θ-dependence of the deconfinement temperature in SU(N) Gauge Theories

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Lorenzo Verzichelli

UNIVERSITÀ DI PISA

Based on [arXiv:2312.12202], by Claudio Bonanno, Massimo D'Elia and Lorenzo Verzichelli

Outline

Polyakov loop and center symmetry

Finite temperature SU(N) theories enjoy a $\mathbb{Z}_N$ symmetry known as center symmetry

On the lattice

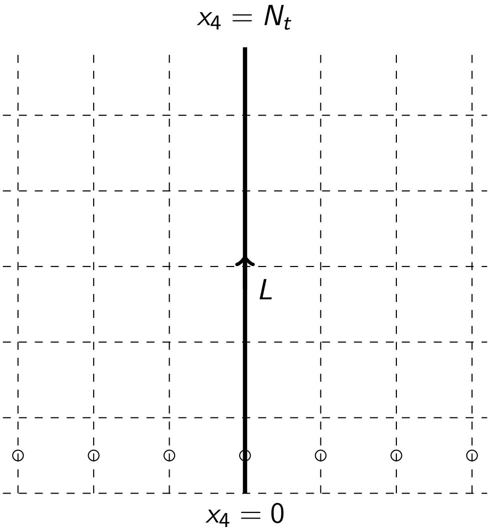
Apply a center symmetry transformation: multiply all the $x_4 = 0$ time-like link variables by $V = \exp(i2k\pi/N) \in \mathbb{Z}_N$, i.e. $U_4(\vec{x}, 0) \to VU_4(\vec{x}, 0)$

The Polyakov loop, L, is defined as

$$L(\vec{x}) = \frac{1}{N_c} \mathrm{Tr} \left[\prod_{x_4=0}^{N_t} U_4(\vec{x}, x_4) \right]$$

Under center symmetry transformations

$$L \to VL$$



Deconfinement in SU(N) theories

If the center symmetry is exactly realized (top panel): $\langle L \rangle = 0$

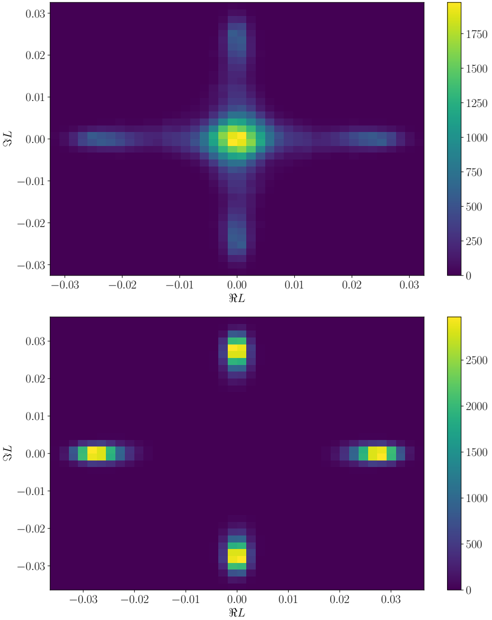
Since, being F the free energy of a static colored source, $\langle |L| \rangle \propto \exp(-F/T)$, exact realization of the center symmetry is interpreted as confinement

At high temperature, the center symmetry spontaneously breaks and L acquires a non zero expectation value (deconfinement, bottom panel)

In 3+1 D, the deconfinement phase transition is first order for $N \geq 3$

$$\frac{T_c(N)}{\sqrt{\sigma}} = 0.5970(38) + \frac{0.449(29)}{N^2}$$

[arXiv:hep-lat/0307017]



Topology on the lattice

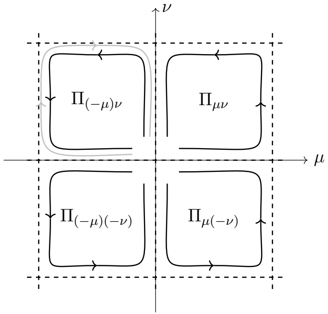
At infinity (in $\mathbb{R}^4$) the gauge field must be $A_\mu \simeq \Omega^{-1}\partial_\mu\Omega$ to have finite action.
One or more SU(2) subgroups can wind non trivially around the S^3 sphere at infinity

The winding number Q (topological charge) can be written as

$$Q = \int d^4x\, q \equiv \int d^4x\, \frac{g^2}{32}\epsilon_{\mu\nu\rho\sigma}\,\mathrm{Tr}\left[F_{\mu\nu}F_{\rho\sigma}\right]$$

