Metadynamics Remedies for Topological Freezing

Francesco Sanfilippo

UNIVERSITY OF Southampton
School of Physics and Astronomy

Mainly based on

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

A.Laio, G.Martinelli, F.S - JHEP 2016(7), 1-21

Summary

The Illness

1. Topological charge
2. Critical Slowing Down

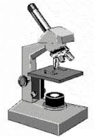
The Treatment

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

Drug Facts
Active ingredient (in each tablet) Purpose
Loratadine 10 mg Antihistamine
Uses temporarily relieves these symptoms due to hay fever or other upper respiratory allergies:
• runny nose • itchy, watery eyes
• sneezing • itching of the nose or throat
Warnings
Do not use if you have ever had an allergic reaction to this product or any of its ingredients.
Ask a doctor before use if you have liver or kidney disease. Your doctor should determine if you need a different dose.
When using this product do not take more than directed. Taking more than directed may cause drowsiness.
Stop use and ask a doctor if an allergic reaction to this product occurs. Seek medical help right away.
If pregnant or breast-feeding, ask a health professional before use.

Side Effects
(and side outcomes!)

1. Measuring the Free Energy
2. Reweighting



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

Winding number

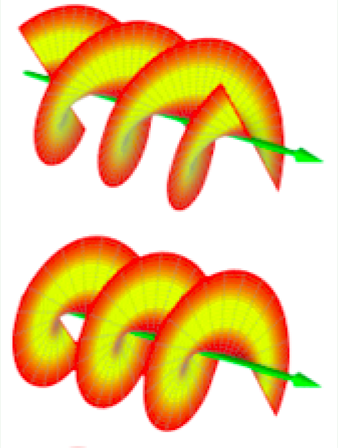
Topological charge **density** in QCD

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

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

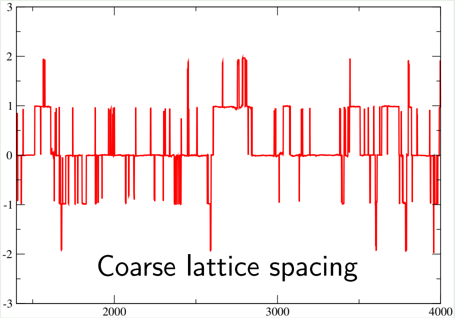
$$Q = \int d^4x \, q(x)$$

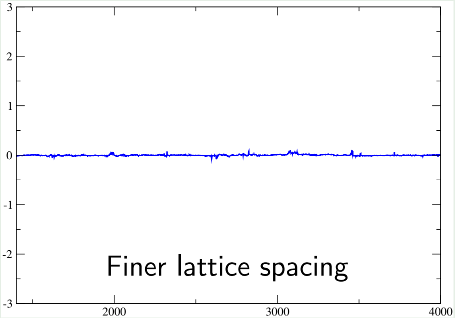
  related to the **winding number** of the field
- Several definitions on the lattice



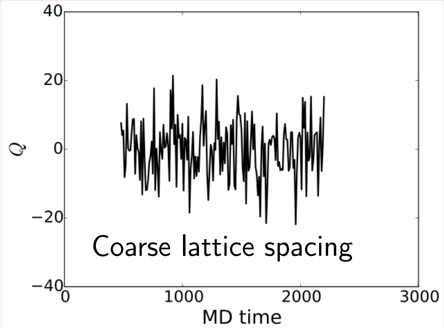
Topological charge slowing down - two examples

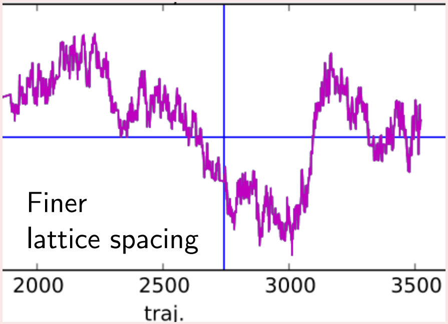
Staggered simulations for Axion Phenomenology (see G.Martinelli talk on Friday@14.20)





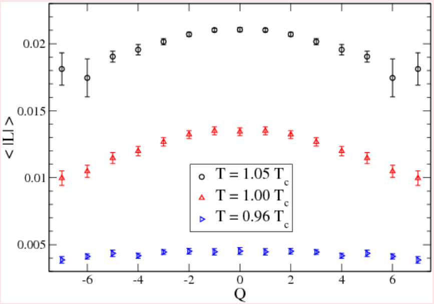
RBC/UKQCD: Domain Wall simulations for Charm (see T.Tsang talk on Friday@14)





Do we have to bother?

Can't we just ignore the problem?



NO!

[see e.g. M.D'Elia, F.Negro, PRD88 (2013)]

- At finite volume, Observables depends on Q
- Bad sampling of Q means to bias observables

Several solutions proposed

- Lattice QCD without topology barriers,
  M.Lüscher, S.Schaefer JHEP 1107 (2011)
- Simulate at strictly fixed topology,
  JLQCD, PRD74 (2006)
- Encourage tunneling on the point x^* where the $|q(x)|$ is the largest,
  P.de Forcrand et al., Nucl.Phys.Proc.Suppl. 63 (1998)
- Dislocation enhancement determinant,
  G.McGlynn, R.Mawhinney, PoS lattice'13 arXiv:1311.3695

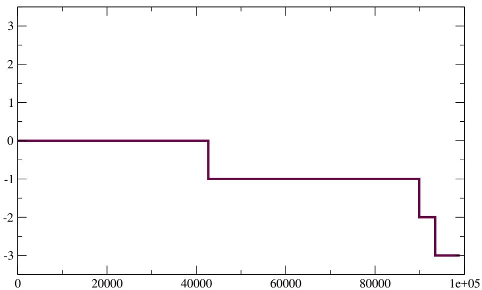
FROZEN

TOPOLOGICAL CHARGE?

