RHEINISCHE FRIEDRICH-WILHELMS-UNIVERSITÄT BONN
TRANSDISCIPLINARY RESEARCH AREA

Normalising-flow-based density of states : 2D U(1) gauge theory with a θ-term

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(quite) recent work in progress with* Lena Funcke

Multi-canonical methods in lattice gauge theories,
@ ECT* Trento

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**special thanks to Julian Urban, Lorenz Von Smekal and Aishwarya Deshpande*

Brief outline

I. Known: Density of states (DoS) method

- for real & complex actions

II. Known: Normalising-flow-based DoS for ϕ^4 theory

III. New: Applied to U(1) lattice gauge theory in 2D

- with and without θ-term

IV. First results: Learn the constraints and compute DoS

Disclaimer : This is early exploratory work. The goal is to share ideas and collect feedback on the NF + DoS approach.

The original approach: DOS for real action

$$Z(\beta) = \int DU e^{-\beta S_e[U]} \longrightarrow U \sim p_\beta(U)$$

Instead of sampling from full Boltzmann distribution
-> split computation in two steps:

Step 1: Compute β-independent DoS

$$\rho(E) = \int DU \delta(S_e[U] - E) \qquad U \sim p_E(U)$$

Step 2: Perform 1D integral to recover partition function

$$Z(\beta) = \int dE\ \rho(E)\, e^{-\beta E}$$

[F. Wang and D. P. Landau (2001)], [K. Langfeld, B. Lucini and A. Rago (2012)]

Generalisation of DOS to complex actions

Sign-problem-afflicted action: $\beta S_e[U] = S_R[U] + i\,h\,S_I[U]$

$$U \sim e^{-\beta S_e[U]}$$

Generalised DoS: $\rho(c) = \int DU\, e^{-S_R[U]}\, \delta(c - S_I[U])$

[K. Langfeld, B. Lucini (2014)]

Recover partition function via a Fourier Transform!

$$Z(\mu) = \int dc\, \rho(c)\, e^{-i\mu c}$$

How does one compute the DoS in practice?

How does one sample: $U \sim \delta(c - S_I[U])$?

Regularise the delta: $\lim_{P\to\infty} e^{-\frac{P}{2}(x-a)^2 - \log N} = \delta(x-a)$

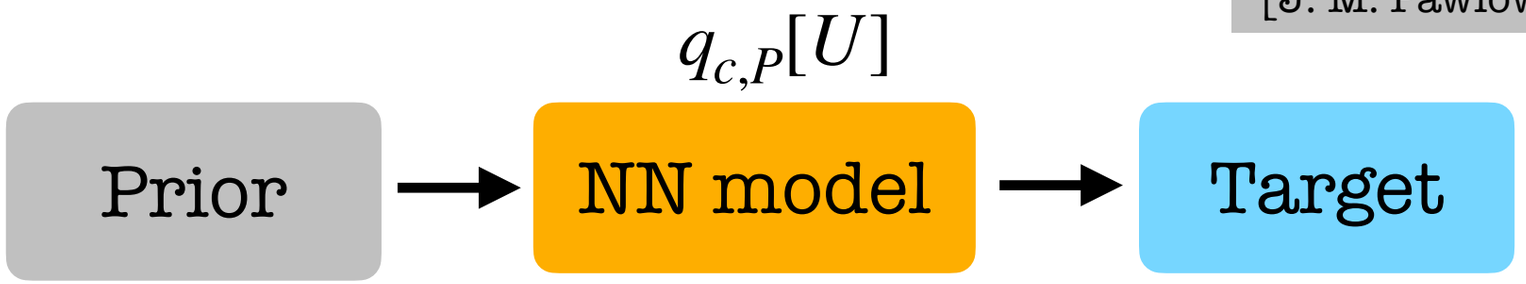
P-dependent DoS*: $\rho_P(c) = \int \mathscr{D}U\, e^{-S_{c,P}[U]}$

where $S_{c,P} = S_r[U] + \frac{P}{2}\left(c - S_I[U]\right)^2 + \log N$

*some discussion on the magnitude of P can be found here S. Borsanyi and D. Sexty (2021)

Method: Using normalising flows to estimate DoS

[J. M. Pawlowski, J. M. Urban (2023)]



$$\rho_P(c) = \int \mathscr{D}U\, e^{-S_{c,P}[U]}$$

Trick: insert identity

K. A. Nicoli et. al., (2021)

$$\rho_P(c) = \int \mathscr{D}U\, q_{c,P}(U)\, \frac{e^{-S_{c,P}[U]}}{q_{c,P}(U)}$$

$$\rho_P(c) \approx \langle e^{-S_{c,P}[U] - \ln q_{c,P}(U)} \rangle_{U \sim q_{c,P}(U)}$$

Theory: 2D U(1) Lattice Gauge Theory

Motivation: Gauge theories in 2D can be exactly solved,
- perfect test bed for new methods!

- 2D U(1) LGT used previously to benchmark equivariant flow-based sampling: reduced freezing of topological charge

[G. Kanwar et. al (2021)], [M. S. Albergo et.al. (2021)]

Recall : $\rho(E) = \int DU\, \delta(S_e[U] - E)$ and $Z(\beta) = \int dE\, \rho(E)\, e^{-\beta E}$

- Can the topological charge freezing be further reduced by β–independent learning of gauge configurations with DoS?

G. Cossu, D. Lancaster, B. Luicni, R. Pellegrini, A. Rago et.al. (2021)

Theory: 2D U(1) LGT with θ-term

$$S_e[U] = S_{Wilson}[U] + i\,\theta\,Q_{top}[U]$$

- Can use Hamiltonian methods - limited by system size
- Lagrangian methods - no direct simulation with real θ

DoS offers the possibility to study larger* systems without analytical continuation from imaginary θ!

[S. Borsanyi, D. Sexty, 2021] [C. Gattringer and O. Orasch, 2020]
[C. Gattringer, M. Giuliani, A. Lehmann, P. T̈orek (2016)]

*than what Hamiltonian methods can currently probe

Considerations for the sign problem :

- However, DoS cannot solve the exponential worsening of the SP with volume…

$$\langle e^{i\phi} \rangle = \frac{\int \mathscr{D}\phi \; e^{-S_R[\phi]+i\mu S_I[\phi]}}{\int \mathscr{D}\phi \; e^{-S_R[\phi]}} = \frac{\int ds \, e^{is\mu}\rho(s)}{\int ds \, \rho(s)}$$

$$\langle e^{i\phi} \rangle = \frac{Z_{full}}{Z_{PQ}} = e^{-V\Delta f}$$

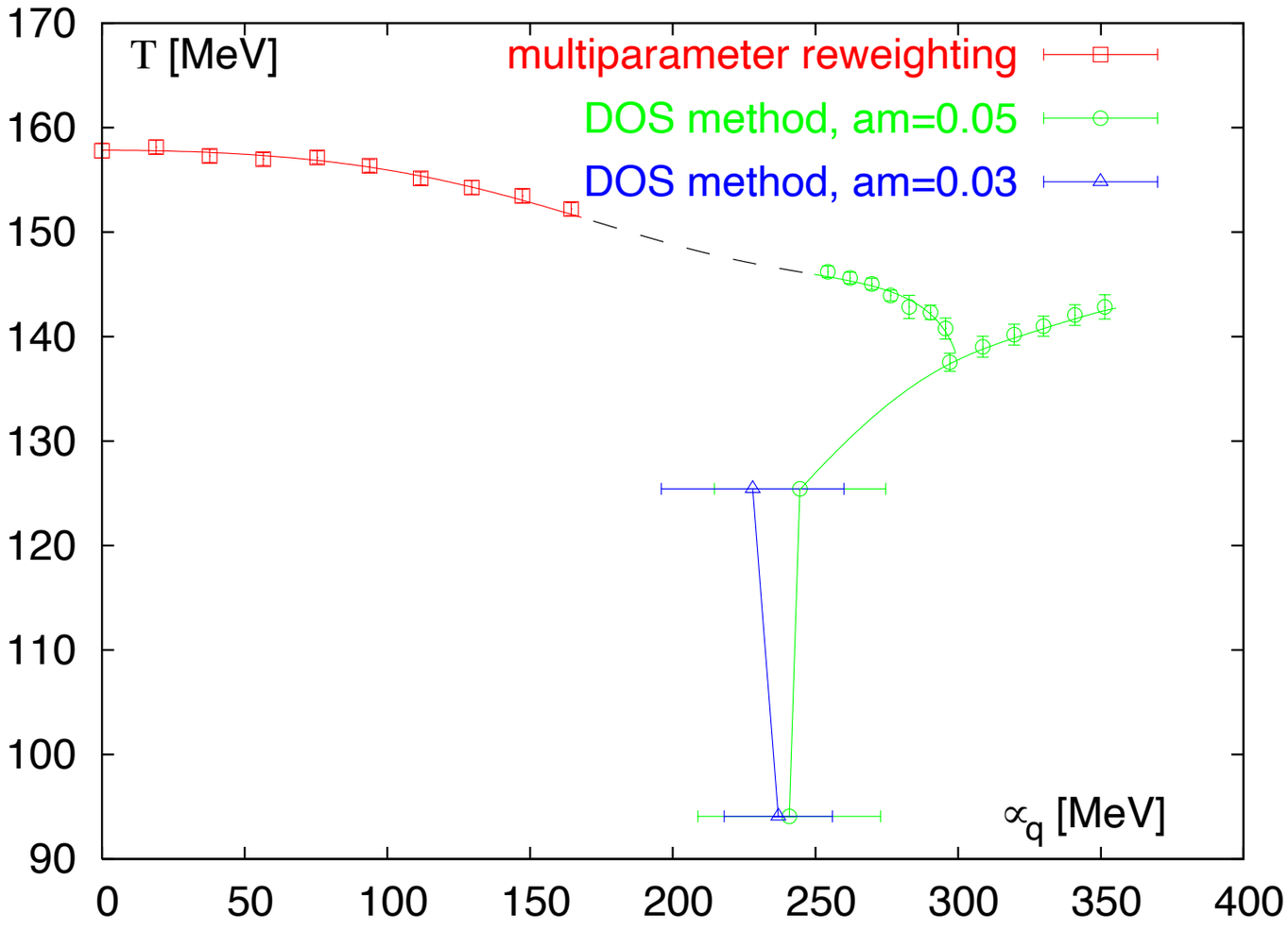
- Re-weighting suffers when the sampling measure misses dominant configurations

