# Topological Susceptibility to High Temperatures via Improved Reweighting

**P. Thomas Jahn**

**with Guy D. Moore and Daniel Robaina**

Institut für Kernphysik
Technische Universität Darmstadt

TECHNISCHE UNIVERSITÄT DARMSTADT

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Strong-interaction matter under extreme conditions

# Outline

- Introduction
  - Why topology at high temperature?
  - Why is it complicated?
- How do we use reweighting to overcome those problems?
- Quenched results at $2.5\ T_\mathrm{c}$ and $4.1\ T_\mathrm{c}$
- Improvement of the reweighting technique
- Conclusions

# Introduction

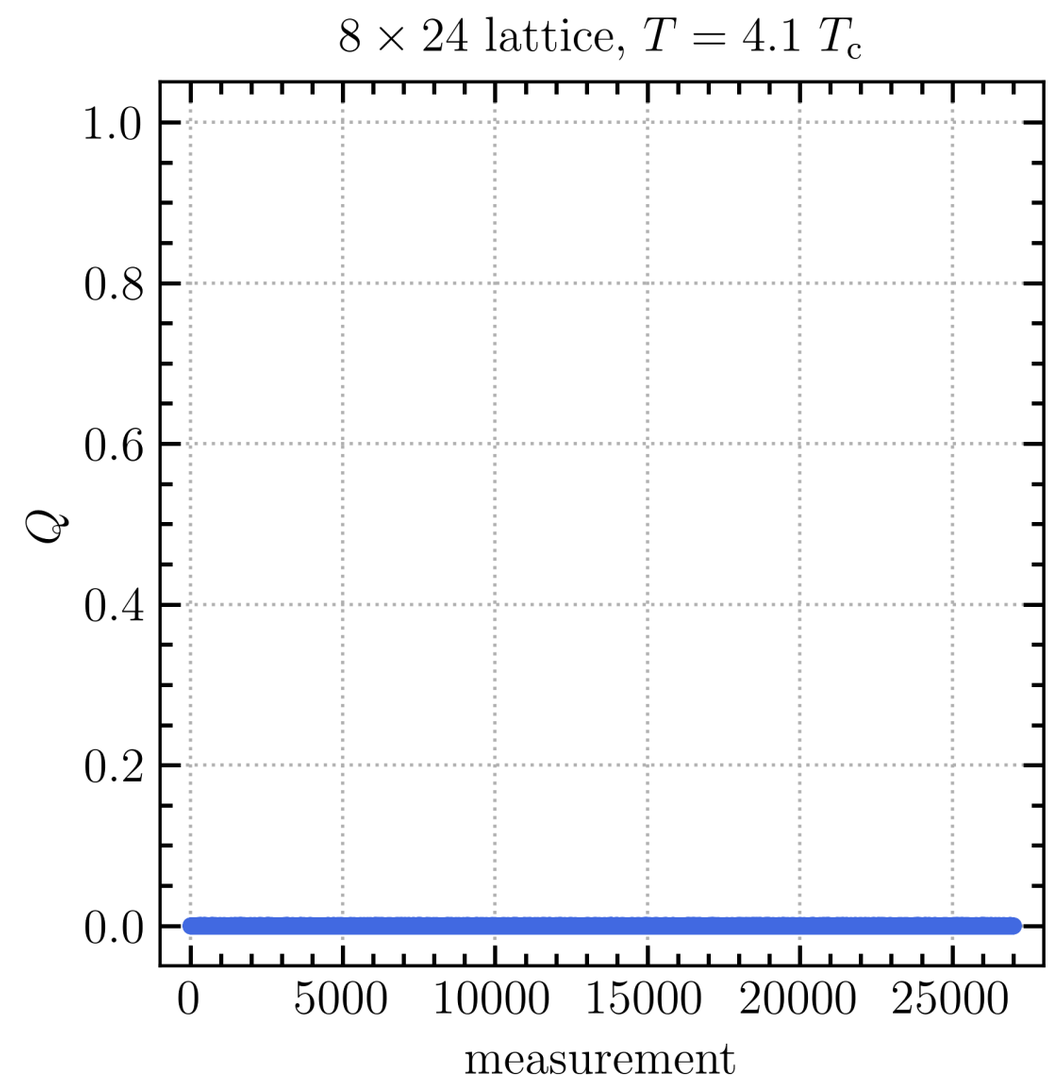
$$\chi_{\text{top}} = \int \mathrm{d}^4x \ \langle q(x)q(0)\rangle = \frac{T}{L^3}\langle Q^2\rangle$$

$$Q = \int \mathrm{d}^4x \ q(x) \in \mathbb{Z}, \qquad q(x) = \frac{1}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}(x)F^a_{\rho\sigma}(x)$$

- properties of QCD axion are sensitive to $\chi_{\text{top}}$ up to ~ $7\ T_{\text{c}}$

  G. Moore, EPJ Web Conf. **175**, 01009 (2018);
  V. Klaer and G. Moore, JCAP **1711**, 049 (2017)

- very suppressed at high temperatures $\quad \mathrm{e}^{-S} = \exp\left(-\frac{8\pi^2\,|Q|}{g^2}\right)$
  - virtually no configs with $|Q| \neq 0$



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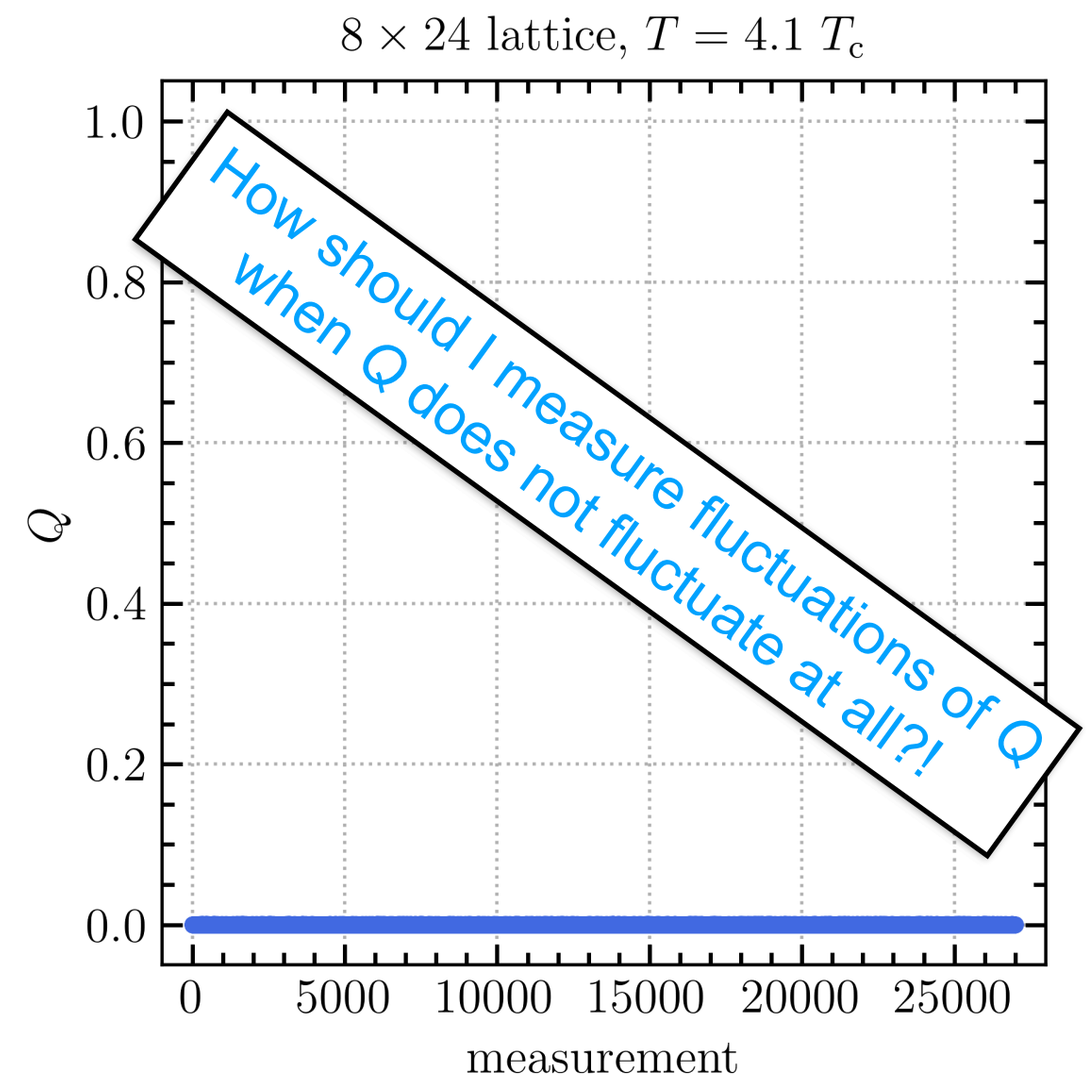
- two possibilities to determine $\chi_{\mathrm{top}}$
  - run forever to get good statistics
  - have a clever idea to artificially enhance the number of instanton configs



# Reweighting
# Basic Idea

B. A. Berg and T. Neuhaus, PLB **267**, 249 (1991); Kajantie, Laine, Rummukainen, Shaposhnikov, Nucl. Phys, **B466**, 189 (1996); M. Laine and K. Rummukainen, Nucl. Phys. **B535**, 423 (1998); F. Wang and D.P. Landau, PRL **86**, 2050 (2001)

## Standard Lattice QCD:

want to calculate $\langle O \rangle = \frac{\int \mathcal{D}A_\mu \, \mathrm{e}^{-S[A]} O[A]}{\int \mathcal{D}A_\mu \, \mathrm{e}^{-S[A]}}$

create *N* configs with weight $\mathrm{e}^{-S[A]}$

$\langle O \rangle_{\mathrm{lat}} = \frac{1}{N} \sum_n O_n$

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$\langle O \rangle = \frac{\int \mathcal{D}A_\mu \; \mathrm{e}^{-S[A]+W(\xi)} \mathrm{e}^{-W(\xi)} O[A]}{\int \mathcal{D}A_\mu \; \mathrm{e}^{-S[A]+W(\xi)} \mathrm{e}^{-W(\xi)}}$

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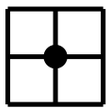
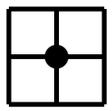
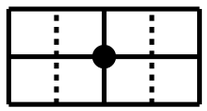
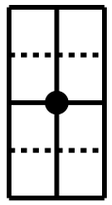
holds for any ***reweighting function*** $W$ and any ***reweighting variable*** $\xi$

if chosen correctly, the number of instantons can be significantly enhanced!

# Reweighting
# Reweighting Variable

natural choice for reweighting variable: $Q = \sum_x -\frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}\left(\hat{F}_{\mu\nu}(x)\hat{F}_{\rho\sigma}(x)\right)$

we use $\mathcal{O}(a^2)$ improved field-strength tensor

$\hat{F}_{\mathrm{clov}} = \frac{1}{4}$  $\Longrightarrow$ $\hat{F}_{\mathrm{imp}} = \frac{5}{12}$  $-\frac{1}{24}\Bigg($  $+$  $\Bigg)$

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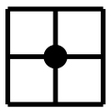
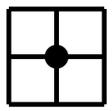
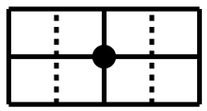
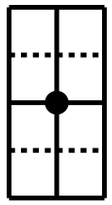
$\hat{F}_{\mathrm{clov}} = \frac{1}{4}$  $\Longrightarrow$ $\hat{F}_{\mathrm{imp}} = \frac{5}{12}$  $-\frac{1}{24}\Bigg($  $+$  $\Bigg)$

**BUT:** UV fluctuations spoil topological charge ⟶ ***gradient flow***

$$\partial_t B_\mu(x,t) = D_\nu[B]F_{\nu\mu}[B], \qquad B_\mu(x,0) = A_\mu(x)$$

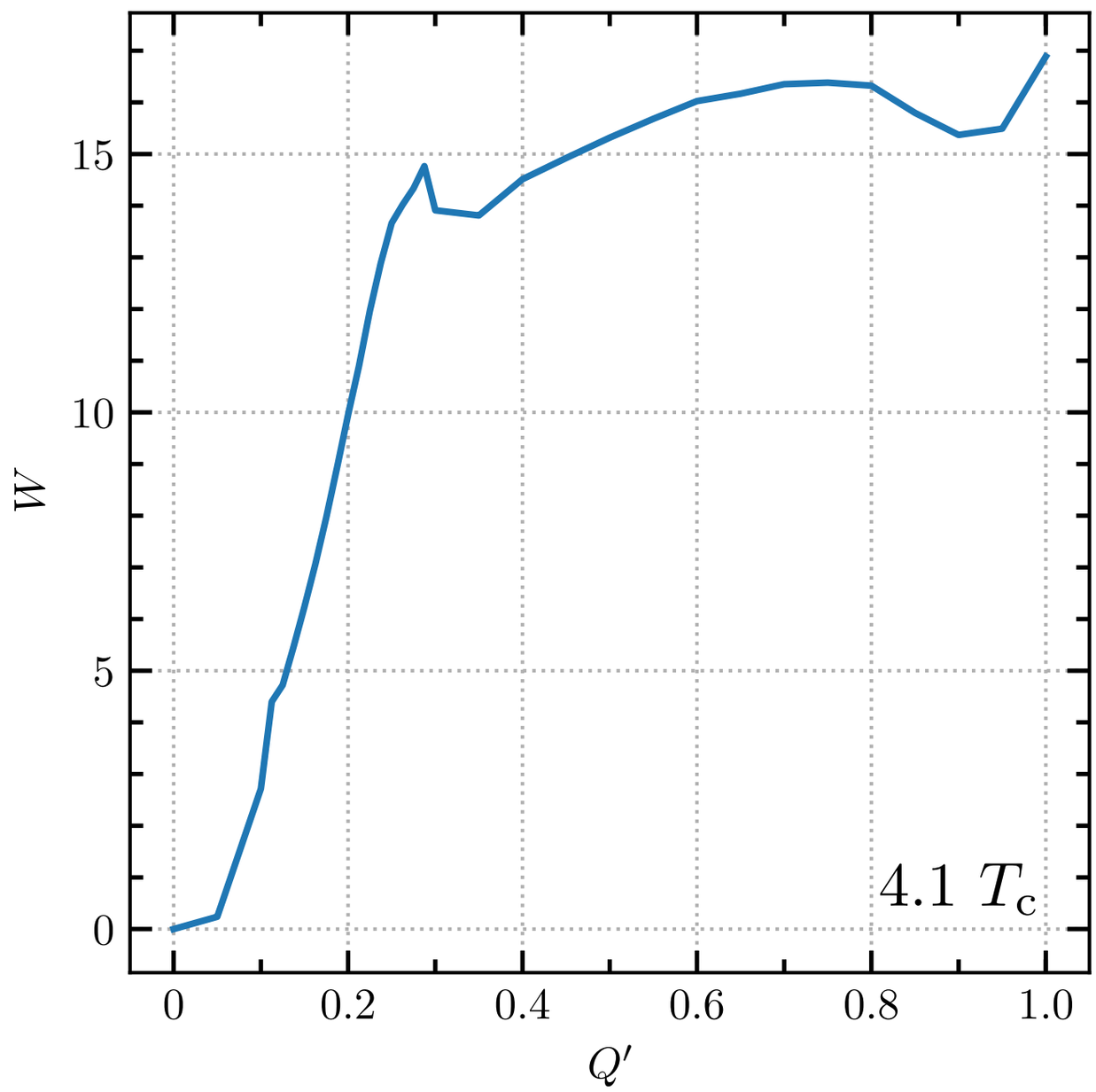
gauge fields are “smeared”, UV fluctuations are removed, $Q$ pushed towards integers

