Numerical Stochastic Perturbation Theory around instantons

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Outline

Introduction:

1. Intantons problem in Quantum Mechanics: the Double Well Potential case
2. Instanton calculus and standard diagrammatic perturbation theory

Basic recap about NSPT:

1. Fundamental assumptions and Langevin dynamics
2. Solving the Numerical Stochastic Perturbation Theory

NSPT around instantons:

1. ABC, non-trivial solutions, zero modes and all that
2. Computing the twisted partition function (I) : Faddeev-Popov method
3. Computing the twisted partition function (II) : the perturbative free energy
4. Preliminary check: a first look to continuum limit
5. Extrapolations, continuum limit and preliminary results

Conclusions:

1. Summary and future prospects

Instantons in Quantum Mechanics : the Double Well Potential case

Starting from a Quantum Mechanical model $S_E[x] = \int dt \Big[\frac{1}{2}m\dot{x}^2 + V(x)\Big]$

we can use PI formalism to compute observables, but more interesting ...

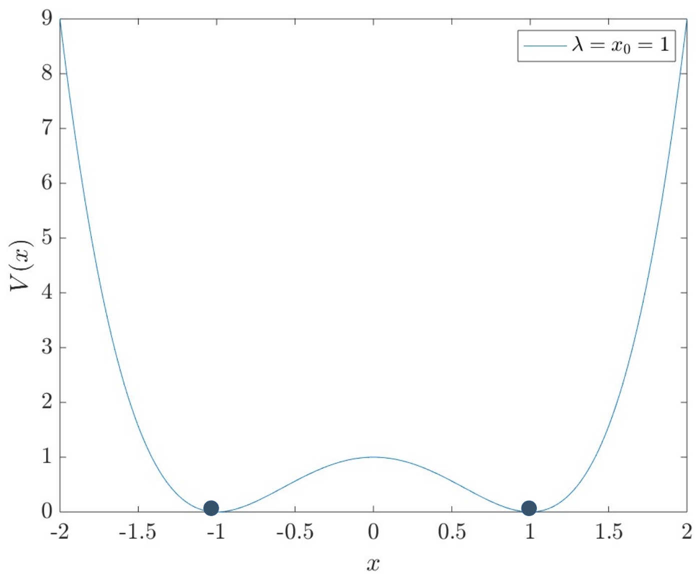
$$Z(\beta) = \int_{PBC} \mathcal{D}x \; e^{-S_E[x]} \qquad \lim_{\beta\to\infty} Z(\beta) \sim e^{-\beta E_0} + \mathcal{O}(e^{-\beta(E_1-E_0)})$$

Many times impossible to compute, but we can use perturbation theory !

$$Z(\beta) = \int_{PBC} \mathcal{D}x \; e^{-S_E^0}\Big(1 + \lambda S_{int} + \dots\Big) = Z^{(0)} + \lambda Z^{(1)} + \lambda^2 Z^{(2)} + \dots$$

We are implicitly choosing a minimum of the action where we expand on. This procedure defines the free theory

However, it can lead to wrong conclusions ...



DWP: $V(x) = \lambda(x^2 - x_0^2)^2$

In this two saddles the same perturbation theory!

Doubly degenerate eigenvalues? ... No !

We know from (standard) Quantum Mechanics that ...

$$E_0(\lambda) = \sum_{n\geq 0} \lambda^n E_0^{(n)} + e^{-\frac{A}{\lambda}} \sum_{n\geq 0} \lambda^n \bar{E}_0^{(n)} + \dots$$

Tunneling (i.e. instantonic) contribution!

Instantons calculus and standard diagrammatic perturbation theory

Again from standard Quantum Mechanics :

$$\hat{H} = \frac{\hat{p}^2}{2m} + \lambda(\hat{x}^2 - x_0^2)^2 \quad \rightarrow \quad [\hat{H}, \hat{P}] = 0 \qquad \hat{P}\psi(x) = \psi(-x) \qquad E_{0,\pm} = E_0 \mp \frac{\Delta E}{2}$$

$$\sim e^{-\frac{A}{\lambda}}$$

Now, turning back to PI formalism ...

$$\lim_{\beta\to\infty} Z(\beta) = \lim_{\beta\to\infty} \int dx \ \langle x|e^{-\beta\hat{H}}|x\rangle \sim e^{-\beta E_{0,+}} + e^{-\beta E_{0,-}} \sim 2e^{-\frac{\beta}{2}(E_{0,+}+E_{0,-})} \cosh\frac{\beta\Delta E}{2}$$

So, if we want the energy splitting in perturbation theory ...

