Topological susceptibility of pure gauge theory using Density of States

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Overview

1. Why is it interesting?
   Axion and its potential, topology, strong CP
2. Why is it hard to calculate?
   Perturbative result, MC sampling
3. How can you calculate it easier?
   Density of States, Proxy charge,
   results, reconstructed histograms, cont. limit

Results from [Borsanyi,Sexty arxiv:2101.03383]

Topology in QCD

Topological charge density:

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

QCD action could be:

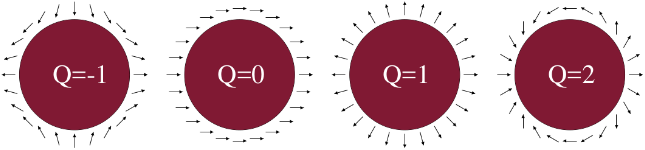
$$S = -\frac{1}{2}\mathrm{Tr}F_{\mu\nu}F^{\mu\nu} + \Theta e^{\mu\nu\alpha\beta}\frac{1}{8\pi^2}\mathrm{Tr}F_{\mu\nu}F_{\alpha\beta} \tag{2}$$

new term is a total derivative $\implies$ classical equations unchanged
new term is a topological constant $\in \mathbb{Z}$
new term breaks P invariance
Θ is an independent parameter of the QCD action

Experiments: electric dipole moment of the neutron is very small $\implies \Theta < 10^{-10}$
Strong CP problem: Why is Θ so small? Fine tuning needed?

Instantons, calorons

The topological charge density has local peaks: field configurations carrying topological charge called **instantons** appear [Belavin et al (1975)]



Their contribution to the FF term in the action:

$$S = |Q| \frac{2\pi}{\alpha_s} \tag{3}$$

Independently of their size. Scale dependence enters through the running coupling.

At finite temperature the size of the temperature axis limits their size. Also, periodic boundary conditions must be respected.
Use "mirror" charges. Defects are now called **Calorons**

Dilute Instanton Gas

Single Instanton has action $2\pi/\alpha_s$, independently of the size
At finite temperature, typical size given by temperature T:

$$\chi(T) \sim T^4 e^{-2\pi/\alpha} \tag{4}$$

Dilute Instanton Gas Approximation (DIGA): Instantons appear independently of each other.
Running of the QCD coupling $d\alpha^2/d\ln\mu^2 = -\alpha^2(11 - 2/3N_f)/(2\pi)$:

$$e^{-2\pi/\alpha_s} \sim T^{-11+2/3N_f} \tag{5}$$

For Yang-Mills theory:

$$\chi(T) \sim T^{4-11} = \frac{1}{T^7} \tag{6}$$

Perturbative treatment with loop corrections: [Gross, Pisarski, Yaffe 1981]
Fermion fields → zero modes complicate picture

Axion

The Θ field is reinterpreted as a particle (phase of a complex scalar)

$$L = f_a^2 \partial_\mu \Theta \partial^\mu \Theta + i\Theta \frac{1}{8\pi^2} \mathrm{Tr}(F_{\mu\nu}\tilde{F}^{\mu\nu}) \tag{7}$$

2nd term gives an effective mass term for the Goldstone particle

$$m_a^2 = f_a^2 \frac{\partial^2 V(\Theta)}{\partial \Theta^2} = f_a^2 \left\langle \frac{Q^2}{V} \right\rangle = f_a^2 \chi \tag{8}$$

At the minimum Θ will be very small
During the early universe axion particles are created before Θ eventually settles in the minimum → **Dark Matter**

Axion tidies two problems: strong CP problem and dark matter

Topological susceptibility

$$\chi(T) = \int d^4x \langle q(x)q(0)\rangle_{T,\Theta=0} = \lim_{\Omega\to\infty} \frac{\langle Q^2\rangle_{T,\Theta=0}}{V}. \tag{9}$$

Perturbation theory: $\chi \sim T^{-7}$

For axion phenomenology, the higher order coefficients of the potential are also needed:

$$V(\Theta, T) = \frac{1}{2}\chi(T)\Theta^2[1 + b_2(T)\Theta^2 + b_4(T)\Theta^4 + \ldots], \qquad b_2 = -\frac{\langle Q^4\rangle - 3\langle Q^2\rangle^2}{12\langle Q^2\rangle}$$

for the DIGA approximation, one expects:

