$$\frac{\delta S_E}{\delta x(\tau)} = 0 \quad \Rightarrow \quad m\ddot{x} = V'(x) \quad \Rightarrow \quad x_I(\tau) = -x_A(\tau) = f \times tgh\left[\frac{\omega}{2}(\tau - \tau_0)\right]$$

where: $\omega = 4f$, τ_0 is the location of the instanton, and satisfies the boundary conditions: $x(\tau \to \pm\infty) = \pm f$. The tunnelling rate is:

$$n_{I+A} = \frac{N_{I+A}}{\beta} \sim e^{-S_0} \text{ , where: } S_0 = \frac{4f^3}{3}$$

Let us work in the semi-classical expansion (considering small fluctuations around the instanton solution), then:

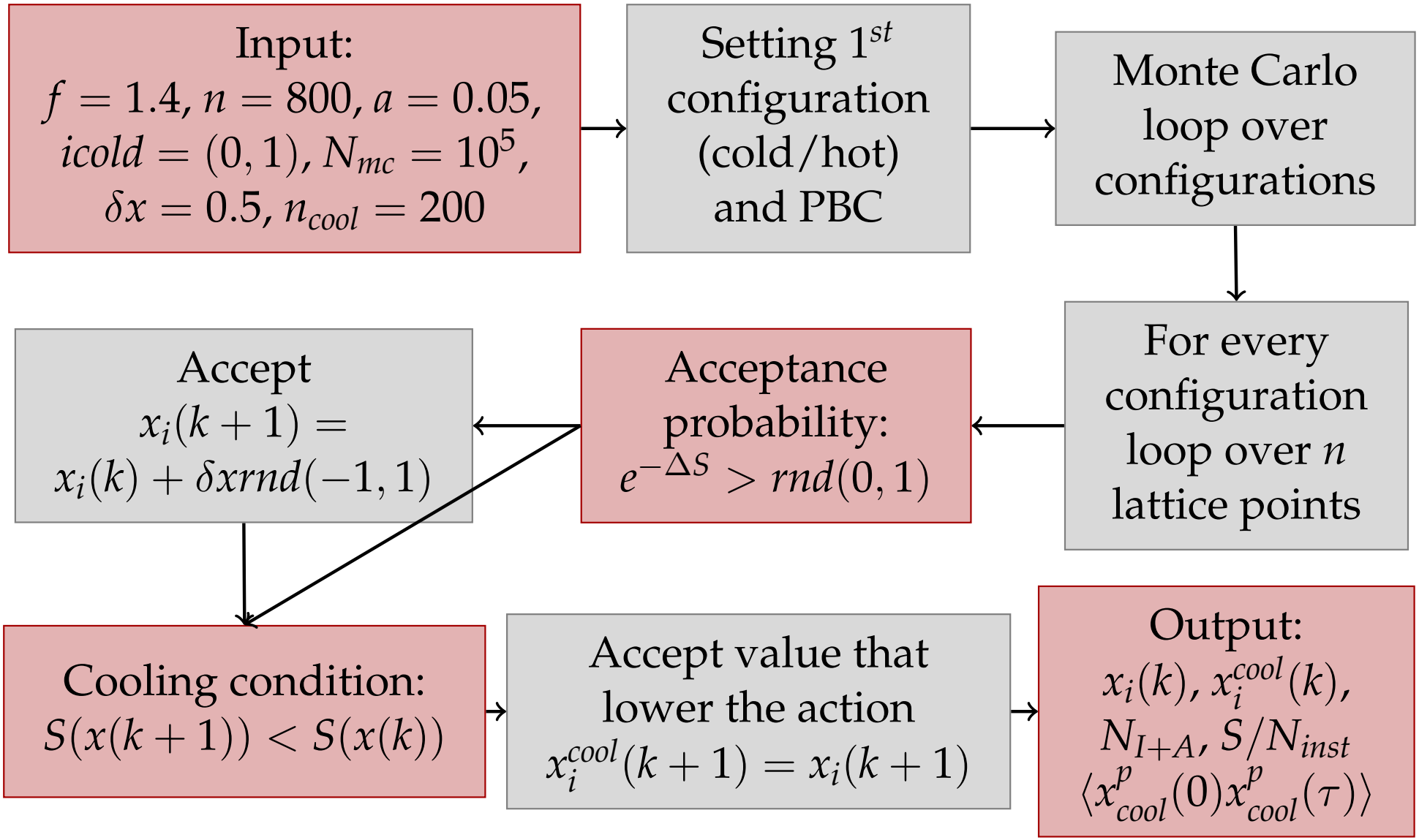
$$n_{I+A} = 8f^{5/2}\sqrt{\frac{2}{\pi}}e^{-S_0 - \frac{71}{72}\frac{1}{S_0}}$$

- The tunneling events can be studied in more detail after removing short distance fluctuations.
  $\Rightarrow$ Cooling method: only accept Metropolis update that lower the action.
- This drives the system towards the nearest classical solution and allows to study the instanton content of a quantum configuration.
- We can extract the instanton and anti-instanton locations from the zero crossings in the Euclidean-path.
- We can consider the cooled configurations as a superposition of tunnelling events:

$$x_{sum} = f\left\{\sum_i Q_i tgh\left[\frac{\omega}{2}(\tau - \tau_i)\right]\right\} \qquad Q_i = \pm 1$$

- We lose agreement with the exact value of the correlation functions, since we are removing fluctuations which play an important role.

qmcool.py


Input:
$f = 1.4, n = 800, a = 0.05,$
$icold = (0,1), N_{mc} = 10^5,$
$\delta x = 0.5, n_{cool} = 200$
Setting 1^{st} configuration (cold/hot) and PBC
Monte Carlo loop over configurations
For every configuration loop over n lattice points
Acceptance probability:
$e^{-\Delta S} > rnd(0,1)$
Accept
$x_i(k+1) = x_i(k) + \delta x rnd(-1,1)$
Cooling condition:
$S(x(k+1)) < S(x(k))$
Accept value that lower the action
$x_i^{cool}(k+1) = x_i(k+1)$
Output:
$x_i(k), x_i^{cool}(k),$
$N_{I+A}, S/N_{inst}$
$\langle x^p_{cool}(0) x^p_{cool}(\tau)\rangle$

