Metadynamics Remedies for Topological Freezing

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School of Physics and Astronomy

(that's where you'll come at the end of July)

Mainly based on arXiv:1508.07270

"Metadynamics Surfing on Topology Barriers: the $CP(N-1)$ ***Case"***

A.Laio, G.Martinelli, F.S

Summary

The Illness

1. Topological charge
2. Critical Slowing Down

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The Treatment

1. Metadynamics
2. A case of investigation: $CP(N-1)$ model

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Side Effects
(and side outcomes!)

1. Measuring the Free Energy
2. Reweighting

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1. Measuring the Free Energy
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Extension and perspectives

1. First checks in QCD
2. Extension of the method

Topological charge

Homotopy group

Topological sector: set of configurations that can be transformed one into the other by means of a continuous deformation

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Winding number

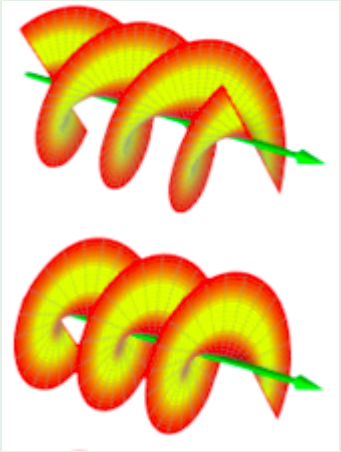
Topological charge **density** in QCD

$$q(x) = \frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}\left[F_{\mu\nu}(x)\,F_{\rho\sigma}(x)\right]$$

- Its volume integral define the **topological charge**

$$Q = \int d^4x\, q(x)$$

  related to the **winding number** of the field
- Several definitions on the lattice



Phenomenology of the topological charge

Topological charge is present in QCD lagrangian

$$\mathcal{L} = \frac{1}{4} F_{\mu\nu} F_{\mu\nu} + \theta q$$

- Strong CP problem
- $\eta - \eta'$ masses
- Instantons interaction
- Dependence of observables on Q

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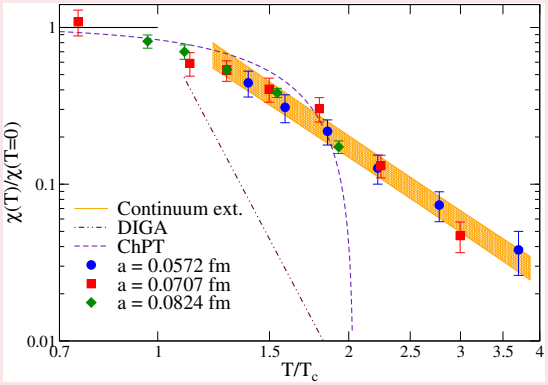
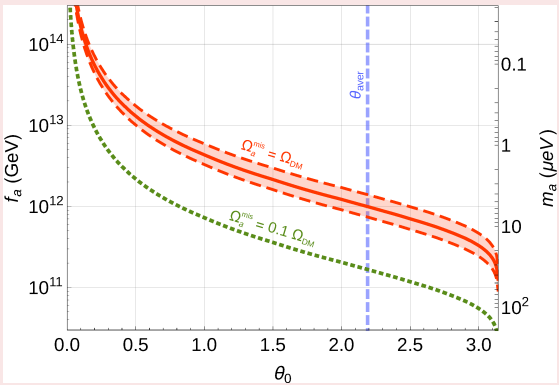
Axion phenomenology - Susceptibility of the topological charge

From arXiv:1512.06746, C.Bonati, M.D'Elia, M.Mariti, G.Martinelli, M.Mesiti, F.Negro, F.S, G.Villadoro





Topological charge on the lattice

Many possibilities

Overlap operator through index theorem

Wilson Flow and field theoretical definition $Q = F_{\mu\nu}\tilde{F}_{\mu\nu}$

Cooling discrete Wilson Flow [as shown by C.Bonati, M.D'Elia PRD89 (2014)]

Stout Wilson Flow with a simpler integration scheme

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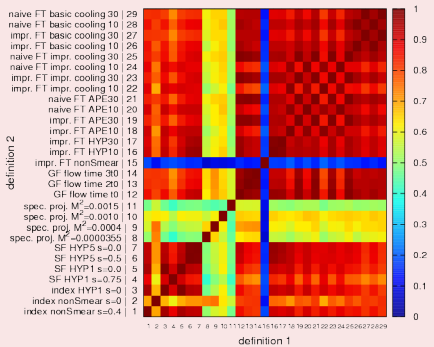
One bottom line

They are all
equivalent
in the
continuum limit

[K.Chichy et al, Lattice'14]



- Different definitions are subject do different cut-off effects
- They can come handy for different reasons...

The history of Topological Charge Slowing Down

1996 - the prophecy: "*Hybrid Monte Carlo and topological modes of full QCD*"

B. Alles, G. Boyd, M. D'Elia, A. Di Giacomo and E. Vicari, Phys.Lett.B389 (1996)

"The hybrid Monte Carlo algorithm has **serious problems decorrelating the global topological charge** [...]. This represents **a warning** which must be seriously considered."

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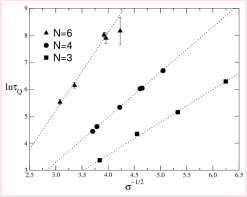
2002: "*θ dependence of $SU(N)$ gauge theories*", L.Del Debbio, H.Panagopoulos, E.Vicari



- Non-gaussianity: $\tau_Q \neq a^{-2}$ is shown for topological charge, at variance with "ordinary" observables
- Empirical behavior: $\tau_Q \sim \exp[-c/a]$ is proposed
- Emergence of "***sizable free-energy barriers separating different regions of the configuration space***" is suggested

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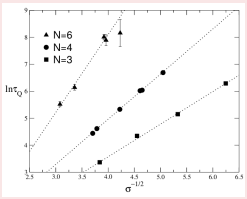

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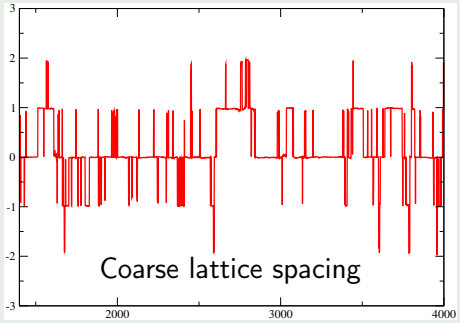
2010 - the revelation: "*Properties & uses of the Wilson flow in LQCD*", M.Lüscher

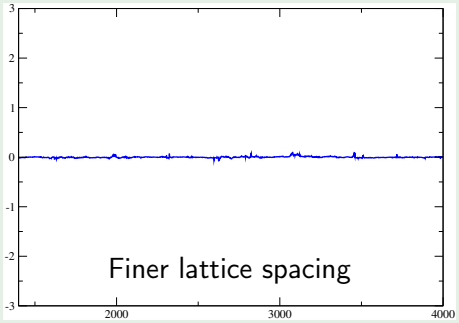
At the Lattice Conference in Sardinia, The Truth is proclaimed:

- Wilson Flow should be used to define the topological charge
- In this way: "***the emergence of the topological (instanton) sectors in the continuum limit becomes transparent***"