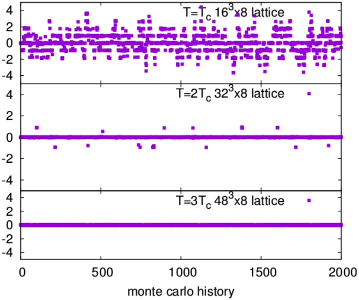
$$V(\Theta, T) = \chi(T)(1 - \cos\Theta) \quad \Longrightarrow \quad b_2 = -1/12,\ b_4 = 1/360 \tag{10}$$

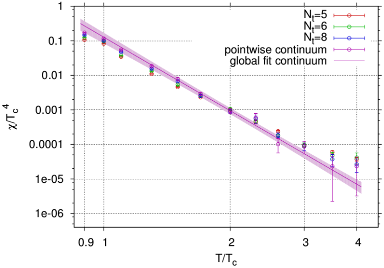
at large T and small V:

$$\langle Q^4\rangle = \langle Q^2\rangle \quad \Longrightarrow \quad b_2 \approx -1/12 \tag{11}$$

Topological susceptibility on the lattice

We can measure Q^2/V using an importance sampling simulation on the lattice





[Wuppertal-Budapest 1508.06917]

At large temperatures, due to the strong suppression of the χ, configurations with $Q \neq 1$ are very rare.

$$p_{Q\neq 0} = V\chi \sim T^{-11} \tag{12}$$

Very hard to collect enough statistics for a reliable measurement of χ
Tunneling rate between different topological sectors are suppressed
Computational effort for a given precision scales with at least T^{11}

Density of States

Consider an action $S[\Phi]$ of fields Φ
We use the partition function: $Z = \int D\Phi e^{-S[\Phi]}$
Insert the Gaussian integral

$$\int_{-\infty}^{\infty} dc\ e^{-\frac{P}{2}(c-a)^2} = \sqrt{\frac{2\pi}{P}} \tag{13}$$

And exchange order of integrations

$$Z = \int D\Phi \int_{-\infty}^{\infty} dc\ e^{-\frac{P}{2}(c-F[\Phi])^2} e^{-S[\Phi]} = \int_{-\infty}^{\infty} dc\ \rho(c) \tag{14}$$

where we defined the 'density of states':

$$\rho(c) = \int D\Phi e^{-S[\Phi]-\frac{P}{2}(c-F[\Phi])^2}. \tag{15}$$

In the limit $P \to \infty$, and $F[\Phi] =$ energy, $\rho(c)$ gives the density of energy levels.
Equality is exact for any P and any $F[\Phi]$

DoS

One can measure any operator A, provided $\langle A\rangle_c$ is measured:

$$\langle A\rangle = \frac{1}{Z}\int_{-\infty}^{\infty} dc \int D\Phi A[\Phi] e^{-S[\Phi]-\frac{P}{2}(c-F[\Phi])^2} = \frac{\int_{-\infty}^{\infty} dc\ \rho(c)\langle A\rangle_c}{\int_{-\infty}^{\infty} dc\ \rho(c)} \tag{16}$$

$$\langle A\rangle_c = \frac{\int D\Phi e^{-S_c[\Phi]} A[\Phi]}{\int D\Phi e^{-S_c[\Phi]}} = \frac{1}{\rho(c)}\int D\Phi e^{-S_c[\Phi]} A[\Phi] \tag{17}$$

How do we get $\rho(c)$?

$$\frac{\partial \ln\rho(c)}{\partial c} = \frac{1}{\rho(c)}\int D\Phi e^{-S[\Phi]-\frac{P}{2}(c-F[\Phi])^2}\left(-P(c-F[\Phi])\right) = \langle -P(c-F[\Phi])\rangle_c, \tag{18}$$

Overall normalization of $\rho(c)$ is fixed to 1. (drops out from results)

We have roughly constant errors for $\ln\rho(c) \to \Delta\rho/\rho \approx \text{const}$
$\to$ exponentially better than measuring histogram: $\Delta\rho \sim \sqrt{\rho} \implies \Delta\rho/\rho \sim 1/\sqrt{\rho}$