On the lattice we used the clover discretization of q which is CP odd by construction

$$q_{clov} = \frac{1}{2^9\pi^2}\sum_{\mu,\nu=\pm 1}^{\pm 4}\epsilon_{\mu\nu\rho\sigma}\,\mathrm{Tr}\left[\Pi_{\mu\nu}\Pi_{\rho\sigma}\right]$$



Q_{clov} is related to Q by a finite renormalization [arXiv:1109.6815]

Topological features at the critical point

Topological features change in correspondence of the deconfinement transition [arXiv:1309.6059]

$$\chi = \frac{\langle Q^2 \rangle}{V}$$

In the limit of large N, χ at zero temperature is finite (Witten-Veneziano solution to the U(1) problem)

For $T < T_c$, χ is approximately constant

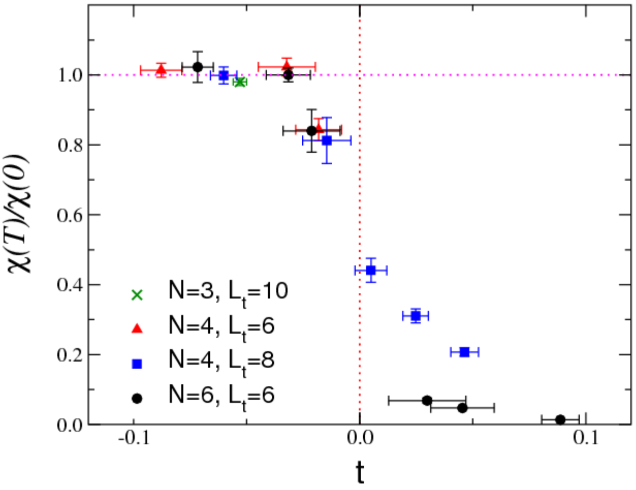


Image from arXiv:1309.6059

In the deconfined phase χ is suppressed exponentially in N

Topological features at the critical point

For $T < T_c$: topological feature similar to $T = 0$

For $T > T_c$: rapidly approach to the prediction of Diluted Instanton Gas Approximation (DIGA)

DIGA allows to predict moments of the distribution of Q beyond χ at high temperature

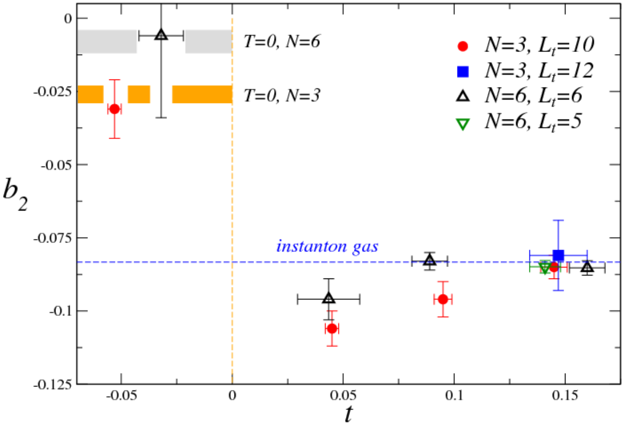


Image from arXiv:1309.6059

Also DIGA is in agreement with the exponential suppression of χ in the large N limit

The θ-T phase diagram

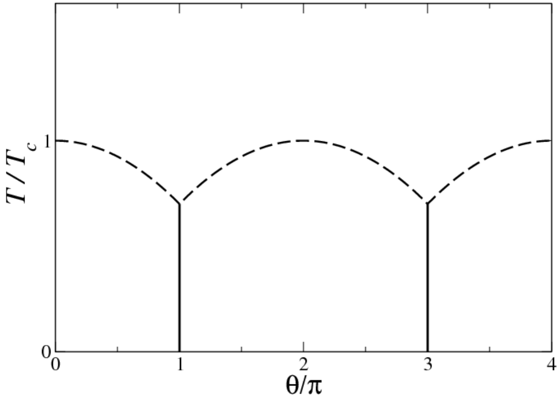
Let us introduce the topological charge density in the Lagrangian, coupled to a parameter θ:

$$q = \frac{g^2}{32}\epsilon_{\mu\nu\rho\sigma}\,\mathrm{Tr}\,[F_{\mu\nu}F_{\rho\sigma}]$$

