Reweighting for Topology at High-T

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- What's QCD topology and why is it interesting?
- How can the lattice have topology and why is it hard?
- What's interesting but extra hard at high temperatures?
- Reweighting: methodology, efficacy
- Reweighting: limitations and prognosis

Action and Pure Glue QCD

Covariant derivative $D_\mu = \partial_\mu - iA_\mu$, field strength $F_{\mu\nu} = i[D_\mu\, ,\, D_\nu]$.

Action Hermitian, scalar, dim-4. Two pure-glue terms:

$$\mathcal{L} = \frac{1}{2g^2}\,\mathrm{Tr}\, F_{\mu\nu}F^{\mu\nu} + \frac{\Theta}{32\pi^2}\,\mathrm{Tr}\,\epsilon^{\mu\nu\alpha\beta}F_{\mu\nu}F_{\alpha\beta}$$

First term: most of standard QCD.

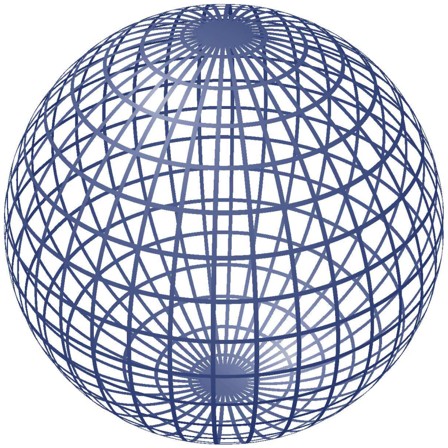
Second term: pure divergence: $\mathrm{Tr}\,\epsilon_{\mu\nu\alpha\beta}F^{\mu\nu}F^{\alpha\beta} = \partial_\mu K^\mu$

$$\int d^4x\, \mathcal{L} = \frac{1}{g^2}(\text{nontrivial}) + \int_\Sigma K_\mu d\Sigma^\mu$$

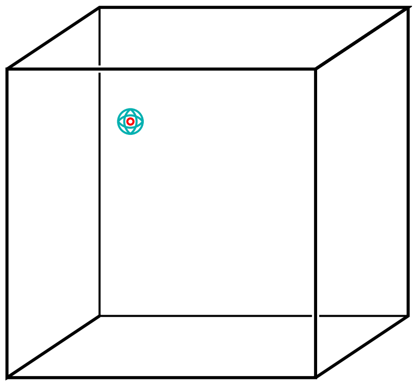
Gauge singularities and Topology

A^μ: *coordinate choice* on connection

Coord not always singularity-free



A^μ defined after we excise one point



Surface around cutout $= S^3$.

$A^\mu = \Omega^{-1}\partial^\mu\Omega$ pure-gauge on this surface.

$\pi_3(SU(N)) = \mathcal{Z}$, index $N_I = \int K_\mu d\Sigma^\mu = \int d^4x \frac{1}{16\pi^2}\,\mathrm{Tr}\, F\tilde{F}$

Instantons

On compact, no-boundary space,

$$\int d^4x \, \frac{1}{32\pi^2} \, \mathrm{Tr} \, \epsilon_{\mu\nu\alpha\beta} F^{\mu\nu} F^{\alpha\beta} = N_I \in \mathcal{Z}$$

Introduces CP, $\mathbf{T}$ violating phases into path integral

$$\exp\left[i\Theta \int d^4x \, \frac{1}{32\pi^2} \, \mathrm{Tr} \, \epsilon_{\mu\nu\alpha\beta} F^{\mu\nu} F^{\alpha\beta} \right] = \exp\left[i\Theta N_I \right].$$

$$Z_{\mathrm{eucl}}[\Theta] = \int \mathcal{D}A_\mu \, e^{-\frac{1}{2g^2} \int d^4x \, \mathrm{Tr} \, F^2} \times e^{i\Theta N_I}$$

Severely constrained experimentally.

$\Theta \to 0$ under axion mechanism. But cosmological details require we compute $F[\Theta] = -\ln Z_{\mathrm{eucl}}(T)$ for $T \sim 1\,\mathrm{GeV}$.