Topological charge slowing down - two examples

Pisa Collaboration: Staggered simulations for Axion Phenomenology





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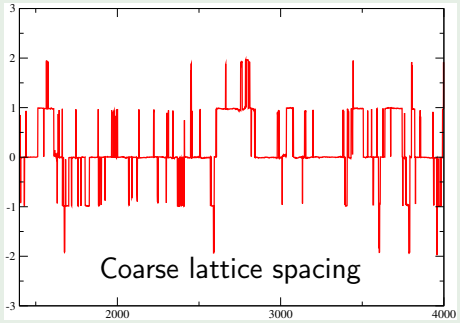
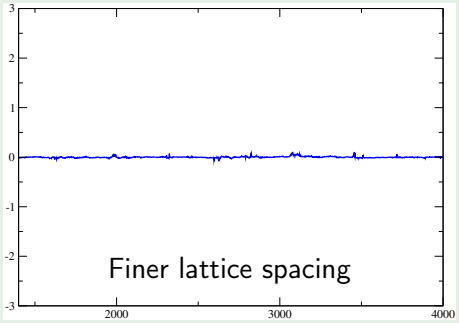
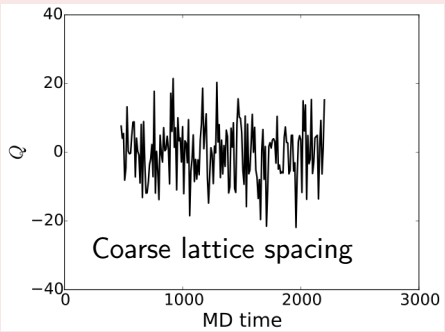
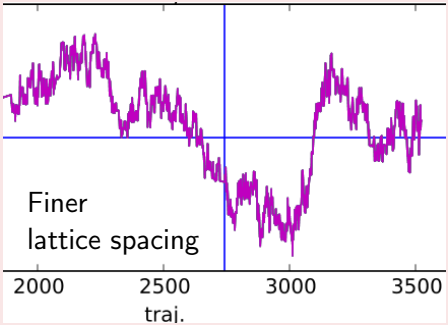




RBC/UKQCD: Domain Wall simulations for Charm physics





A PUZZLING QUESTION

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How can the system
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Topological sectors are ill defined at finite lattice spacing

- Assignment of a configuration not unique, depends on the method
- The assignment gets clearer and clearer as we proceed to the continuum limit
- Some configurations are **particularly difficult** to assign

"Slow Down yourself, please! Why does the system tunnel in the first place?"

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The system can tunnel by passing through **topologically ill defined configurations**

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The tunneling mechanism

The system can tunnel by passing through **topologically ill defined configurations**

In the continuum limit the "breaches" are closed

- Topologically ill-defined configurations have zero measure in the continuum limit
- The tunneling gets more and more suppressed as we proceed towards the continuum

Do we have to bother?

Can't we just ignore the problem?

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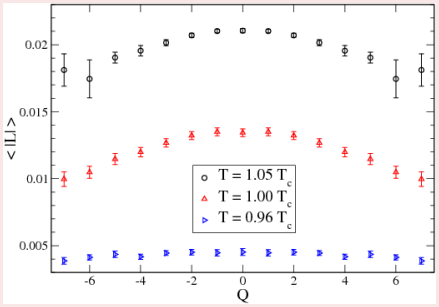

NO!

[see e.g. M.D'Elia, F.Negro, arXiv:1306.2919]

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- Bad sampling of Q means to bias observables

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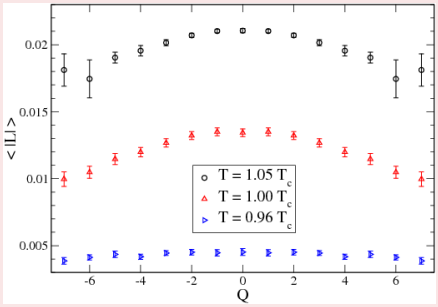

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Can't we get rid of topological sectors?

2011: "*Lattice QCD without topology barriers*", M.Lüscher, S.Schaefer

Open the boundary on one side of the lattice

- ✓ Topological objects free to flow in/out from the system
- ✗ Loose translation invariance
- ✗ Volume effects are expected to be minimized with periodic boundaries

Other ideas

Simulate at strictly fixed topology

[JLQCD, PRD74 (2006)]

- ✓ In the infinite volume limit, all sectors are equivalent
- ✗ Nontrivial effects at finite volume, e.g:

$$\lim_{m \to 0} \langle q\bar{q} \rangle_{Q=0} \quad = \quad 0 \qquad \text{at fixed } V$$

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Encourage tunneling on the point x^* where the $|q(x)|$ is the largest

$$\Delta S = -\alpha \exp\left[-q^2(x^*)\right]$$

[P.de Forcrand et al., Nucl.Phys.Proc.Suppl. 63 (1998)]

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- ✗ Not addressing large scale topological structures

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Torturing the configuration by causing dislocations

"Increase the transitions rate between topological sectors by **encouraging more zero-modes**"

[G.McGlynn, R.Mawhinney, PoS lattice'13 arXiv:1311.3695]

- ? Is it working? (question for the authors in the audience)
- ? What about the scaling to the continuum?

NEW FRIENDS

CP(N-1) MODELS

$CP(N-1)$ models in a nutshell

In the continuum - 2D space

- Commutating complex field $\vec{z} = (z_1 ... z_N)$ of norm 1
- $U(1)$ gauge symmetry, covariant derivative: $D_\mu = \partial_\mu + iA_\mu$ with $A_\mu \in \mathcal{R}$

$$S = \beta N \int d^2x \sum_{\mu=1}^{2} |D_\mu \vec{z}(x)|^2 , \qquad \boxed{N = 21}$$

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Like QCD...

- There is a topology Q
- There is a mass gap $M \sim 1/\xi$
- The beta-function is negative
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But simpler!

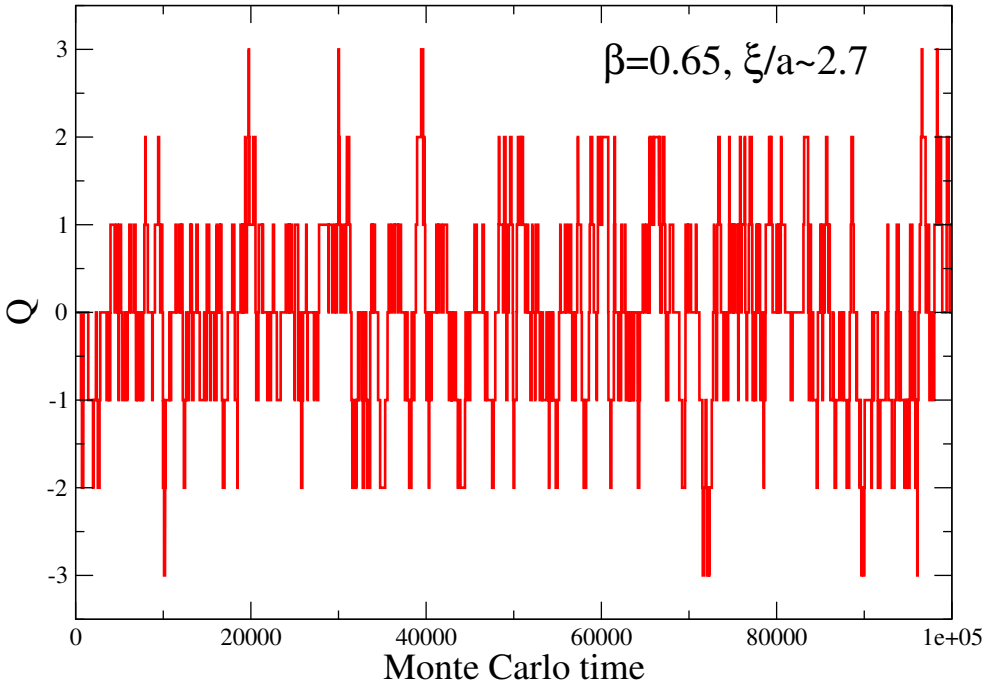
- Simulations can be run on a laptop! (actually: Ulisse cluster at Sissa)
- Excellent framework to test new algorithms