on the lattice: *Wilson Flow* R. Narayanan and H. Neuberger, JHEP **03**,64 (2006); M. Lüscher, Comm.Math.Phys. **293**,899 (2010)

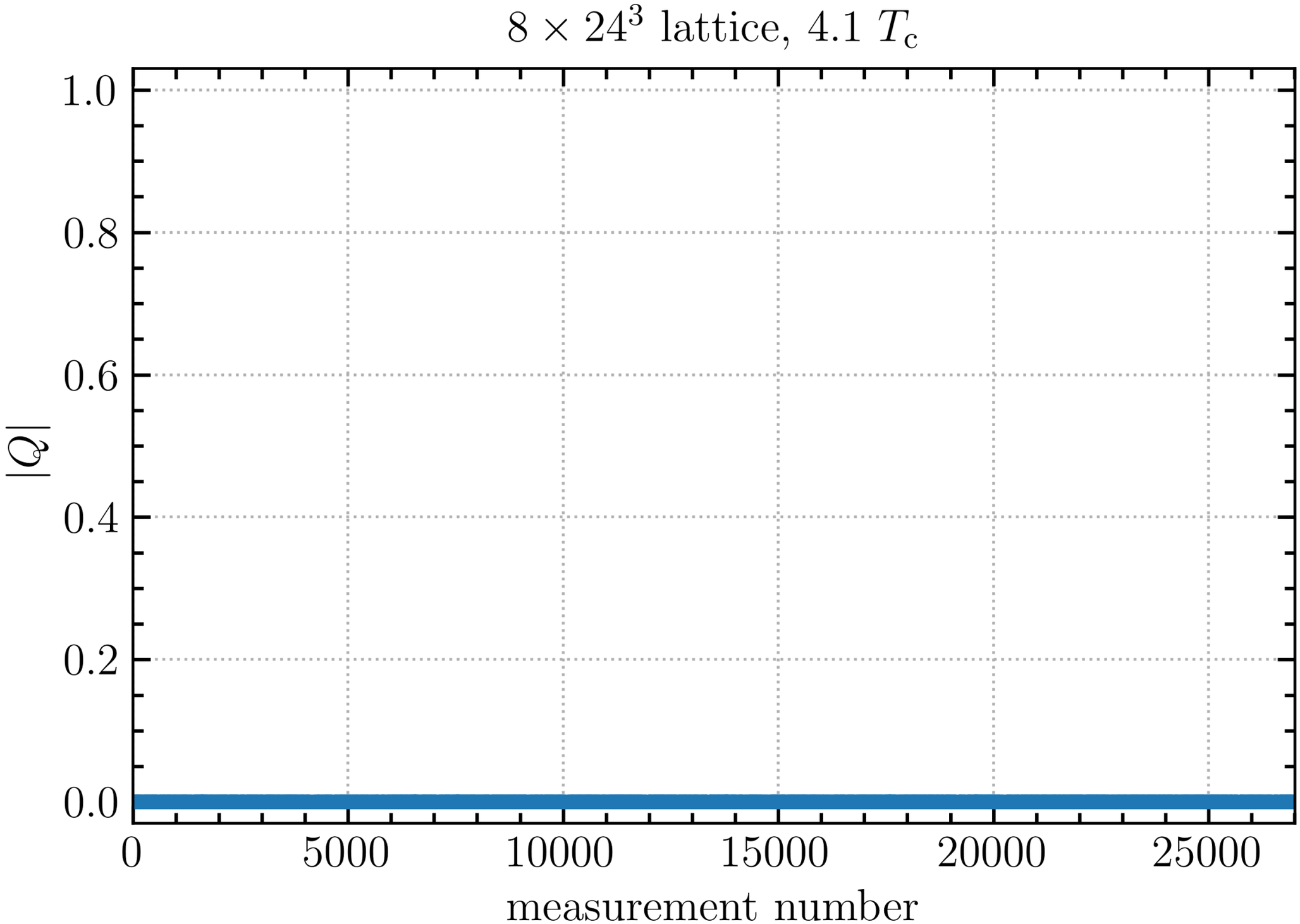
**reweighting variable:** $Q' \equiv (Q \text{ after } \textit{small amount} \text{ of flow})$

# Reweighting
# Reweighting Function

$$\text{weight} \sim \exp\left[W(Q')\right]$$



# Reweighting
# It Works!



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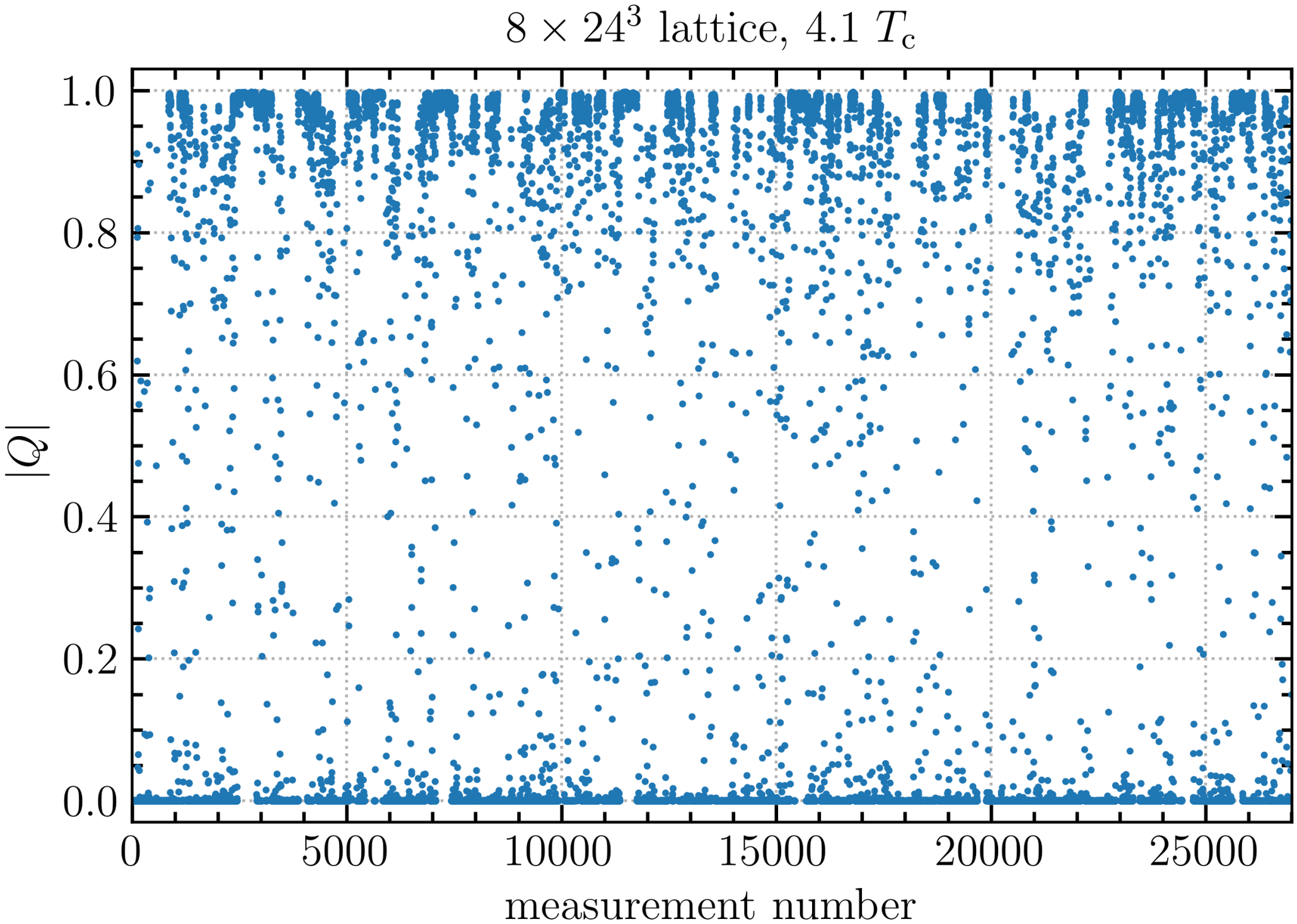
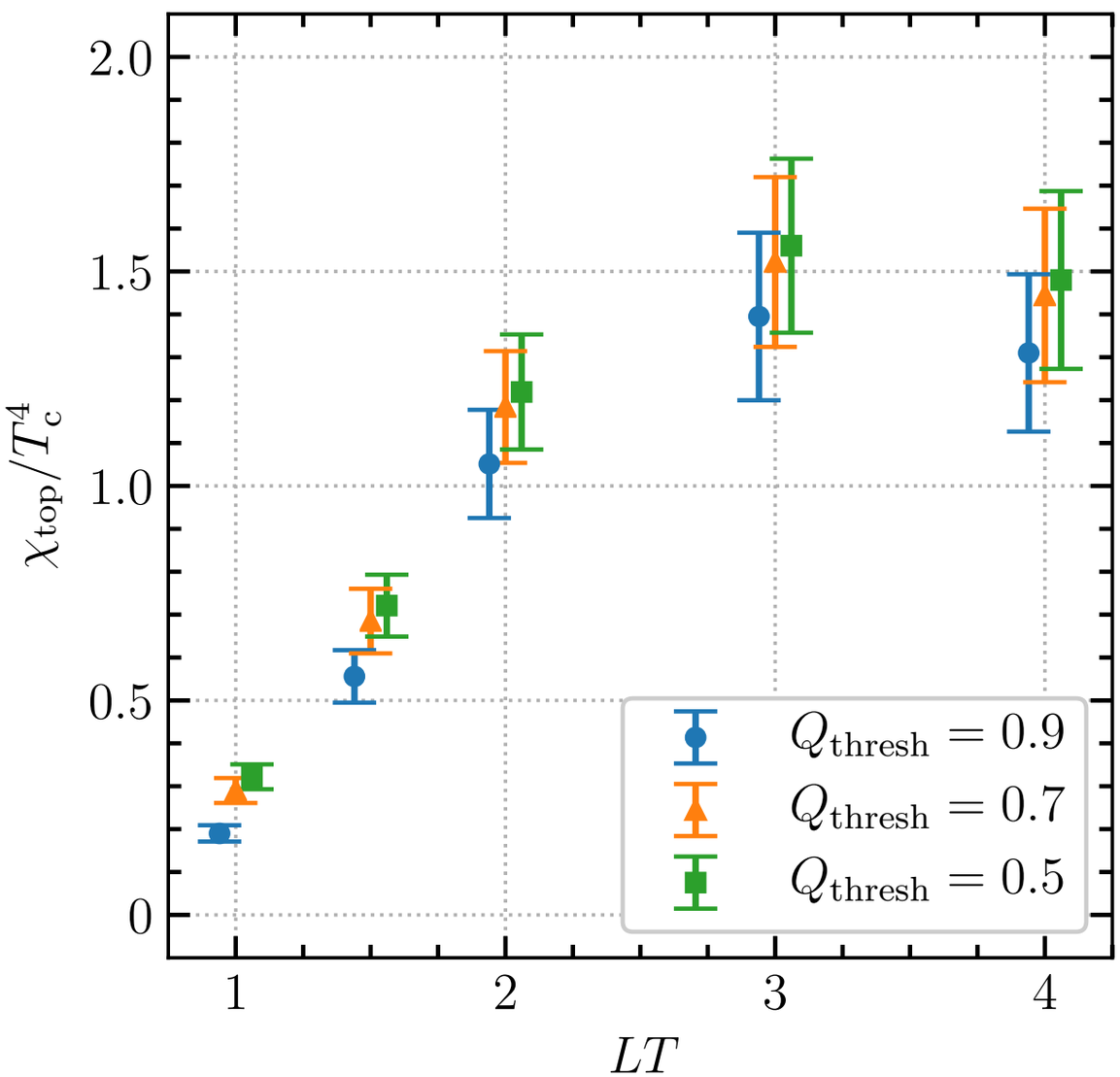


