Continous temperature sampling in a single Monte-carlo Simulation

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CRC-TR 211
Strong-interaction matter under extreme conditions

TECHNISCHE UNIVERSITÄT DARMSTADT

Work done in collaboration with

P. Thomas Jahn, Guy Moore and Daniel Robaina

Multicanonical reweighting for the QCD topological susceptibility

arXiv:2103.01069

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Outline

- Motivation and general idea of the method.
- Application to QCD $\chi_{\text{top}}(\beta)$ at high temperatures.
- Simulation algorithm.
- Results and comparison with the standard method.

Motivation

- Consider a lattice calculation of $\langle \mathcal{O} \rangle_\beta$

$$\langle \mathcal{O} \rangle_\beta = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \, e^{-\beta S[U]} \, \mathcal{O}[U]$$

Single coupling corresponds to single temperature

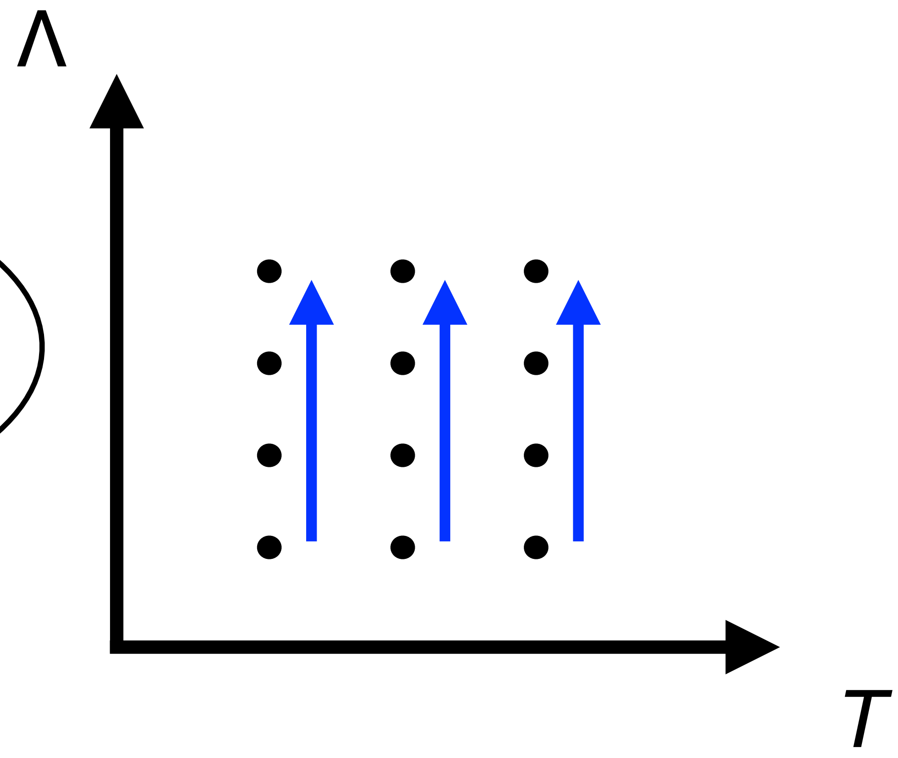
- We are interested in the temperature and cutoff dependence

CRC-TR 211

- Consider a lattice calculation of $\langle \mathcal{O} \rangle_\beta$

$$\langle \mathcal{O} \rangle_\beta = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \, e^{-\beta S[U]} \, \mathcal{O}[U]$$

