Nested Sampling for gauge theories:

- Partition functions
- Unfreezing topology
- First order phase transitions

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Swiss National Science Foundation

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Nested sampling (John Skilling, 2004)

Nested sampling is a **Monte Carlo method** to estimate the **likelihood vs phase space** curve of a theory:

- Gives access to density-of-states / partition function
- Estimates of observables at arbitrary couplings

good for phase transitions

- Cheaper/easier Monte Carlo steps

constrained uniform instead of weighted sampling

- May alleviate topological freezing
- Easily parallelized

benefits of the specific sampling schedule

Nested sampling (John Skilling, 2004)

Bayesian evidence integral:

$$Z = \int \mathscr{L}(\theta)\pi(\theta)d\theta$$

$\pi(\theta)$: prior distribution

$\mathscr{L}(\theta)$: likelihood

Z: evidence

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Transform to 1-dim. integral:

$$dX = \pi(\theta)d\theta$$

$$X(\lambda) = \int_{\mathscr{L}(\theta)>\lambda} \pi(\theta)d\theta$$

such that:

$$Z = \int_0^1 \mathscr{L}(X)dX$$

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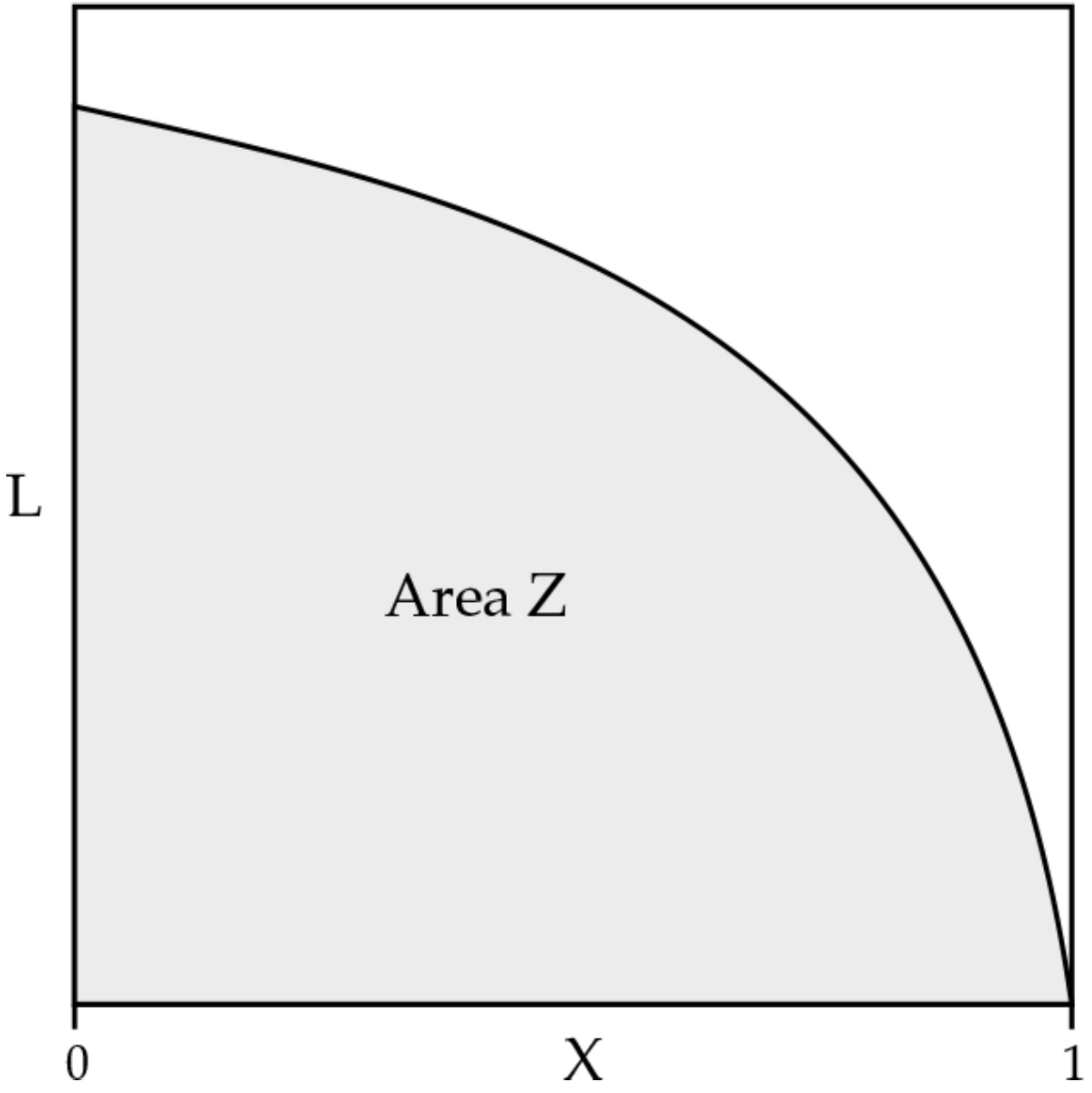
⇒ phase space $X(\lambda)$ contained within likelihood $\mathscr{L} > \lambda$

Nested sampling (John Skilling, 2004)



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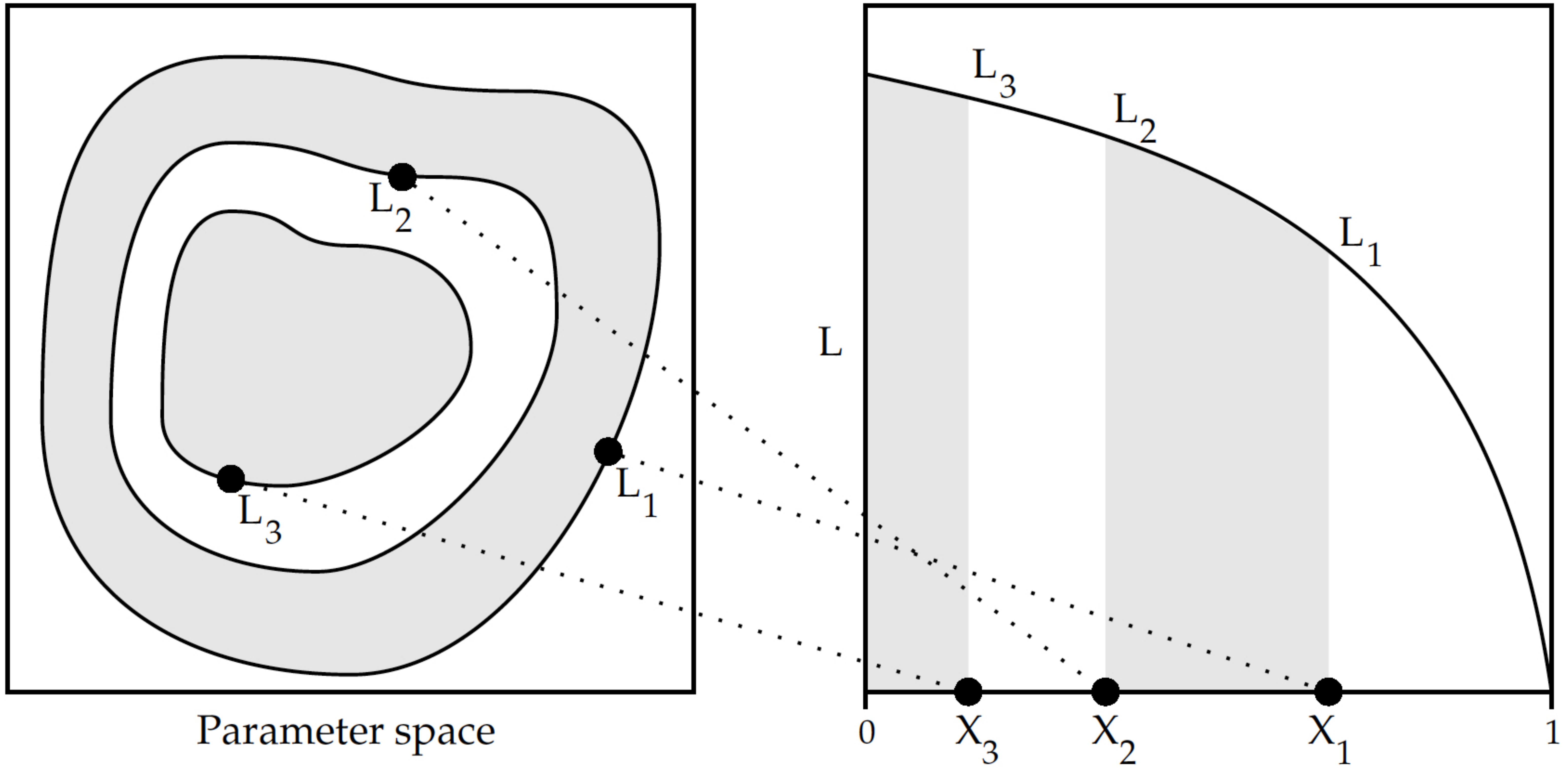
Draw samples uniformly from $\pi(\theta)d\theta$:



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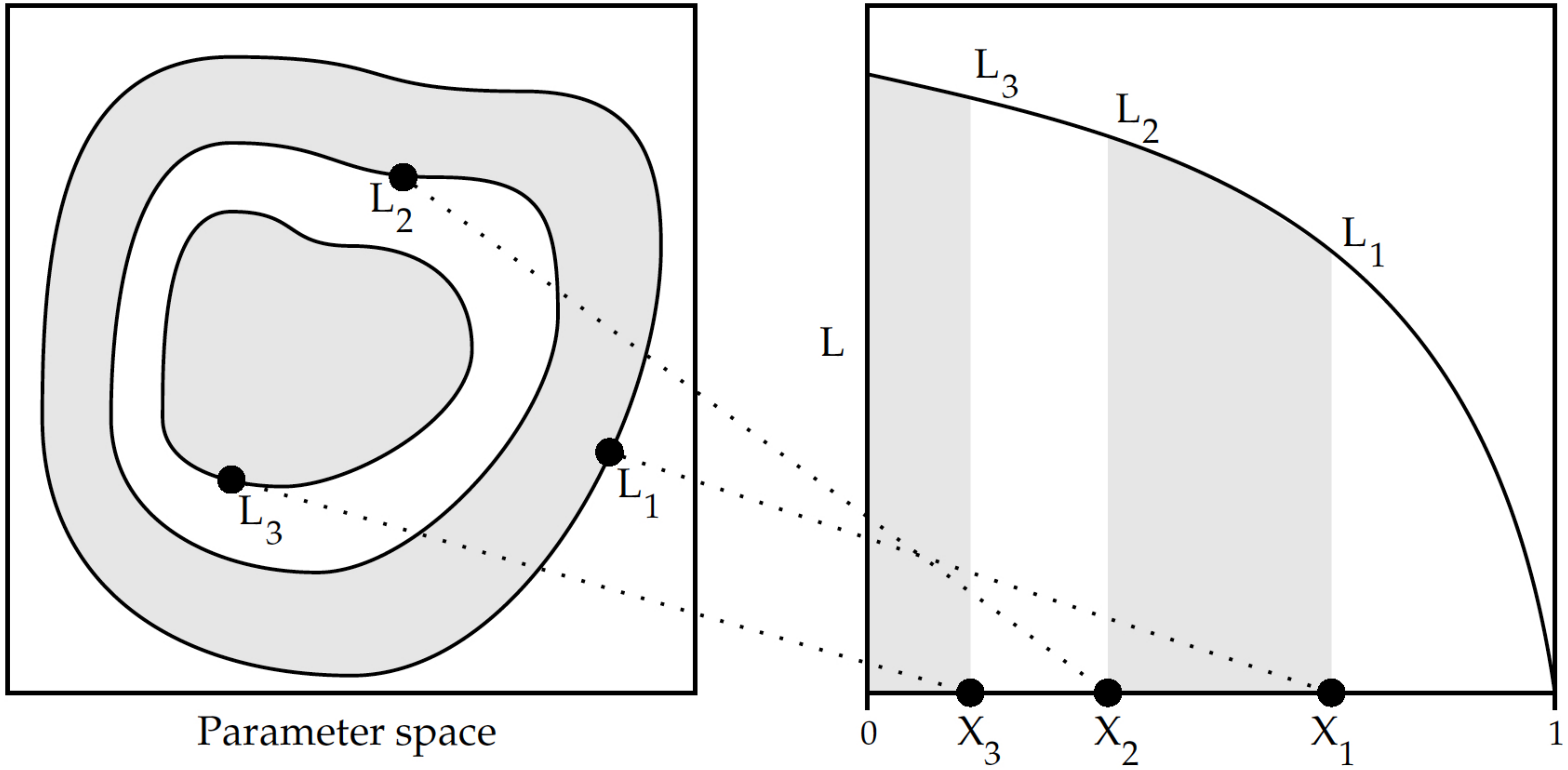

L_i's can be calculated.

X_i's are unknown, but:

$$X_0 = 1, \quad X_i = t_i X_{i-1}$$

$$\Pr(t_i) = N\, t_i^{N-1} \quad \text{in (0,1)}$$

with $\langle \ln t \rangle = -1/N$

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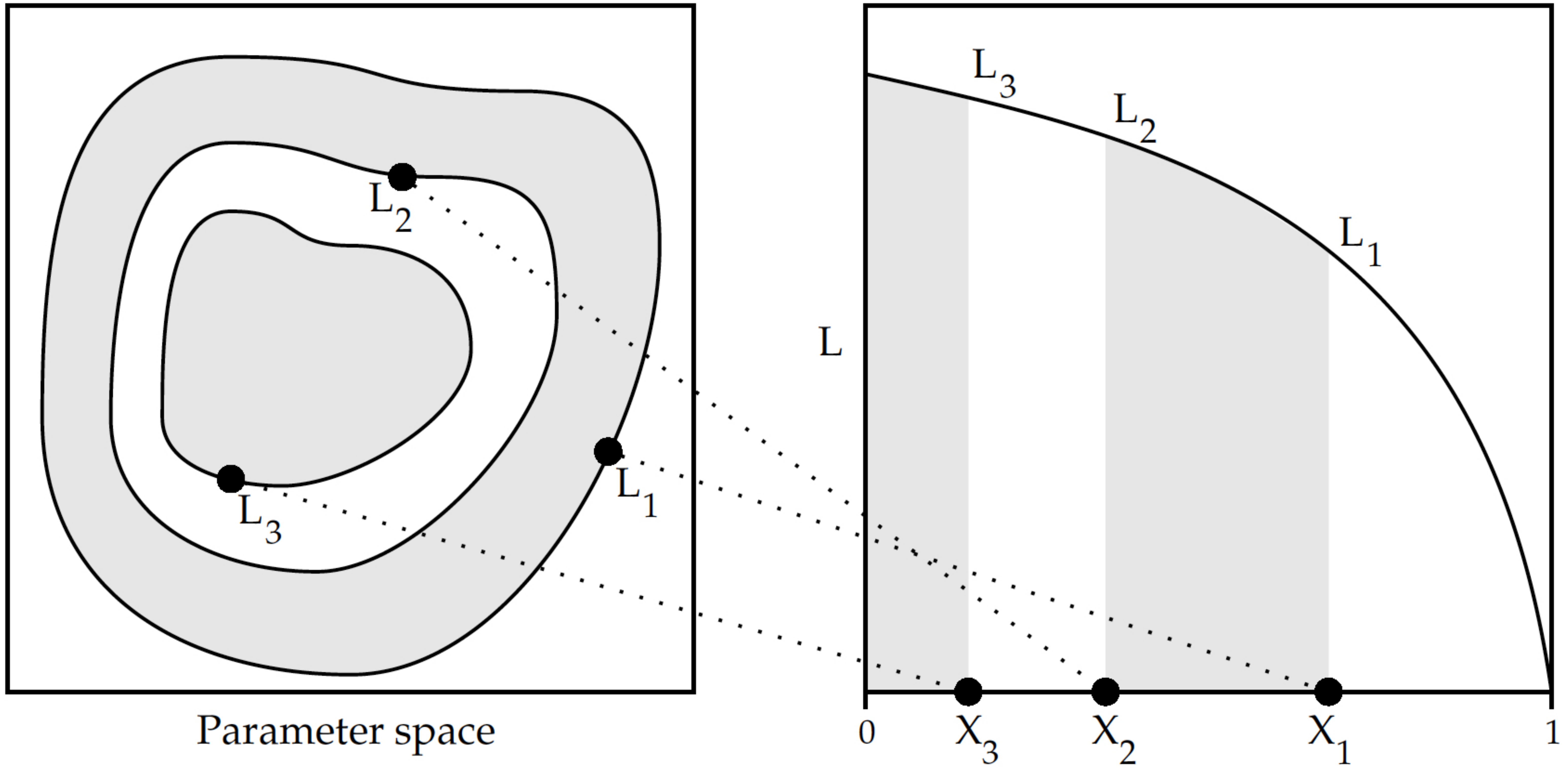

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$\Rightarrow$ Estimate phase space X within contours of constant likelihood $\mathscr{L}$

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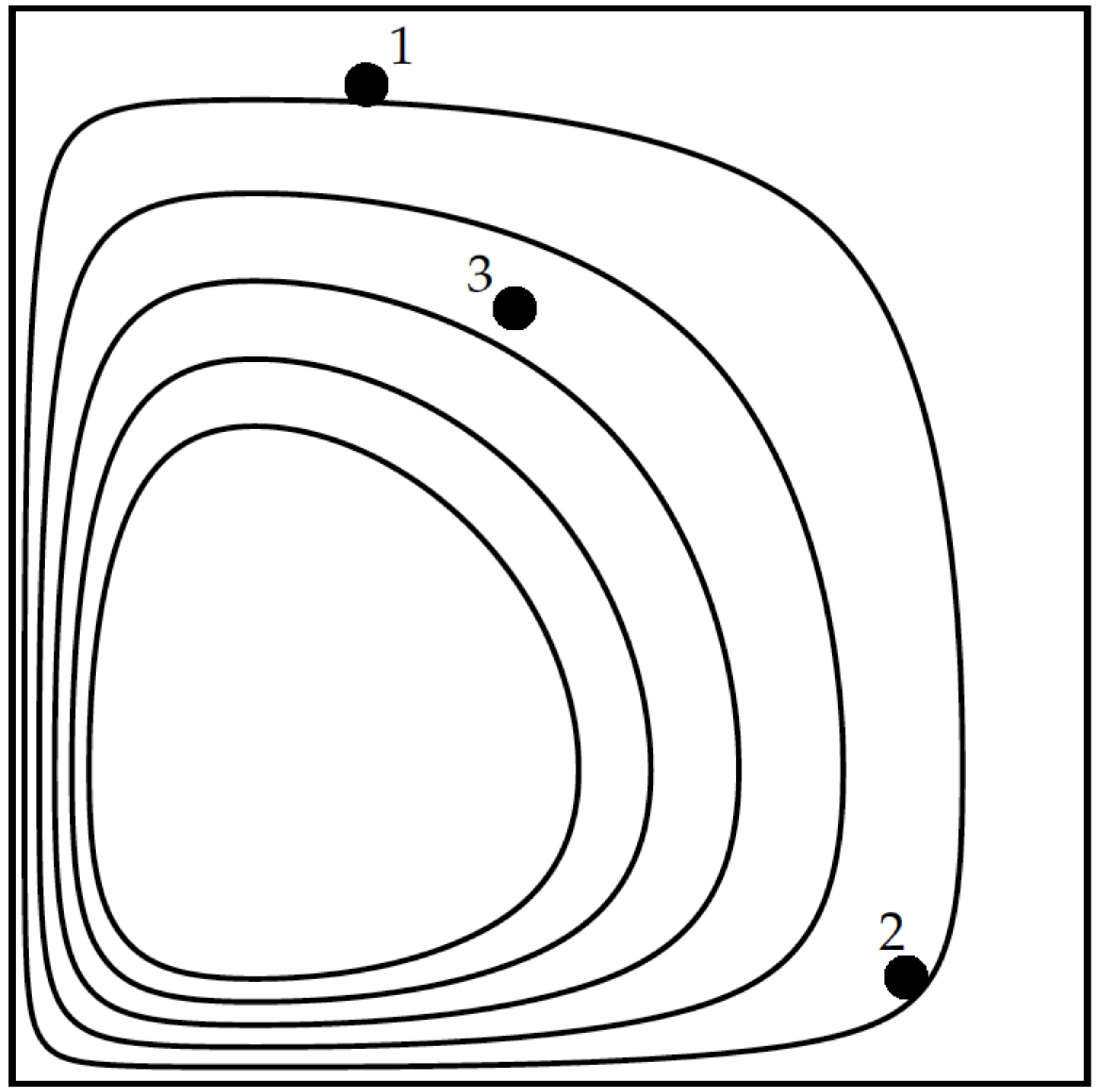
- Initialisation: **sample** N random points θ from $\pi(\theta)d\theta$



Parameter space

Nested sampling (John Skilling, 2004)

