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Nesting sampling: SU(3) confinement transition

Gurtej Kanwar
University of Bern

In collaboration with:
Simone Romiti & Urs Wenger

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Motivation

Nested Sampling is a **particle Monte Carlo method**
to estimate the **action vs phase space** curve of a theory.

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

good for phase transitions

- Cheaper/easier Monte Carlo steps

constrained uniform instead of weighted sampling

- May alleviate topological freezing
- Easily parallelized

benefits of being a particle sampler

Skilling (2004) “Nested sampling”
Skilling (2006) “Nested sampling for general Bayesian computation”

Nested sampling

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Nested sampling

Estimate phase space X within contours of constant likelihood $L = e^{-S}$

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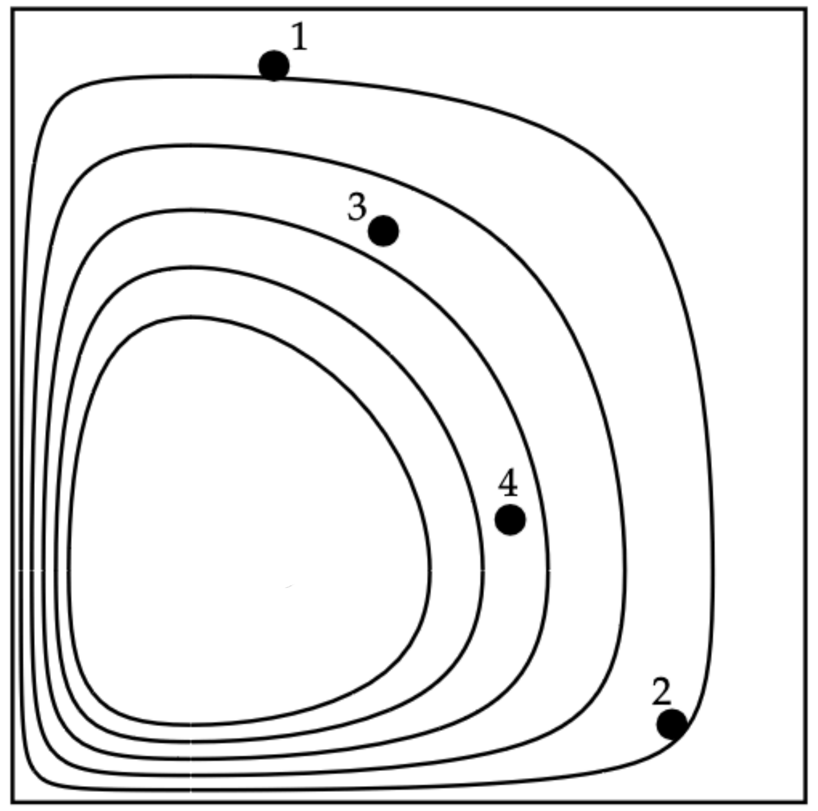

Configuration space

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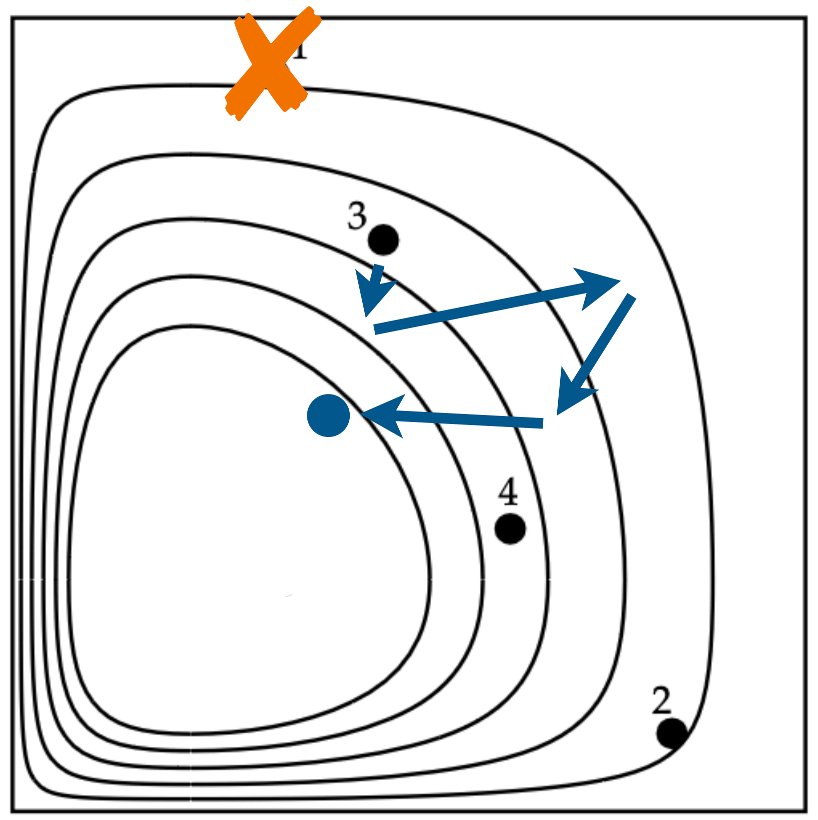

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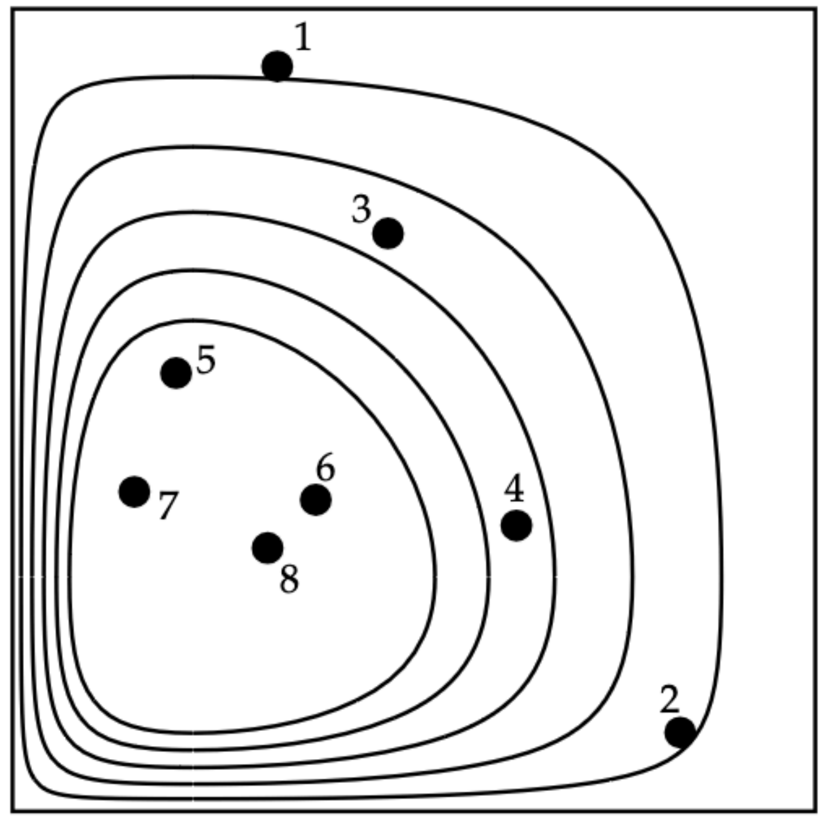
- Step i: **record** largest action S_i, **drop** this sample, **resample** uniformly within $S < S_i$
- Analysis: **Compression factor** X_{i+1}/X_i follows a Beta distribution
  bootstrap or central value to build $L(X)$ curve

$$t \equiv X_{i+1}/X_i \in [0,1]$$
$$p(t) \propto t^{N_{\text{live}}-1}$$



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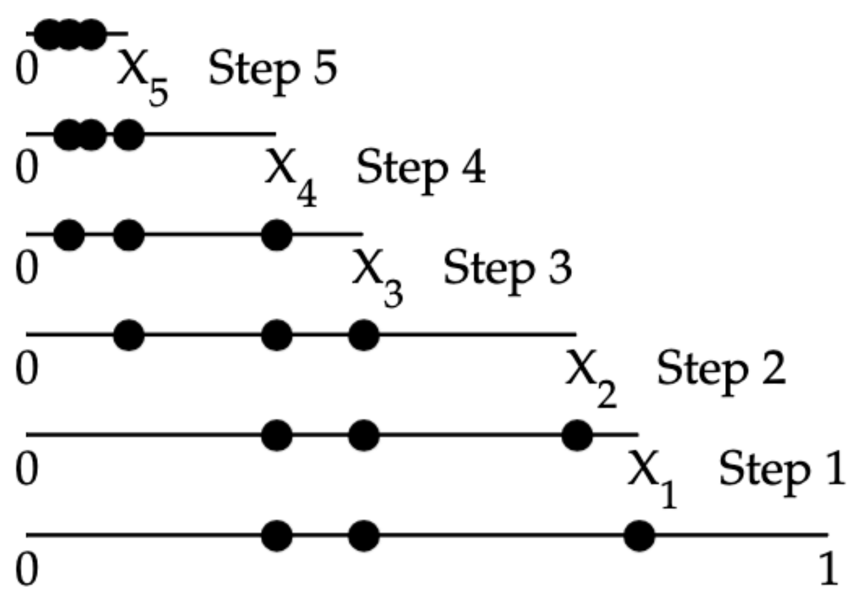

Enclosed phase space X

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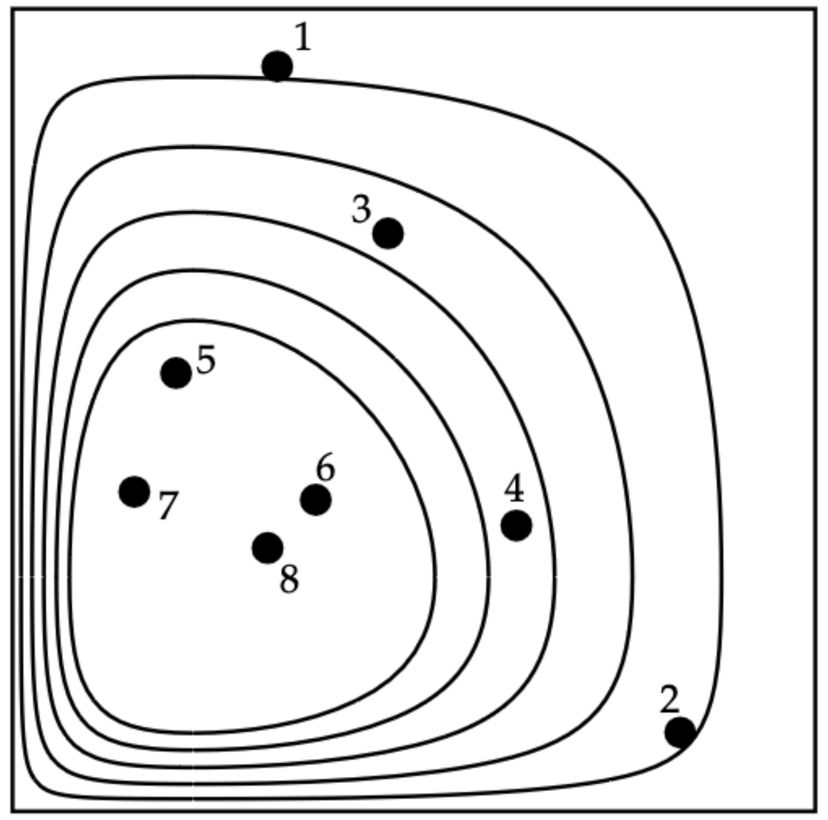

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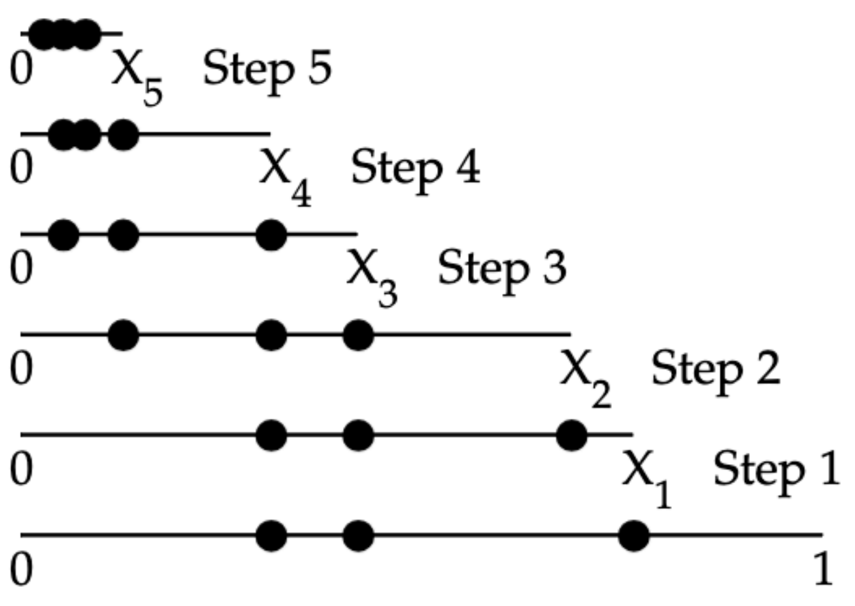