Are instantons big? Common?

Triangle inequality

$$\left| \mathrm{Tr}\, \epsilon_{\mu\nu\alpha\beta} F^{\mu\nu} F^{\alpha\beta} \right| \leq 2\, \mathrm{Tr}\, F_{\mu\nu} F^{\mu\nu}$$

Action of an instanton is at least

$$N_I = 1 \quad \Longrightarrow \quad \frac{1}{2g^2}\, \mathrm{Tr}\, F_{\mu\nu} F^{\mu\nu} \geq \frac{8\pi^2}{g^2}$$

giving $e^{-2\pi/\alpha_{\mathrm{s}}}$ suppression. Size distribution:

$$\chi \equiv V^{-1} \langle N_I^2 \rangle \sim \int \frac{d\rho}{\rho^5} \exp\left(-\frac{2\pi}{\alpha(\bar{\mu} \sim \rho^{-1})} \right)$$

Asymptotic freedom: Large $\rho \sim \Lambda_{\mathrm{qcd}}^{-1}$ instantons dominate

Small instantons *steeply* suppressed at small size ρ

Hi-T: $\rho \leq T^{-1}$. Very few instantons, $\chi \propto T^{-7-N_{\mathrm{f}}/3}$

Instantons, chiral symmetry

Chiral anomaly means instantons help violate axial current:

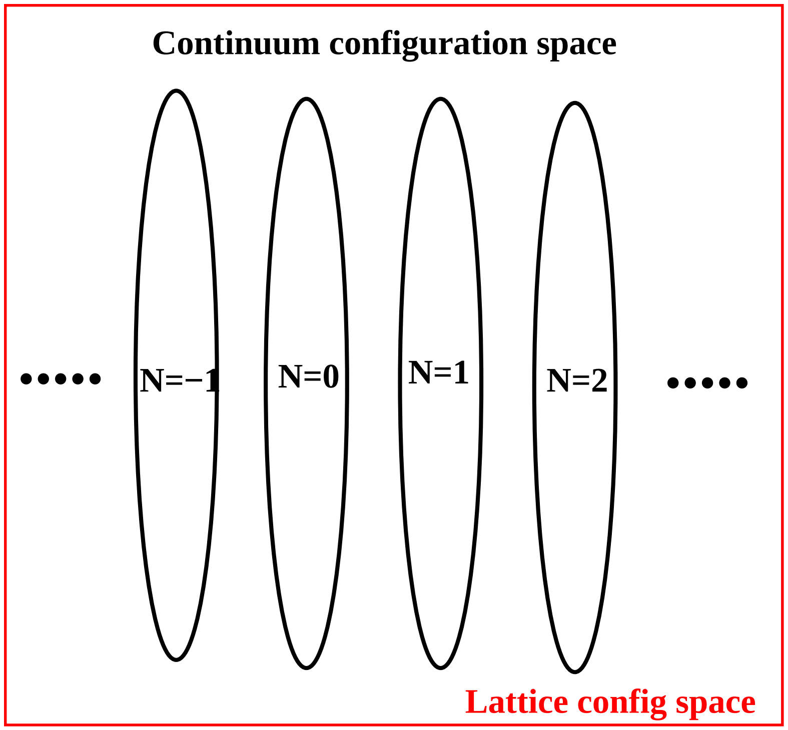
$$J^\mu_{5,u} = \bar{u}\gamma^\mu\gamma^5 u\,; \qquad \partial_\mu J^\mu_{5,u} = m_u \bar{\psi}\psi + \frac{1}{32\pi^2}\,\mathrm{Tr}\epsilon_{\mu\nu\alpha\beta}F^{\mu\nu}F^{\alpha\beta}$$

Instanton number $=$ number of chiral zero-modes of $\not{D}$.

Banks-Casher: density of near-zero modes $=$ Chiral Condensate.

Instantons related to chiral symmetry breaking, phase structure.