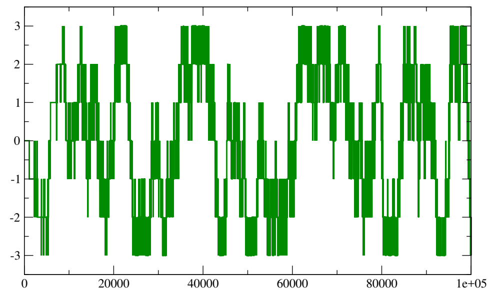
Metadynamics Elixir

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

Before

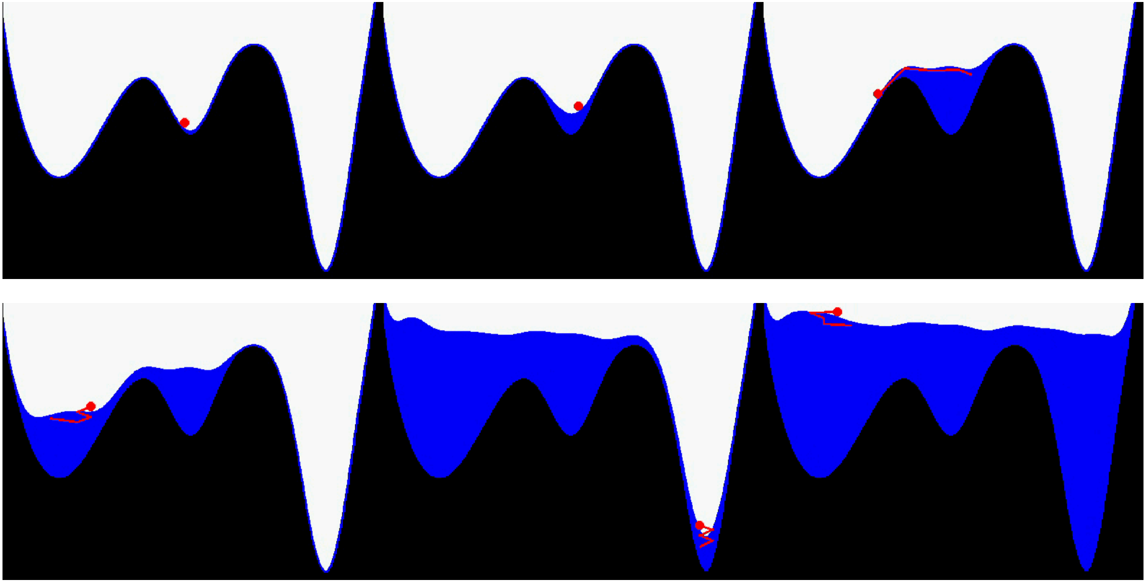


After the treatment



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...)

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 $A_\mu \in \mathcal{R}$

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

Gauge field A_μ has no kinetic term and could be integrated away, but we'd rather keep it

On the lattice

$$S = \beta N \sum_{n \in L^2} \sum_{\mu=1}^{2} |D_\mu \vec{z}_n|^2 , \quad D_\mu z_n = \Lambda_{n,\mu} z_{n+\hat{\mu}} - z_n$$

Like QCD...

- There is a topology Q
- There is a mass gap $M \sim 1/\xi$
- The beta-function is negative
- β sets the scale: $a \xrightarrow{\beta \to \inf} 0$

But simpler!

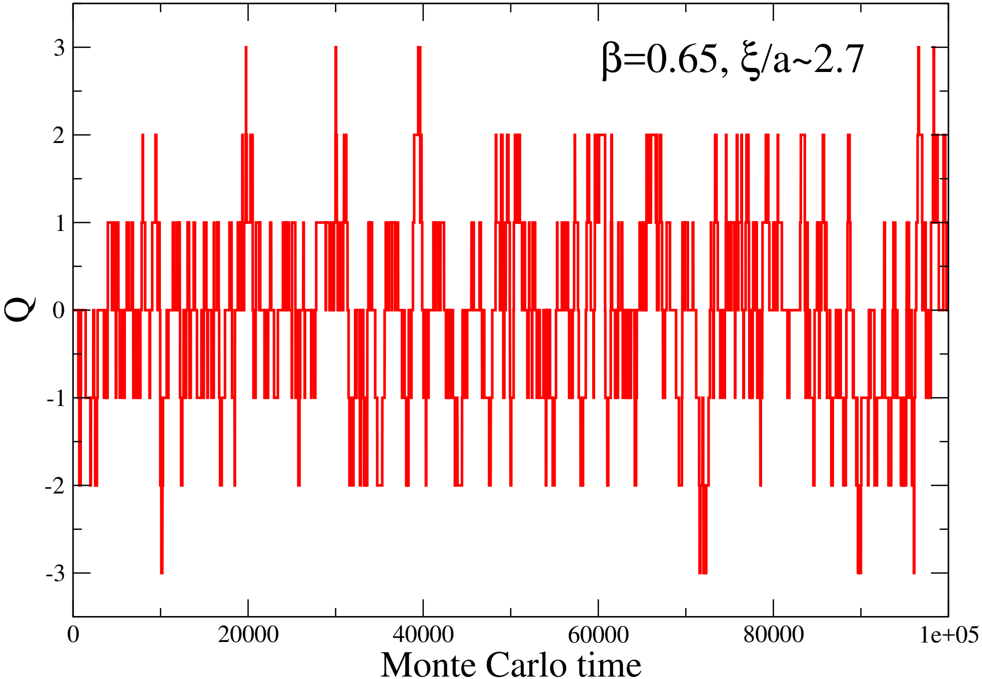
- Simulations can be run on a laptop! (actually: Ulisse cluster at Sissa)
- Excellent framework to test new algorithms