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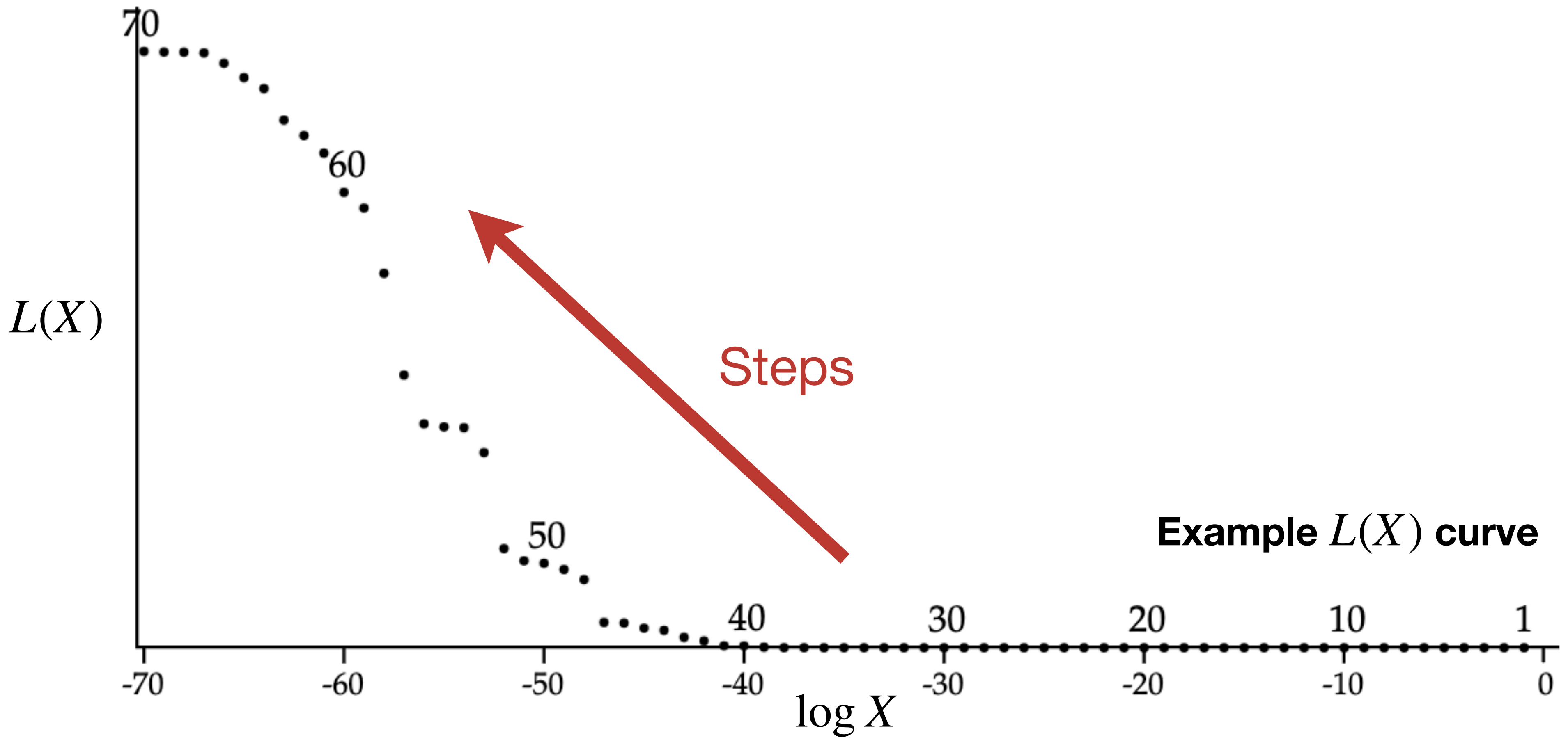

Example $L(X)$ curve

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Nested sampling

Estimate phase space X within contours of constant likelihood $L = e^{-S}$

- Partition function and observables at multiple choices of β

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

  - Relevant region of L (and X) depends on β See previous talks by S. Romiti, U. Wenger

- Density of states $\rho(S) = \dfrac{dX}{dS} = -\dfrac{dX}{d\log L}$

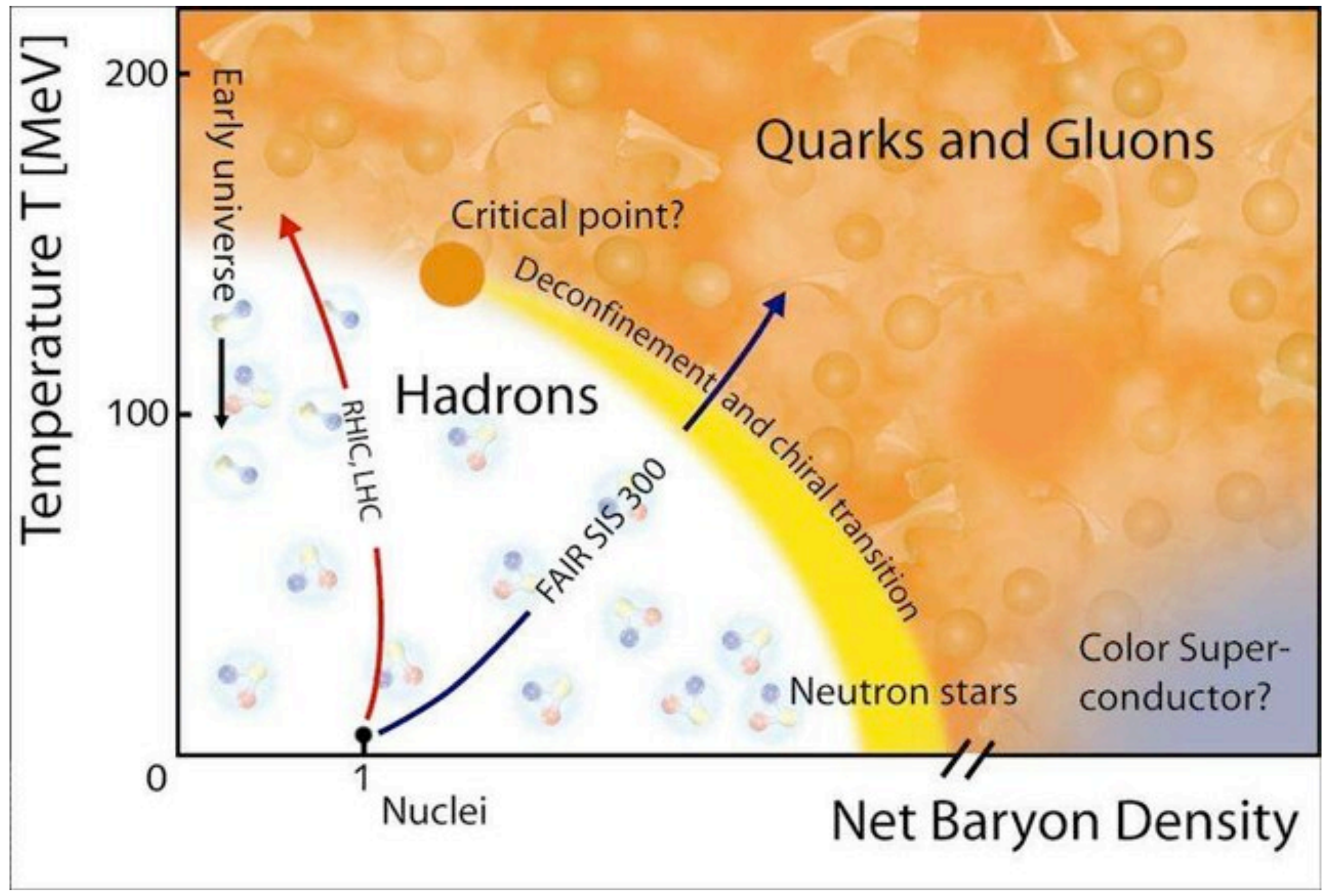
  - Universal function independent of β

- Useful to restrict sampling to important regions to improve statistics

SU(3) confinement transition

Aarts, et al. 1412.0847

First-order transition in full QCD



Center symmetry

Rotate temporal links on one timeslice by $z = e^{2\pi i k/3} \in \mathbb{Z}_3$

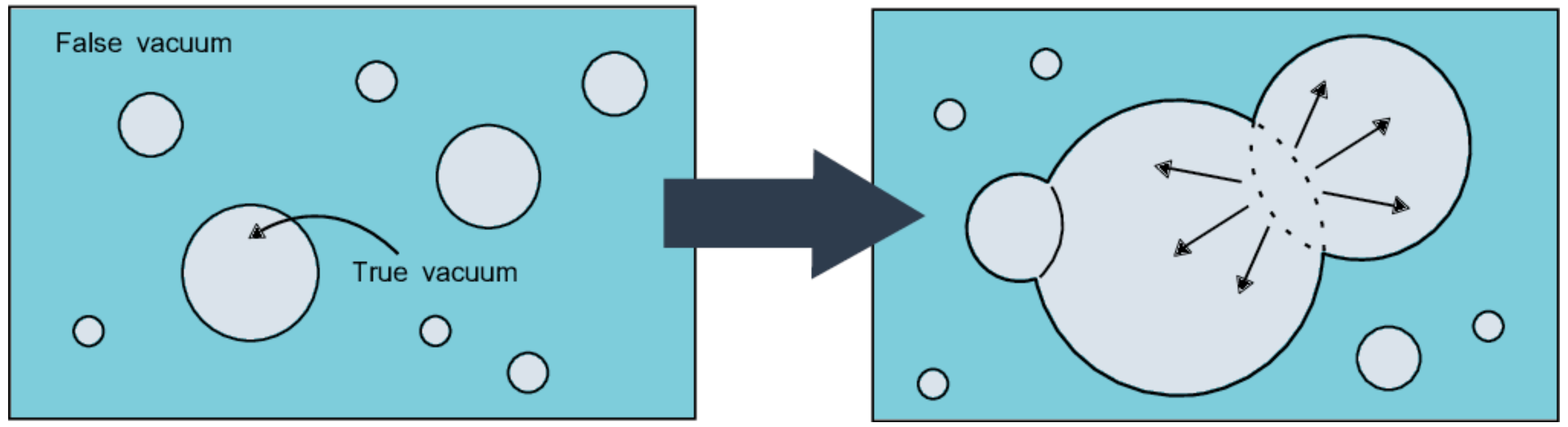
Polyakov loop is a good order param

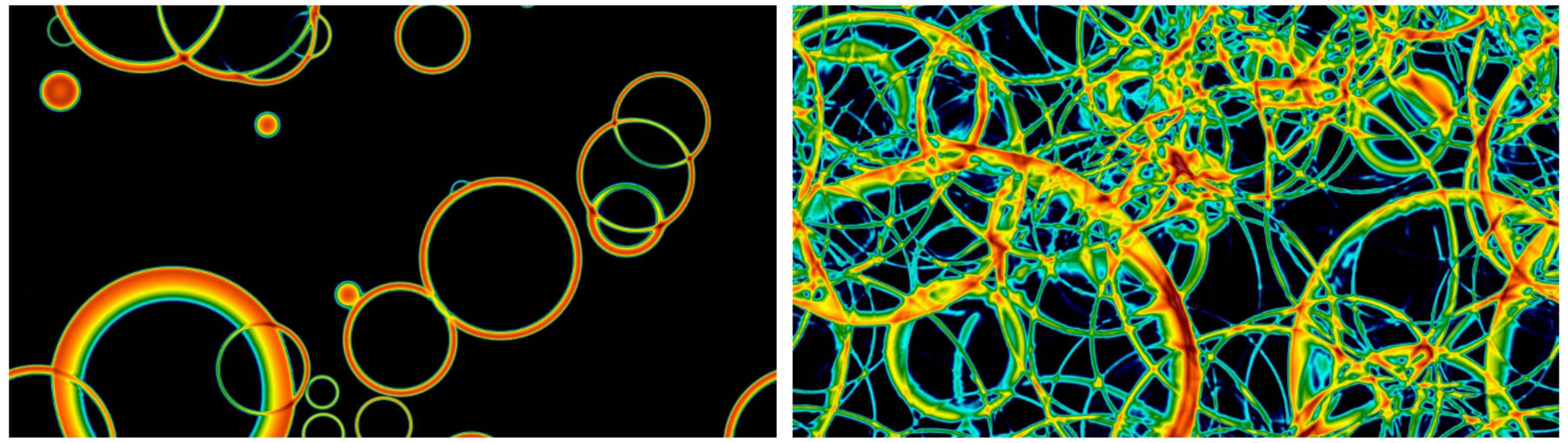
$$\ell(\vec{x}) \equiv \frac{1}{N_c}\mathrm{Tr}[\prod_t U_0(\vec{x},t)] \longrightarrow P \equiv \frac{1}{N_s^3}\sum_{\vec{x}} \ell(\vec{x})$$