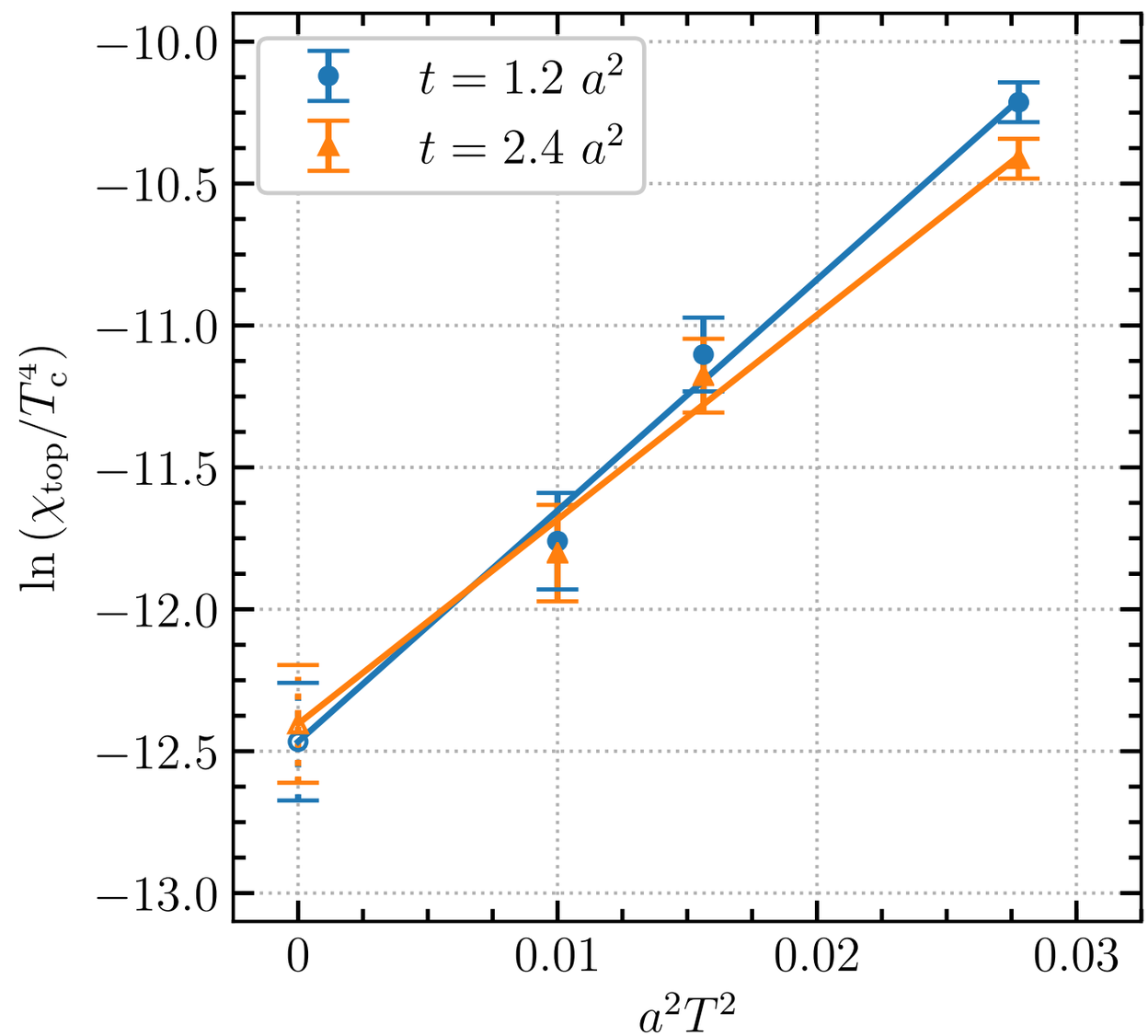
# Quenched Results @ 2.5 and 4.1 Tc

PTJ, G.D. Moore, D. Robaina, PRD**98**, 054512 (2018)

$$\chi_{\text{top}} = \frac{T}{L^3} \frac{\sum_{\text{configs}} \mathrm{e}^{-W(Q')} \, Q^2_{\text{flowed}}}{\sum_{\text{configs}} \mathrm{e}^{-W(Q')}}$$

we use the topological charge after gradient flow, thresholded to be an integer and compare 3 thresholds and 2 flow depths



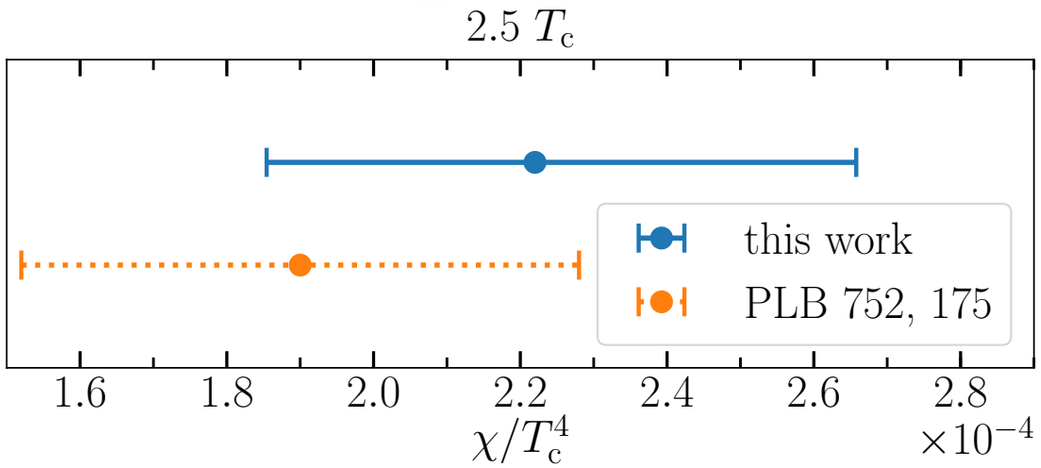



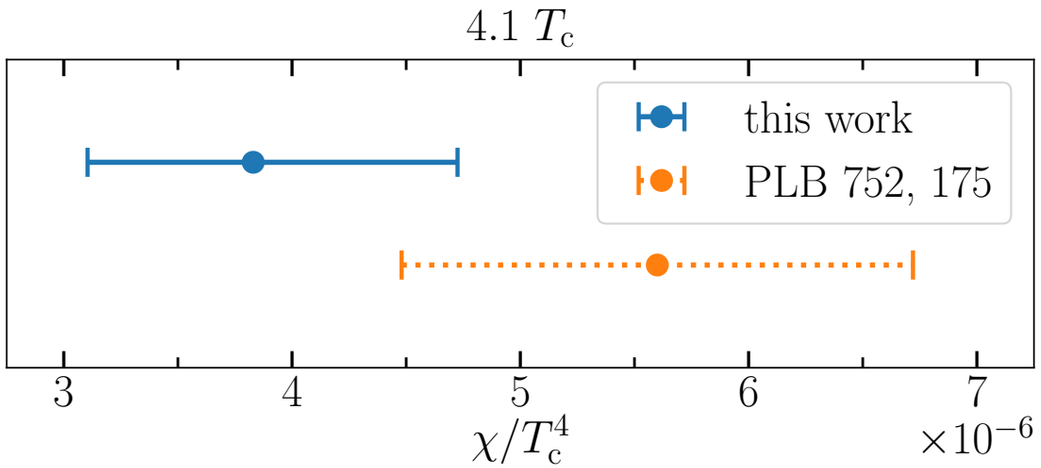
# Quenched Results @ 2.5 and 4.1 Tc Final Numbers and Comparison

PTJ, G.D. Moore, D. Robaina, PRD**98**, 054512 (2018)

S. Borsanyi *et al.*, PLB **752**, 175 (2016):

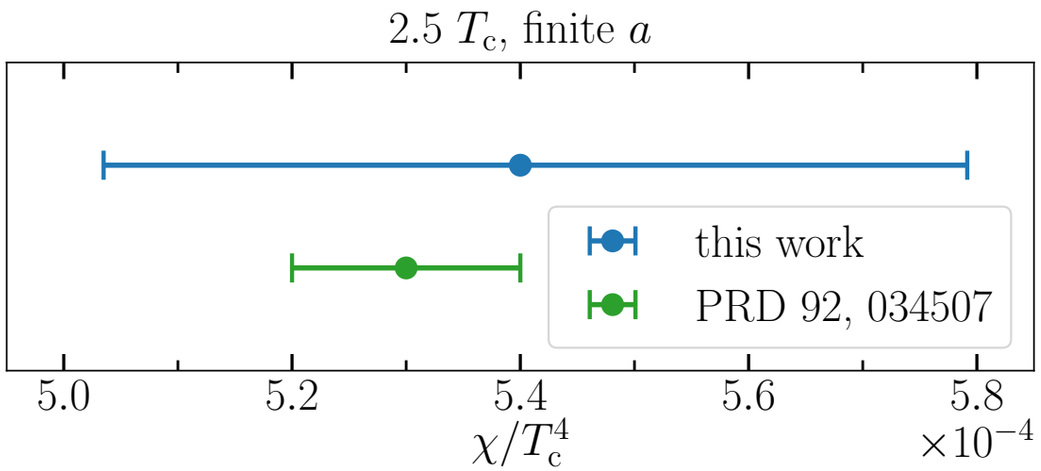
conventional calculation with
heat bath/overrelaxation algorithm
up to $4\ T_c$ , much more statistics,
grand fit to all continuum extrapolated data



