Fighting topological freezing in the two-dimensional CP^{N-1} model

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Continuum limit of a lattice theory

Determine $1/\xi(\beta) = ma$ from decay of correlation functions on the lattice; setting m equal to the experimentally known mass of the particle
$\Longrightarrow$ $a(\beta)$, where β is a parameter of the action

Continuum results are obtained for $a(\beta) \to 0$

Asymptotically free theories:
errors on physical quantities vanish with some power of a

Costs of Monte Carlo simulations increase:

- For fixed physical volume, number of sites increases a^{-d}
- On top critical slowing down a^{-z}

Sometimes much worse; In lattice QCD: topological sectors can not be changed when going below a certain value of a_{freeze}

What should we do?

- Maybe nothing; Results obtained for $a \geq a_{freeze}$ are accurate enough ? In lattice QCD $a_{freeze} \approx 0.05$ fm
- Try to extract physics from fixed topological sectors
- Overcome topological freezing by algorithmic improvement

The CP^{N-1} model

Square lattice with sites $x = (x_0, x_1)$, where $x_i \in \{0, 1, 2, ..., L_i - 1\}$.
The lattice spacing is set to $a = 1$
Periodic or open boundary conditions in 0-direction
Periodic boundary conditions in 1-direction

$$S = -\beta N \sum_{x,\mu} \left(\bar{z}_{x+\hat{\mu}} z_x \lambda_{x,\mu} + z_{x+\hat{\mu}} \bar{z}_x \bar{\lambda}_{x,\mu} - 2 \right) \ ,$$

- z_x is a complex N-component vector with $z_x \bar{z}_x = 1$
- $\lambda_{x,\mu}$ is a complex number with $\lambda_{x,\mu} \bar{\lambda}_{x,\mu} = 1$

Toy model of (lattice) QCD

- asymptotically free
- $1/N$-expansion computed to $O(1/N)$
- Stable instanton solutions
- Problem shared with lattice QCD: topological freezing

Topological susceptibility

Topological charge

$$Q_{plaq} = \frac{1}{2\pi} \sum_x \theta_{plaq,x}$$

where

$$\theta_{plaq,x} = \theta_{x,\mu} + \theta_{x+\hat{\mu},\nu} - \theta_{x+\hat{\nu},\mu} - \theta_{x,\nu} - 2n\pi \quad , \qquad \mu \neq \nu$$

where $\theta_{x,\mu} = \arg\{\bar{z}_x z_{x+\hat{\mu}}\}$ and n is such that $-\pi < \theta_{plaq,x} \leq \pi$.

$$\chi_t = \frac{1}{V} \langle Q^2 \rangle$$

Basic algorithm: hybrid of local

- Heatbath/Metropolis (spin/gauge fields) sweeps
- $n_{ov} \propto \xi$ Overrelaxation sweeps

In 2D XY model: dynamical critical exponent $z \approx 1$

CP^{N-1} model, periodic boundary conditions in both directions: autocorrelation times of the topological modes increase very rapidly with the correlation length ξ. Looks like an exponential increase.

We can go up to $\xi \approx 23$, 6, 2.4 for $N = 10$, 21, and 41

Periodic boundary conditions:

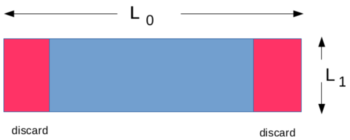
Continuum: disconnected sectors characterized by their charge Q

Finite lattice spacing:

Free energy barriers increase with increasing correlation length.

Markov chain Monte Carlo algorithms become non-ergodic

M. Lüscher and S. Schaefer (2011) Open boundary conditions (lattice QCD)



Here $L_0 = 4L_1$, $L_1 \approx 15\xi_{2nd}$, discard $l_0 \approx 10\xi_{2nd}$

Autocorrelation function

$$\rho(t) = \frac{\langle A_i A_{i+t} \rangle - \langle A \rangle^2}{\langle A^2 \rangle - \langle A \rangle^2}$$