Why topology is "impossible" on lattice



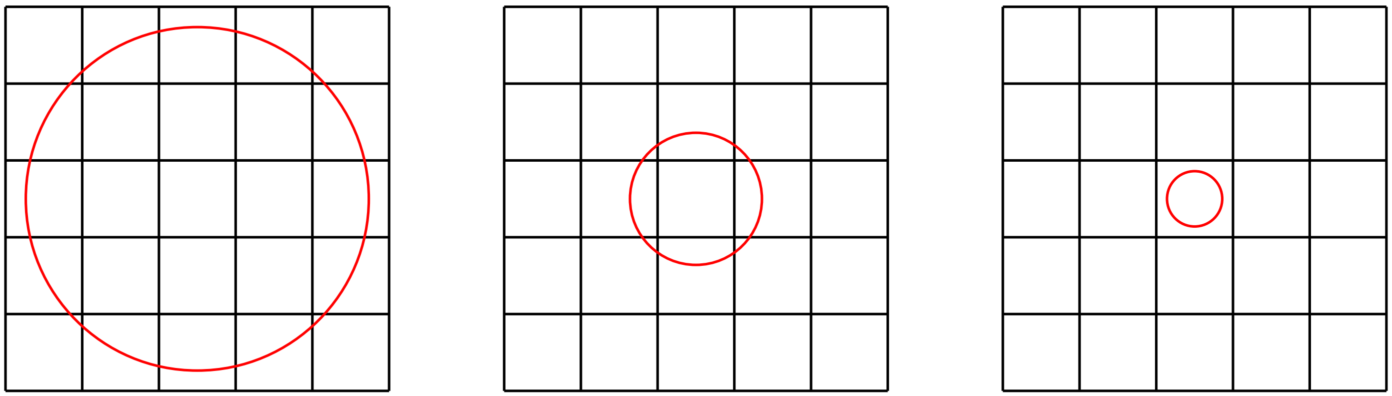
Continuum: each N_I value is a disconnected region of configuration space.

Lattice config. space $[SU(3)]^{4N_tN_xN_yN_z}$ is simply connected.

Lattice configurations must somehow "fill in gaps" between distinct topologies.

Why topology is possible on lattice

Think about different sizes of instantons on a lattice:



Big instanton: definitely there. Should have $N_I = 1$.

Smaller than latt-spacing: should *not* be there, $N_I = 0$

1-2 latt spacings across: now what? Ambiguous!

Topology changes because of “instantons” 1-2a across...

Why topology is hard on the lattice

- Continuum limit: small instantons have large $2\pi/\alpha_{\rm s}$ value, and are rare. Get rarer with $a^{-7-N_f/3}$.
- High temperatures: all instantons are small, $\rho < 1/T$. Get rarer with $T^{-7-N_f/3}$.

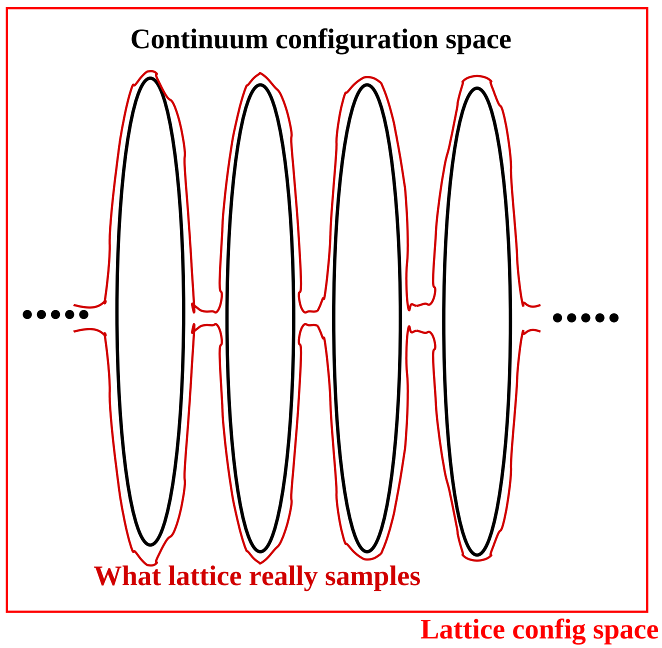
Continuum limit: hard to *move between* instanton sectors. **Poor sampling.**

High temperature: rare to *sample* $N_I \neq 0$ sectors. **Poor statistics** even if you *could* get between sectors.