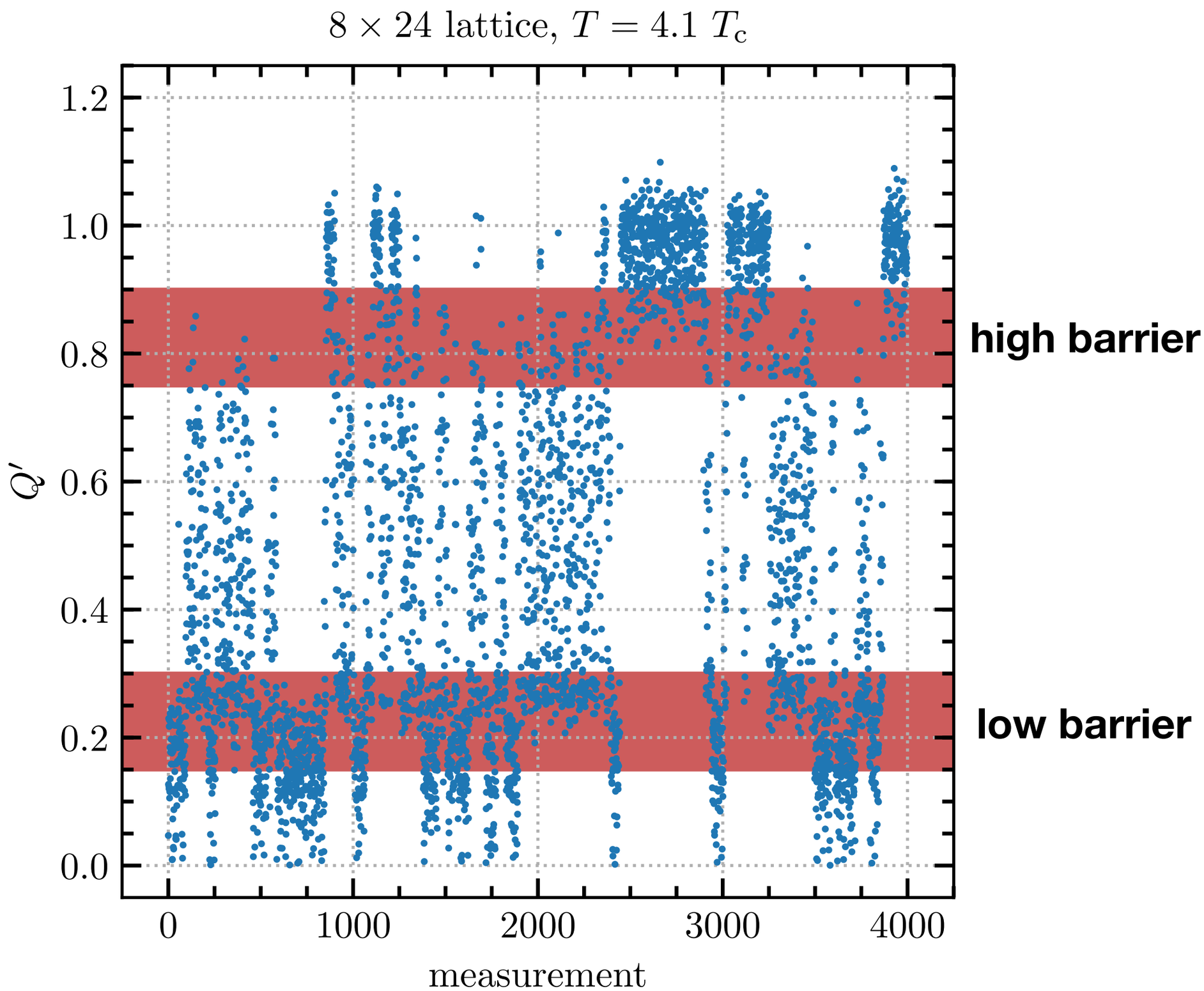




E. Berkowitz *et al.*, PRD **92**, 034507 (2015):

conventional calculation up to
$2.5\ T_c$ , no continuum extrapolation



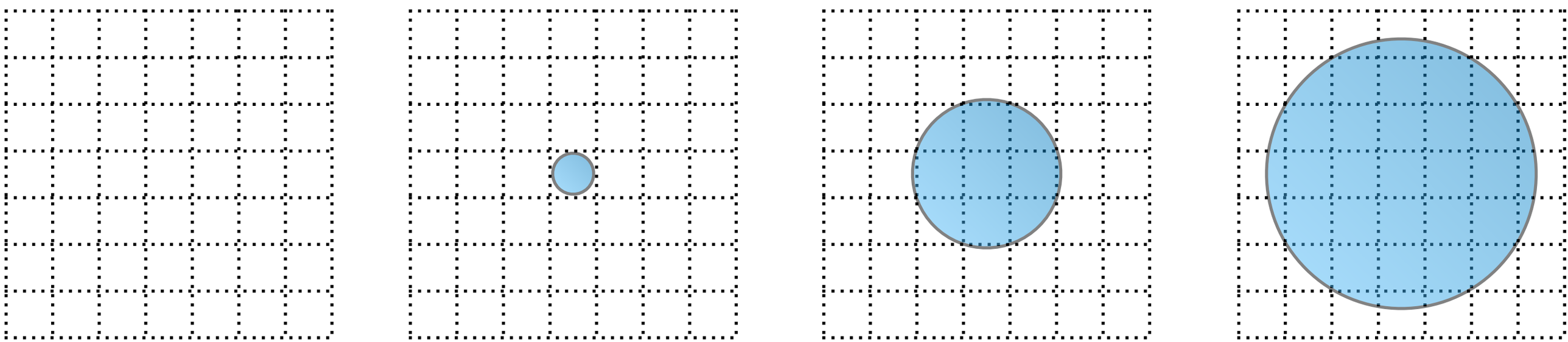
# Still Some Problems…



# Still Some Problems…

**aim of reweighting: moving back and forth**

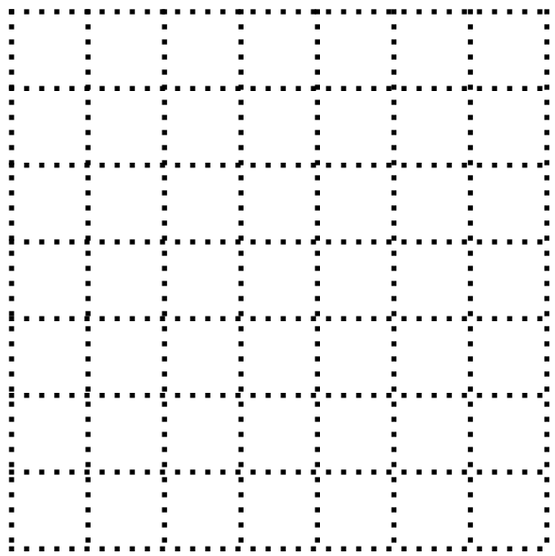
$Q = 0$ $\quad$ $0 < Q < 1$ $\quad$ $Q = 1$



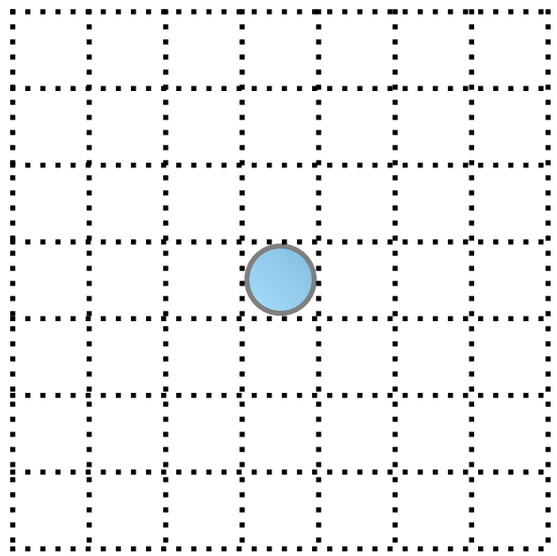
**trivial topology** $\quad$ **dislocation** $\quad$ **small caloron** $\quad$ **genuine caloron**

**low barrier** $\quad$ **high barrier**

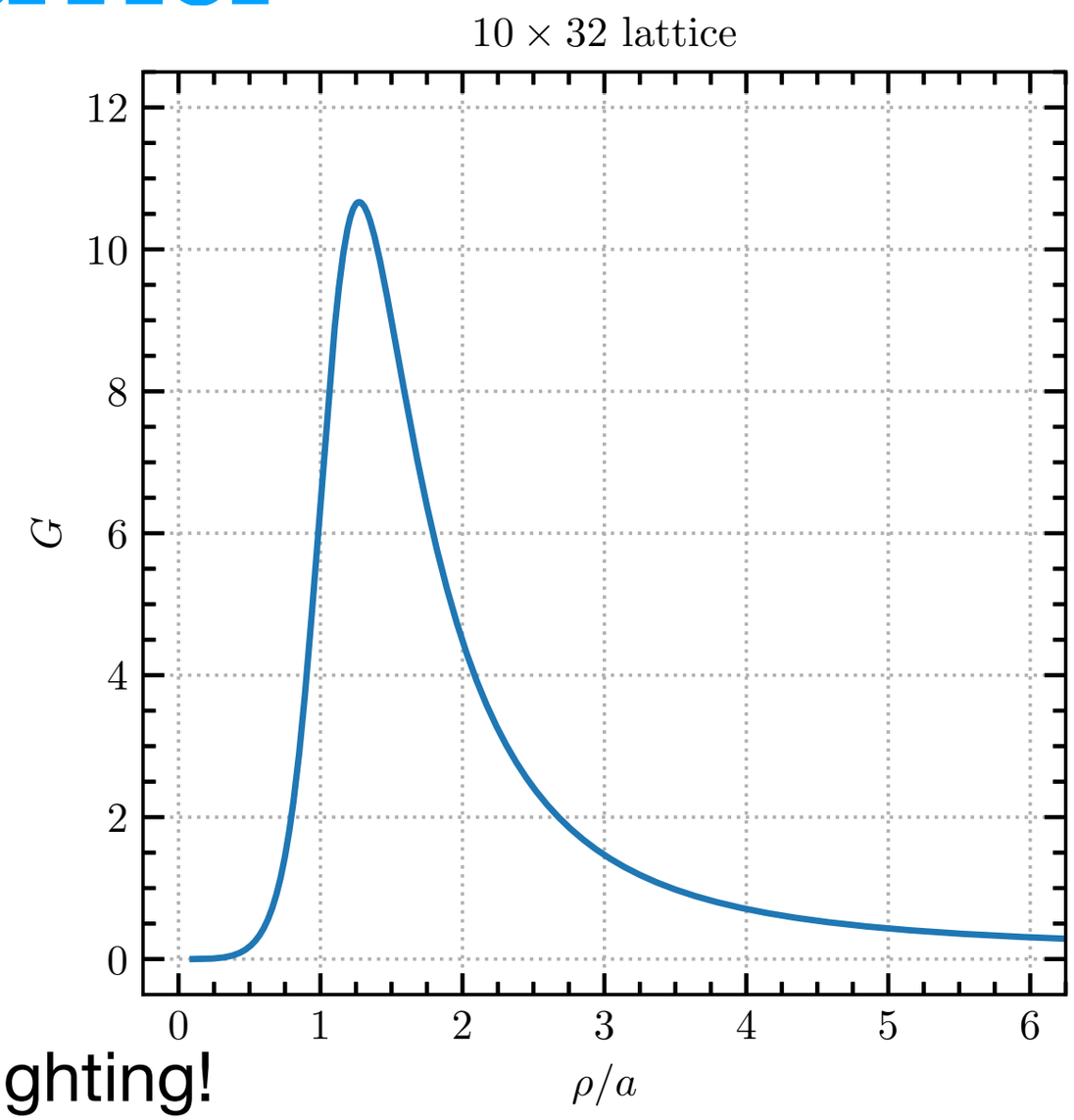
# Low Barrier



**trivial topology**



**dislocation**



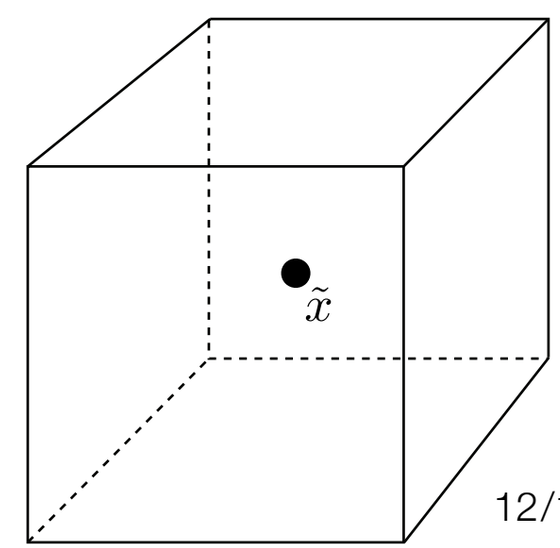

**Problem:** Algorithm has problems to move between trivial topology and dislocations

**Idea:** enhance tunneling by additional reweighting!

→ need quantity "globbiness" to distinguish both…

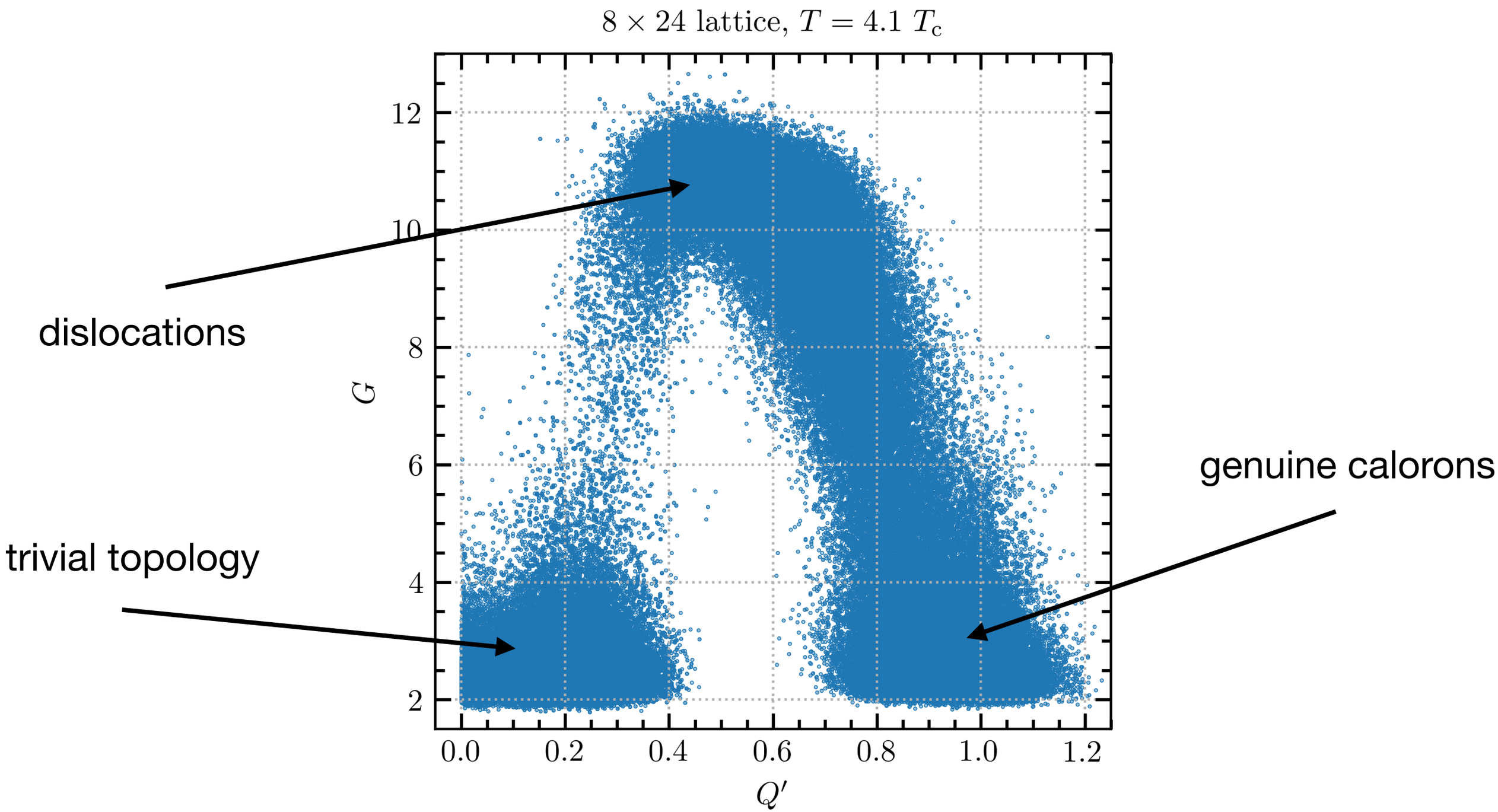
**peak action density:**

$$G \equiv \max\{S(\tilde{x})\}\,, \qquad S(\tilde{x}) = \sum_{P(\tilde{x})} \mathrm{Re}\ \mathrm{tr}\,(1 - P(\tilde{x}))$$



