ETH zürich

Institute for Theoretical Physics

Towards the Application of Skewed Detailed Balance in Lattice Gauge Theories

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The 39th International Symposium on Lattice Field Theory

Outline

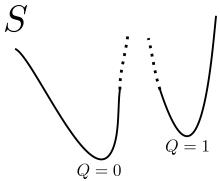
Topological Freezing

- Poor sampling as we approach the continuum limit;
- Affects QCD but also other theories with non-trivial vacuum structure;
- Non local updating algorithms may solve this problem (e.g. Wolff cluster algorithm for $O(N)$ models in $N-1$ dimensions);

  Wolff, U. (1989). Phys. Rev. Lett. 62 361.

- "Naive" generalizations will not solve the problem for certain systems.

  Caracciolo, S.; Edwards, R. G.; Pelissetto, A.; and Sokal, A. D. (1993). Nuclear Physics B, 403(1-2), 475-541.



- Can breaking detailed balance help?

Algorithmic Improvements by Breaking Detailed Balance

- Ising

  Elçi, E. M.; Grimm, J., Ding, L., Nasrawi, A.; Garoni, T. M.; and Deng, Y. (2018). Physical Review E, 97(4), 042126.

  Suwa, H. (2022). arXiv:2206.13881

- Potts model and quantum spins

  Suwa, H.; and Todo, S. (2010). Physical Review Letters, 105(12), 120603.

- Hard spheres

  Bernard, E. P.; Krauth, W., and Wilson, D. B. (2009). Physical Review E, 80(5), 056704.

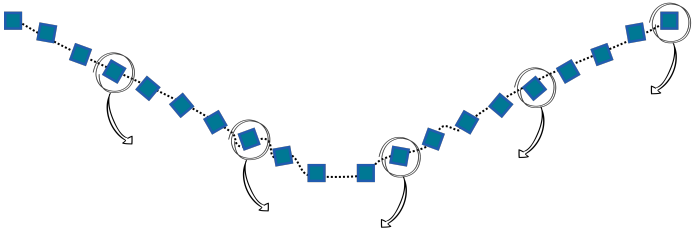
- ($SU(3)$ pure gauge

  Cossu, G., Boyle, P.; Christ, N., Jung, C., Jüttner, A.; and Sanfilippo, F. (2018). In EPJ Web of Conferences (Vol. 175, p. 02008). EDP Sciences.)

- and more ...

Detailed Balance $\Rightarrow$ Global Balance

- Phase space Ω
- Configuration $c \in \Omega$
- Probability distribution $\pi(c)$
- Transition probabilities $T_{cc'}$



$$\pi(c) = \sum_{c' \in \Omega} \pi\left(c'\right) T_{cc'}$$

$$\Uparrow$$

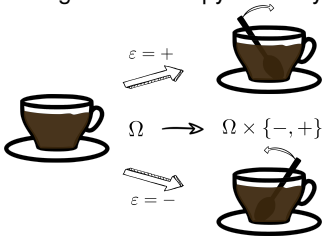
$$\pi(c)\, T_{cc'} = \pi\left(c'\right) T_{c'c}$$

- Most used algorithms satisfy detailed balance with some "mild" exceptions (e.g. sequential updating).

Outline

Lifting and Skewed Detailed Balance

Lifting: enlarged phase space by creating a double copy of the system



Diaconis, P.; Holmes, S.; Neal, R. M. Ann. Appl. Probab. 2000, 10, 726-752.