Simulate at every temperature and cutoff

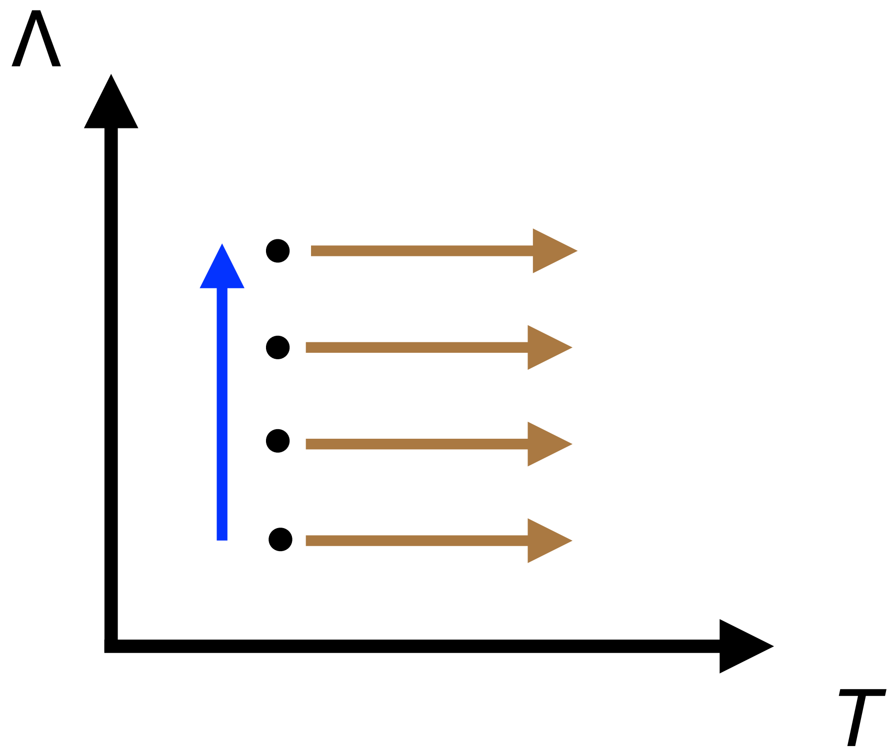


Could be expensive if the temperature range is really large

Perhaps there is a better way ?

Temperature reweighting

- A novel way …. Sample temperatures continuously !
- Employ a reweighting in temperature at a fixed cutoff



Could be very cost effective

Temperature reweighting

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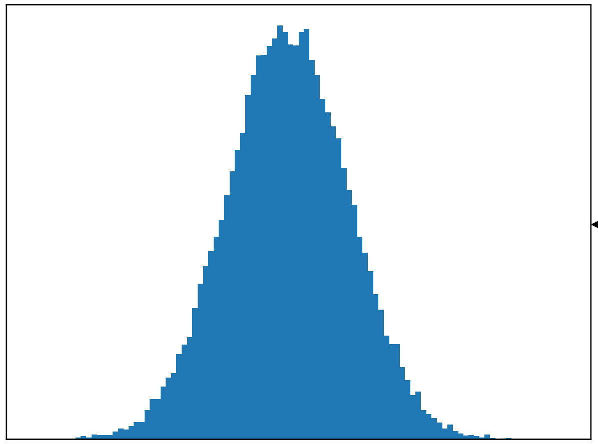
Single β simulates single temperature



Action histogram approx gaussian

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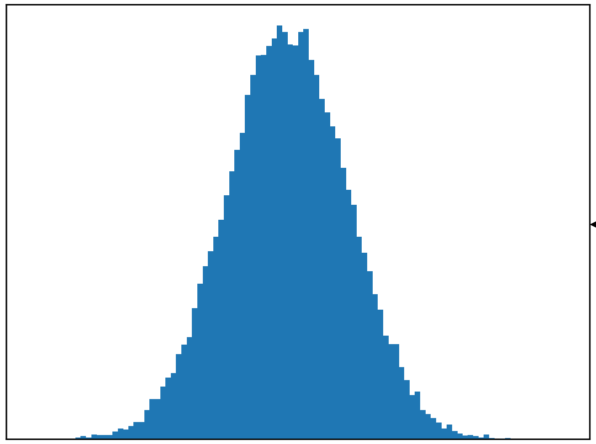
Single β simulates single temperature

