Large-N SU(N) pure-gauge theories with milder topological freezing via parallel tempering on boundary conditions

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Talk based on:

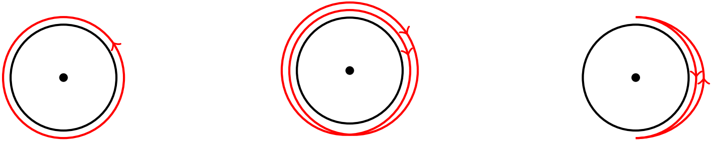
- CB, M. D'Elia, B. Lucini, D. Vadacchino, "*Towards glueball masses of large-N SU(N) pure-gauge theories without topological freezing*", Phys. Lett. B **833** (2022) 137281, arXiv:2205.06190 [hep-lat].
- CB, C. Bonati, M. D'Elia, "*Large-N SU(N) Yang–Mills theories with milder topological freezing*", JHEP **03** (2021) 111, arXiv:2012.14000 [hep-lat].
- M. Berni, CB, M. D'Elia, "*Large-N expansion and θ-dependence of 2d CP^{N-1} models beyond the leading order*", Phys. Rev. D **100** (2019) 11, 114509, arXiv:1911.03384 [hep-lat].

The topological charge in $4d$ non-abelian gauge theories

The topological charge of the finite-action gauge field $A_\mu(x)$

$$Q = \frac{1}{64\pi^2} \int d^4x \, \varepsilon^{\mu\nu\rho\sigma} G^a_{\mu\nu}(x) G^a_{\rho\sigma}(x) \in \mathbb{Z}$$

is a gauge-invariant integer quantity corresponding to the number of windings of $A_\mu(x)$ around the group manifold at $x \to \infty$.



$Q = 1$ $Q = -2$ $Q = 0$

The topological charge can be coupled to the ordinary action of the model S_0 via the dimensionless parameter $\theta \in [0, 2\pi)$:

$$S_0 \to S(\theta) = S_0 + \theta Q.$$

Such coupling introduces a **non-trivial dependence on** θ.

Physical relevance of θ-dep. in QCD and related theories

The study of θ-dependence of QCD and QCD-like gauge theories is prominent both for theoretical and phenomenological reasons.

- **Beyond Standard Model**: non-zero $\theta \to$ breaking of CP symmetry, e.g., non-zero neutron Electric Dipole Moment (nEDM). Experiments: nEDM is well compatible with zero $\implies$ $\theta \sim 0$ within 10^{-10}. No strong-CP violation $\implies$ fine-tuning problem on θ: **strong-**CP **problem**.

- **Hadron physics**: Q **breaks** the $\mathrm{U}(1)_{\mathrm{A}}$ flavor symmetry through **anomaly** $\implies$ large mass of η' meson. Physical parameters of the η' related to θ-dependence of large-N $\mathrm{SU}(N)$ gauge theories.

- **θ-dep. of lower dim. theories**: $2d$ CP^{N-1} models. Extensively studied both **analytically** (large-N limit) and on the **lattice** (cheaper to simulate) as test-beds for validation of numerical methods.

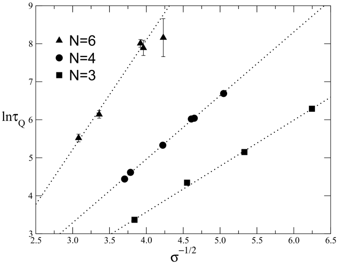
Topological properties and θ-dependence are intrinsically non-perturbative $\implies$ the lattice is a natural tool to explore these topics.

Critical Slowing Down and topological freezing

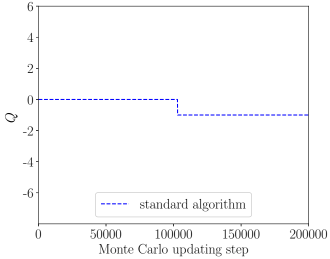
Approaching the continuum limit $a \to 0$, Monte Carlo Markov Chains experience a **Critical Slowing Down** (CSD) when local updating algorithms (e.g., heat-bath) are employed.

CSD = autocorrelation time $\tau(\mathcal{O})$, i.e., number of updating steps to generate two gauge configurations with uncorrelated values of $\mathcal{O}$, grows with $1/a$.