MOST IMPORTANT

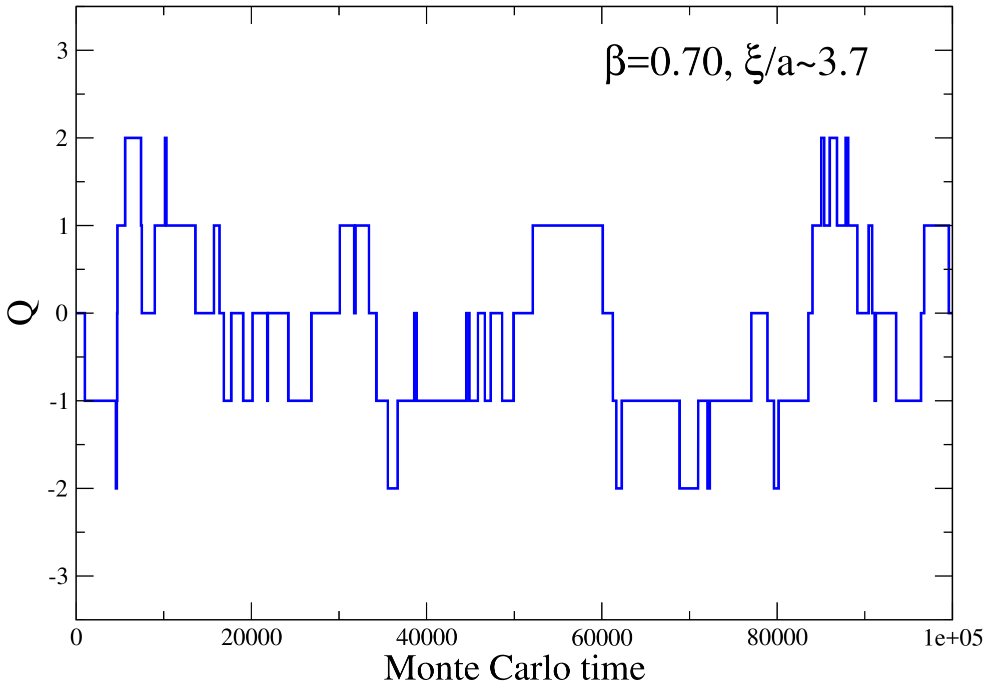
it suffers
from

TOPOLOGICAL
FREEZING

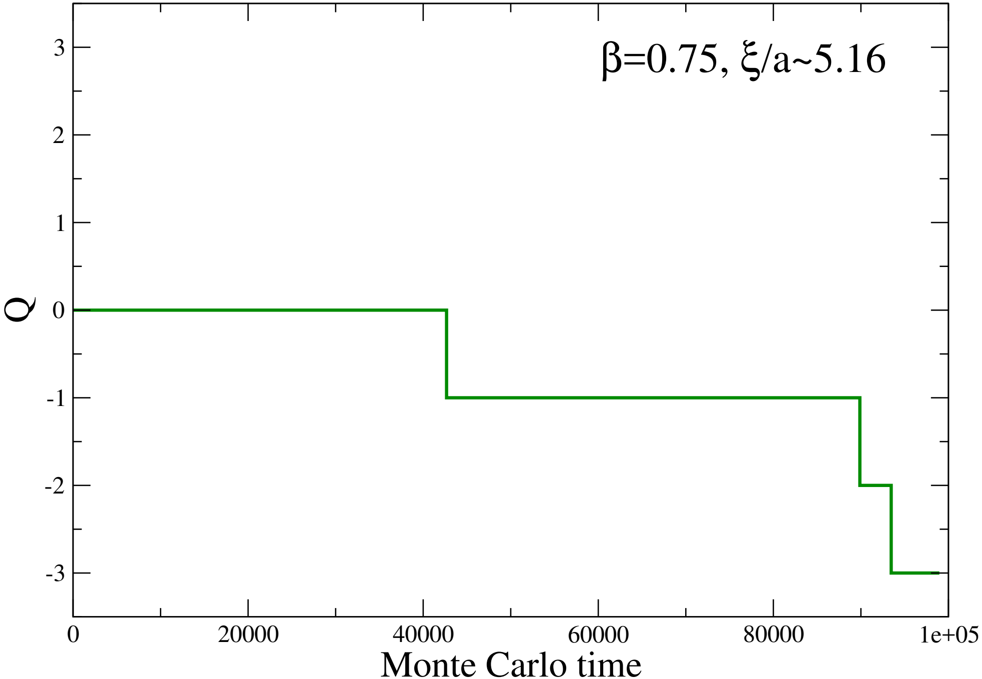
Topological charge evolution



Evolution on a finer lattice spacing (same scales)

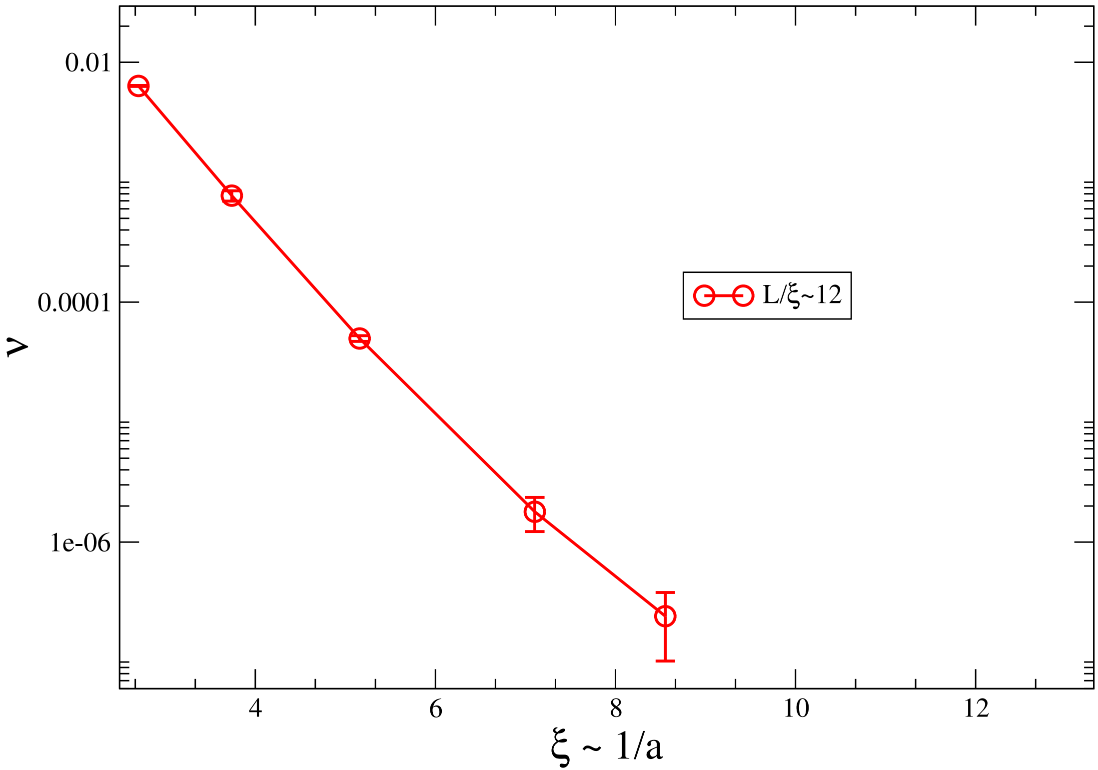


Going even finer

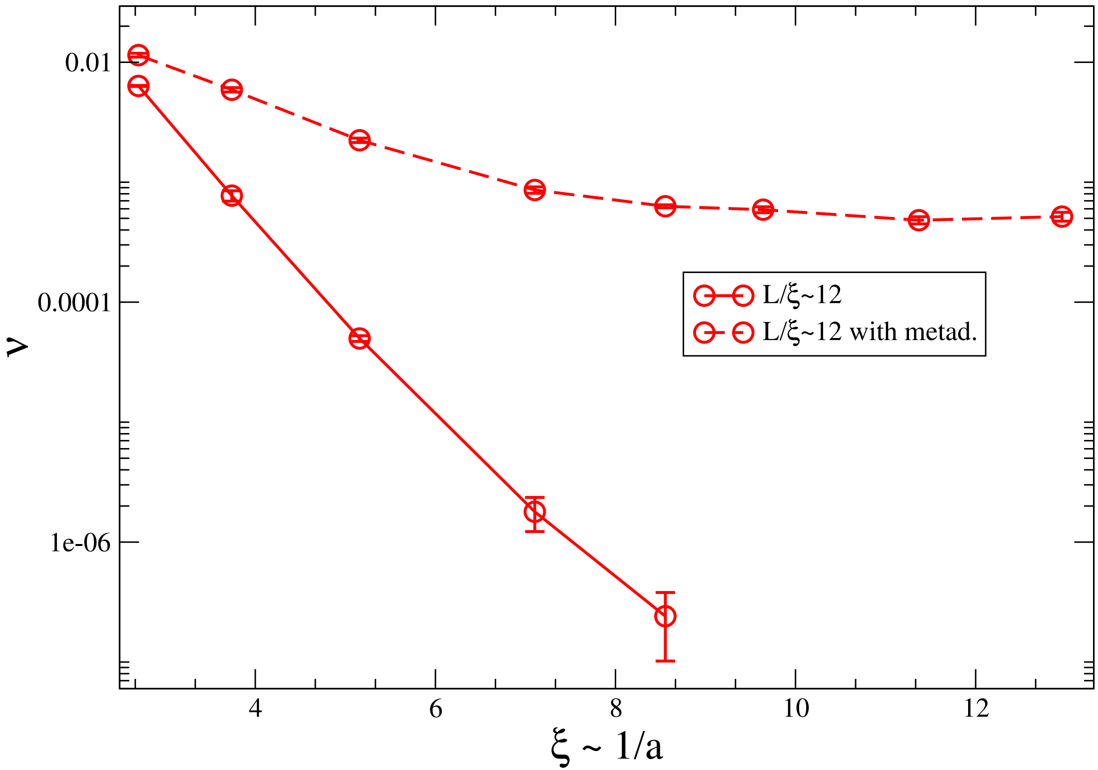


DOES METADYNAMICS WORK?

