QCD Topological Susceptibility at high-T via Reweighting

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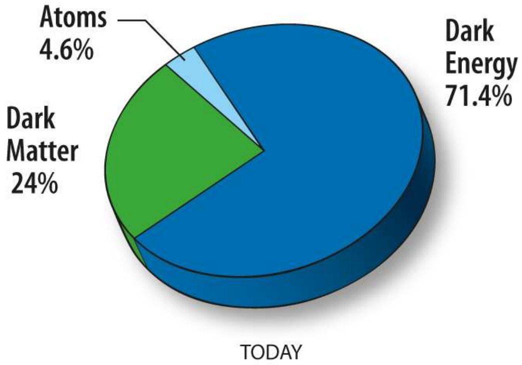
- What's QCD topology and why is it interesting?
- How can the lattice have topology and why is it hard?
- What's interesting but extra hard at high temperatures?
- Reweighting: methodology, efficacy
- Reweighting: limitations and prognosis

Dark Matter: a Cosmic Mystery



Atoms: Standard Model.

Dark Energy: Cosmological Constant.

Strange value, but possible

Dark Matter: MYSTERY! NOT SM!

We only know 3 things about dark matter:

- It's **Matter**: gravitationally clumps.
- It's **Dark**: negligible electric charge, interactions too feeble to be detected except by gravity
- It's **Cold**: negligible pressure by redshift $z = 3000$

Another mystery: **T**-symmetry in QED and **QCD**

T symmetry: "when you run a movie backwards, the *microphysics* is correct."

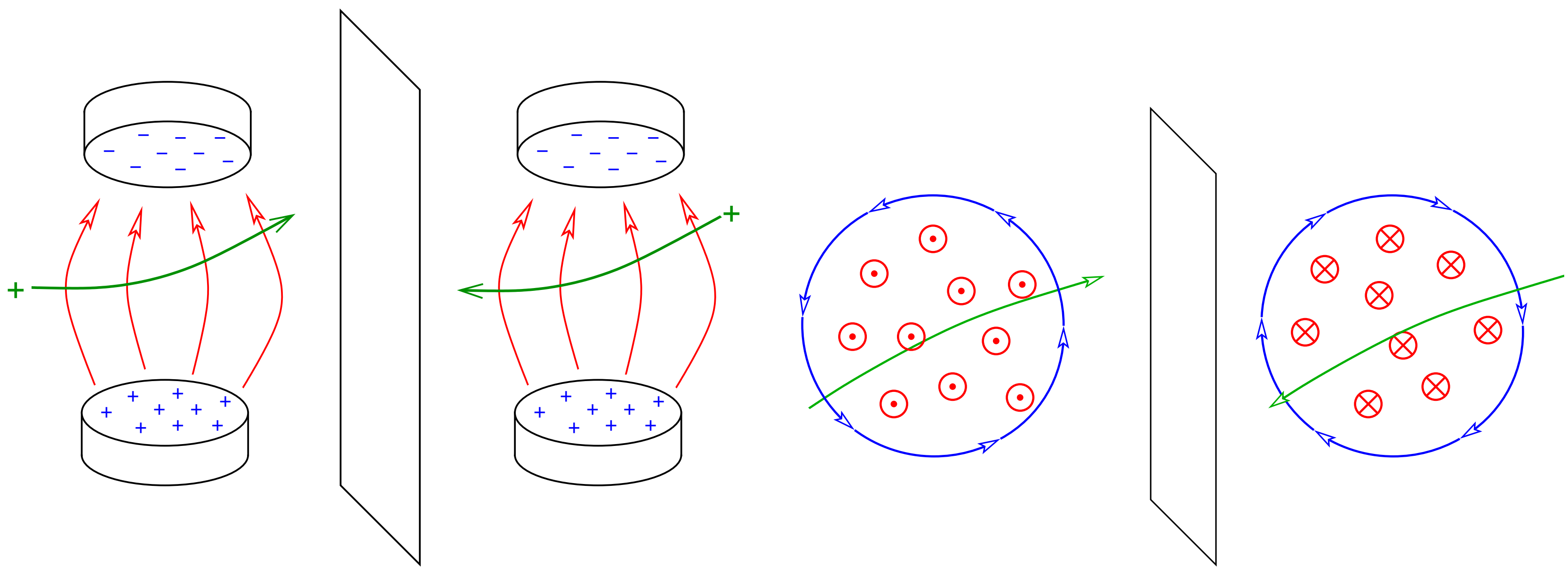
Statistical mechanics breaks **T**.
But microphysics very nearly obeys it!