The Gibbs weight of a field configuration will be multiplied by a phase $\exp(i\theta Q)$, with $Q \in \mathbb{Z}$

Since θ alters the distribution of Q, it is natural to think that it will alter the deconfinement temperature, T_c

Physical quantities are even functions of θ because q is CP odd while $\mathcal{L}_{YM}$ is even



Conjectured θ-T phase diagram from arXiv:1306.2919

We will be mainly interested in the curvature R of the deconfinement transition line in the θ-T phase diagram:

$$T_c(\theta) = T_c(0)\,[1 - R\theta^2 + O(\theta^4)]$$

The θ-T phase diagram

Since θ is coupled to $Q \in \mathbb{Z}$ in the action, θ dependence is 2π-periodic

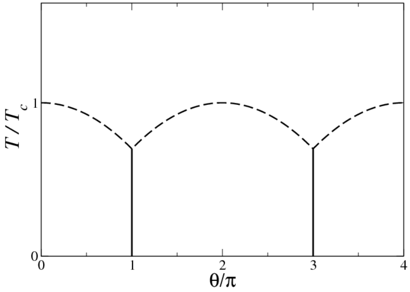
In the large N limit we expect the free energy to be a function of the kind

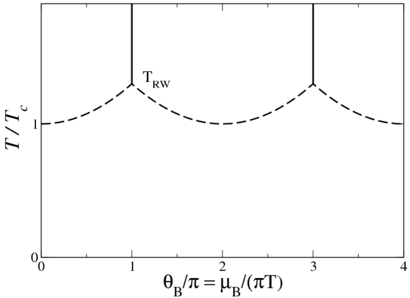
$$f(\theta) = N^2 h(\theta/N) \simeq N^2 \bar{f}(0) + \frac{1}{2}\chi \min_k(\theta + 2k\pi)^2$$

In the confined phase ($\chi \neq 0$), this means first order phase transition a $\theta = (2k+1)\pi$.
Unfortunately large real values of θ are hard to simulate (sign problem)

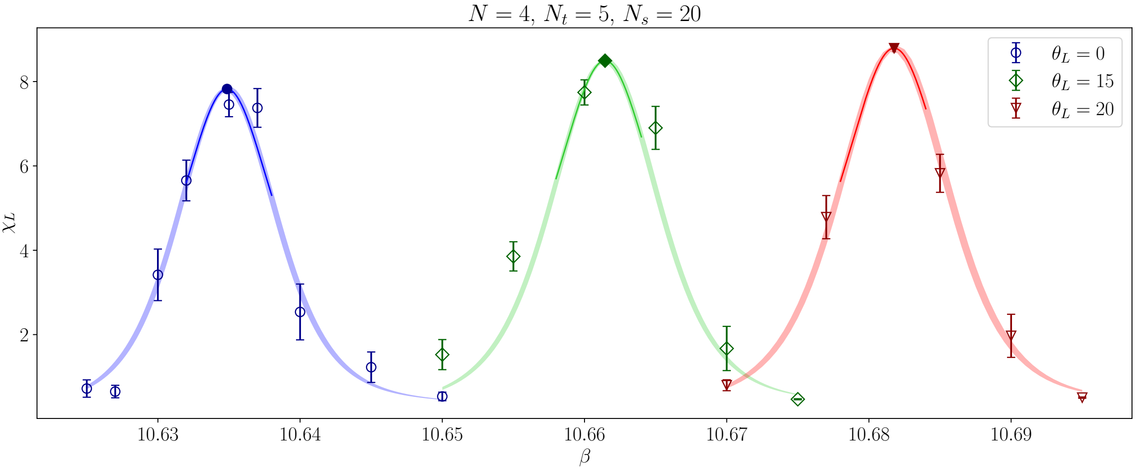
Similarity with the dependence on an imaginary chemical potential in a theory with fermions