- DoS avoids this by estimating the weight of each s-slice directly, but it does not remove the exponential cancellation inherent in the sign problem

*for a nice discussion see O. Francesconi, PhD thesis, 2016

Considerations for the sign problem :

- Is there any benefit w.r.t sign problem from re-weighting? - probably - theory dependent



Z. Fodor, S. Katz and C. Schmidt (2007)

Typical Workflow for NF-Based DoS

Prerequisite: NF setup for the original theory with S_e

I. Define constraint, define new target action $S_{c,P}[U]$ with suitable P, and learn target with NF ✓

II. Compute DoS with $\rho_P(c) \approx \langle e^{-S_{c,P}[U] - \ln q_{c,P}(U)} \rangle_{U \sim q_{c,P}(U)}$ using flow-based samples $U \sim q_{c,P}(U)$ ✓

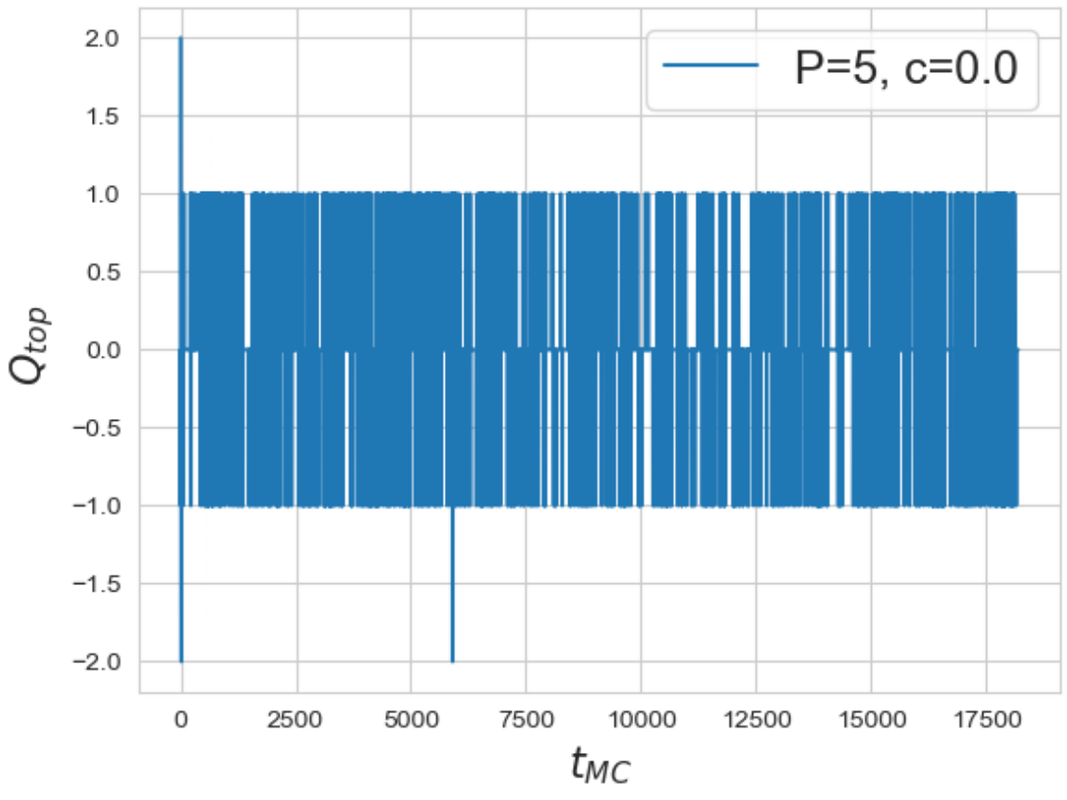
III. Once DoS is computed on fine grid of constraints - compute $Z(\beta)$ ($Z(\theta)$) with 1D integral (Fourier Transform)

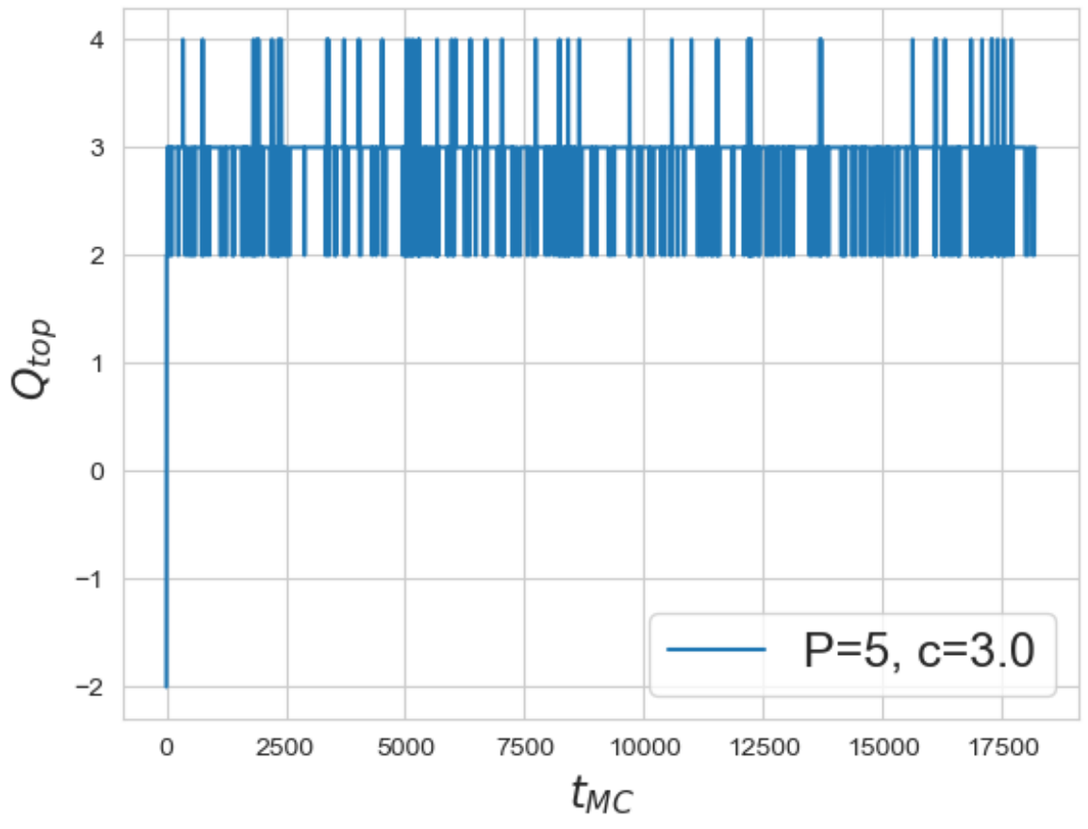
Learning the constraints: 2D U(1) with θ–term