MOST IMPORTANT

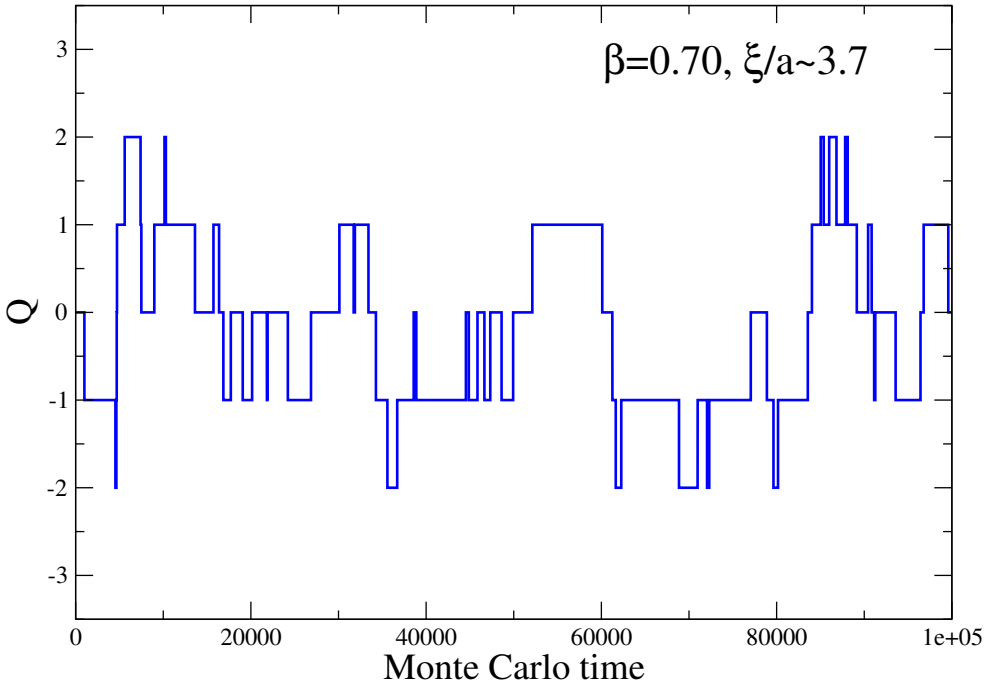
it suffers
from

TOPOLOGICAL
FREEZING

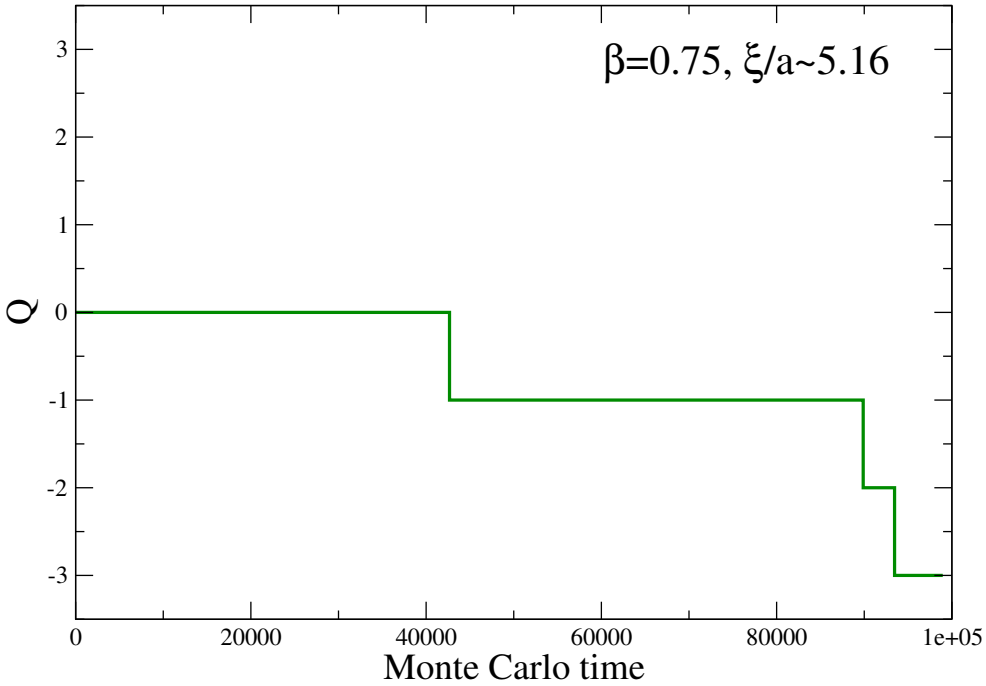
Topological charge evolution



Evolution on a finer lattice spacing (same scales)



Going even finer

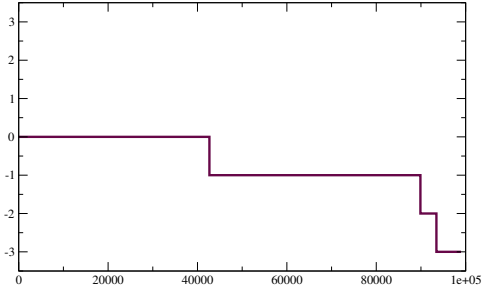


TOPOLOGICAL CHARGE?

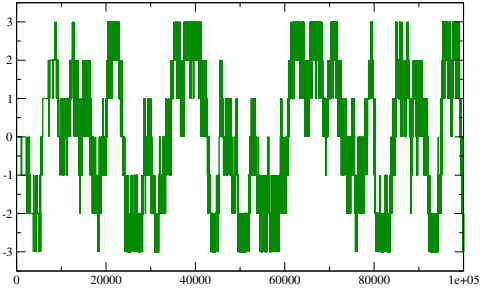
Metadynamics Elixir

"For an *immediate relief*
of your topological ~~paralysis~~ freezing!"