Conjectured θ-T and μ_B-T phase diagrams from arXiv:1306.2919





Computing R from imaginary-θ simulations

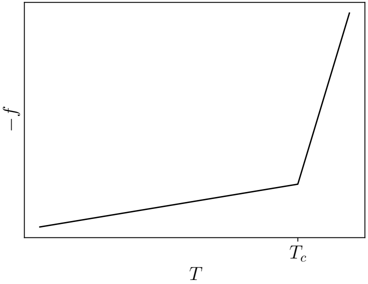


We can find the critical temperature for different imaginary values of $\theta = i\theta_I$ then perform a fit assuming

$$T_c(\theta_I)/T_c(0) = 1 + R\,\theta_I^2$$

A Clausius-Clapeyron-like equation

$$f(T,\theta) = \begin{cases} f_c(T,0) + \frac{1}{2}\chi_c\theta^2 + O(\theta^4) & T < T_c \\ f_d(T,0) + \frac{1}{2}\chi_d\theta^2 + O(\theta^4) & T > T_c \end{cases}$$



At the phase transition the two vacua cross:

$$f_c(T_c(\theta),\theta) = f_d(T_c(\theta),\theta)$$

Using $T_c(\theta) = T_c(0)[1 - R\,\theta^2]$ and expanding up to $O(\theta^2)$:

$$f_c(T_c(0)[1 - R\,\theta^2],0) + \frac{1}{2}\chi_c\,\theta^2 = f_c(T_c(0)[1 - R\,\theta^2],0) + \frac{1}{2}\chi_c\,\theta^2$$

$$\cancel{f_c(T_c(0),0)} + T_c(0)\,s_c\,R\,\theta^2 + \frac{1}{2}\chi_c\,\theta^2 = \cancel{f_d(T_c(0),0)} + T_c(0)\,s_d\,R\,\theta^2 + \frac{1}{2}\chi_d\,\theta^2$$

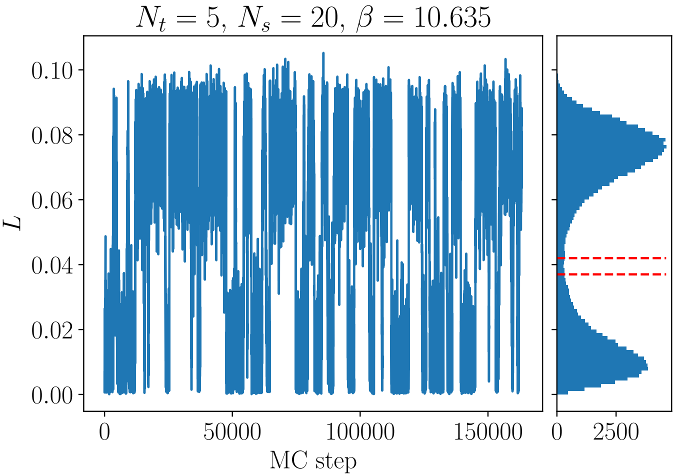
$$R = \frac{\chi_c - \chi_d}{2\,T_c(0)\,(s_d - s_c)} \equiv \frac{\Delta\chi}{2\,\Delta\epsilon}$$

where $s_{c/d}$ is the entropy $(-\partial f/\partial T)$ at $\theta = 0$, $T = T_c$ of the confined/deconfined phase

Lattice computation of $\Delta\epsilon$ and $\Delta\chi$

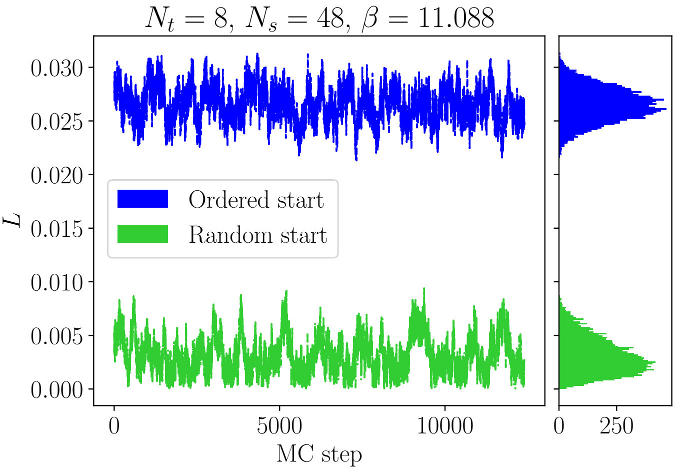
$\Delta\epsilon$ and $\Delta\chi$ can be computed from $\theta = 0$ simulations at $T = T_c$, separating the sampled configurations between the two phases, setting two cut-offs on $|L|$

In [arXiv:2212.08684] the Clausius-Clapeyron-like equation was verified for SU(3):
R (from latent heat) $= 0.0168(27)$, in agreement with
R (from imaginary-θ) $= 0.0178(5)$ found in [arXiv:1205.0538]