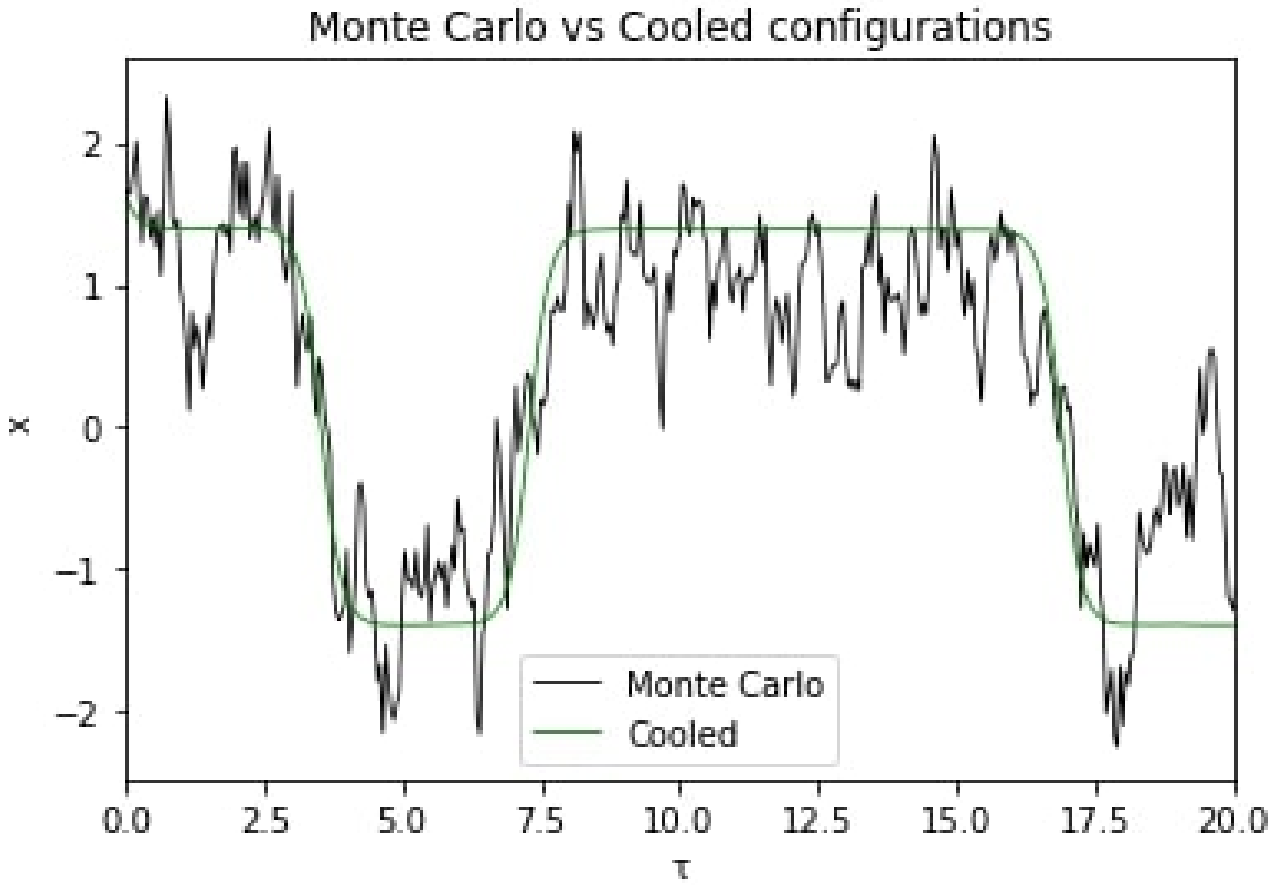


Figure 5: Typical euclidean path obtained in a Monte Carlo simulation of the discretized euclidean action of the double well potential for $f = 1.4$. The lattice spacing in the euclidean time direction is $a = 0.05$ and the total number of lattice points is $n = 800$. The green curve shows the corresponding smooth path obtained by running 100 cooling sweeps on the original path

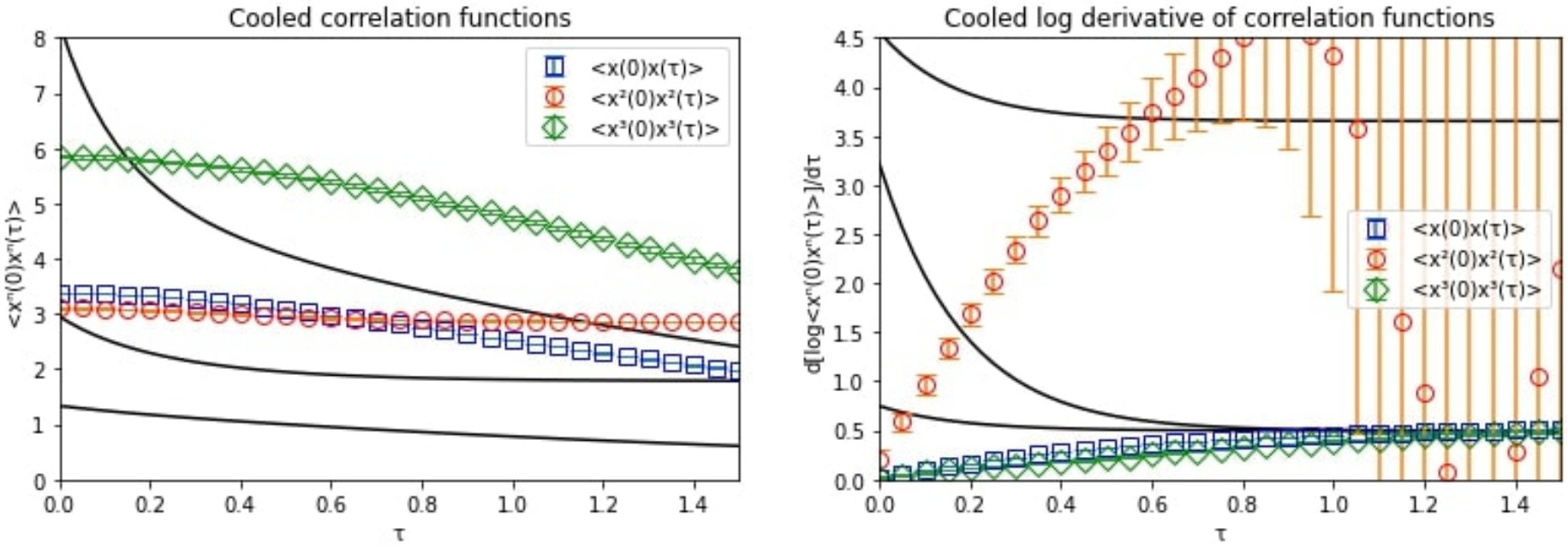


Figure 6: Cooled correlation functions and logarithmic derivative correlation functions, for 200 cooling sweeps (ncool).

- Short distance fluctuations are eliminated by cooling.
- When τ increases the solution become the classical one.

Instanton density

- The net topological charge is well defined as the number of instantons minus the number of anti-instantons.
- Cooling method might be used to estimate the total density of instantons and anti istantons:
  $\rightarrow$ we cannot distinguish between a large quantum fluctuation and a very close instanton, anti-instanton pair $\rightarrow$ dependence on n_{cool}.
- Instanton density well defined in the semi-classical limit
  $\rightarrow$ exponentially large separation of scales between τ_{tun} and τ_{osc}.

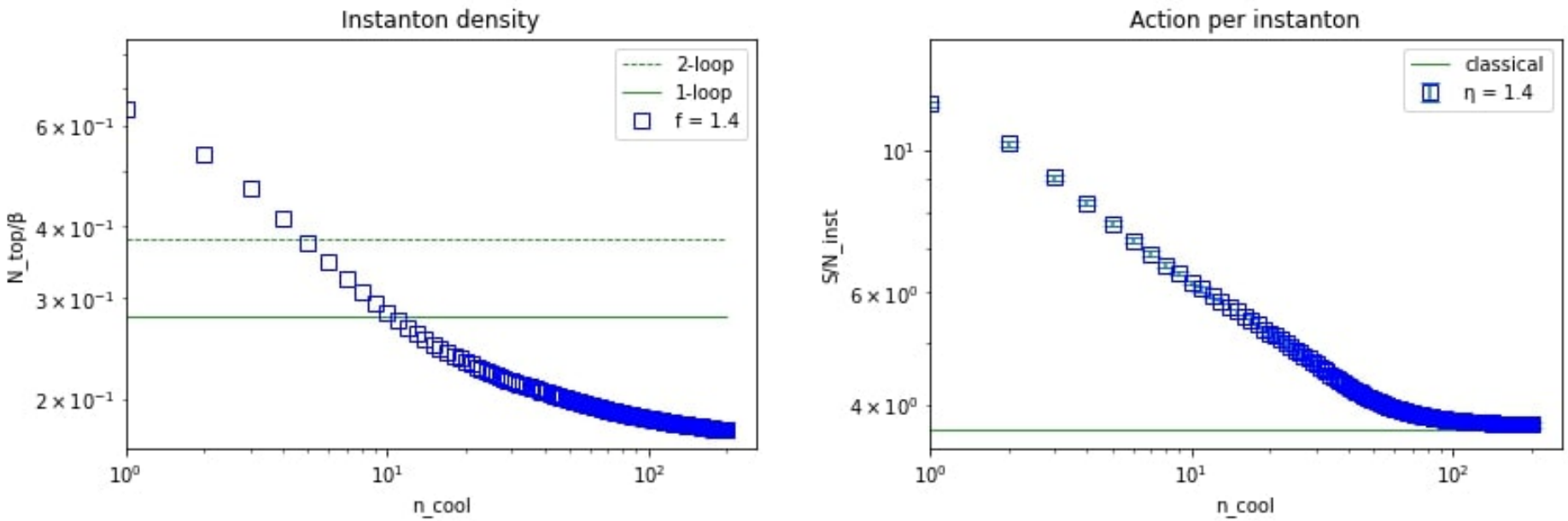


Figure 7: Instanton density and instanton action as a function of the number of cooling sweeps for $f = 1.4$.