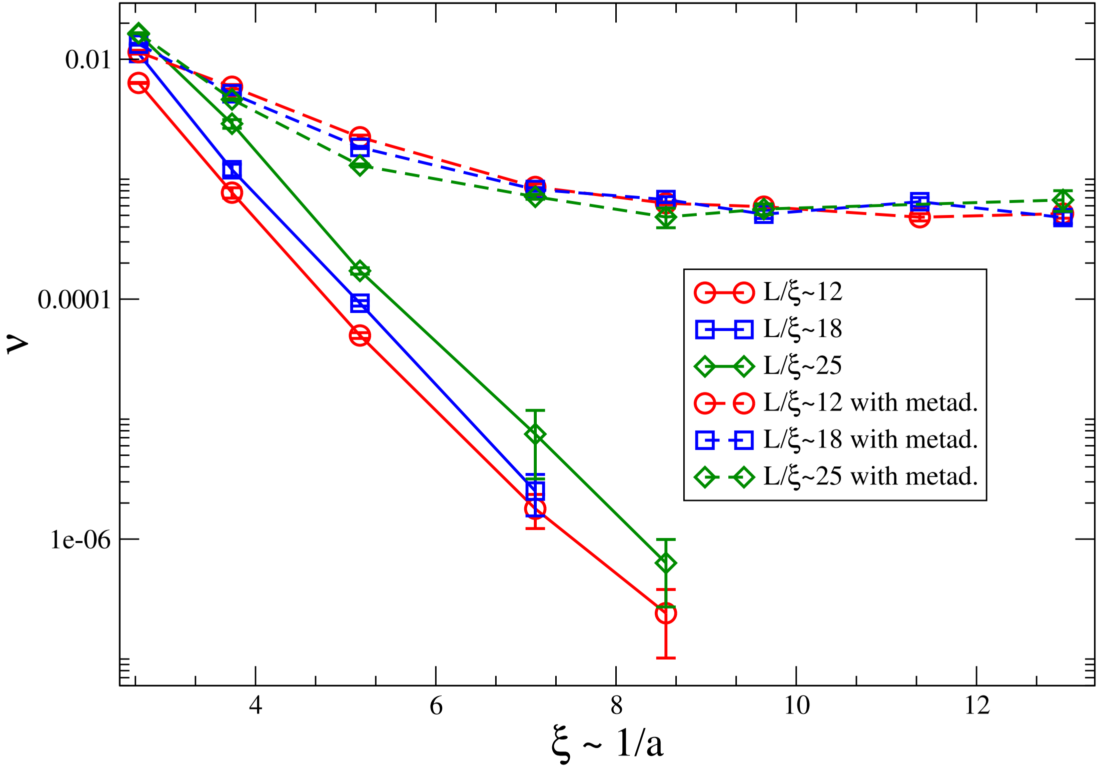
Transition frequency vs lattice spacing - HMC



And in Metadynamics



It works at various volumes



IT WORKS!!
BUT HOW?

How does it work?

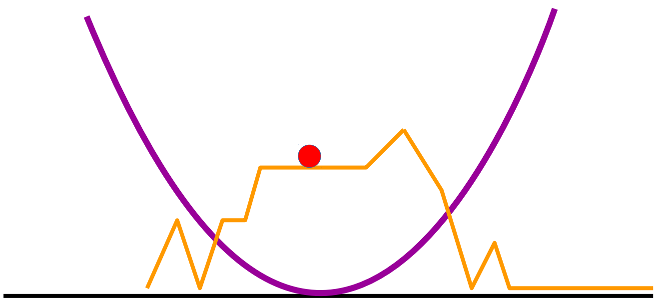
Action dependent on **simulation time** $S(t) = S(0) + V_{bias}(t)$

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**



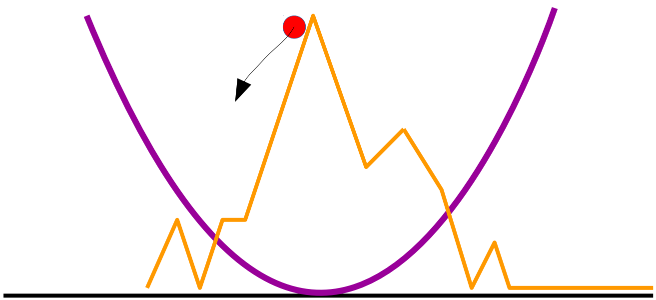
How does it work?

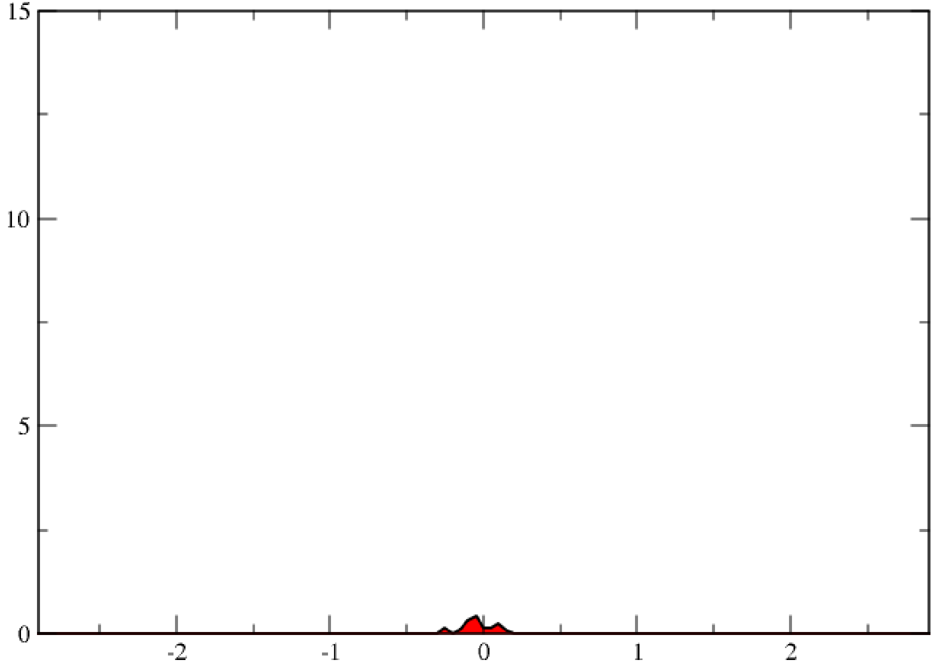
Dynamics

- The induced force $F = -\partial_U V_{bias}$ drives the system **away** from previous values of Q
- V_{bias} **reduces** the probability of occupying previous states
- At large simulation time V_{bias} fills the free energy wells