Confined phase:
$|P| = 0$

1st order transition

Deconfined phase:
$|P| \neq 0, P \propto \{1, z, z^2\}$





First-order transition generating bubble dynamics in the early universe

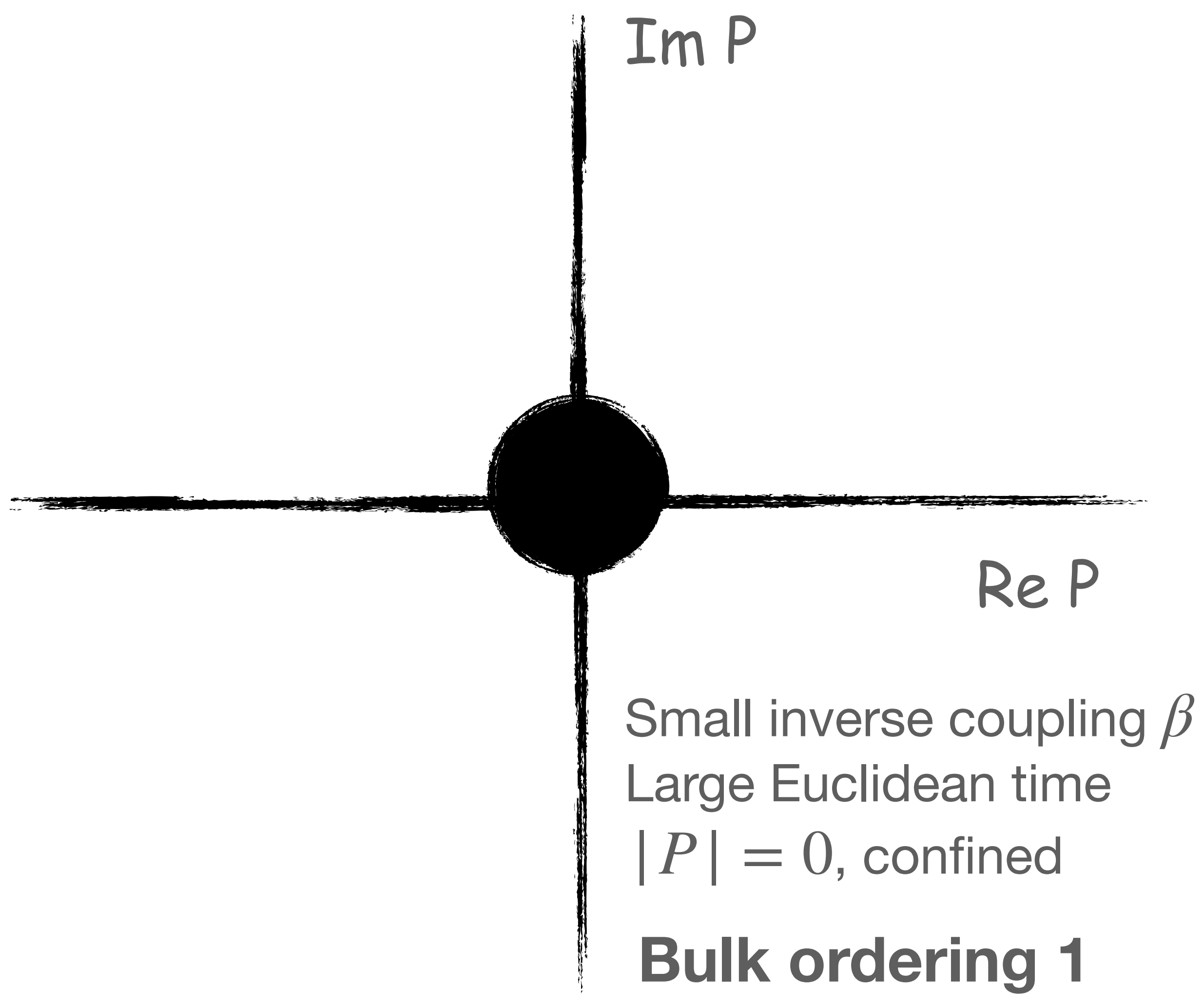
D. Weir (2023) 1705.01783

SU(3) confinement transition

First order phase transition ($N_c > 2$)

- **Bulk ordering 1:** Polyakov loops disordered
  Entropically favored, **energetically** disfavored

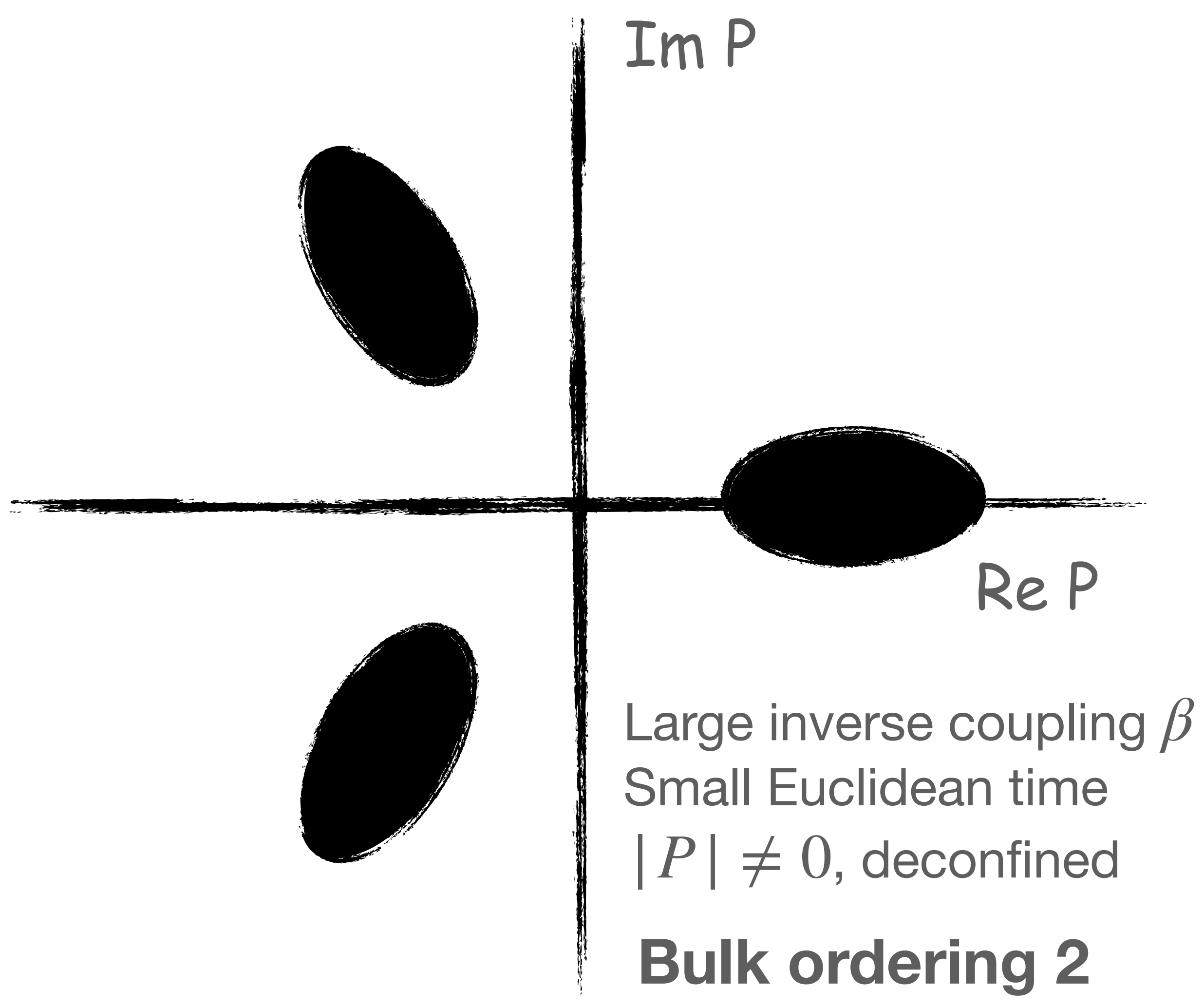
- **Bulk ordering 2:** Polyakov loops ordered
  Energetically favored, **entropically** disfavored



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
  Wed 12:15 D. Mason
- Shifted BCs
  Fri 14:15 L. Virzi



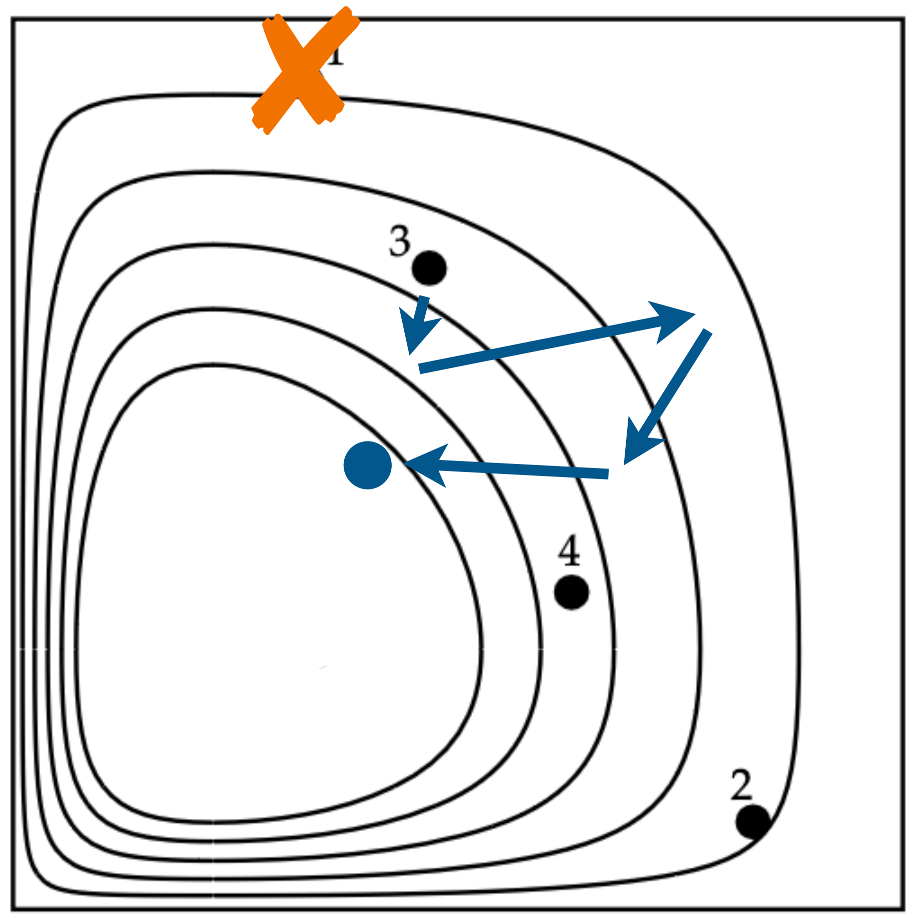
Nested sampling for SU(3)

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)



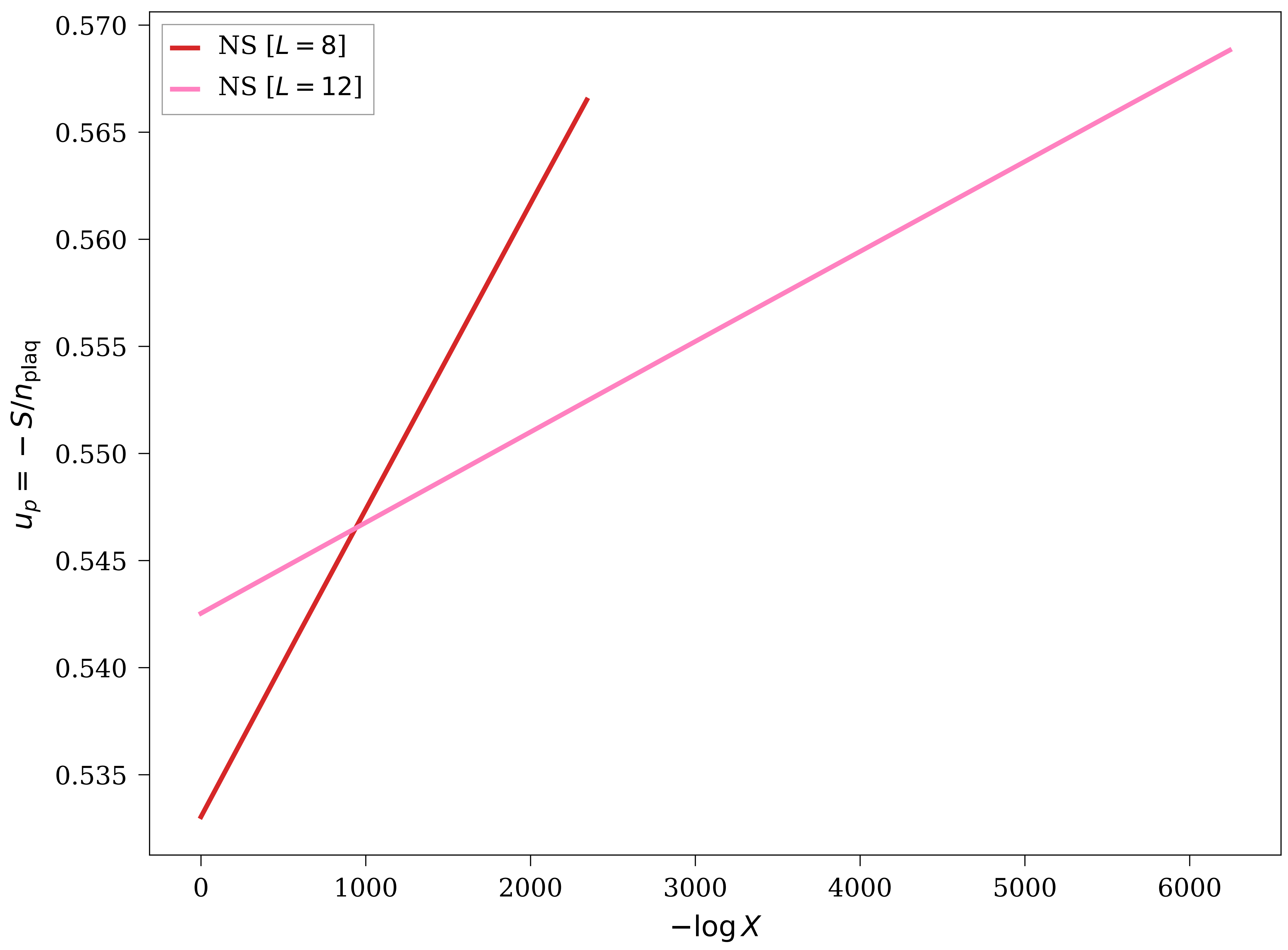
Configuration space

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)