... seems to be more appropriate the Twisted Partition Function

$$\lim_{\beta\to\infty} Z_a(\beta) = \lim_{\beta\to\infty} \int dx \ \langle x|e^{-\beta\hat{H}}|-x\rangle \sim e^{-\beta E_{0,+}} - e^{-\beta E_{0,-}} \sim 2e^{-\frac{\beta}{2}(E_{0,+}+E_{0,-})} \sinh\frac{\beta\Delta E}{2}$$

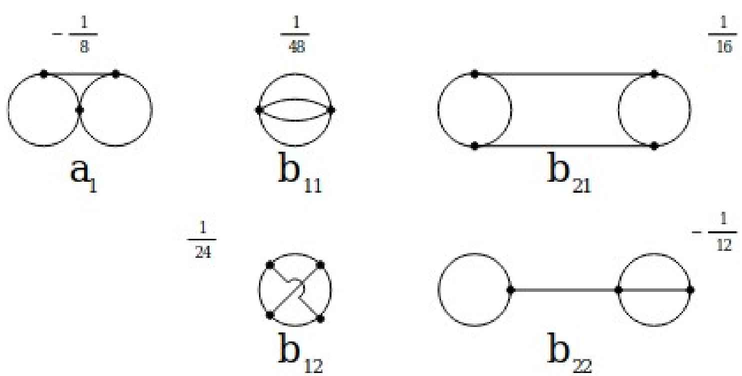
or, to do even better:

$$\boxed{\lim_{\beta\to\infty} \frac{Z_a(\beta)}{Z(\beta)} \sim \frac{\beta\Delta E}{2}}$$

Compute the TPF in PT:

1. find the solutions for the (euclidian) equation of motion with ABC (the instanton!)
2. expand the action around this solution, find propagators and new interaction vertices
3. do the standard diagrammatic perturbation theory

Practically speaking, it becomes difficult already at the third order!



$$\lim_{\beta\to\infty} \frac{Z_a(\beta)}{Z(\beta)} = e^{-S[x_c]} K\Big(1 + \lambda z_1 + \lambda^2 z_2 + \dots\Big)$$

Wöhler and Shuryak, Physics Letters B (333) 1994

Escobar-Ruiz, Shuryak and Turbiner, Phys. Rev. D (92 - 025046) 2015

Fundamental assumptions and Langevin dynamics

Langevin equation for stochastic evolution

$$\boxed{\frac{\partial x_j(\tau)}{\partial \tau} = -\frac{\partial S_E[x]}{\partial x_j(\tau)} + \eta_j(\tau)}$$

$$\langle \eta_j(\tau) \rangle_\eta = 0 \qquad \langle \eta_j(\tau)\eta_k(\tau') \rangle_\eta = 2\delta_{jk}\delta(\tau - \tau')$$

Fokker-Planck equation

$$\frac{\partial \mathcal{P}}{\partial \tau}(x,\tau) = \sum_j \frac{\partial}{\partial x_j}\Big(\frac{\partial S_E}{\partial x_j} + \frac{\partial}{\partial x_j}\Big)\mathcal{P}(x,\tau)$$

Equilibium ..

$$\mathcal{P}_{eq.} = \mathcal{P}(x) = \frac{e^{-\mathcal{S}_E[x]}}{\mathcal{N}}$$

$$\lim_{\tau\to\infty} \langle \mathcal{O}[x_\eta(\tau)] \rangle_\eta = \langle \mathcal{O}[x] \rangle$$

We solve the Langevin equation numerically ...

$$x_j(\tau + \Delta\tau) = x_j(\tau) - \Delta\tau \frac{\partial S_E[x(\tau)]}{\partial x_j(\tau)} + \sqrt{\Delta\tau}\,\eta_j(\tau) \qquad \langle \eta_j(\tau) \rangle_\eta = 0 \qquad \langle \eta_j(\tau)\eta_k(\tau') \rangle_\eta = 2\delta_{jk}\delta_{\tau\tau'}$$

Now additional sistematic error $\longrightarrow$ Looking for a continuum stochastic process extrapolation

($\Delta\tau \to 0$ extrapolation)

Solving the Numerical Stochastic Perturbation Theory

$$\frac{\partial x_j(\tau)}{\partial \tau} = -\frac{\partial S_E[x(\tau)]}{\partial x_j(\tau)} + \eta_j(\tau)$$

$$\boxed{x_j(\tau) = x_j^{(0)}(\tau) + \sum_{n>0} \lambda^n x_j^{(n)}(\tau) \quad \forall j}$$

- Set of hierarchical equations
- Exact at any order in perturbation theory
- Perturbative expansion of observables

Not our approach!