Before

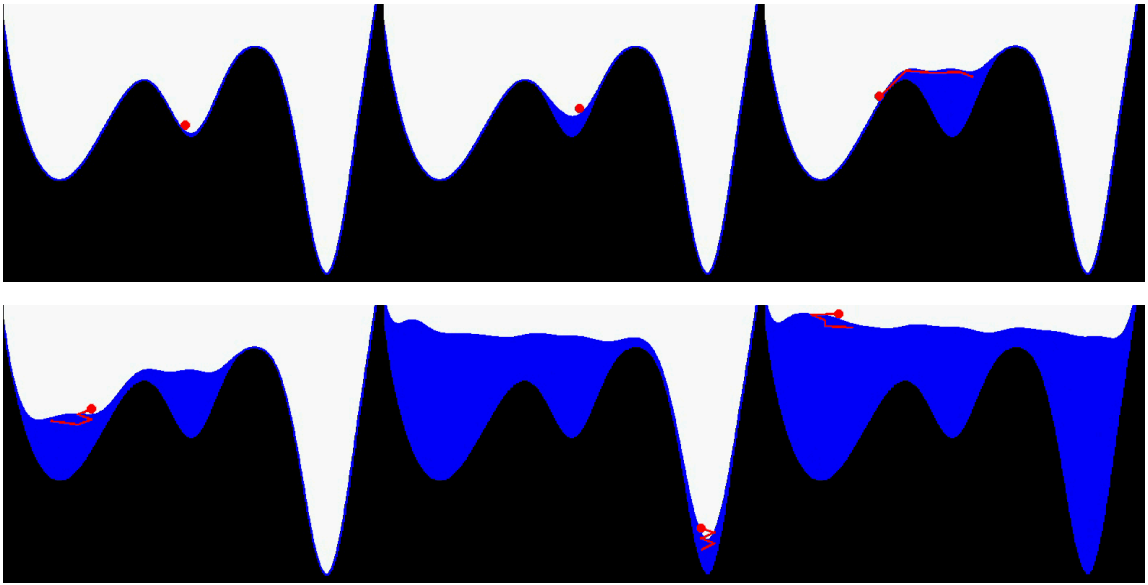


After the treatment



Metadynamics

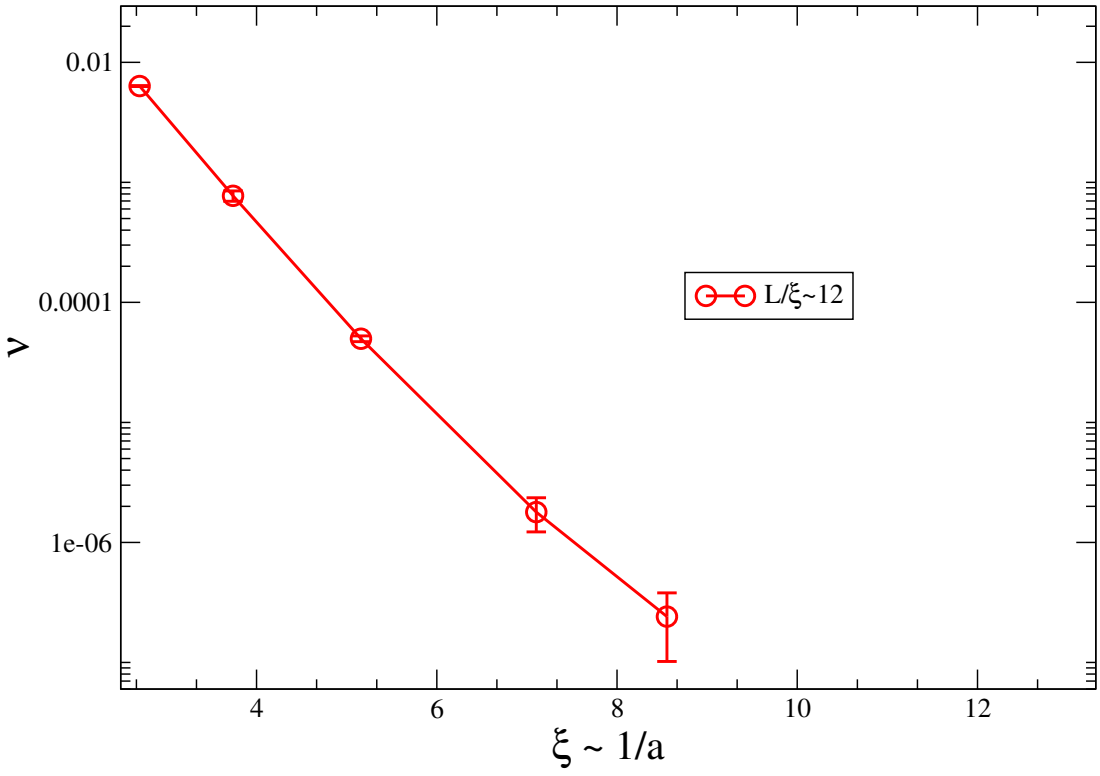
A. Laio, M. Parrinello, "Escaping free-energy minima" (2002)



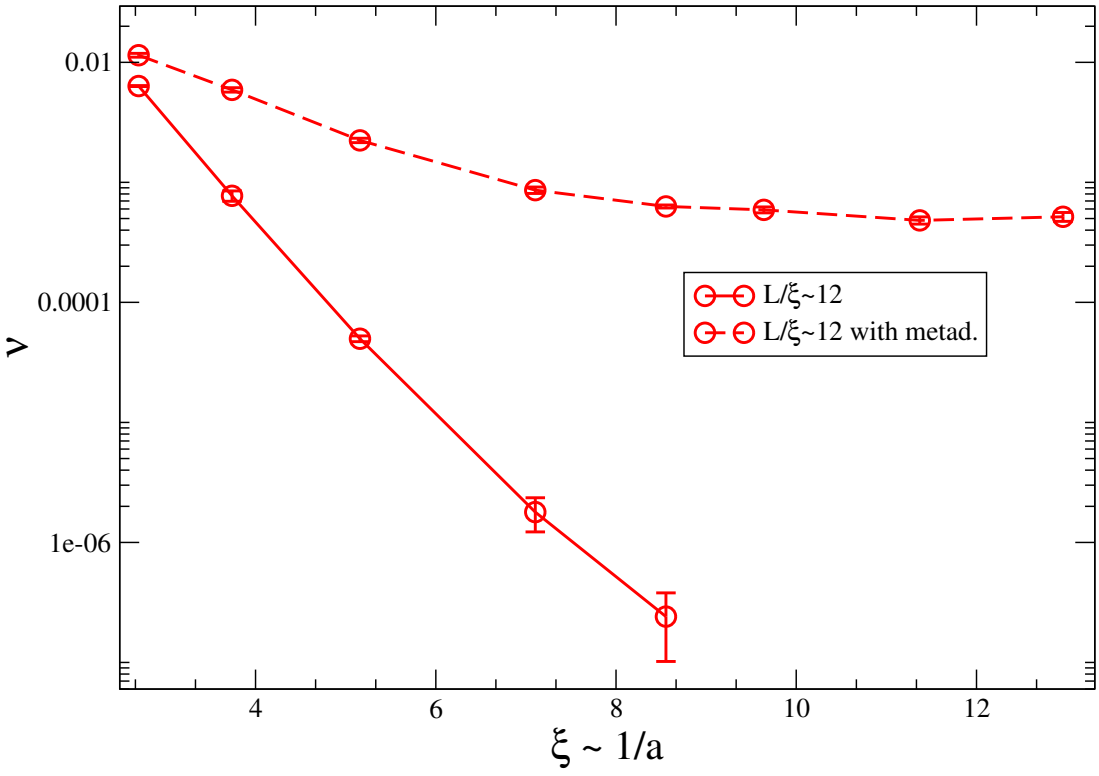
Similar in spirit to Wang Landau (2001) but applied to Molecular Dynamics
Widely adopted in biochemistry (protein folding, docking, dissociation...)

DOES IT WORK?

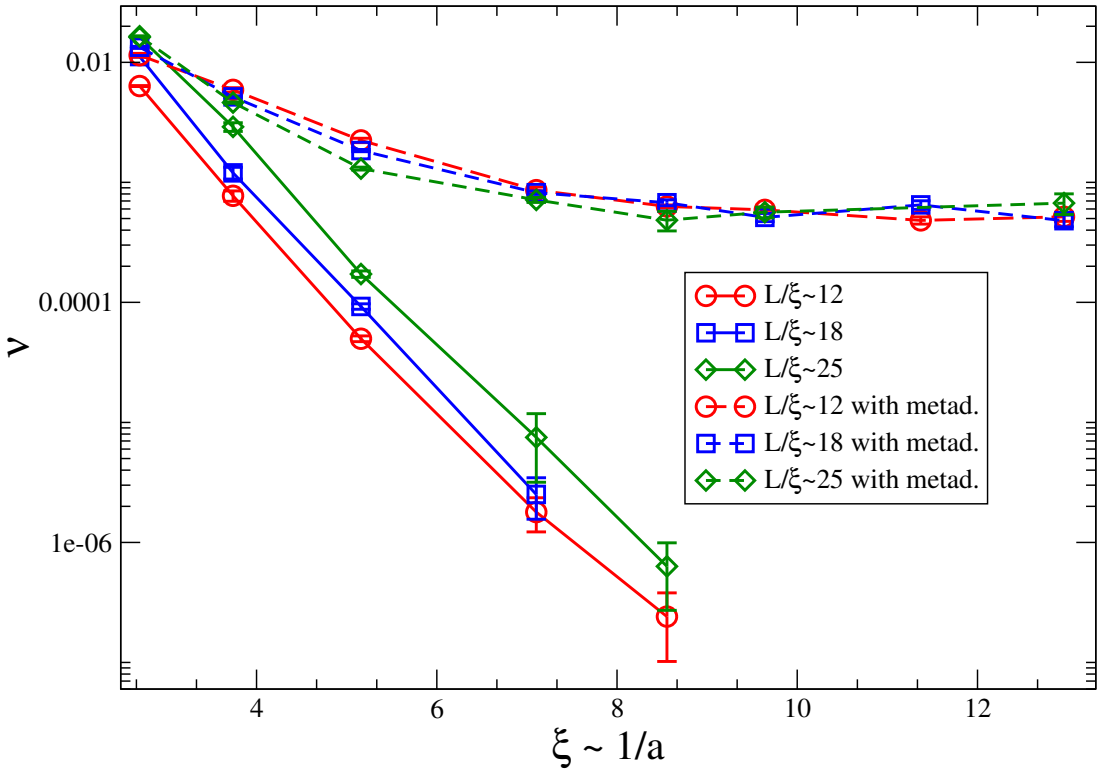
Transition frequency vs lattice spacing - HMC



And in Metadynamics



It works at various volumes



IT WORKS!!
BUT HOW?