DoS for topology

Can we use DoS for topology?
We can choose $F[\Phi] = Q$, but Q is integer, so $\rho(c) = \sum A_n \delta(c-n)$ (in the $P \to \infty$ limit)
$\implies$ hard to measure ρ_c from $\partial_c \ln \rho$

We need a **proxy charge** Q_P

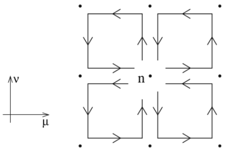
1. It should be able to have continous values
2. It should be close to integer topological charge $Q \approx Q_P$
3. Since we want to have an HMC code, it should be a differentiable function of the fields

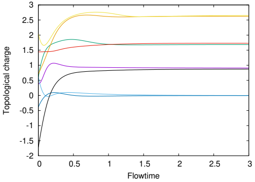
Topological charge

How do we measure the topological charge, anyway? Various definitions using gauge fields and fermionic fields (using index theorem) are available.

$$q(x) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \mathrm{Tr}(F_{\mu\nu}(x) F_{\rho\sigma}(x)) \,. \qquad (19)$$

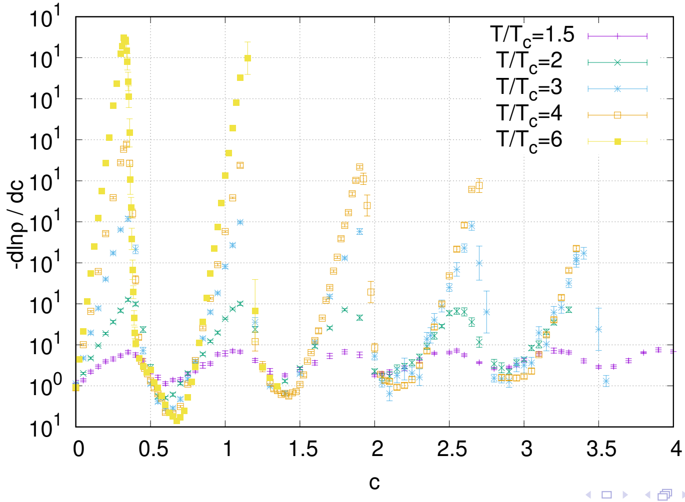
We can discretise this using the "clover" discretisation





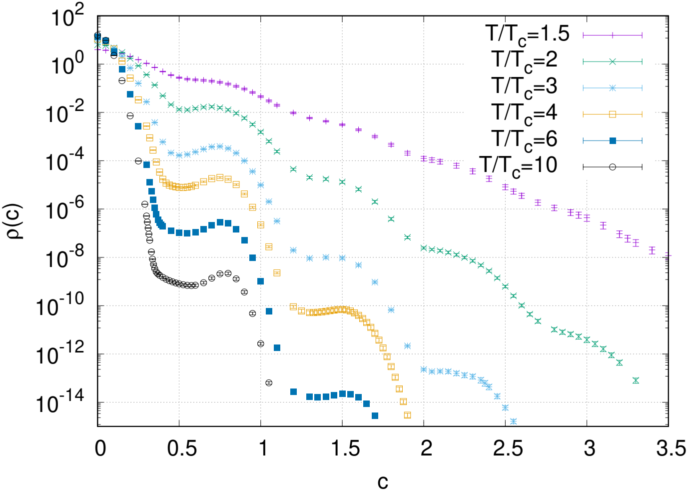
Measuring the clover Q on a configuration does not usually give close to integers, some cooling is needed [de Forcrand, Garcia Perez, Stamatescu (1996)]
nowadays called Gradient Flow [Lüscher (2010)]
proxy charge Q_P
Do a few stout smearing steps ($\approx$ gradient flow), flowtime $= n\rho$
and measure charge using the clover discretisation
Typically we use $n = 4, \; \rho = 0.1 \quad \Longrightarrow \quad$ flowtime=0.4

Pure gauge with Symanzik action, most results at
$N_T = 6, N_S = 24,\ n = 4,\ \rho = 0.1,\ P = 1000$
First we measure $d \ln \rho(c)/dc$