Expected number of instantons:

$$N_I(n_{cool}) = N_{osc} e^{-n_{cool} a/\tau_{osc}} + N_{tun} e^{-n_{cool} a/\tau_{tun}}$$

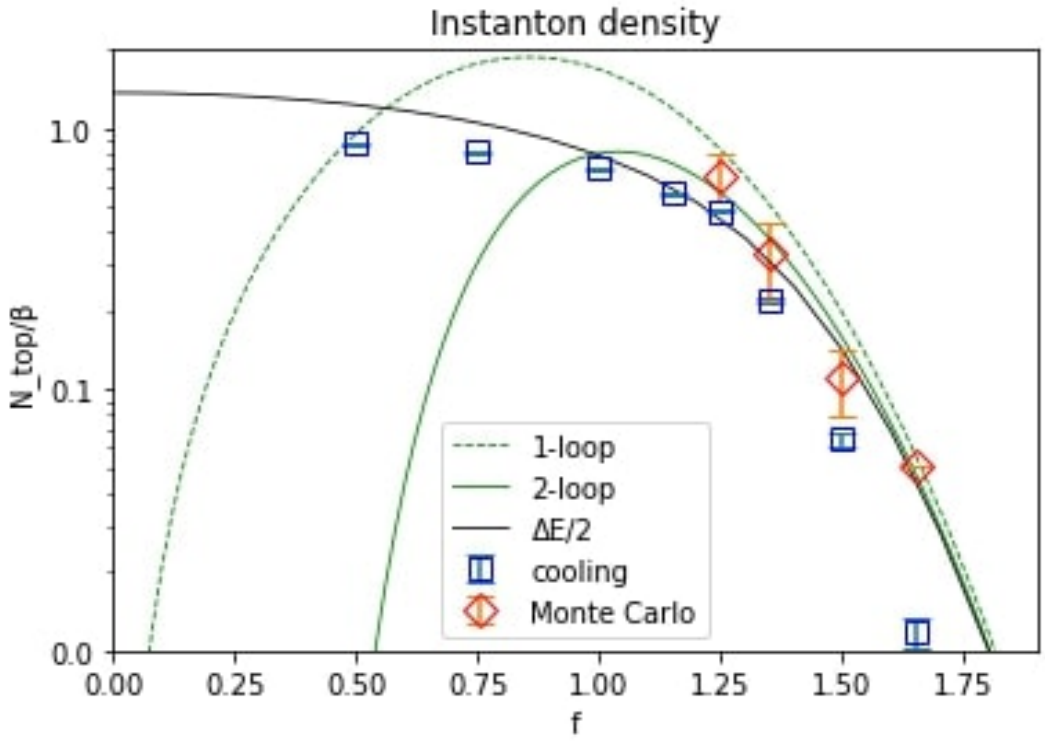


Figure 8: Instanton density as a function of f ($S_0 > 3$ for MC simulations)

- the one-loop result is given by: $n_{I+A} = 8f^{5/2}\sqrt{\frac{2}{\pi}}e^{-S_0}$
- the 2-loop result is given by: $n_{I+A} = 8f^{5/2}\sqrt{\frac{2}{\pi}}e^{-S_0-\frac{71}{72}\frac{1}{S_0}}$
- $\Delta E/2$ was computed by `qmdiag.py` considering the difference in energy between the ground and the first excited state.

qmidens.py

- The 1-loop calculation is based on solving the quadratic expansion: $S = S_0 + \frac{1}{2}\int d\tau \delta x(\tau) \frac{\delta^2 S}{\delta x^2}\big|_{x_I(\tau)} \delta x(\tau) + ...$
- We can introduce again S_α:
  $\rightarrow$ it interpolates between the full action and the Gaussian approximation $S_\alpha = S_{gauss} + \alpha \Delta S$, with $\Delta S = S - S_{gauss}$.
- Quantum weight of an instanton can be obtained integrating over α:

$$n = n_{gauss} exp\Big[- \int_0^1 d\alpha \big(\langle \Delta S \rangle_\alpha^{(1)} - \langle \Delta S \rangle_\alpha^{(0)} \big) \Big]$$

  where $\langle . \rangle_\alpha^{(n)}$ is an expectation value in the n-instanton sector at coupling α.
- The program *qmidens.py* computes:
  - Zero-instanton sector configurations
  - One-instanton sector configurations
  - Details of the adiabatic switching procedure.