While for most observables $\tau(\mathcal{O}) \sim (1/a)^\alpha$ with α small, for topological observable it is observed to be much more severe.



(Fig. from Del Debbio et al., 2002)



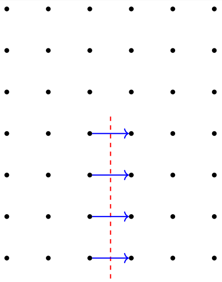
Example for $N = 6$, $a \simeq 0.0842$ fm

Plenty of numerical evidence that $\tau(Q)$ diverges as $\sim \exp N$ at fixed a and vice versa

Parallel tempering on boundary conditions

Proposed for $2d$ CP^{N-1} models (Hasenbusch, 2017; Berni, CB et al., 2019), recently implemented for $4d$ $\mathrm{SU}(N)$ pure-gauge theories (CB et al., 2021, 2022)

- consider a collection of N_r lattice replicas
- replicas differ for boundary conditions on **small** sub-region: *the defect*
- each replica is updated with standard methods
- after updates, propose swaps among configurations via Metropolis test
- other ingredients: hierarchic updates + translation of periodic replica



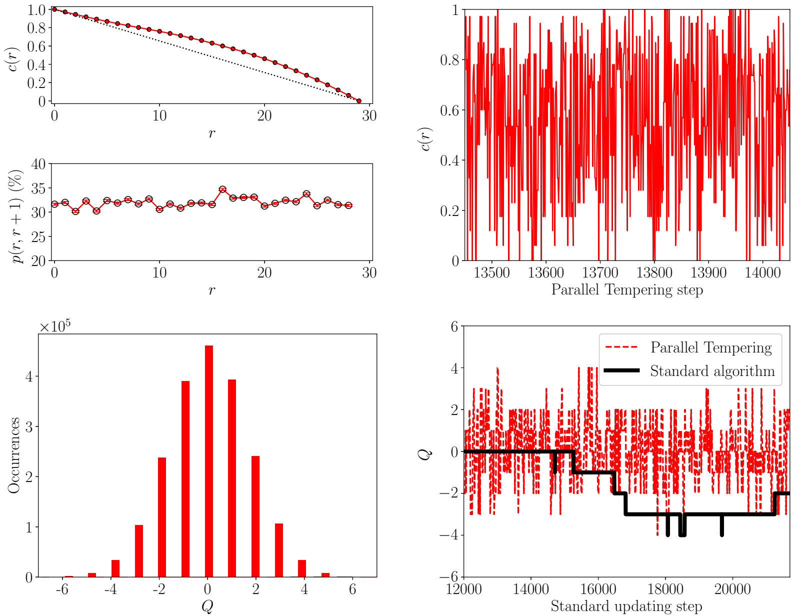
Links crossing the defect: $\beta \to \beta \cdot c(r)$.

Periodic: $c(0) = 1$. Open: $c(N_r - 1) = 0$. Interpolating replicas: $0 < c(r) < 1$.

Decorrelation of Q improved thanks to open boundaries copy, where Q is decorrelated faster.

Observables computed on periodic replica $\to$ easier to have finite-size effects under control.

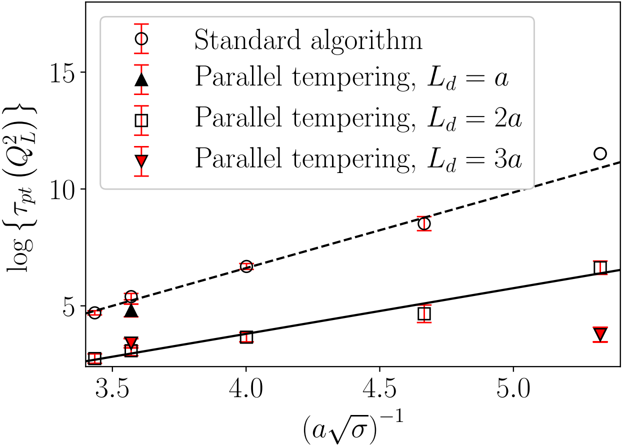
Setup and improvements - SU(6), $a \simeq 0.0938$ fm



Scaling towards the continuum

$\tau_{\rm pt}(Q^2) \equiv N_r\, \tau(Q^2) \sim \exp(1/a)$ if defect size L_d/a is fixed as $a \to 0$, however with a **much smaller** slope compared to the standard algorithm.