Weak physics breaks **T**, but only through very small CKM effects. Observed in handful of experiments, all involving neutral meson oscillation.

No evidence for **T** viol in E&M or Strong interactions.

$\mathbf{T}$ in E&M

How do E, B fields change when you run movie backwards?



Q's unchanged, but J's flip. E same, but B flips.

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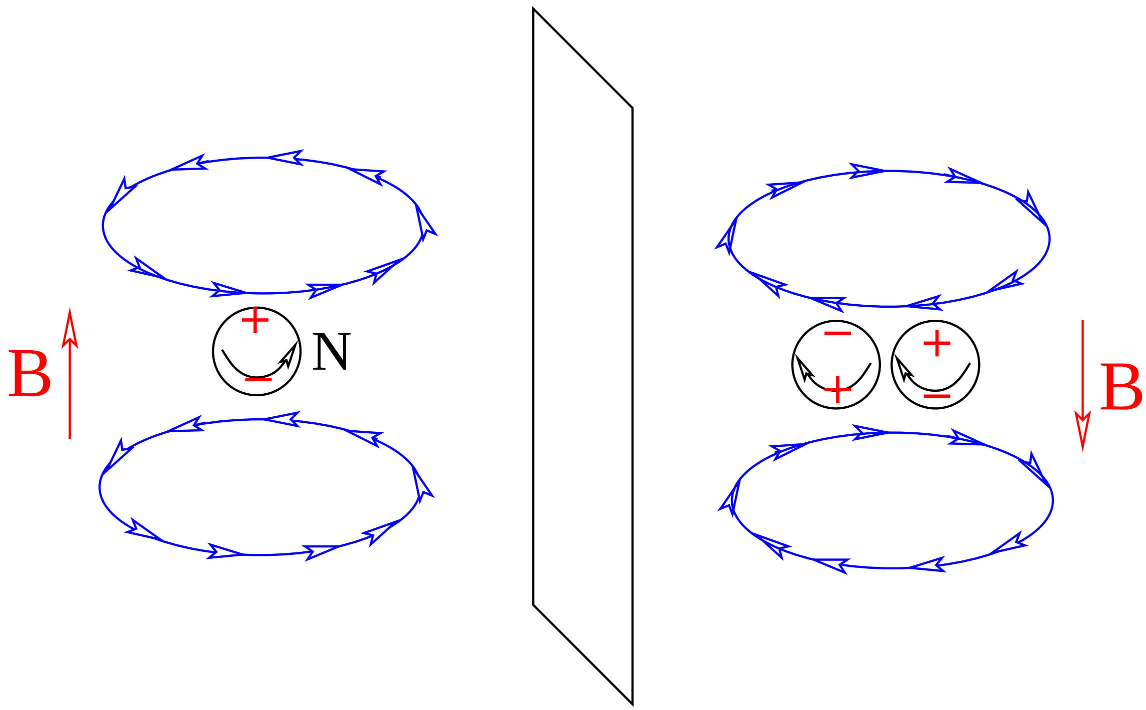
Looking for $\mathbf{T}$: Neutron EDM

Put neutron in $\vec{B}$ field – spin lines up with $\vec{B}$.



Is there an Electric Dipole Moment (EDM) aligned with spin?

If so: looks different when movie runs backwards, $\mathbf{T}$ viol!

Null results down to $3 \times 10^{-26}\ e\,cm$

$\mathbf{T}$ in QCD

QCD field strength $F_a^{\mu\nu}$ group-adjoint, rank-2 tensor.