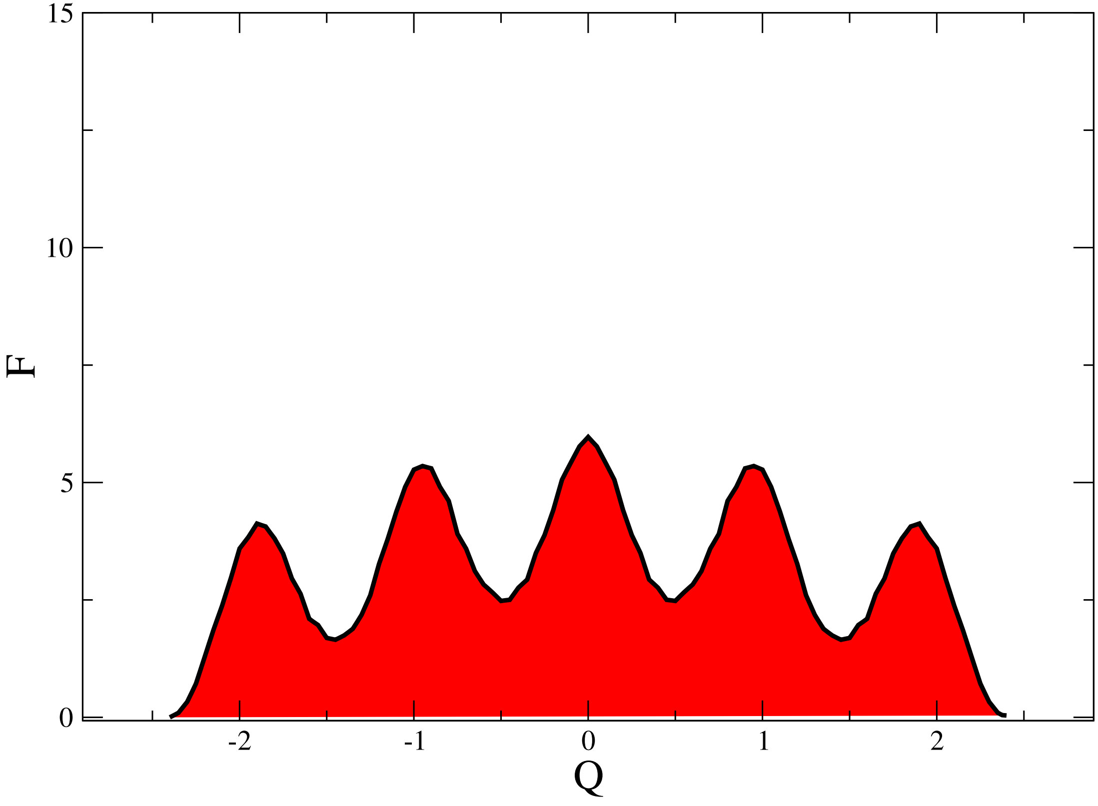
At convergence (long simulated time)