How does it work?

Hamiltonian dependent on **simulation time** $H(t) = H(0) + V_{bias}(t)$

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Bias potential

- V_{bias} built in terms of previous values of a **collective variable**, here taken to be Q
- Example of a possible form of the potential:

$$V_{bias}(t + dt) = V_{bias}(t) + c \cdot \exp\left[-\frac{1}{2}\left(\frac{Q - Q(t)}{\sigma}\right)^2\right]$$

To avoid evaluating too many "exp" we actually use **triangles on a grid**

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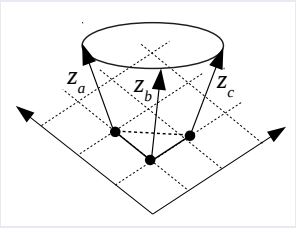
At convergence (long simulated time)

- V_{bias} provides a negative image of the free energy $F(Q) = -\log Z(Q)$
- The dynamics of the system is completely flat w.r.t Q

Which definition of Q?

Geometrical: sum of the solid angle between z on all triangles



$$Q_g = \frac{1}{2\pi} \sum_{\nabla,\Delta} \arg\left[(\vec{z}_a, \vec{z}_b)\,(\vec{z}_b, \vec{z}_c)\,(\vec{z}_c, \vec{z}_a)\right]$$

This is matemagically an integer number

✓ **perfect** to measure the actual topological charge

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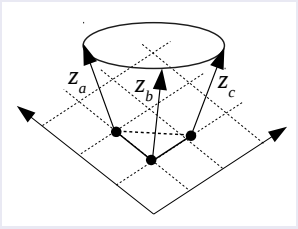

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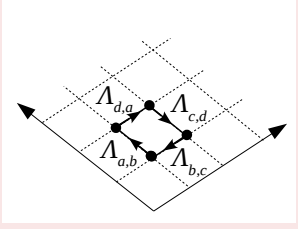
Gauge definition: plaquette of Λ



$$Q = \frac{1}{2\pi} \sum_{\square} \mathrm{Im}\square = ZQ_g + \eta$$ - Not an integer number

✗ **not ideal** to measure the actual topological charge
✓ **useful** as a collective variable: $F_\Lambda = -\partial_\Lambda V^Q_{bias} \propto \partial_\Lambda Q \neq 0$

- Field Λ must be smoothed, so that $\sqrt{\langle \eta^2 \rangle} \lesssim 1$ and $Z \sim 1$
- Analytical smoothing easily differentiable: **stout smearing**

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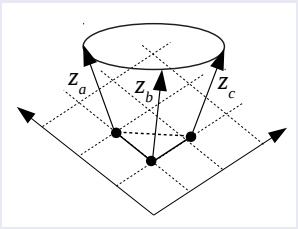

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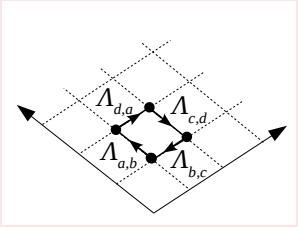

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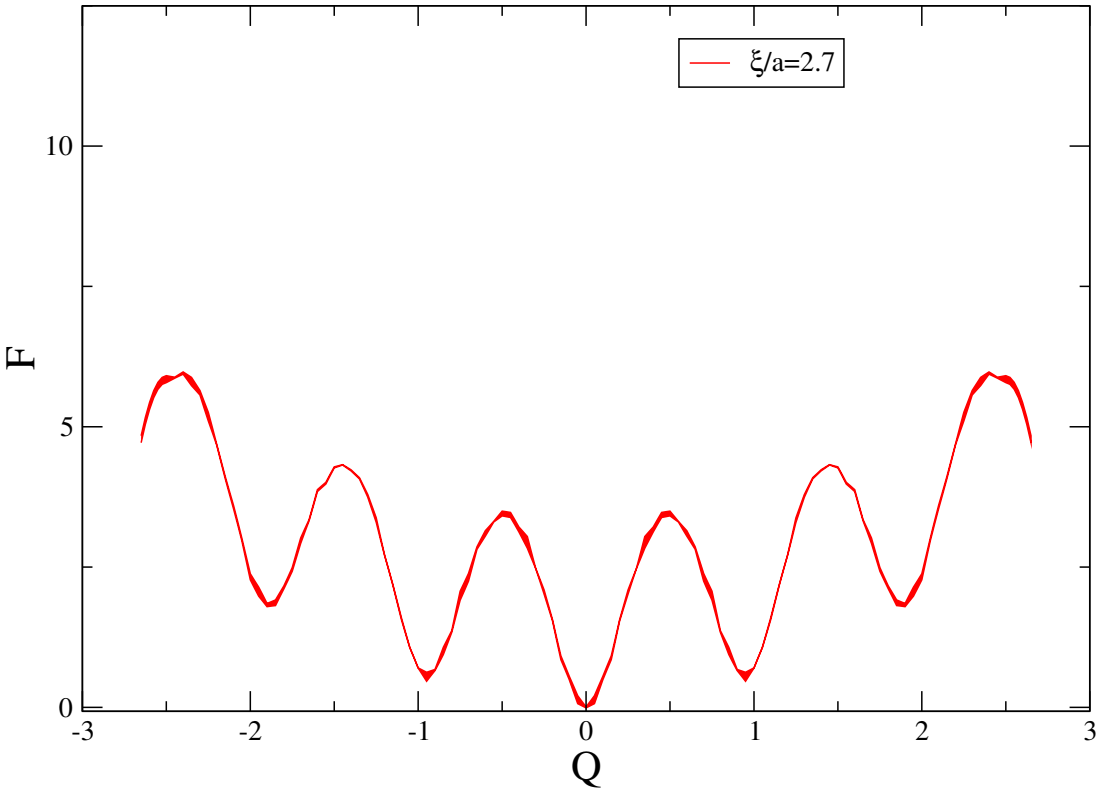
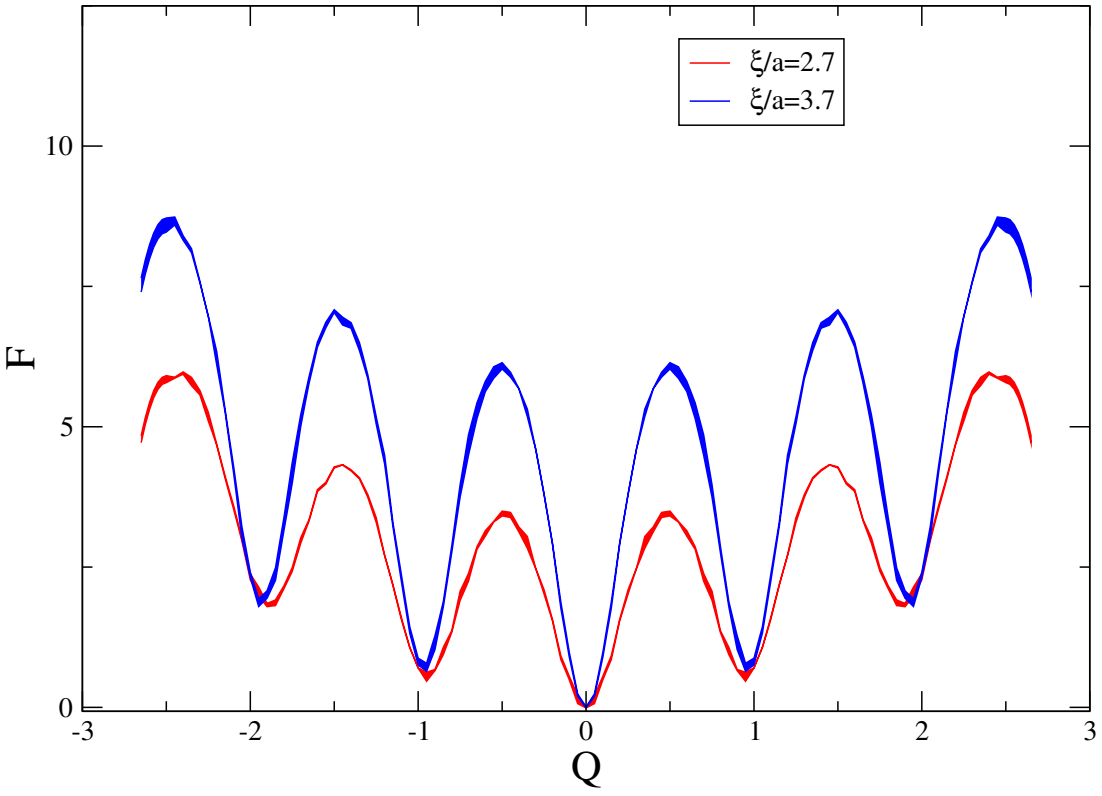
What's the shape of $F(Q)$?