To simulate continuous temperatures, we need to simulate continuous β



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- Replace the weight βS

$$Z(\beta) = \int \mathcal{D}U \, e^{-\beta S} \qquad W(S) = \beta \, S$$

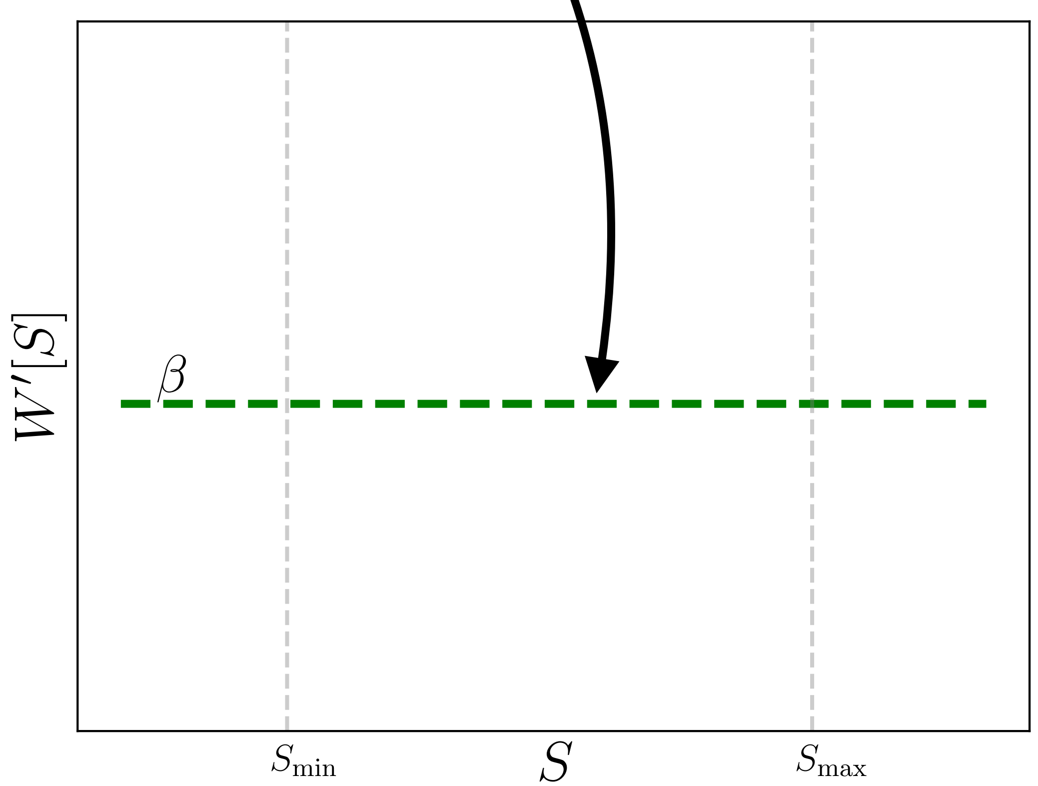
$$\downarrow$$

$$\int \mathcal{D}U \, e^{-W(S)} \qquad W'(S) = \frac{\mathrm{d}W(S)}{\mathrm{d}S} = \beta$$