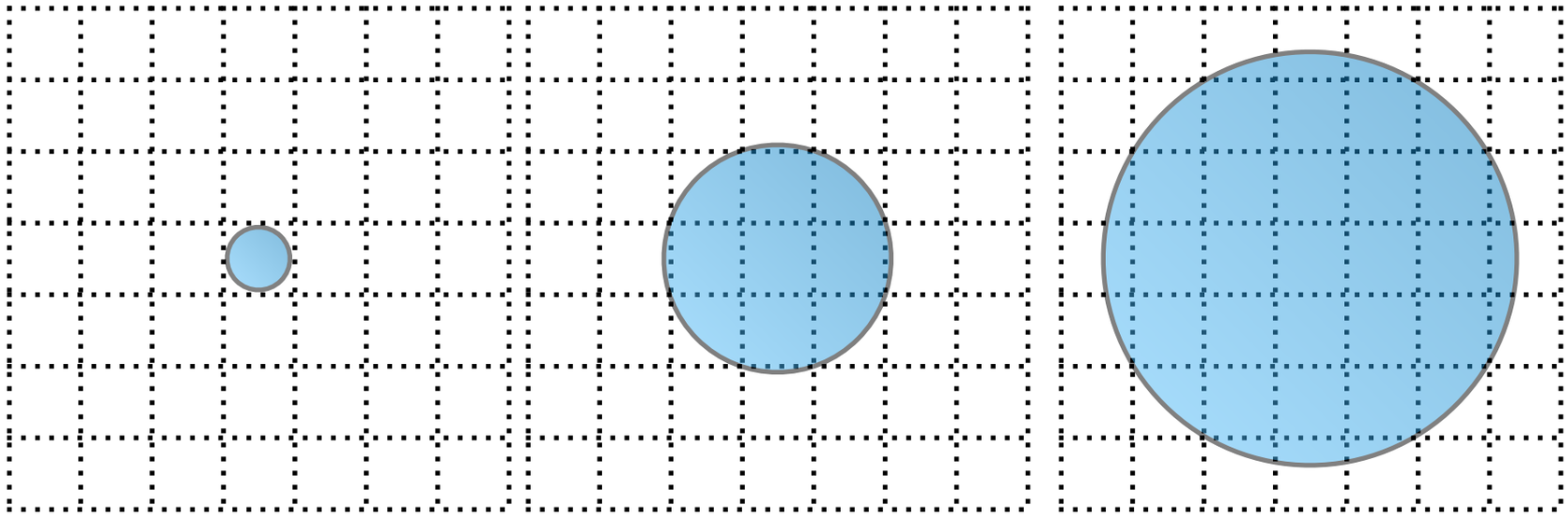

**small for trivial topology, large for dislocations**

# Low Barrier

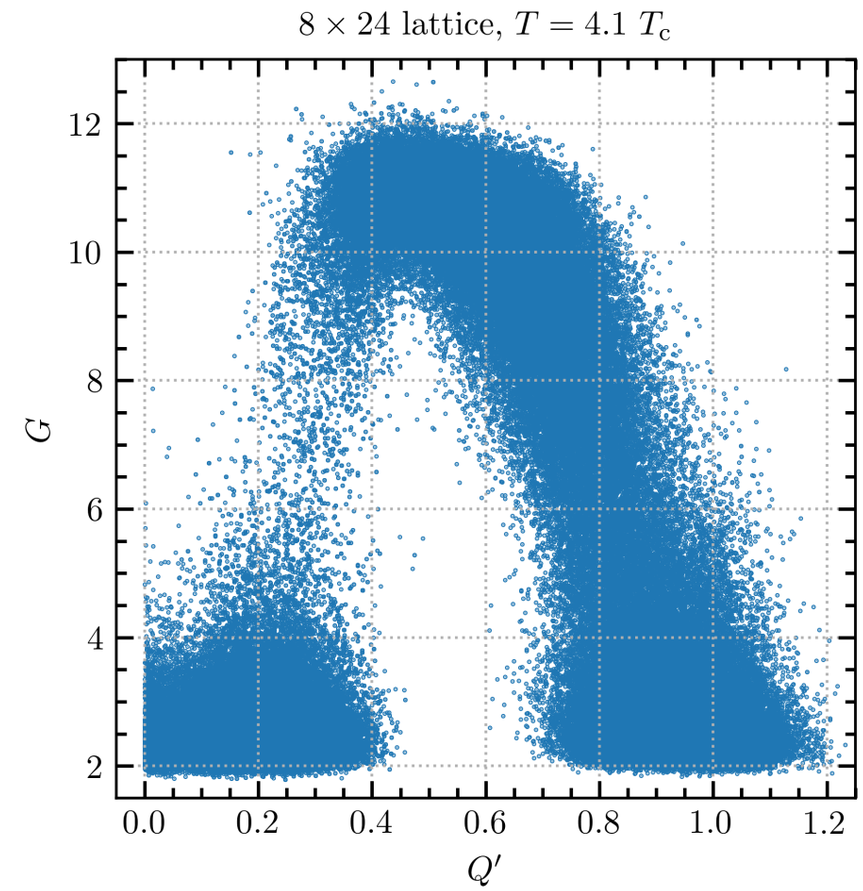



→ Reweighting in terms of $W_{\text{low}} \equiv W_{Q'}(Q') + W_G(G)$

# High Barrier



dislocation small caloron genuine caloron

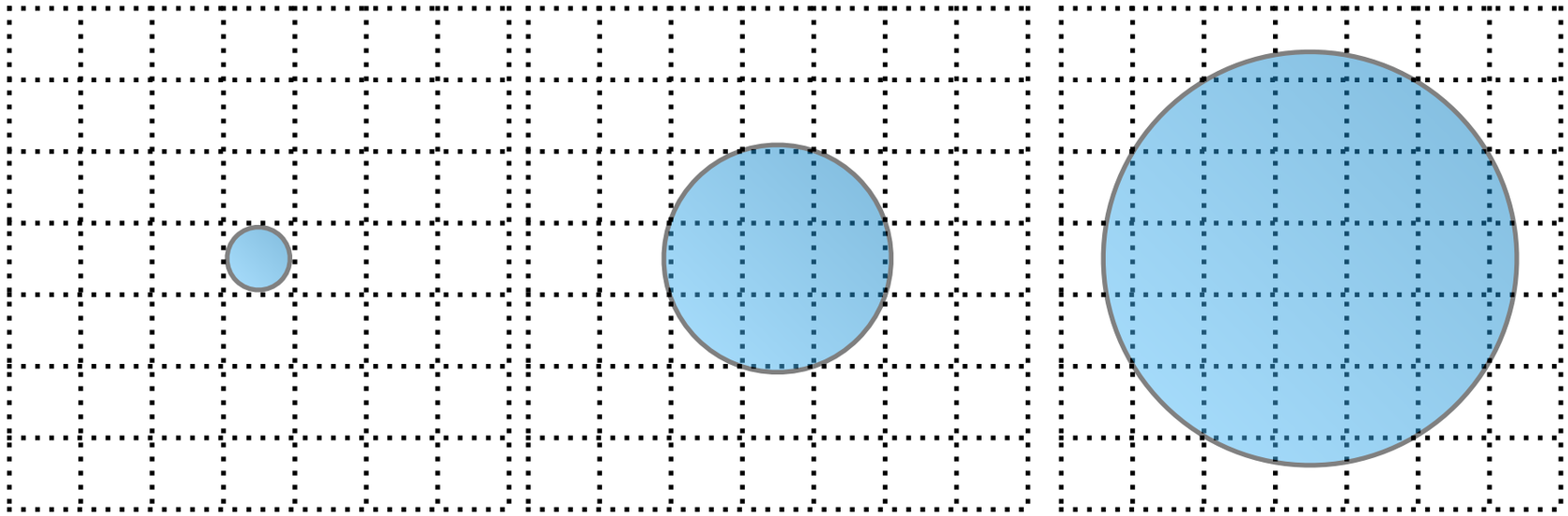



**Problem:** here globbiness does not work…

**BUT:** barrier can be overcome by using more gradient flow and larger HMC steps

→ Reweighting in terms of $Q_2'$ with $W_{\text{high}}(Q_2')$

# High Barrier



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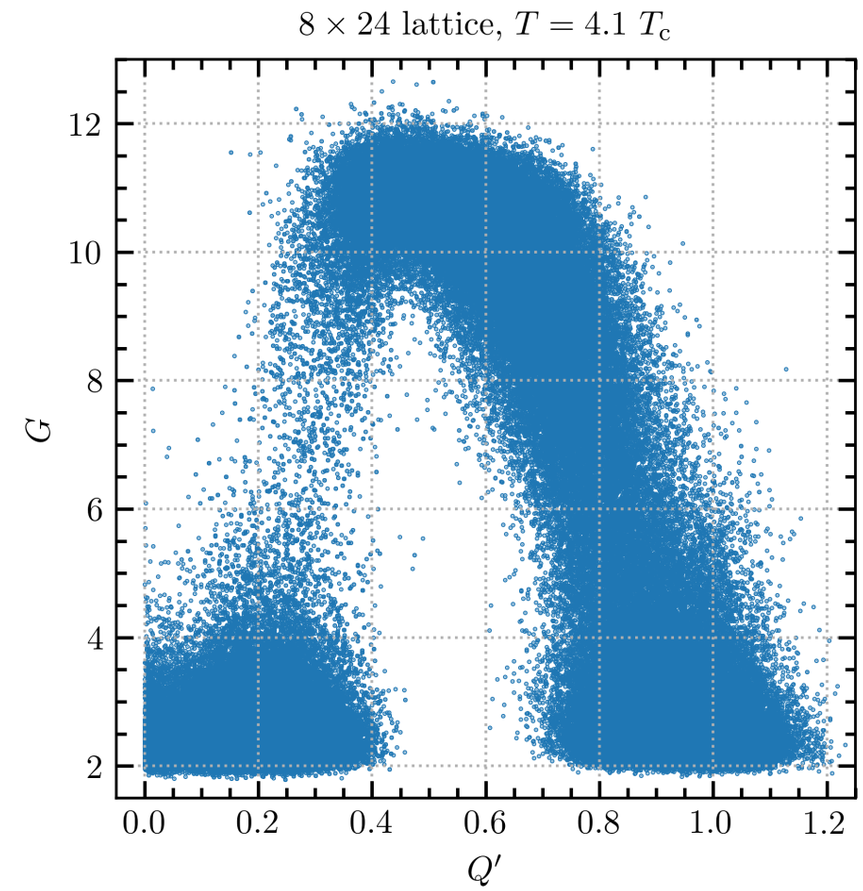


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**BUT:** barrier can be overcome by using more gradient flow and larger HMC steps

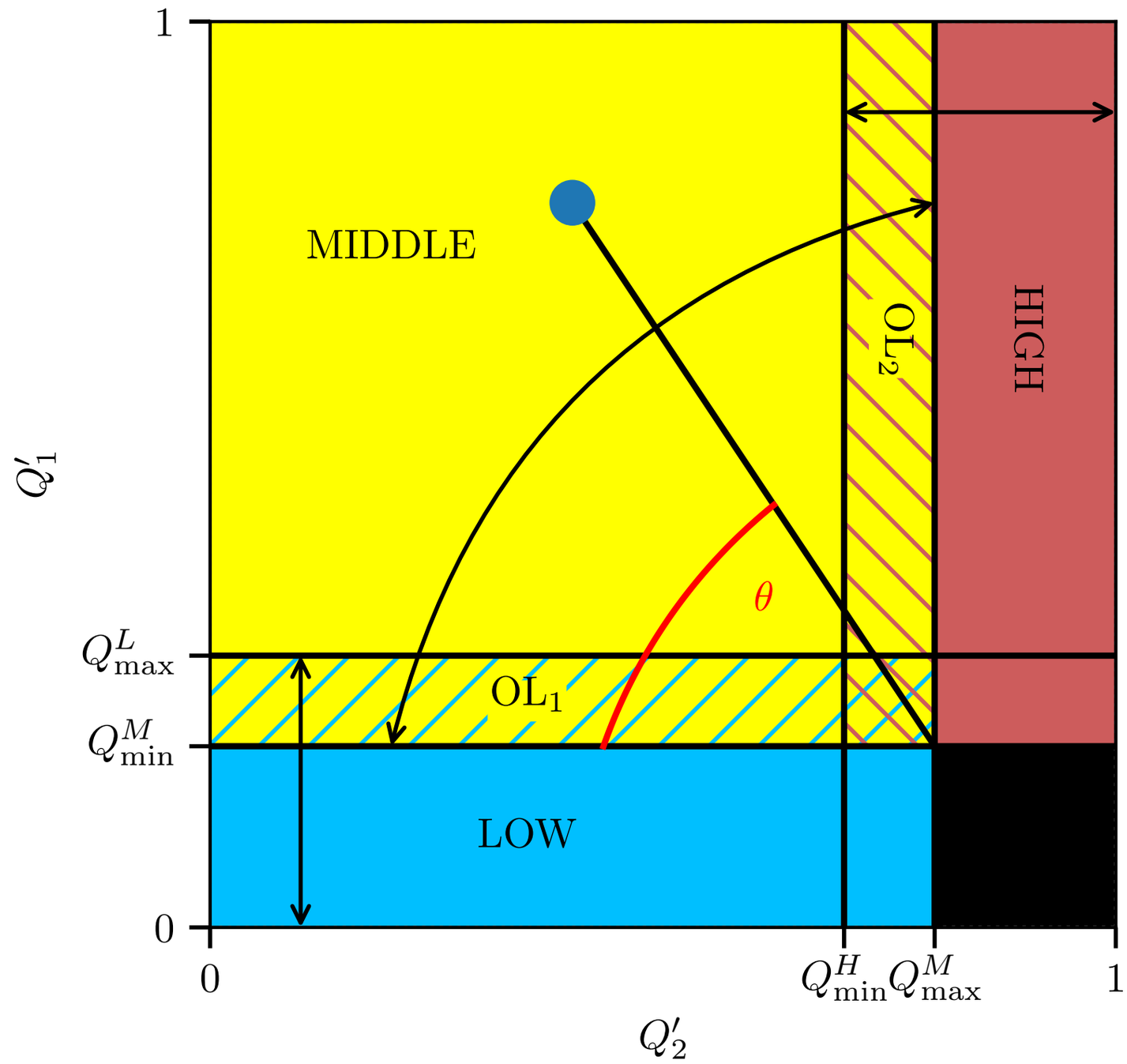
→ Reweighting in terms of $Q_2'$ with $W_{\text{high}}(Q_2')$