Following Fokker-Planck formalism

$$\mathcal{P}(x,\tau) = \sum_{n\geq 0} \lambda^n \mathcal{P}_n(x,\tau)$$

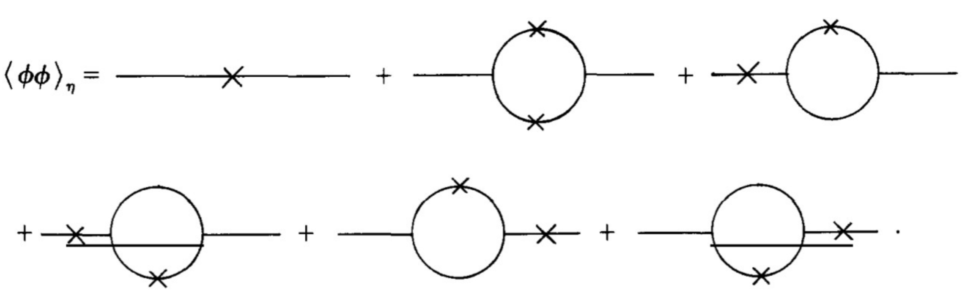
- $\lim_{\tau\to\infty} \mathcal{P}_0(x,\tau) = \mathcal{P}_0^{eq.} = \frac{e^{-S_E^0[x]}}{Z_0}$
- $\mathcal{P}_k(x,\tau) \to_{\tau\to\infty} \mathcal{P}_k^{eq}(x)$

Free theory + Schwinger-Dyson eq.

Floratos-Iliopoulos, Nucl.Phys. B 214 (1983) 392

$$\begin{aligned}\mathcal{O}(x) &= \mathcal{O}^{(0)}(x^{(0)}) + \lambda \mathcal{O}^{(1)}(x^{(0)}, x^{(1)}) + \ldots \\ &= \mathcal{O}^{(0)} + \sum_{n>0} \lambda^n \mathcal{O}^{(n)}\end{aligned}$$

Diagrammatic Stochastic Perturbation Theory



Getting the (usual) Feynman diagrams
in the long-stochastic time limit

Damgaard-Huffel, Phys Rept 152 (1987) 227

Numerical Stochastic Perturbation Theory

Numerically solve the (perturbative) Langevin equation up to a fixed perturbative order

$$\begin{cases} x_j^{(0)}(\tau+\Delta\tau) &= x_j^{(0)}(\tau) - \Delta\tau \left[\frac{\partial S_E[x]}{\delta x_j}(\tau)\right]^{(0)} + \sqrt{\Delta\tau}\,\eta_j(\tau) \\ x_j^{(1)}(\tau+\Delta\tau) &= x_j^{(1)}(\tau) - \Delta\tau \left[\frac{\partial S_E[x]}{\delta x_j}(\tau)\right]^{(1)} \\ & \ldots\ldots \end{cases}$$

Di Renzo, Marchesini, Onofri Nucl. Phys. B 426 (1994) 675

ABC, non-trivial solutions, zero modes and all that

We use the lattice theory

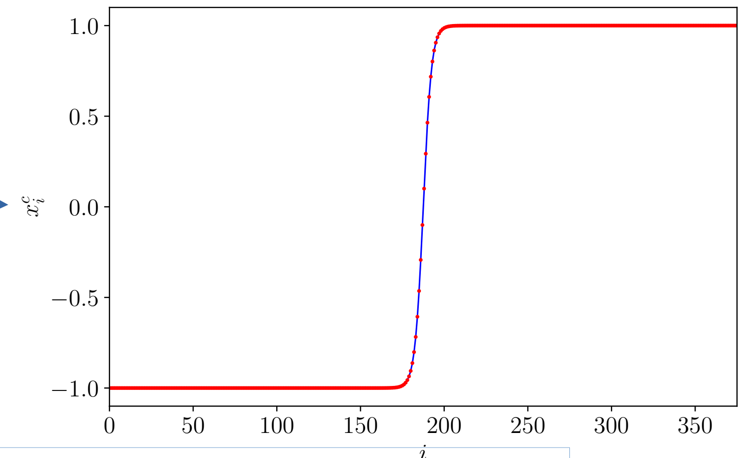
$$\mathcal{S}_E[x] = \int dt \left[\frac{1}{2}m\dot{x} + \lambda(x^2 - x_0^2)^2\right] \longrightarrow \mathcal{S}_E[x_i] = \sum_{i=1}^{L} \left[\frac{1}{2}\tilde{m}(\tilde{x}_{i+1} - \tilde{x}_i)^2 + \tilde{\lambda}(\tilde{x}_i^2 - \tilde{x}_0^2)^2\right]$$

But we want the theory around the instanton solutions! We find it numerically by means of :

$$\dot{x}_j = -\frac{\partial \mathcal{S}[x]}{\partial x_j}$$

with *ABC*

define x_i^c

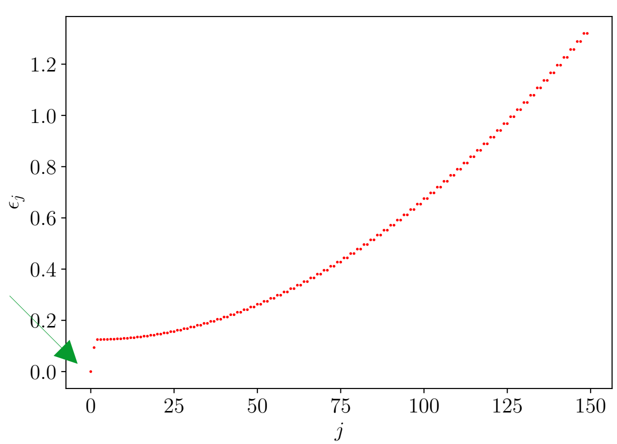


Expanding the action around instantons ...