Lagrangian must be group-singlet, Lorentz scalar. 2 possible:

$$S = \int dt \int d^3x \left(\frac{1}{4g^2} F_a^{\mu\nu} F^a_{\mu\nu} + \frac{\Theta}{64\pi^2} \epsilon_{\mu\nu\alpha\beta} F_a^{\mu\nu} F_a^{\alpha\beta} \right)$$

Two unknowns g^2, Θ. Good news: second term a total deriv.

$$\frac{1}{64\pi^2} \epsilon_{\mu\nu\alpha\beta} F_a^{\mu\nu} F_a^{\alpha\beta} = \partial^\mu K_\mu \,,$$

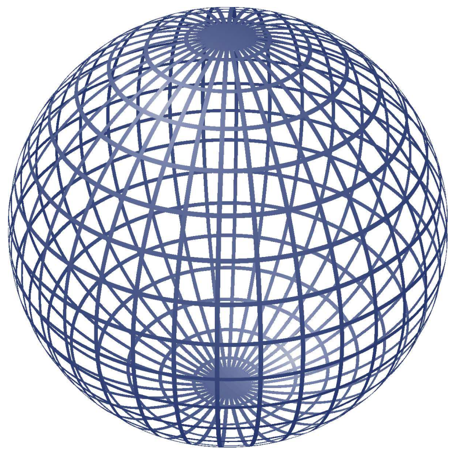
$$2K_\mu = \epsilon_{\mu\nu\alpha\beta} \left(A_a^\nu F_a^{\alpha\beta} + \frac{f_{abc}}{3} A_a^\nu A_b^\alpha A_c^\beta \right)$$

Violates $\mathbf{T}$! But, integrates to a boundary term.

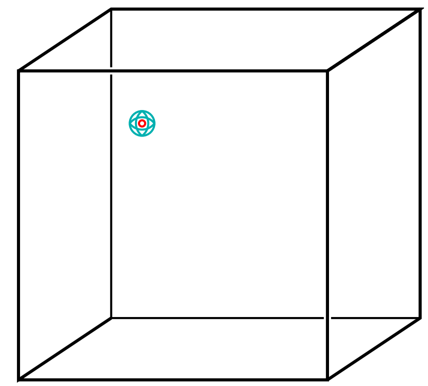
Gauge singularities and Topology

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 "Instanton number"

$$N_I = \int K_\mu d\Sigma^\mu = \int d^4x \frac{1}{64\pi^2} \epsilon_{\mu\nu\alpha\beta} F_a^{\mu\nu} F_a^{\alpha\beta}$$

Axions

QCD needs to be **T** invariant, eg, $\Theta = 0$. Mechanism?

Introduce complex scalar φ, U(1)-breaking potential

$$\mathcal{L}_\varphi = \partial_\mu \varphi^* \partial^\mu \varphi + \frac{m_r^2}{8 f_a^2} \left(2\varphi^* \varphi - f_a^2 \right)^2 + \ldots$$

whith . . . heavy DOF which gives effective interaction

$$\mathcal{L}_{\varphi,QCD} = \frac{1}{64\pi^2} \epsilon_{\mu\nu\alpha\beta} F_a^{\mu\nu} F_a^{\alpha\beta} \, \mathrm{Arg}\, \varphi$$

Replaces Θ with Arg(φ) which is dynamical

QCD dynamics prefer the **T** respecting value.

and Arg(φ) = Axion is CDM candidate!

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Axion dynamics

Axion likely starts in random (space-nonuniform?) state.
Dynamics: requires **QCD** $\epsilon_{\mu\nu\alpha\beta} F_a^{\mu\nu} F_a^{\alpha\beta}$ physics at high-T

Long story short: want to know

$$\chi(T) = \frac{T}{V} \langle N_I^2 \rangle$$

as function of temperature for $T \in [3T_c, 7T_c]$.

Dominated by well-localized gauge-field clumps with
$\int \epsilon_{\mu\nu\alpha\beta} F_a^{\mu\nu} F_a^{\alpha\beta} = \pm 1$ "Calorons"