**Consequence:** now we use different amounts of gradient flow in high and low regions

→ **need a middle region to connect them!**

# Middle Region

Choose middle region such that it has a ~10% overlap with both high and low regions




→ Reweighting in terms of

$$\theta = \arctan\left(\frac{Q'_1 - Q^M_{\min}}{Q^M_{\max} - Q'_2}\right) \in [0, \pi/2] \quad \text{with} \quad W_{\mathrm{mid}}(\theta)$$

# Reweighting with Multiple Regions

$$\chi_{\text{top}} \sim \frac{\int \mathcal{D}U \mathrm{e}^{-\beta S[U]} \Theta(Q)}{\int \mathcal{D}U \mathrm{e}^{-\beta S[U]}} \simeq \frac{\sum_i \mathrm{e}^{-W[Q'_i]} \Theta(Q_i)}{\sum_i \mathrm{e}^{-W[Q'_i]}}$$

"standard" reweighting

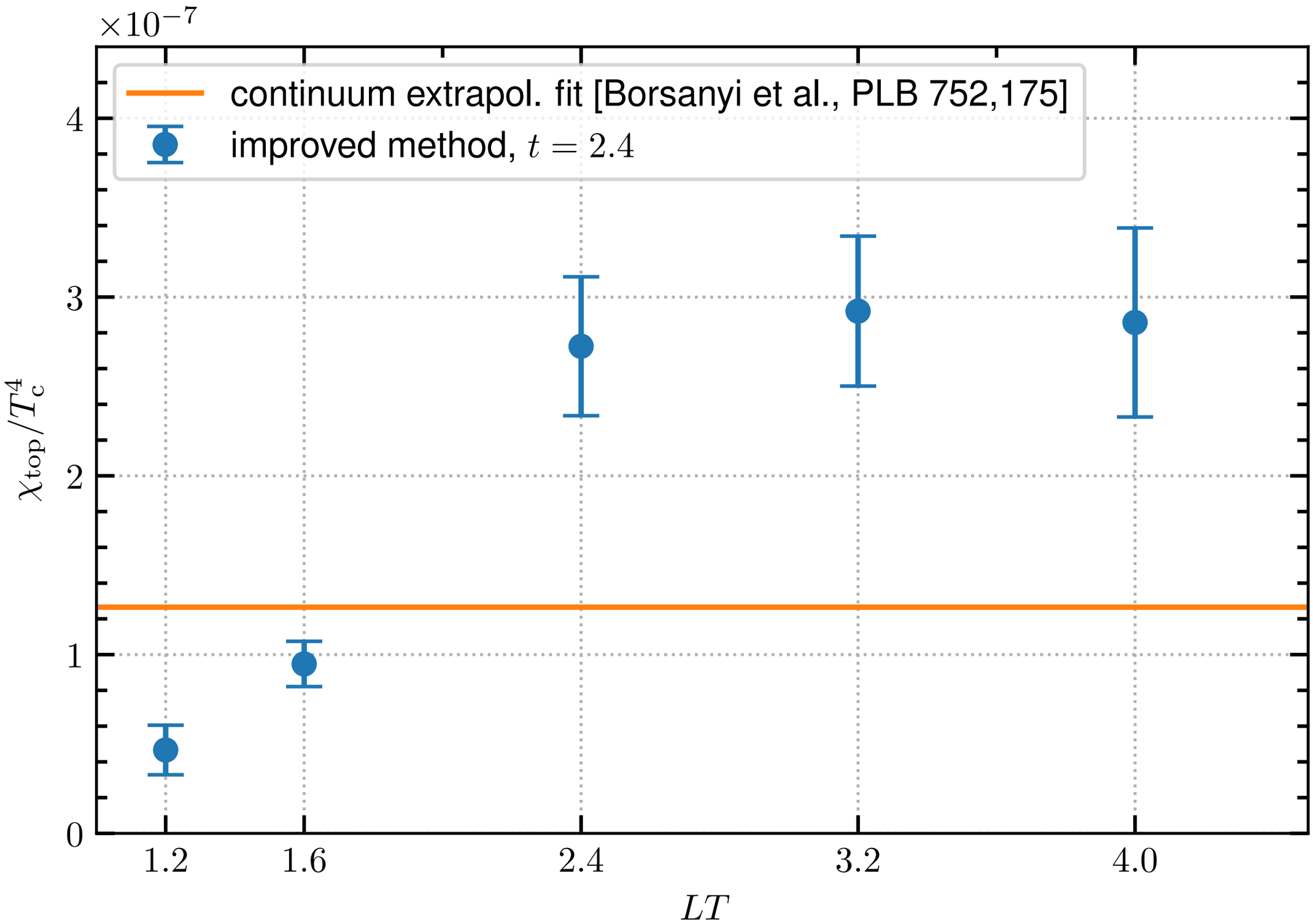
$$\simeq \frac{\sum_{\text{High}} \mathrm{e}^{-W_{\text{high}}[Q'_i]} \Theta(Q_i)}{\sum_{\text{Low}} \mathrm{e}^{-W_{\text{low}}[Q'_i, G_i]}}$$

all topology is in the high region, all weight is in the low region

$$\simeq \frac{\sum_{\text{High}} \mathrm{e}^{-W_{\text{high}}[Q'_i]} \Theta(Q_i)}{\sum_{\text{OL}_2} \mathrm{e}^{-W_{\text{high}}[Q'_i]}} \times \frac{\sum_{\text{OL}_2} \mathrm{e}^{-W_{\text{mid}}[\theta_i]}}{\sum_{\text{OL}_1} \mathrm{e}^{-W_{\text{mid}}[\theta_i]}} \times \frac{\sum_{\text{OL}_1} \mathrm{e}^{-W_{\text{low}}[Q'_i, G_i]}}{\sum_{\text{Low}} \mathrm{e}^{-W_{\text{low}}[Q'_i, G_i]}}$$

each ratio is computed in its on Monte Carlo sample!

# Finite Volume Study @ 7 Tc



# Conclusions

- QCD topological susceptibility at high temperatures relevant for axion cosmology
- however, very hard to measure at high temperatures due to bad statistics and topological freezing
- reweighting overcomes both problems and allows for direct measurements of $\chi_{\mathrm{top}}$ at high temperatures [ PTJ, G.D. Moore, D. Robaina, PRD**98**, 054512 (2018) ]
- results in quenched approximation agree well with literature up to $4.1\ T_{\mathrm{c}}$
- improvement of reweighting yields even better performance
- we see no conceptual problems in following the same philosophy with fermions [C. Bonati et al., JHEP (2018) 2018, 170]
- **ongoing:** measurement of topological susceptibility up to $7\ T_{\mathrm{c}}$ with improved technique

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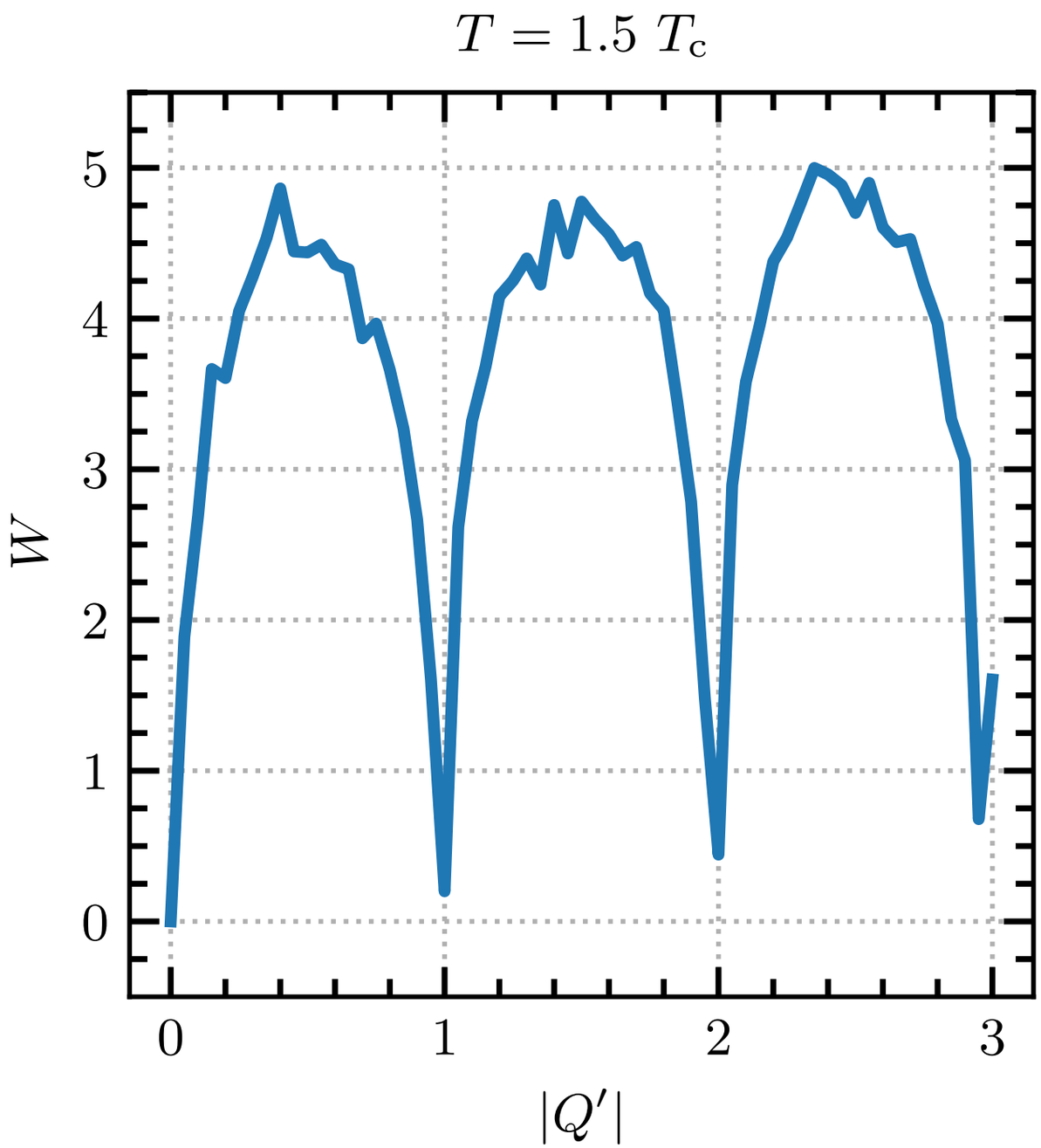
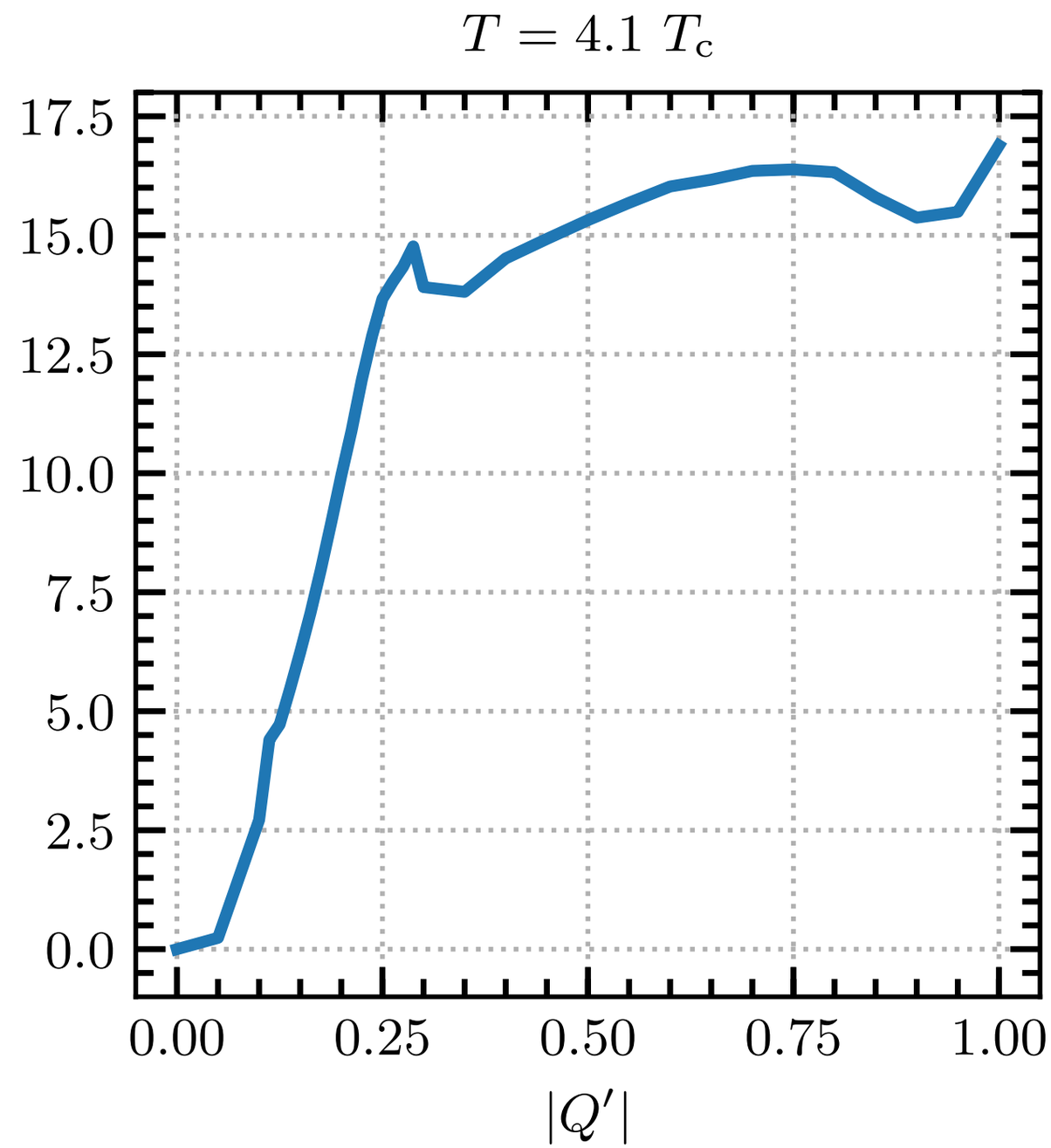
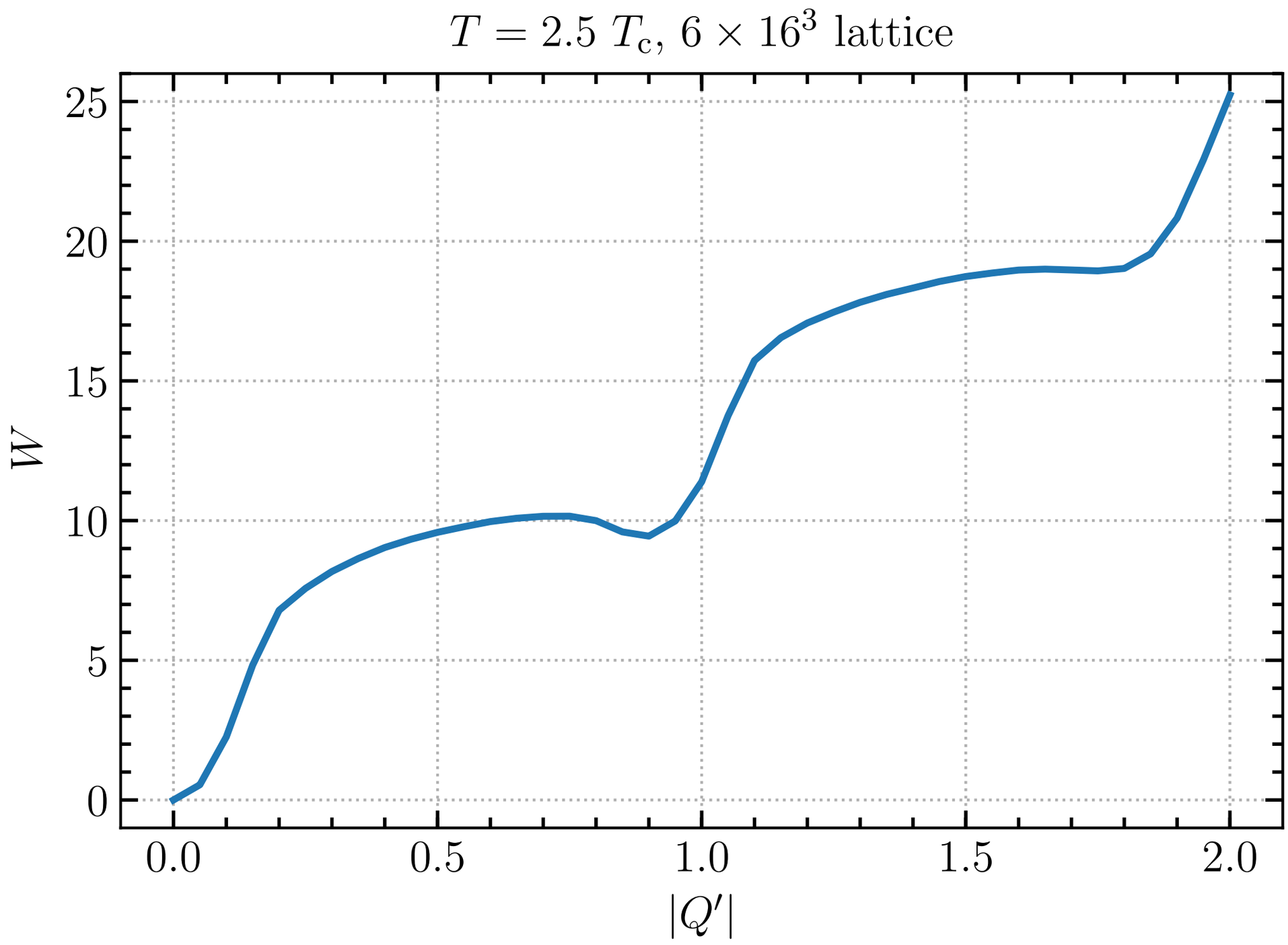
Thank You!