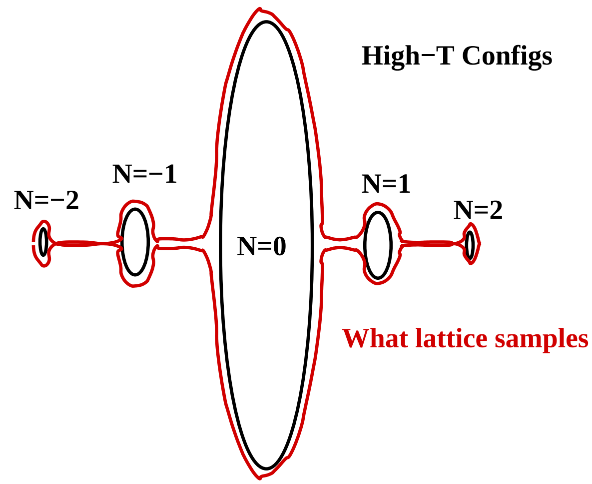
I will try to study topology at $T \gg T_c$!

Configuration space

Configurations at small spacing:



Configurations at high T:



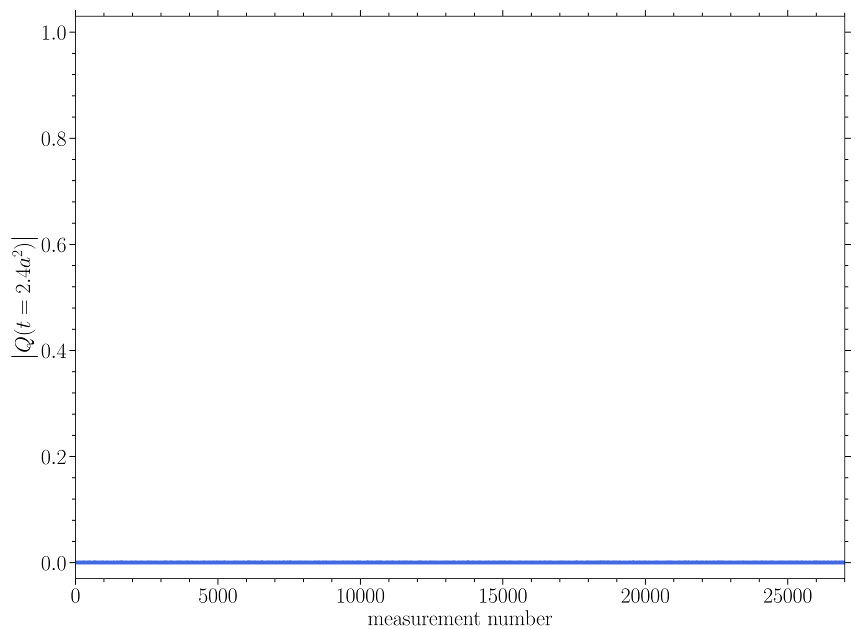
Lattice effectively provides narrow "bridges" between N_I sectors. Small a: narrower. Hi T: $N \neq 0$ is smaller.

How to measure $\chi(T)$ at $T \gg T_c$

Sample?? $$\chi = \frac{1}{V} \frac{\int \mathcal{D}A_\mu e^{-\int d^4x \,\mathrm{Tr}\, F^2/2g^2} \Theta(N_I^2 - N_{\mathrm{thresh}}^2)}{\int \mathcal{D}A_\mu e^{-\int d^4x \,\mathrm{Tr}\, F^2/2g^2}}$$

$$= \frac{\sum_i \Theta(N_I^2 - N_{\mathrm{thresh}}^2)}{V \sum_i 1}$$

That didn't work!!!