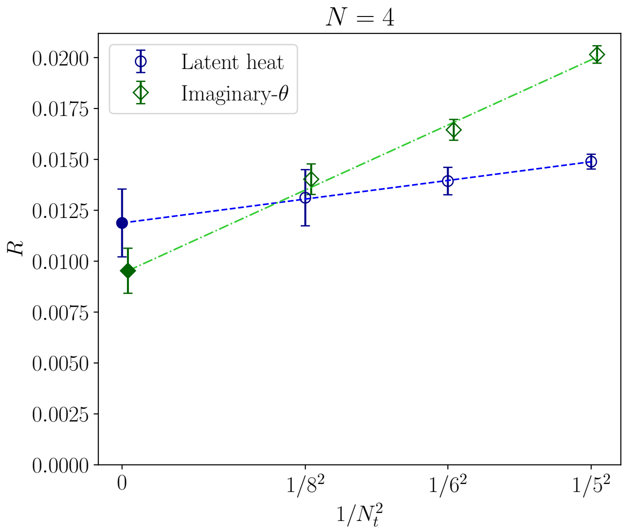


Lattice computation of $\Delta\epsilon$ and $\Delta\chi$

If the volume is large enough (at least for $N > 3$), the system will not tunnel between the two phases and it is possible to sample each phase separately



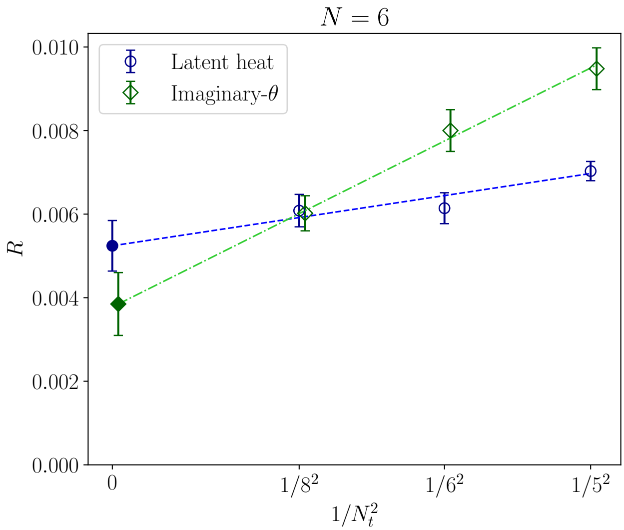
SU(4) results



$N = 4$			
Latent heat			Imaginary-θ
N_s	N_t	$R = \dfrac{\Delta\chi}{2\Delta\epsilon}$	R (from fit)
20	5	0.01489(36)	0.0202(4)
36	6	0.01385(67)	0.0165(5)
48	8	0.0131(14)	0.0140(8)
cont.		0.0095(11)	0.0119(16)

Combined fit: 0.01025(92),
$\chi^2/n\,d.o.f. = 2.3/3$, p-value $= 52\%$

SU(6) results

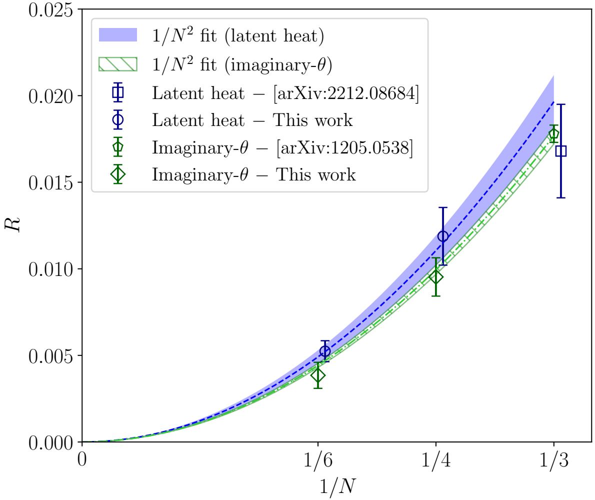


$N = 6$			
Latent heat			Imaginary-θ
N_s	N_t	$R = \frac{\Delta\chi}{2\Delta\epsilon}$	R (from fit)
10	5	0.00703(22)	0.00948(50)
12	6	0.00614(37)	0.00800(50)
16	8	0.00608(39)	0.00598(39)
cont.		0.00524(61)	0.00385(75)