If instead L_d is kept fixed in physical units, scaling is **tremendously improved**: $\tau_{\rm pt}$ obtained for $L_d = 2a$ and $L_d = 3a$ for smaller lattice spacing are compatible within the errors.



The θ-Dependence of Large-N SU(N) Yang–Mills Theories

The θ-dependence of the Yang–Mills vacuum energy

The θ-dependence of the vacuum energy is defined in Euclidean time as

$$E_{\rm YM}(\theta) = -\frac{1}{V}\log\int[d\overline{\psi}d\psi dA]e^{-S_{\rm YM}+i\theta Q}, \quad E_{\rm YM}(\theta) = \frac{1}{2}\chi\theta^2\left(1+\sum_{n=1}^{\infty}b_{2n}\theta^{2n}\right).$$

Taylor coefficients are related to cumulants of the $\theta = 0$ charge distribution:

$$\chi = \frac{\langle Q^2\rangle}{V}\bigg|_{\theta=0}, \qquad b_2 = -\frac{1}{12}\frac{\langle Q^4\rangle - 3\langle Q^2\rangle^2}{\langle Q^2\rangle}\bigg|_{\theta=0}, \qquad b_{2n} \propto \frac{\langle Q^{2n+2}\rangle_c}{\langle Q^2\rangle}\bigg|_{\theta=0}.$$

At large N: actual expansion parameter θ/N and $E_{\rm YM} \sim O(N^2)$:

$$\Longrightarrow \; E_{\rm YM}(\theta, N) \underset{N\to\infty}{\sim} N^2 f\left(\frac{\theta}{N}\right) + O\left(\frac{1}{N^2}\right).$$

$$\chi = \bar{\chi} + O(1/N^2)$$

Witten–Veneziano argument: $m^2_{\eta'} = (4N_f/f^2_\pi)\,\bar{\chi} \implies \bar{\chi} \simeq (180\ \text{MeV})^4$

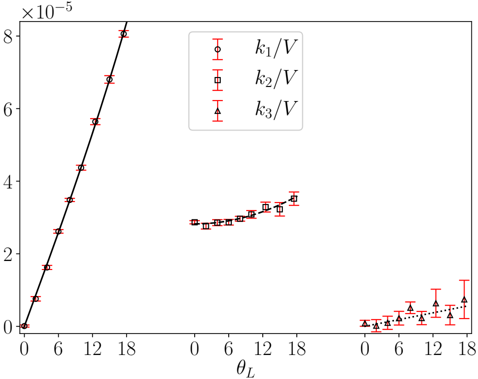
$$b_{2n} = \frac{\bar{b}_{2n}}{N^{2n}}\left\{1 + O\left(\frac{1}{N^2}\right)\right\}$$

Higher-order cumulants and imaginary-θ simulations

Signal-to-Noise Ratio (SNR) of b_{2n} (higher-order cumulants) decades with the volume
$\Longrightarrow$ large statistics required to keep finite-size effects under control

Imaginary-θ simulations: θ-term acts as a source term for Q, enhancing SNR of higher-order cumulants $k_n \equiv \langle Q^n \rangle_c$

$$S \to S + \theta_I Q, \quad \theta_I \equiv i\theta \qquad \Longrightarrow \qquad k_n \to k_n(\theta_I) = \langle Q^n \rangle_c (\theta_I) \propto \frac{d^n E_{\mathrm{YM}}(\theta_I)}{d\theta_I^n}$$



Imaginary-θ fit: information on χ and b_{2n} encoded in θ_I-dependence of lower-order cumulants
$\Longrightarrow$ extract χ and b_{2n} from combined fit of θ_I-dependence of cumulants k_n:

$$\frac{k_1}{V}(\theta_I) = \frac{\langle Q \rangle}{V}(\theta_I) \quad = \chi(\theta_I - 2b_2\theta_I^3 + \dots)$$