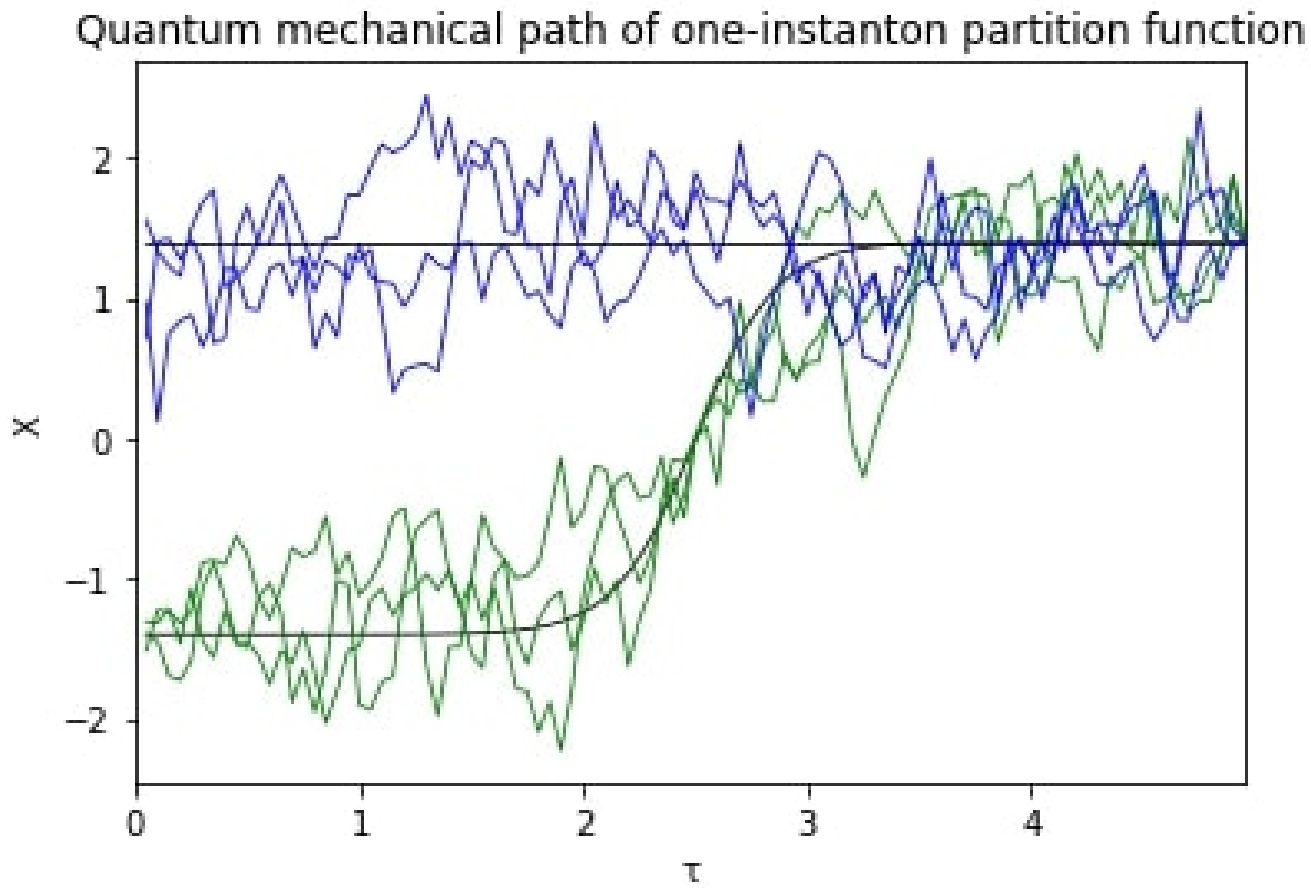
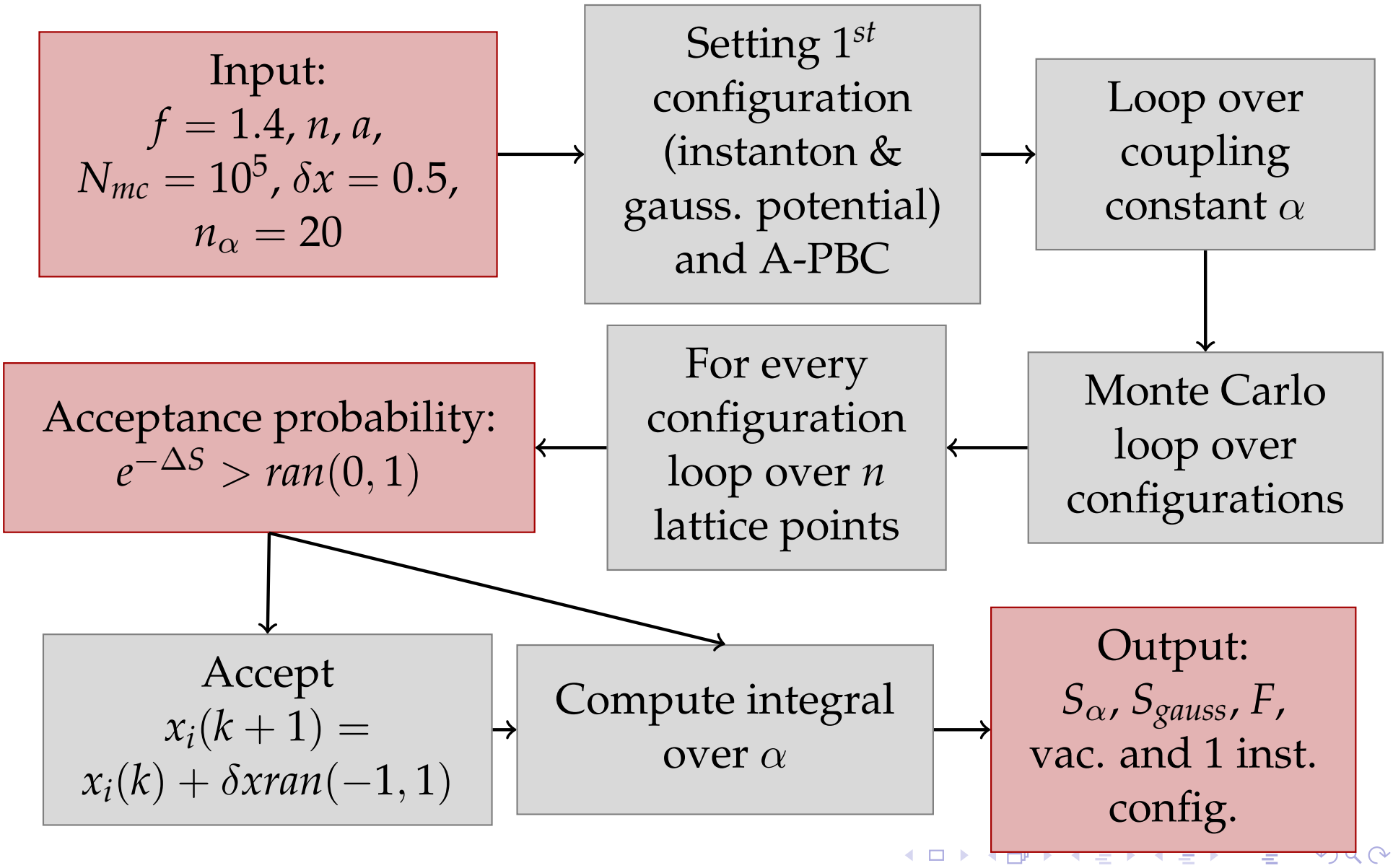
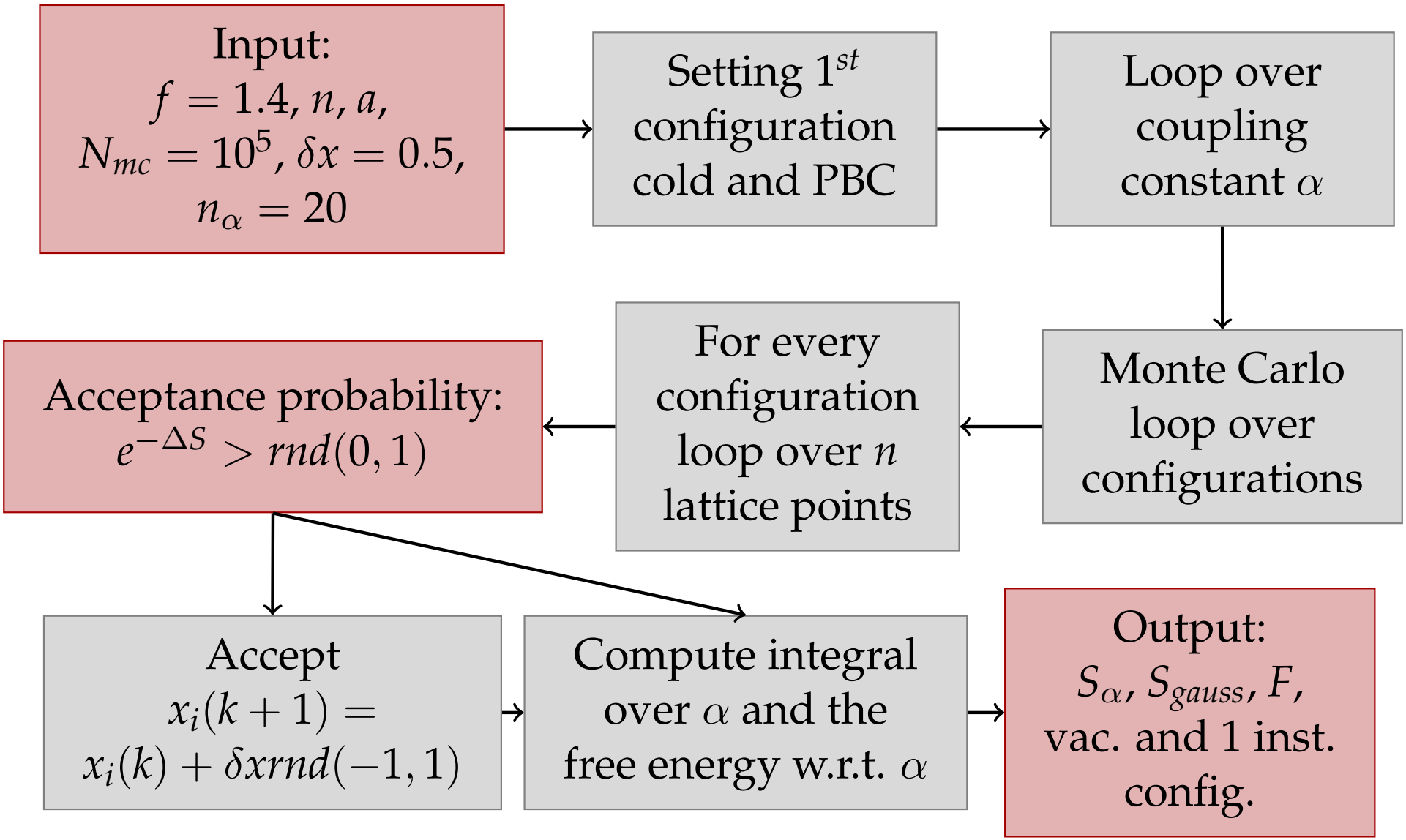


Figure 9: Quantum mechanical paths in Monte-Carlo calculation of the one-instanton partition function. The calculation involves adiabatic switching between the Gaussian effective potential and the full potential. The smooth curves are the initial configurations. The Monte Carlo updates in the one-instanton sector involve a constraint which keeps the instanton location fixed.

qmidens.py (I)


Input:
$f = 1.4, n, a,$
$N_{mc} = 10^5, \delta x = 0.5,$
$n_\alpha = 20$
Setting 1^{st} configuration (instanton & gauss. potential) and A-PBC
Loop over coupling constant α
Monte Carlo loop over configurations
For every configuration loop over n lattice points
Acceptance probability:
$e^{-\Delta S} > ran(0,1)$
Accept
$x_i(k+1) = x_i(k) + \delta x ran(-1,1)$
Compute integral over α
Output:
$S_\alpha, S_{gauss}, F,$
vac. and 1 inst. config.

qmidens.py (II)



Random instanton model

Let's study correlation function in semi-classical approximation.