Combined fit: 0.00469(47),
$\chi^2/n\,d.o.f. = 3.18/3$, p-value = 37%

For $N_t = 8$ the parallel tempering on boundary conditions was exploited

Large N scaling and comparison with Latent Heat



Both determinations lead to a very precise $1/N^2$ scaling, $N \geq 3$

$$R(N) = \frac{0.177(14)}{N^2}, \qquad \text{(from latent heat)}$$

$$R(N) = \frac{0.159(4)}{N^2}, \qquad \text{(from imaginary-}\theta\text{)}$$

In the large N limit one could use

$\Delta\epsilon/T_c^4$ from [arXiv:hep-lat/0206029]

$\chi(T=0)/\sigma^2$ from [arXiv:0803.1593]

$T_c/\sqrt{\sigma}$ from [arXiv:hep-lat/0502003]

And estimate

$$R = \frac{0.253(56)}{N^2}$$

Conclusions

- From the imaginary-θ fit method we found

$$R(N) = \frac{0.159(4)}{N^2}$$

- Results from latent heat method are compatible (after taking the continuum limit)
  This is consistent with our interpretation of the role of topology in the deconfinement transition

- Results of SU(3) are already consistent with the large N scaling within our uncertainties

BACKUP

At high temperature, DIGA leads to
$f(T,\theta) \approx f(T,0) + \chi(T)(1-\cos(\theta))$ and
$\chi(T) \approx T^4 \exp\left(-8\pi^2/g^2(T)\right) \sim T^{-11N_c/3+4}$

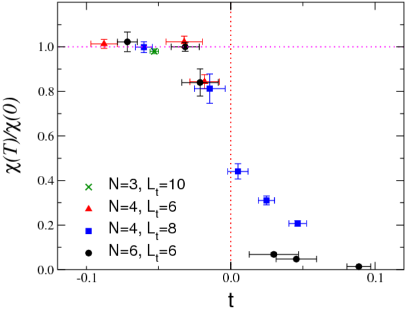
The coefficients in the expansion
$f(\theta) = f(0) + (1/2)\chi_Q\theta^2\left(1+\sum b_{2i}\theta^{2i}\right)$ are determined
in particular $b_2 = -1/12$ in the high T limit

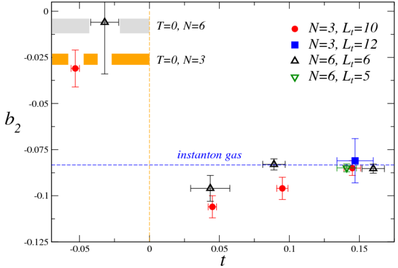
In the confined phase

$$\frac{\chi}{\sigma^2} = 0.0221(14) + \frac{0.055(18)}{N^2}$$

[arXiv:hep-th/0204125]

In this phase b_{2i} coefficients scale as N^{-2i}
$b_2 = -0.23(2)/N_c^2 + O(N^{-4})$ [arXiv:1309.6059]

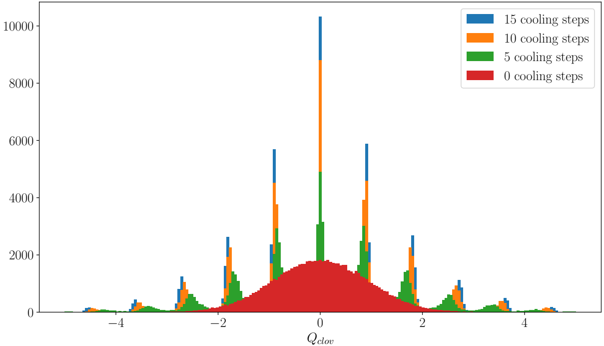




Images from arXiv:1309.6059

Topology on the lattice: smoothing

Q_{clov} has in general non-integer values
Indeed it is affected by UV fluctuations
Those can be removed for example with the cooling procedure
We performed 50 cooling steps on each configuration, but the results are stable after ~ 10



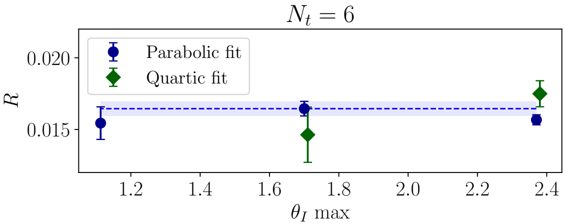
The topological charge Q_{cold} of the cooled configuration is still not an integer, but its histogram presents peaks close to integer values