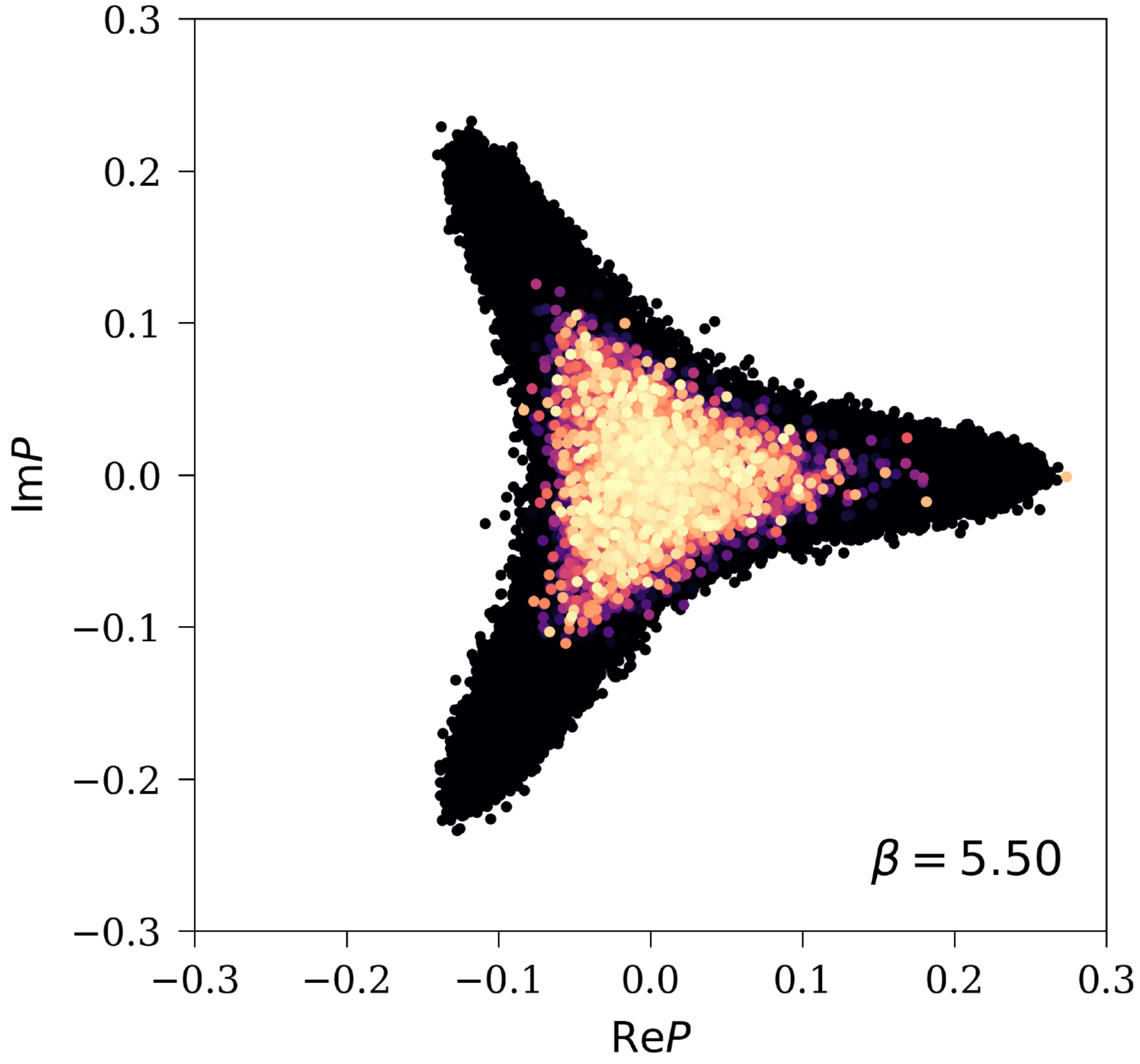
All measurements of P during NS run

Color based on weight in NS integral:

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

↓

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



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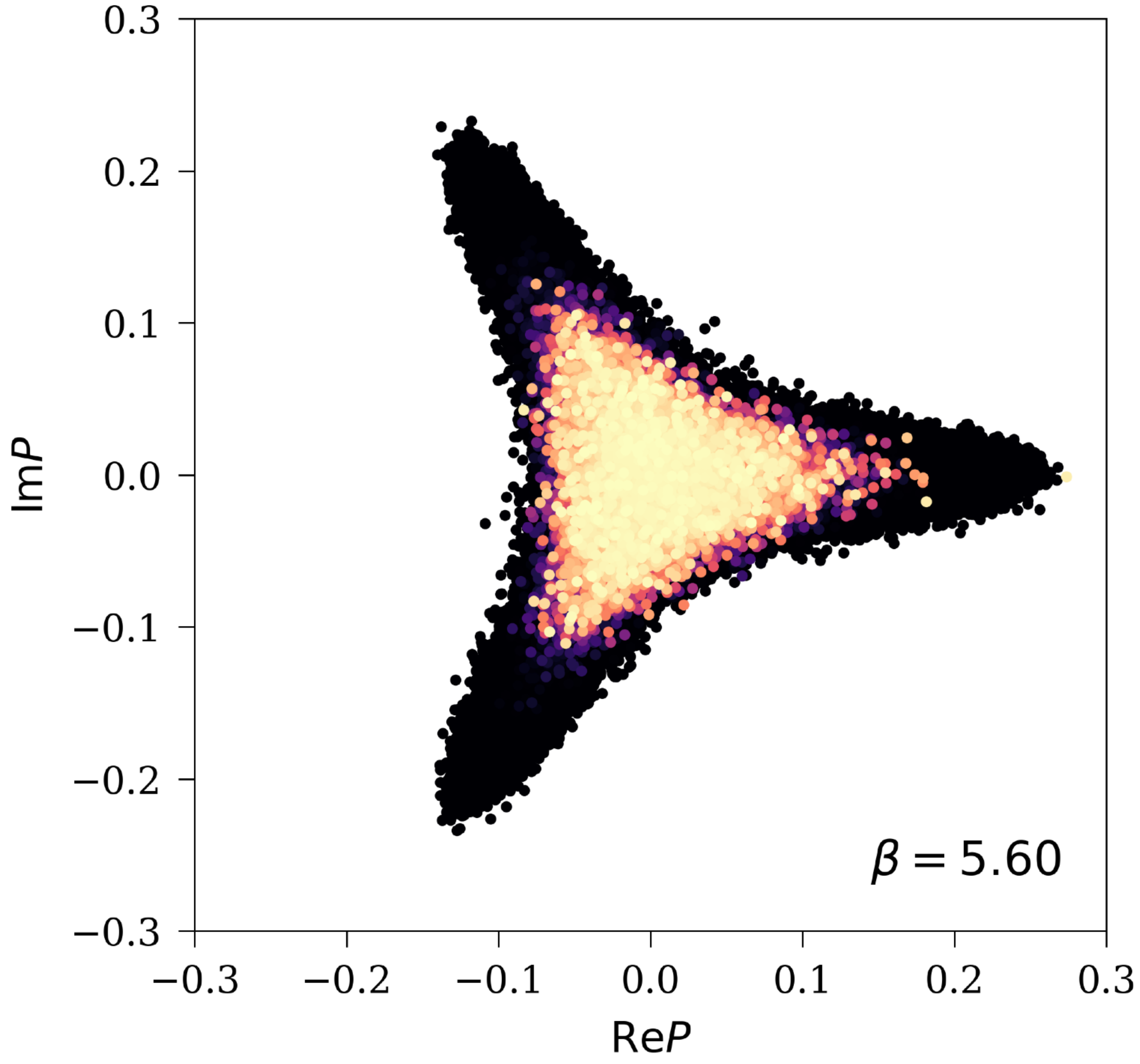

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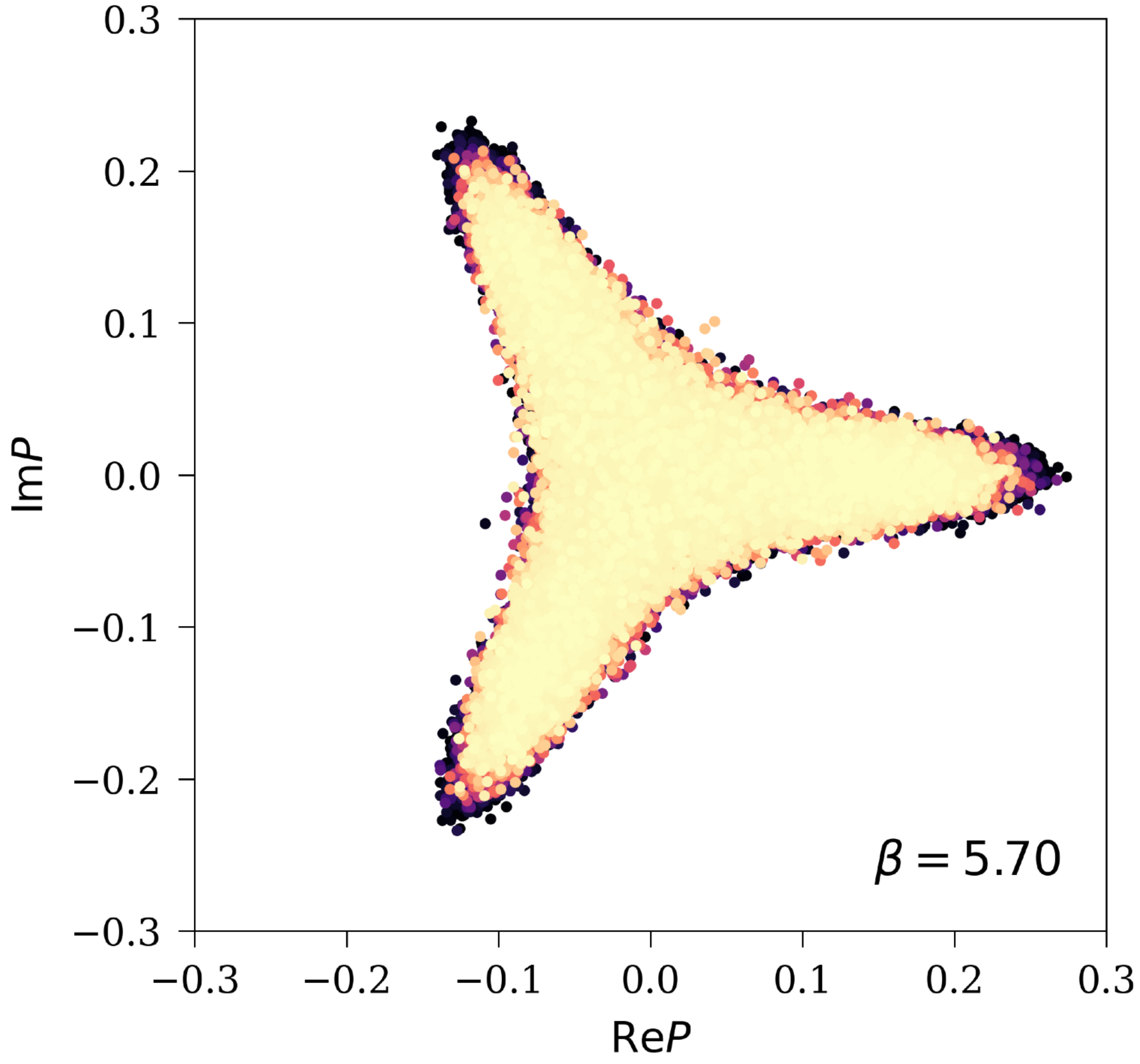