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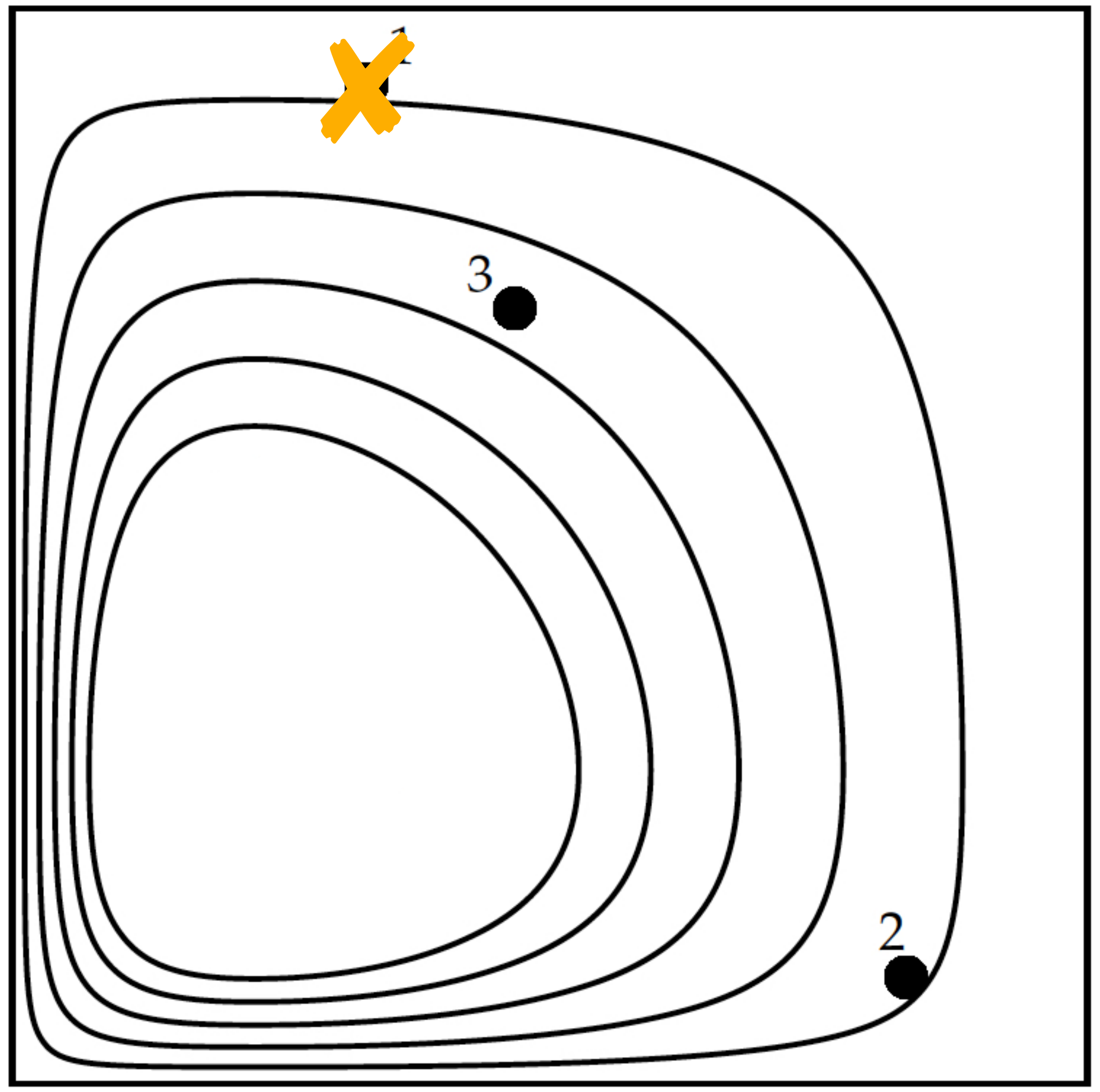

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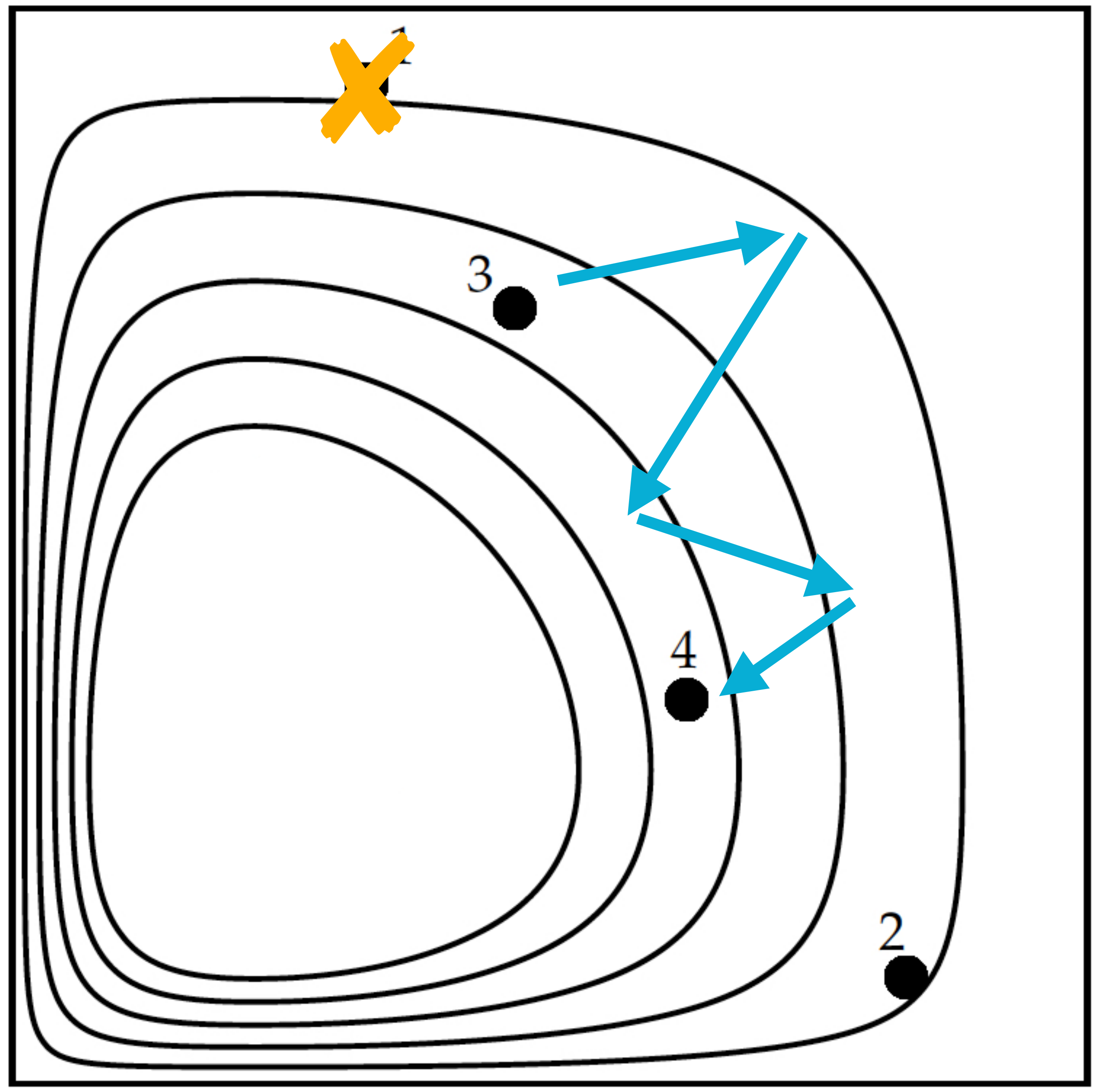

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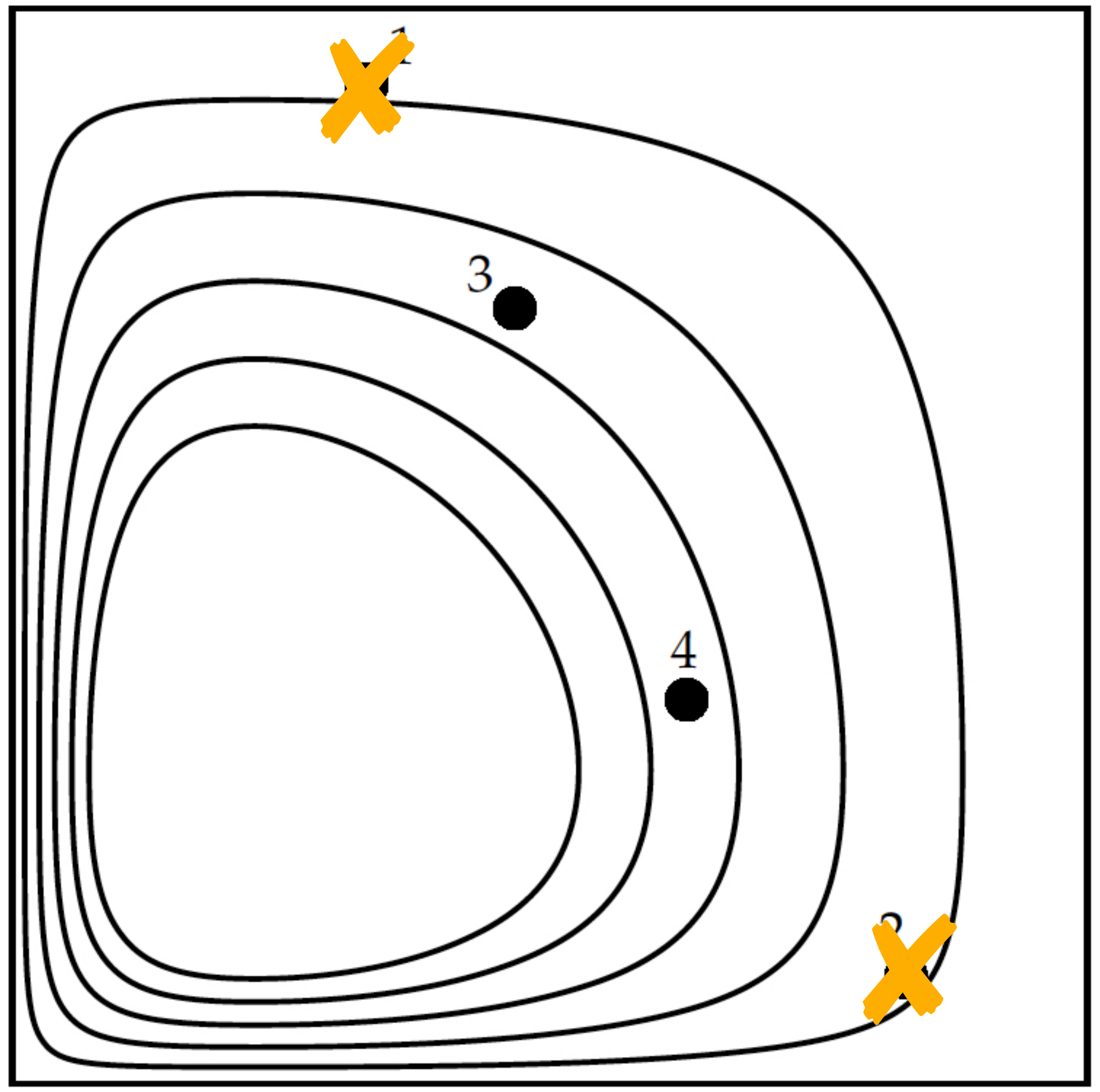

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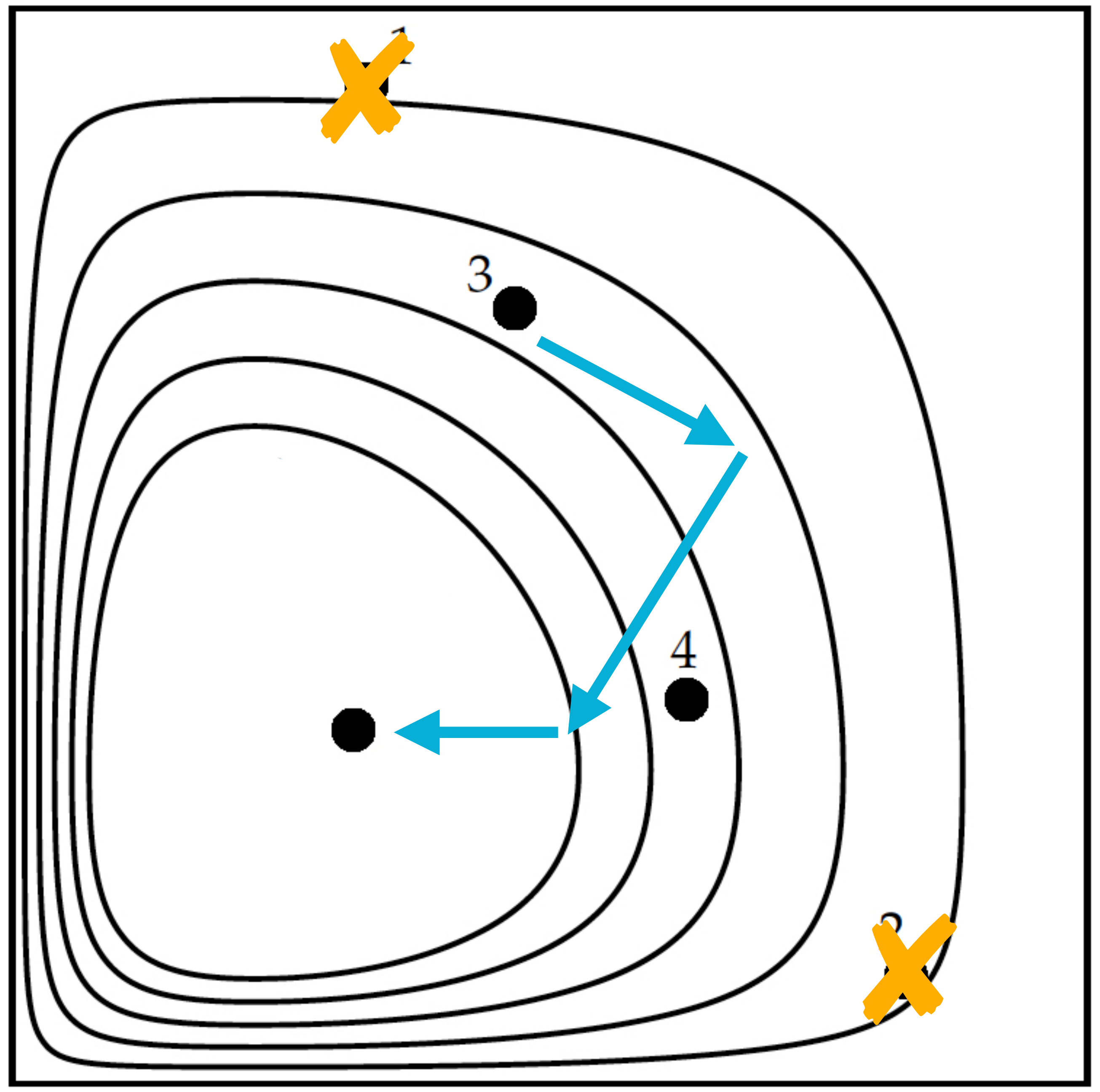

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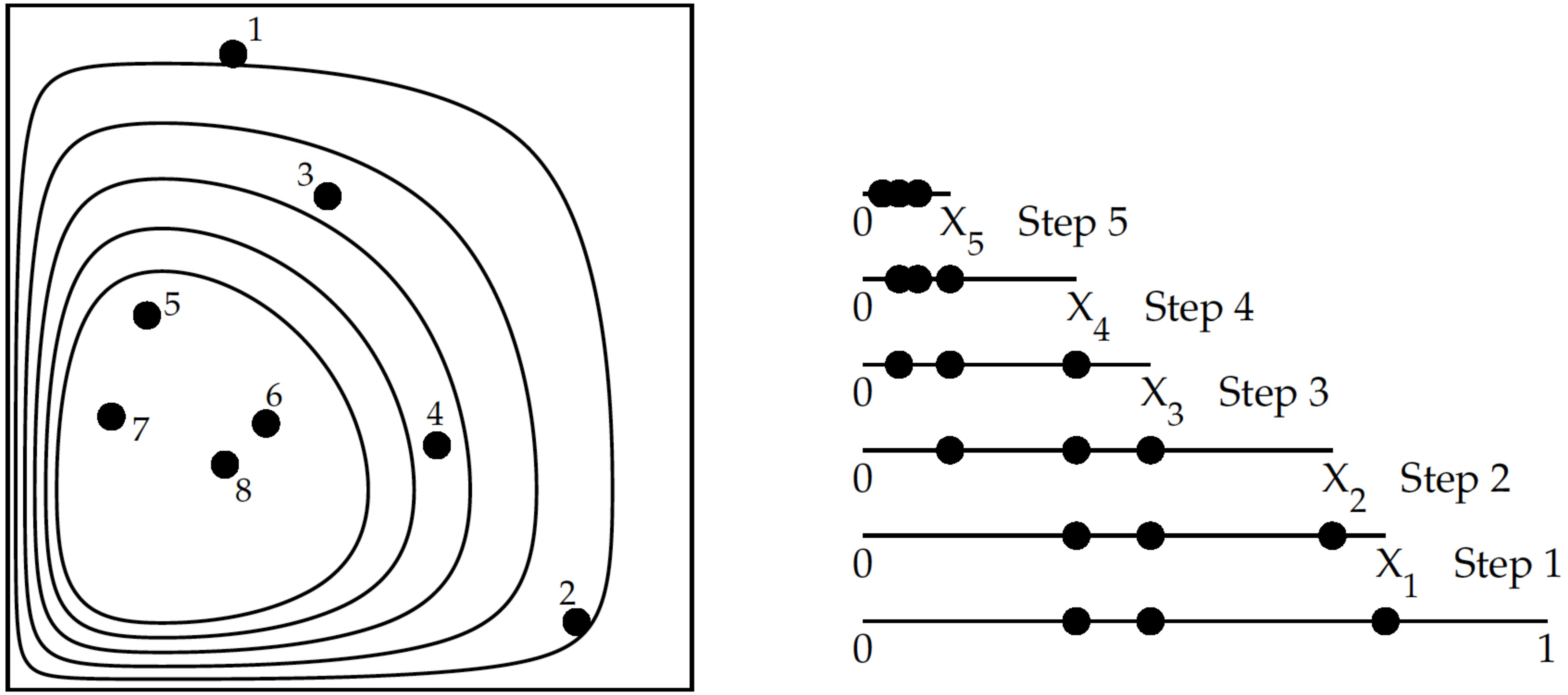

Parameter space

Enclosed prior mass X

Nested sampling (John Skilling, 2004)