Continuous Temperatures → Continuous gauge couplings β's → Continuous $W'(S)$

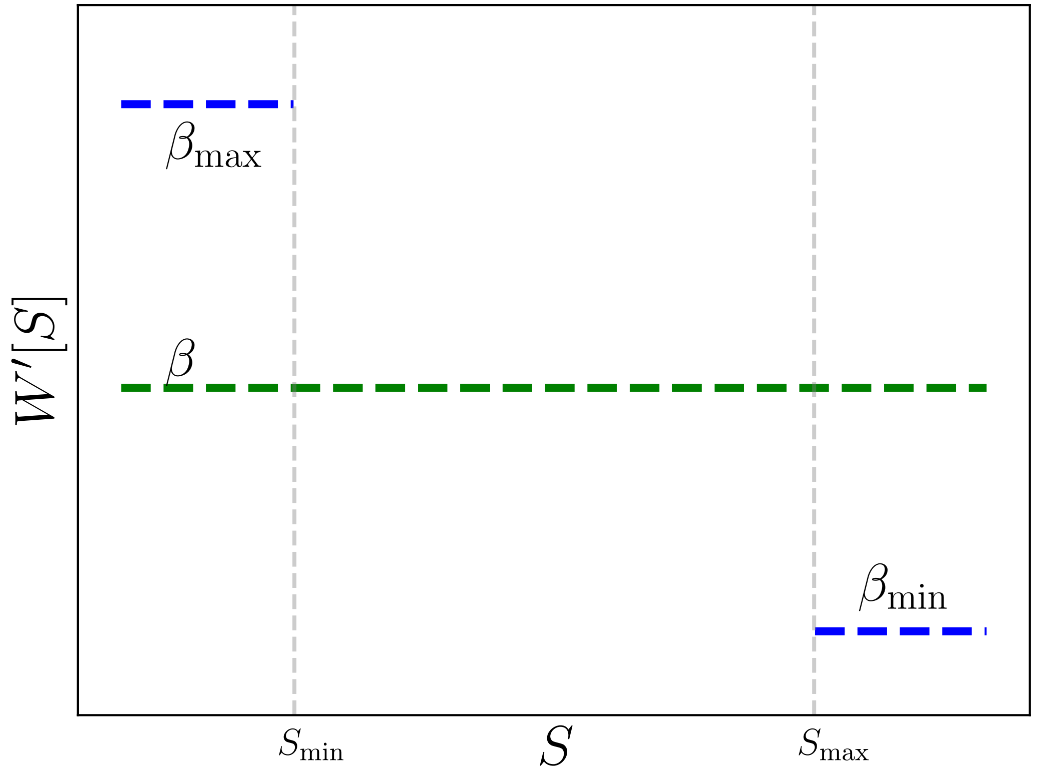
Temperature reweighting

- Standard single temperature/coupling MC



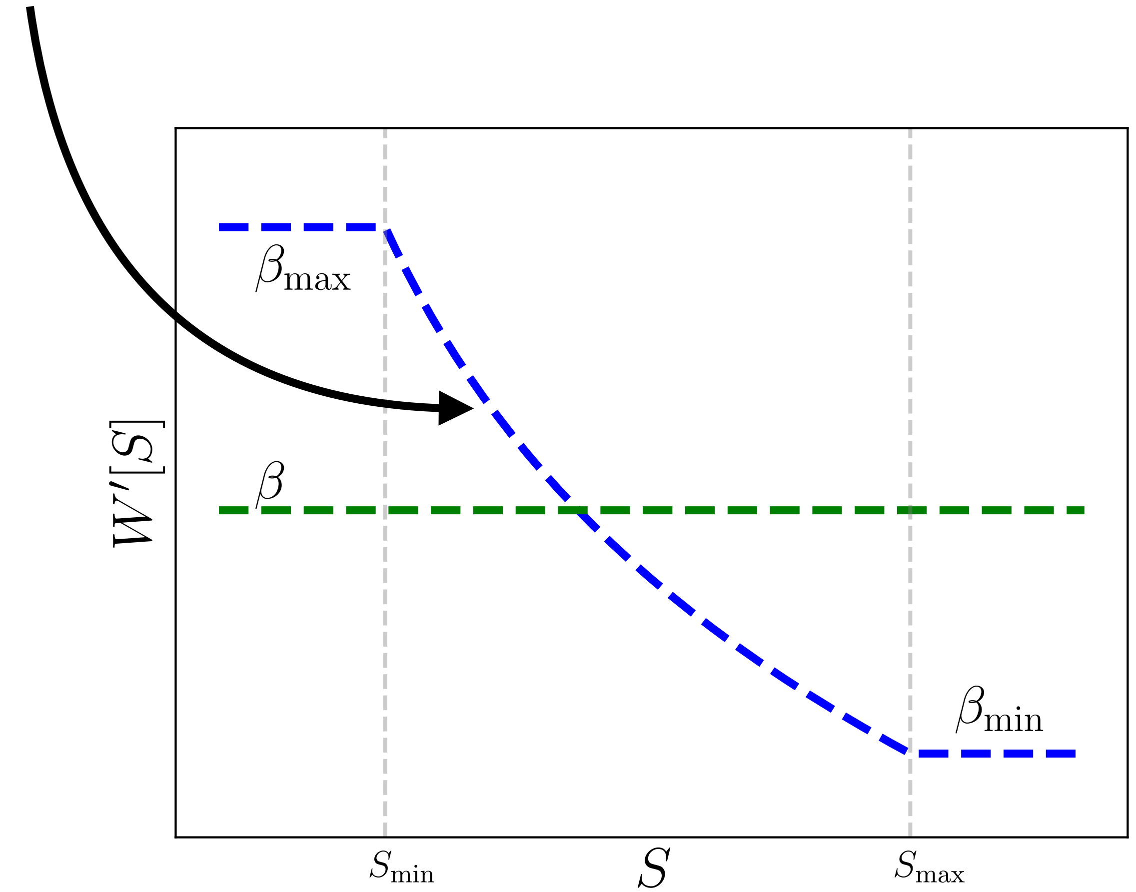
Temperature reweighting

- Standard single temperature/coupling MC
- Define the range for continuous temperatures



Temperature reweighting

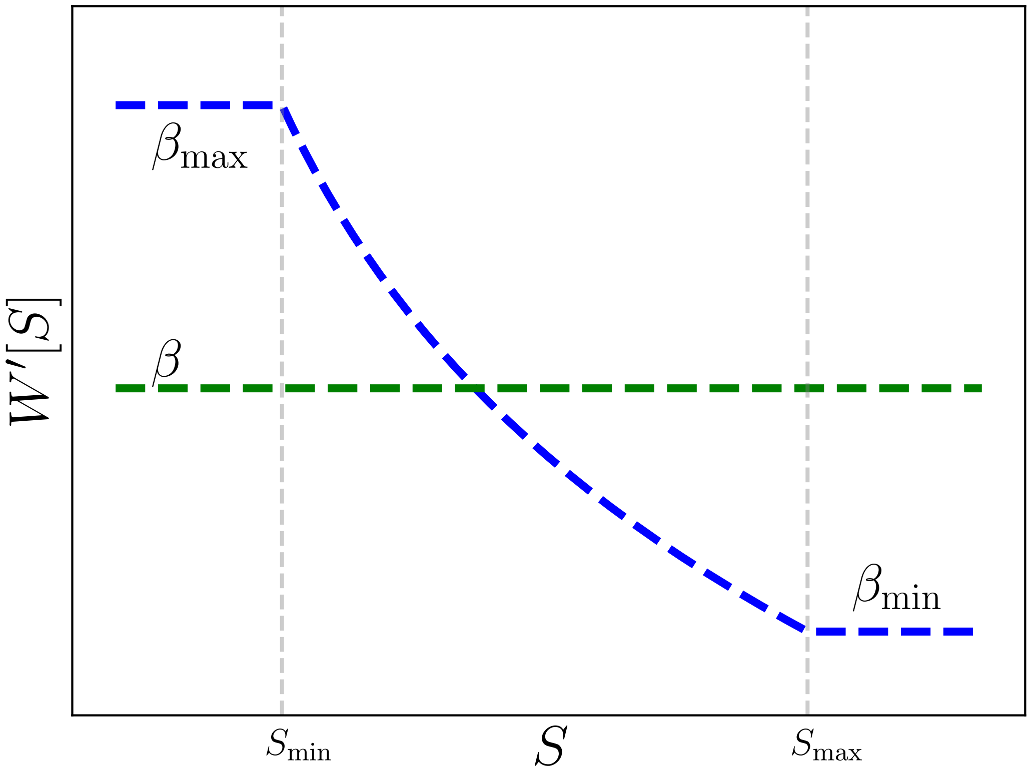
- Standard single temperature / β MC
- A continuous sampling in S *within the range* samples continuous β