- Begin with the classical path contribution

$$Z = \sum_{n_I, n_A} \frac{\delta_{n_I, n_A}}{n_I! n_A!} \left(\prod_i \int d\tau_i \right) e^{-S}.$$

- Coordinate correlation function given by

$$\prod_{cl}(\tau) = \langle x_{cl}(0) x_{cl}(\tau) \rangle$$

  $\langle . \rangle \rightarrow$ average over collective coordinates τ_i.
- Ignoring interactions $\rightarrow$ **Instanton Gas Model** (**Random Instanton Approximation**):
  - $S = (n_I + n_A) S_0$
  - Random distribution of collective coordinates

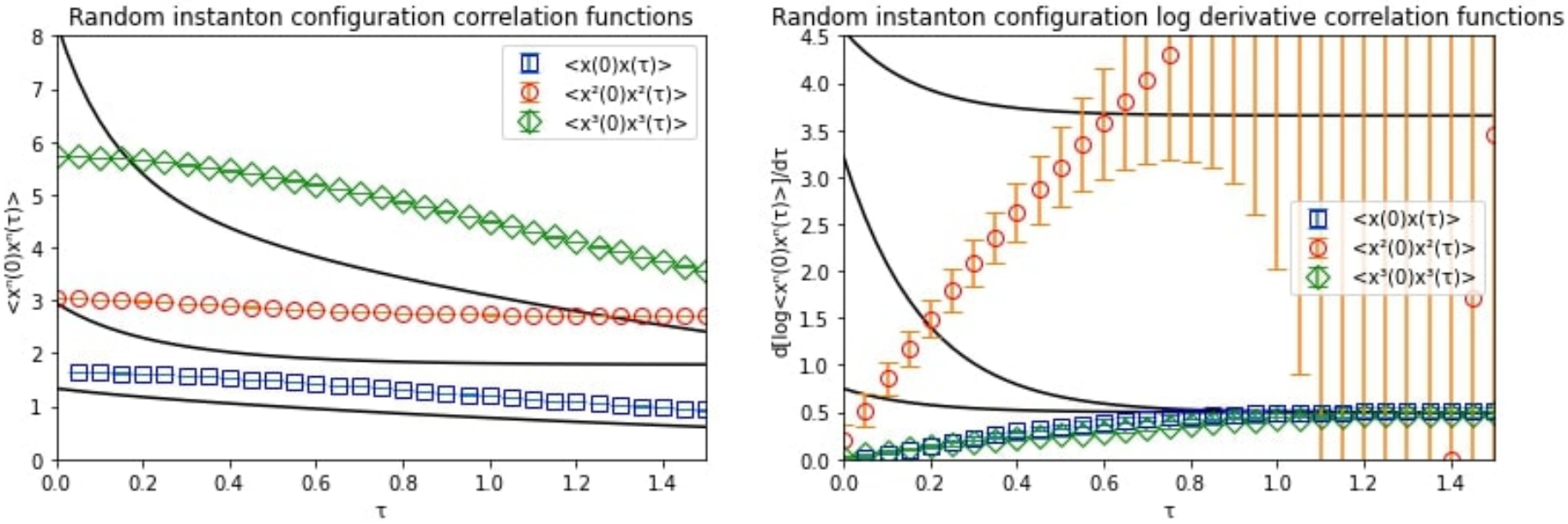
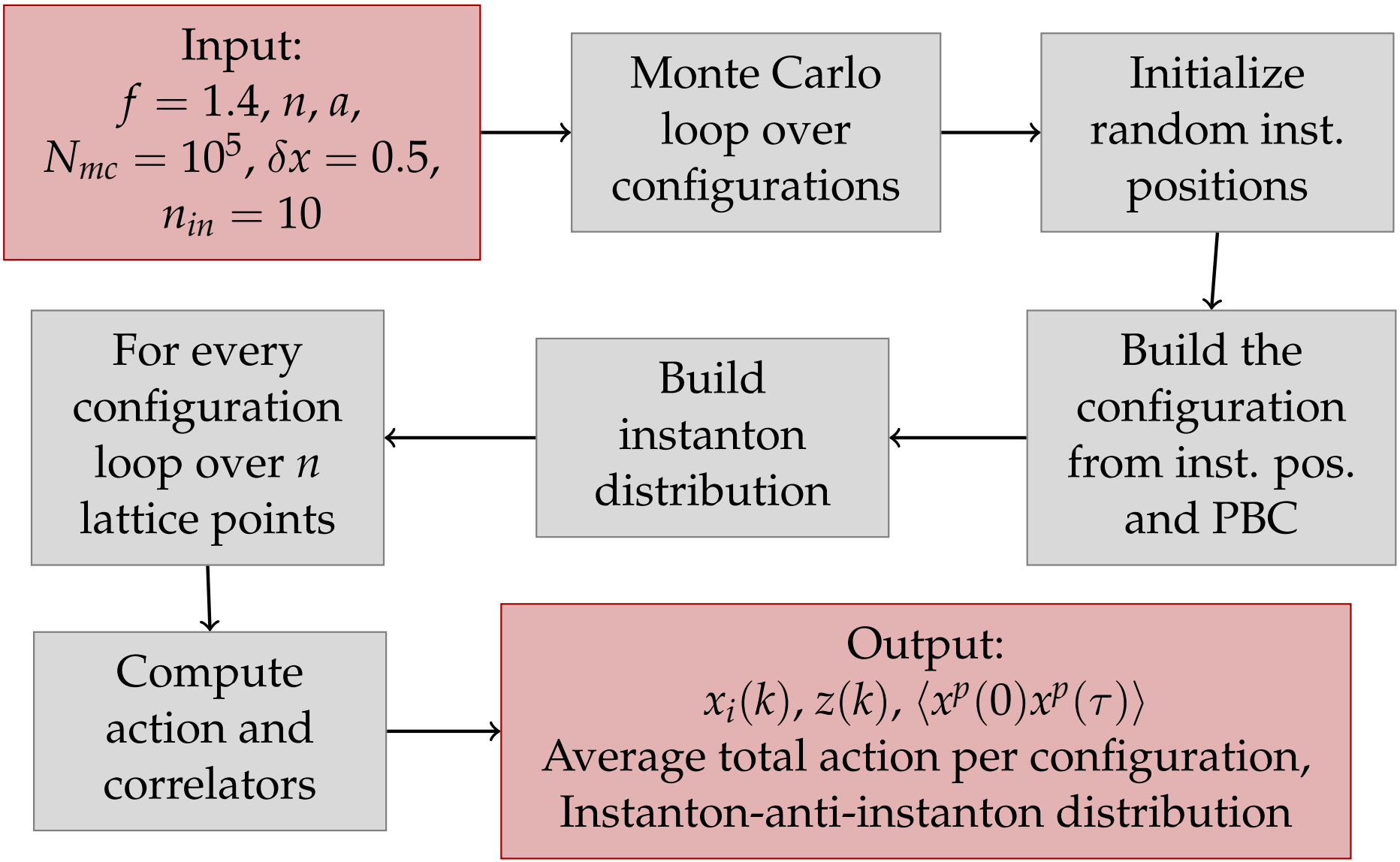


Figure 10: Correlation functions and logarithmic derivative correlation functions evaluated from a random instanton configuration.

- Correlation functions in the random instanton model are very similar to the cooled correlation functions.
- Splitting between ground state and first excited state is good, but not for other aspects.

rilm.py


Input:
$f = 1.4, n, a,$
$N_{mc} = 10^5, \delta x = 0.5,$
$n_{in} = 10$
Monte Carlo loop over configurations
Initialize random inst. positions
Build the configuration from inst. pos. and PBC
Build instanton distribution
For every configuration loop over n lattice points
Compute action and correlators
Output:
$x_i(k), z(k), \langle x^p(0)x^p(\tau)\rangle$
Average total action per configuration,
Instanton-anti-instanton distribution

Quantum Fluctuation

- Quantum fluctuations determine the pre-exponential factor in the tunneling rate

$$n_{I+A} = 8f^{5/2}\sqrt{\frac{2}{\pi}}e^{-S_0-\frac{71}{72}\frac{1}{S_0}}$$

- Path can be written as:

$$x(\tau) = x_{cl}(\tau)+\delta x(\tau) \quad \rightarrow \quad S = S_0+\frac{1}{2}\int d\tau \delta x(\tau)\frac{\delta^2 S}{\delta x^2}\Big|_{x_I(\tau)}\delta x(\tau)+\dots$$

- Correlation function can be computed analytically for a single instanton, but in the case of an ensemble we will do it numerically, using the "heating" method.
- Starting from a classical path determine the Gaussian effective potential for small fluctuations around the path.