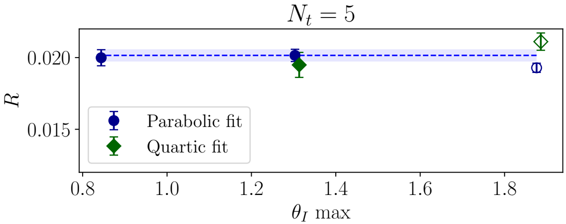
We considered as the actual topological charge $Q_{int} = \text{round}(\alpha Q_{cold})$ where α minimizes $\sum(Q_{int} - \alpha Q_{cold})^2$

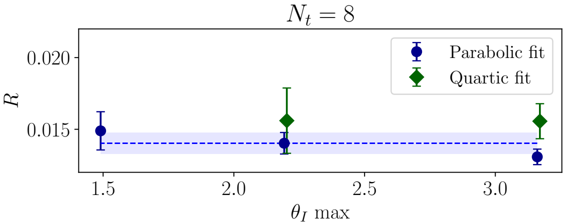
The actual charge Q is related to Q_{clov} (coupled to θ_L): $Q_{clov} \approx ZQ$
Z depends on β and can be computed at 0 temperature as $Z(\beta) = \frac{\langle Q_{clov} Q_{int} \rangle_\beta}{\langle Q_{int}^2 \rangle_\beta}$

Especially on coarse lattice, T_c corrections $O(\theta^4)$ can become relevant

We repeated the parabolic fit reducing the range of θ considered and compared the values of R with the results of a fit including θ^4 corrections

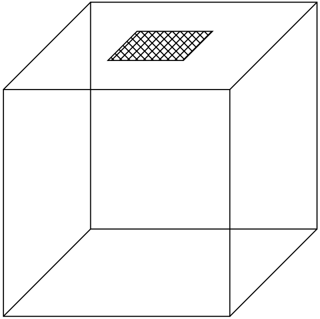






Parallel tempering on boundary conditions

Proposed in [arXiv:1706.04443] for CP^N models, described in [arXiv:2012.14000] for SU(N) theories



When N is large enough, approaching the continuum limit, the topological sector become very separated and standard update algorithms become ineffective in sampling Q (Topological slowing down, [arXiv:hep-th/0204125])

$n_{replica}$ copies of the lattice are simulated and swapped during the simulation with a Metropolis test

All the replica have the same action, except for a 3-dimensional cubic defect, where links orthogonal to the defect enter the action with a $K^{(r)}$ factor.
$K^{(r)}$ for $r = 0, 1, ..., n_{replica} - 1$ interpolate between $K^{(0)} = 1$ and $K^{(n_{replica}-1)} = 0$

In the last replicum, open boundary conditions in the defect disrupt the topology of the configuration, making easier to alter the value of Q in an update

Latent heat formulas

To extract the latent heat we actually compute the difference in trace anomaly between the two phases

$$\frac{\epsilon - 3p}{T^4} = T\frac{\partial}{\partial T}\left(\frac{p}{T^4}\right) = T\frac{\partial}{\partial T}\left(\frac{1}{VT^4}\log(\mathcal{Z})\right)$$

On the lattice we can compute

$$\frac{\epsilon - 3p}{T^4} = N_t^4 \frac{\partial\beta}{\partial\log[a(\beta)/\sqrt{\sigma}]}\frac{\langle S_W\rangle}{V\beta}$$

The latent heat is

$$\frac{\Delta\epsilon}{T_c^4} = \left(\frac{N_t}{N_s}\right)^3 \frac{-\partial\beta}{\partial\log[a(\beta)/\sqrt{\sigma}]}\bigg|_{\beta_c} \sum_{x,\mu>\nu} \Re\,\mathrm{Tr}[\langle\Pi_{\mu\nu}\rangle_d - \langle\Pi_{\mu\nu}\rangle_c]$$

$$R = \frac{\Delta\chi}{2\Delta\epsilon} = \frac{-\partial\beta}{\partial\log[a(\beta)/\sqrt{\sigma}]}\bigg|_{\beta_c} \frac{\left\langle Q^2\right\rangle_c - \left\langle Q^2\right\rangle_d}{2\sum_{x,\mu>\nu}\Re\,\mathrm{Tr}[\langle\Pi_{\mu\nu}\rangle_d - \langle\Pi_{\mu\nu}\rangle_c]}$$