- Standard single temperature / β MC
- Computing $Z(\beta_0)$ from $\int \mathcal{D}U\, e^{-W(S)}$ Assuming *W(S)* is known

$$Z(\beta_0) = \int \mathcal{D}U\, e^{-W(S)}\; e^{W(S)-\beta_0 S}$$

$$\propto \sum_i e^{W(S_i)-\beta_0 S_i}$$



- Overall normalisation unknown
- Regularisation issues of $Z(\beta_0)$

Topological Susceptibility

- Compute QCD $\chi_{\text{top}}(\beta)$ at high temperatures :

$$\chi_{\text{top}}(\beta) a^4(\beta) = \frac{1}{V_L} \frac{Z_1(\beta)}{Z_0(\beta)}$$

- Actually compute ratios of $\chi_{\text{top}}(\beta)$

$$\frac{\chi(\beta_{\text{h}}) a^4(\beta_{\text{h}})}{\chi(\beta_{\text{c}}) a^4(\beta_{\text{c}})} = \underbrace{\frac{Z_1(\beta_{\text{h}})}{Z_1(\beta_{\text{c}})}} \underbrace{\frac{Z_0(\beta_{\text{c}})}{Z_0(\beta_{\text{h}})}}$$

Allows two fixed topology simulations

Topological Susceptibility

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- Ratio in temperature reweighting :

$$\frac{\chi_{\text{top}}(\beta_h)a(\beta_h)^4}{\chi_{\text{top}}(\beta_c)a(\beta_c)^4} = \frac{Z_1(\beta_h)}{Z_1(\beta_c)}\frac{Z_0(\beta_c)}{Z_0(\beta_h)} = \left(\frac{\left(\sum_{iQ} e^{W_Q[S_{iQ}]}e^{-\beta_h S_{iQ}}\right)\left(\sum_i e^{W[S_i]}e^{-\beta_c S_i}\right)}{\left(\sum_{iQ} e^{W_Q[S_{iQ}]}e^{-\beta_c S_{iQ}}\right)\left(\sum_i e^{W[S_i]}e^{-\beta_h S_i}\right)}\right)$$

How to simulate continuous temperatures

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$$\mathcal{H}(\pi, U) = \sum_{\mu,x} \frac{1}{2}(\pi_\mu(x))^2 + W(S[U])$$

Initial W(S) obtained from interpolation

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Initial W(S) obtained from interpolation

- Solve the Hamilton's EOM :

$$\frac{\mathrm{d}U}{\mathrm{d}t} = -i\pi U \qquad \frac{\mathrm{d}\pi}{\mathrm{d}t} = iU^\dagger \frac{\partial W[S[U]]}{\partial U} = iU^\dagger \frac{\partial W[S[U]]}{\partial S[U]} \frac{\partial S[U]}{\partial U}$$

β changes during trajectory evolution

- Metropolis accept/reject step :

$$\Delta\mathcal{H} = \mathcal{H}(\pi_f, U_f) - \mathcal{H}(\pi_i, U_i)$$

How to compute *W(S)*

- W(S) needs to be computed in a separate simulation :
- Initial W(S) obtained from interpolation :

$$(\beta_{\text{min}}, \beta_{\text{mid}}, \beta_{\text{max}}) \longrightarrow (S_{\text{max}}, S_{\text{mid}}, S_{\text{min}})$$

- Action S is split in N intervals $(S_1, S_2 ... S_N)$

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$$W(S) = \begin{cases} W_i + s_r x(W_{i+1} - W_i), & S_{\text{max}} < S_i < S_{\text{min}} \\ \beta_{\text{max}} S, & S < S_{\text{min}} \\ \beta_{\text{min}} S, & S > S_{\text{max}} \end{cases}$$

- After S traverses all intervals and back, s_r is reduced
- Separate simulation needed for Q=0,1