$$S_e[U] = S_{Wilson}[U] + i\,\theta\,Q_{top}[U]$$

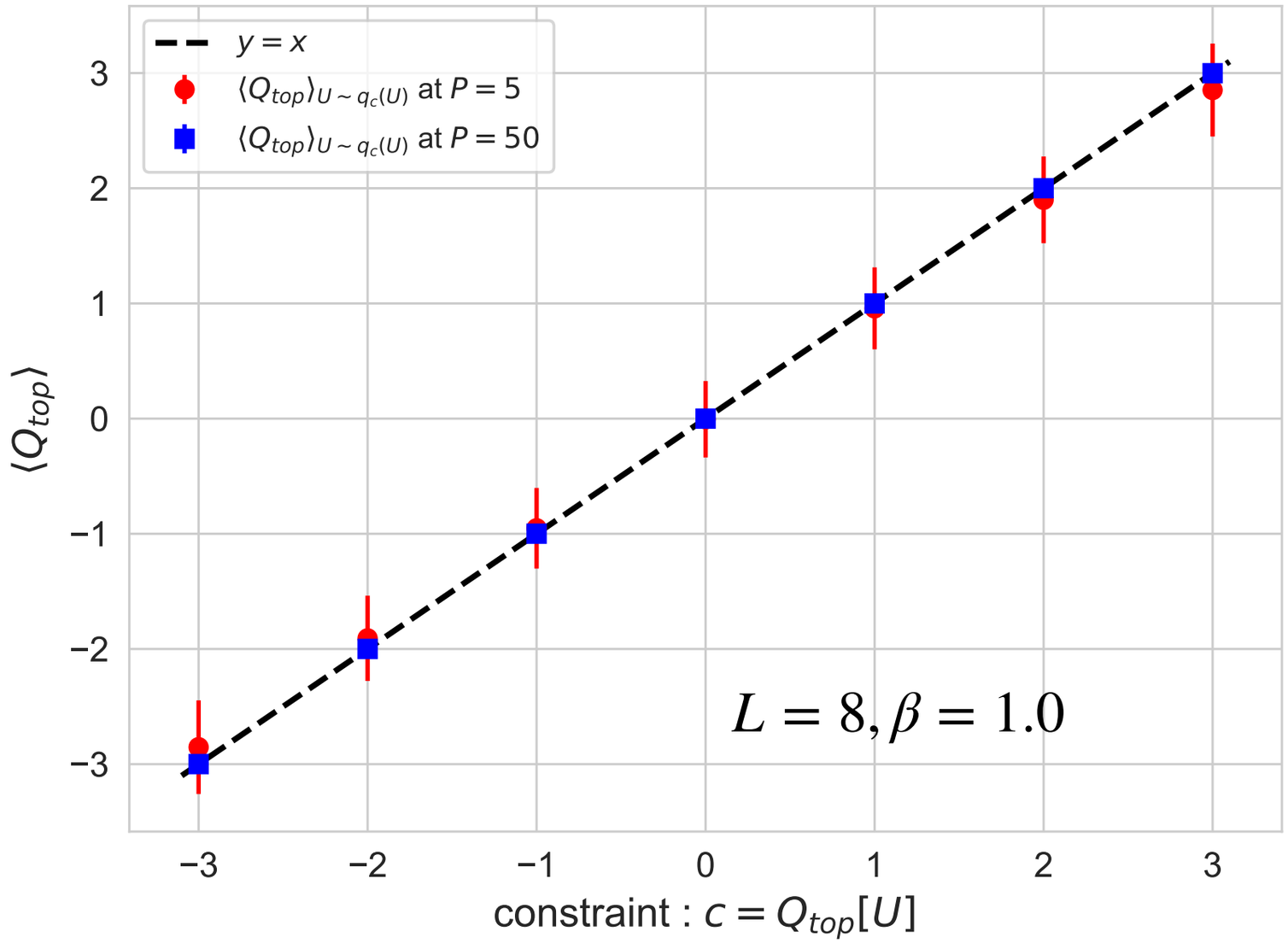
$$S_{c,P}[U] = S_{Wilson}[U] + \frac{P}{2}\left(c - Q_{top}[U]\right)^2 + \log N$$

- Currently, training independent flows for each c





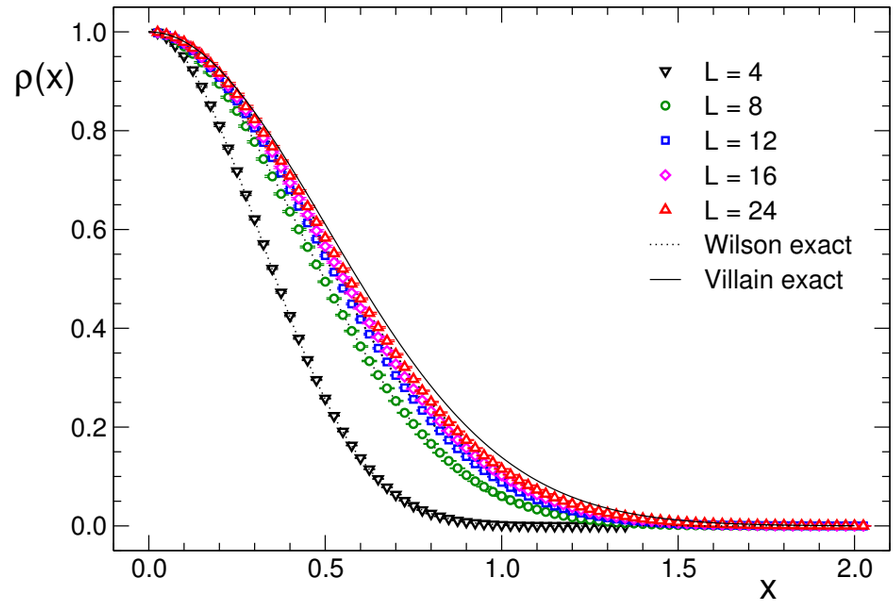
Learning the constraints: 2D U(1) with θ–term



P–dependence of constraint

$$\rho^{(per)}(x) \propto \sum_{n \in \mathbb{Z}} e^{-2\frac{\pi^2}{R} n^2} \delta(x - n)$$