Integrated autocorrelation time

$$\tau_{int,A} = \frac{1}{2} + \sum_{t=1}^{\infty} \rho(t)$$

Statistical error

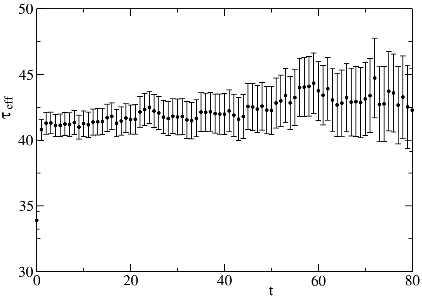
$$\epsilon = \sqrt{\frac{2\tau_{int,A}\sigma^2(A)}{N}}$$

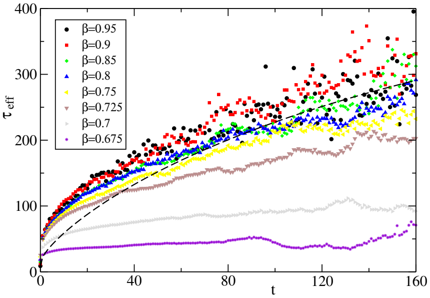
Effective autocorrelation time of the topological susceptibility

$$\tau_{eff,s,A}(t) = -s/\ln[\rho_A(t+s)/\rho_A(t)]$$

periodic b.c. $N = 10$,
$\beta = 0.96$, $\xi_{2nd} = 12.87(1)$

open b.c., N=21,
ξ_{2nd} up to 18.242(2)





G. McGlynn and R. D. Mawhinney (2014)
Effective model for diffusion of instantons:

$$\rho(t) \propto \sum_n c_n \exp\left(-\frac{n^2}{\tau_{exp}} t\right) \;,$$

Dashed line in our plot, ad hoc:
$c_n \propto 1/n$, $\tau_{exp} = 455$

Parallel tempering: a short reminder

C. J. Geyer in *Computer Science and Statistics: Proc. of the 23rd Symposium on the Interface*, edited by E. M. Keramidas (Interface Foundation, Fairfax Station, 1991), p. 156; K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. **65**, 1604 (1996)

Related: E. Marinari and G. Parisi, *Simulated Tempering: A New Monte Carlo Scheme*, [arXiv:hep-lat/9205018], Europhys. Lett. **19**, 451 (1992).

A prototype problem: study of spin-glasses

At low temperature:
ragged free energy landscape $\Longrightarrow$ large autocorrelation times

Introduce N_t copies of the system, each at a different value of the inverse temperature $\beta_i = \frac{1}{k_B T_i}$.

Simple choice $\beta_i = \beta_0 + i \Delta\beta$ with $\Delta\beta = \frac{\beta_{max} - \beta_0}{N_t - 1}$

Simulations at β_0 have small autocorrelation times

Steps of the algorithm:

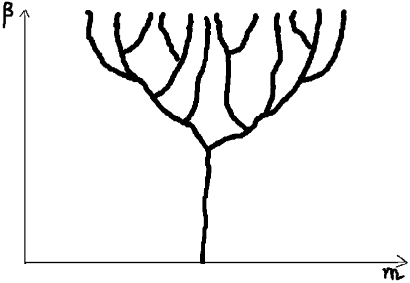
-Standard updates of the individual systems for each β_i

-Swap configurations X_i and X_{i+1} between β_i and β_{i+1}:
Accept with Metropolis probability

$$A_{swap} = \min\left[1, \exp\left(-\Delta\beta \left[H(X_i) - H(X_{i+1})\right]\right)\right]$$

$\Delta\beta$ has to be chosen such that (very roughly) $A_{swap} \approx 50\%$

Minima of the free energy in some macroscopic parameter m plotted versus β.

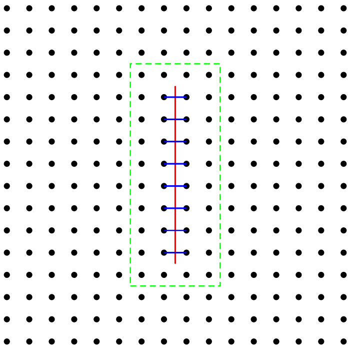


- Idea can be generalized to other parameters of the action
- Additional systems might have no physical meaning
- Introduced only for the purpose of the algorithm

Parallel tempering in a line defect

$$S = -\beta N \sum_{x,\mu} c_{t,x,\mu} \ \left(\bar{z}_{t,x+\hat{\mu}} z_{t,x} \lambda_{t,x,\mu} + z_{t,x+\hat{\mu}} \bar{z}_{t,x} \bar{\lambda}_{t,x,\mu} - 2\right)$$

where $c_{t,x,\mu} = c_r(t)$ for x, μ on the defect line and $c_{t,x,\mu} = 1$ else.