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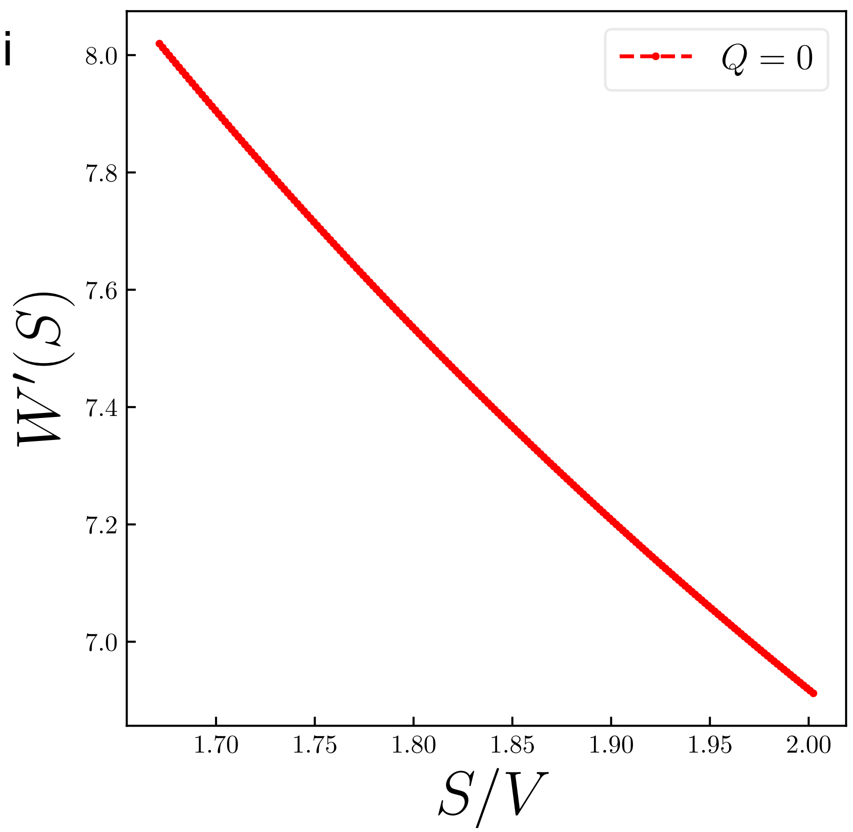
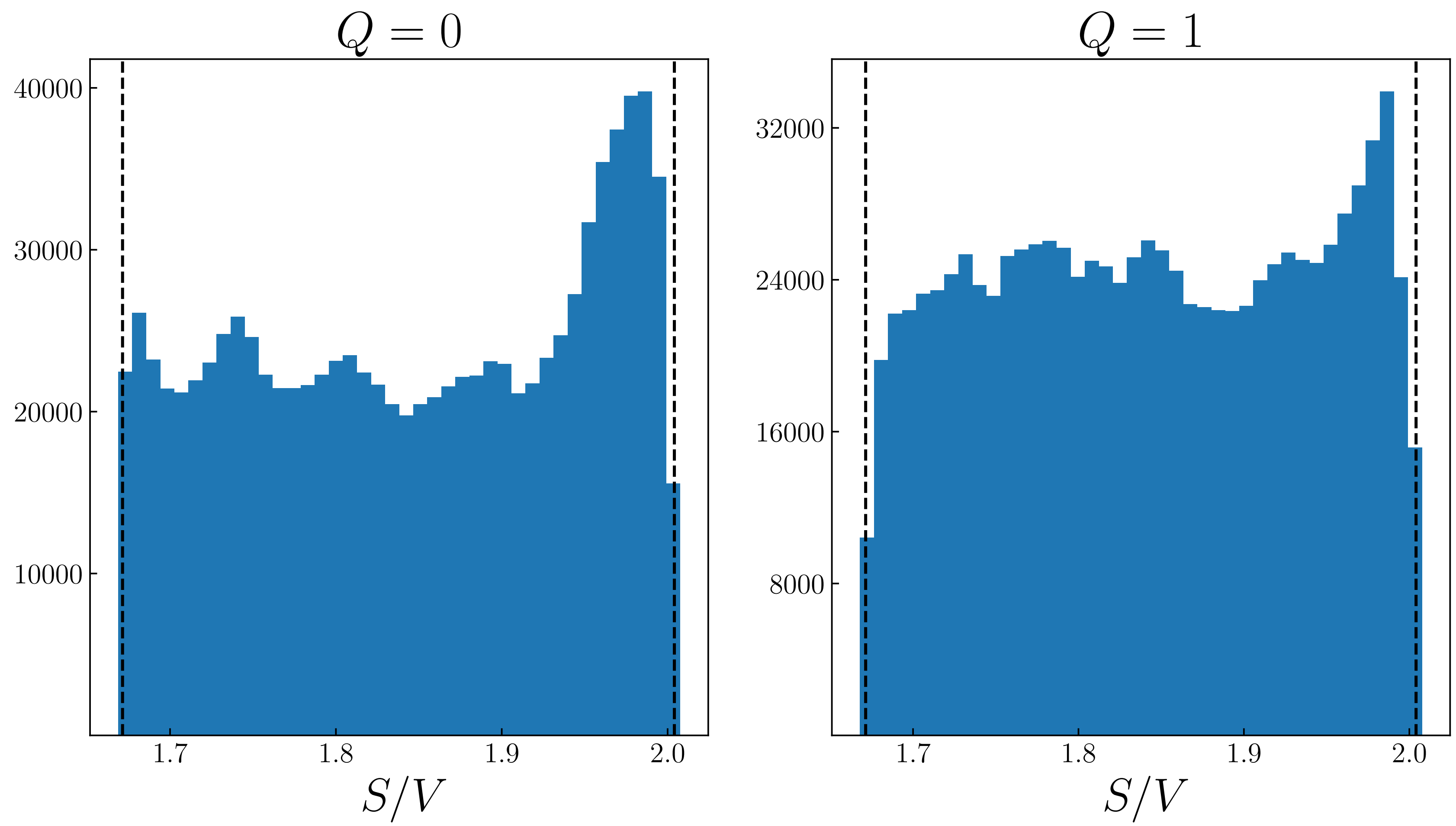