At this temperature: nonperturbative. need lattice QCD

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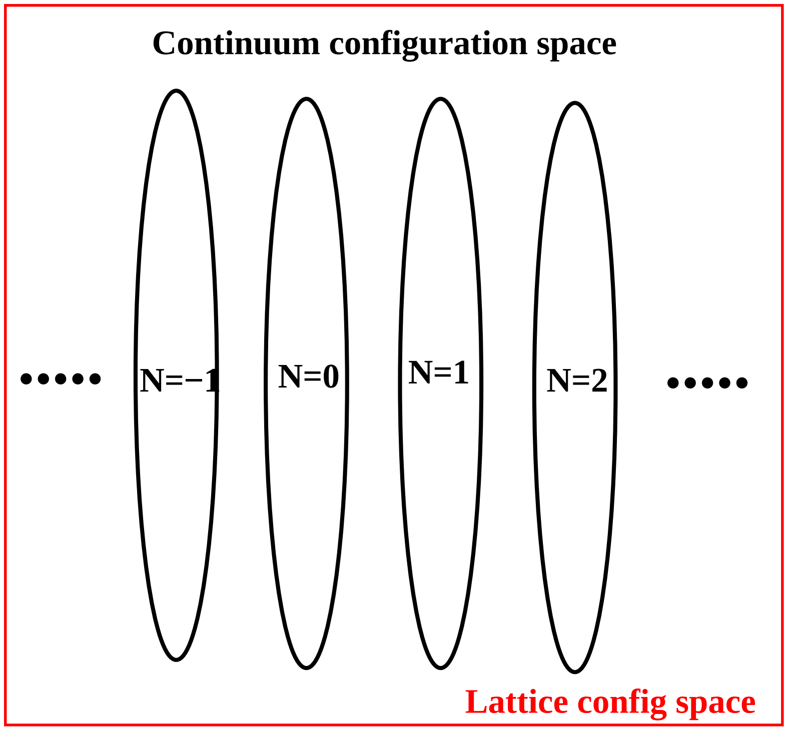
Why topology is “impossible” on lattice



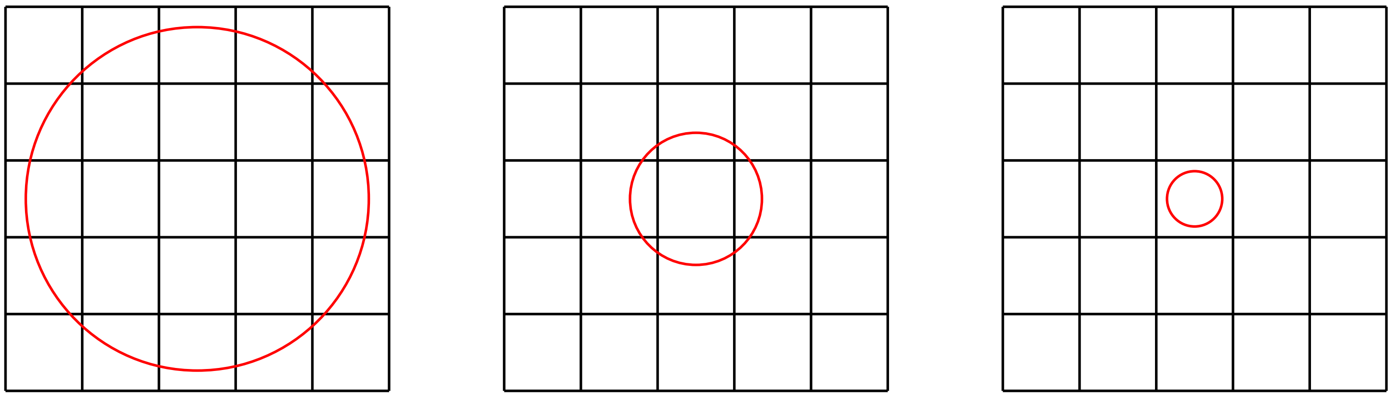
Continuum: N_I is integer. each N_I value: disconnected region of config. space.

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 calorons on a lattice:



Big caloron: 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 "calorons" 1-2a across...