$$\rho^{(open)}(x) \propto e^{-2\frac{\pi^2}{R} x^2}$$

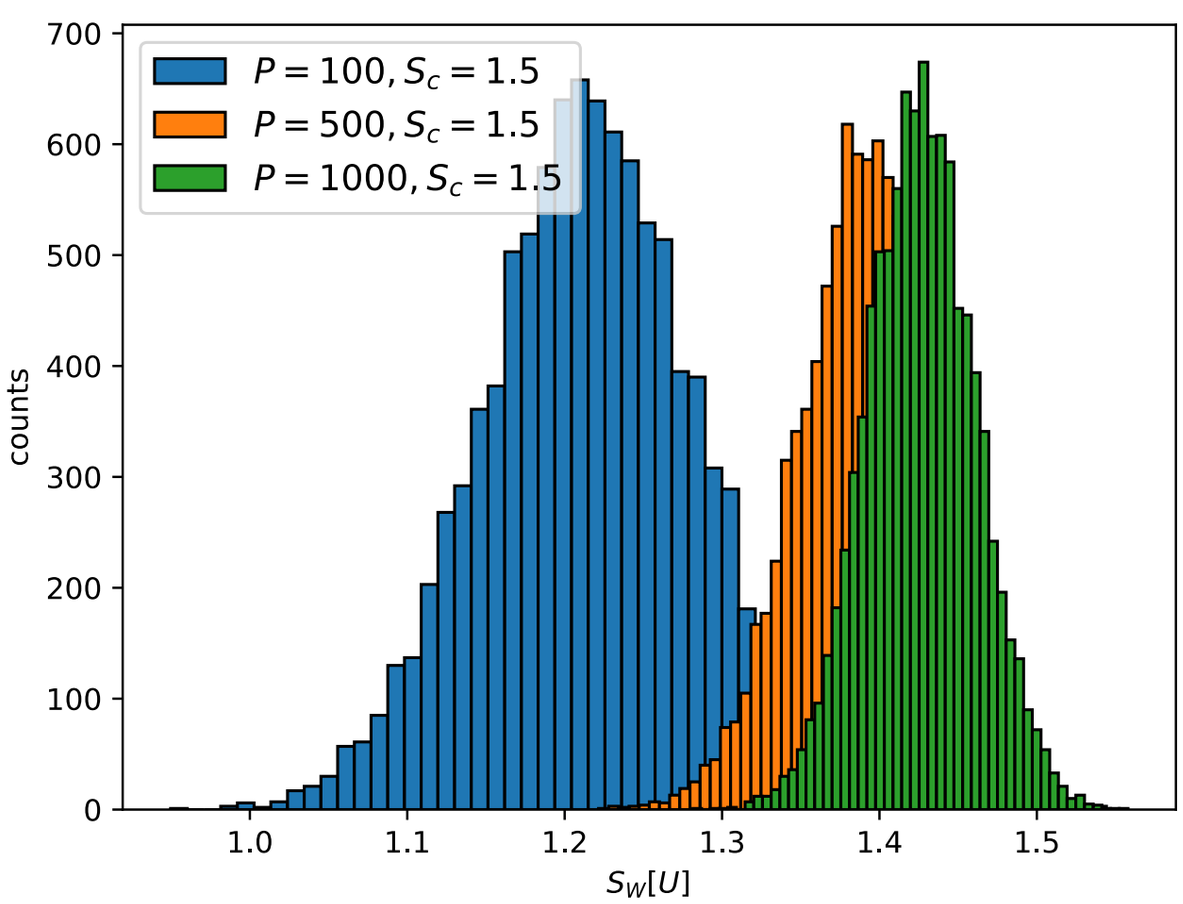


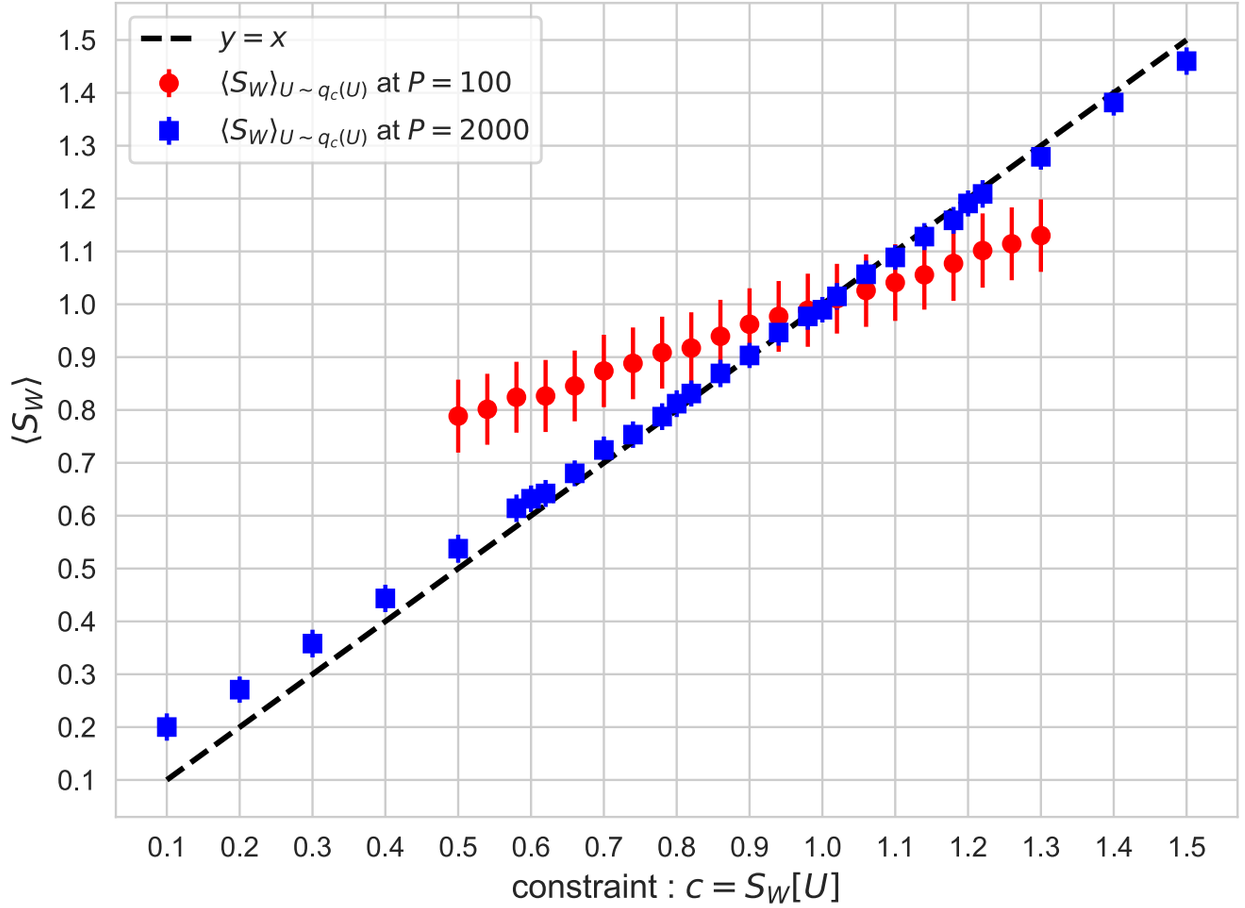
C. Gattringer and O. Orasch, 2020

Learning the constraints II: 2D U(1) w/o θ-term

$$S_{c,P}[U] = \frac{P}{2}\left(c - S_{Wilson}[U]\right)^2 + \log N \qquad S_{Wilson}[U] = \sum_p \left(1 - \left[U_p + U_p^\dagger\right]\right)/N_p \in [0,2]$$

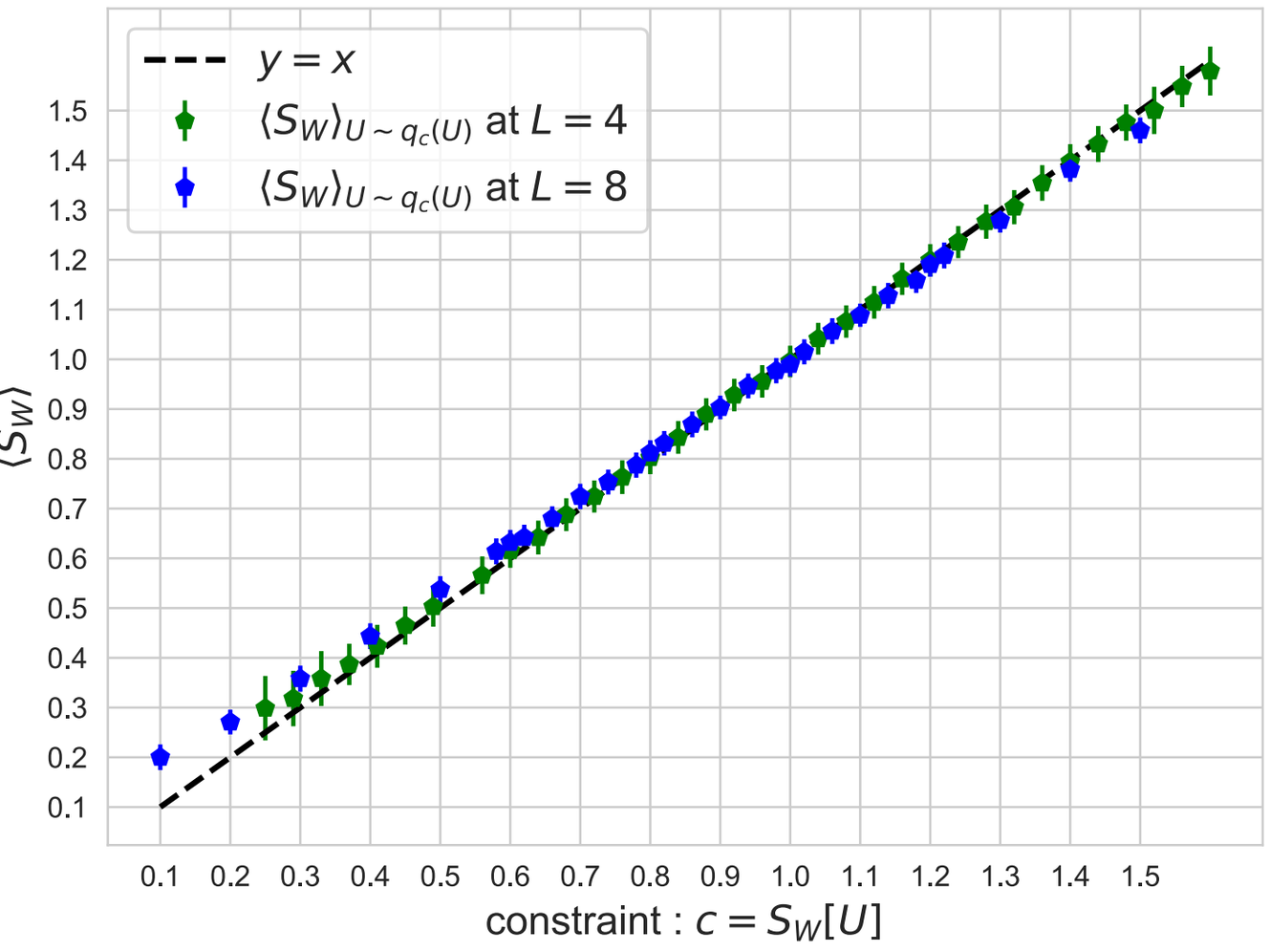
Action constraint only works at large P!!