$$\tilde{x}_i = \tilde{x}_i^c + \tilde{\xi}_i = \tilde{x_0} \cdot \bar{x}_i + \tilde{\xi}_i \quad , \quad \tilde{x_0} = \sqrt{\frac{\tilde{m}\tilde{\omega}^2}{8\tilde{\lambda}}}$$

$$\boxed{\mathcal{S}_E[\xi_j] = \mathcal{S}_E[x_j^c] + \sum_{i=1}^{L}\left[\frac{1}{2}\tilde{m}(\tilde{\xi}_{i+1} - \tilde{\xi}_i)^2 + \frac{1}{2}\tilde{m}\tilde{\omega}^2\left(\frac{3}{2}\bar{x}_i^2 - \frac{1}{2}\right)\tilde{\xi}_i^2 + \sqrt{2\tilde{\lambda}\tilde{m}\tilde{\omega}^2}\bar{x}_i\tilde{\xi}_i^3 + \tilde{\lambda}\tilde{\xi}_i^4\right]}$$

In analogy with the continuum theory, now we have a zero mode for the operator $\left.\dfrac{\partial^2 S_E[\tilde{\xi}]}{\partial\tilde{\xi}_j \partial\tilde{\xi}_k}\right|_{\tilde{\xi}=0}$



- we fail to keep first order evolution under control
- higher orders will also be compromised
- we will manage the observables in order to evolve only fluctuations without zero mode

(revisited Faddev-Popov procedure)

ABC, non-trivial solutions, zero modes and all that

We evolve with (the discrete version of) Langevin equation the fluctuations *(order by order)*

$$\tilde{\xi}_j(\tau+\Delta\tau) = \tilde{\xi}_j(\tau) - \Delta\tau\Big[\tilde{m}(2\tilde{\xi}_j - \tilde{\xi}_{j+1} - \tilde{\xi}_{j-1}) + \tilde{m}\tilde{\omega}^2\Big(\frac{3}{2}\bar{x}_j^2 - \frac{1}{2}\Big)\tilde{\xi}_j + \sqrt{18\tilde{\lambda}\tilde{m}\tilde{\omega}^2}\,\bar{x}_j\tilde{\xi}_j^2 + 4\tilde{\lambda}\tilde{\xi}_j^3\Big]$$

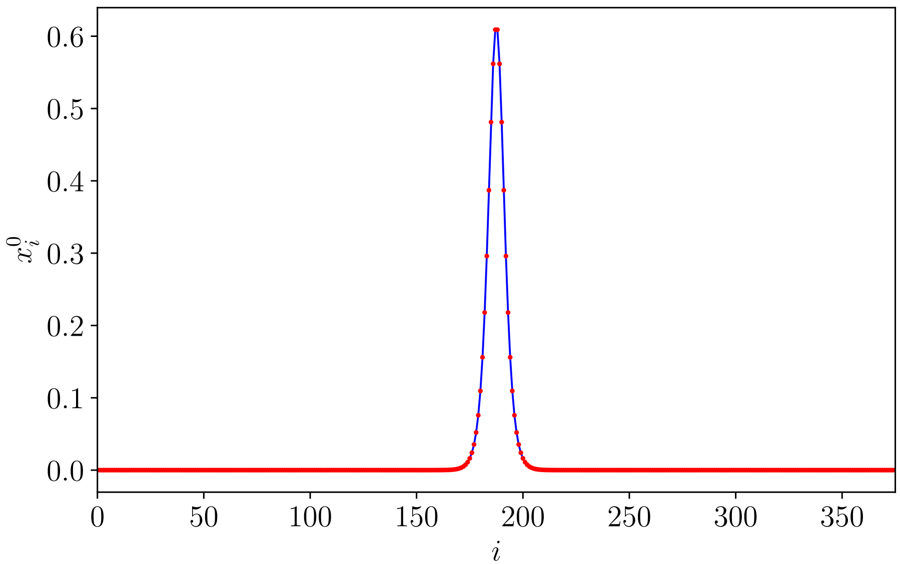
with anti-periodic boundary conditions

But, for what mentioned above, we propagate in this way also the zero mode.
How can we eliminate this component from the fluctuations?
At the end of each iteration, we can compute ..

$$c_0 = \sum_i \tilde{\xi}_i x_i^0$$

using the decomposition

$$\tilde{\xi}_j = c_0 x_j^0 + \tilde{\xi}_j^\perp \rightarrow \boxed{\tilde{\xi}_j^\perp = \tilde{\xi}_j - c_0 x_j^0}$$



The eigenvector with zero eigenvalue under the action of the operator

$$\left.\frac{\partial^2 S_E[\tilde{\xi}]}{\partial\tilde{\xi}_j\partial\tilde{\xi}_k}\right|_{\tilde{\xi}=0}$$

Now MonteCarlo evolution under control!