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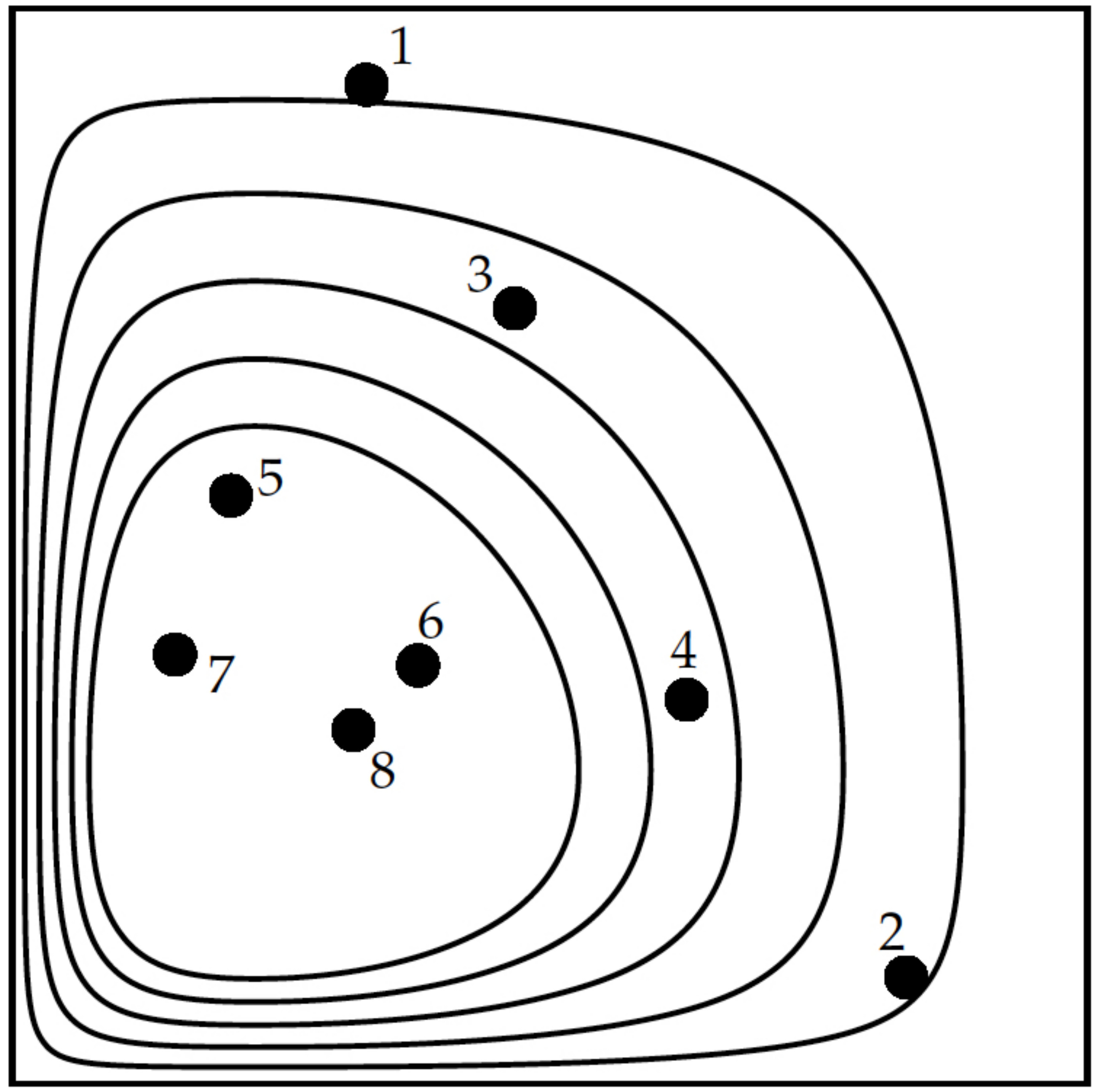
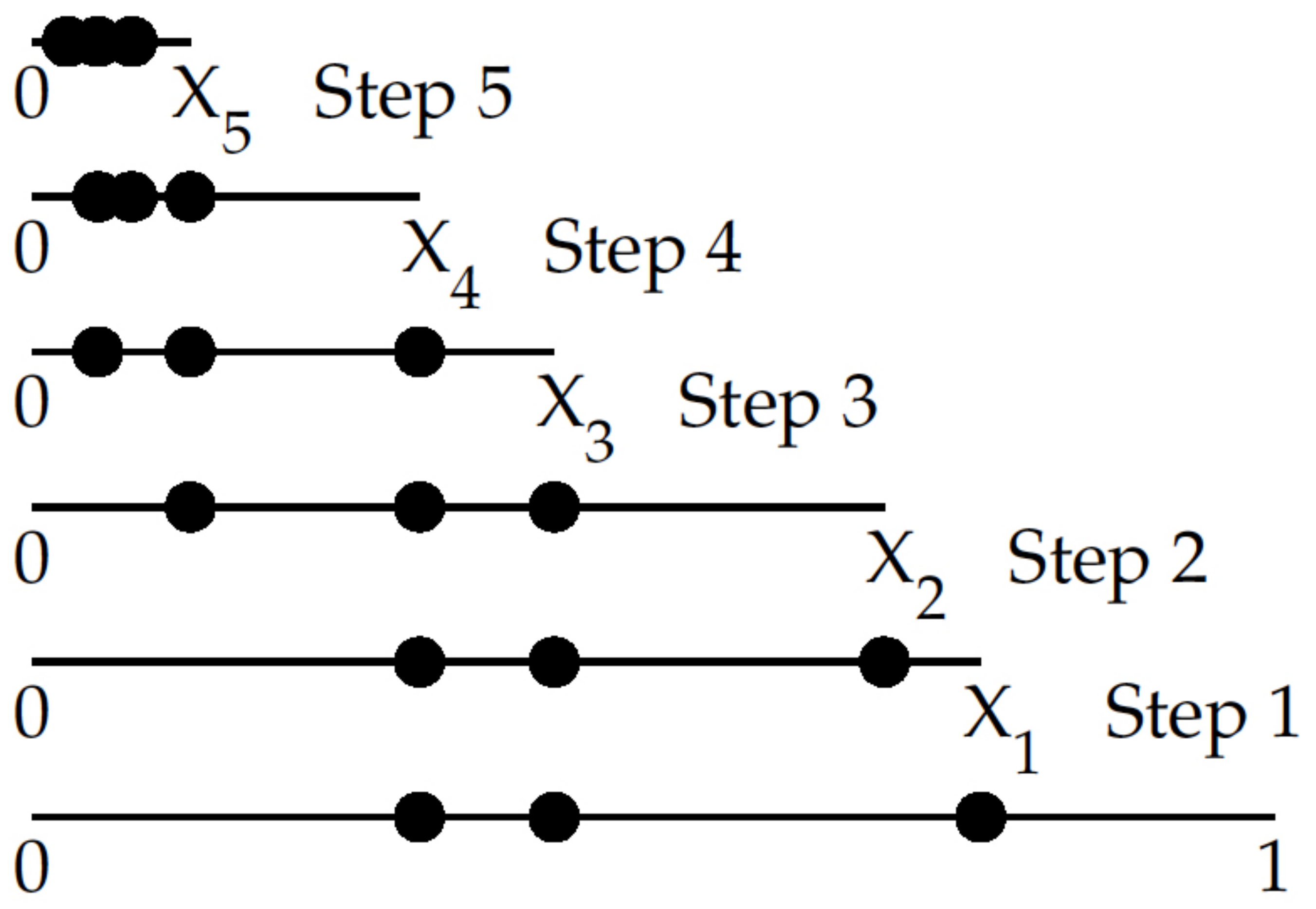
- Initialisation: **sample** N random points θ from $\pi(\theta)d\theta$
- Step i: **record** smallest likelihood $\mathscr{L}_i$, **drop** the point, **resample** uniformly within $\mathscr{L} > \mathscr{L}_i$
- Analysis: **compression factor** $t_i = X_i / X_{i-1}$ follows Beta distribution $p(t) \propto t^{N-1}$



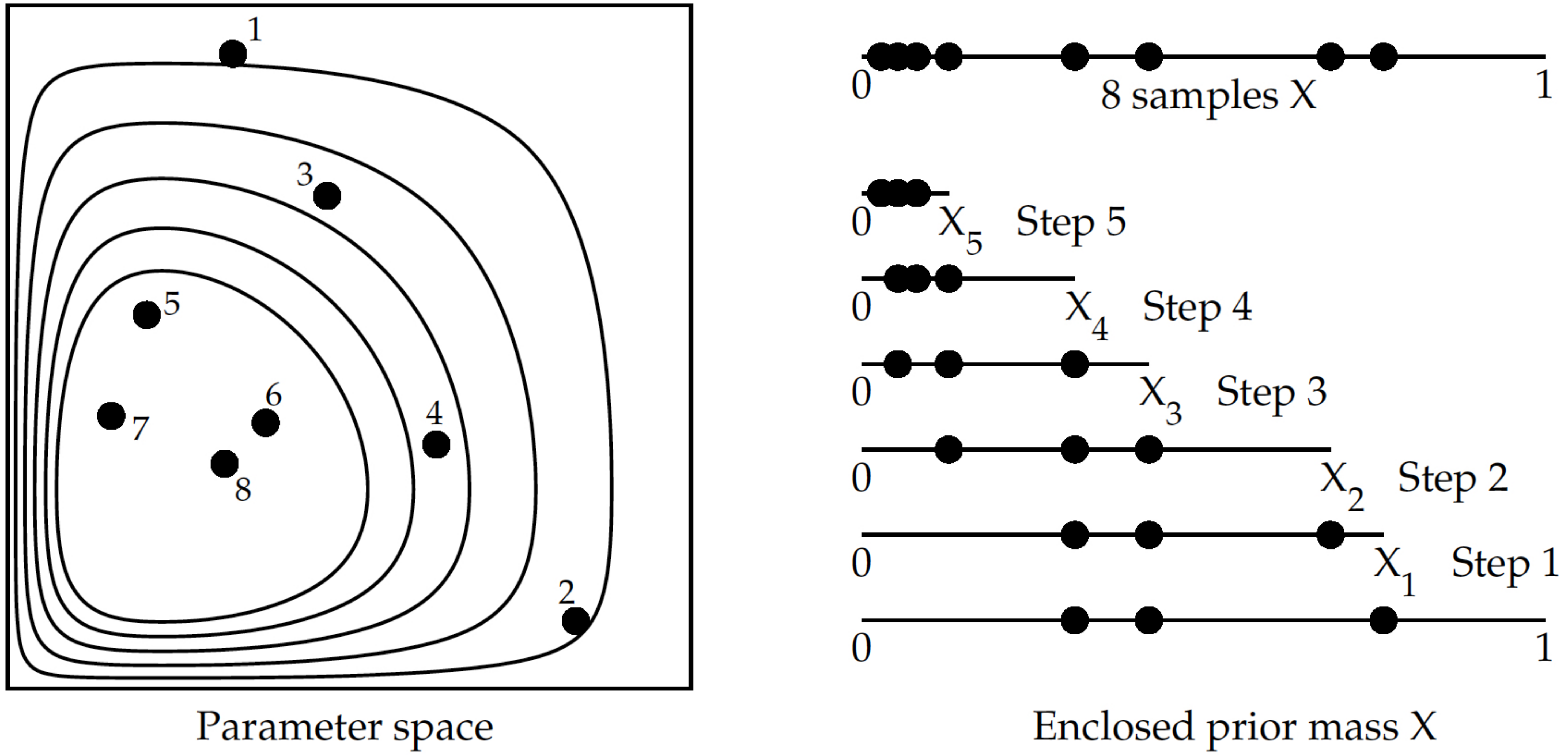
Parameter space



Enclosed prior mass X

Nested sampling (John Skilling, 2004)

Result from simulation ⇒ ordered list of $\{X_i, \mathscr{L}_i\}$



Nested sampling (John Skilling, 2004)

⇒ Estimate phase space X within contours of constant likelihood $\mathscr{L}$

- Partition function and observables for any value of β, e.g., with $\mathscr{L} = e^{-S}$:

$$Z(\beta) = \int_0^1 dX\, \mathscr{L}(X)^\beta \qquad\qquad \langle O \rangle_\beta = \frac{1}{Z(\beta)} \int_0^1 dX\, \mathscr{L}(X)^\beta \, \langle O \rangle_{\mathscr{L}(X)}$$

⇒ *a posteriori* !

- Density of states ⇒ universal function independent of β:

$$\rho(S) = \frac{dX}{dS} = -\frac{dX}{d\ln\mathscr{L}} \qquad\qquad Z(\beta) = \int dS\, \rho(S)\; e^{-\beta S}$$

- Possible to restrict sampling to important regions in phase space (or energy)

Application to gauge field theories

Parameters θ $\Rightarrow$ gauge fields U

Likelihood $\mathscr{L}$ $\Rightarrow L = \exp(-S[U])$

Prior $\pi(\theta)$ $\Rightarrow$ Haar measure on gauge group

Example applications:

2d quenched U(1) (Schwinger model)

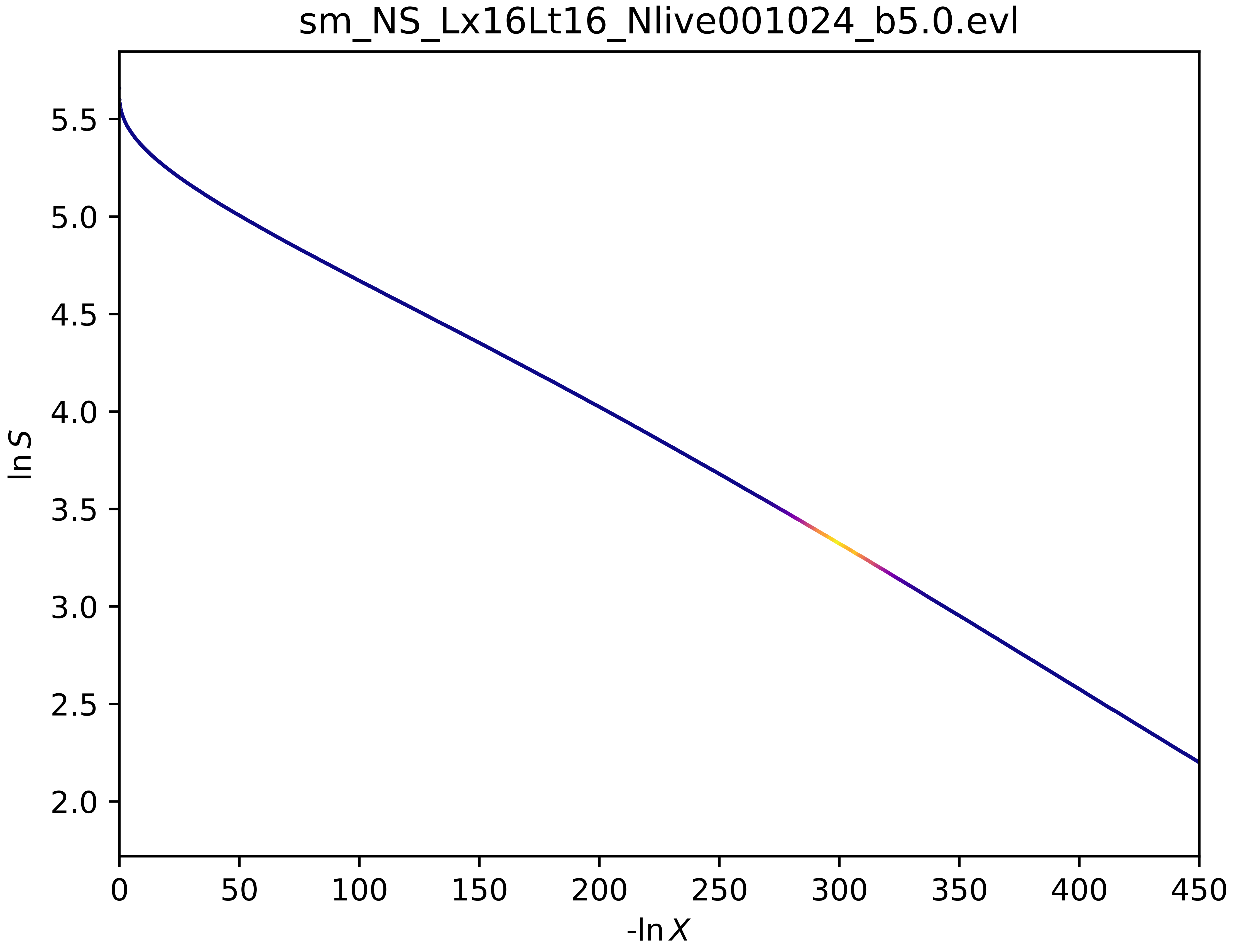
$\Rightarrow$ topological freezing

4d quenched SU(3)

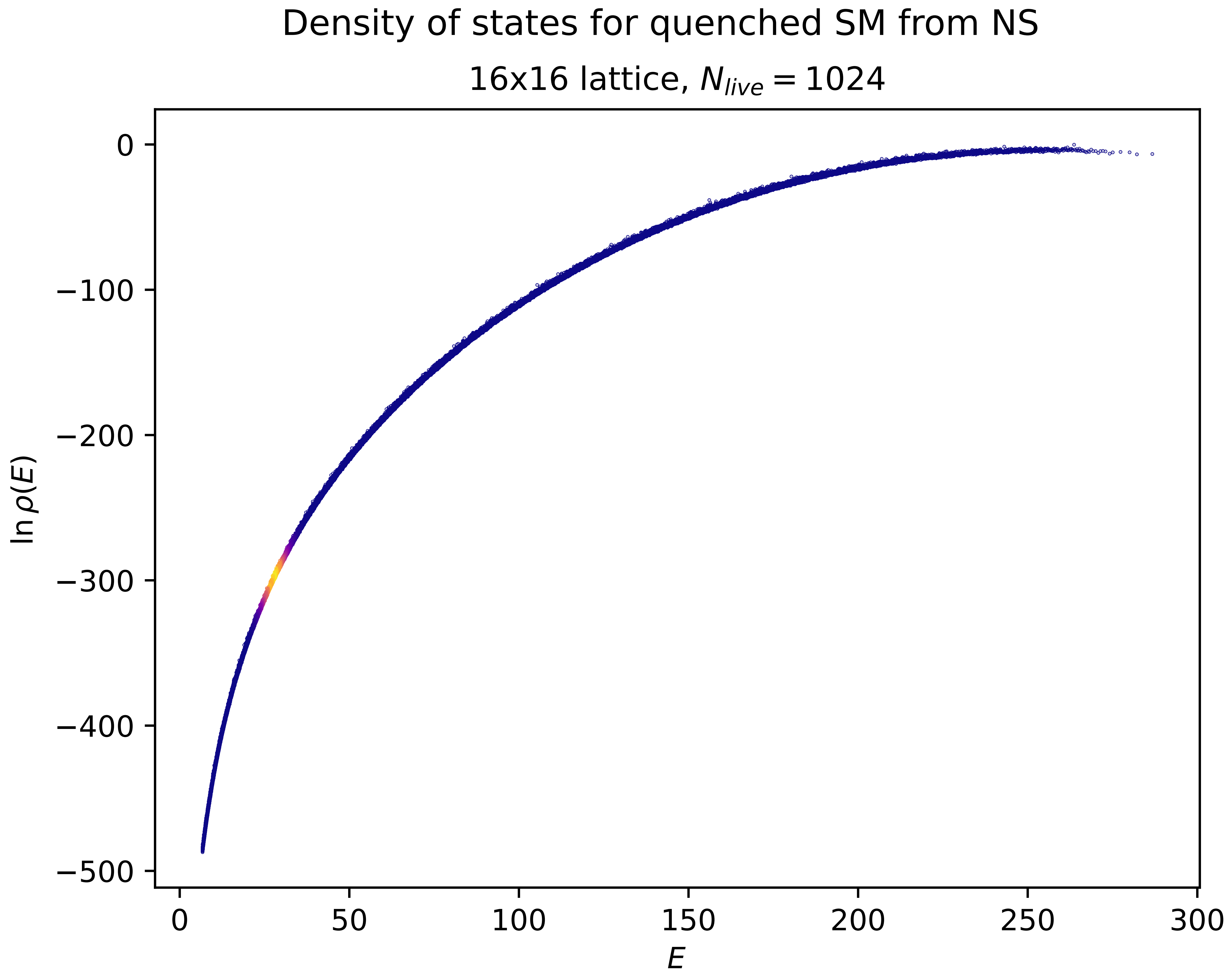
$\Rightarrow$ first order phase transition

Likelihood L vs. prior volume X and density of states

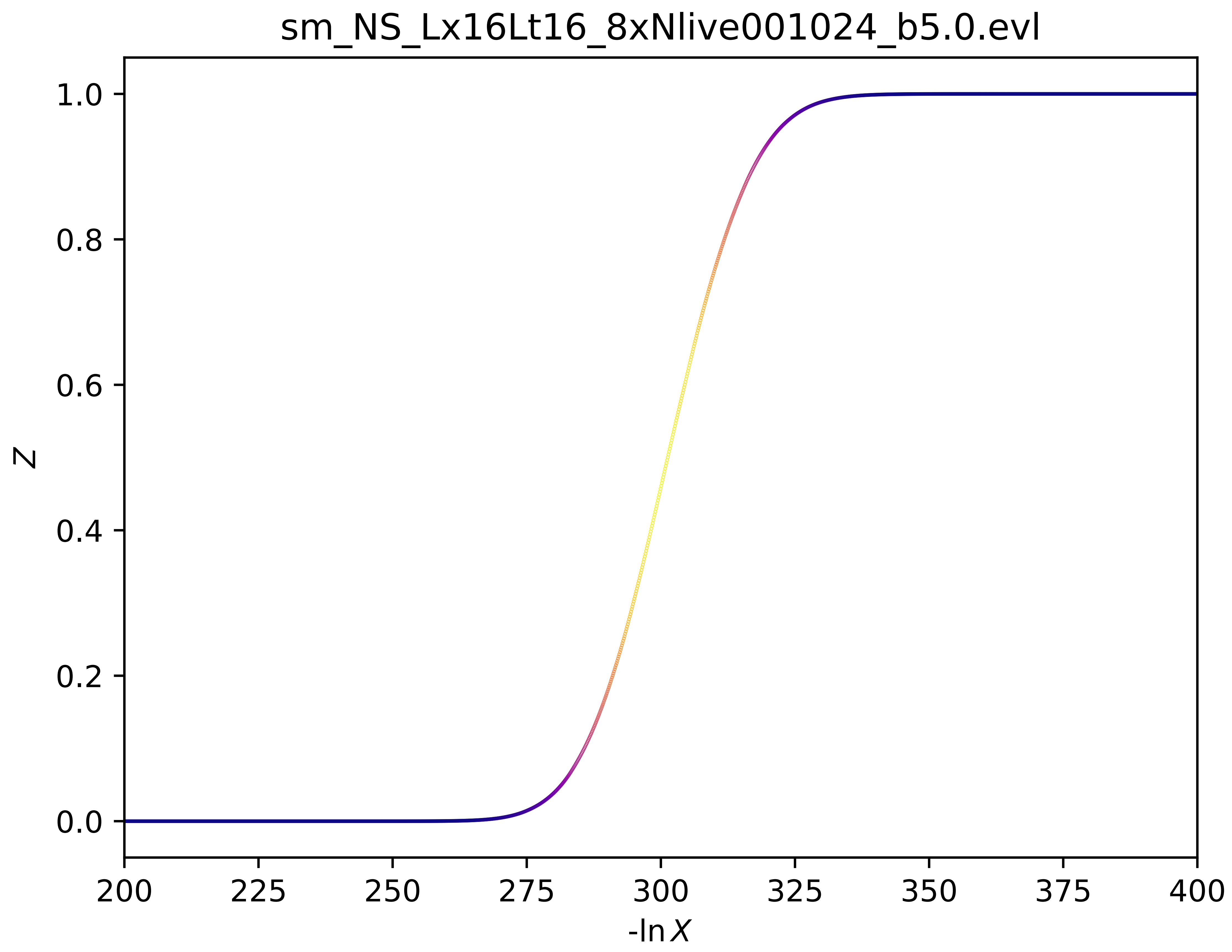
…or better $-\ln L = S$ and $\ln S$ vs $-\ln X$:

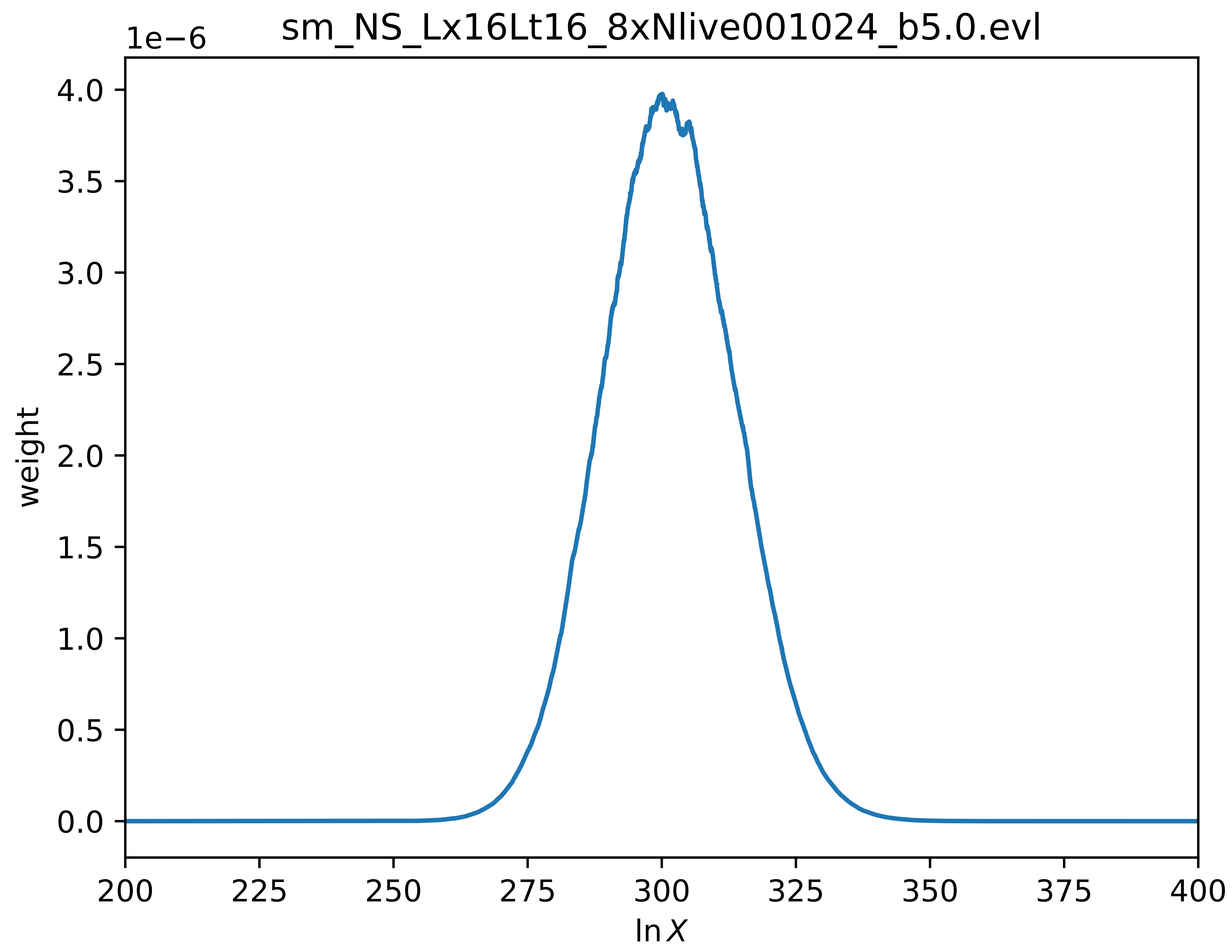


…or $\rho(E) = dX/dE$ and $\ln \rho(E) = -X\, d\ln X/d\ln L$:

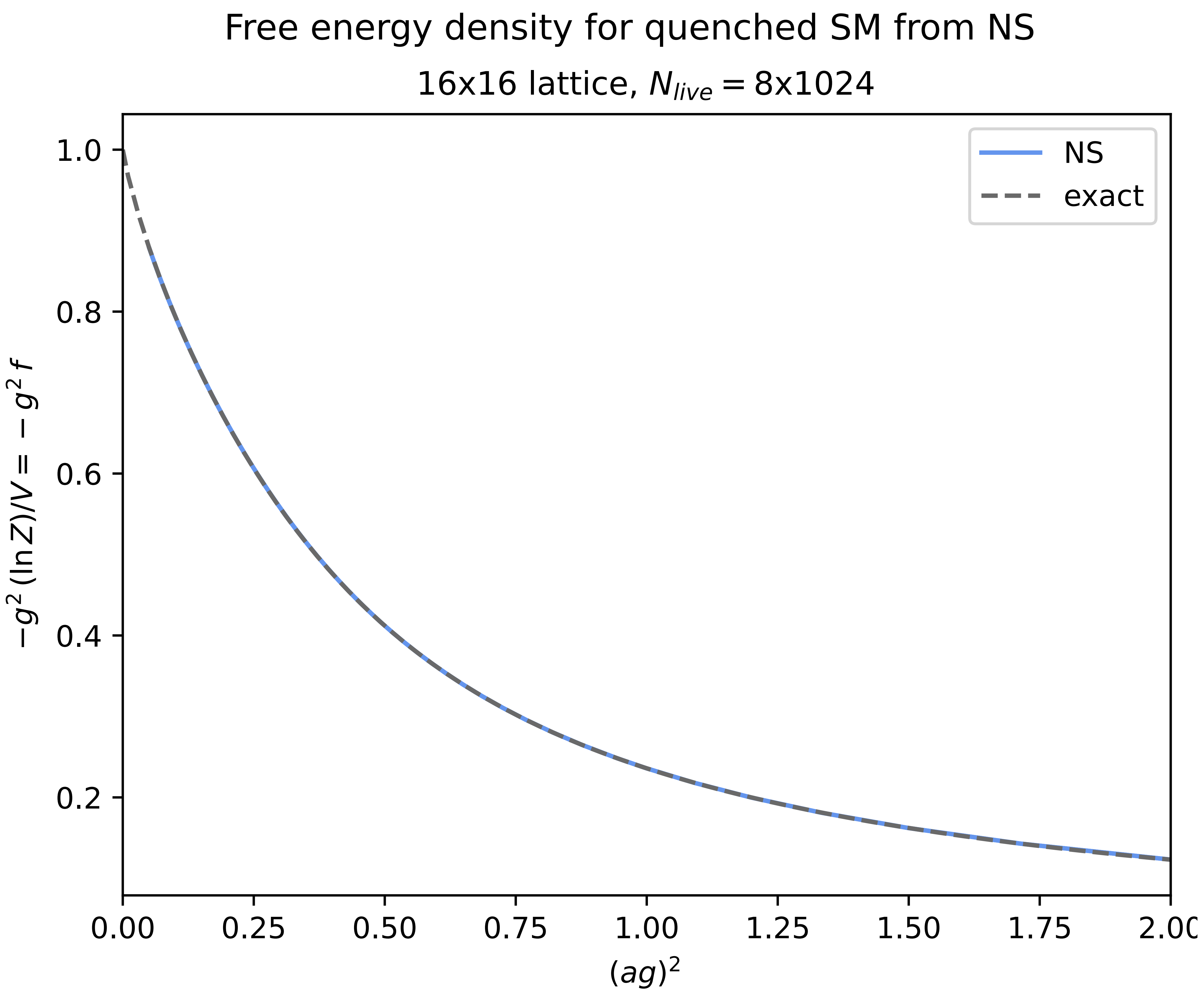


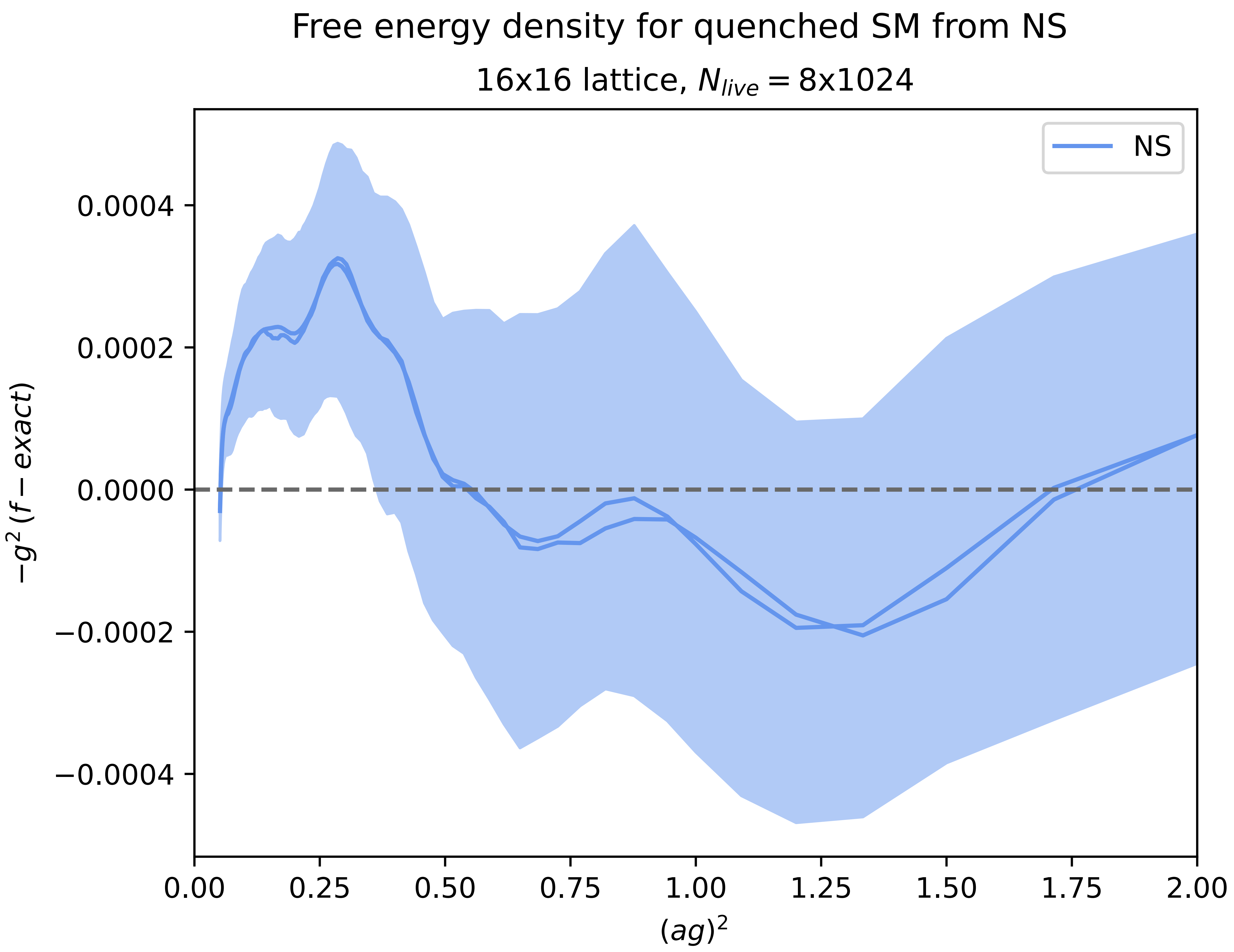
Partition function Z with weights at $\beta = 5.0$