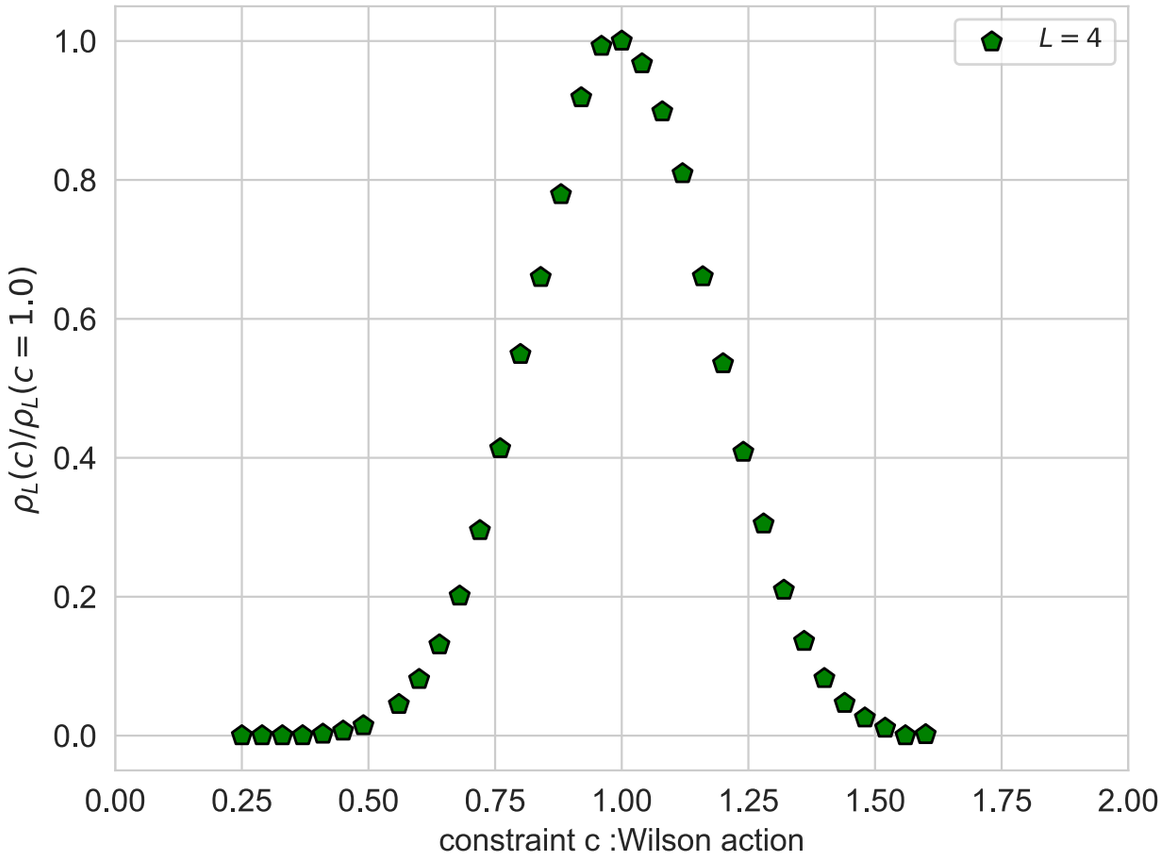
Computing the DoS: 2D U(1) without θ–term

$$S_{Wilson}[U] = \sum_p \Big(1 - \cos(\phi_p)\Big)/N_p \in [0,2]$$



Checking constraints for
$L = 4,8$ and $P = 2000$

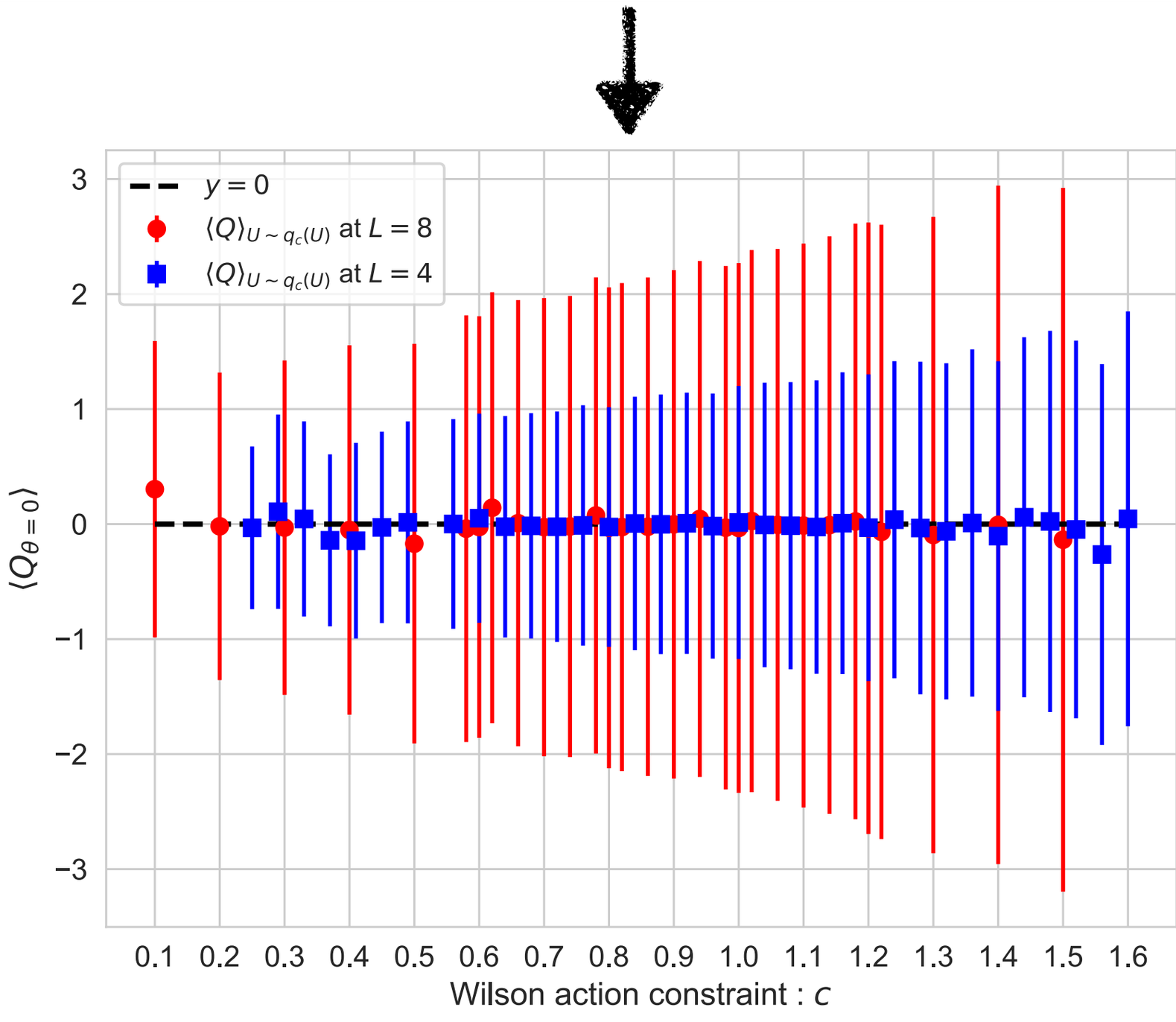
$$\frac{\rho_L(c)}{\rho_L(c = 1.0)}$$



Most states contribute to
$S_{Wilson}[U] = 1.0$

Learning the constraints I : Wilson action

Sanity check : Simulating without θ–term equivalent to setting $\theta = 0$, all sectors must be sampled giving a net $\langle Q \rangle \approx 0$



Summary & outlook

- NF-based DoS method applied to 2D U(1) LGT
- Successfully learned action constraints and computed DoS (preliminary)
- Learned configurations with fixed topological charge