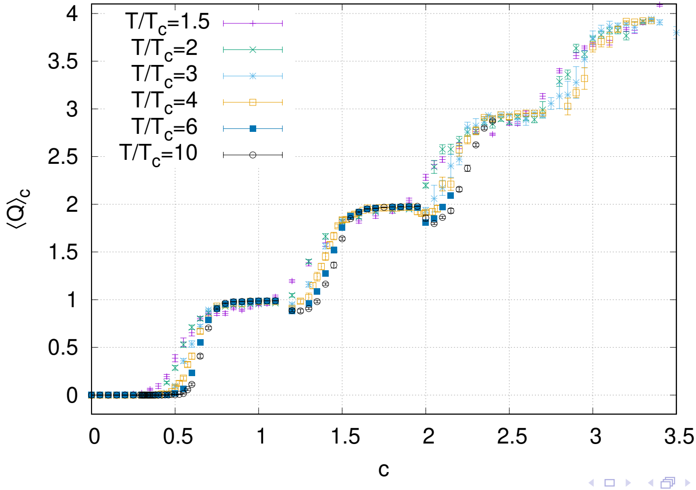
Results

Than we reconstruct $\rho(c)$:



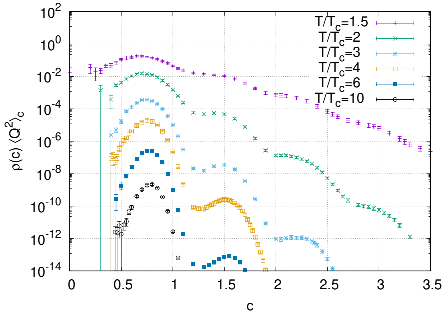
Charge average

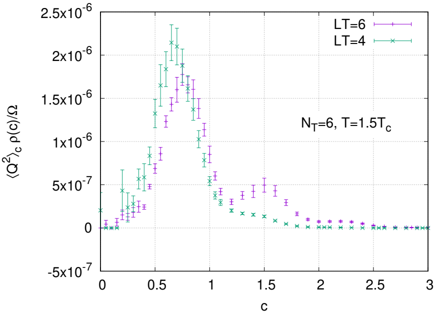
Plateaus at integer charges
in the middle regions one has many tunnelings.
c is typically slightly smaller than Q – effect of discretisation, small flow time



Susceptibility integrand

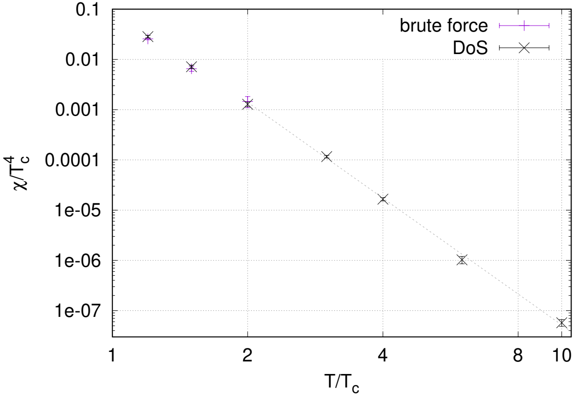
The integral of $\rho(c)\langle Q^2\rangle_c$ gives the susceptibility ($\rho(c)$ is normalized to 1)
The contribution of the higher sectors ($|Q| \geq 2$) is small already at $T = 1.5T_c$
This statement is volume dependent: $\chi = \langle Q^2\rangle/V$
Comparing two volumes at $T = 1.5T_c$ $\rightarrow$ $Q = 2$ sector contributes at larger volume





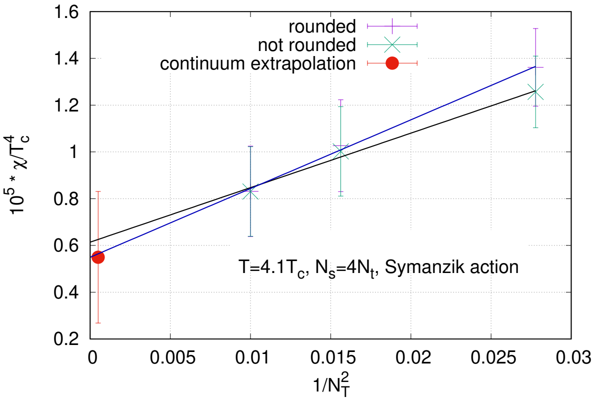
$\chi(T)$

Measureing the susceptibility at various temperatures
Perturbation theory + DIGA: $\chi \sim T^{-7}$
Fitted exponent: ≈ -6.3
Discretisation is always $N_T = 6$, continuum extrapolation needed