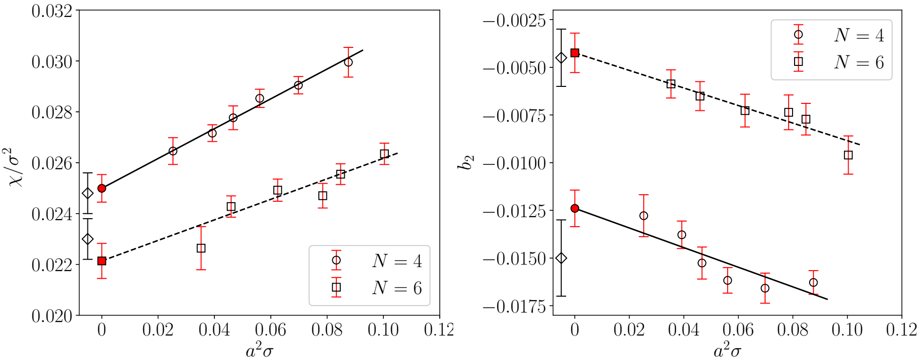
$$\frac{k_2}{V}(\theta_I) = \frac{\langle Q^2 \rangle_c}{V}(\theta_I) = \chi(1 - 6b_2\theta_I^2 + \dots)$$

$$\frac{k_3}{V}(\theta_I) = \frac{\langle Q^3 \rangle_c}{V}(\theta_I) = \chi(-12b_2\theta_I + \dots)$$

Continuum limit of χ and b_2 for $N = 4, 6$

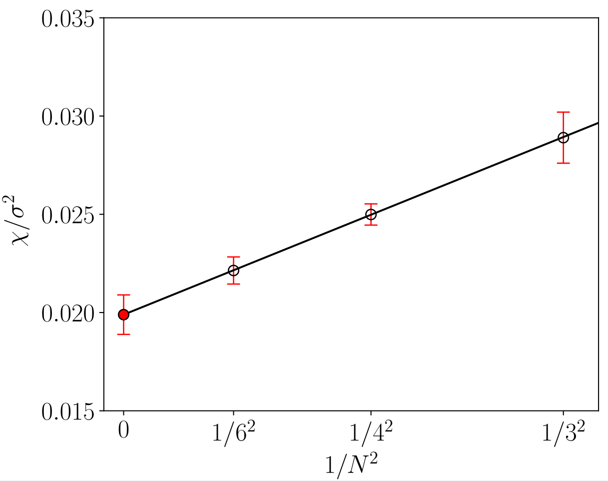
Parallel tempering + imaginary-θ method dramatically **improve** continuum limit of topological quantities at large N compared to standard methods.

Note that earlier result for $b_2(N = 6)$ was not a continuum extrapolation but just a confidence interval: first continuum extrapolation performed in CB, Bonati, D'Elia, 2021 (arXiv:2012.14000).



Continuum limits: diamond points (Bonati et al., 2016), full points (CB, Bonati, D'Elia, 2021).

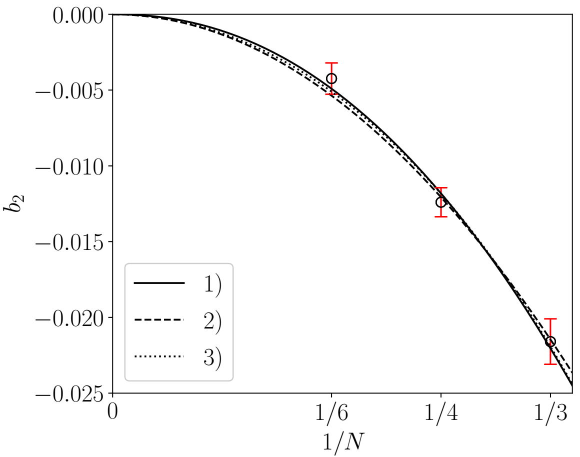
Large-N limit of χ in SU(N) pure-gauge theories



Witten–Veneziano: $\bar{\chi}^{1/4} \simeq 180$ MeV $+ O(1/N^2)$. Fit results:

$$\chi/\sigma^2 = 0.0199(10) + 0.08(2)(1/N^2)$$

$$\bar{\chi}/\sigma^2 = 0.0199(10) \implies \bar{\chi}^{1/4} = 173(8) \text{ MeV}$$



Dilute Instanton Gas Approximation (DIGA):

$b_2 = -1/12 \simeq -0.0833$

Dilute Gas of Fractional $1/N$ Instantons:

$b_2 = (-1/12)/N^2$

$\Longrightarrow \; \bar{b}_2 \simeq -0.0833$

Large-N prediction: $b_2 = \bar{b}_2/N^2 + O(1/N^4)$. Fit results:

1) $b_2 = \bar{b}_2/N^\gamma \quad \to \quad \gamma = 2.17(26)$

2) $b_2 = \bar{b}_2/N^2 \quad \to \quad \bar{b}_2 = -0.19(1)$

3) $b_2 = \bar{b}_2/N^2 + \bar{b}_2^{(1)}/N^4 \quad \to \quad \bar{b}_2^{(1)} = -0.17(35)$

Glueball Masses and Topology of Large-N $\mathrm{SU}(N)$ Yang–Mills Theories

Physical motivations

Glueball states are predicted on the basis of **QCD confinement** and are currently searched in collider experiments. Refinement of QCD theoretical predictions about glueball masses is thus of utmost importance in this respect.

Determining glueball masses from numerical lattice QCD simulations is a long-standing problem that has been widely investigated.
Main computational framework: large-N SU(N) pure-gauge theories:

- large-N is "close" to $N = 3$, as corrections are suppressed as powers of $1/N$
- **no quarks** + $N = \infty \implies$ all glueballs are exactly non-interacting and with ∞ lifetime

Overall, this framework provides acceptable approximation of real-world QCD, and an interesting theoretical ground to provide useful predictions.

Although glueball masses are not topological quantities, topological freezing may have a non-negligible impact in their lattice determination.

Glueball masses and topology

Computing a glueball mass M on a finite volume and in a **fixed topological sector**, i.e., in the presence of topological freezing, leads to a bias (Brower et al., 2002; Aoki et al., 2007)

$$M_Q = M + \frac{1}{2}\frac{d^2 M}{d\theta^2}\bigg|_{\theta=0}\frac{1}{V\chi} = M + O\left(\frac{1}{N^2 V}\right)$$

- $S_{\mathrm{YM}}(\theta) = S_{\mathrm{YM}}^{(\theta=0)} + i\theta Q$
- $E_{\mathrm{YM}}(\theta, N) \underset{N\to\infty}{\sim} N^2 f\left(\frac{\theta}{N}\right) + O\left(\frac{1}{N^2}\right)$
- M_Q = Glueball mass in fixed topological sector Q
- M = Glueball mass averaged over all topological sectors
- $\chi \equiv \frac{\langle Q^2 \rangle}{V}$ $\longrightarrow$ **Topological Susceptibility**

No satisfactory check of possible systematics related to fixed topology due to topological freezing at large N so far.

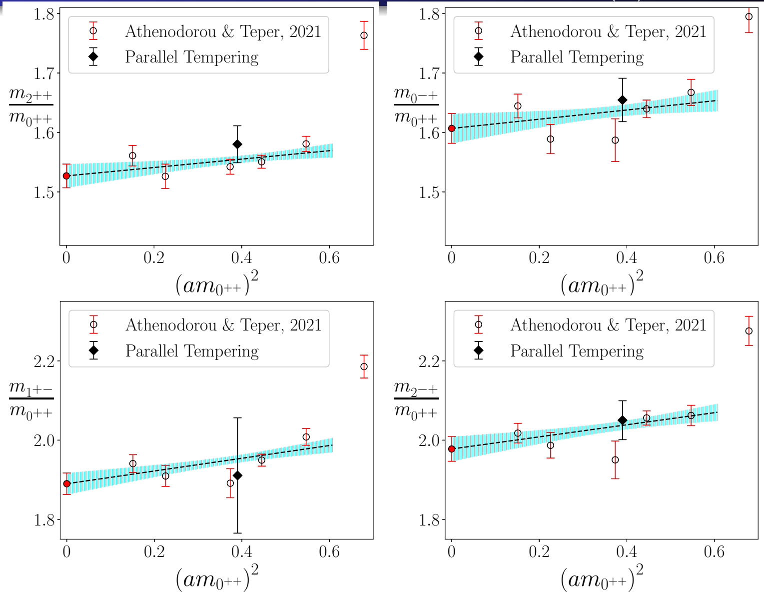
Recap of state-of-the-art methods for glueball masses

(Berg et al., 1983; Teper et al., 1987; Morningstar et al., 1999; Lucini et al., 2001, 2004, 2010; Hong et al., 2017, Bennett et al., 2020; Athenodorou et al., 2020, 2021; and many more. . .)