Reweighting: general idea

Identity:

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\varphi e^{-S[\varphi]} \mathcal{O}[\varphi]}{\int \mathcal{D}\varphi e^{-S[\varphi]}} = \frac{\int \mathcal{D}\varphi e^{-S[\varphi]} e^{+W[Q[\varphi]]} e^{-W[Q[\varphi]]} \mathcal{O}[\varphi]}{\int \mathcal{D}\varphi e^{-S[\varphi]} e^{+W[Q[\varphi]]} e^{-W[Q[\varphi]]}}$$

Here $\mathcal{O}$ is desired operator, Q is *some* other operator.
How to use it: use $e^{-S[\varphi]} e^{W[Q]}$ as sampling weight!

$$\langle \mathcal{O} \rangle = \frac{\sum_i e^{-W[Q_i]} \mathcal{O}_i}{\sum_i e^{-W[Q_i]}} \qquad \text{Sample-weight: } e^{-S} e^{+W[Q]}$$

No matter how ugly $Q[\varphi]$ is, Metropolis always works!
Pick Q and W so you sample the things you need.

Plan to use reweighting

Choose function Q, weight $W[Q]$ such that we spend about equal time sampling:

- Ordinary $N_I = 0$ configurations
- Interesting $N_I = \pm 1$ configurations
- Small instantons ("dislocations") you need to get between $N_I = 0$ and $N_I = \pm 1$

Need a way to tell these 3 things apart.

Aside about $\epsilon_{\mu\nu\alpha\beta}F^{\mu\nu}F^{\alpha\beta}$

Not hard to find lattice implementation. (Clover). But:

$$F_{\mu\nu}\tilde{F}^{\mu\nu}_{\mathrm{latt}} = F_{\mu\nu}\tilde{F}^{\mu\nu}_{\mathrm{contin}} + c_1 a^2 D^\mu D^\mu F_{\mu\nu}\tilde{F}^{\mu\nu}_{\mathrm{contin}} + c_2 a^4 \ldots$$

Contaminated. $F\tilde{F}$ integrates to integer, others add garbage.

Garbage from short-distance fluct. Remove with gradient flow.

Gradient flow $\tau_{\mathrm{F}} > 1$: kill fluctuation *and* small instantons.

Less flow $\tau_{\mathrm{F}} \sim 0.4$: less fluctuation; small instanton $N_I \sim 1/2$.

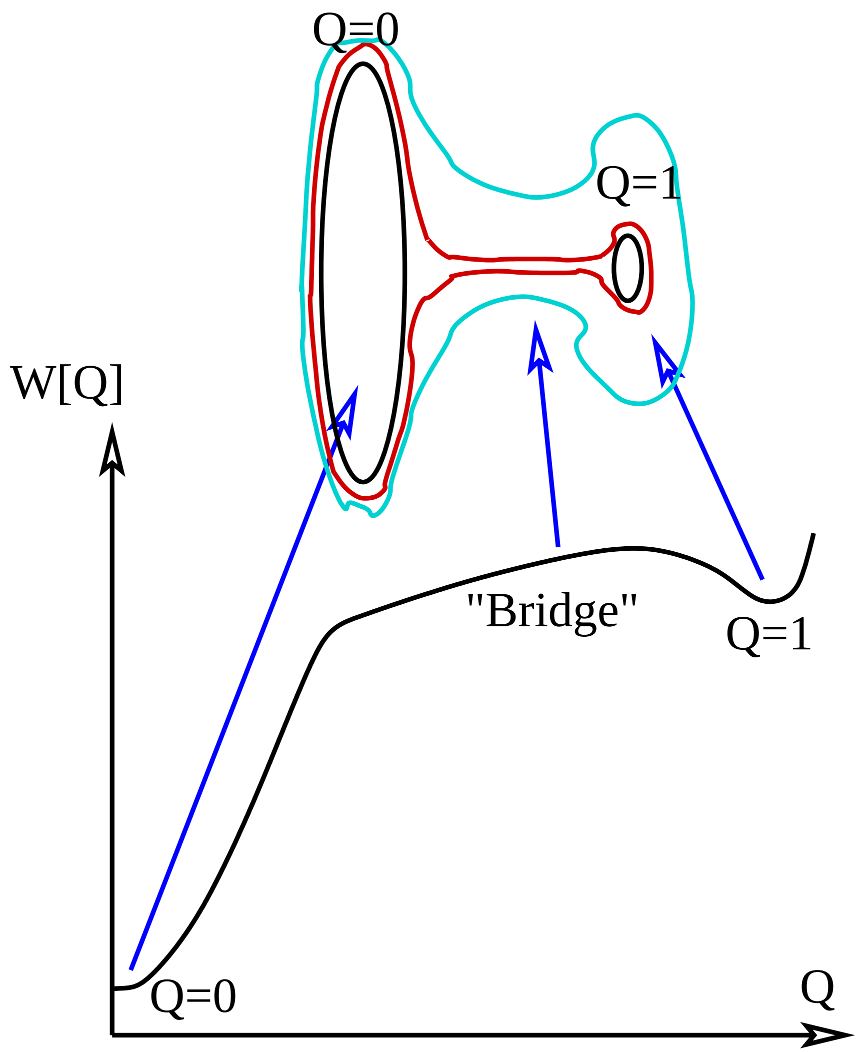
Use "incomplete" gradient flow to tell no instanton from small instanton from full instanton.