- For a single instanton:

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

- One zero mode:

$$\delta x(\tau) = -S_0^{-\frac{1}{2}} \frac{dx_{cl}(\tau - \tau_I)}{d\tau_I} \text{ (translation of the instanton solution)}$$

- the corresponding non-Gaussian fluctuations can be eliminated imposing a constraint on the location of the instanton, by the use of the identity: $1 = \int \delta(x(\tau_I))|\dot{x}(\tau_I)|$
- Heated random instanton path lacks large excursions from the minima of the potential that do not lead to a tunnelling event

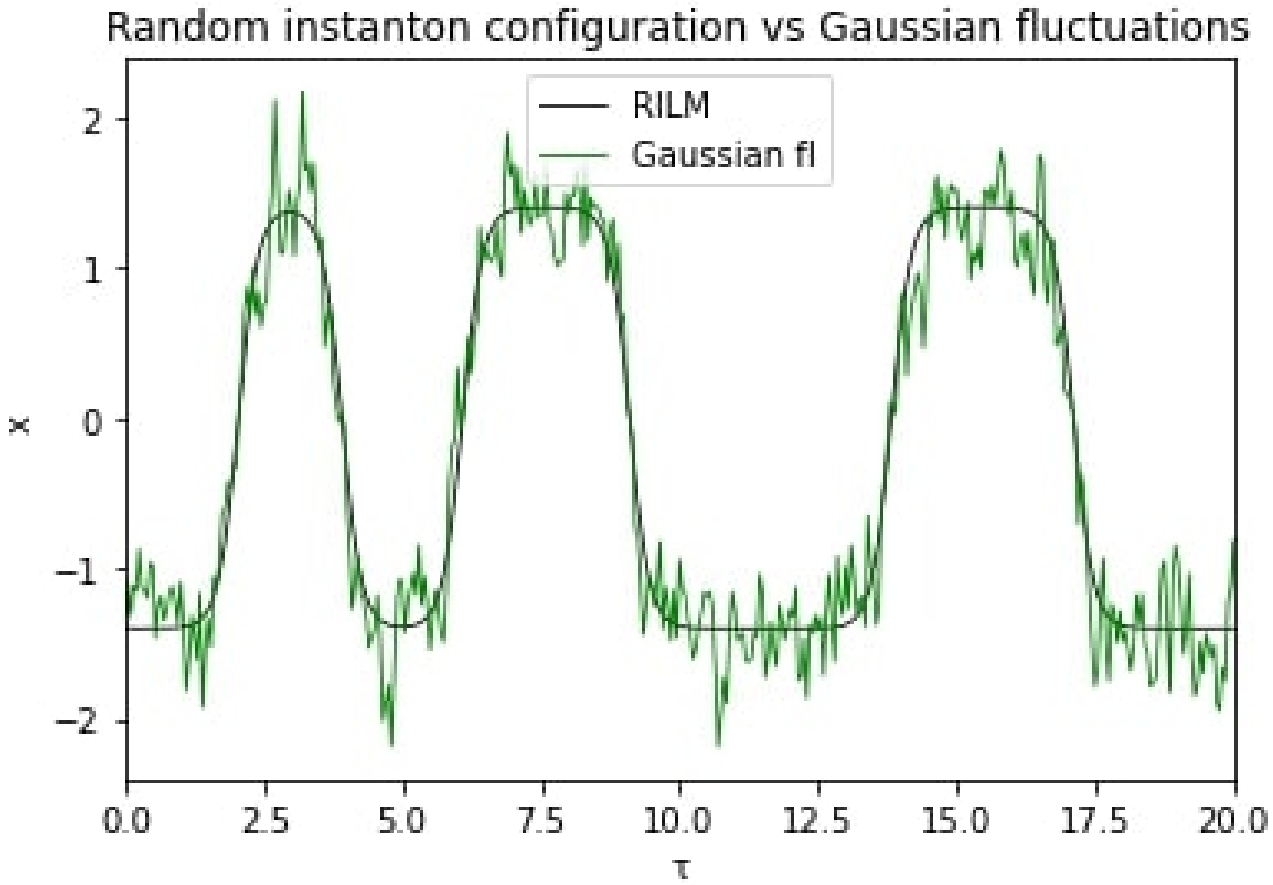
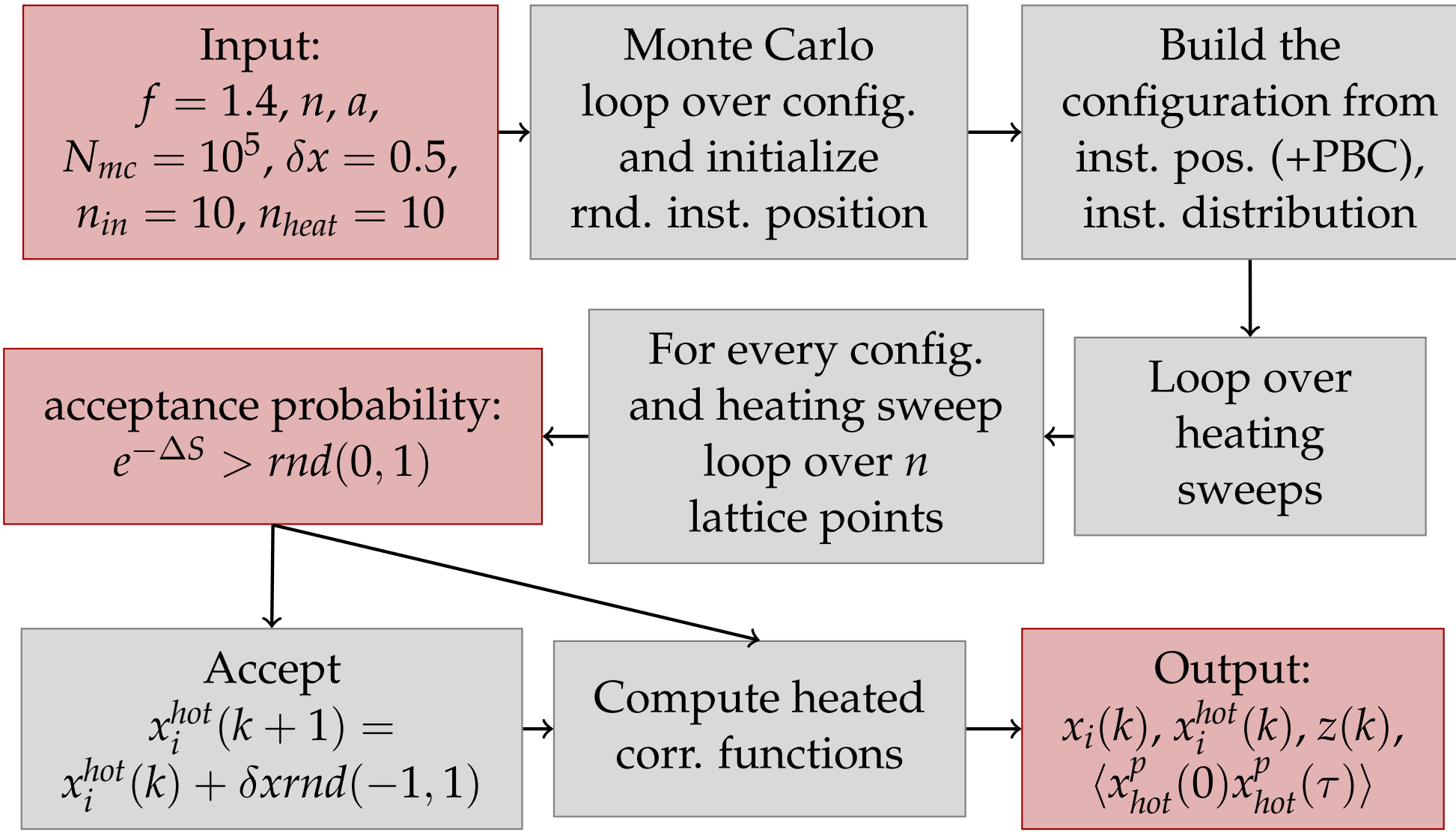


Figure 11: Typical random instanton configuration and the same configuration with Gaussian fluctuations. The noisy path generated using 10 heating sweeps in the Gaussian potential around the classical path.

rilm_gauss.py



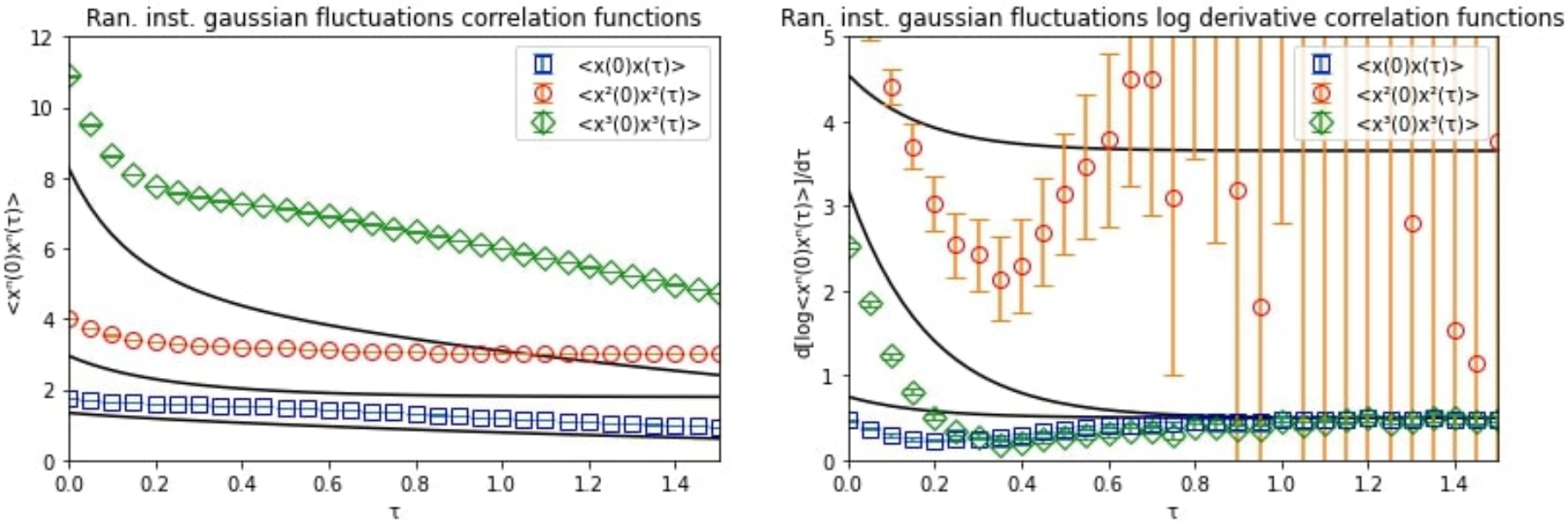


Figure 12: Correlation functions evaluated in a random instanton ensemble with Gaussian fluctuations.