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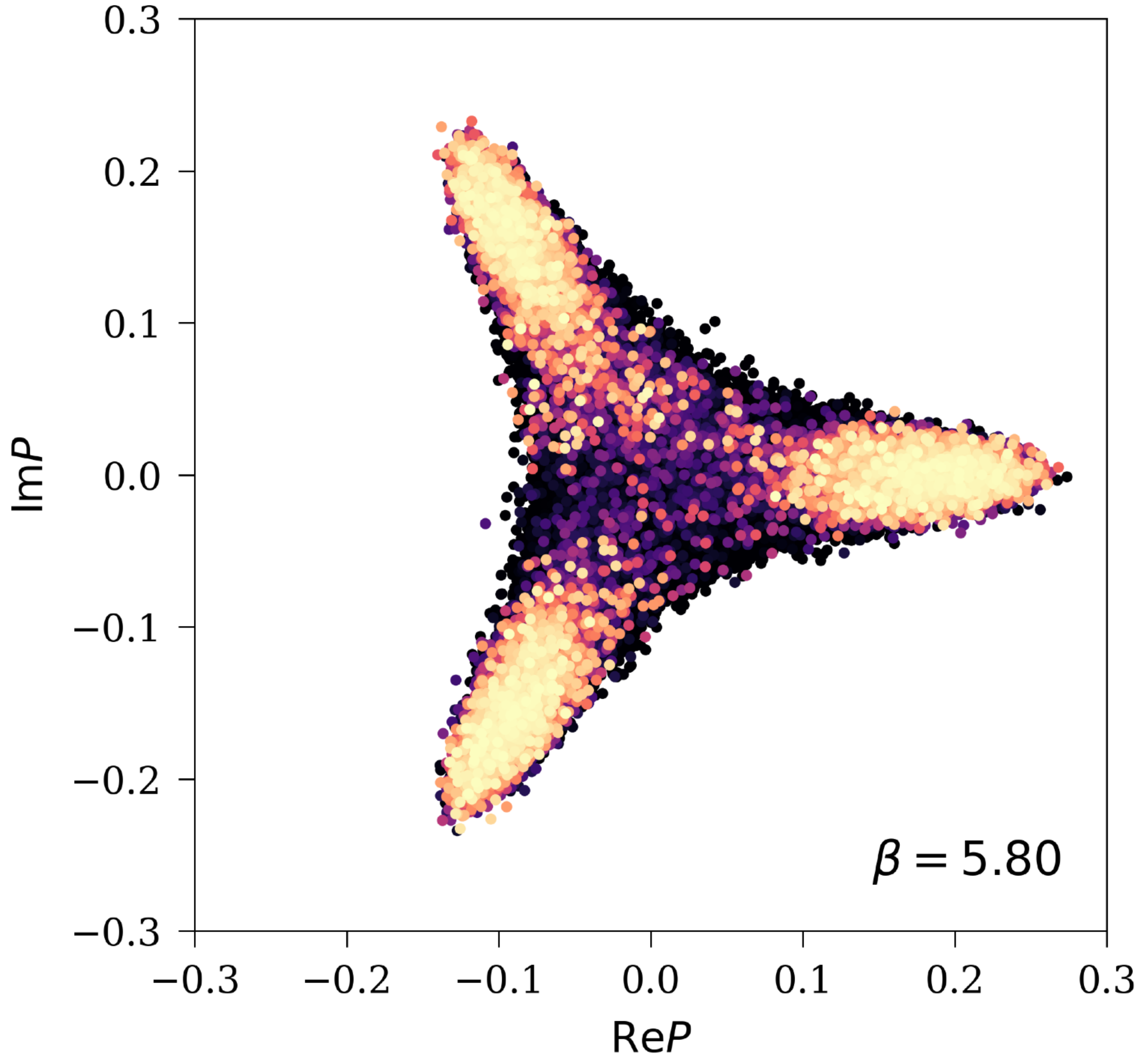

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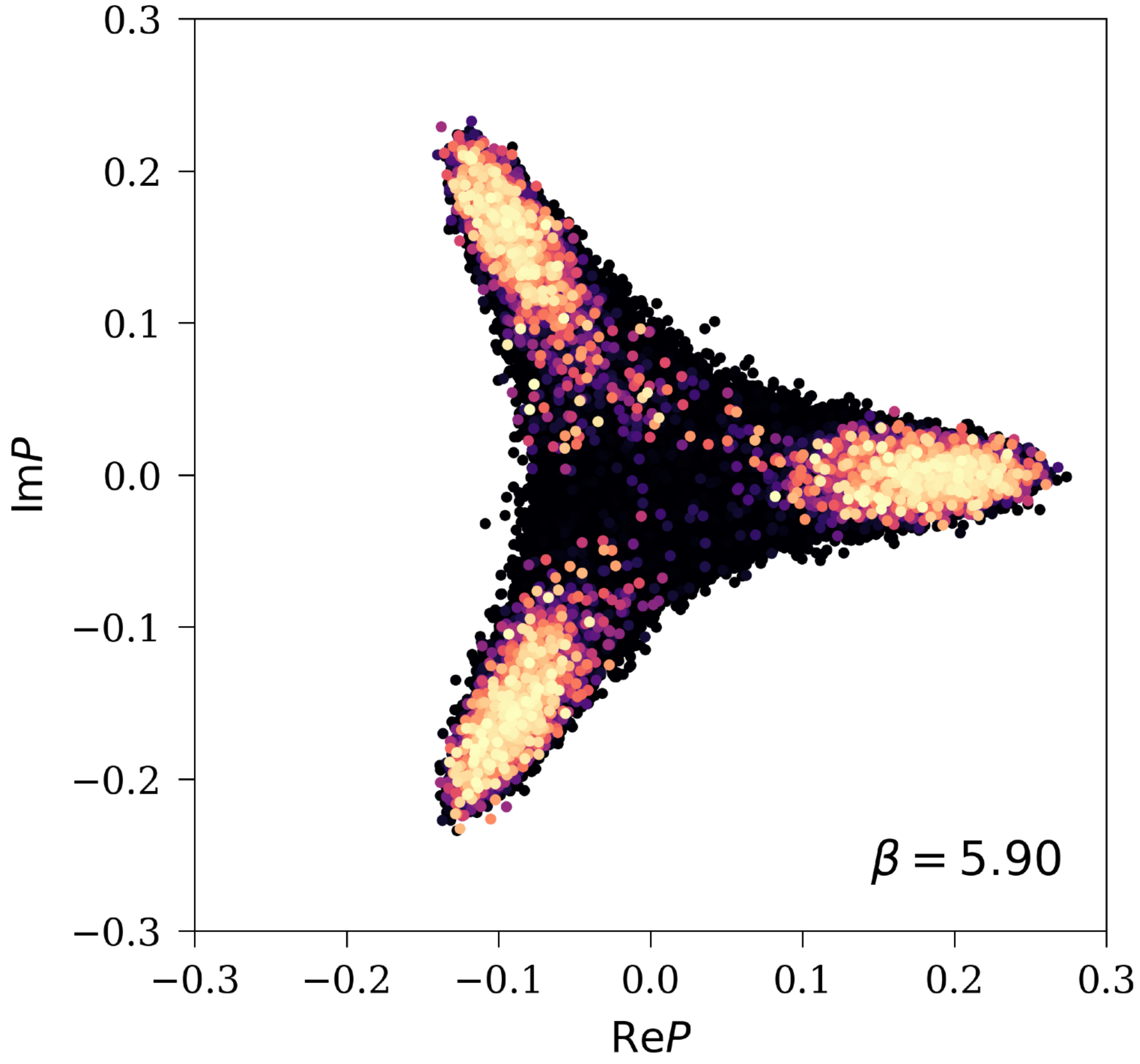

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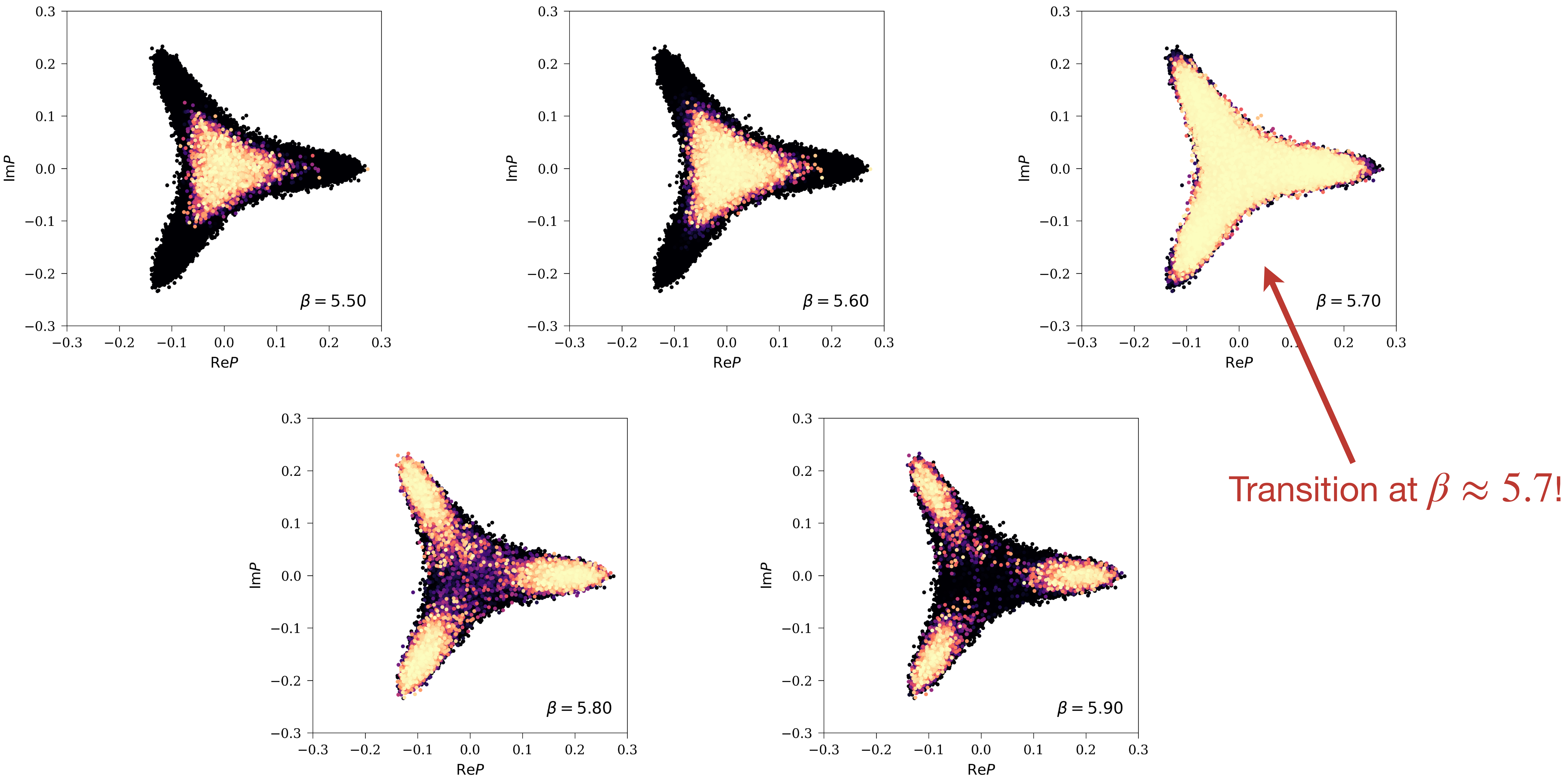
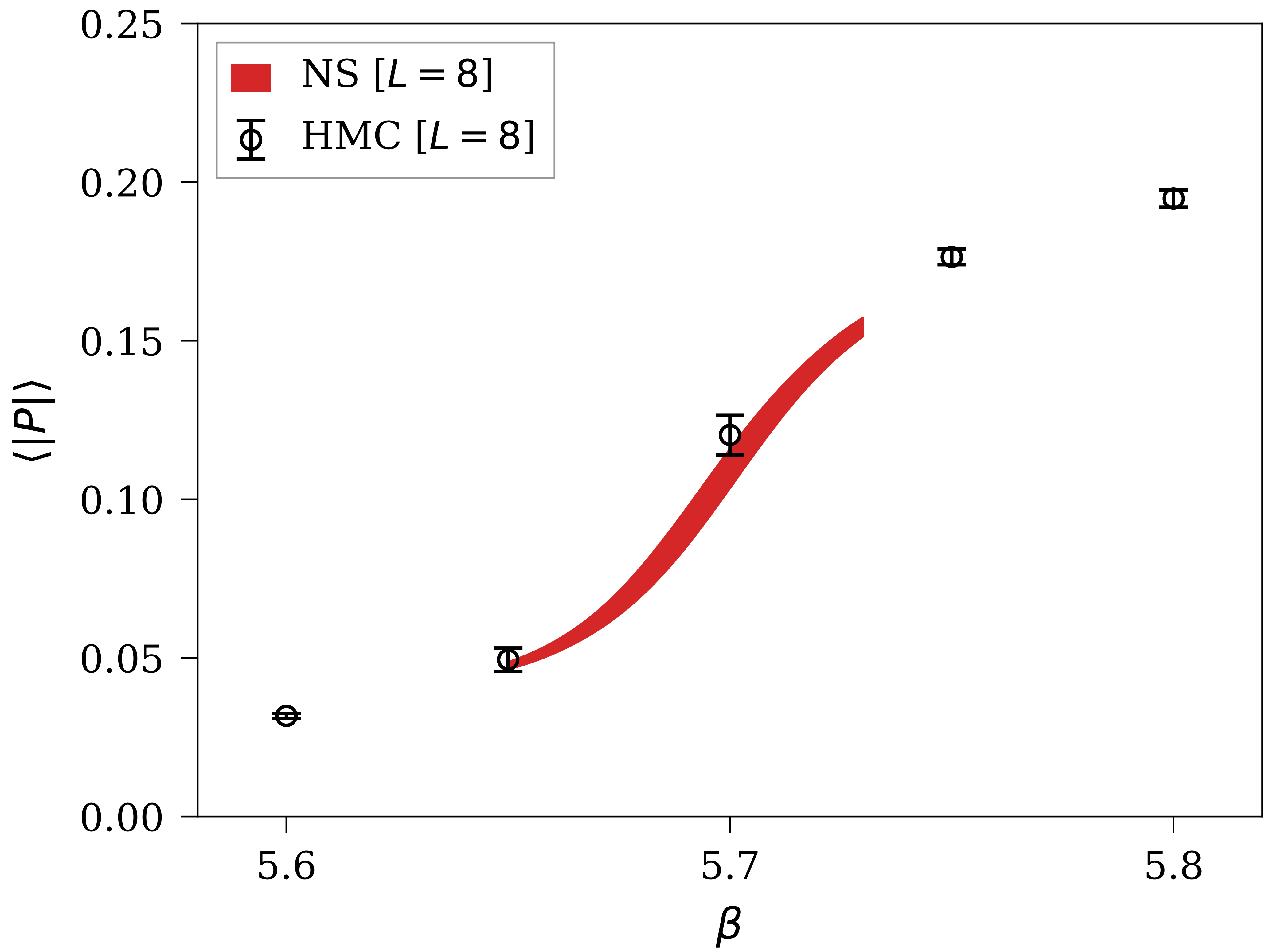
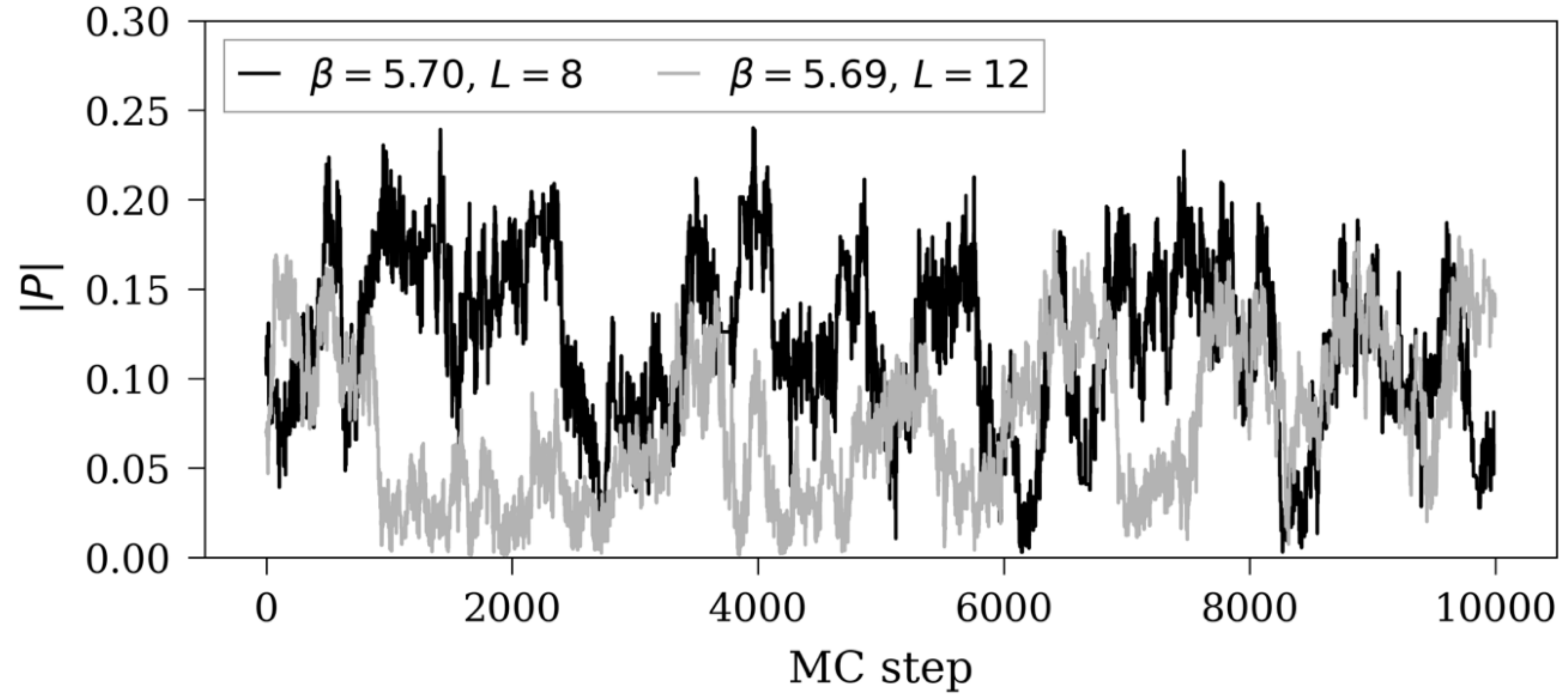