ξ/a=2.7
F
Q
10
5
0
-3
-2
-1
0
1
2
3


ξ/a=2.7
ξ/a=3.7
F
Q
10
5
0
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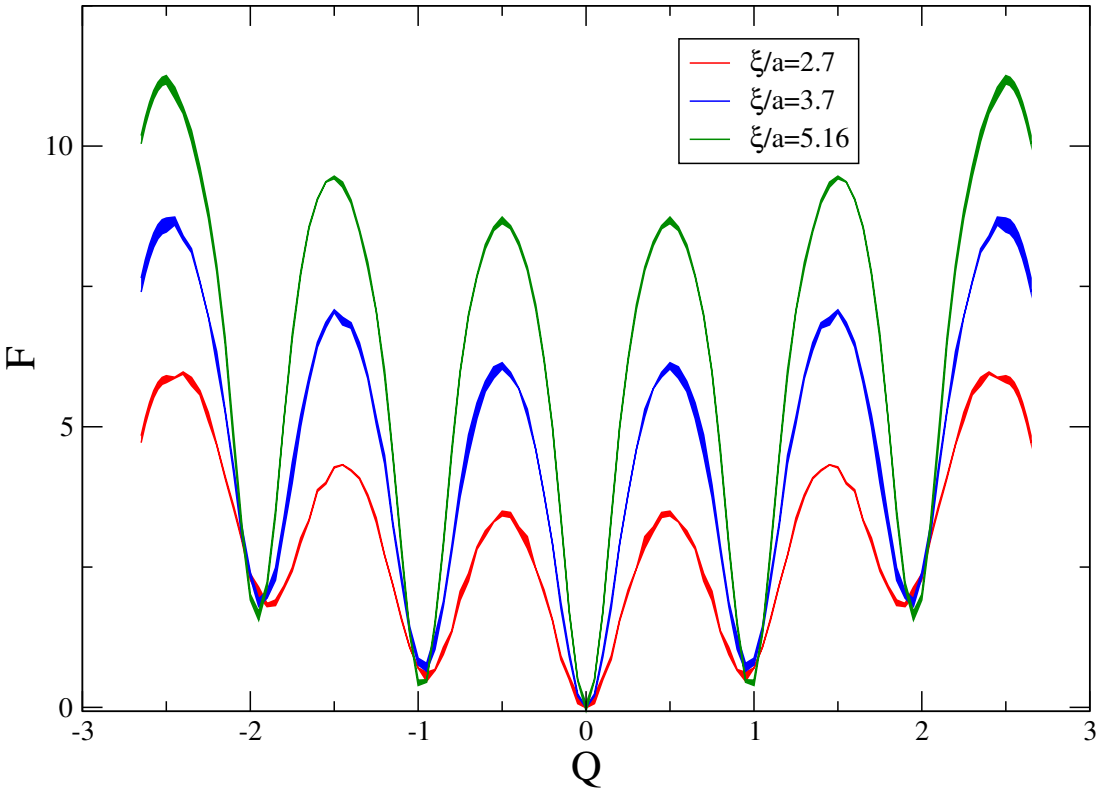
-1
0
1
2
3


ξ/a=2.7
ξ/a=3.7
ξ/a=5.16
F
Q
0
5
10
-3
-2
-1
0
1
2
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"What about the **sampled distribution** of Q?"

At convergence

By construction $F(Q) = -\log Z(Q)$ which means that

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in the generated sample

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"So you are sampling a different distribution!!!"

$F(Q)$ can be used to **reweight** the distribution:

$$\langle O \rangle = \frac{\sum_i O_i \exp\left[-F(Q_i)\right]}{\sum_j \exp\left[-F(Q_j)\right]}$$

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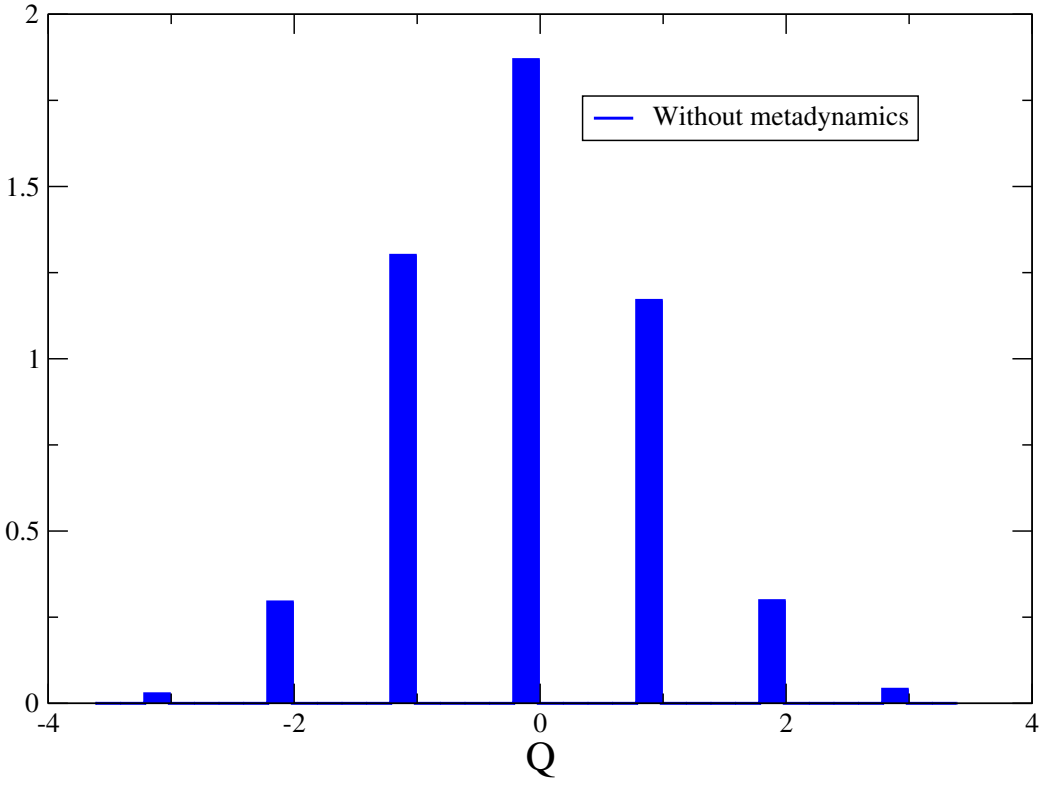
Reweighting costs