Why topology is hard on the lattice

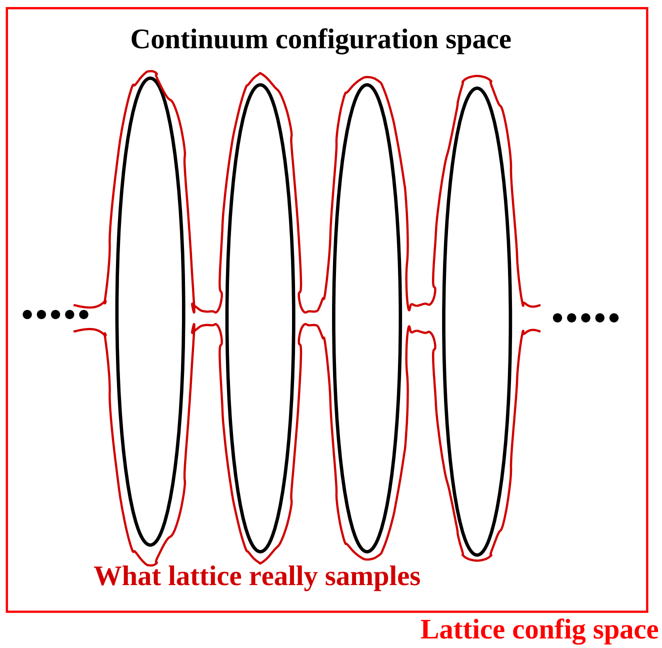
- Continuum limit: small calorons have large $2\pi/\alpha_{\mathrm{s}}$ value, and are rare. Get rarer with $a^{-7-N_f/3}$.
- High temperatures: all calorons are small, $\rho < 1/T$. Get rarer with $T^{-7-N_f/3}$.

Continuum limit: hard to *move between* caloron sectors.
Poor sampling.
High temperature: rare to *sample* $N_I \neq 0$ sectors. **Poor statistics** even if you *could* get between sectors.

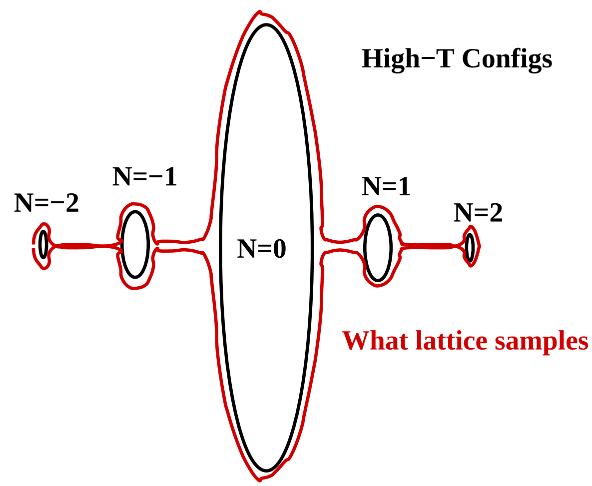
I will try to study topology at $T \gg T_c$!

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.

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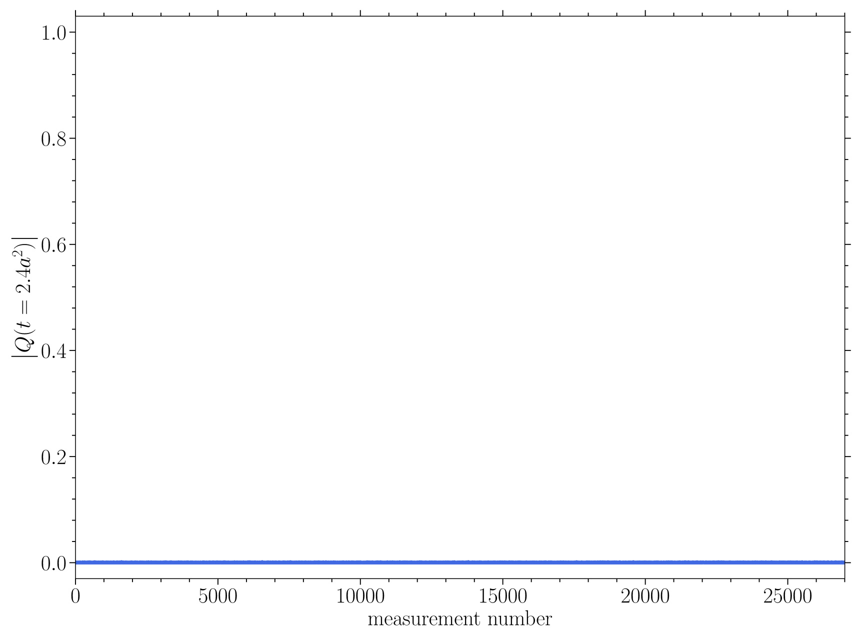
How to measure $\chi(T)$ at $T \gg T_c$

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!!!



