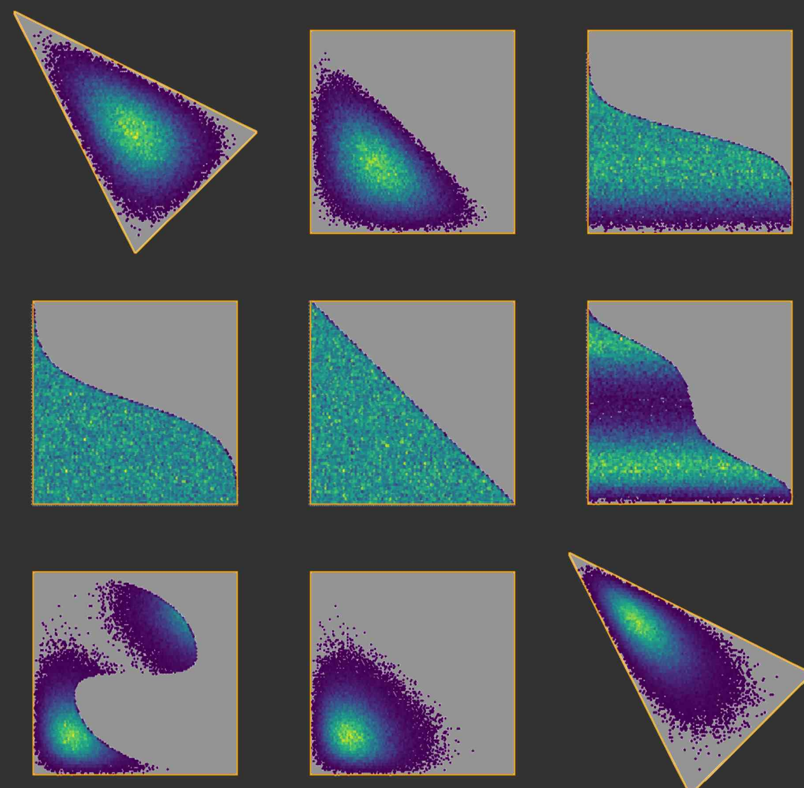
Constructing approximate semi-analytic and machine-learned trivializing maps for lattice gauge theory



Julian M. Urban

lettucefield.org

MIT / IAIFI

Collaborators

Phiala Shanahan

Daniel Hackett

Denis Boyda

Fernando Romero-Lopez

Ryan Abbott

JMU

DeepMind

Danilo Rezende

Sebastien Racaniere

Ali Razavi

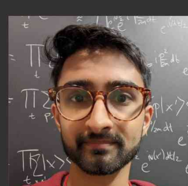
Alexander Matthews

Aleksandar Botev

UNIVERSITÄT BERN

AEC ALBERT EINSTEIN CENTER FOR FUNDAMENTAL PHYSICS

Gurtej Kanwar



NYU

Michael Albergo

THE UNIVERSITY of WISCONSIN MADISON

Kyle Cranmer

Talks by collaborators

Thursday, 15:10

Practical applications of machine-learned flows on gauge fields

Daniel Hackett

Denis Boyda

Enhancing expressivity in machine learning: application of normalizing flows in LQCD

Thursday, 14:50

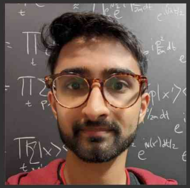
Ryan Abbott

Multiscale normalizing flows for gauge theories

Monday, 16:20

Monday, 10:00

Flow-based sampling for lattice field theories



Gurtej Kanwar

Basic concepts

- Change of variables $Z = \int \mathrm{d}U \, e^{-S} = \int \mathrm{d}V \, e^{-S + \log |J|}$

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  - $S' \equiv S_{\mathrm{defect}}$ $\longrightarrow$ restoration of topological ergodicity (cf. Dan Hackett's talk)

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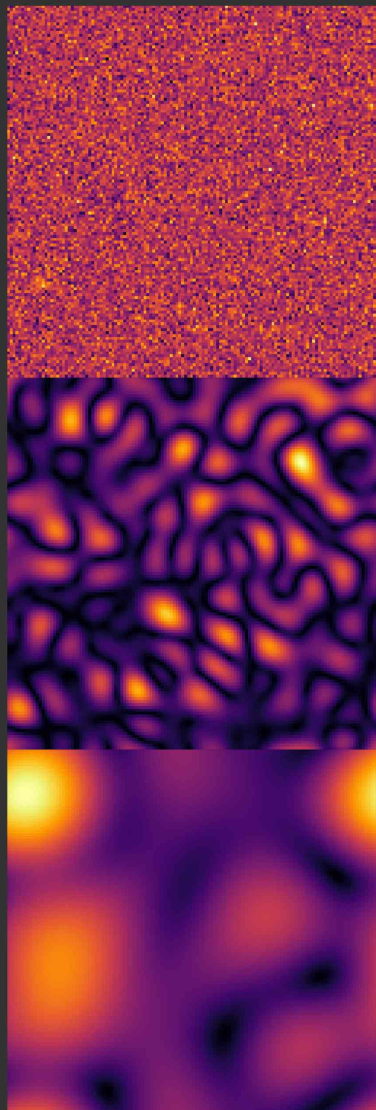
  - $S' \equiv S_{\mathrm{defect}}$ $\longrightarrow$ restoration of topological ergodicity (cf. Dan Hackett's talk)
  - $S' \equiv S_{\Lambda}$ $\longrightarrow$ renormalization group interpretation (cf. backup slides)