# Reweighting Functions



# Need of Higher Topological Sectors

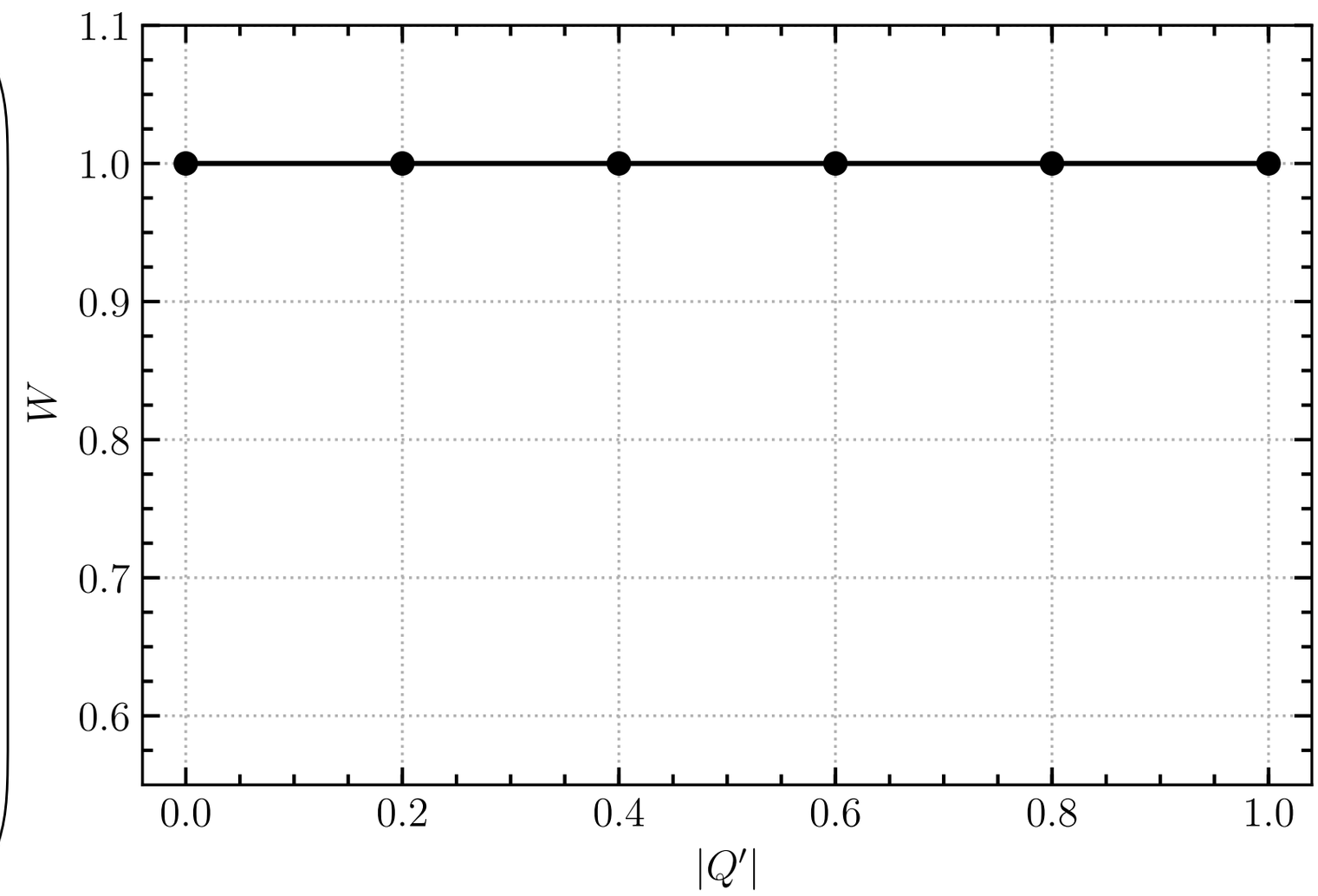


# Building the Reweighting Function Step by Step

constrain to $|Q'| \in [0, 1]$ and perform extra Markov chain for building W

similar to M. Laine and K. Rummukainen, Nucl. Phys. **B535**, 423 (1998); F. Wang and D.P. Landau, PRL **86**, 2050 (2001)

discretize W on this interval and make it piecewise linear



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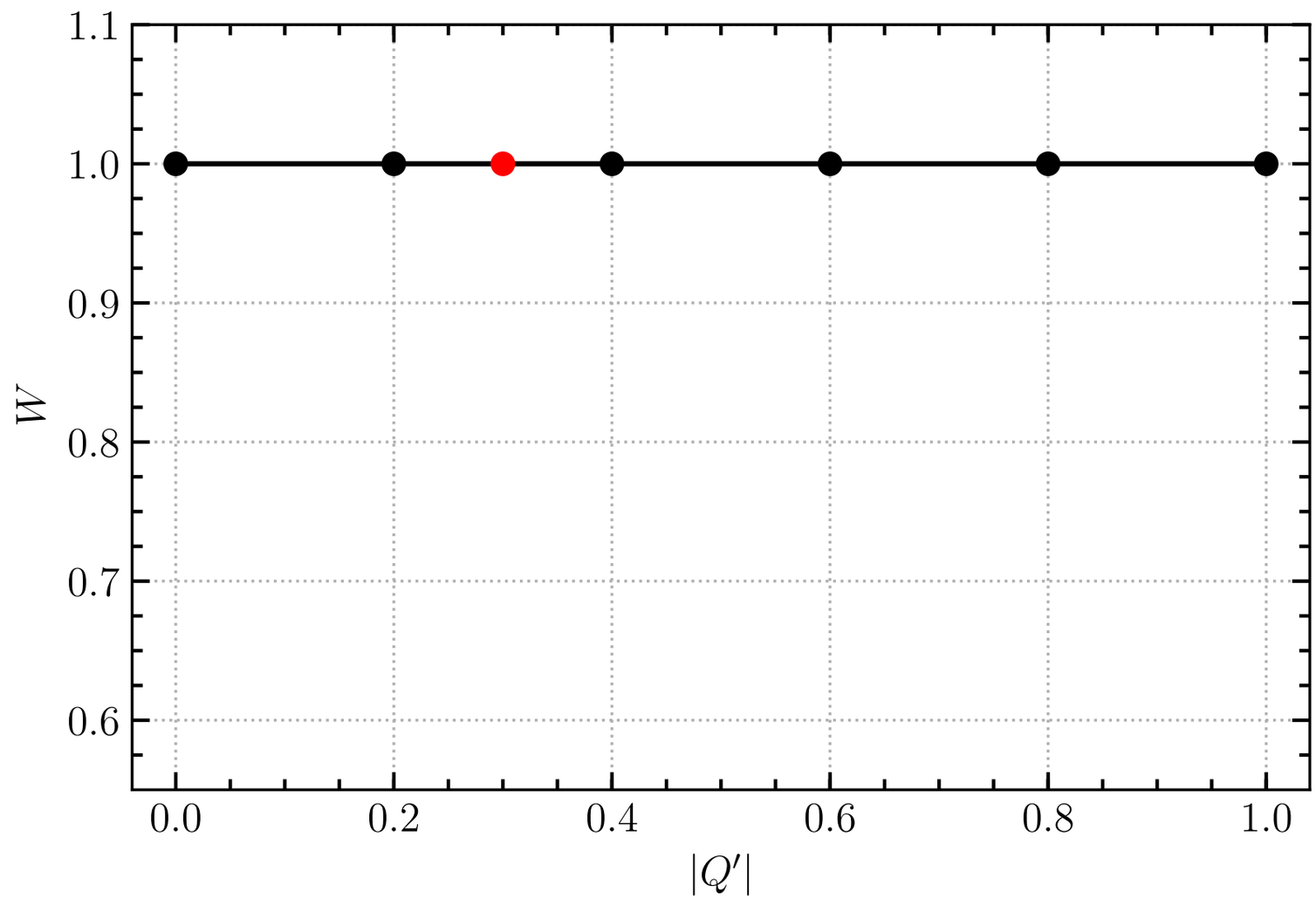