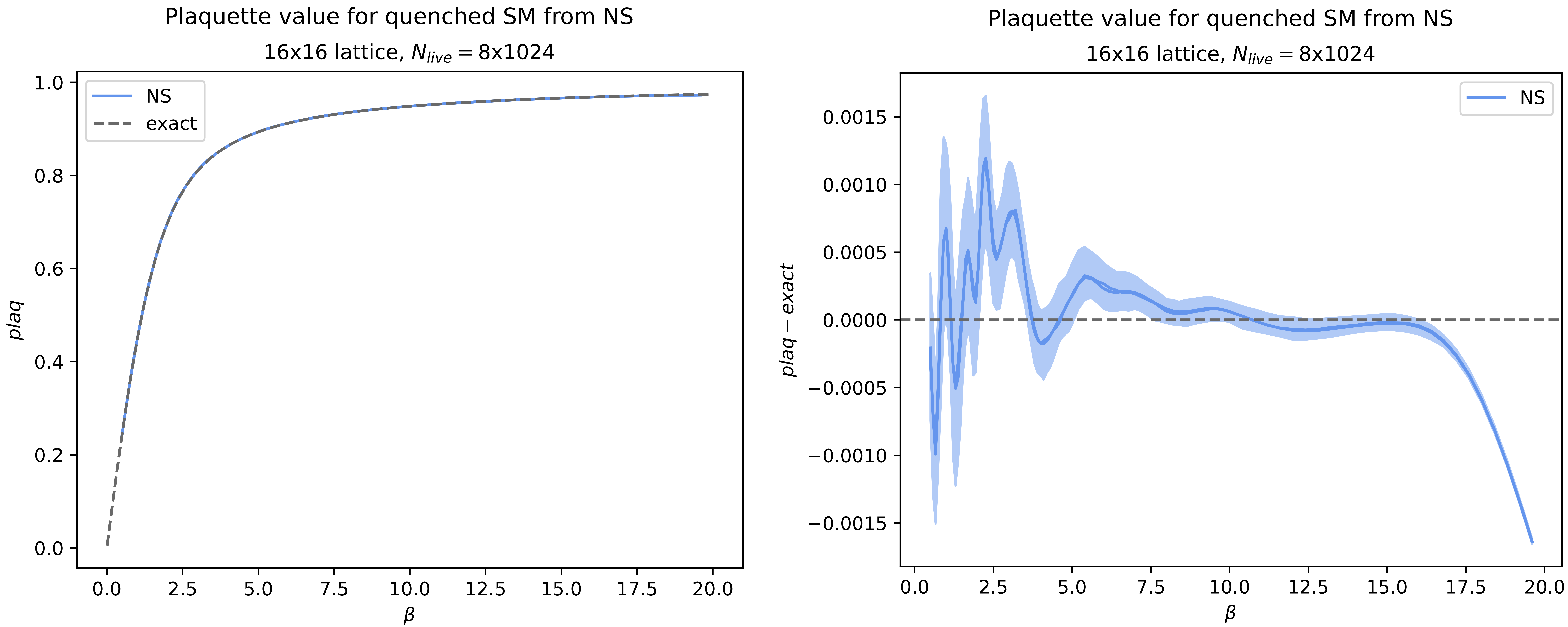


Free energy density, continuum limit

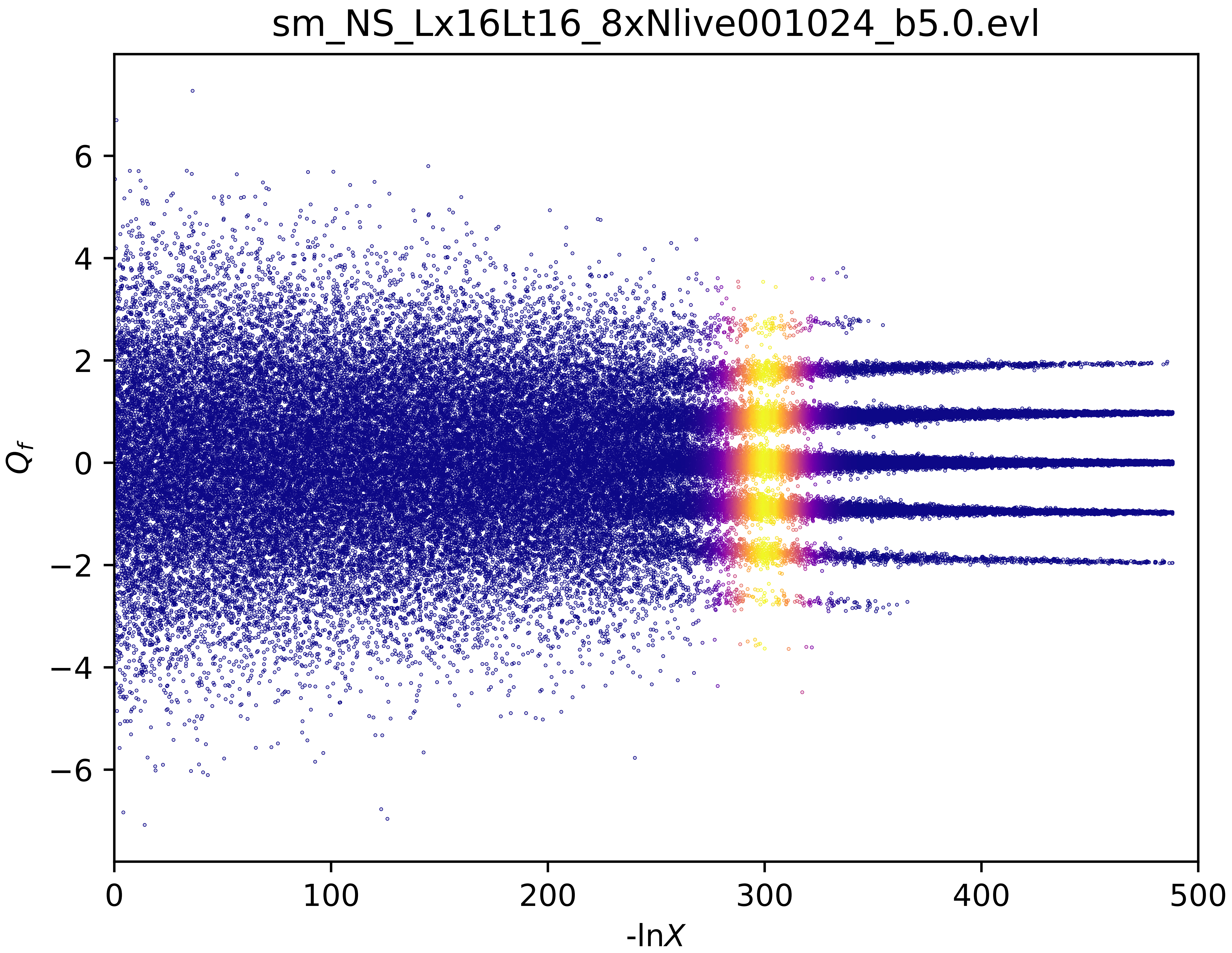




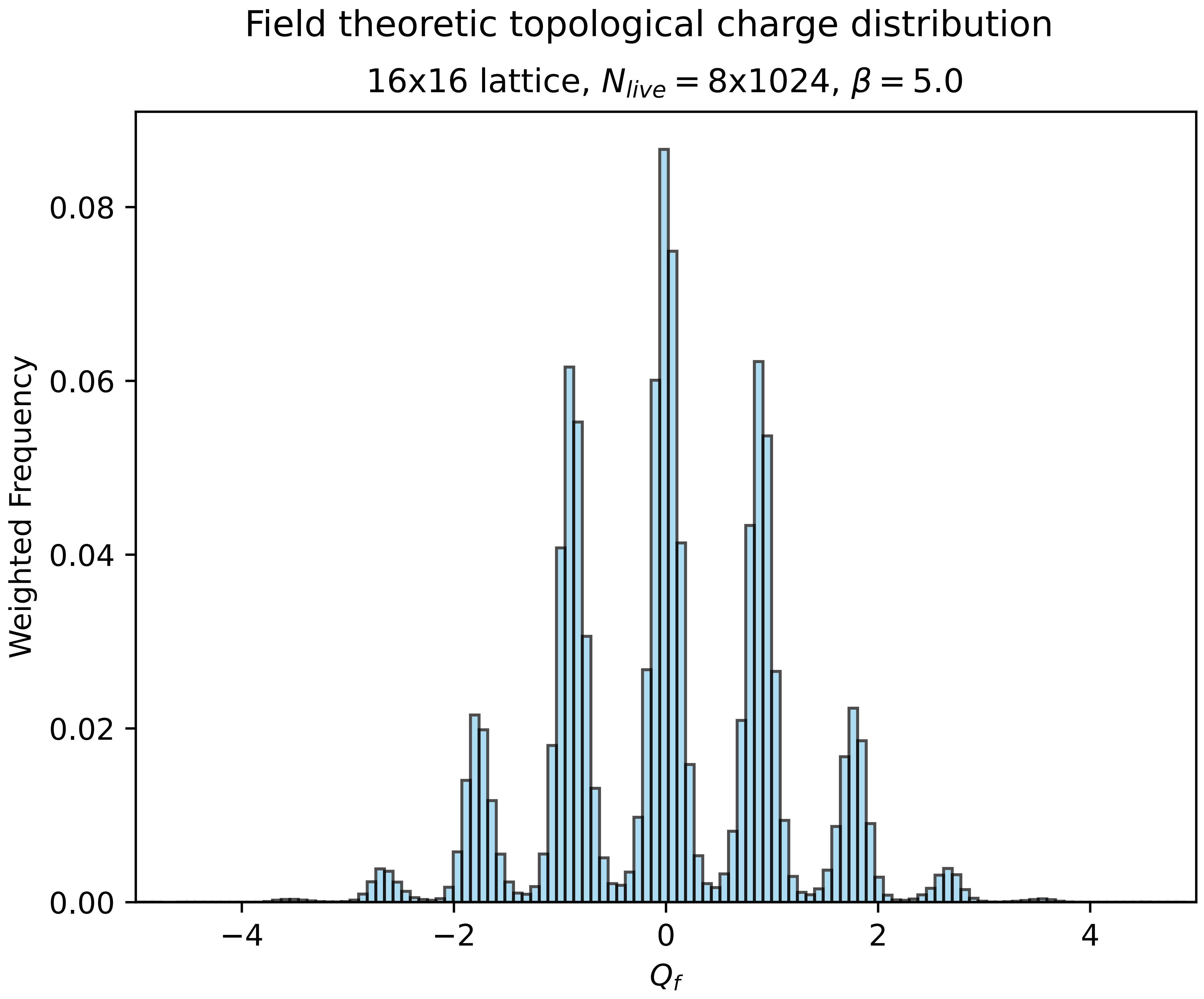
Plaquette value vs β

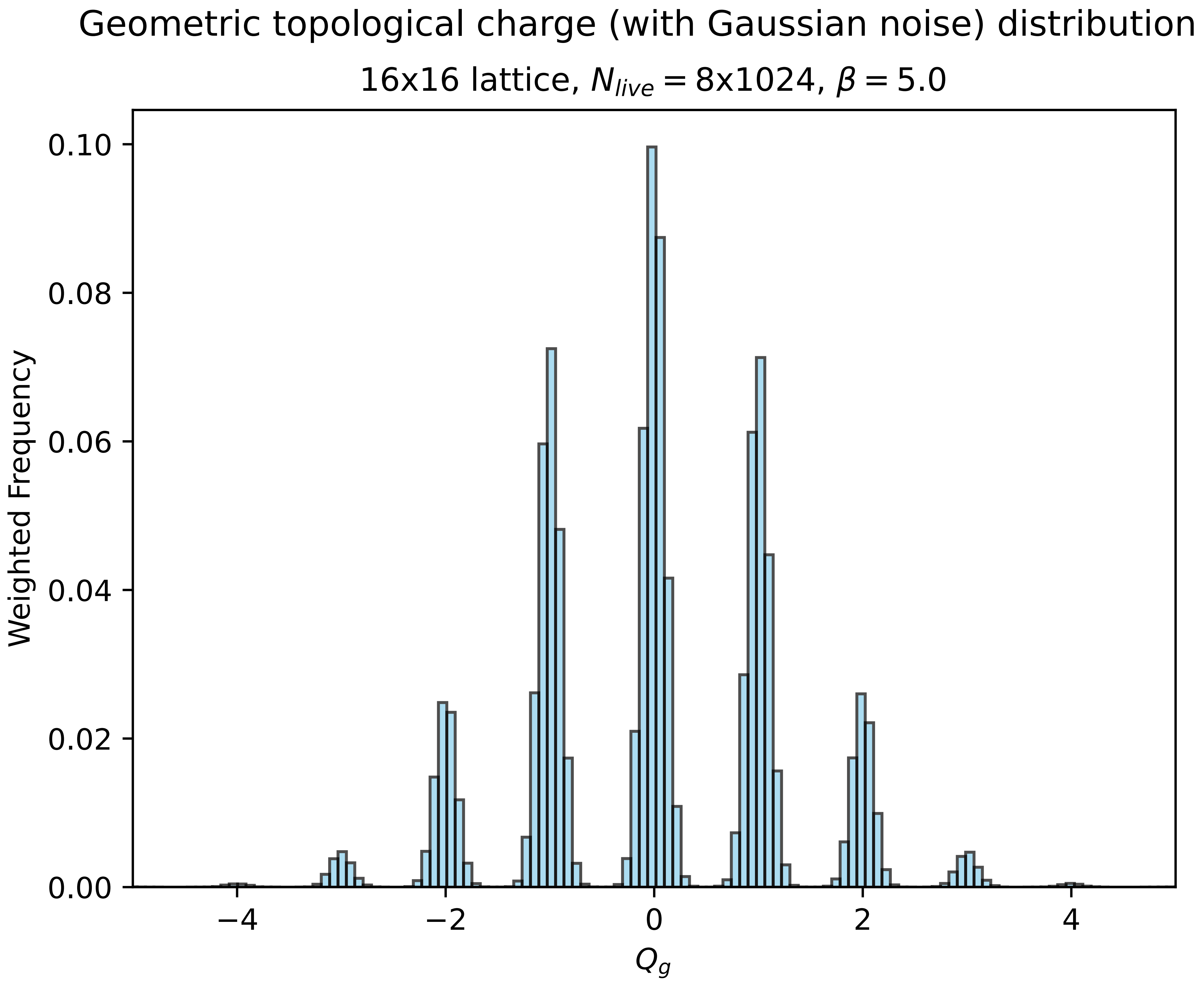


Topological charge with weights at $\beta = 5.0$

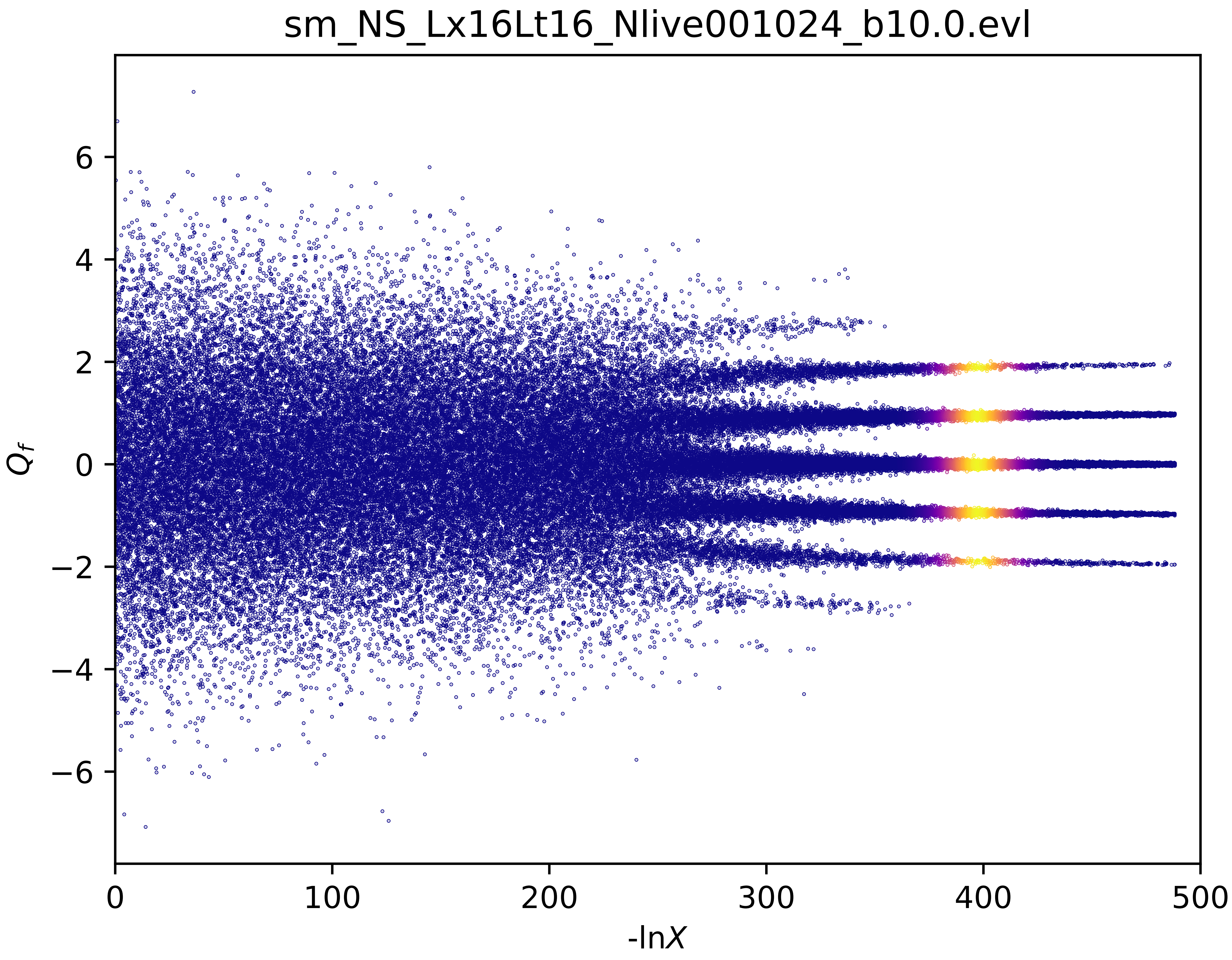


Topological charge distribution





Topological charge with weights at $\beta = 10.0$



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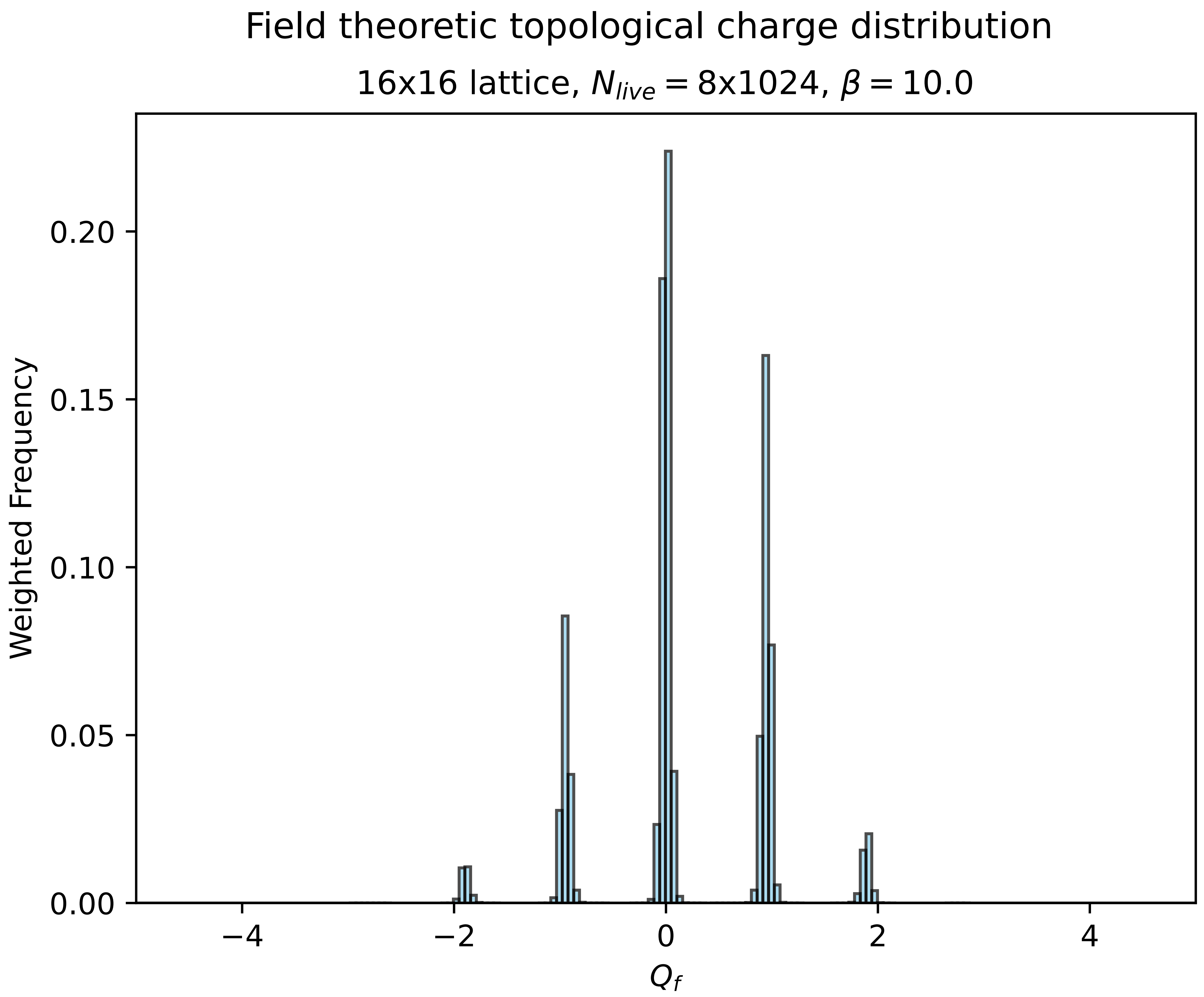
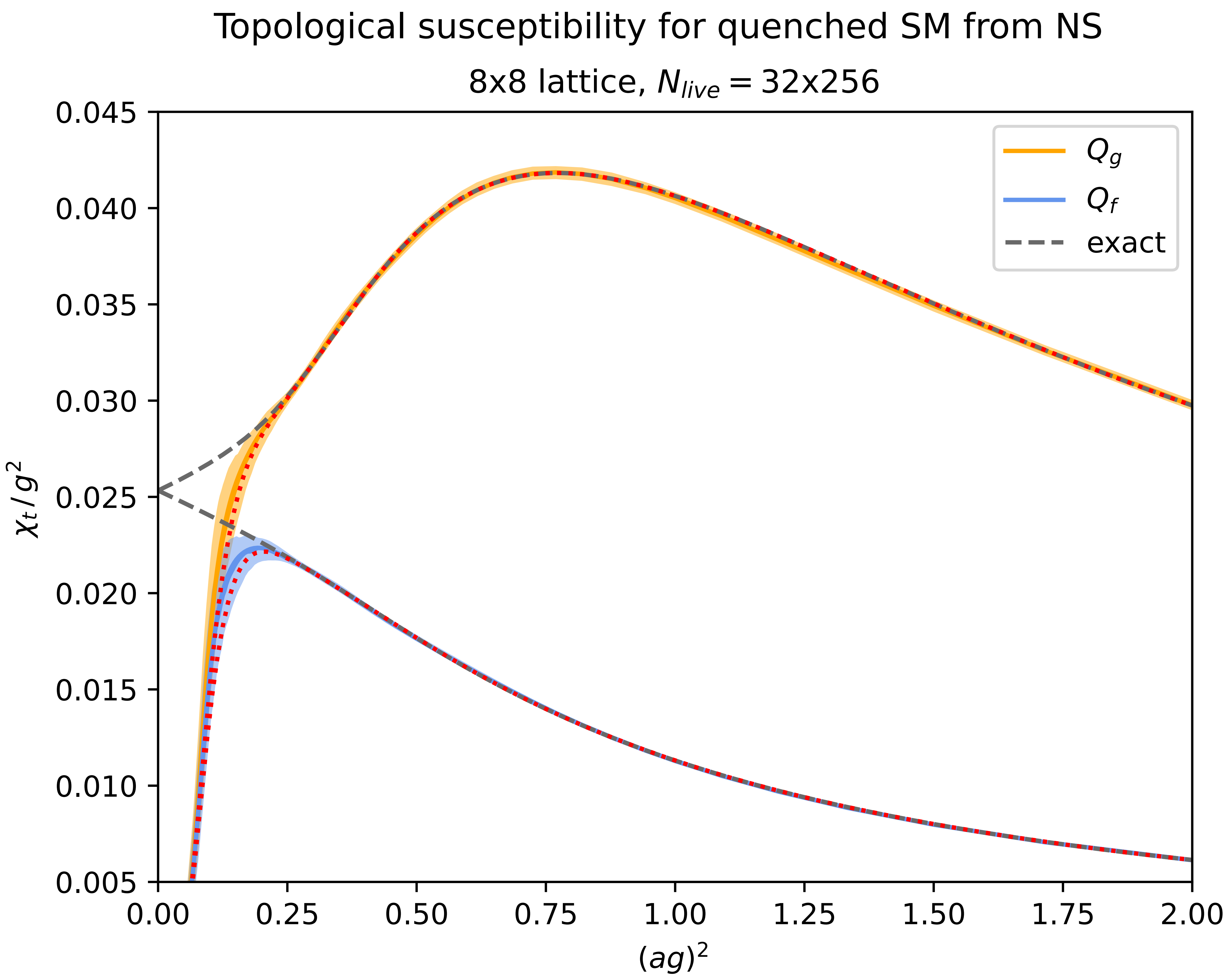
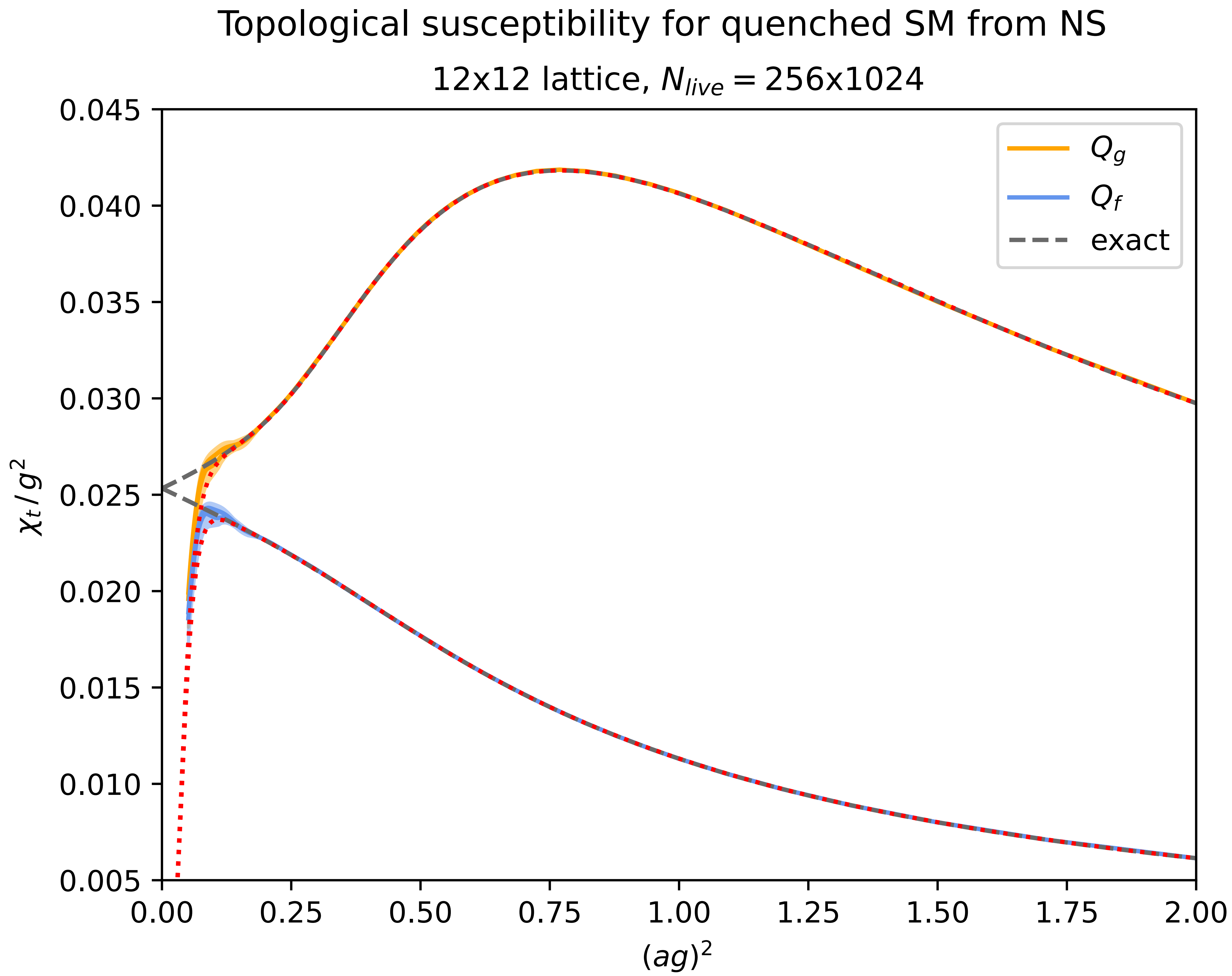