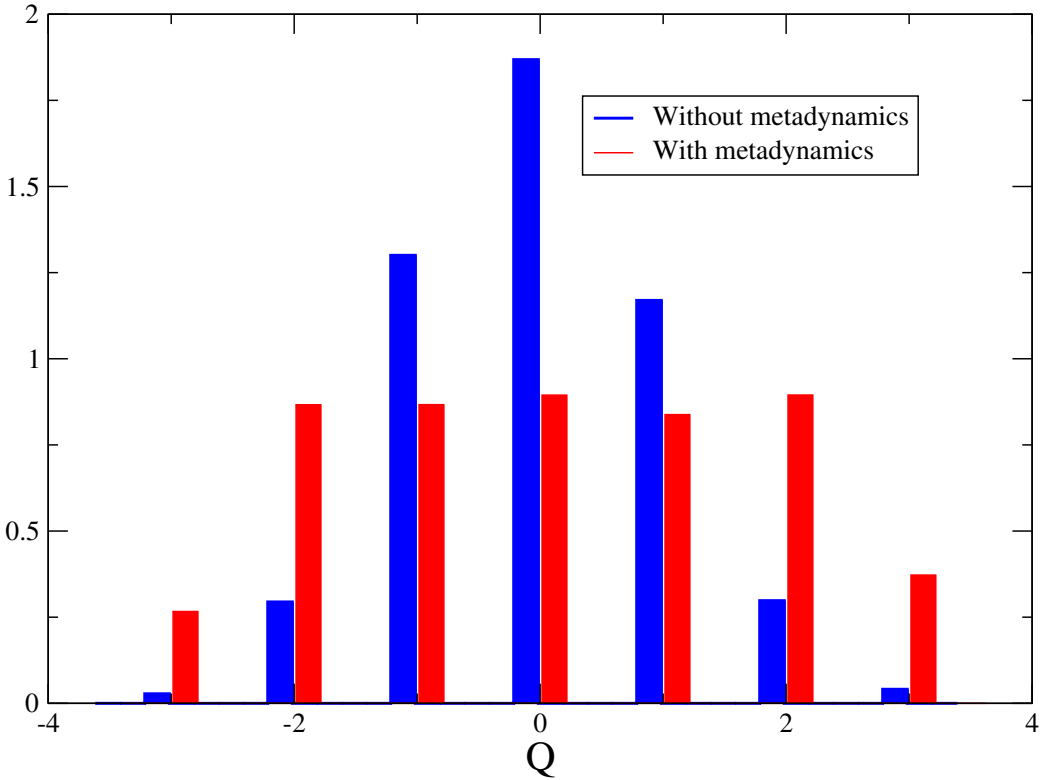
- By reweighting we suppress configurations with non-integer charge
- Nonetheless the configurations generate by metadynamics are uncorrelated
  - We agree with HMC where it works, but we achieve increasingly large speed-up as $a \to 0$
  - We obtain sensible results at reasonable cost, even when the HMC is completely frozen

The associated costs seems to scale well with a and V (see next plots)

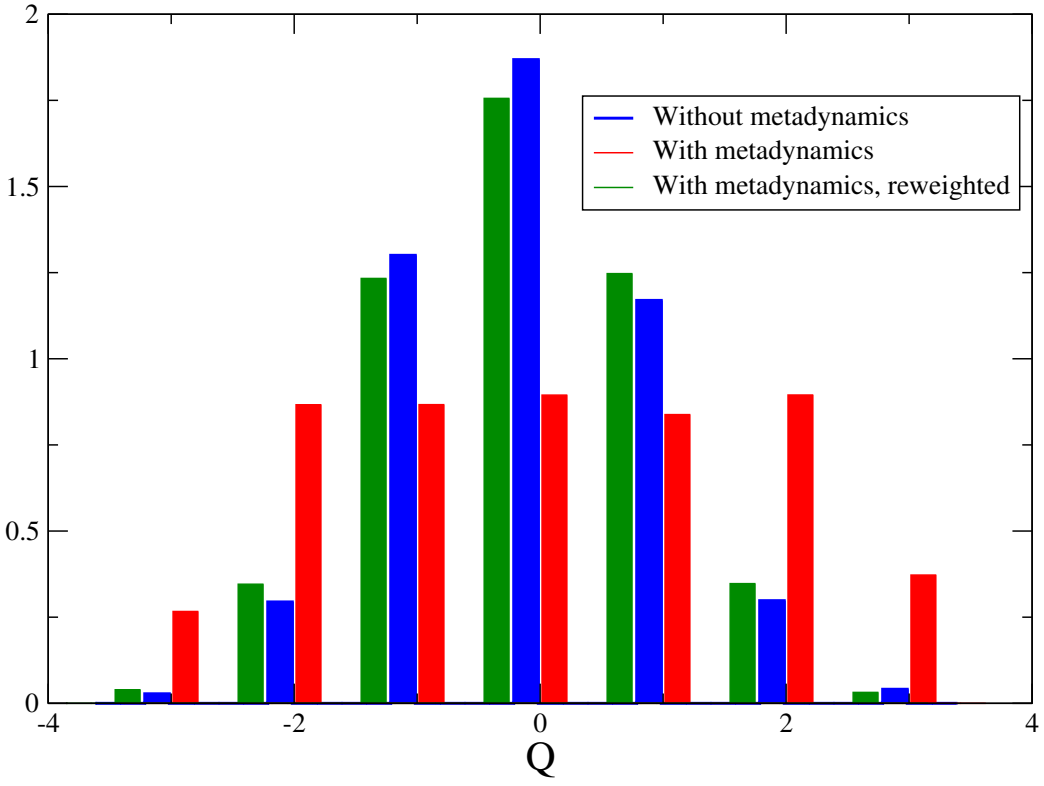
$\rho(Q)$, HMC (40M painful trajectories, $\beta = 0.75$, $\xi/a \sim 5.16$, $L/a = 60$)



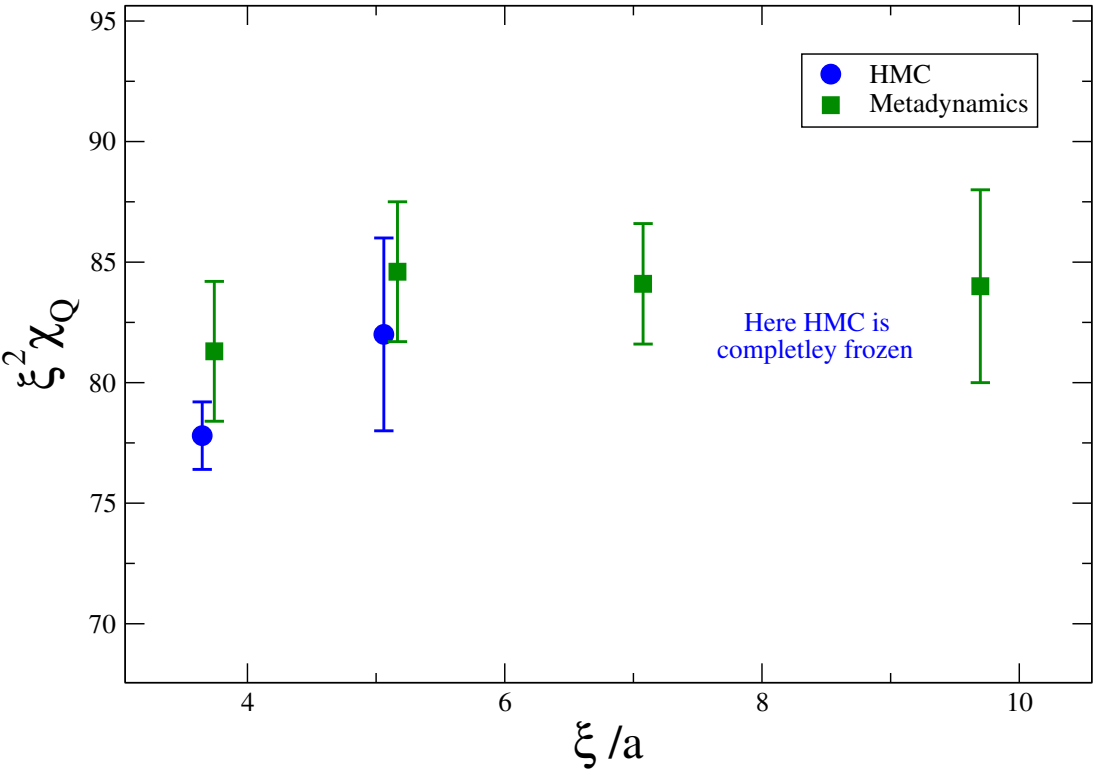
$\rho(Q)$, metadynamics (700k trajectories)