Results: Polyakov order param



Challenges for HMC:

- Long autocorrelation times
- Hysteresis near transition



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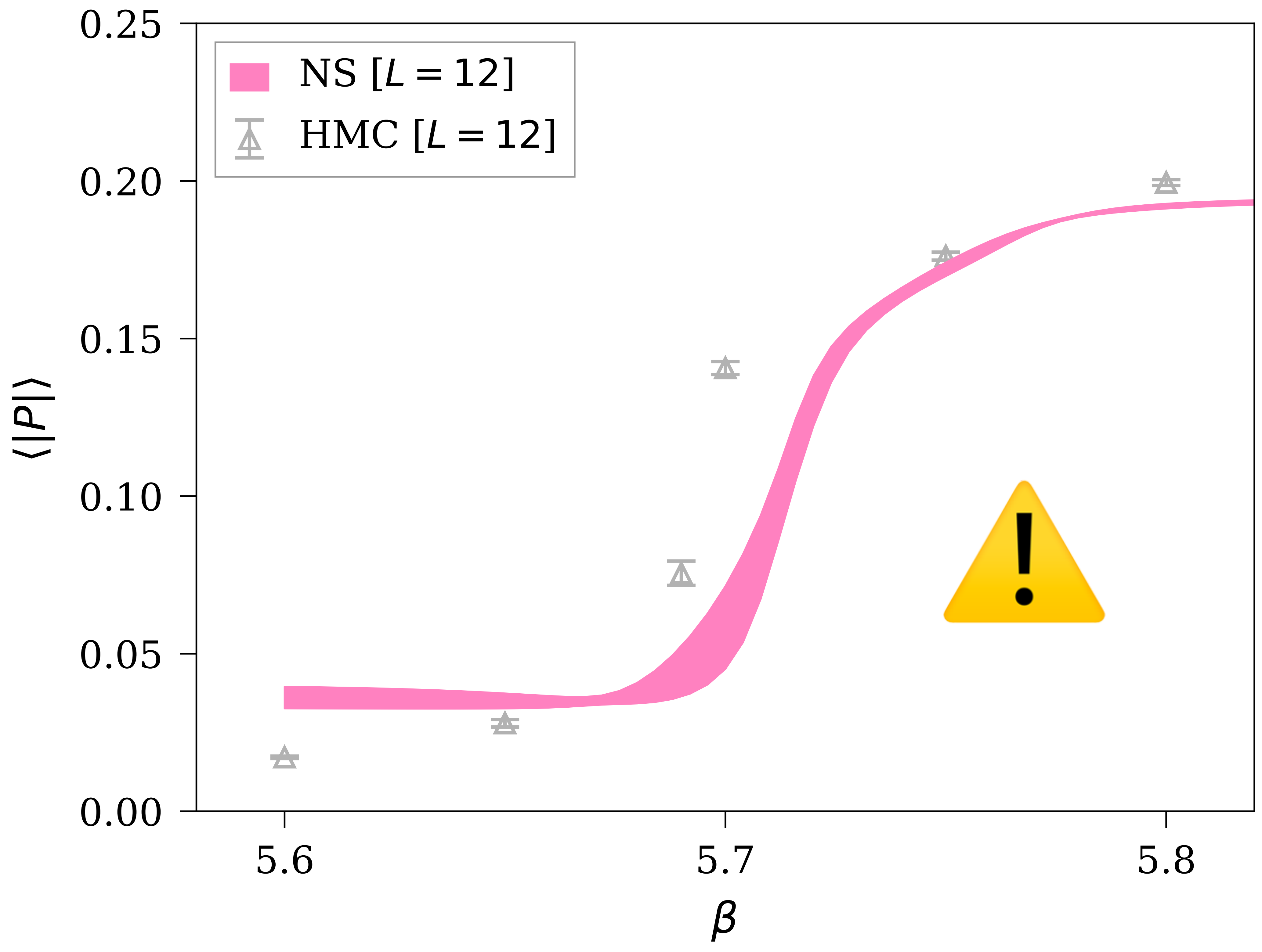

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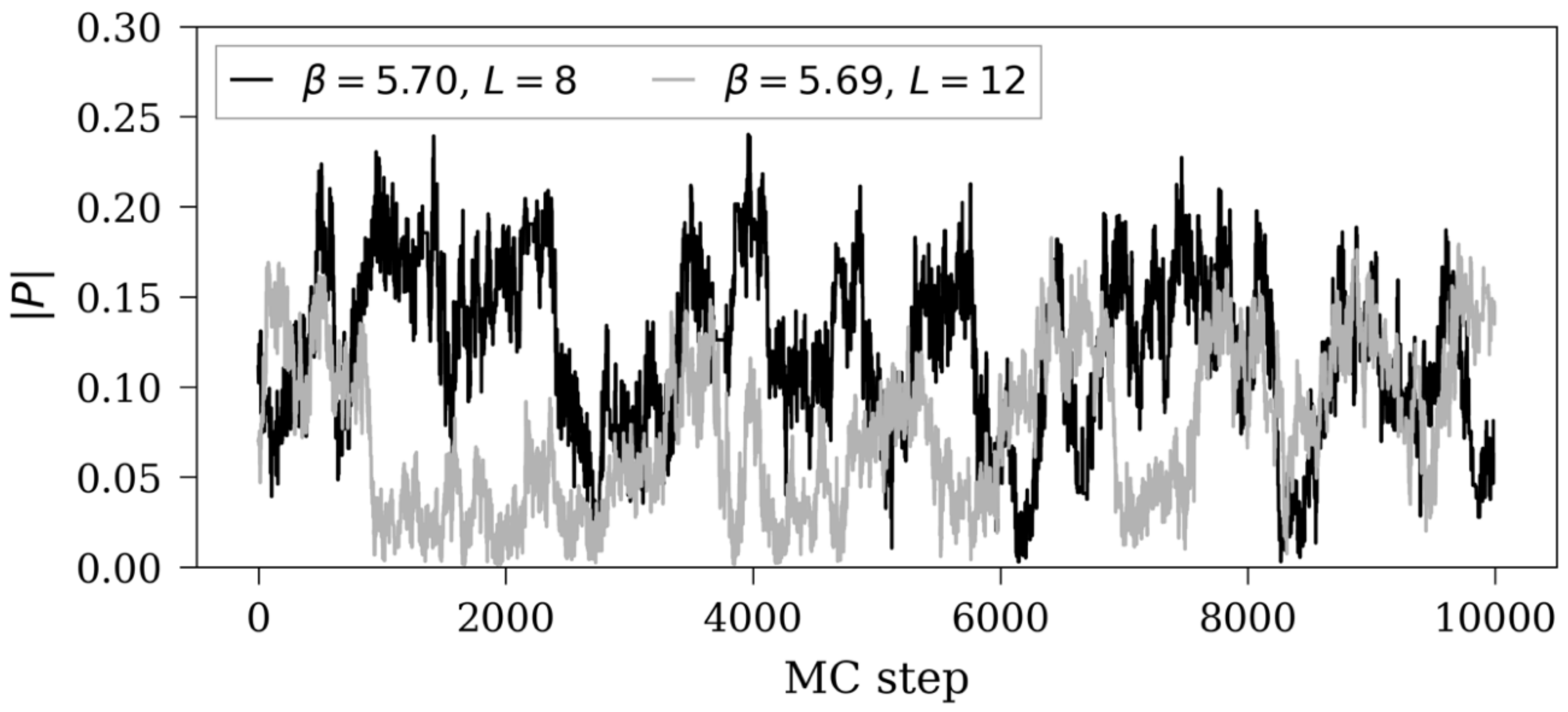
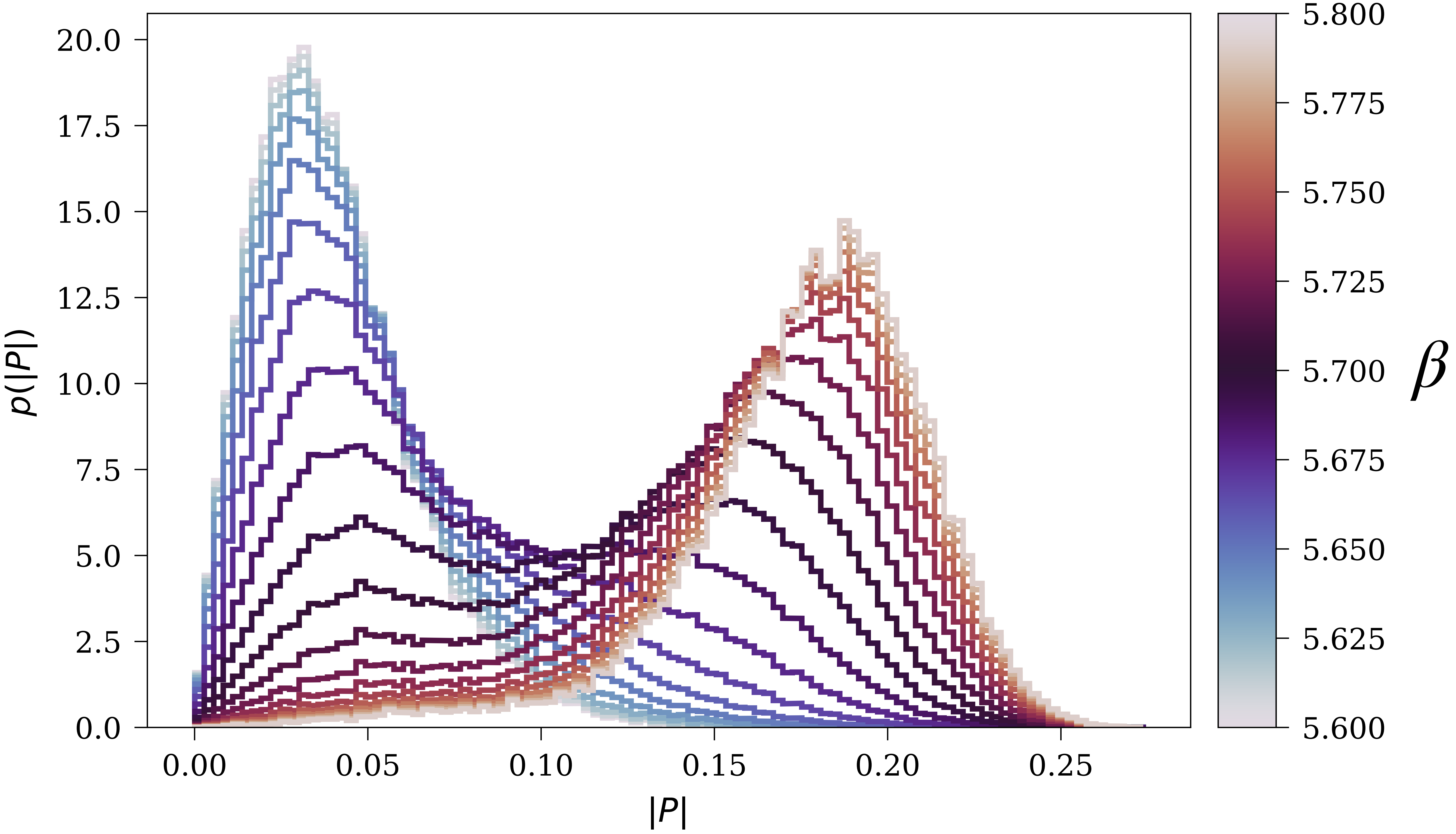