Topological susceptibility continuum limit





Summary

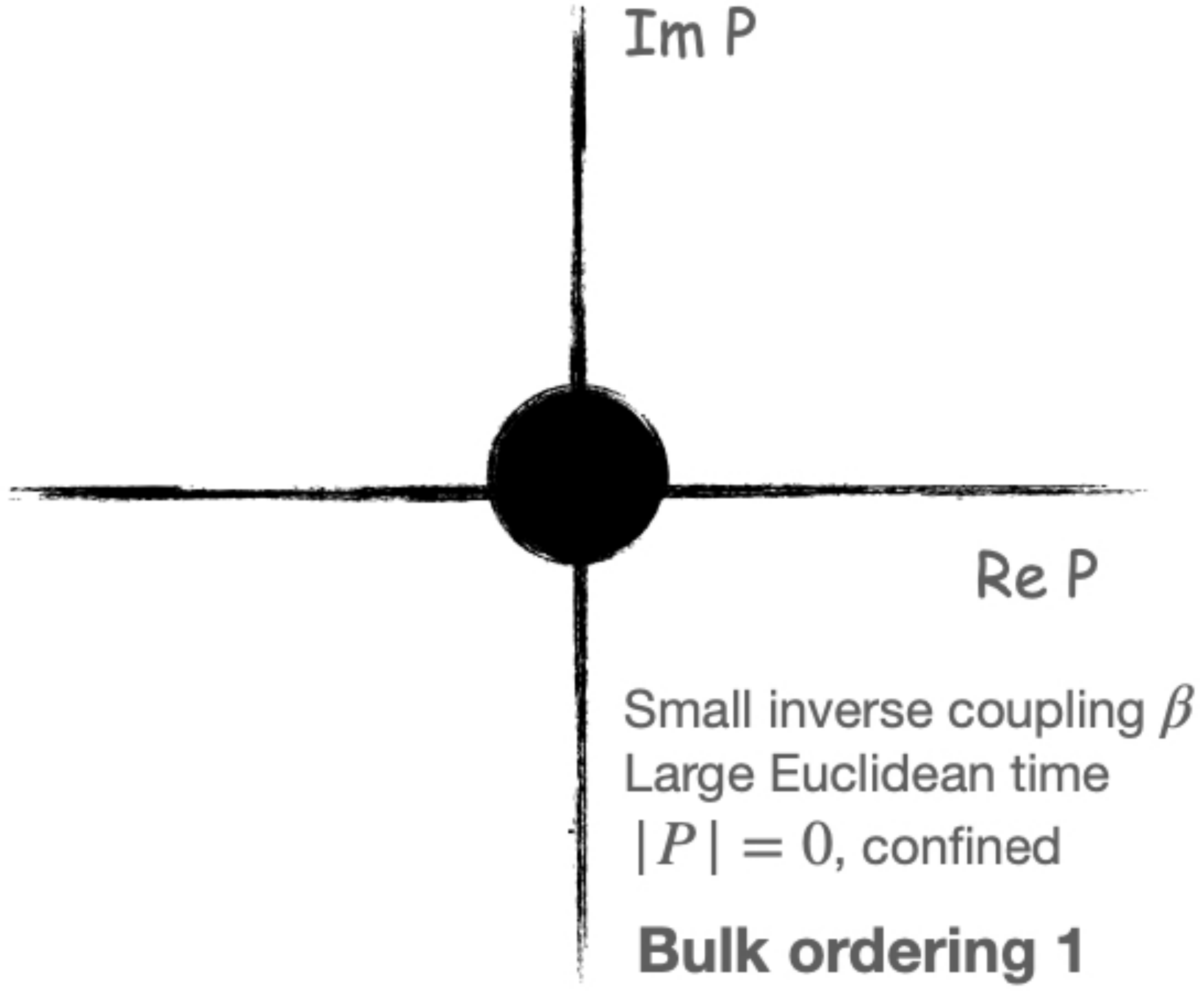
- Nested sampling has the potential to unfreeze topology
- Nested sampling parallelizes trivially
- Scaling with V needs to be investigated in detail

- Application to 1st order phase transitions

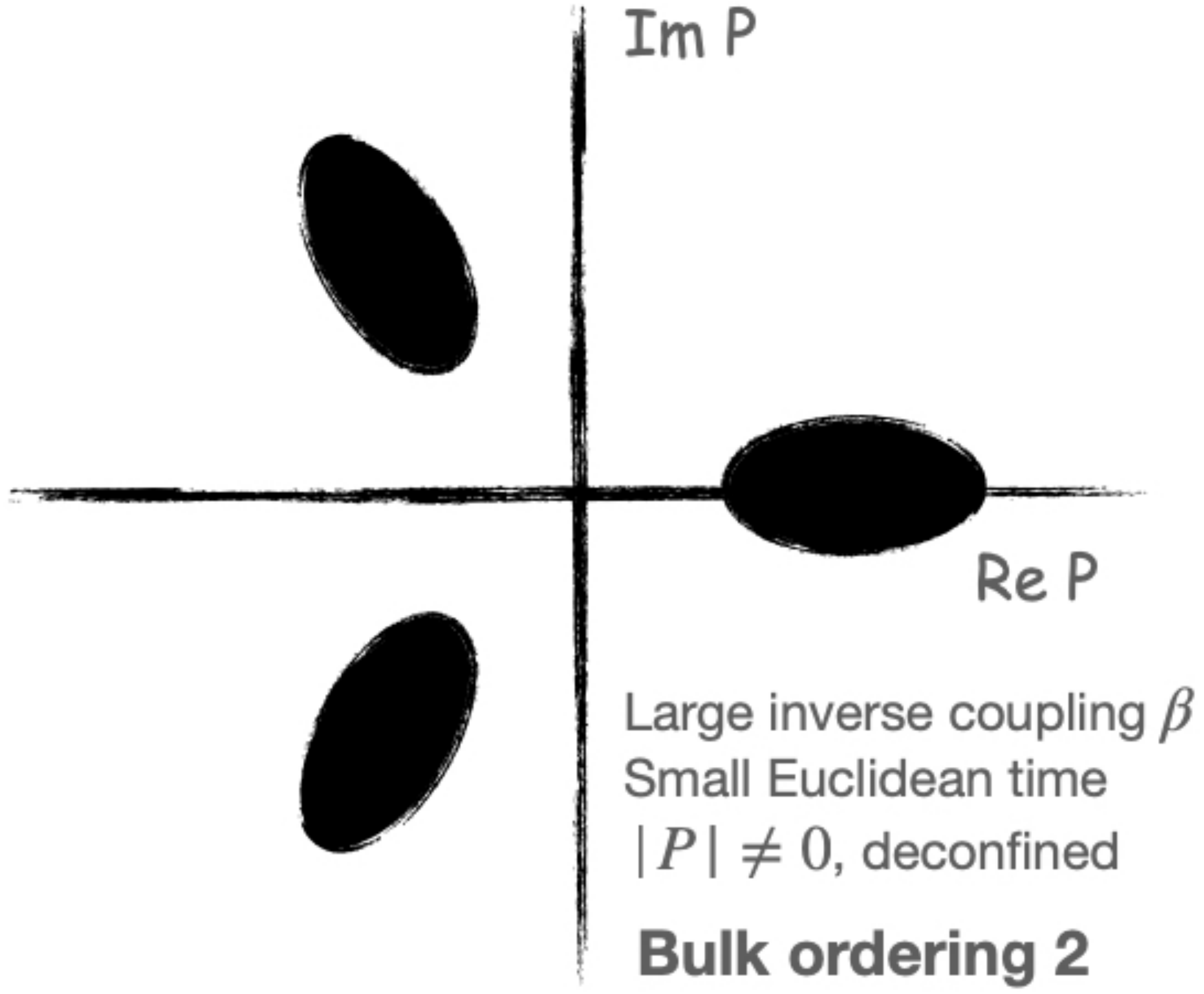
SU(3) confinement transition

First order phase transition ($N_c > 2$)

- **Bulk ordering 1:** Polyakov loops disordered
  Entropically favored, energetically disfavored
- **Bulk ordering 2:** Polyakov loops ordered
  Energetically favored, entropically disfavored



Study using thermodynamic lattices ($N_s^3 \times N_t$, $N_t < N_s$) with varying inverse coupling β



Various existing lattice results

- Standard MC
  Kajantie, et al. (1981)
  Çelik, et al. (1983)
  Gottlieb, et al. (1985)
  …
- Parallel tempering
  Borsanyi, et al. 2202.05234
- LLR method
  Lucini, et al. 2305.07463
- Shifted BCs

Nested sampling for SU(3)

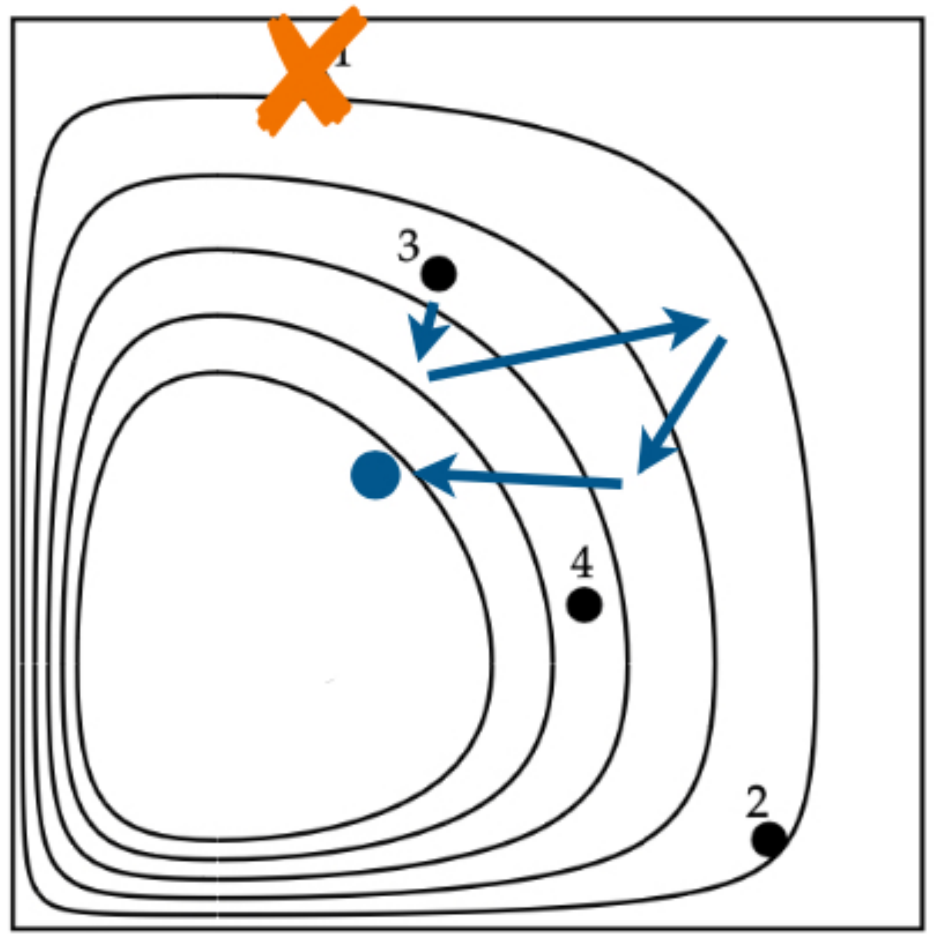
Executed 16 fully independent “streams”

- $N_{\text{live}} = 8192$ walkers for high-stats $L = 8$, $L_t = 4$ run
- $N_{\text{live}} = 256$ walkers for exploratory $L = 12$, $L_t = 4$ run
- Bootstrap over streams for Monte Carlo errors, compression errors still required

Constrained Monte Carlo $p(U) \propto \Theta(S^* - S(U))$

- Initialize each resampling step copying another walker in stream
- Local constrained Metropolis updates mix sufficiently well
- Constrained HMC also possible

Betancourt (2010) 1005.0157
Skilling (2012)



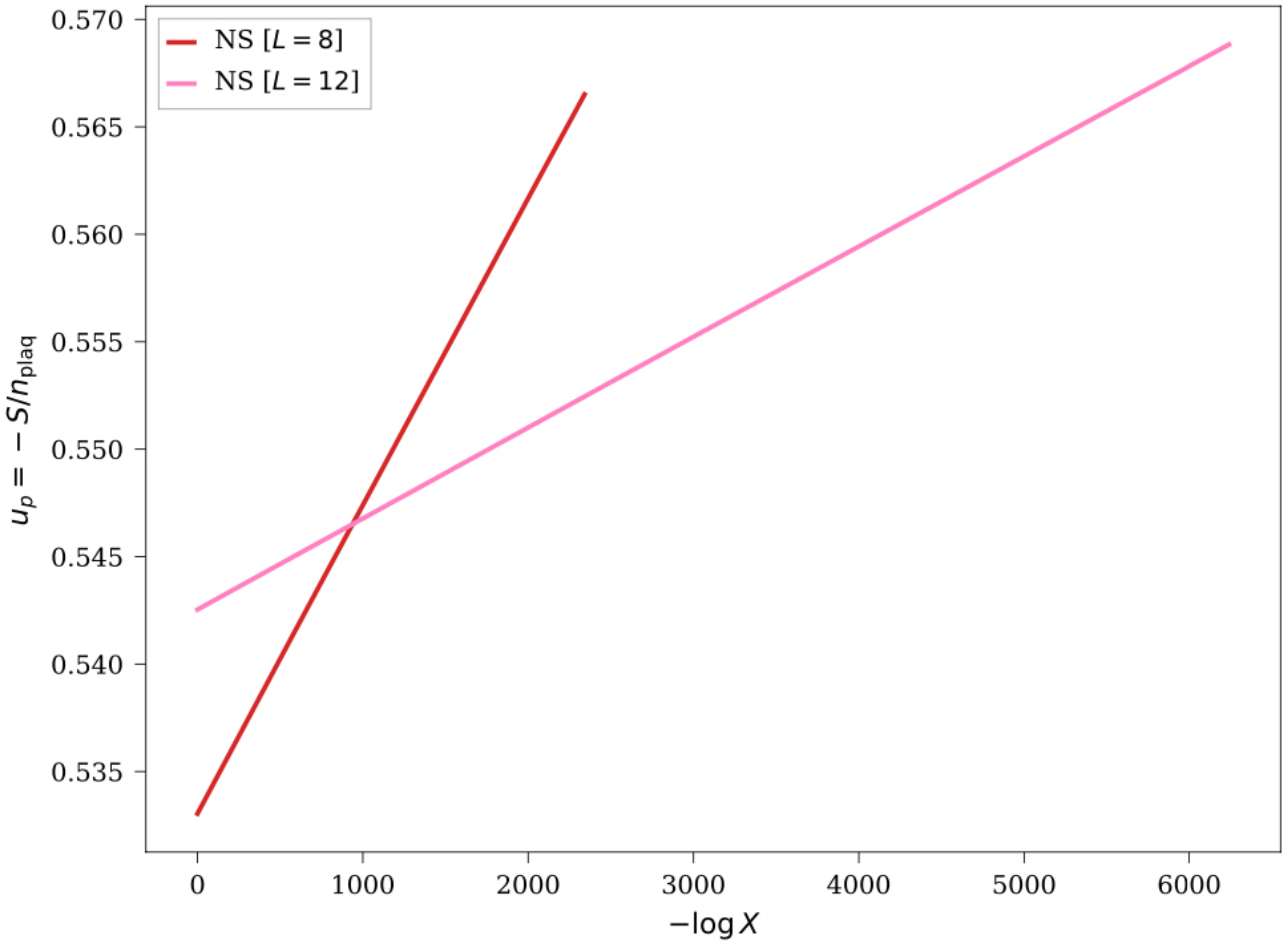
Configuration space

Results: Action vs phase space

- Smooth movement through action values

- Nearly linear vs $-\log X$

- MCMC appears to be performing well



Results: Polyakov evolution vs beta (L=8)

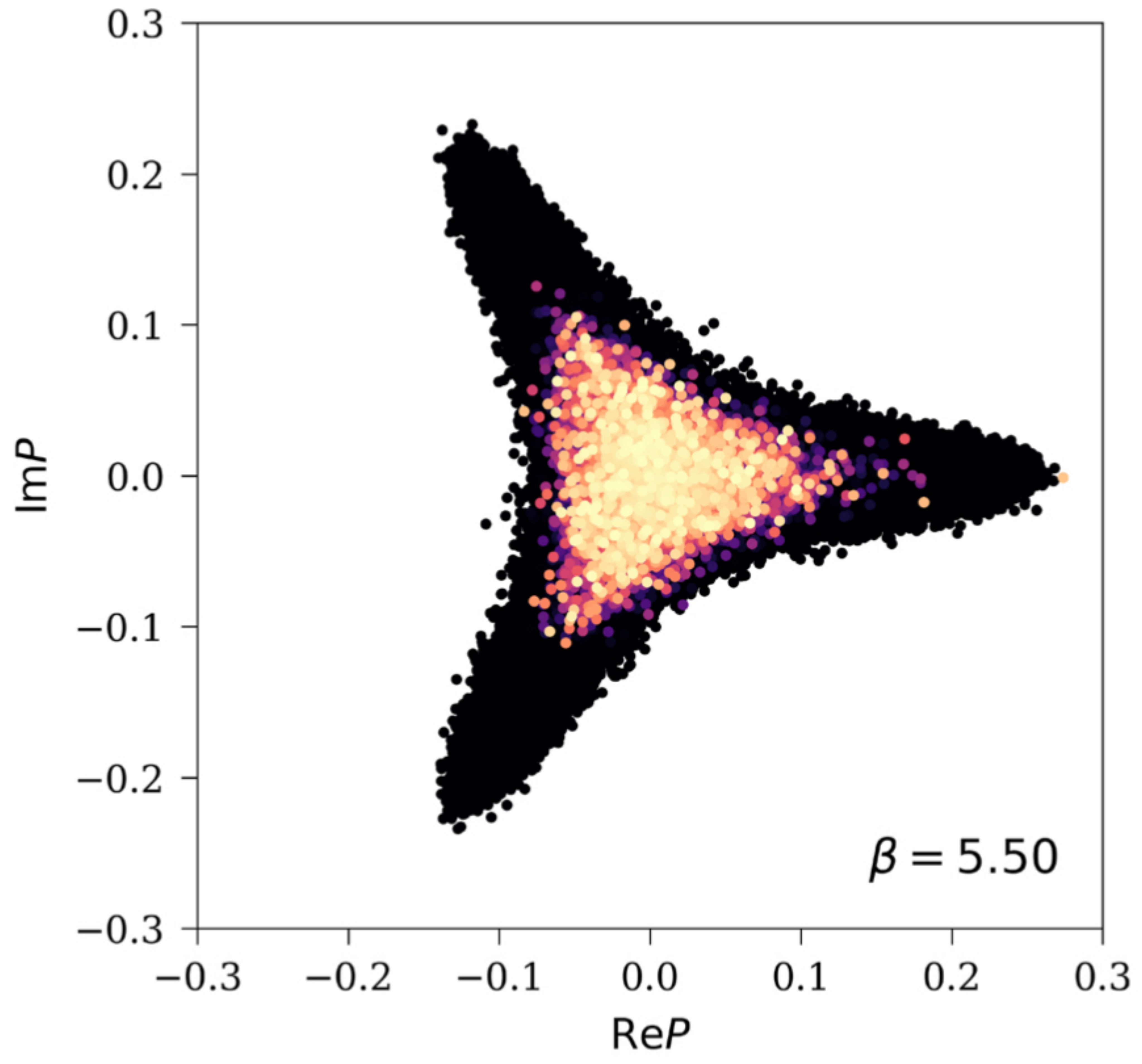
All measurements of P during NS run

Color based on weight in NS integral:

$$\langle O(\theta)\rangle_\beta = \frac{1}{Z(\beta)}\int_0^1 dX L(X)^\beta \langle O\rangle_{L(X)}$$

$$\downarrow$$

$$w_i \propto (X_{i+1} - X_i)e^{-\beta S_i}$$



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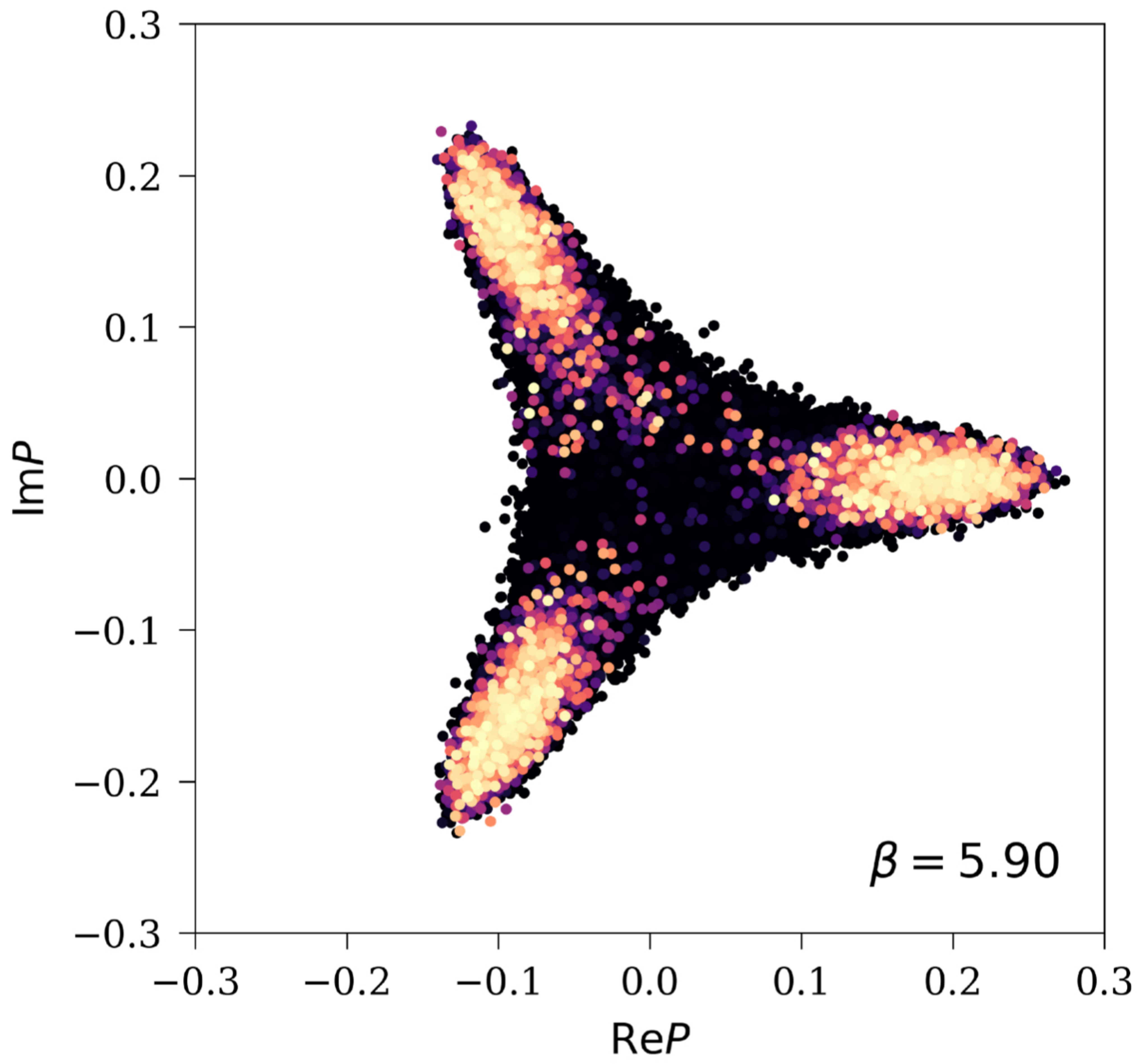