Reweighting: summary

- I perform a Markov-chain Monte-Carlo over configurations
- Metropolis step to make some Q-values more common
- Sample is now *enriched* in $N_I = \pm 1$ configs
- Also enhances "tunneling" between topologies
- Good statistics!
- But I **know** the level of over-sampling. Still get correct expectation values.

Reweighting: cartoon

Reweighting enhances sampling of both the "bridge" between $Q = 0$ and $Q = 1$ configs, and the $Q = 1$ configs.



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But how do you choose $W[Q]$?

Key feature: how much do I "reweight" to emphasize $N_I = 1$ configs?

Answer: until I sample $N_I = 1$, $N_I = 0$ roughly equally.

But that's roughly the thing I am trying to learn!

If I choose $W[Q = 1] - W[Q = 0]$ too big, I will *only* sample $N_I = 1$ and miss $N_I = 0$ – also a problem.

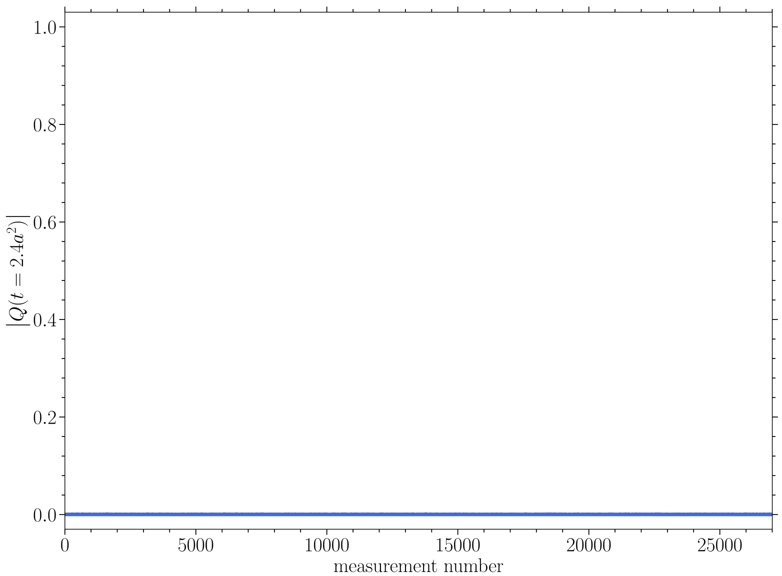
Need some *iterative, self-consistent* approach.
Key: reduce $W[Q]$ wherever you sample a lot.