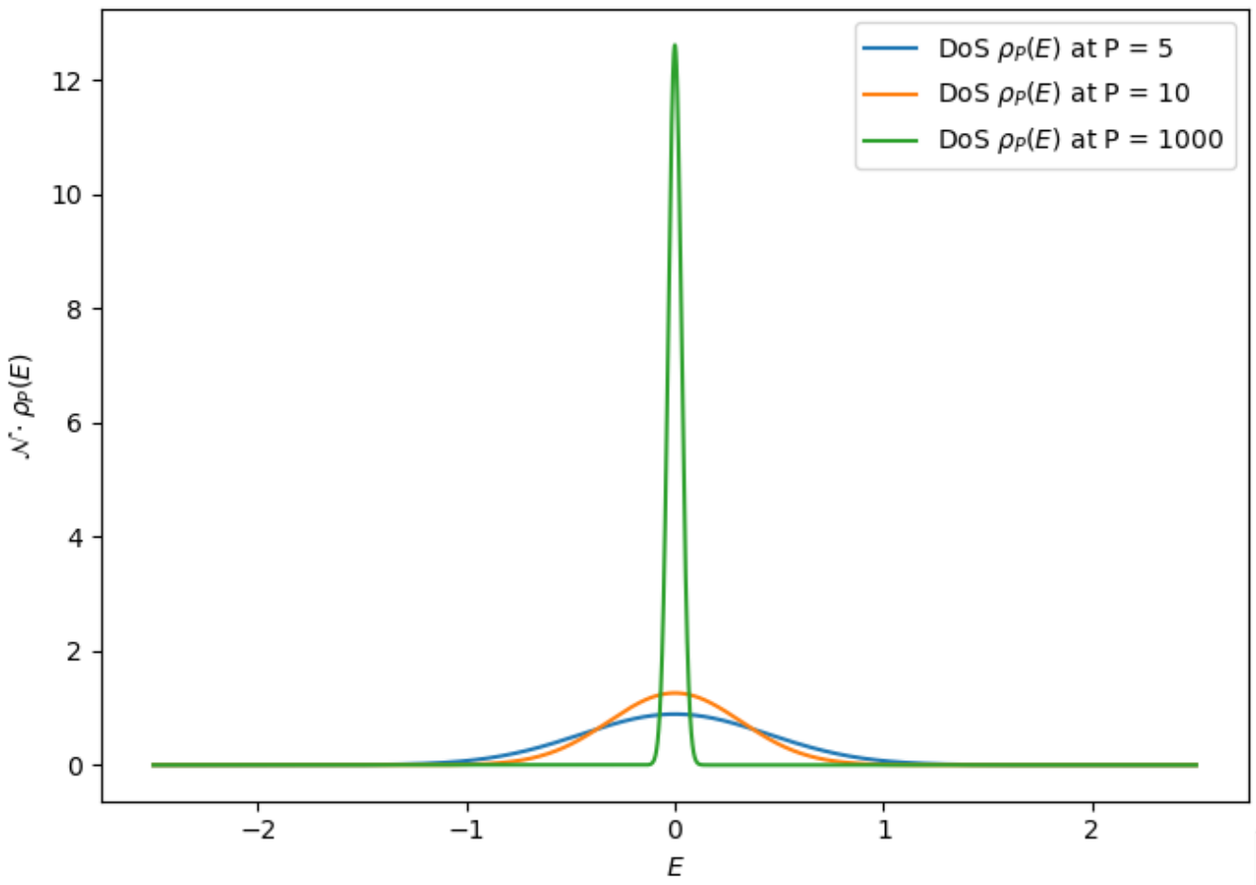
Next Steps

- Explore more expressive architectures for 2D U(1)
- Compute DoS for 2D U(1) with θ–term to reconstruct $Z(\theta)$
- Extend the method beyond 2D to study the de-confinement phase transition (like in [A. Bazavov, B. A. Berg, Daping Du, Y. Meurice (2012)])
- Also in the works: Hubbard model with a chemical potential

Thank you for your attention !

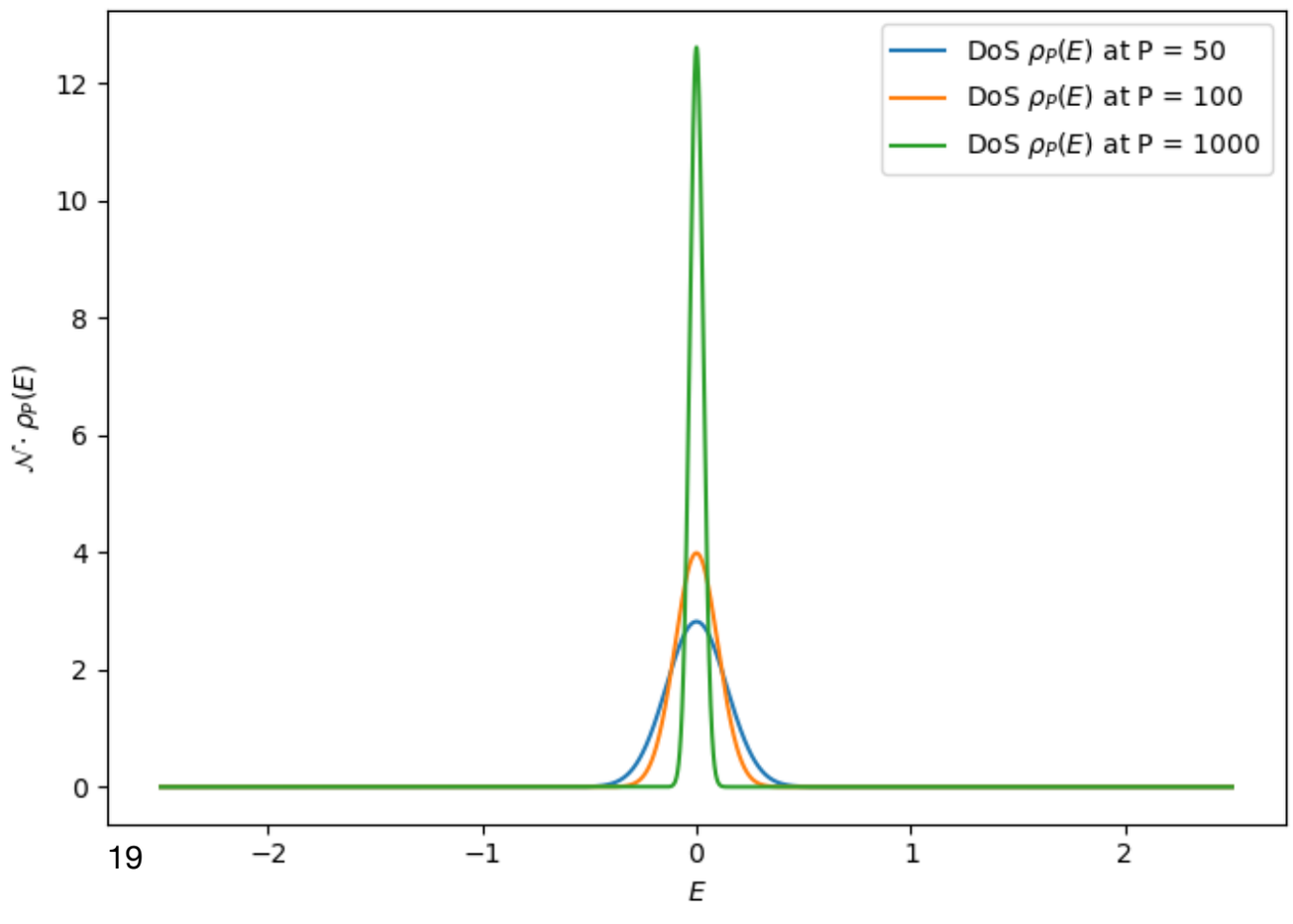
BACKUP SLIDES

Gaussian limit of Dirac delta



- most papers use $P \sim 1000$
- Used $P \sim 5 \,\&\, 50$ for theta term

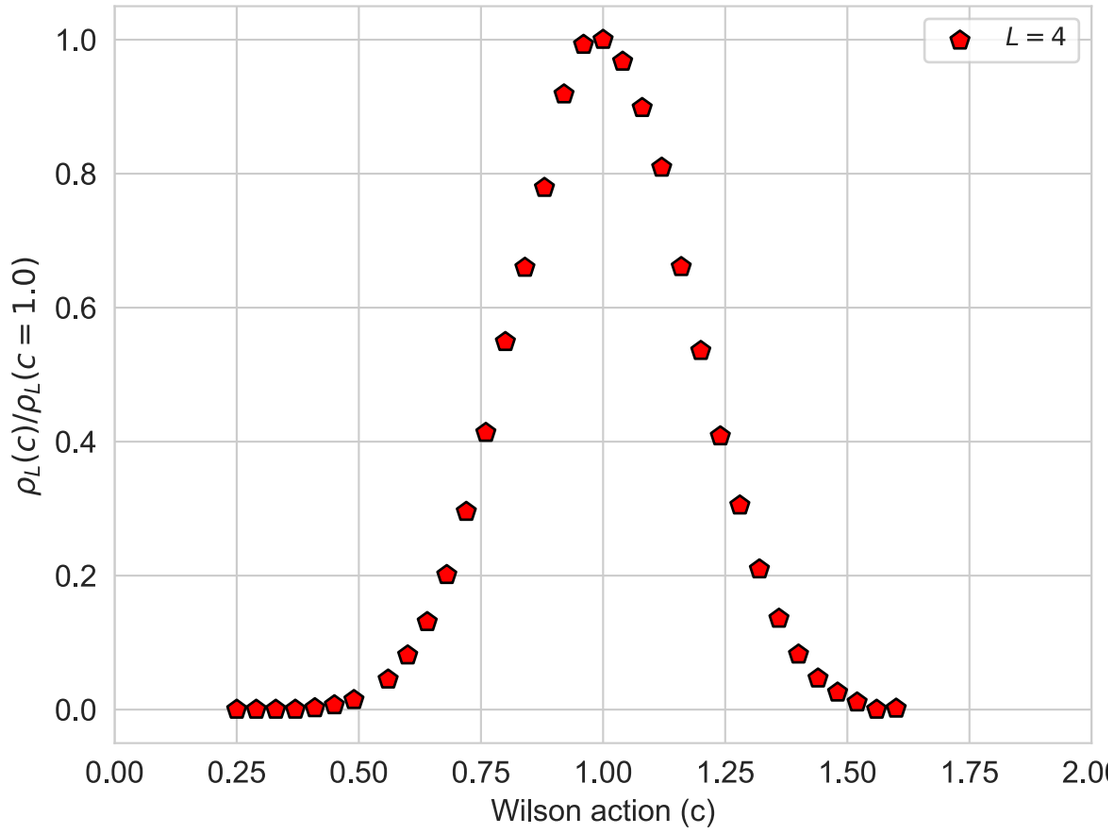
- Used $P \sim 2000$ for pure Wilson gauge theory