- 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

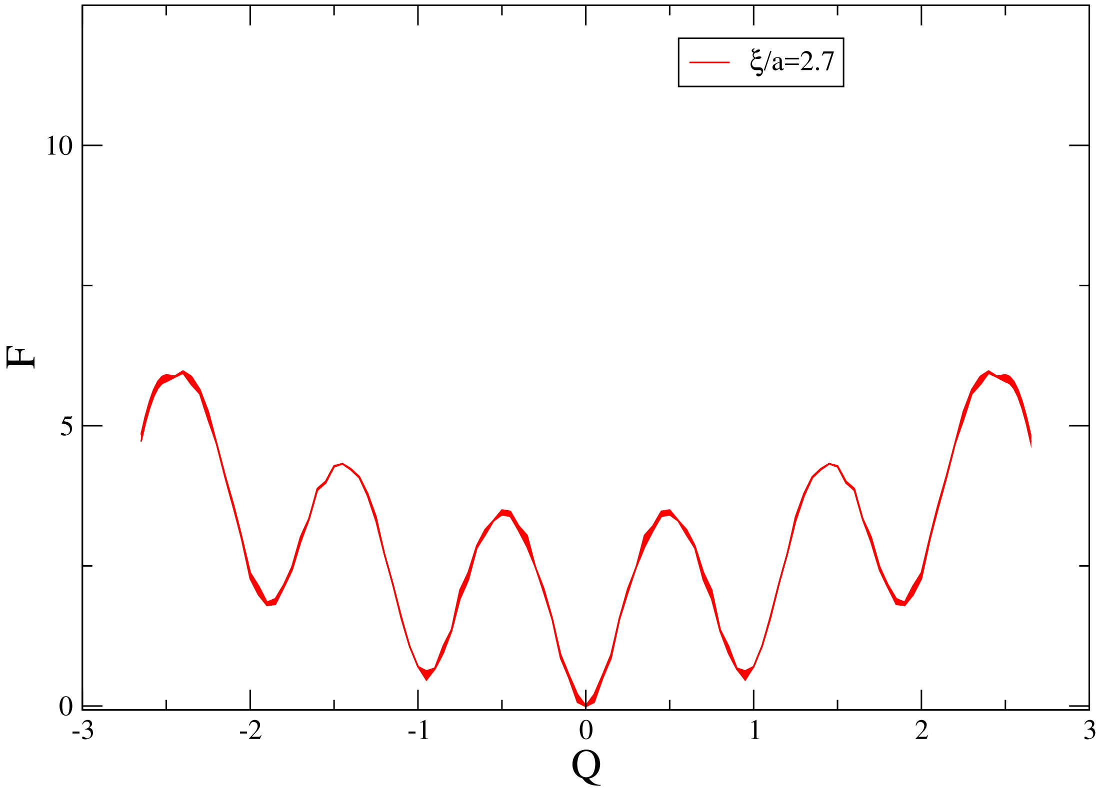




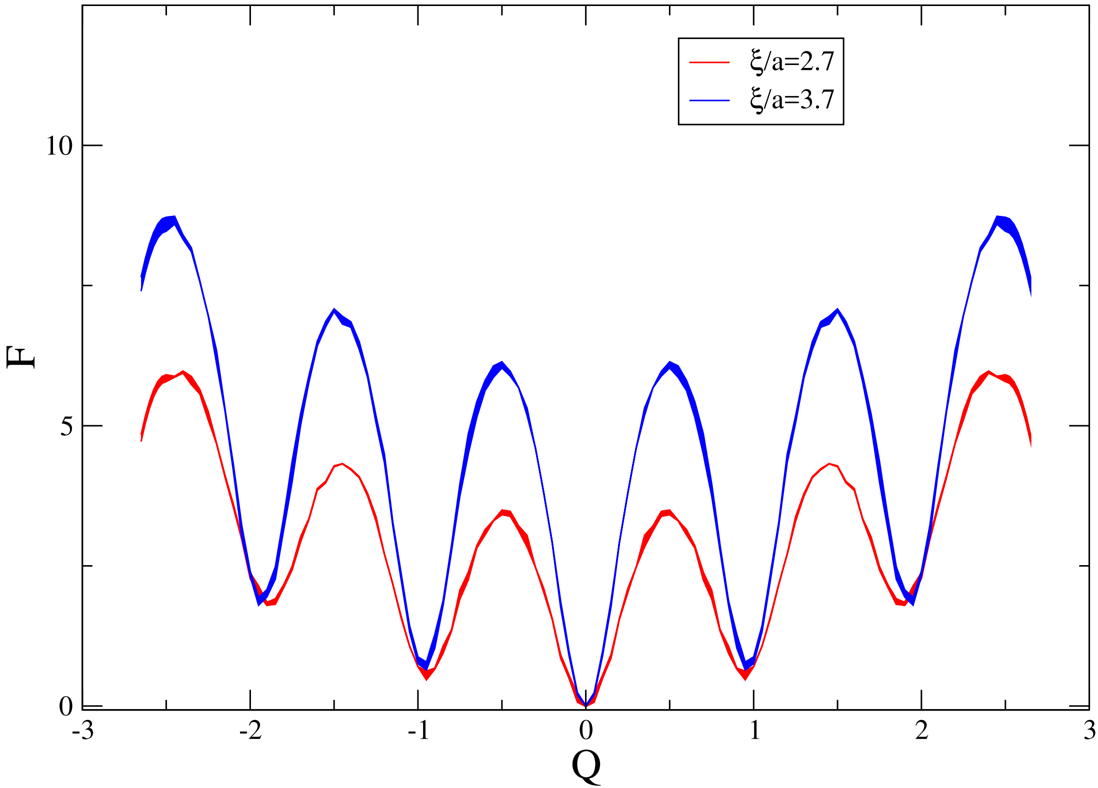
15
10
5
0
-2
-1
0
1
2



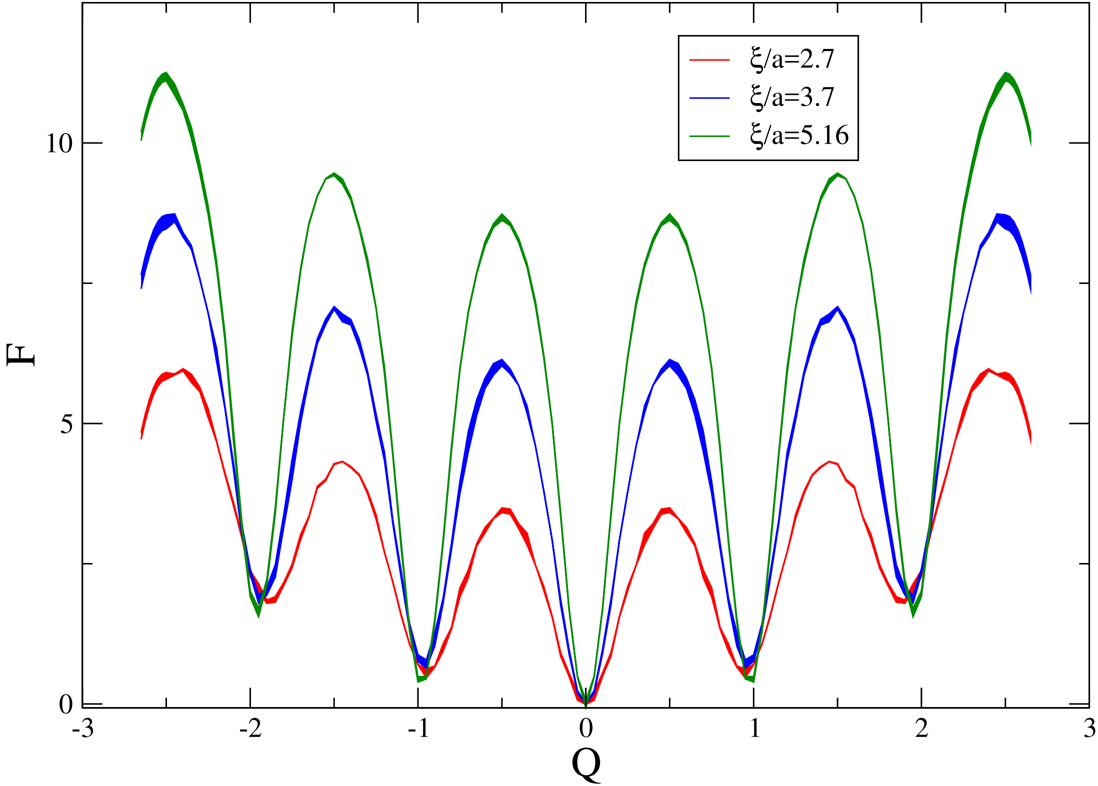
15
10
5
0
F
-2
-1
0
1
2
Q



ξ/a=2.7
F
Q
0
5
10
-3
-2
-1
0
1
2
3



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



ξ/a=2.7
ξ/a=3.7
ξ/a=5.16
F
Q
0
5
10
-3
-2
-1
0
1
2
3

"What about the **sampled distribution** of Q?"

At convergence

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

$$P(Q) = \text{const}$$

in the generated sample

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

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

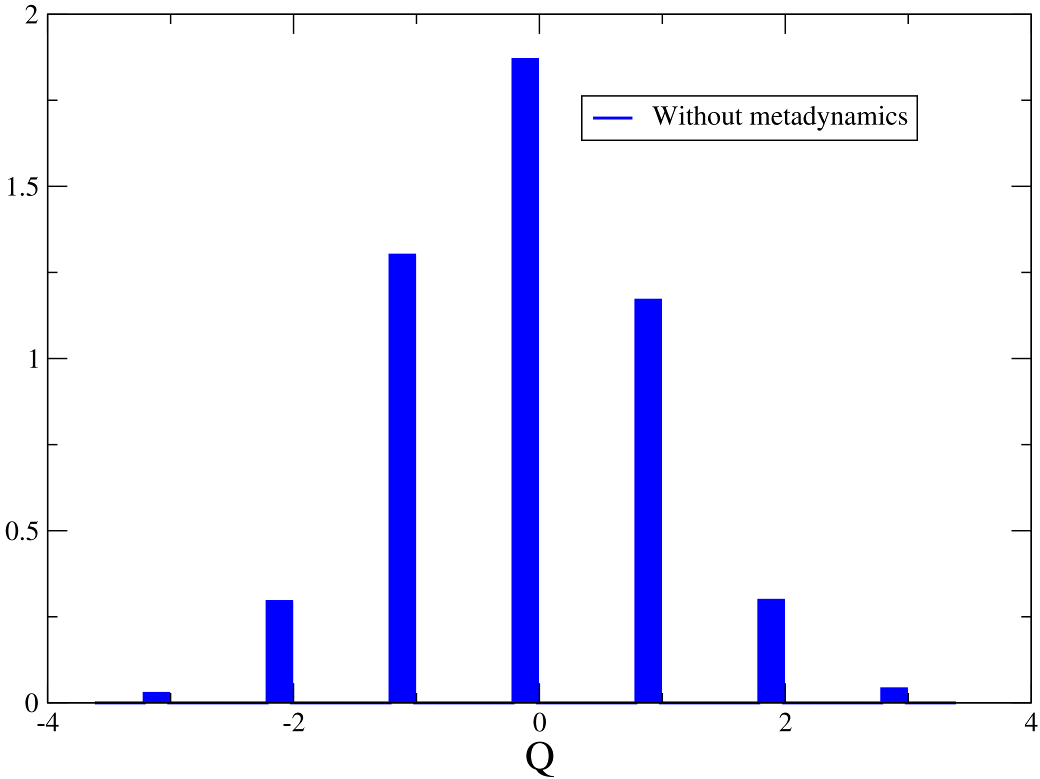
$$\langle O \rangle = \frac{\sum_i O_i \exp\left[-F(Q_i)\right]}{\sum_j \exp\left[-F(Q_j)\right]}$$