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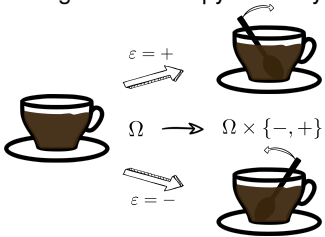

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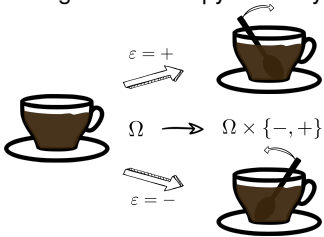

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- $T^{\varepsilon}_{cc'}$: probability of transitioning to c', ε
- $\Lambda^{c}_{\varepsilon,-\varepsilon}$: probability of transitioning to $c, -\varepsilon$

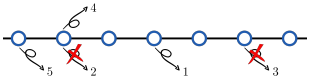
Outline

Skewed Detailed Balance in the Potts Model

$$H = -J \sum_{\langle i,j \rangle} \delta_{s_i, s_j}, \quad s_i \in \{1, \ldots, q\}$$

- skewed detailed balance aids the local algorithm;

  1. choose random site i;
  2. choose a spin according to the probability distribution $p\left(s_i \to s_i'\right)$;
  3. accept it with probability $\frac{1+\varepsilon\delta \operatorname{sign}\left(s_i' - s_i\right)}{1+\delta} \in \{1, \frac{1-\delta}{1+\delta}\}$
  4. if rejected, propose the flip $\varepsilon \to -\varepsilon$ with the appropriate probability;



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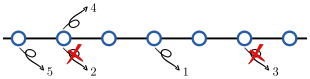

- $\delta \in [0, 1]$;
  - $\delta = 0$: satisfies detailed balance;
  - $\delta = 1$: "maximizes" detailed balance violation.

Skewed Detailed Balance in the Potts Model

How much MC time do we need to get the correct magnetization average?

- $q = 4$ states Potts model;
- $m = \frac{1}{L}\sum_x s_x \;\rightarrow\; \langle m \rangle = 5/2.$
- $C_m(\tau) = \frac{E[m(t+\tau)m(t)] - E[m(t)]^2}{E\left[m(t)^2\right] - E[m(t)]^2}$

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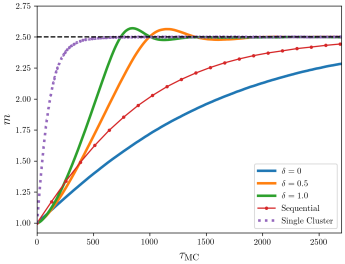

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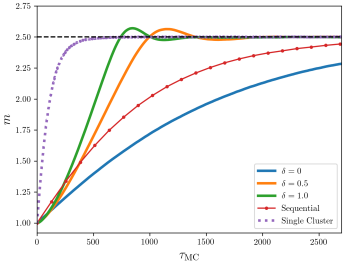

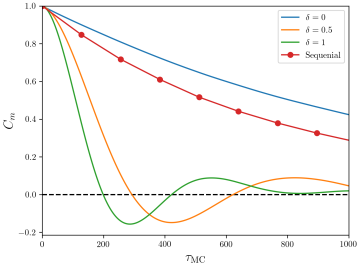

$H = -J\sum_{\langle i,j \rangle} \delta_{s_i,s_j}$, $L = 128$, $J = 2$

See also Faizi, F.; Deligiannidis, G., and Rosta, E. (2020). Journal of Chemical Theory and Computation, 16(4), 2124-2138.

Outline

Biasing Towards Specific Topological Sectors

- Challenges:
  - local updates do not change the topological sector;
  - infinite (or very large) number of topological sectors;
  - (dealing with continuous variables);

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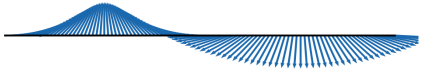
A cartoon of the 1-d $O(2)$ model: an angle defined at every site $\theta_x \in [0, 2\pi)$

$Q = 0$

$Q = 1$



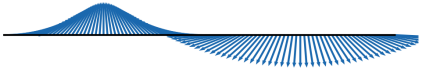
$Q = 2$

$Q = 4$

Instanton Background Lifting

- Consider a "instanton background", which can have positive or negative charge $I_\varepsilon(x)$;

$I_+(x)$



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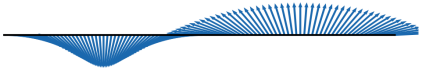

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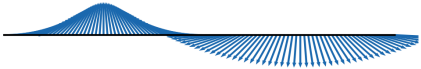