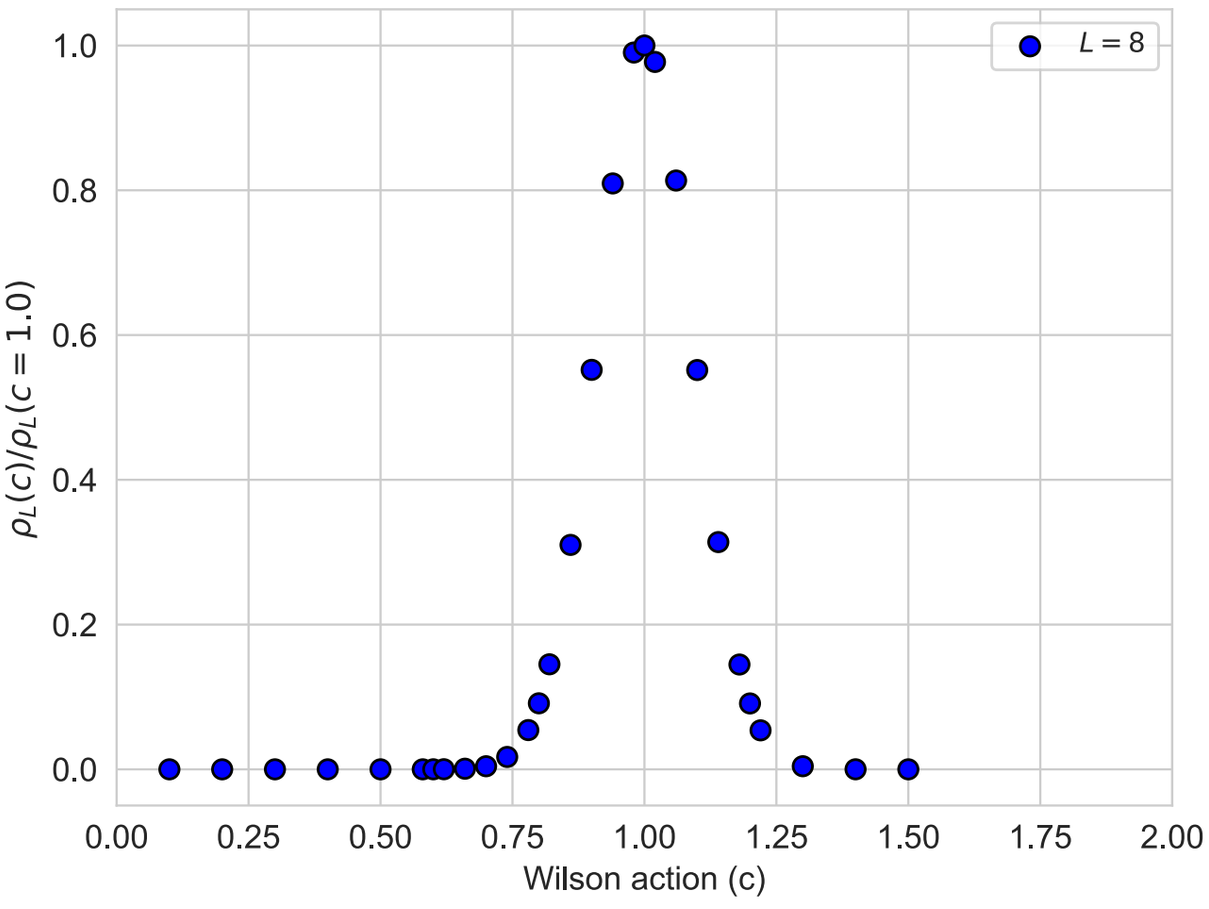


First results on DoS of wilson action

Some first results on :