Computing the twisted partition function (I) : Faddeev-Popov method

What is the price to pay to be able to handle only with transverse fluctuations $\xi^{\perp}$?

→ It is not just a problem of MonteCarlo simulatios, in fact ...

$$Z_a = \int_{ABC} \prod_i dx_i \; e^{-S_E[x_j]} \approx e^{-S_E[x_i^c]} \int_{ABC} \prod_i d\xi_i \; e^{-S_E[\xi_j]} \approx e^{-S_E[x_i^c]} \mathcal{N} \underbrace{\boxed{(\det M)^{-\frac{1}{2}}}}_{\text{Zero Eigenvalue}} (1 + \mathcal{O}(\lambda))$$

In analogy with the continuous theory, we use the Faddeev-Popov procedure

- we start considering the tunnelling point τ_0 that parameterizes $x_j^c(\tau_0)$
- using a suitable rewriting of the identity

$$1 = \int d\tau_0 \underbrace{\delta\Big[\sum_i (x_i - x_i^c(\tau_0)) x_i^0(\tau_0)\Big]}_{=\delta(c_0)} \Big(-\sum_i \dot{x}_i^c(\tau_0) x_i^0(\tau_0) + \sum_i (x_i - x_i^c(\tau_0) \dot{x}_i^0\Big)$$

- now we can integrate out the zero mode and compute the (perturbative) TPF
- extra (perturbative term): the Faddeev-Popov term

$$Z_a = \frac{e^{-S[x^c]} \beta \sqrt{S}}{\sqrt{2\pi}} \int_A \prod_\sigma \boxed{d\xi_\sigma^{\perp}} \Big[1 + \boxed{\sqrt{\frac{\lambda}{S'}} \sum_k \boxed{\xi_k^{\perp}} \frac{(x_{k-1}^0 - x_k^0)}{a}} \Big] e^{-S[\boxed{\xi_l^{\perp}}]}$$

- usually, the continuum perturbation theory starts here
- we have some extra work to do: we can measure only expectation values

Computing the twisted partition function (II) : the perturbative free energy

Using the (perturbative) TPF without zero mode :

$$Z_a = \frac{e^{-S[x^c]}\beta\sqrt{S}}{\sqrt{2\pi}} \underbrace{\langle 1 + \sqrt{\frac{\lambda}{S'}} \sum_k \xi_k^{\perp} \frac{(x_{k-1}^0 - x_k^0)}{a} \rangle}_{\text{now a perturbative observable}} Z_a^{\perp}$$

We have a partition function again. But trying to get around the problem (at least in PT) ...

$$Z_{a,\perp} = Z_{a,\perp}(\lambda) \rightarrow \frac{d}{d\lambda} \ln Z_{a,\perp} = \frac{1}{\lambda} \underbrace{\langle -\frac{1}{2}\sqrt{\lambda} S_1[\xi_j] - \lambda S_2[\xi_j] \rangle}_{=\lambda b_1 + \lambda^2 b_2 + \lambda^3 b_3 + \ldots} \rightarrow Z_{a,\perp} = Z_{a,\perp}^{(0)} \boxed{\exp \sum_n \lambda^n \frac{b_n}{n}}$$

Perturbative Free energy

The same is true in periodic theory (remembering we only want ratios of partition functions)!

$$Z = Z^{(0)} \exp \sum_n \lambda^n \frac{c_n}{n}$$

Finally we can go back to the start and consider :

$$\boxed{\frac{Z_a}{Z} = \frac{e^{-S[x^c]}\beta\sqrt{S}}{\sqrt{2\pi}} \left(\frac{Z_{a,\perp}^{(0)}}{Z^{(0)}}\right) \langle 1 + \sqrt{\frac{\lambda}{S'}} \sum_k \xi_k^{\perp} \frac{(x_{k-1}^0 - x_k^0)}{a} \rangle \exp \sum_n \frac{\lambda^2}{n} (b_n - c_n) \sim \frac{\beta \Delta E}{2}}$$