Large N systematics

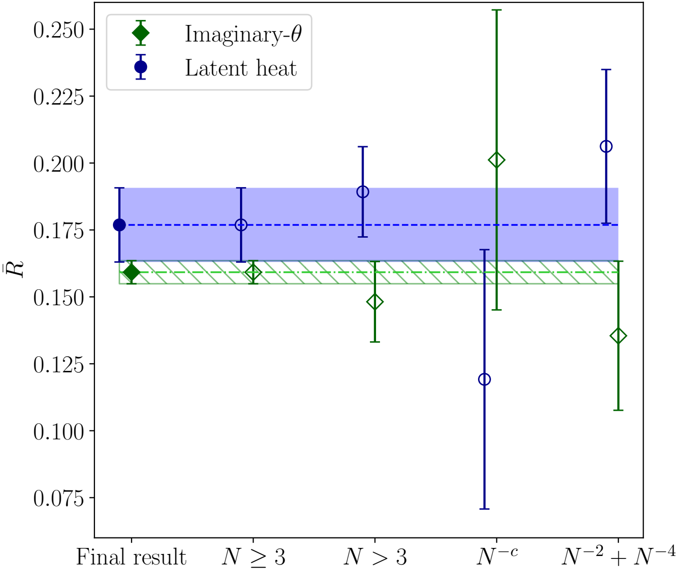
We fitted $R(N)$ with different ansätze:

$$R = \frac{\bar{R}}{N^2}, \;\; N \geq 3$$

$$R = \frac{\bar{R}}{N^2}, \;\; N > 3$$

$$R = \frac{\bar{R}}{N^c}$$

$$R = \frac{\bar{R}}{N^2} + \frac{\bar{R}^{(1)}}{N^2}$$



Multi-histogram: reweighting numerical data

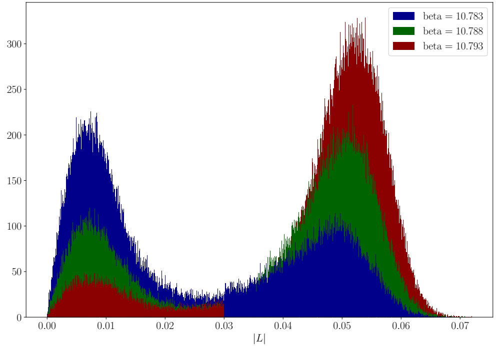
We simulated the system at some values of β. We would like to use the results to compute the mean value of an observable $\mathcal{O}$ at different values of β, in particular interpolating between the simulated ones

The key observation is that the states of the system are the same, but the probability distribution is different. We can reweight the states we generated at a give β, to obtain the probability distribution at a different one

$$\langle \mathcal{O} \rangle_\beta = \frac{1}{Z(\beta)} \sum_{O,E} \rho(O,E)\, O \exp(-\beta\, E)$$

$\rho(O,E)$ is the density of states of the system with value O of the observable $\mathcal{O}$ and E of the action
Z is the partition function:
$Z(\beta) = \sum \rho(O,E) \exp(-\beta\, E)$

$\rho(O,E)$ can be estimated from any simulation
The best estimation is obtained combining all the performed simulations



Multi-histogram: formulas

Notation: the i-th simulation was performed at β_i, generating N_i different configurations and finding $n_i(O,E)$ times the values O and E for the observable and the action
$O_{i,s}$ and $E_{i,s}$ are the values of the observable and the action for the s-th configuration of the i-th simulation

The best estimation of $\rho(O,E)$ is

$$\rho(E,O) = \frac{\sum_i n_i(E,O)}{\sum_j N_j \exp(-\beta_j E)/Z_j}$$

Thus can be found

$$\langle \mathcal{O} \rangle_\beta = \frac{1}{Z(\beta)} \sum_{i,s} \frac{O_{i,s}}{\sum_j N_j Z_j^{-1} \exp[(\beta - \beta_j) E_{i,s}]}$$

$$Z(\beta) = \sum_{i,s} \frac{1}{\sum_j N_j Z_j^{-1} \exp[(\beta - \beta_j) E_{i,s}]}$$

Z_j are the values of $Z(\beta_j)$ that make the last equation consistent