Bootstrap determination of $W[Q]$

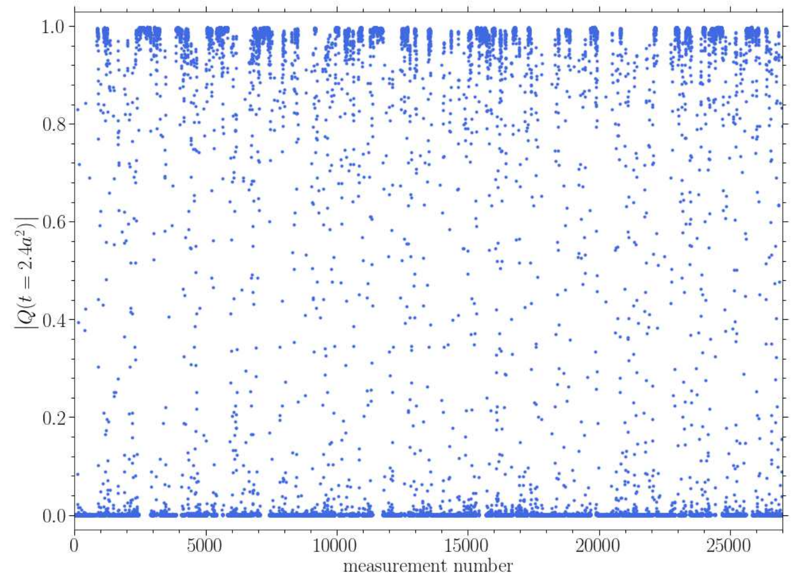
Piecewise-linear $W[Q]$
MC evolution
Each step: lower W at
current Q-value
Reduce rate-of-change
with time

Then, *fix* $W[Q]$ and do a Monte-Carlo "for keeps"

Does it work?



Before



After

Monte-Carlo can now see both $Q = 0$ and $Q = 1$

Transitions between Q-values control statistical power

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Does it work?