for what we have seen the main contribution

Anti periodic theory

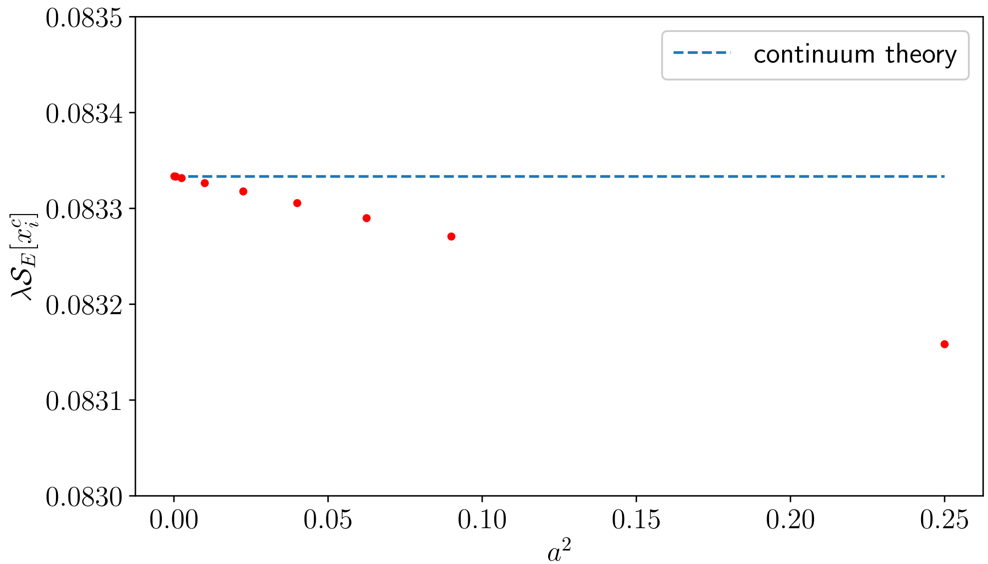
Periodic theory

They are already know

Preliminary check: a first look to continuum limit

$$\frac{Z_a}{Z} = \boxed{\frac{e^{-S[x^c]}\beta\sqrt{S}}{\sqrt{2\pi}}\left(\frac{Z^{(0)}_{a,\perp}}{Z^{(0)}}\right)} \langle 1 + \sqrt{\frac{\lambda}{S'}}\sum_k \xi_k^{\perp}\frac{(x^0_{k-1}-x^0_k)}{a}\rangle \exp\sum_n \frac{\lambda^2}{n}(b_n - c_n) \sim \frac{\beta\Delta E}{2}$$

Leading order



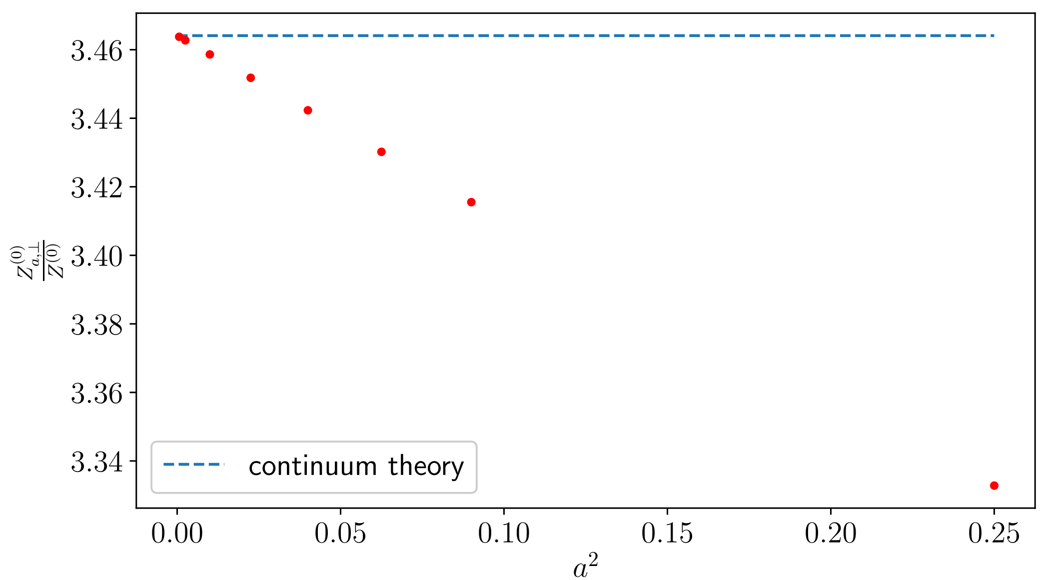
The system seems to approach the continuum theory very well at leading order