- Choose a proper variational basis $\mathcal{B} = \{\mathcal{O}_i(t)\}$ of operators with compatible quantum numbers with respect to the desired channel
- Operators $\mathcal{O}(t) = \sum_{\vec{x}} \mathcal{O}(\vec{x}, t)$: zero-momentum gauge-invariant operators built in terms of traces of product of links along closed spatial paths
- Compute the correlation matrix $C_{ij}(t) = \langle \mathcal{O}_i(t)\mathcal{O}_j(0)\rangle$ and solve the **Generalized Eigenvalue Problem** $C_{ij}(t)v_j = \lambda(t, t')C_{ij}(t')v_j$
- For the ground state in the selected channel, it is sufficient to consider eigenvector $\overline{v}_i$ related to the largest eigenvalue $\overline{\lambda}(t, t')$
- The best overlapping correlator between the vacuum and the desired glueball state is $C_{\text{best}}(t) \equiv C_{ij}(t)\overline{v}_i\overline{v}_j \underset{t\to\infty}{\sim} \exp\{-amt\}$
- Extract the glueball state mass looking for a plateu in

$$am_{\text{eff}}(t) \equiv -\log\left(\frac{C_{\text{best}}(t+1)}{C_{\text{best}}(t)}\right)$$

Results for low-lying glueball masses - SU(6)



Perfect agreement within precision with results of (Athenodorou & Teper, 2021) obtained with standard algorithms, also in channels with same quantum numbers of Q

Conclusions

Relevant take-home messages

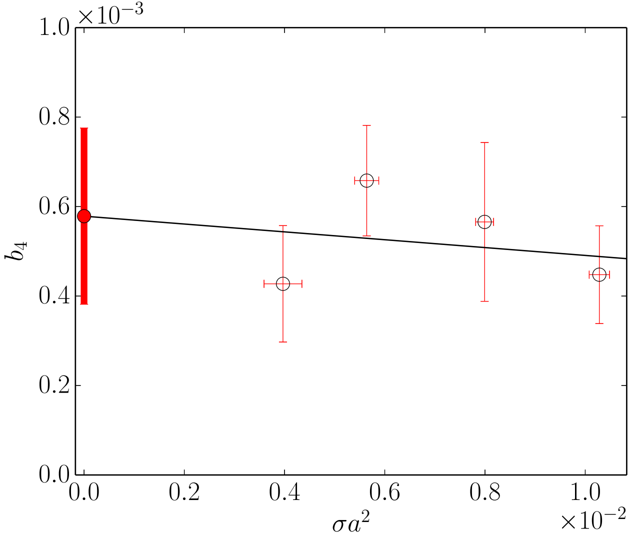
- Parallel tempering on boundary conditions is an affordable and viable solution to fight topological freezing, especially at large N
- Combining Parallel tempering and imaginary-θ it is possible to accurate study θ-dependence at large-N beyond the leading order
- Our percent results for $b_2(N)$ perfectly fit leading-order large-N predictions; no evidence for dilute instanton gas (nor integer or fractional)
- First computation of glueball masses at large N without topological freezing does not detect any effect from fixed topology at our percent level

Some future outlooks

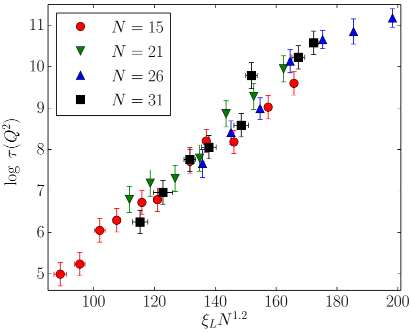
- Bias on computation of M_{glueball} due to fixed topology related to $\frac{d^2 M_{\text{glueball}}}{d\theta^2}\Big|_{\theta=0}$. Direct computation of this quantity?
  Only reported result in the literature: $N = 3$ for 0^{++} state. Possible improvements from imaginary-θ method + parallel tempering.
- Recently, tensions on lattice determinations of Λ_{QCD} in SU(3) pure-gauge theory have been pointed out: what's the impact of fixed topology?