$I_-(x)$

- Construct an algorithm that takes the background into account;
  1. choose random site x;
  2. choose an angle according to the probability distribution $p(\theta_x \to \theta'_x)$;
  3. accept it with probability

$$\frac{1+\varepsilon\delta\,\mathrm{sign}\left(\cos\left(\theta'_x - I_\varepsilon(x)\right) - \cos\left(\theta_x - I_\varepsilon(x)\right)\right)}{1+\delta}$$

  4. if rejected, propose the flip $\varepsilon \to -\varepsilon$ with the appropriate probability;

Equilibrating Topological Charge in the 1-d $O(2)$ model

How much time do we need to get rid of some initial topological charge?

- Consider an initial instanton configuration
- Topological charge $Q = 1$;
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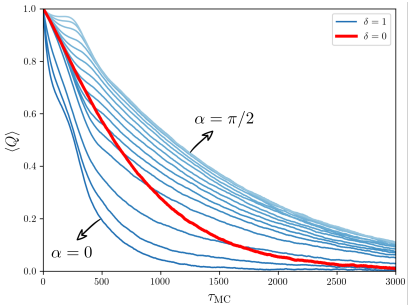

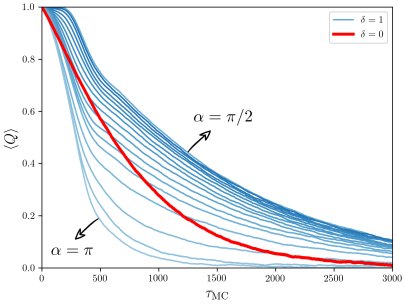

Equilibration is accelerated only when $\alpha \lesssim 0.2 \bmod \pi$.

Conclusions

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Can breaking detailed balance improve simulations of lattice gauge theories, in general, and QCD, in particular?

Most likely yes!

Skewed Detailed Balance Condition and Transitions

For a given configuration in the enlarged phase space, c, ε:

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A possible choice is the Turitsyn-Chertkov-Vucelja (TCV) type

$$\Lambda^{c}_{\varepsilon,-\varepsilon} = \max \left\{ 0, \sum_{c' \neq c} \left(T^{-\varepsilon}_{cc'} - T^{\varepsilon}_{cc'} \right) \right\}$$

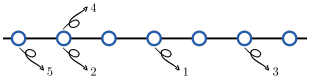
Turitsyn, K. S.; Chertkov, M.; Vucelja. Physica D 2011, 240, 410-414.

If the probability of total transitions at ε is low, then the transition $\varepsilon \to -\varepsilon$ becomes likely.

Simulating the q-states Potts Model

$$H = -J \sum_{\langle i,j \rangle} \delta_{s_i, s_j}, \quad s_i \in \{1, \ldots, q\} \qquad \rightarrow \qquad q \text{ ground states}$$

- local updating algorithms may have difficulty going from one ground state to other;
  1. choose random site i;
  2. choose a spin according to $p\left(s_i \rightarrow s_i'\right)$ satisfying detailed balance;



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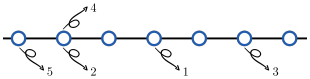
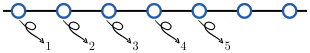


- sequential updating is better (and breaks detailed balance);



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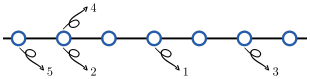

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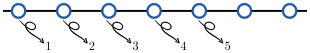

- cluster algorithm performs much better;

Autocorrelation Function under SDB

Eigenvalues of the transition matrix are not necessarily real

$$C(t) = Ae^{-t/\tau_1} + B\cos(\omega t + \phi)\, e^{-t/\tau_2}$$

Turitsyn, K. S.; Chertkov, M.; Vucelja, M. (2011). Irreversible Monte Carlo algorithms for efficient sampling. Physica D: Nonlinear Phenomena, 240(4-5), 410-414.

Vucelja, M. (2016). Lifting—a nonreversible Markov chain Monte Carlo algorithm. American Journal of Physics, 84(12), 958-968.

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