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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!

$$\langle \mathcal{O} \rangle = \frac{\sum_i e^{-W[Q_i]} \mathcal{O}_i}{\sum_i e^{-W[Q_i]}}$$

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 calorons ("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 $\epsilon_{\mu\nu\alpha\beta} F_a^{\mu\nu} F_a^{\alpha\beta}$

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

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

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

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

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

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

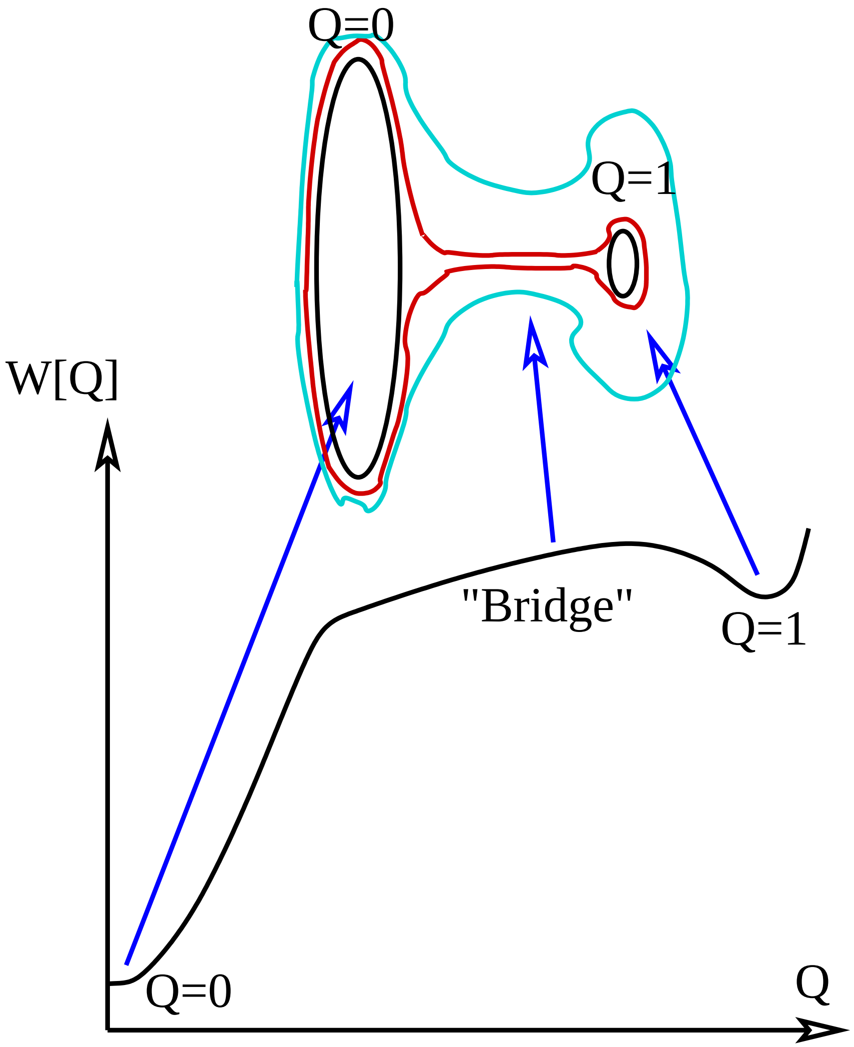
Use “incomplete” gradient flow to tell no caloron from small caloron from full caloron.

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 $W[Q]$?

Question: how much to "reweight" to emphasize $N_I = 1$ configs?

Answer: until $N_I = 1$, $N_I = 0$ roughly equal in sample

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.