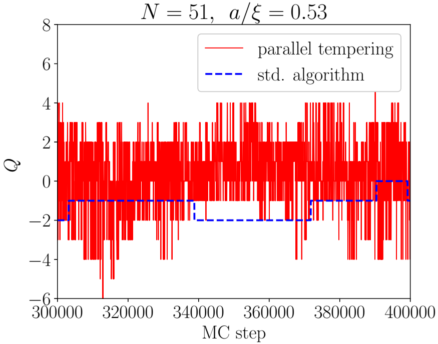
Back-up Slides

Continuum-extrapolated results for b_4 for SU(2) Yang–Mills theory

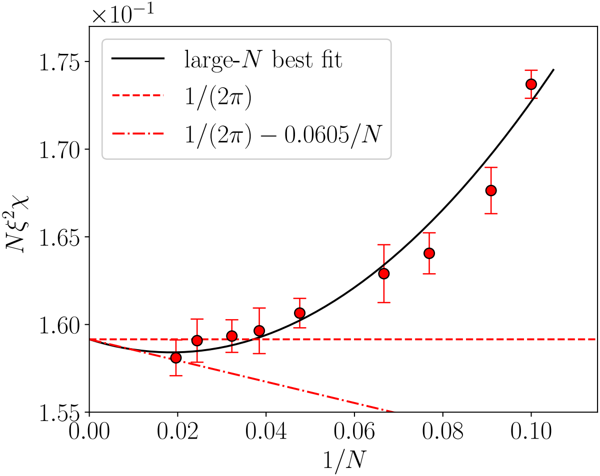


Topological freezing at large N - $2d$ CP^{N-1} models





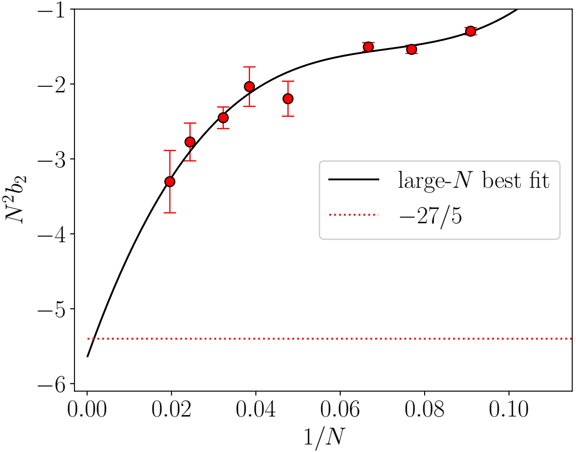
Large-N behavior of $N\xi^2\chi$ in $2d$ CP^{N-1} models



Fit results up to $O(1/N^2)$ terms, $N \in [11, 51]$

$$N\xi^2\chi = 1/(2\pi) - 0.08(2)(1/N) + 2.2(3)(1/N^2)$$

Large-N behavior of $N^2 b_2$ in $2d$ CP^{N-1} models

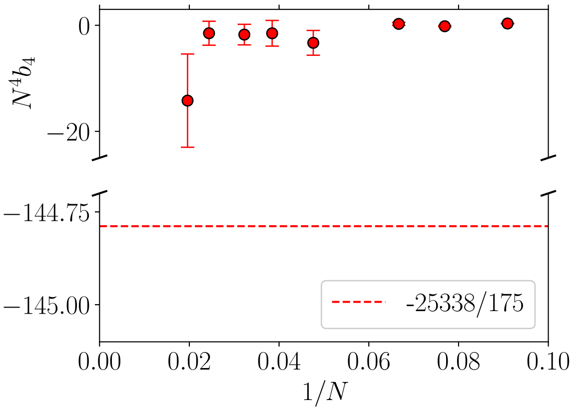


Fit results up to $O(1/N^3)$ terms, $N \in [11, 51]$

$$\bar{b}_2^{(\mathrm{theo})} \equiv \lim_{N\to\infty} N^2 b_2 = -27/5 = -5.4,$$

$$(N^2 b_2)_{\mathrm{fit}} = -5.7(1.1) + 160(60)(1/N) + \dots$$

Large-N behavior of $N^4 b_4$ in $2d$ CP^{N-1} models



In our large-N simulations b_4 was always compatible with zero, except for $N = 9$ and 11.

We find $|\bar{b}_4| \sim |N^4 b_4| \lesssim 20$, but large-$N$ analytic computation yields $\bar{b}_4 = -25338/175 \simeq -144.788571\dots$