- Separate simulation needed for Q=0,1

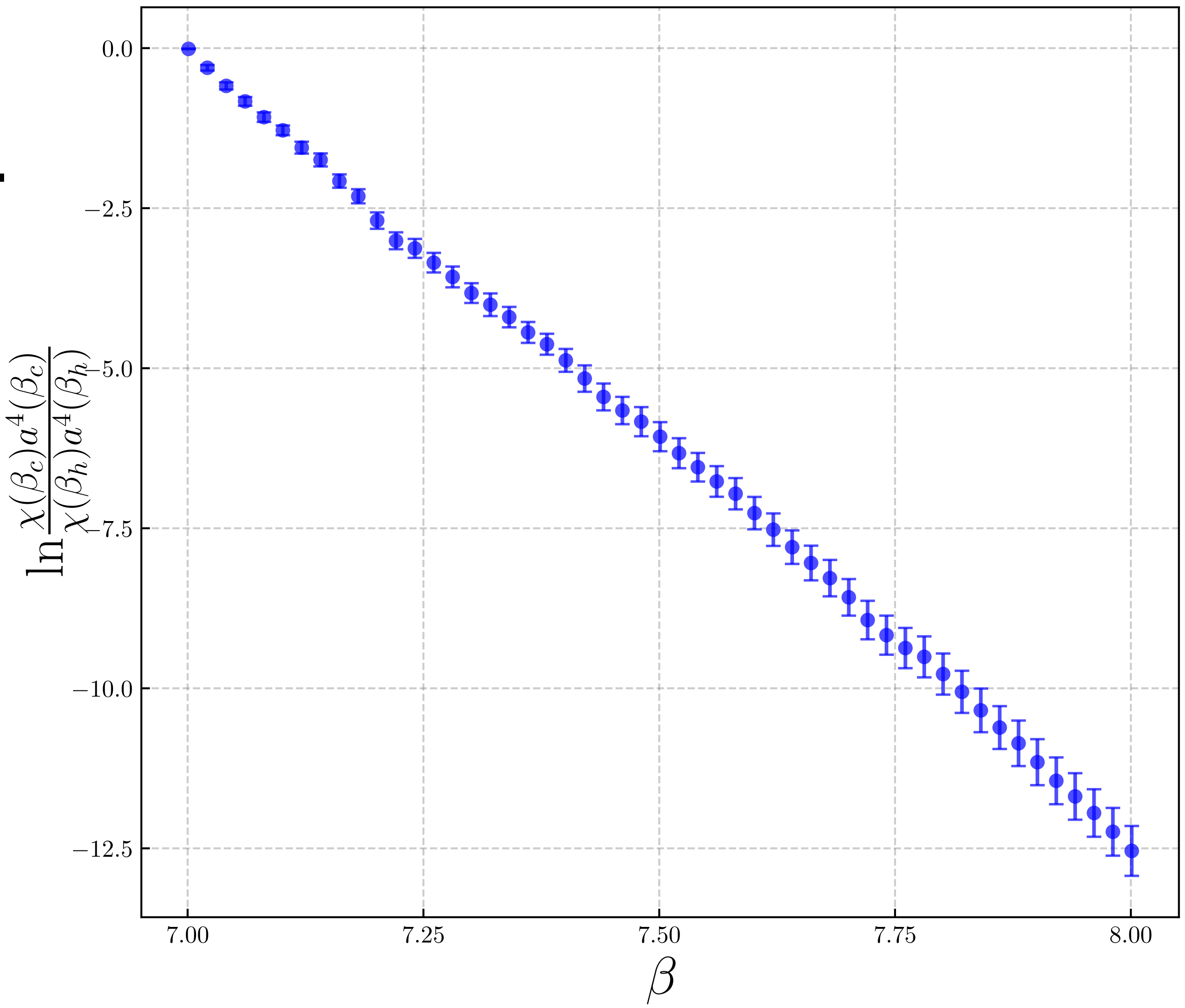
Results for the Action distribution

- Simulation with Wilson gauge action
- Temperature range $2.5T_c \ - \ 9.4T_c$
- Lattice geometry $N_t \times N_{x,y} \times N_z = 10 \times \ 32^2 \times 36$