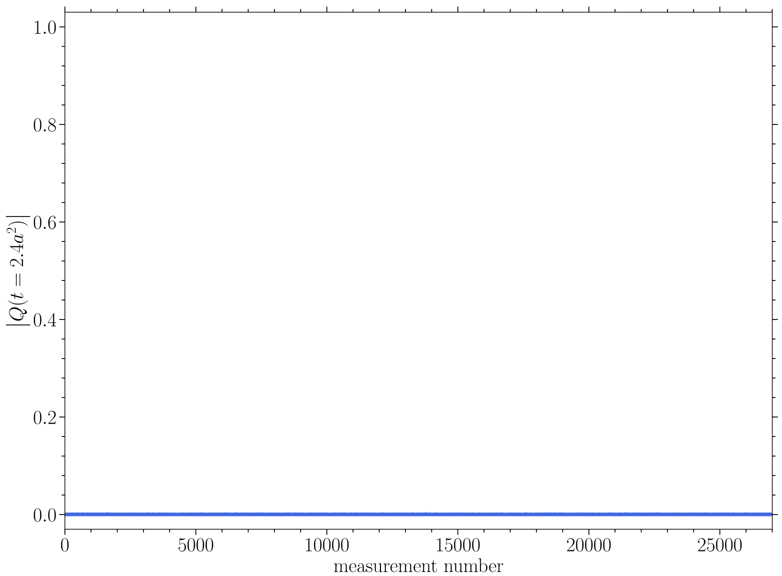
Need some *iterative, self-consistent* approach.
Key: reduce $W[Q]$ wherever you sample a lot.

Bootstrap determination of $W[Q]$

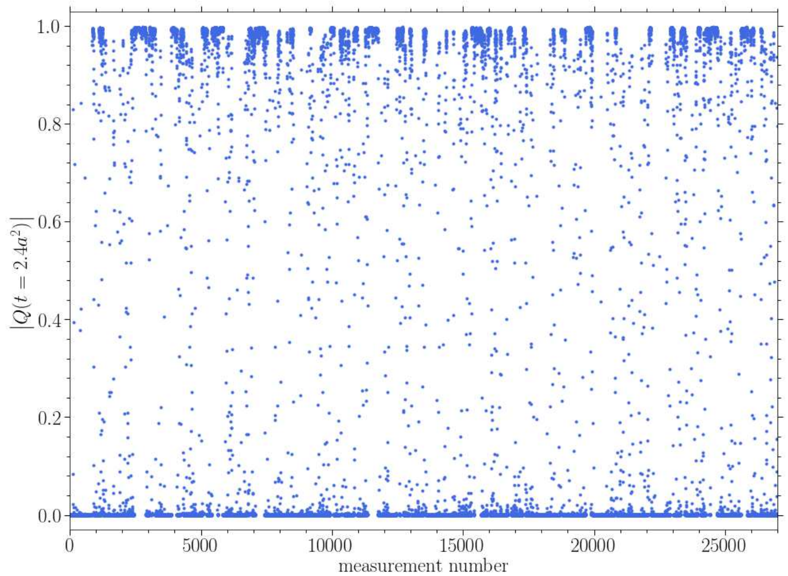
Piecewise-linear $W[Q]$
MC evolution
Each step: lower W at
current Q-value
Reduce rate-of-change
with time

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

Does it work?