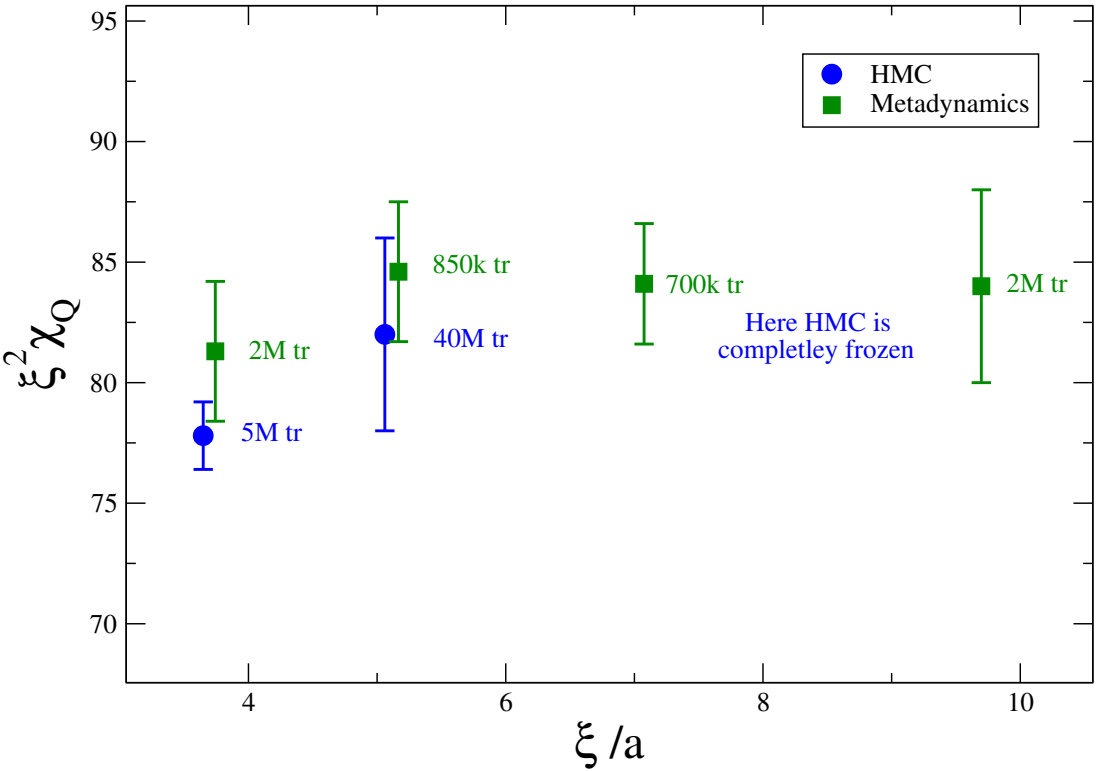
Reweighting



Topological susceptibility



Topological susceptibility - The cost



Other comments

"The algorithm is not ergodic!"

- Left to itself, the algorithm would explore with equal probability **all topological sectors**
- We don't want to sample sectors with **too large charge** (suppressed after reweighting)
- We **constrain** the dynamic in the range $[-Q_{max}; +Q_{max}]$
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"You are violating the sacred principles of Monte Carlo methods!"

- In fact the algorithm does not build a Markov Chain of configurations $[z, \Lambda]$ at all!
- You have to think in terms of the enlarged configuration space $\{[z, \Lambda] \otimes V_{bias}\}$
- Indeed it was rigorously shown that:

The correct sampling of the configuration space is obtained

after reweighting

[*Equilibrium Free Energies from Nonequilibrium Metadynamics*,
G.Bussi, A.Laio, M.Parrinello, PRL96 (2006)]

Extension to QCD

No conceptual difference

It amounts to simulate with a time-dependent (imaginary) $V_{bias} = \theta_{QCD} Q^{stout}$ where

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- Compute a new force term $\propto \partial_U Q$
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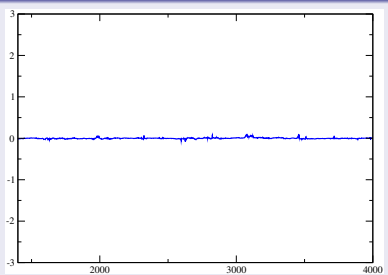
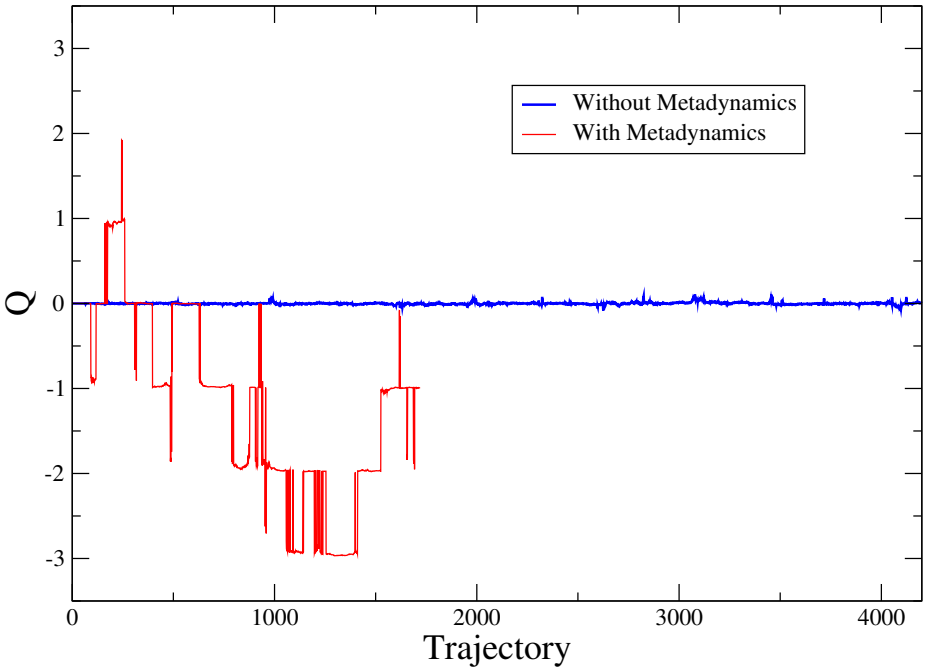
A first taste - In collaboration also with M.D'Elia, C.Bonati

Can we unfreeze this? $\longrightarrow$

- $\beta = 4.36$
- $a = 0.0397\,\mathrm{fm}$
- $M_\pi \sim 135\,\mathrm{MeV}$
- $L/a = 40$
- staggered
- $N_f = 2+1$
- small volume
- totally frozen



It looks promising...



Future improvements

Squeezing the best from the algorithm

- Make use of $Q \rightarrow -Q$ symmetry
- Make use of $Q \rightarrow Q + 2k\pi$ symmetry?
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More than topology?

- Can it be used to study **Gribov copies** problem in Gauge Fixing?
- Can it help computing **Spectral Density**?
- Can it be used to study **Finite Density**!?

Conclusions

Topology

- Different definitions of the Topological charge can be **useful for different reasons**
- Dependency on the topological sector is **non trivial**
- Simulations get frozen close to the continuum limit (**a long history**)

Metadynamics

Coupling **the past** history to reduce the occupancy of already explored states

- Bias potential inducing a force driving "**away from the past**"
- Topological charge gets **unfrozen**
- Distribution of Q at Long Simulation Time is **flat**: $P(Q) = 1$
- Reweighting restores the proper distribution
- Several parameters to tune...

The future

- Use all the available **symmetries**
- Further test **QCD** simulations
- Apply to **other problems**

...THANKS...

...FOR YOUR ATTENTION!!!