Continuum extrapolation

continuum extrapolation at $T = 4.1T_c$
(to compare with [Jahn,Moore,Robaina] : we get consistent results)



We can build histograms of the topological sectors in a direct simulation:

$$h(n) = \langle \delta_{Q,n} \rangle = \int dc \rho(c) \langle \delta_{Q,n} \rangle_c, \qquad \sum_n h(n) = 1 \tag{20}$$

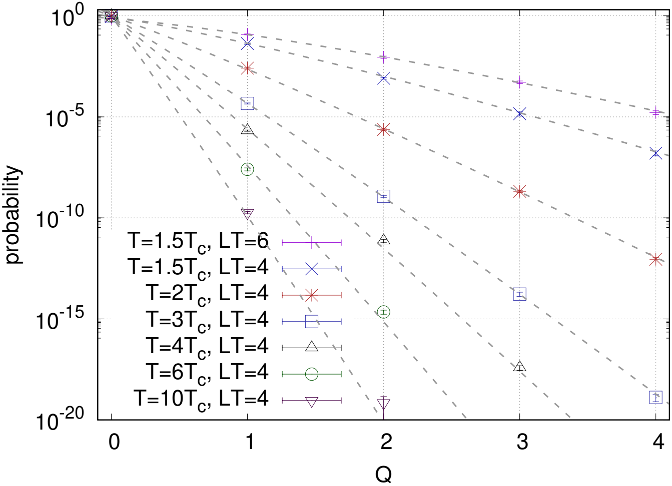
which we reconstruct from the DoS simulations

What we expect for **independent instantons**:
Number of defects follows a Poisson distribution. Each defect has a random sign.
Equivalently: The number of positive defects n_+ and the number of negative defects n_- both follow an independent Poisson distribution.
Skellam distribution:

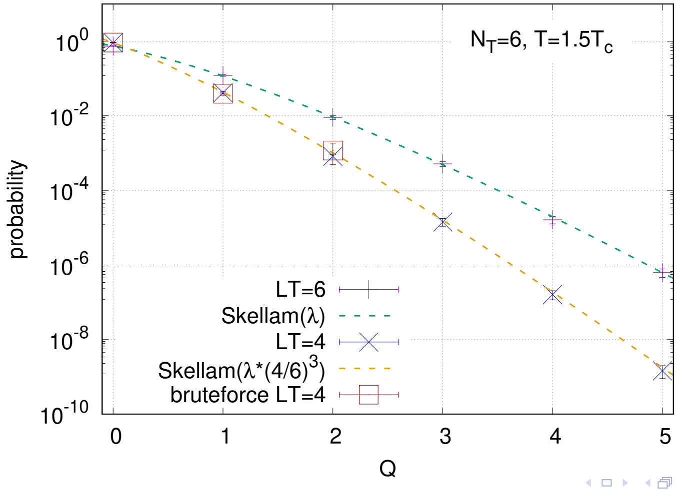
$$p_k = e^{-2\lambda} I_k(2\lambda) \tag{21}$$

with I_k, the modified Bessel function of the first kind

Fitted the λ of the Skellam distribution



at $T = 1.5T_c$, using 2 different volumes
λ scales with the volume, as expected
with brute force, only the first few values are possible



Conclusions, outlook

- DoS is applicable to the problem calculating the topological susceptibility using the proxy charge
- Simulations are feasible at high temperatures, here results up to $10T_c$
- inclusion of fermions poses no additional conceptual problem
- Volume dependence of χ is checked,
  Histograms of a direct importance sampling simulation are reconstructed,
  results consistent with DIGA already at $T = 1.5T_c$,
  with charge sectors going up to $|Q| = 5$

Extra slides