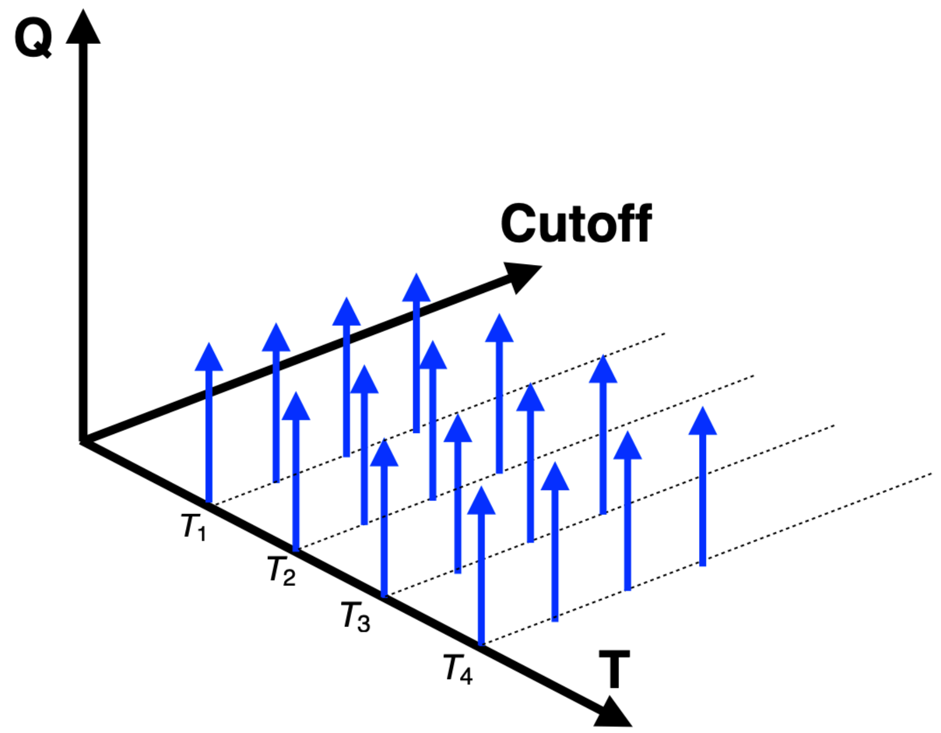
Results for Topological Susceptibility

- Method accomplishes continuous sampling of temperatures.
- Results in agreement with topological reweighting.
- Scale agnostic determination.
- Method comparable to current methods for high statistics determination.
- Inefficient for less precise determination



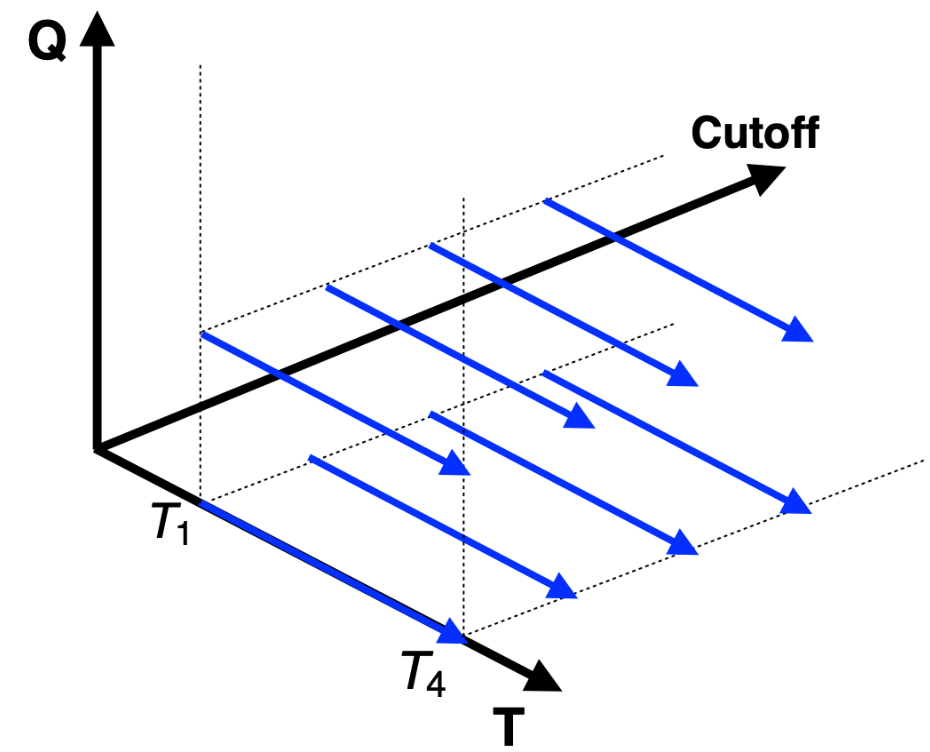
Outlook

Topological Reweighting



- Needs to be simulated at every cutoff and temperature.
- No of simulations = x
- Simulation for reweighting function cheap
- Cheaper for lower statistics

Temperature Reweighting



- Needs to simulated at two topologies and every cutoff.
- No of simulations = x / 2
- Simulation for reweighting function very expensive
- Expensive for lower statistics

The End.

Thank you for your attention !