Pure Glue

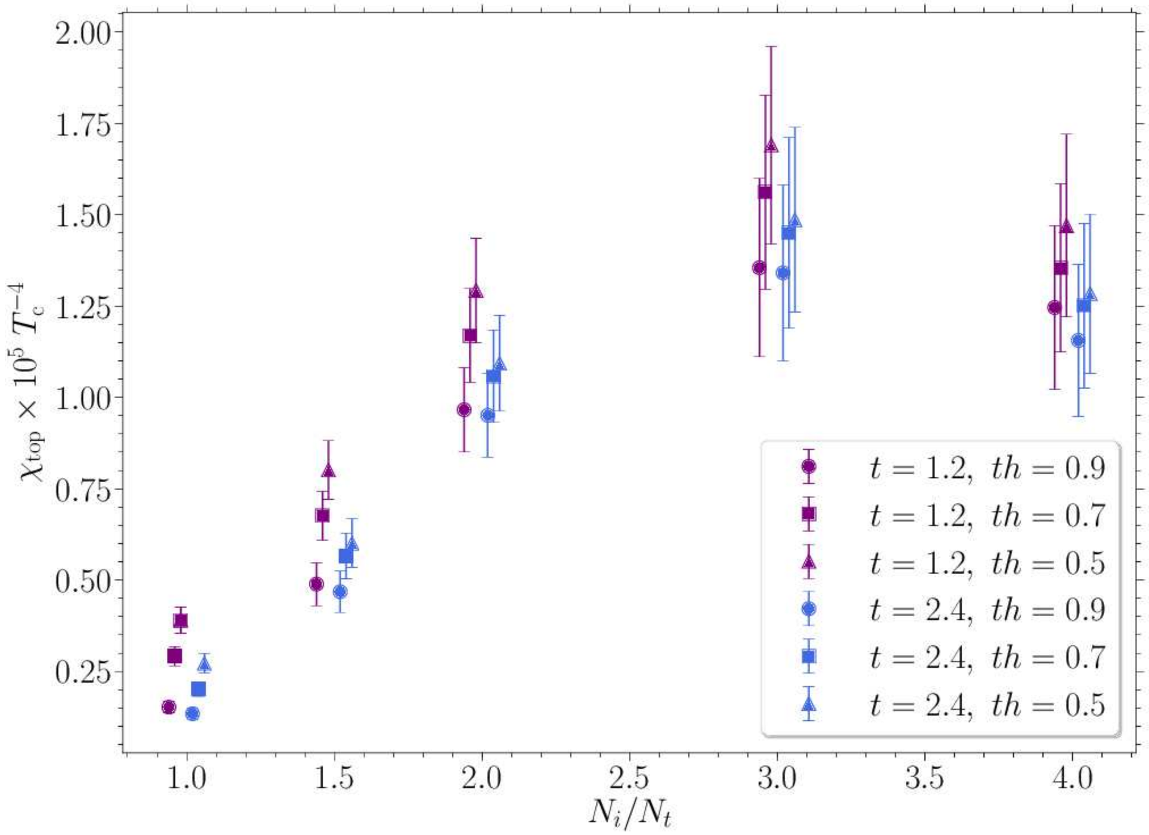
$T = 4.1 T_c$

At this T,

$\chi \sim 10^{-5} T_c^4$

1 config in 10^6

has topology



$N_t = 8$, exploring flow depth, Q-threshold, aspect ratio

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Is this a silver bullet?

Still has limitations!

- Requires very short HMC trajectories, Q-measurement (numerically inefficient)
- Becomes inefficient at large aspect ratio
- Becomes inefficient in continuum (large N_t) limit
- Unquenched theory not yet explored – expect issues at high-T with near-zero modes of Dirac operator

Multicanonical method?

Reweight in S

(Technically easier)

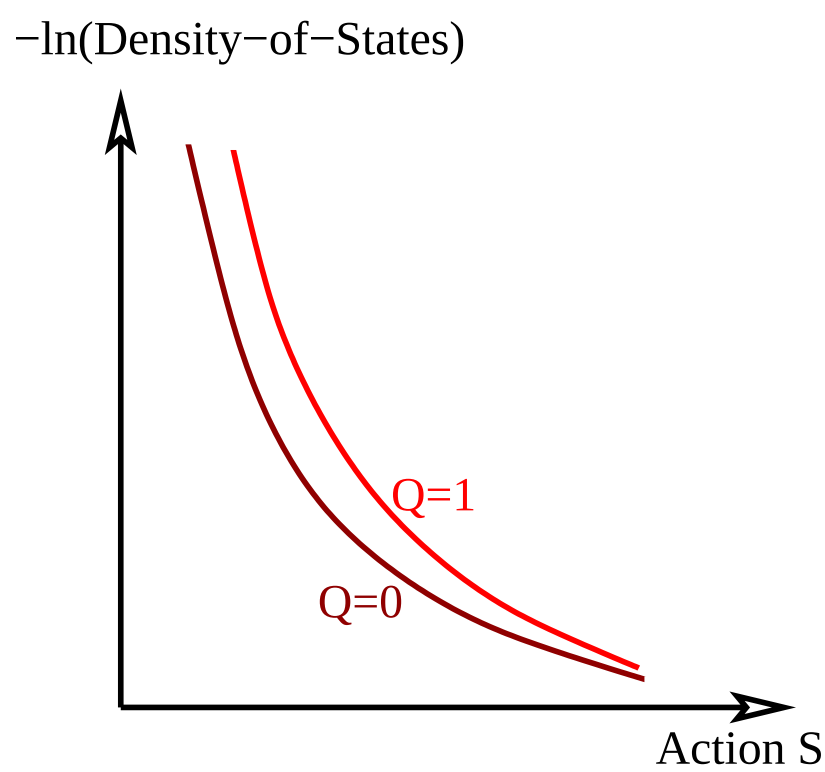
For $Q = 0$ *and* $Q = 1$

(No transitions needed)

Conceptually similar to

1606.07175 Frison et al,

1606.07494 Borsanyi et al



Curve difference $\Rightarrow$ probability ratio, $Q = 1/Q = 0$

Need explicit calculation at *one* T-value

Future plans

- Implement multicanonical approach (still quenched)
- Cross-check: reweight at two T-values
  vs Multicanonical difference between them
- How high-T can we reweight in *unquenched*?
- Deal with near-0 modes in unquenched?
- Quark masses in multicanonical approach?

Conclusions

- Topology is hard for 2 reasons:
  - Can't get *between* topologies at small a
  - Can't get *to* $Q \neq 0$ at high-T
- Reweighting – nice general-purpose approach
- Q after modest gradient flow is good reweighting variable
- Overcomes *both* limitations, but
- Not quite a "silver bullet"