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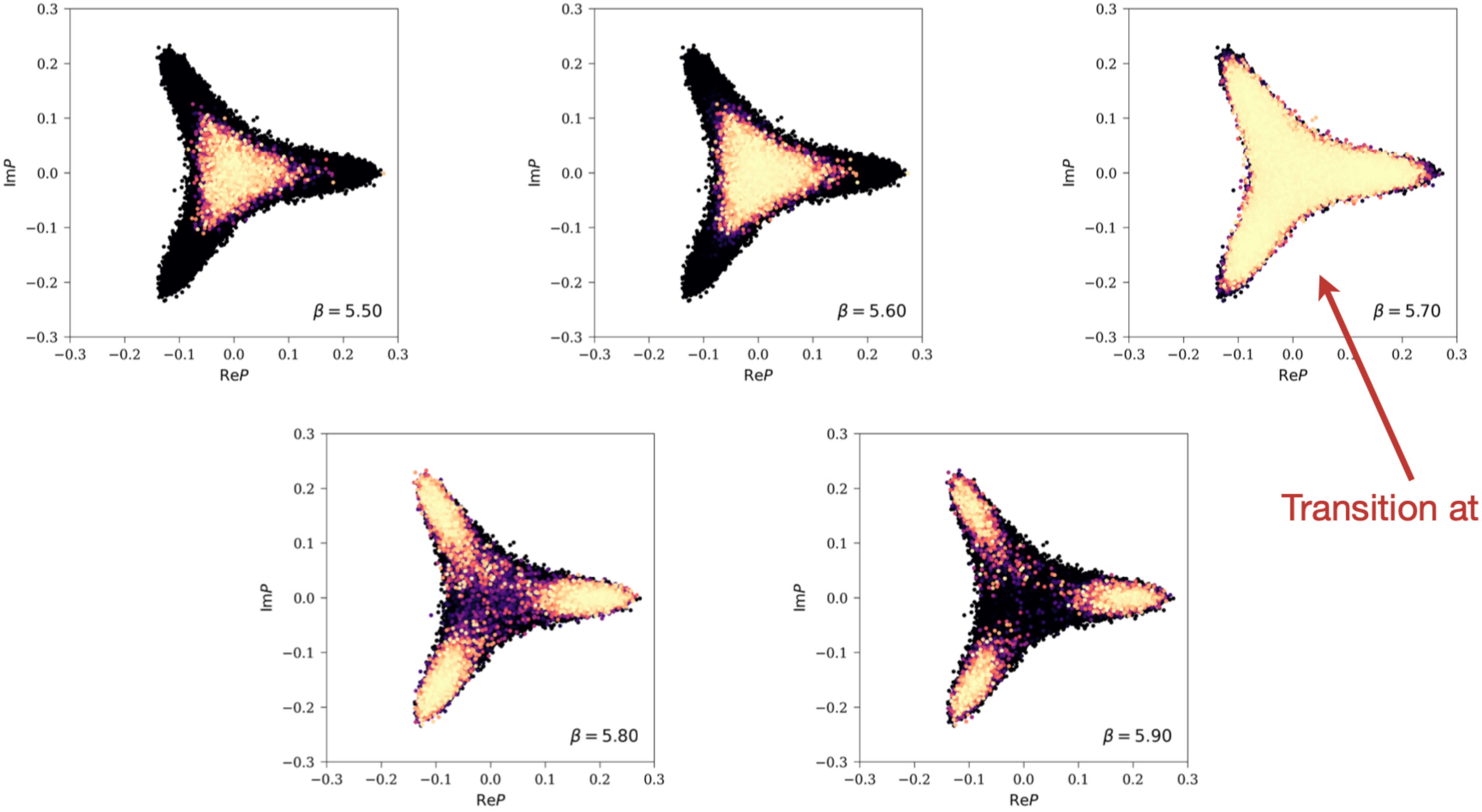
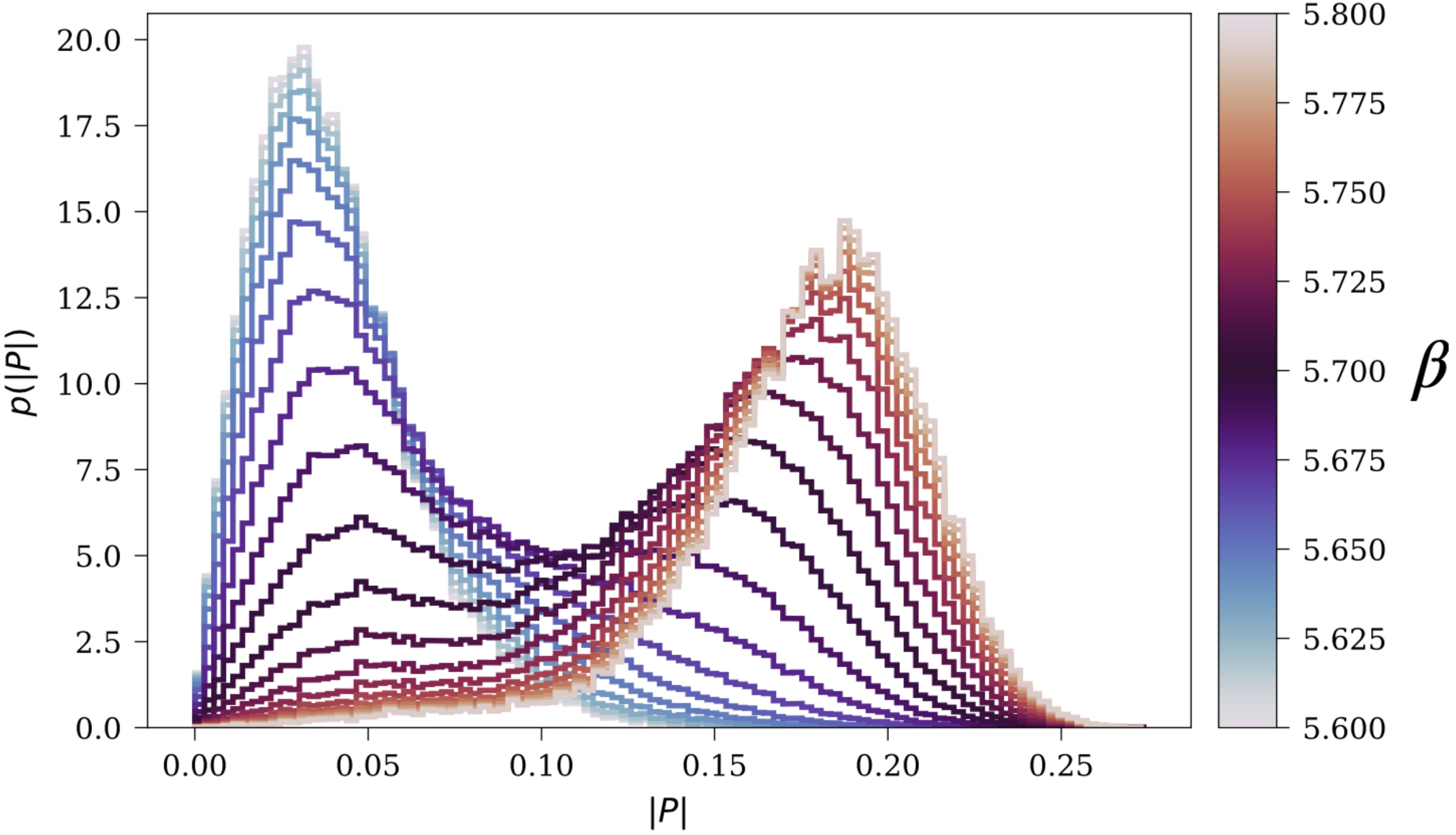


Transition at $\beta \approx 5.7$!

Results: Polyakov histograms (L=8)



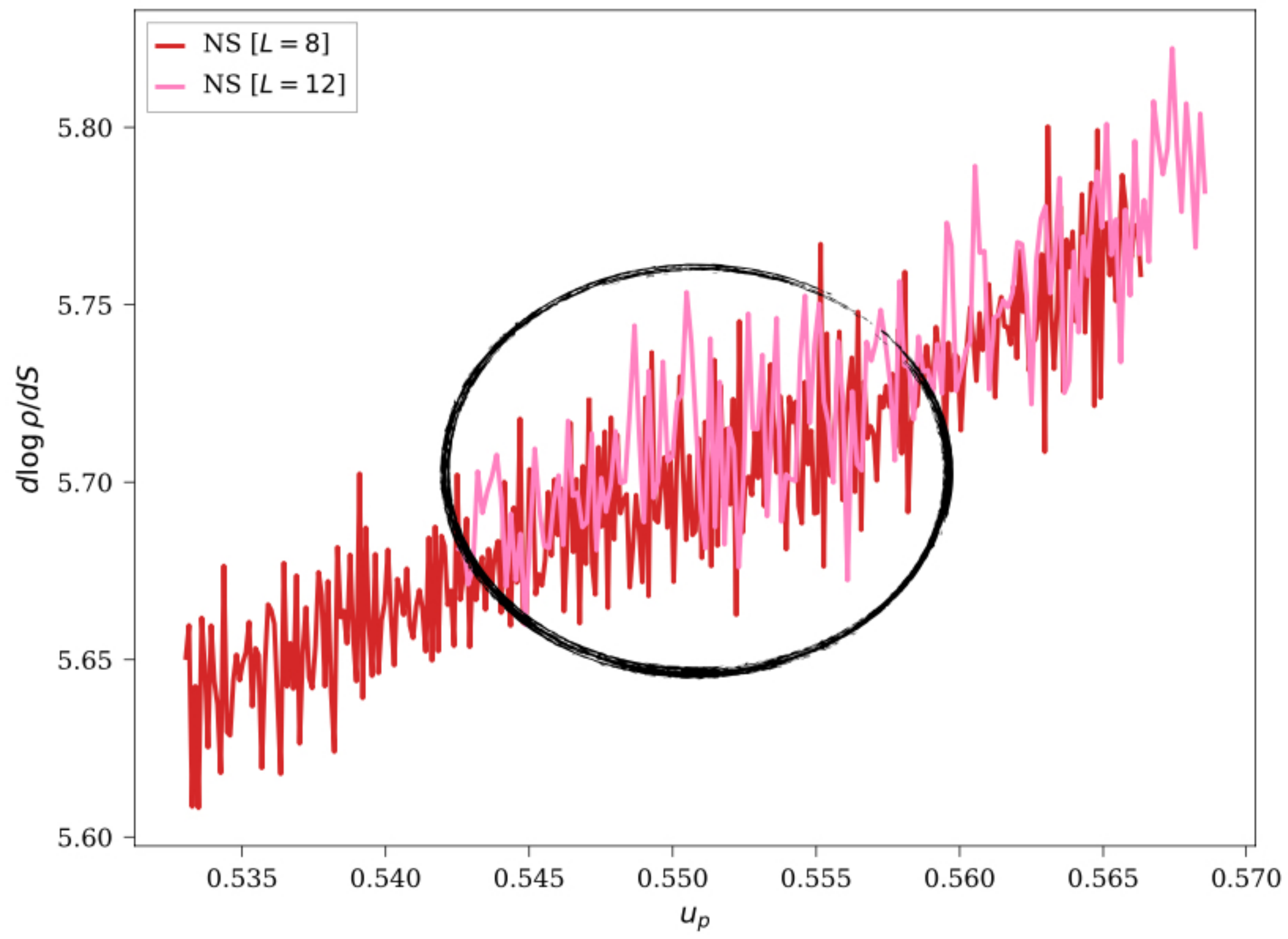
Results: Density of states

Density of states:

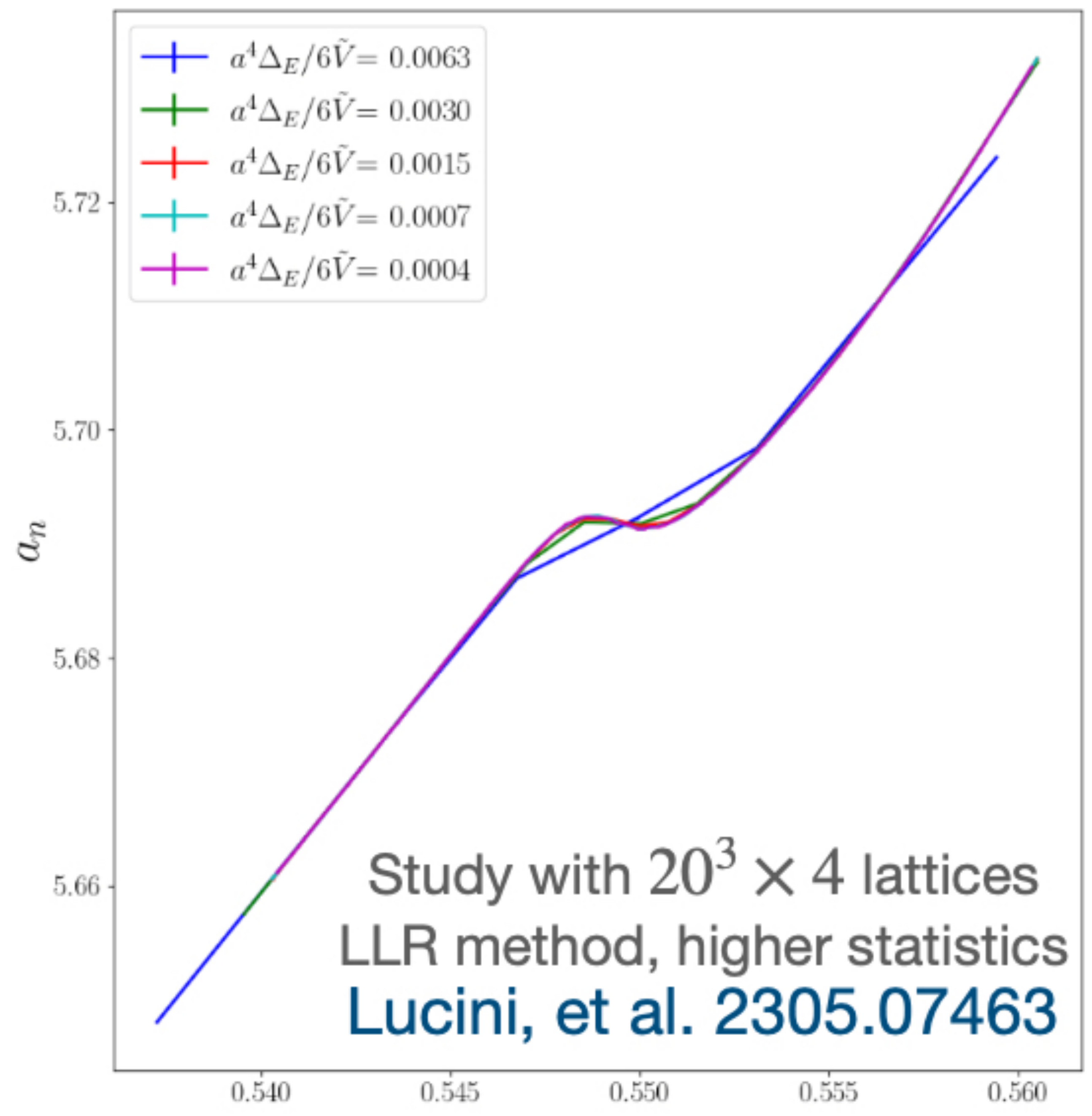
$$\rho(S) = \frac{dX}{dS} = -\frac{dX}{d\log L}$$