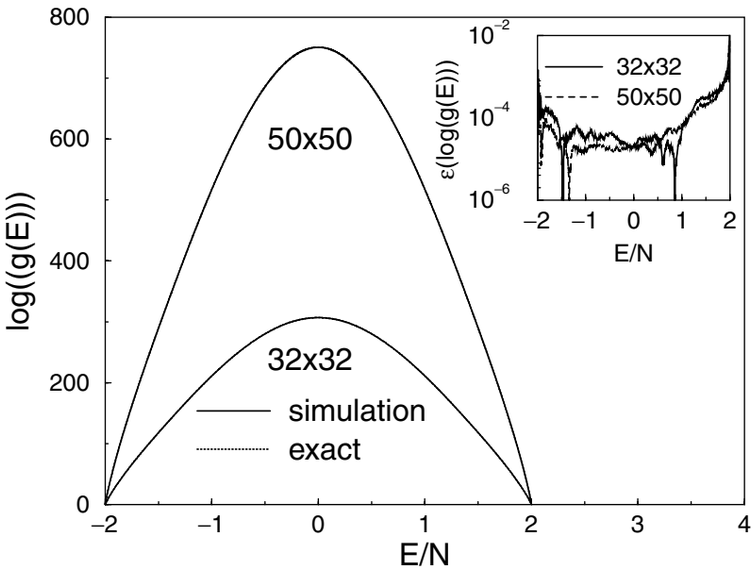
$$\frac{\rho_L(c)}{\rho_L(c=1.0)}$$

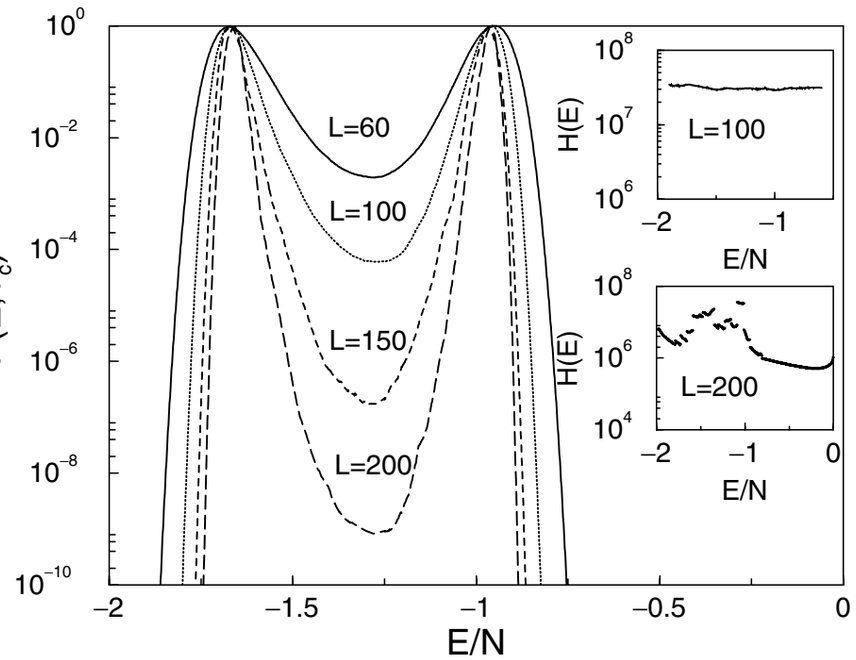




Intuitively makes sense - most states contribute to $S_{Wilson}[U] = 1.0$

Original motivation for DoS: Efficient simulations near criticality

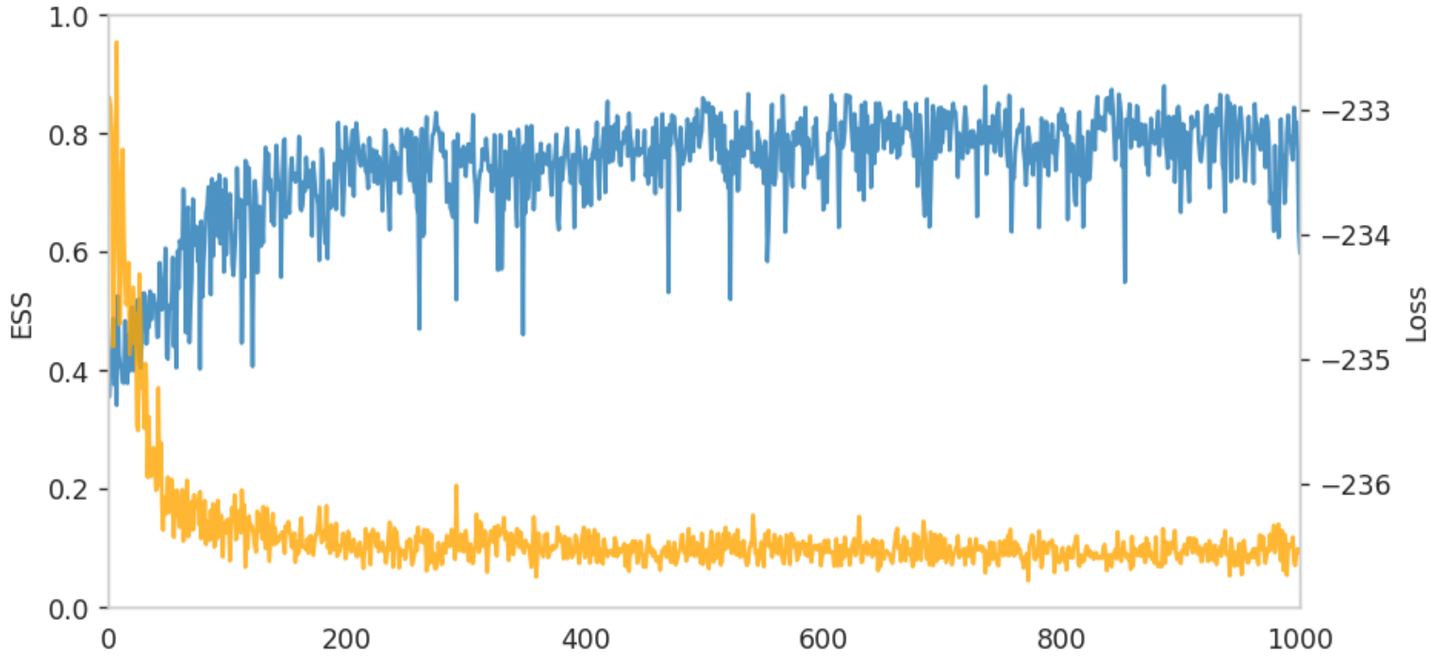




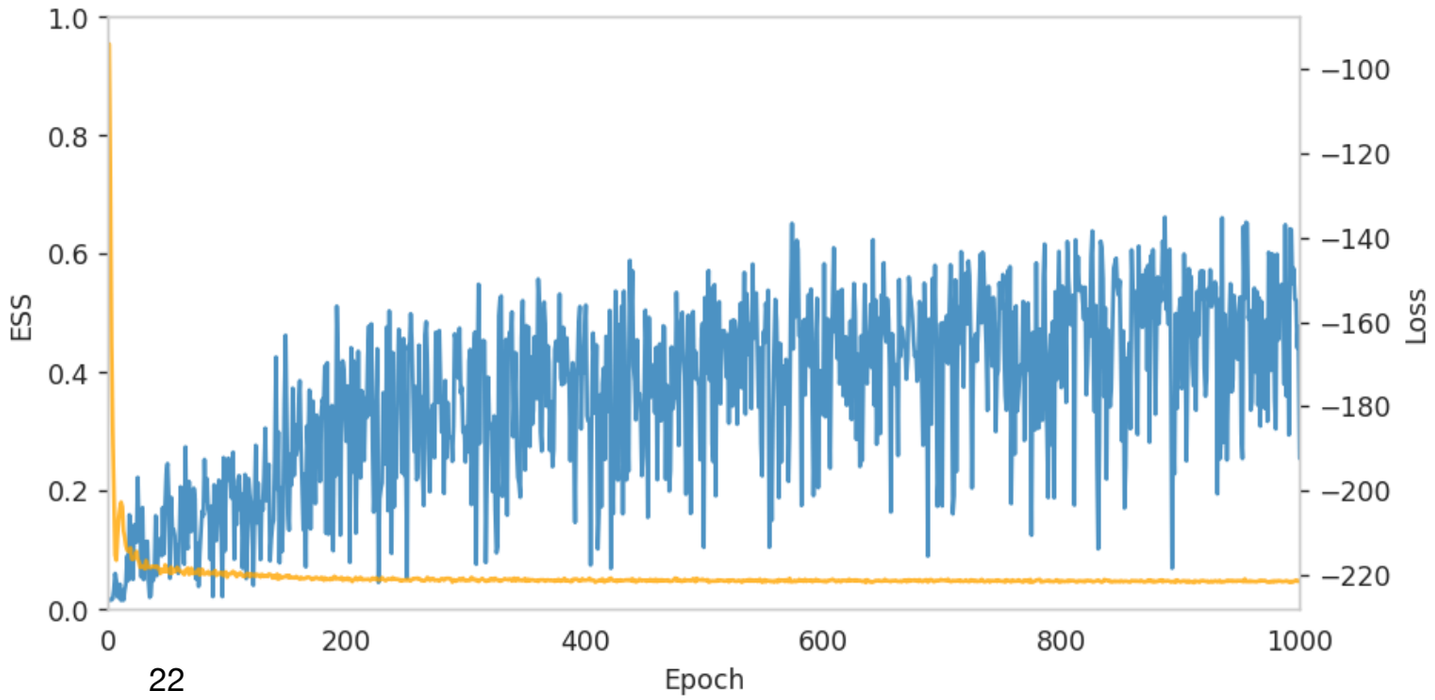
[F. Wang and D. P. Landau (2001)]

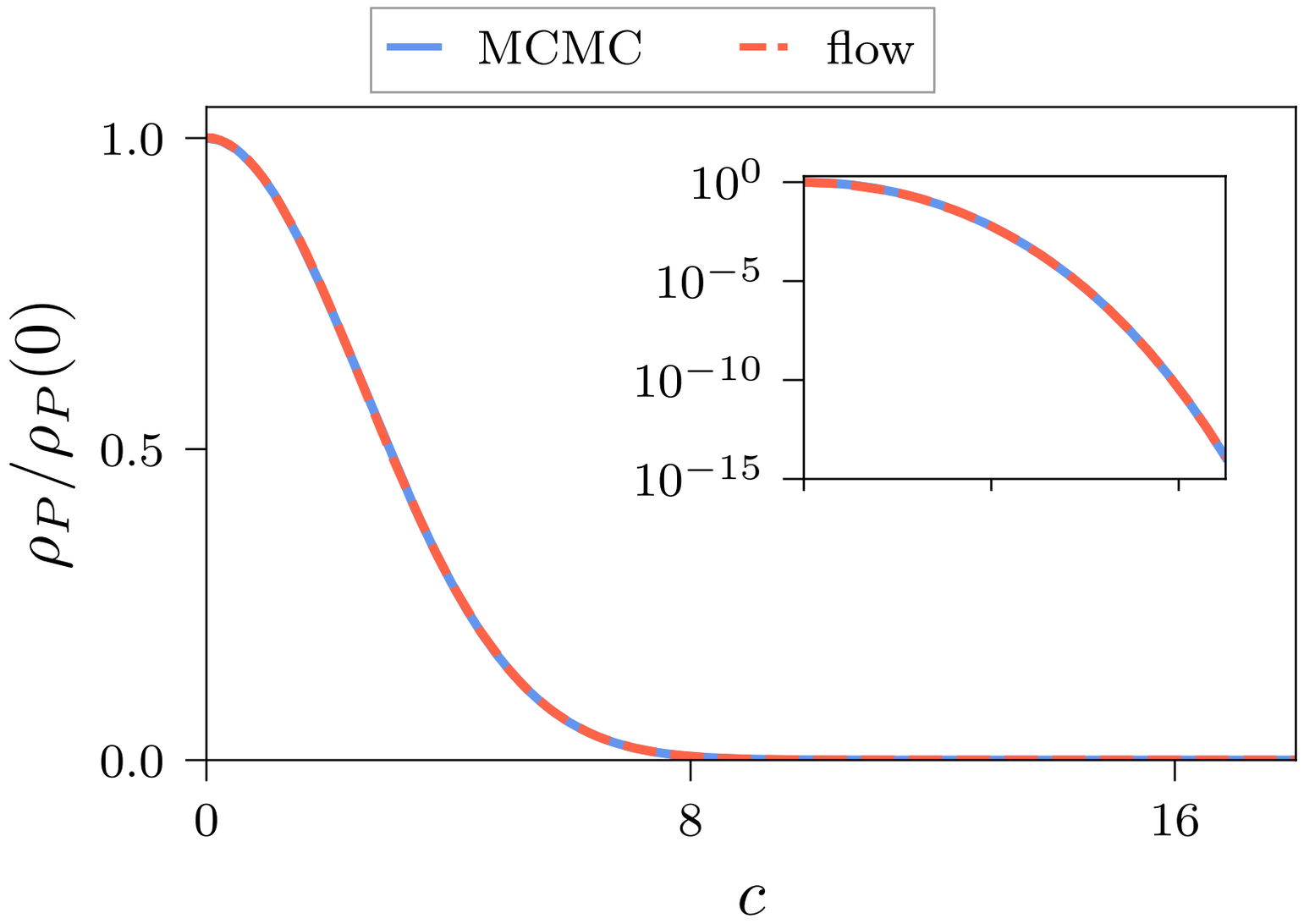
Now the challenges : ESS drops with increasing β, moving away from the constraint where most states contribute, and increasing P

$$P = 1000\,, S_E = 1.0\ , L^2 = 8 \times 8$$



$$P = 1000\,, S_E = 1.5\ , L^2 = 8 \times 8$$





(a)

[J. M. Pawlowski, J. M. Urban (2023)]