Reweighting costs

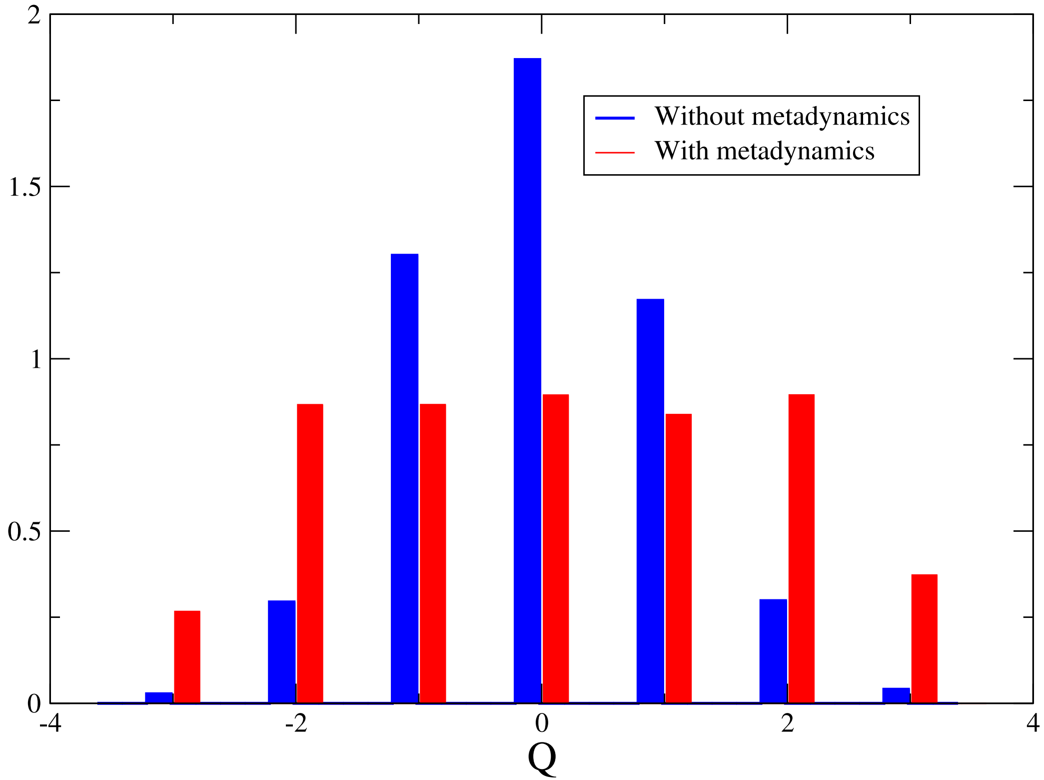
- By reweighting we suppress configurations with non-integer charge
- Nonetheless the configurations generate by metadynamics are uncorrelated
  - We agree with HMC where it works, but we achieve increasingly large speed-up as $a \to 0$
  - We obtain sensible results at reasonable cost, even when the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

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

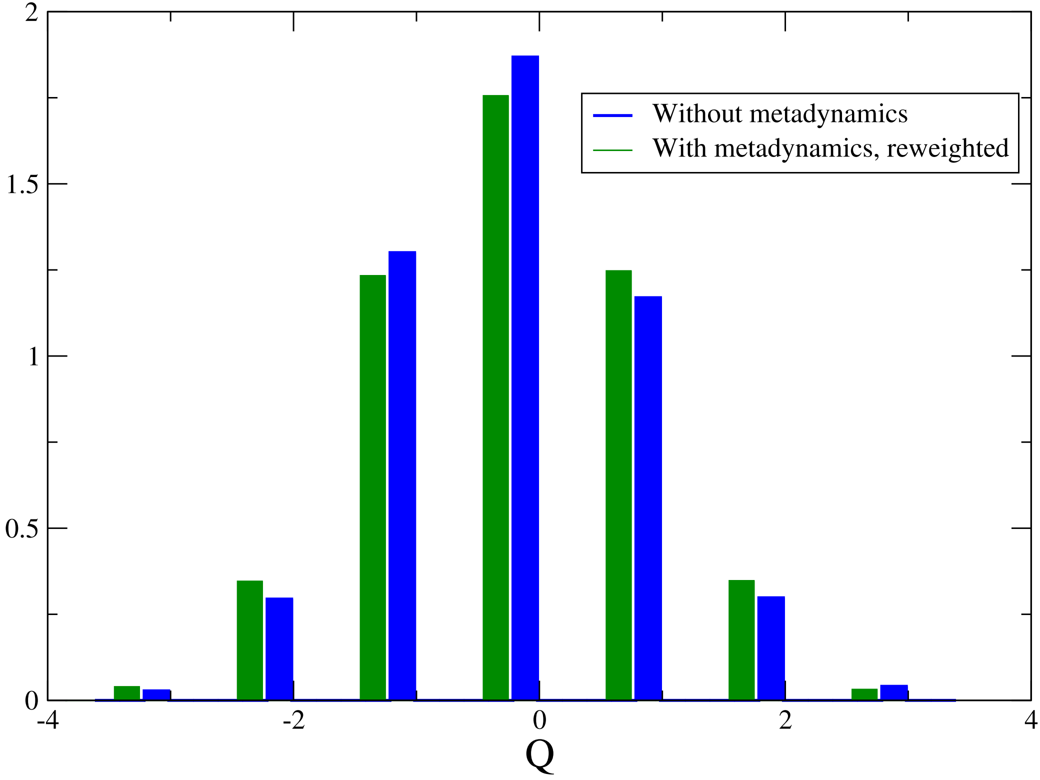
$\rho(Q)$, HMC (40M painful trajectories, $\beta = 0.75$, $\xi/a \sim 5.16$, $L/a = 60$)