CL: $\lambda(S_E[x_i^c] - S_E[x_{cl}]) \approx -2\cdot 10^{-7}\lambda$

A direct consequence of

$$\sum_i |x_i^c - x_0 \tanh\frac{\omega}{2}t_i|^2 \to 0$$

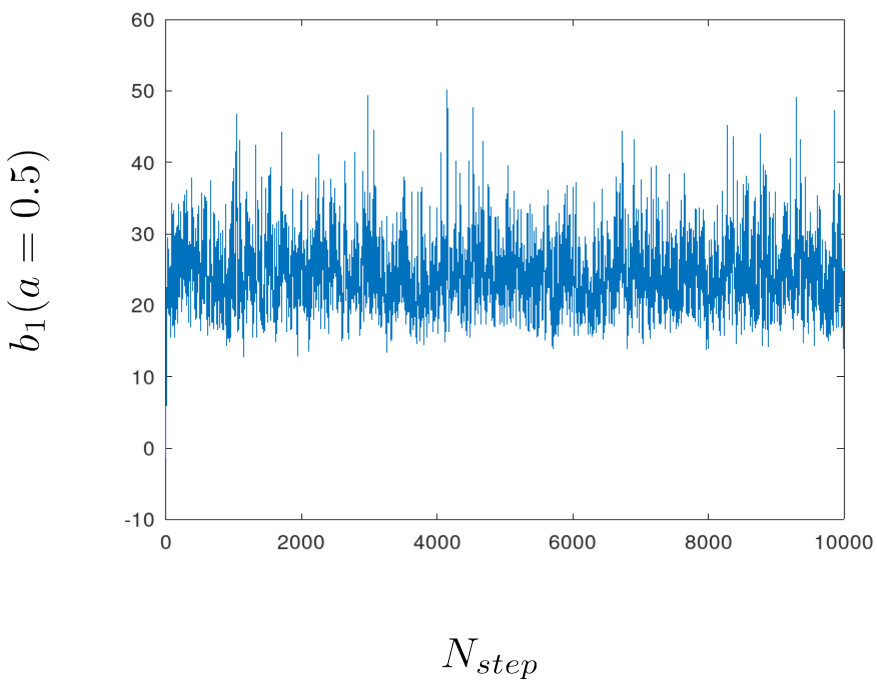
for $a \to 0$

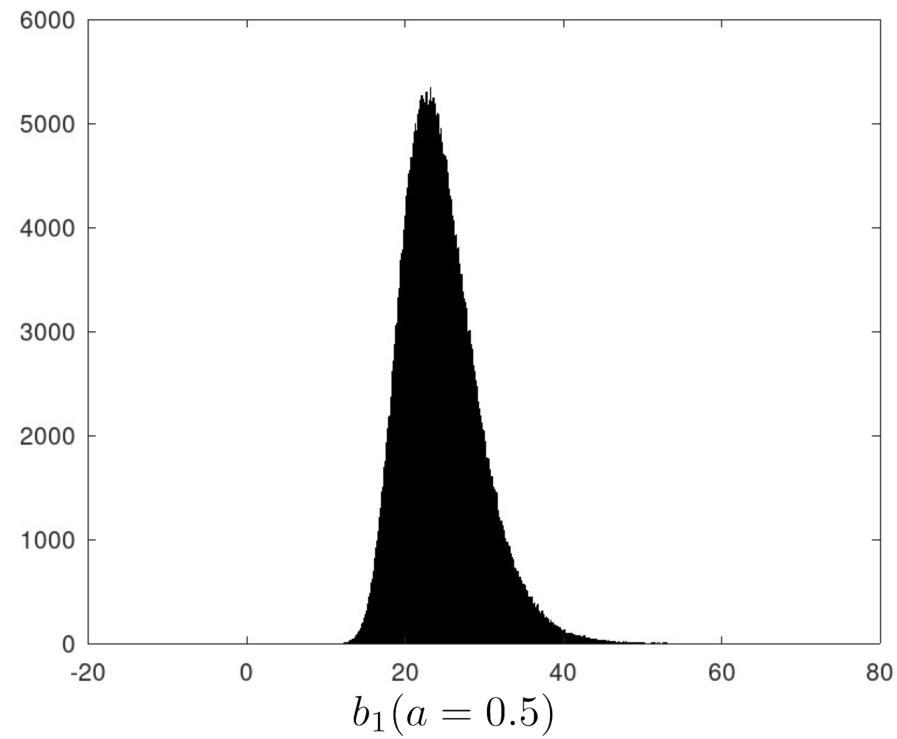


Extrapolations, continuum limit and preliminary results

$m = \omega = 1$

a	$\Delta\tau$			
0.75	0.01	0.02	0.03	
0.60	0.01	0.02	0.03	
0.50	0.01	0.02	0.03	
0.40	0.01	0.015	0.02	0.03
0.30	0.01	0.015	0.02	