Results: Polyakov histograms (L=8)



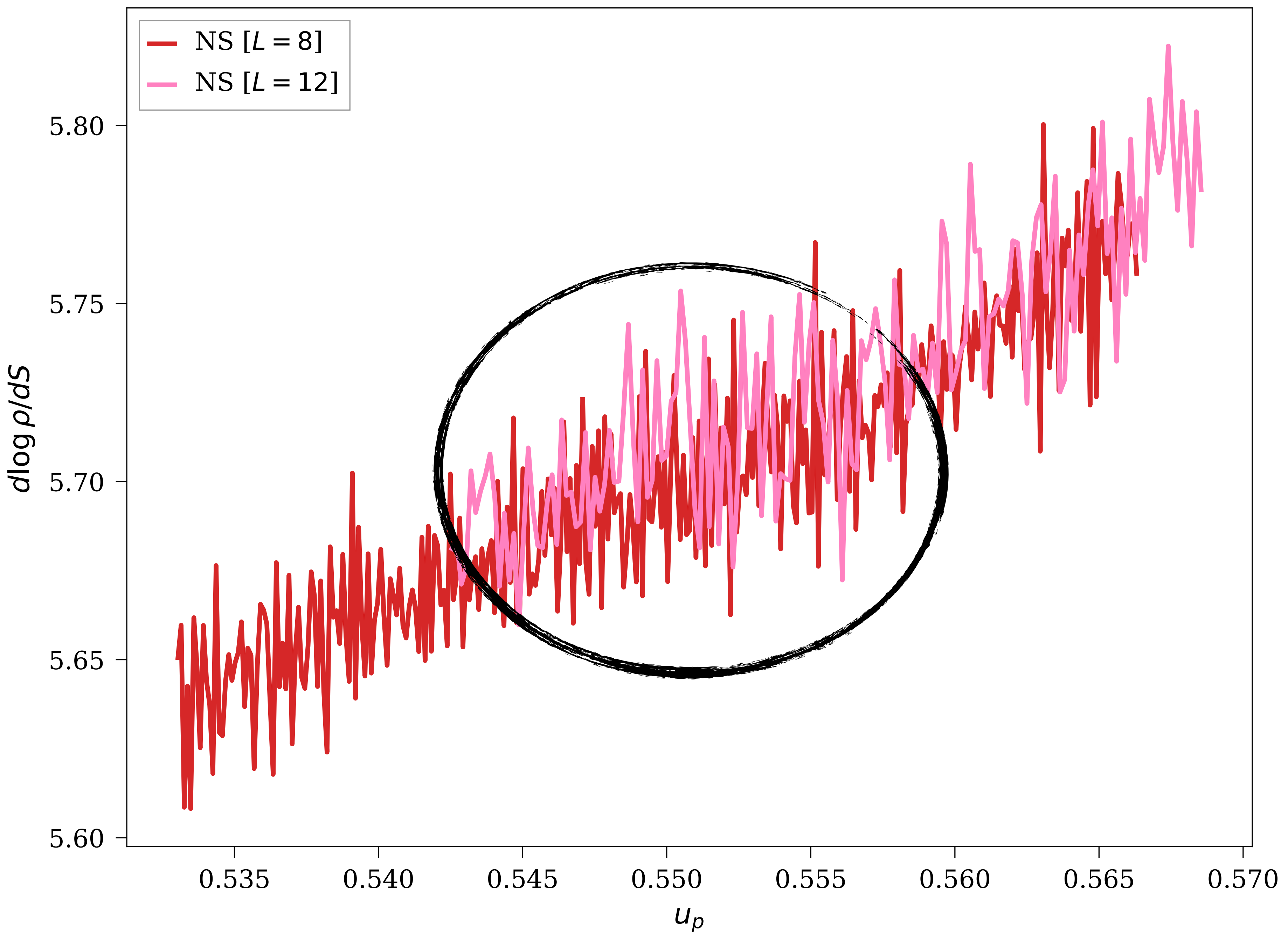
Results: Density of states

Density of states:

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

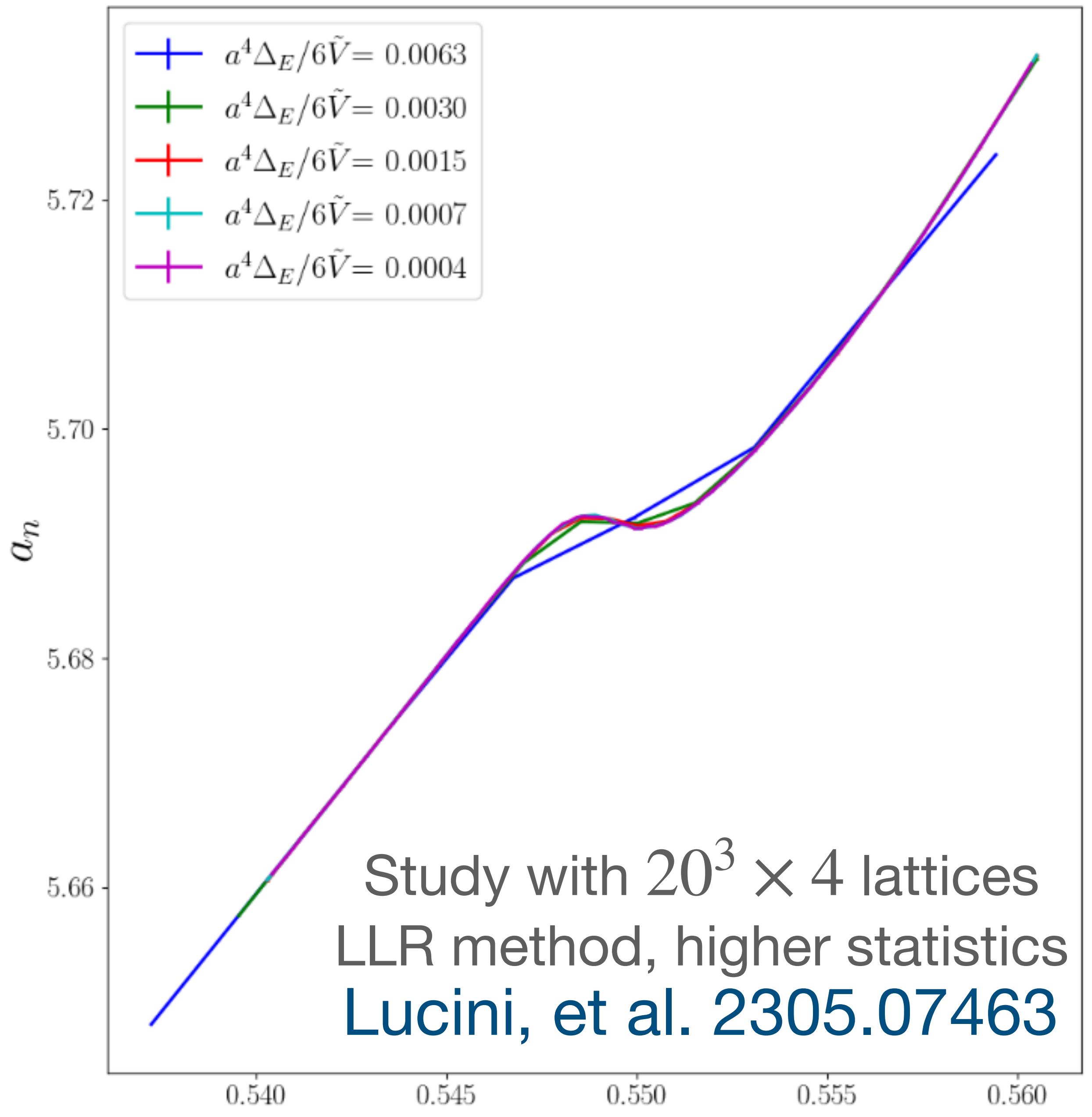
Microcanonical temperature:

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



$L \to$ large

FUTURE WORK



Comments: Monte Carlo challenges

1. Local Metropolis was much easier to tune than HMC

- Acceptance rate remains relatively constant over whole run
- Hard constraint for HMC requires (a) costly reflection calculation or (b) higher rejection rate unless $d\tau$ tuned well Betancourt (2011)
- Soft constraint for HMC possible Habeck (2015)

2. Even with many live walkers, fluctuations between 3 degenerate modes of broken symmetry phase are large

- Not a problem for relevant observables, such as $|P|$
- Relevant if inequivalent modes (e.g. instanton sectors) See previous talk by U. Wenger

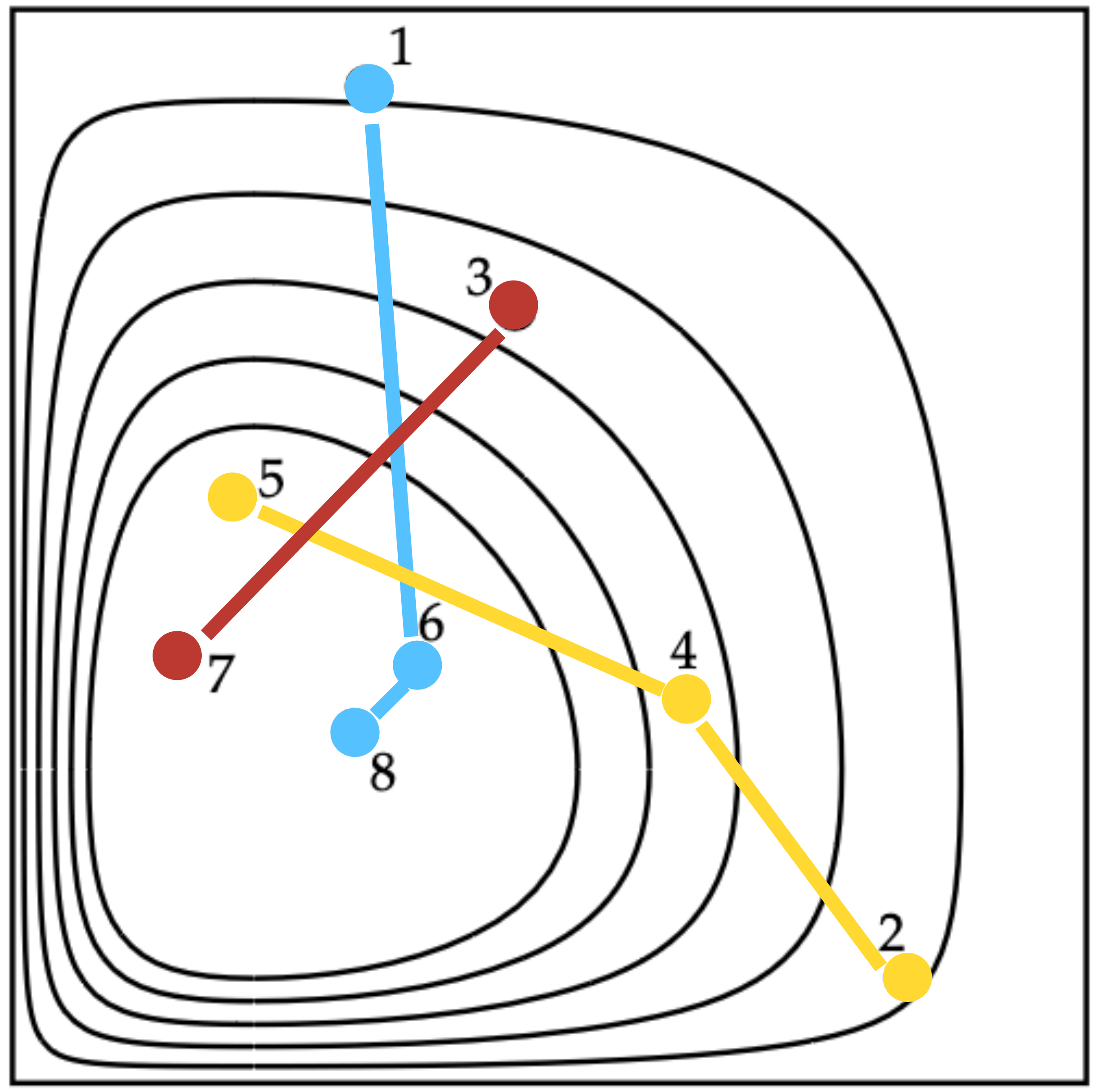
Comments: Parallelization

1. Nested sampling splits into independent "threads"

Higson, et al. (2018)

- Each resampled U' only depends on action S_i of deleted U_i
- Other walkers still useful as a resource to initialize resampling, but $k < N_{\mathrm{live}}$ can be deleted and resampled in parallel