We expect a better result than in the random or cooled case, since we have added some Gaussian fluctuations → we have not only a good description of the energy splitting between the ground state and the first excited state, but also of the second excited state.

Instanton Interactions

- By now we have neglected the tunnelling events due to the interaction between instantons:
  - In QCD is known that instantons' interactions, in particular the ones mediated by fermions lead to qualitative changes in the instanton ensemble
  - In our case these interactions are only short range and lead to relatively small effects
- A first guess to study theirs interactions is to construct a trial function and compute its action, e.g. we can start from the sum-ansatz.
  Let us call: $\tau_{IA} = |\tau_I - \tau_A|$, then we can argue that:
  - $\tau_{IA} \to \infty$ (no interaction) $S_{IA} = 2S_0 \left(1 - 6e^{-f\tau_{IA}} + \ldots\right)$
  - $\tau_{IA} \to 0$ (strong interaction) they annihilate each other $S_{IA} = 0$

Streamline (Valley) Method

Let us notice that exist one almost flat direction along which the action slowly varies between our 2 asymptotic limits in the space of all the instanton-anti-instanton paths (while all the other paths corresponds to perturbative fluctuations).
To force the instanton-anti-instanton path to go along the almost flat direction, we add a Lagrange multiplier:

$$S_\xi = \xi(\lambda) \int d\tau \left[x(\tau) - x_\lambda(\tau)\right] \frac{dx_\lambda(\tau)}{d\lambda}$$

Where $\xi(\lambda)$ is an arbitrary function (we should have reparametrization invariance).
To find the streamline configuration we start from a separated IA pairs and let the system evolve following the principle of the steepest descendent, i.e. :

$$\xi(\lambda)\frac{dx_\lambda(\tau)}{d\lambda} = \left.\frac{\delta S}{\delta x(\tau)}\right|_{x=x_\lambda} \qquad \text{BC: } x_{\lambda=0}(\tau) \simeq x_{sum} \text{ (well separated IA pairs)}$$

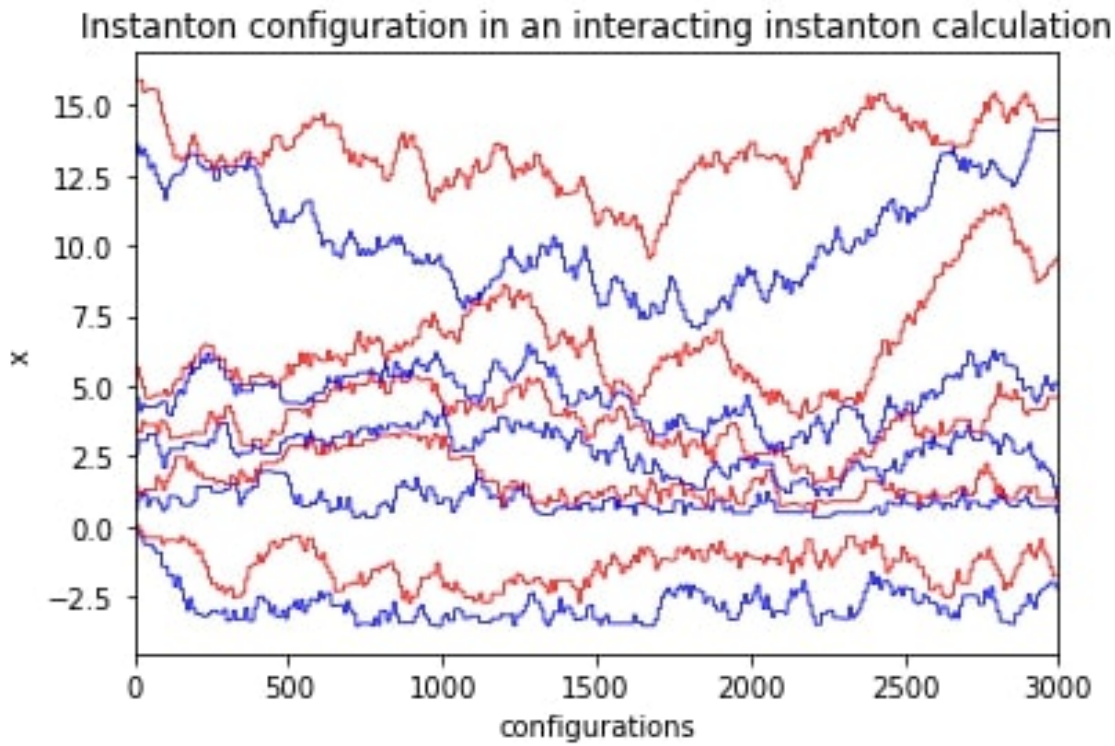


Figure 13: Typical instanton configuration in an interacting instanton calculation. The figure shows the location x of the first 10 instantons (blue) and anti-instantons (red) over a period of 3000 configurations.

To reproduce the hard-core repulsing interaction

$\rightarrow S_{core}(\tau_{IA}) = A_c e^{\frac{\tau_{IA}}{\tau_c}}$, where $A_c = 3$ and $\tau_c = 0.3$

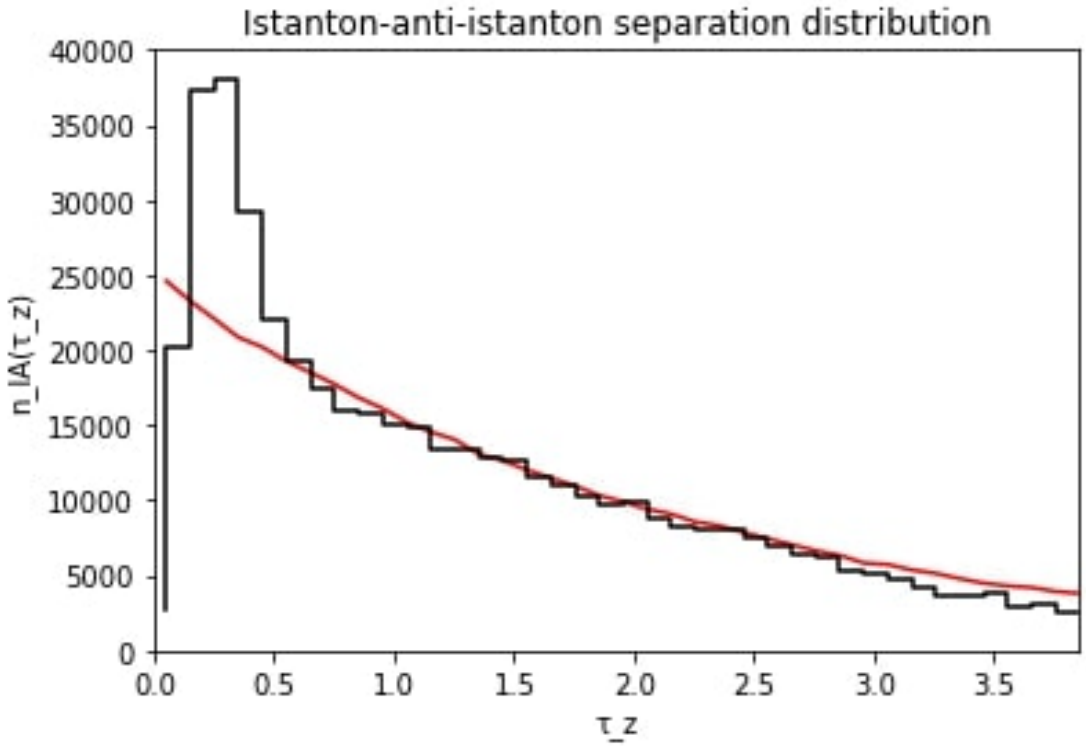


Figure 14: Distribution of IA separations after 10 cooling/heating sweeps.