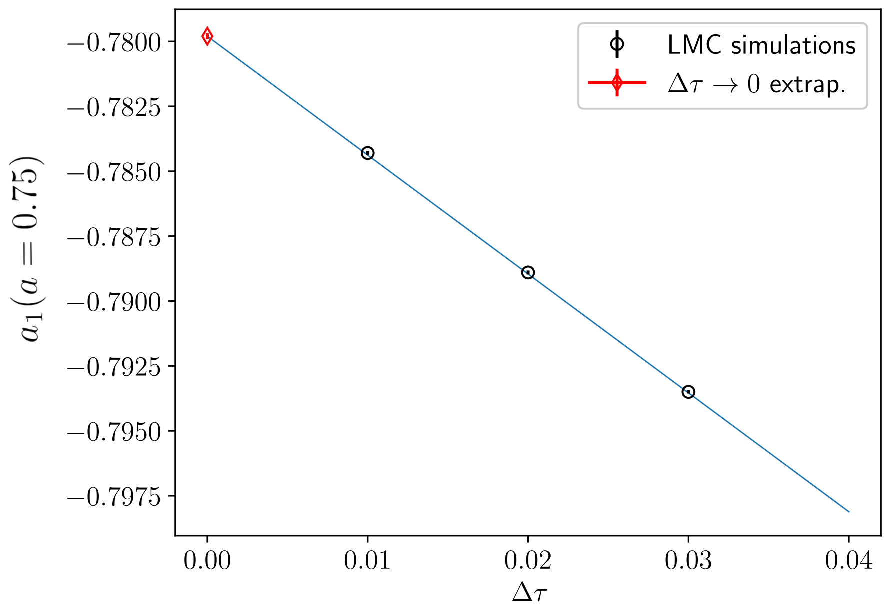


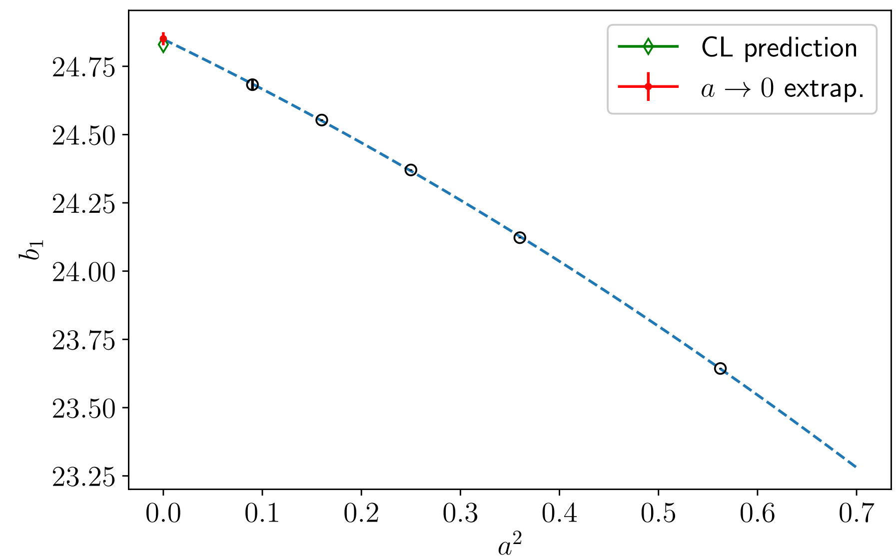


Extrapolations, continuum limit and preliminary results

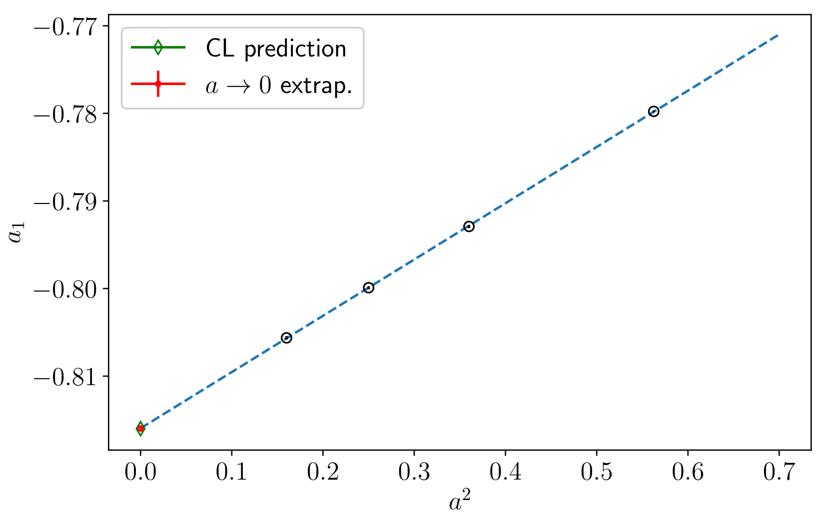
Removing the systematic error of the discrete stochastic process:

- a continuum stochastic time extrapolation for each lattice spacing
- not an order by order extrapolation : we have (also) cross-correlations





$$z_1 = a_1 + (b_1 - c_1)$$



Continuum PT	*This work*
$-71/72 \approx -0.986$	$-0.966(25)$

this seems to encourage us!

But still a lot of work to be done ...
First of all: smaller lattice spacing simulations

Conclusions

Summary:

- In this presentation we saw the spirit behind the idea of NSPT computations around instantons

- Even if it's only preliminary work, I given you a brief account for the first order

- On the other hand, this simple system already presents some difficulties
  1. *We have to measure small differences (large relative errors)*
  2. *Statistical errors can be magnified by the exponentiation of free energy*
  3. *Different scaling regions for different observables: we have to extract carefully the CL*

Future prospects:

- Smaller lattice spacing simulations
- High order computations
- Switch from Quantum Mechanics to QFT

Thank you for your attention!