Pure Glue

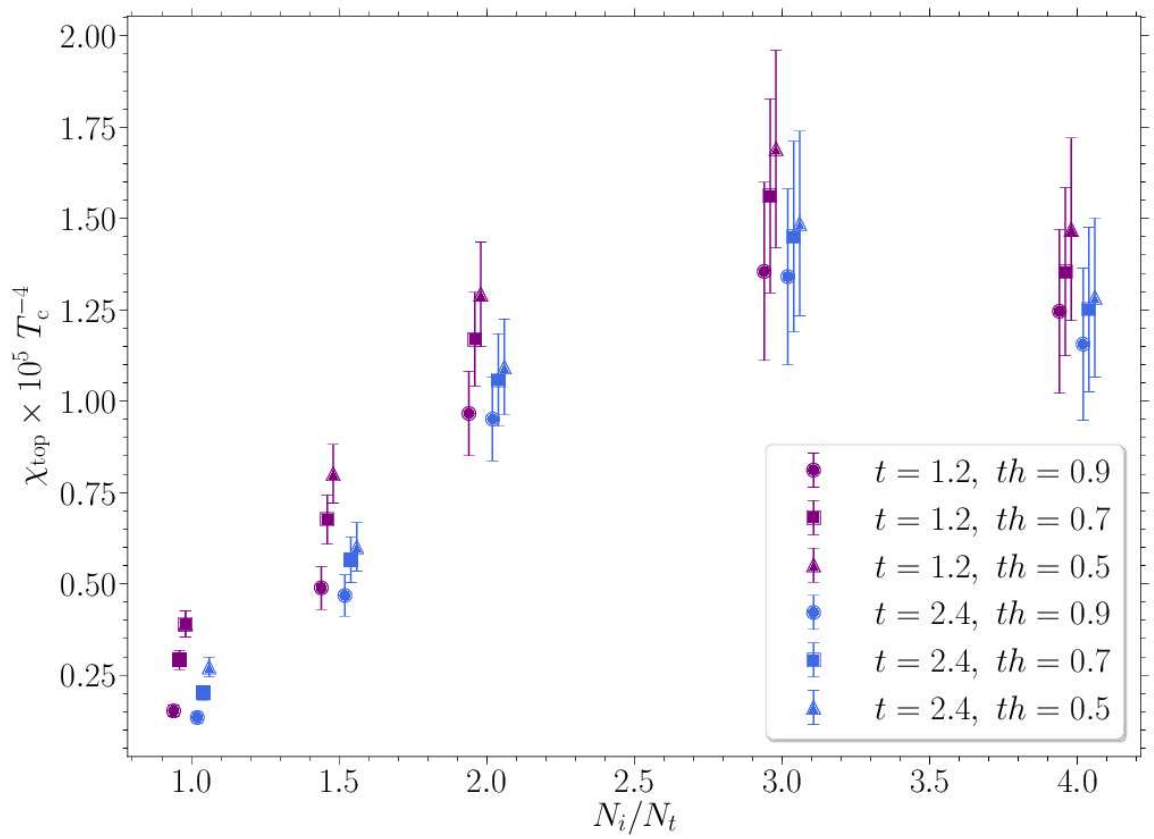
$T = 4.1T_c$

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

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"

Multicanonical method?

Reweight in S

(Technically easier)

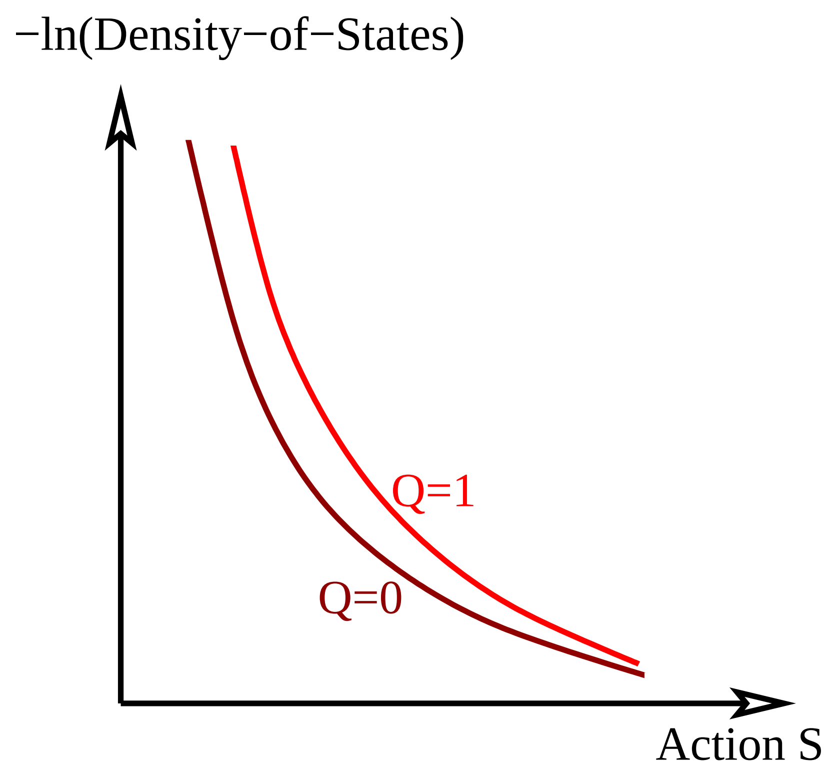
For $Q = 0$ *and* $Q = 1$

(No transitions needed)

Conceptually similar to

1606.07175 Frison et al,

1606.07494 Borsanyi et al



Curve difference ⇒ 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?