Note: In contrast to existing literature, we resample with respect to distinct $S*$ values per deleted walker, avoiding loss of resolution



Configuration space

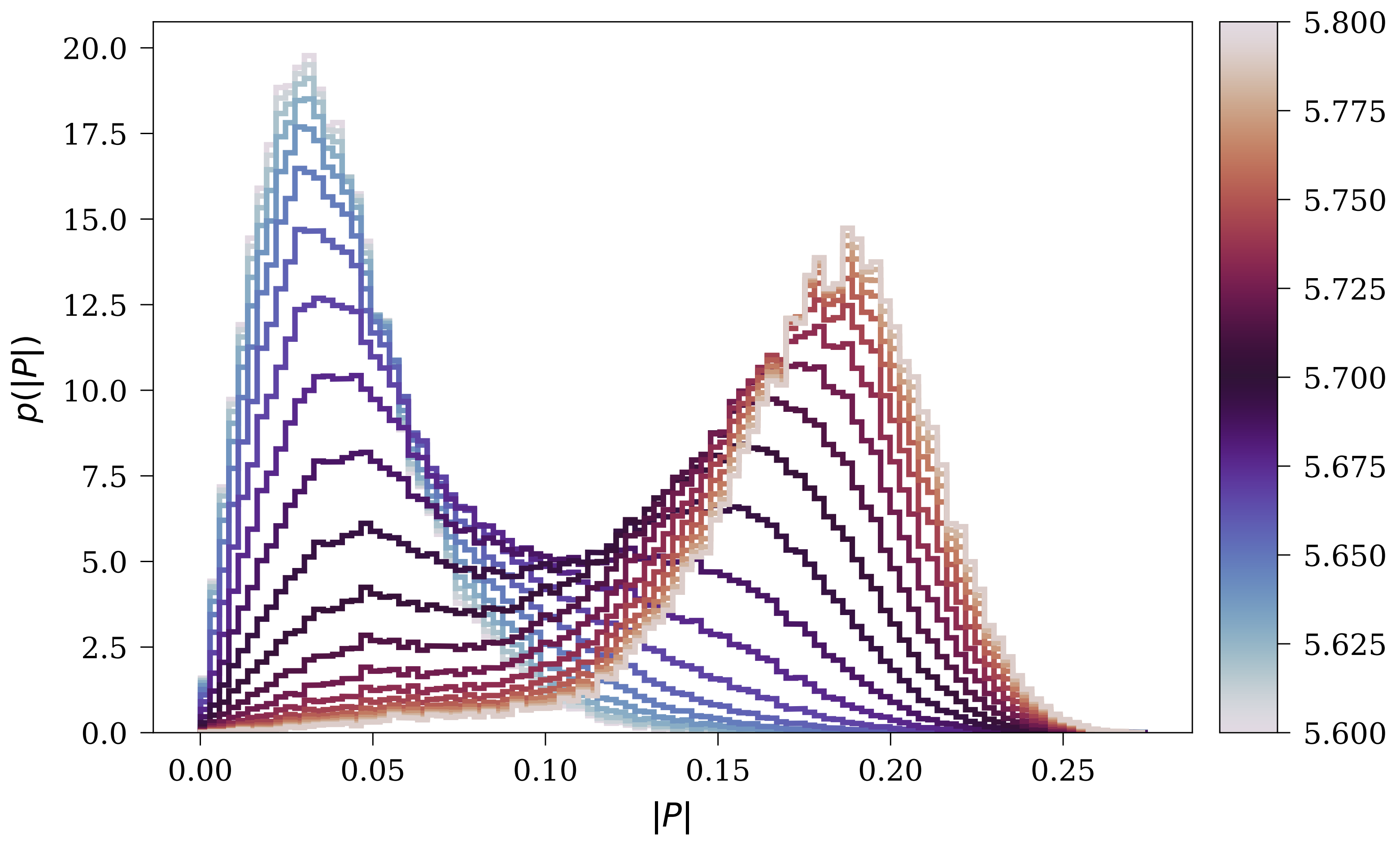
2. Threads can be combined post-hoc

- Binning and bootstrapping over threads for error estimates even with only one stream
- Statistics can be incrementally generated as usual

Summary / outlook

1. Nested sampling is a promising new Monte Carlo method
   - Particularly useful for phase transitions
   - Very different sampling strategy (uniform within contours)

2. Early results for $SU(3)$ confinement transition



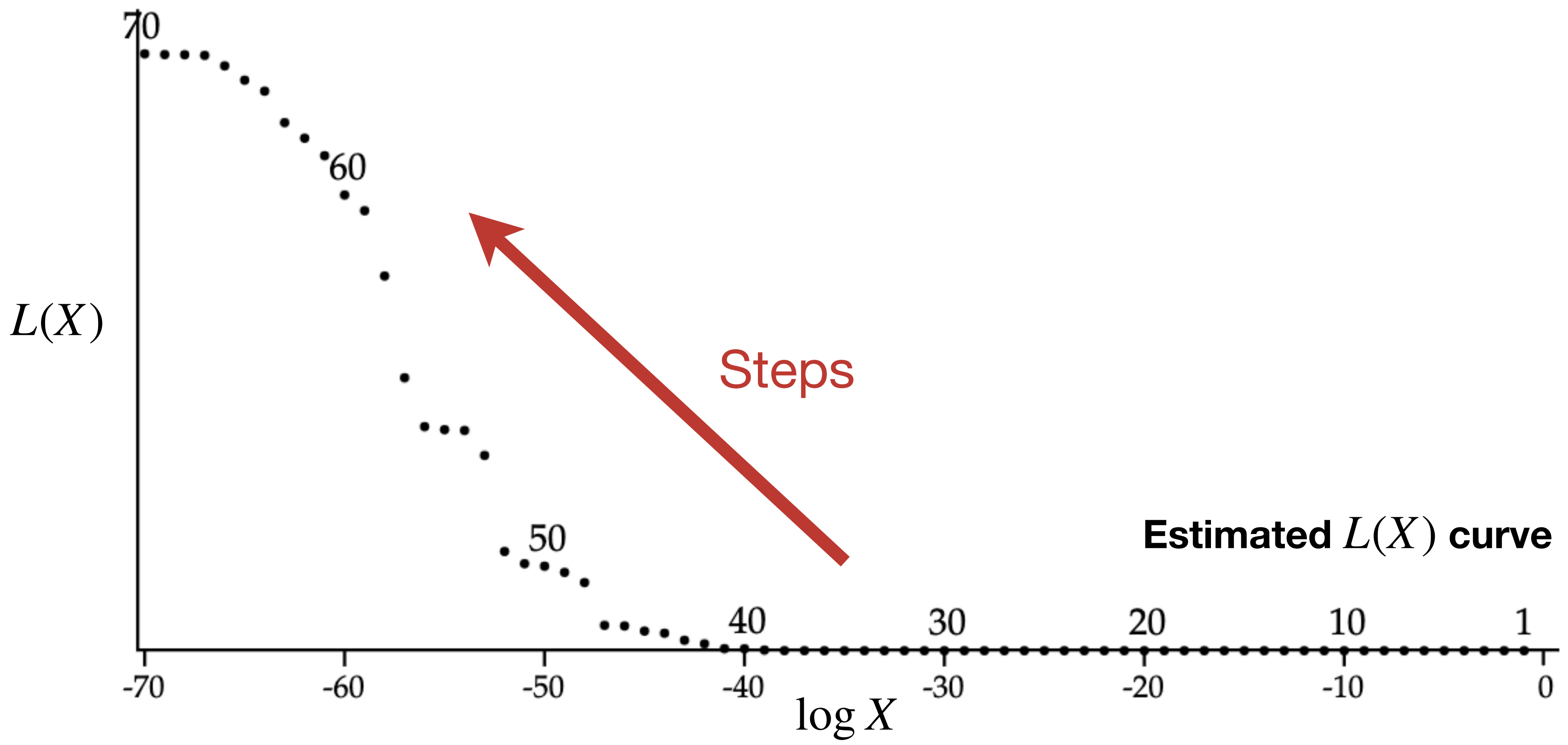
3. More developments to be done
   - Continue to control statistical and systematic error
   - Better understand volume scaling

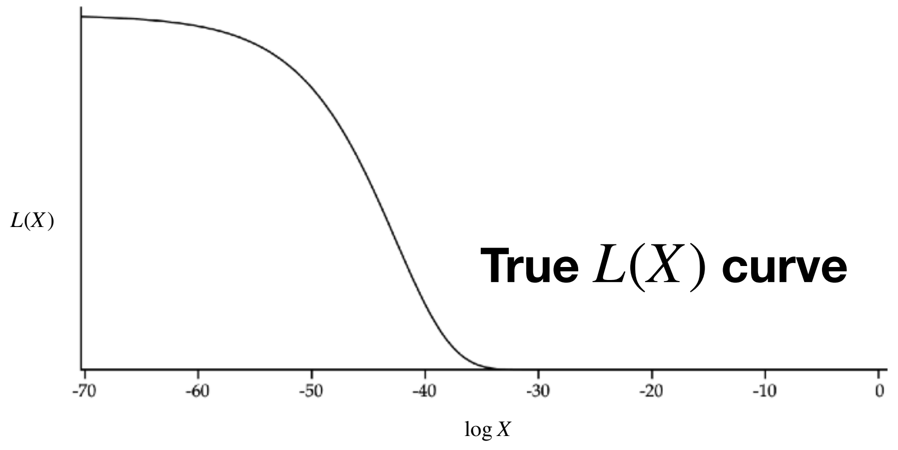
Backup slides

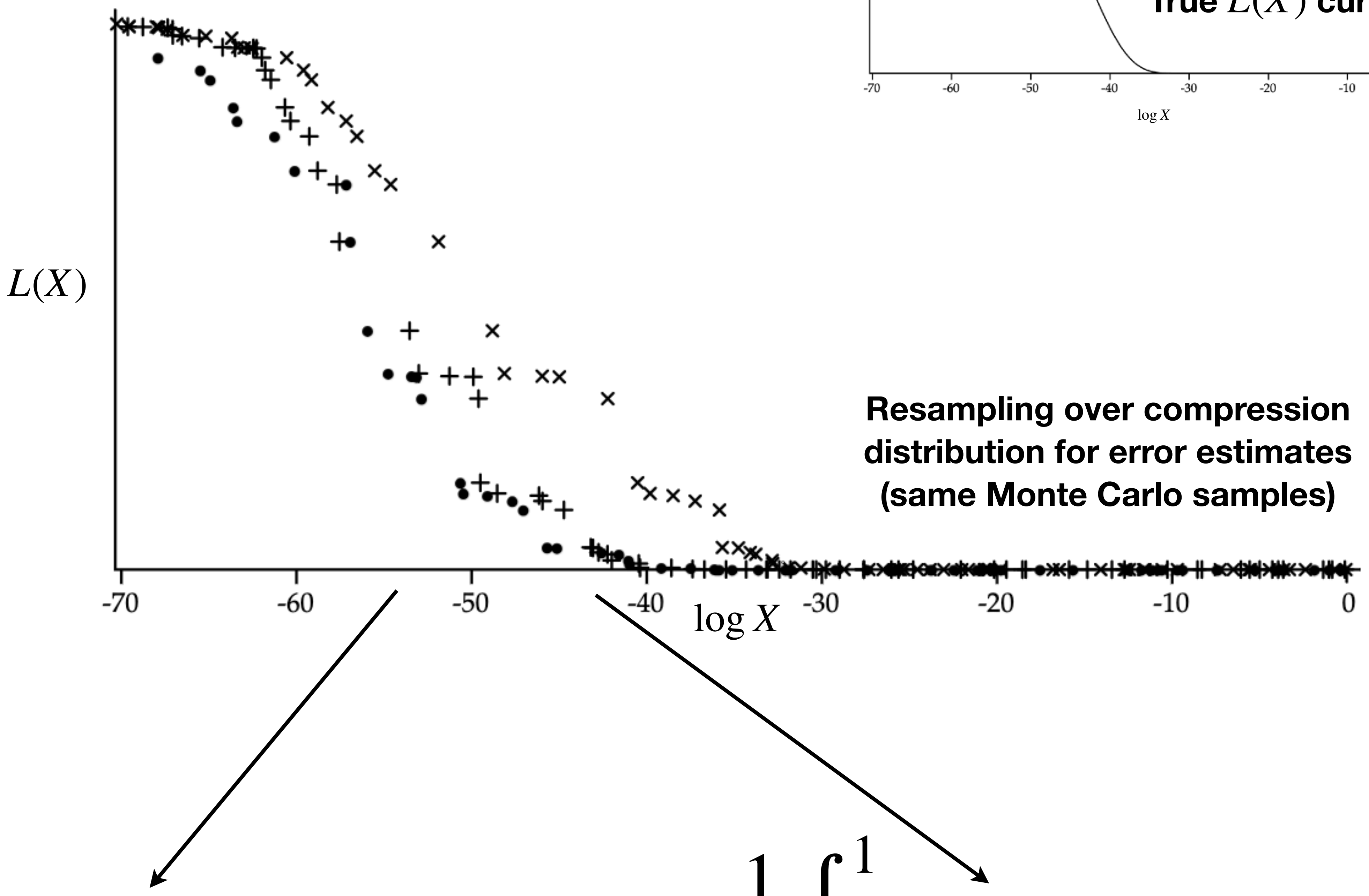
Nested sampling details

Estimate phase space X within contours of constant likelihood $L = e^{-S}$

- Example: N-dim Gaussian $L(\theta) = e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{N}\theta_i^2}$







- Partition function and observables

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

Undersampling is apparent for L=12