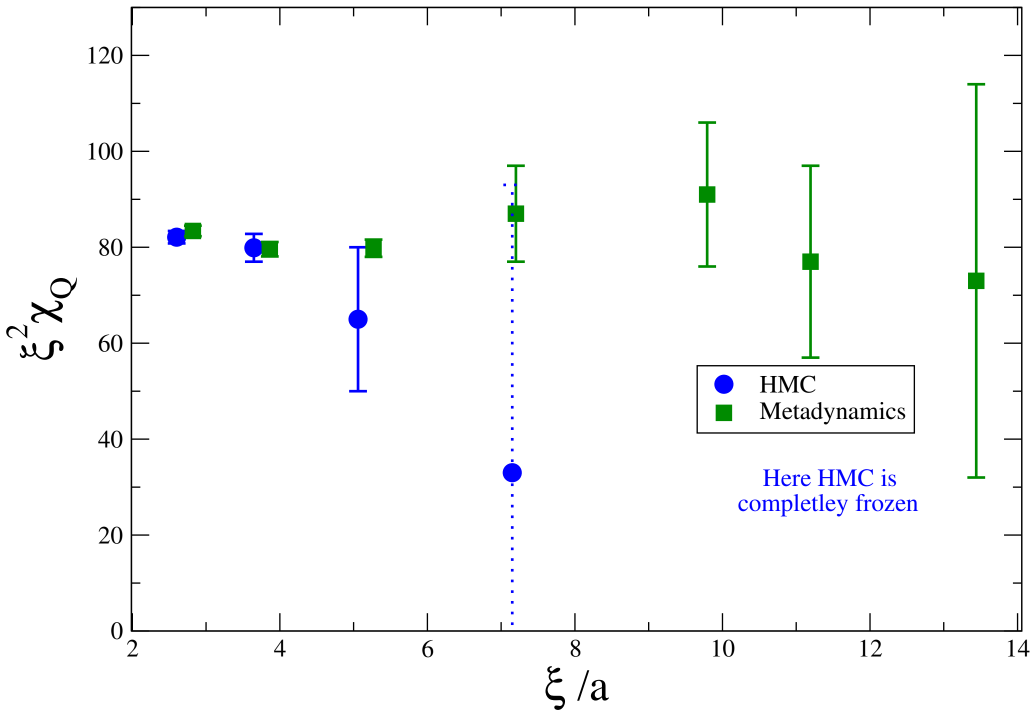
$\rho(Q)$, metadynamics (700k trajectories)



Reweighting



Topological susceptibility - 3M trajectories $L/\xi_g \sim 12$



Extension to QCD

No conceptual difference

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

$$\theta_{QCD}(t) = i\, F\left[Q^{stout}(t)\right]$$

Tune the ∼5 parameters on the basis of the $CP(N-1)$ experience

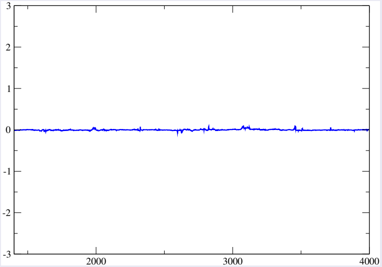
Ingredients

- Compute a new force term $\propto \partial_U Q$
- Stout smear the configuration (several levels, $\mathcal{O}(10)$ needed)
- Remap the force iteratively $F^{non-stout} \rightarrow F^{1-stout} \rightarrow \ldots F^{N-stout}$

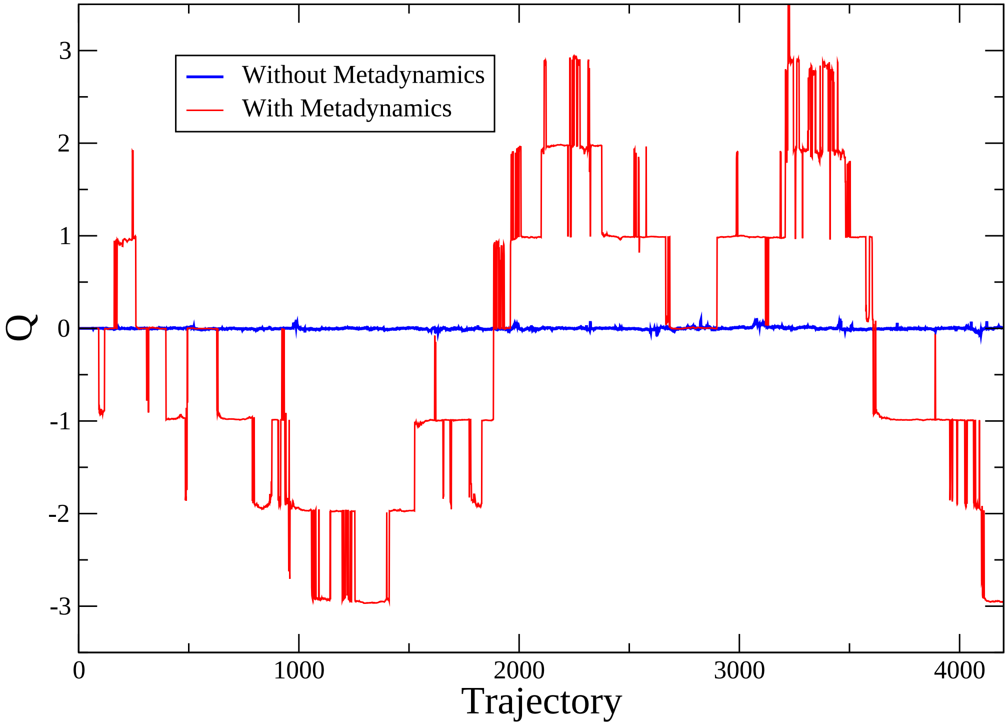
A first taste - In collaboration also with M.D'Elia, C.Bonati

Can we unfreeze this? ⟶

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



It looks promising...



Future improvements

Squeezing the best from the algorithm

- Make use of $Q \to -Q$ symmetry
- Make use of $Q \to Q + 2k\pi$ symmetry?
- Precondition the algorithm, feeding-in the information on $F(Q)$
- Improve the convergence starting from a guess of V_{bias}
- Include other collective variables

Extending to QCD

- No conceptual problems, just a bit of pain to implement
- Preliminary test shows encouraging results
- Needs more stout: 30-40% overhead (less important towards the continuum limit)

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**

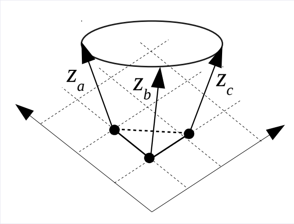
...THANKS...

...FOR YOUR ATTENTION!!!

BACKUP

Which definition of Q?

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



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

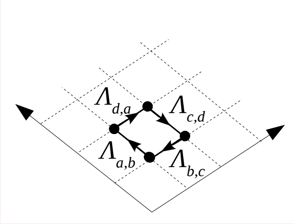
This is matemagically an integer number

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

✗ **useless** as a collective variable!

In fact $F_z = -\partial_z V^g_{bias} \propto \partial_z Q_g = 0$: the bias would induce no force on the system

Gauge definition: plaquette of Λ



$$Q = \frac{1}{2\pi} \sum_{\Box} \mathrm{Im}\Box = Z Q_g + \eta$$ - 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**

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

Other comments

"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)]