- at small distance we have an enhancement of close IA pairs, which correspond to an attractive IA potential, which however is short range;
- the rapid decreasing when the distance goes to 0 is given by the approximation of rigid spheres (used to avoid divergences).

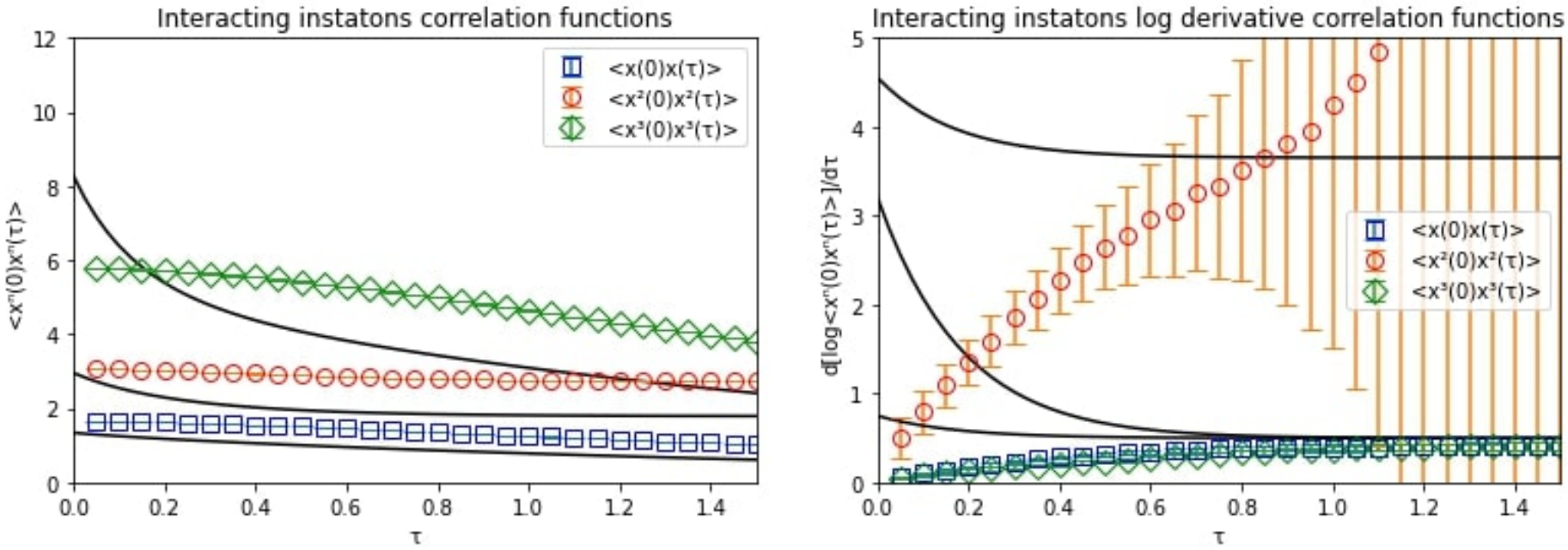
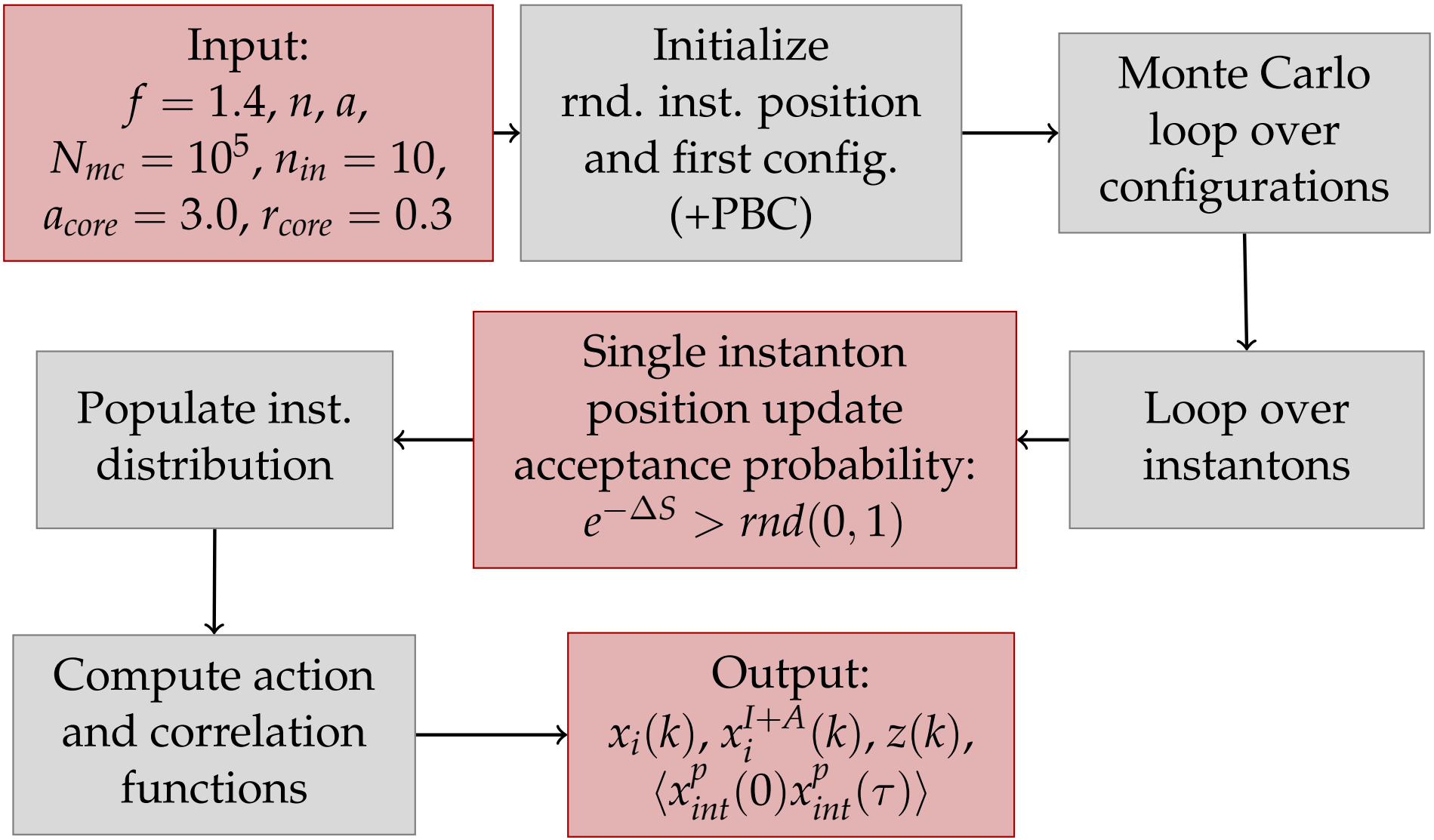


Figure 15: Correlation functions evaluated in an interacting instanton ensemble.

The correlation functions are similar to the random instanton ensemble because the interaction is small and only short range.

iilm.py


Input:
$f = 1.4, n, a,$
$N_{mc} = 10^5, n_{in} = 10,$
$a_{core} = 3.0, r_{core} = 0.3$
Initialize
rnd. inst. position
and first config.
(+PBC)
Monte Carlo
loop over
configurations
Loop over
instantons
Single instanton
position update
acceptance probability:
$e^{-\Delta S} > rnd(0,1)$
Populate inst.
distribution
Compute action
and correlation
functions
Output:
$x_i(k), x_i^{I+A}(k), z(k),$
$\langle x_{int}^p(0) x_{int}^p(\tau) \rangle$

Conclusions

- The methods in this context are very poor, since from the exact diagonalization we get the entire spectrum of the anharmonic oscillator, but in more complex cases, where we do not have only a parameter (f) which regulates the dynamics these methods are useful.
- We focused on $S_0 \sim 3$, since:
  - if $S_0 >> 1$: we can identify easily the instantons, but with a low tunnelling rate
  - if $S_0 \sim 1$: instantons are very abundant and is hard to determine an instanton density
- In QCD our simple model have a great application, but the things gets further more complicated than in the case analyzed