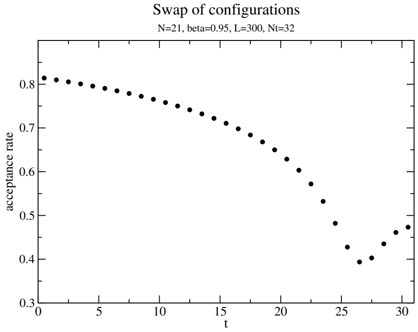


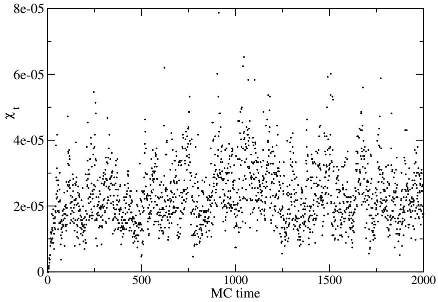
$t \in \{0, 1, ..., N_t - 1\}$ labels the points of the tempering chain. In our simulations we take $c_r(t) = 1 - t/(N_t - 1)$

$A_{swap} = \min[1, \exp(-\beta N$
$[c_r(t_1) - c_r(t_2)] [E_r(t_2) - E_r(t_1)])]$

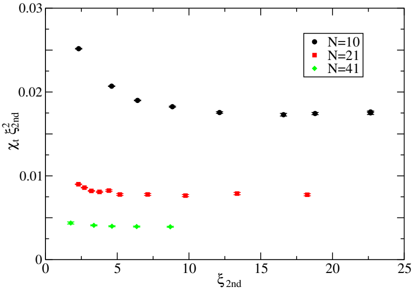
```
Sweeps over the full lattice; replica ex.; transl.;
  for(i1=0;i1<n1;i1++)
    {
    Sweeps over box(l_1); replica ex.; transl.; measure;
    for(i2=0;i2<n2;i2++)
      {
      Sweeps over box(l_2); replica ex.; transl;
      for(i3=0;i3<n3;i3++)
        {
        Sweep over box(l_3); replica ex.; transl.;
        .
        .
        .  until l_i = 1
    } } ...}
```

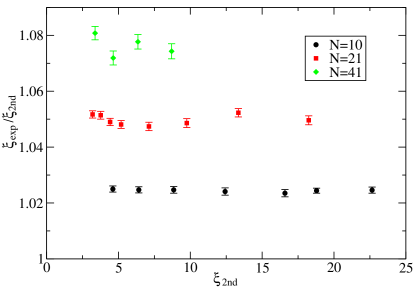
$N = 21$, $\beta = 0.95$, $L = 300$, $l_d = 16$, Largest box: 80×64
Tempering cycle $n_1 = 24$, $n_2 = n_3 = n_4 = 3$, and $n_5 = n_6 = 2$.
The number of overrelaxation updates: 28, 14, 7, 7, 3, and 3 at levels 1, 2, 3, 4, 5, and 6. 4849 config. exchange updates per cycle.
50370 update cycles, 25 days on a CPU with 4 cores.





$\tau_{int,pos} = 1.875(13)/72$, $\chi_t = 0.00002305(16)$, $\tau_{int,\chi_t} = 7.2(5)$,
$\tau_{exp} \approx 16$





$$\chi_t \xi_{2nd}^2 = \frac{1}{2\pi N}\left(1 - \frac{0.38088...}{N}\right) + O\left(N^{-3}\right)$$

$$\frac{\xi_{2nd}}{\xi_{exp}} = \sqrt{\frac{2}{3}} + O\left(N^{-2/3}\right)$$

$$\sqrt{\frac{3}{2}} = 1.2247...$$

Conclusions and outlook

- open boundary conditions avoid topological freezing (as expected)
- Dynamical critical exponent of hybrid overrelaxation $z \approx 1$
- Parallel tempering of line defect looks fine; with respect to the error of χ_t slightly better than standard simulation with open boundary conditions
- Does it work for lattice QCD?

M. H., [arXiv:1706.04443], Phys.Rev. D96 (2017) 054504
M. H., [arXiv:1709.09460]

Thanks for your attention!