Microcanonical temperature:

$$\frac{1}{t} = \frac{d\log\rho}{dS}$$



$L \to$ large



Results: Density of states

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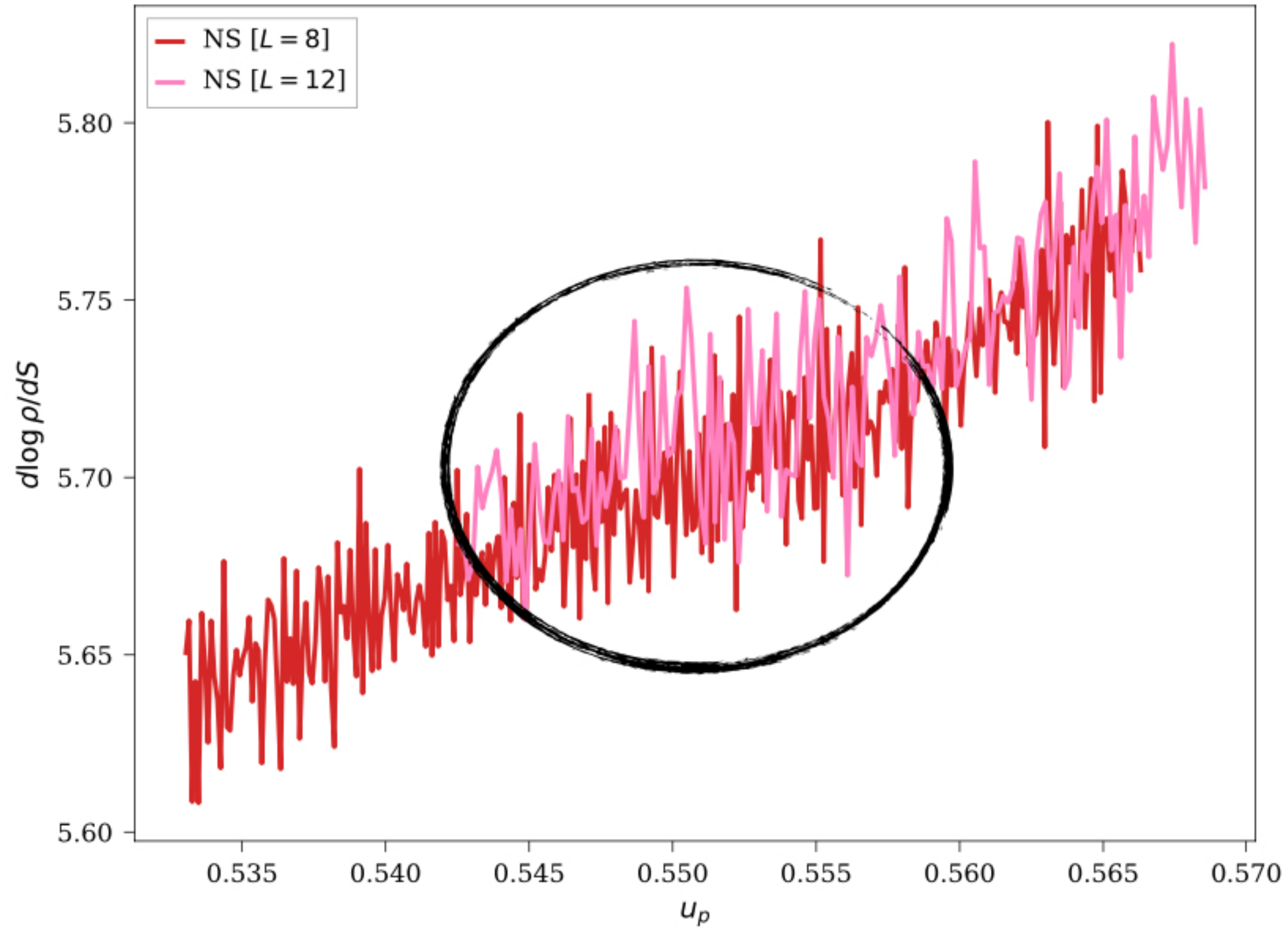
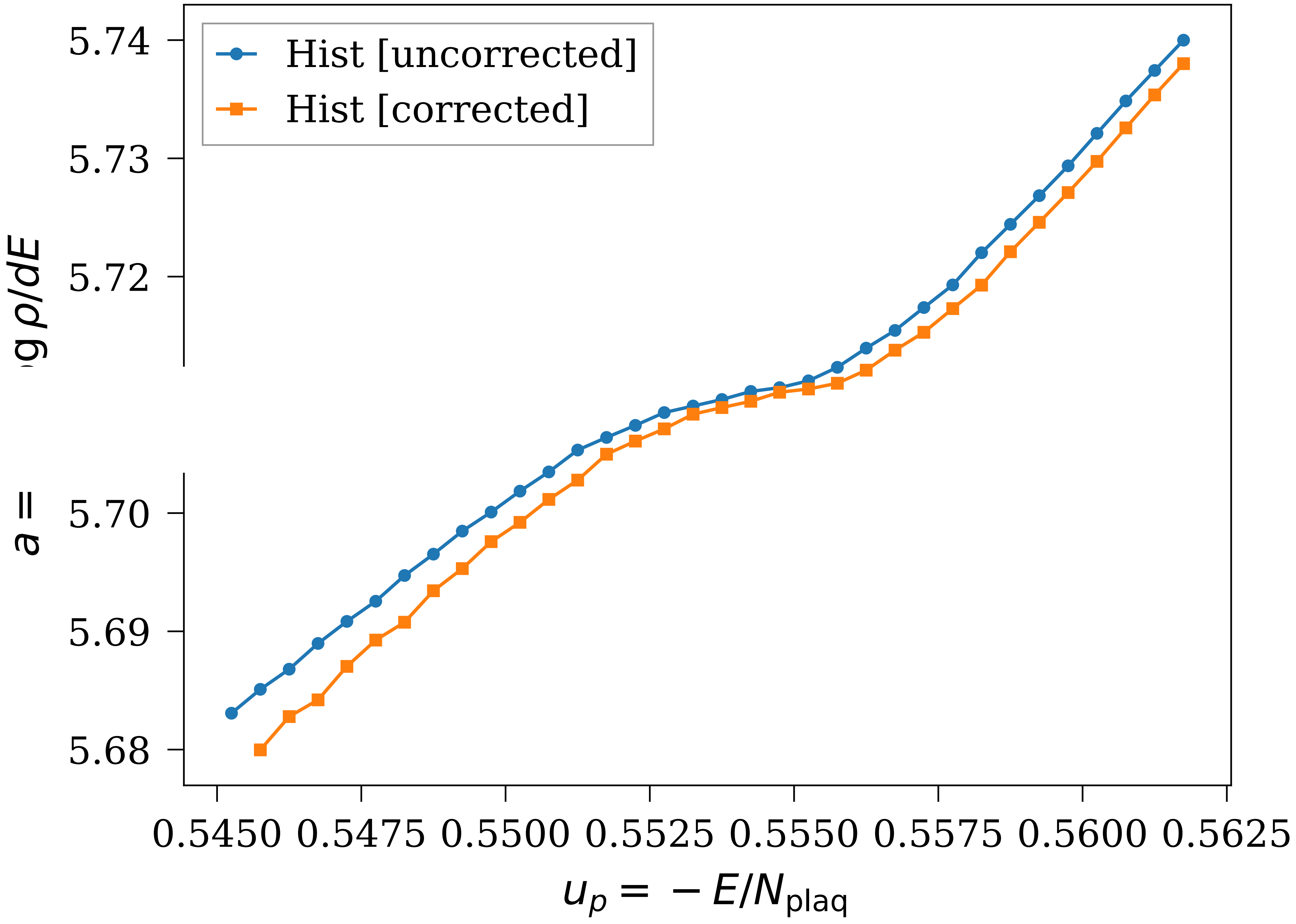
$$\rho(S) = \frac{dX}{dS} = -\frac{dX}{d\log L}$$

Improvement achieved using:

- modified prior $\pi(U) \sim \exp\{-\beta S[U]\}$ with $\beta \sim \beta_c$
- Savitsky-Golay filtering

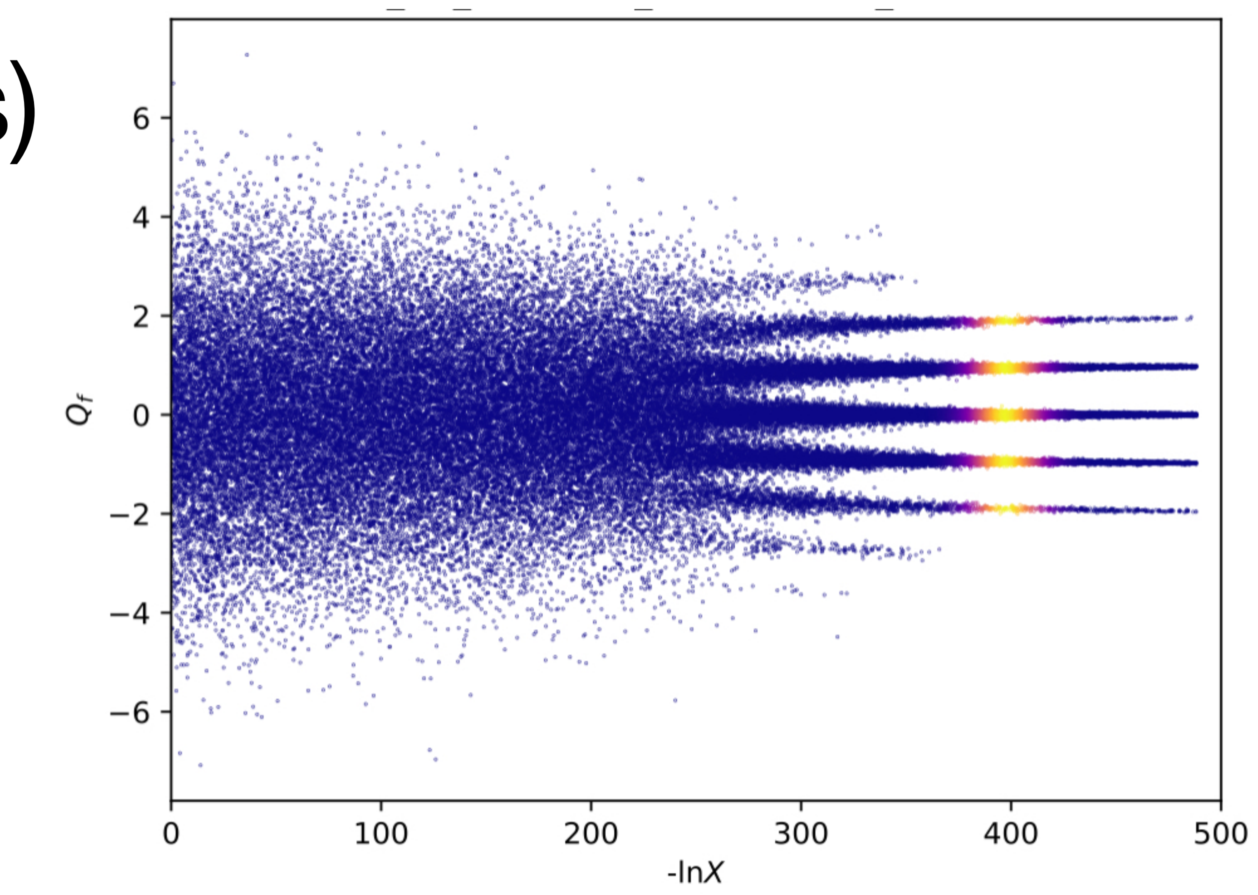




Conclusions

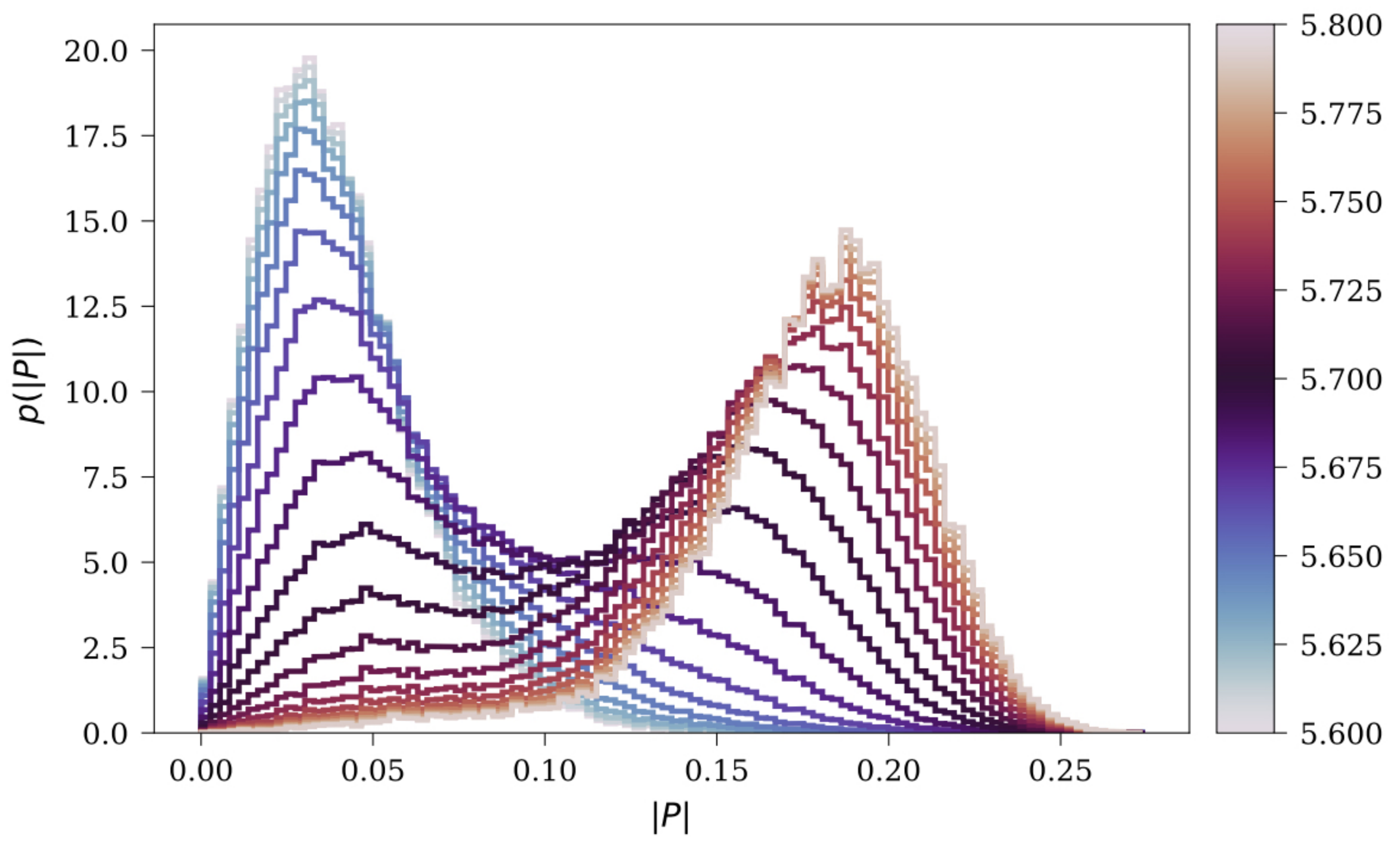
Nested sampling is a promising alternative Month Carlo method:

- very different sampling strategy (uniform within contours)
- it has the potential to unfreeze topology
- it can alleviate the suppression of
  tunnelling in 1st order PT
- it parallelizes trivially



Challenges and outlook:

- Scaling with V needs to be investigated
- inclusion of fermions

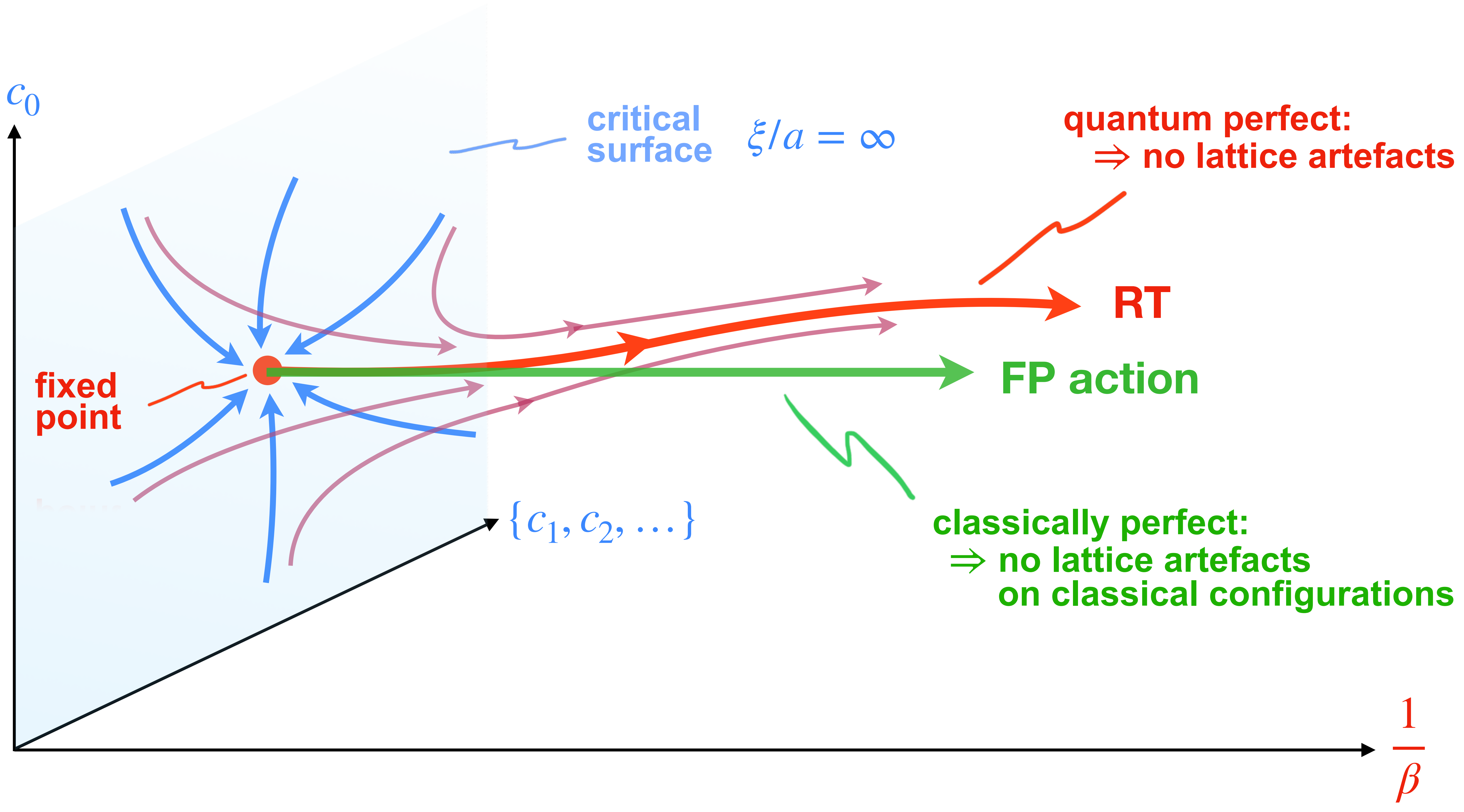


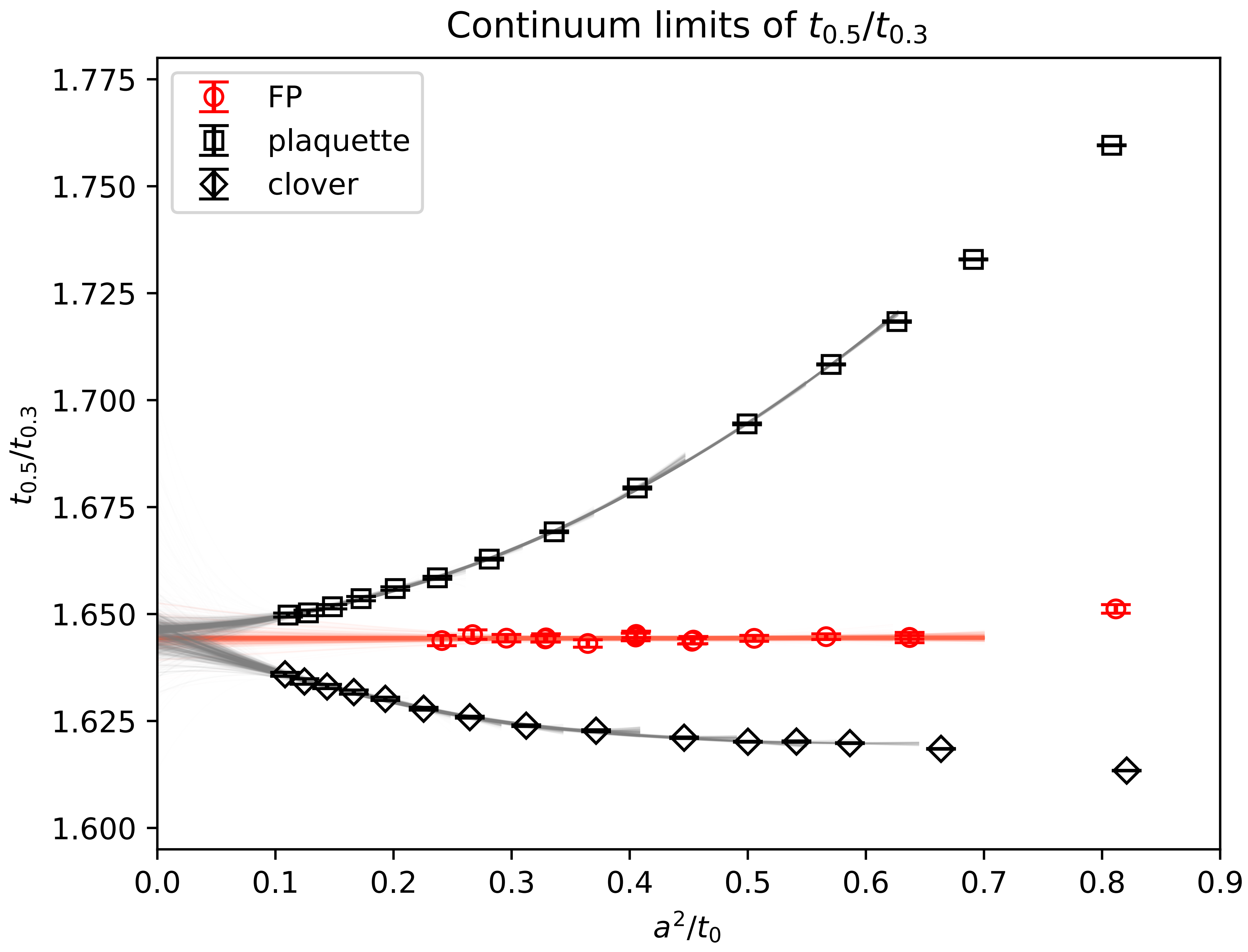
Alternative approach [Ipp, Müller, Holland, Wenger, 2401.06481 & 2501.XXXXX]

to avoid critical slowing and topological freezing

Use highly improved actions and simulate at coarse lattice spacing

$\Rightarrow$ physics informed flow (based on RG)





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Fakher Assaad (Würzburg)
Shailesh Chandrasekharan (Duke)
Jens Eisert (FU Berlin)
Lena Funcke (Bonn)
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SIGN 25
10th International Workshop on the sign problem in QCD and beyond
20-24 January 2025
AEC Bern, Switzerland
Registration deadline: 15 December
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