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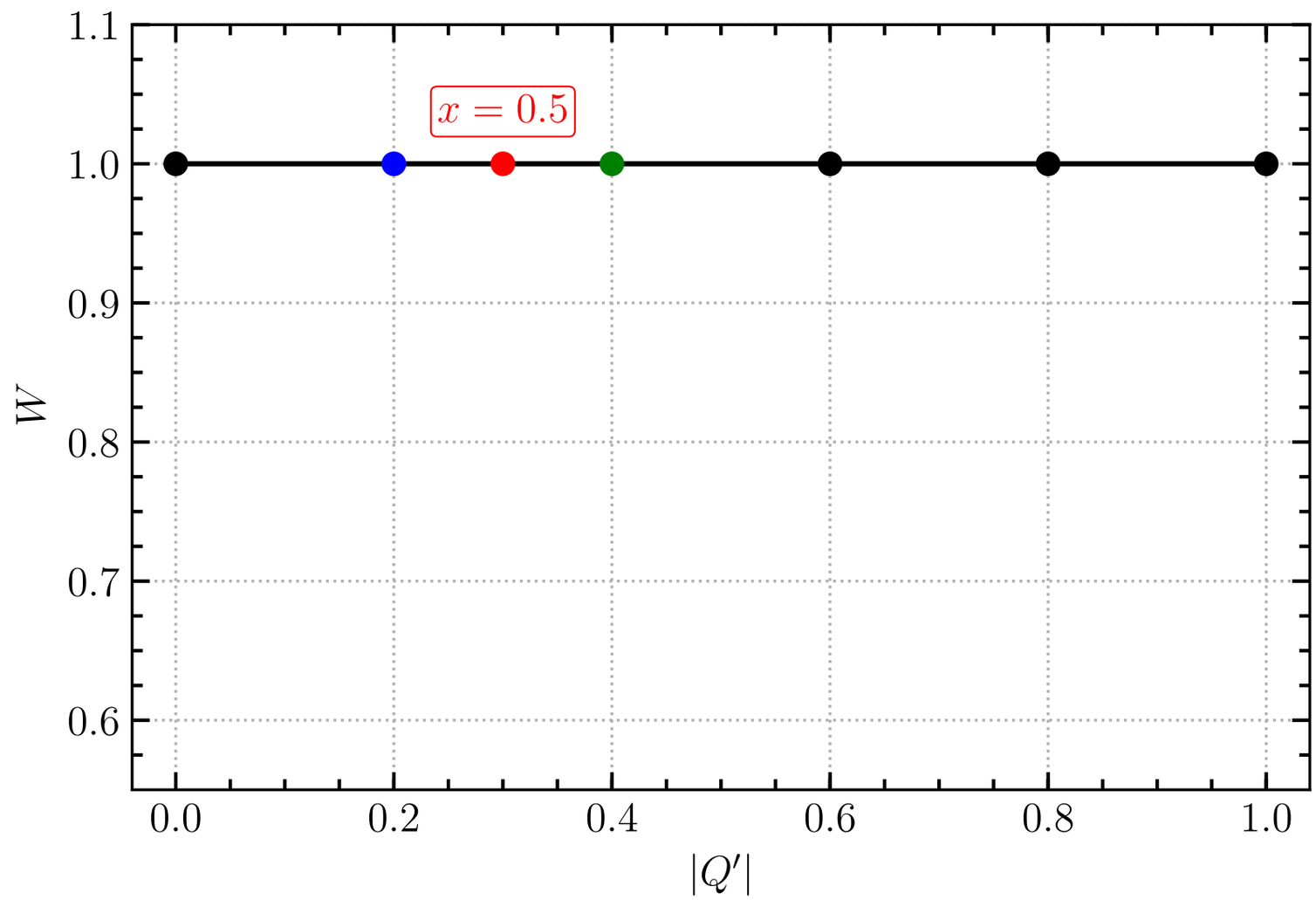

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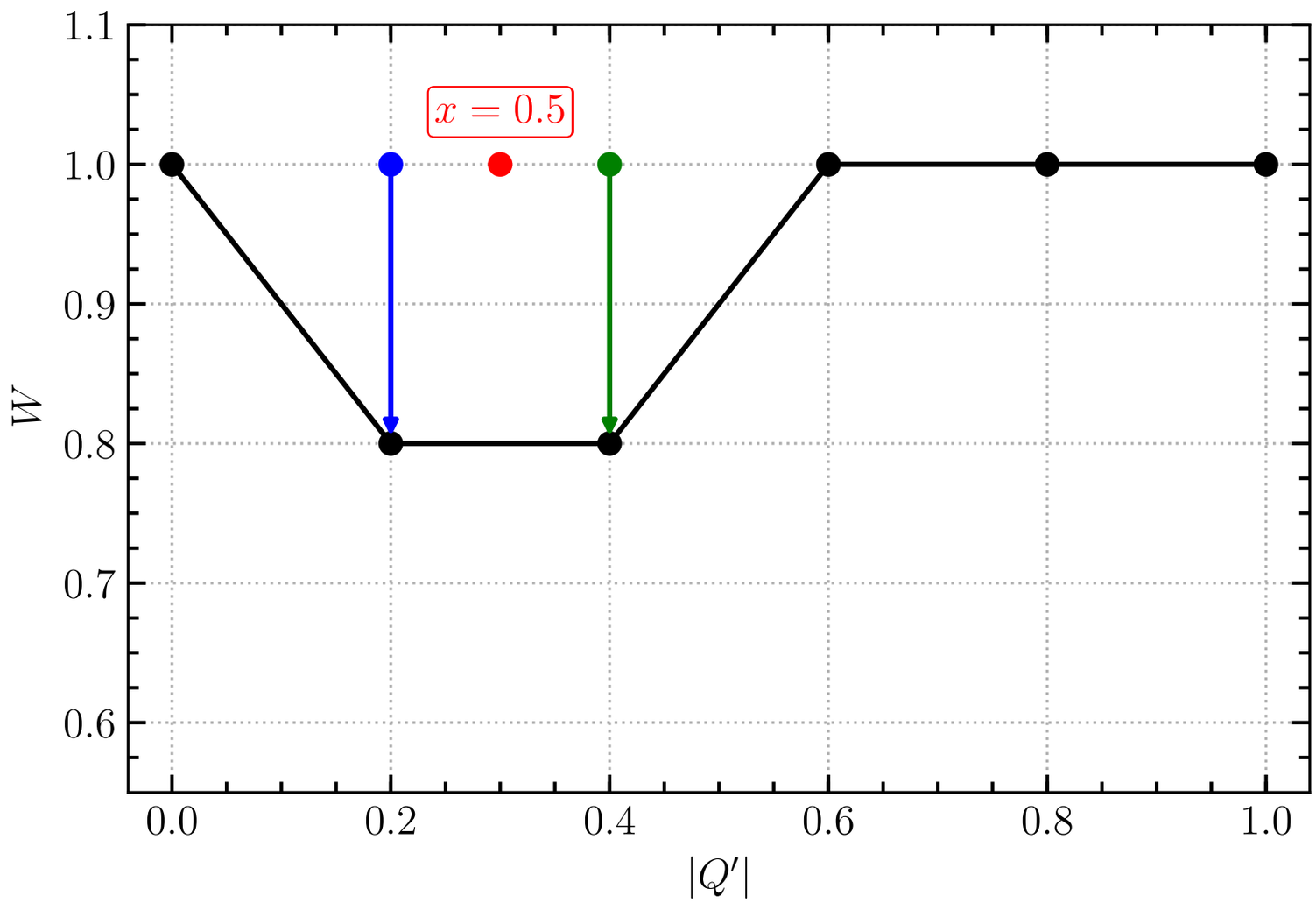

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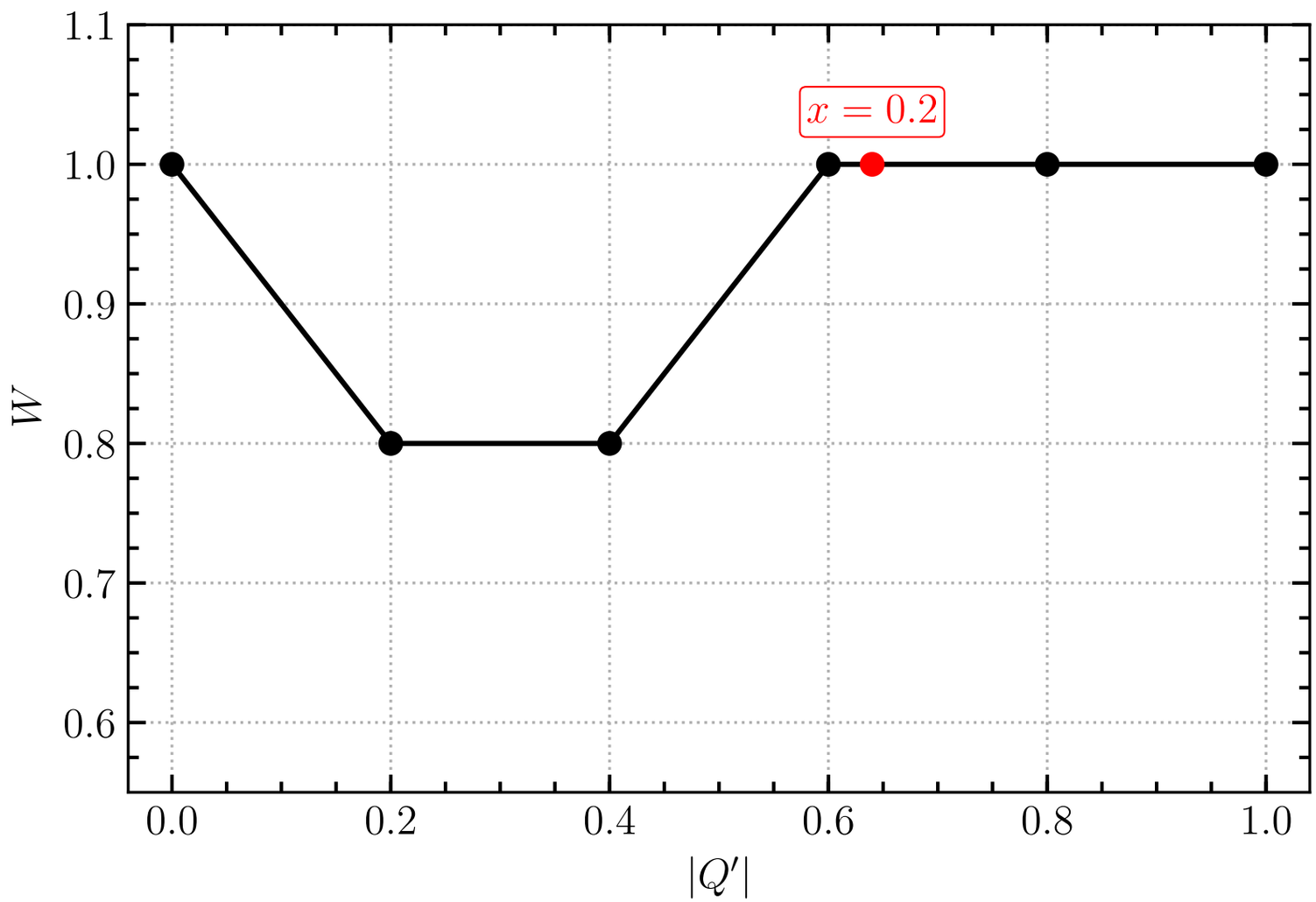

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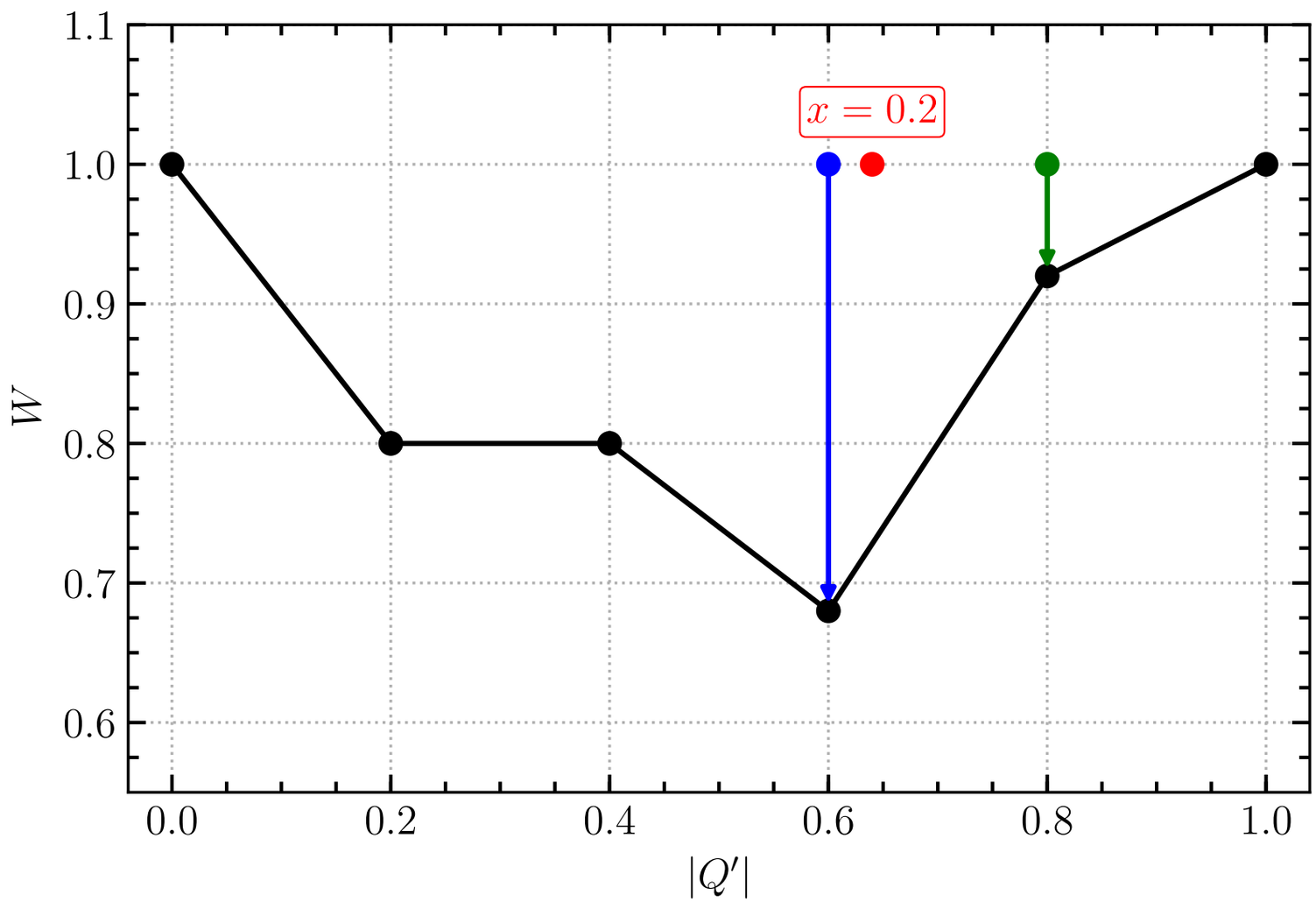

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5. if W does not change much any more, stop building