Lüscher [arXiv:0907.5491]

(f) *Renormalization group.* By composing the trivializing map $U = \mathcal{F}_1(V)$ in the Wilson theory with its inverse at another value of the gauge coupling, one obtains a group of transformations whose only effect on the action is a shift of the coupling. The locality properties of these transformations are not transparent, however, and could be quite different from the ones of a Wilsonian "block spin" transformation.

Wilson vs Kadanoff

Huang, *Statistical Mechanics*



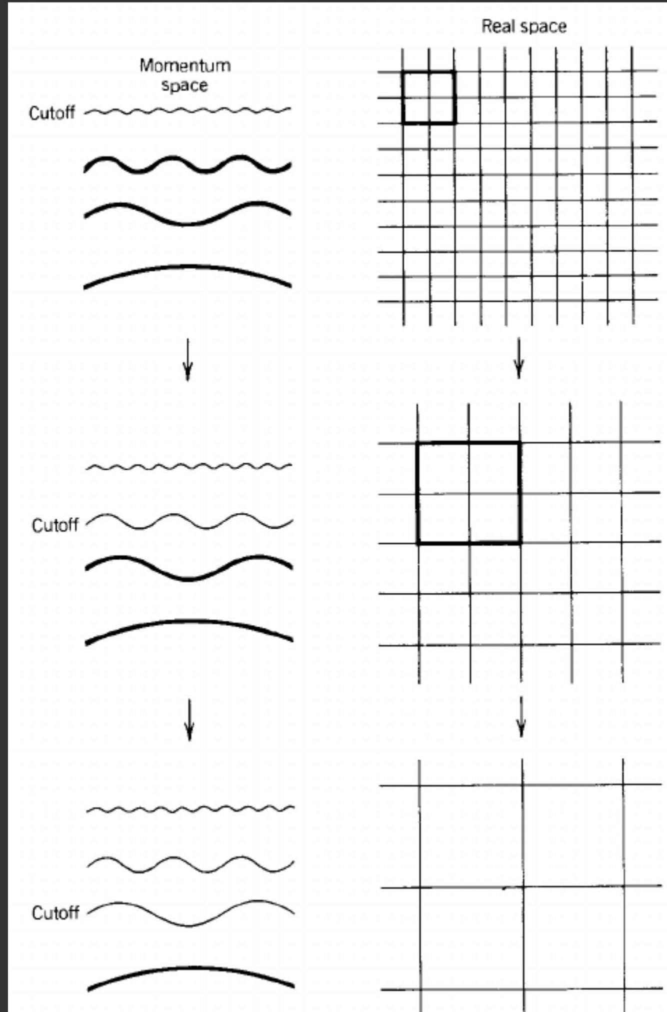
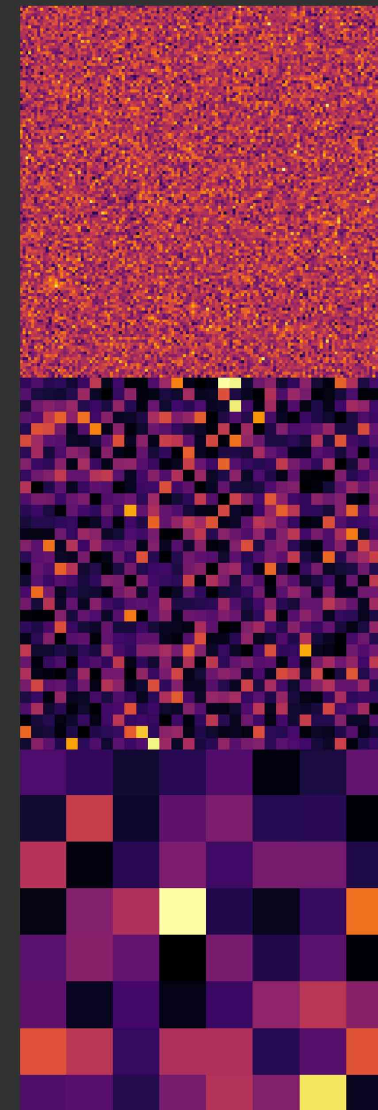
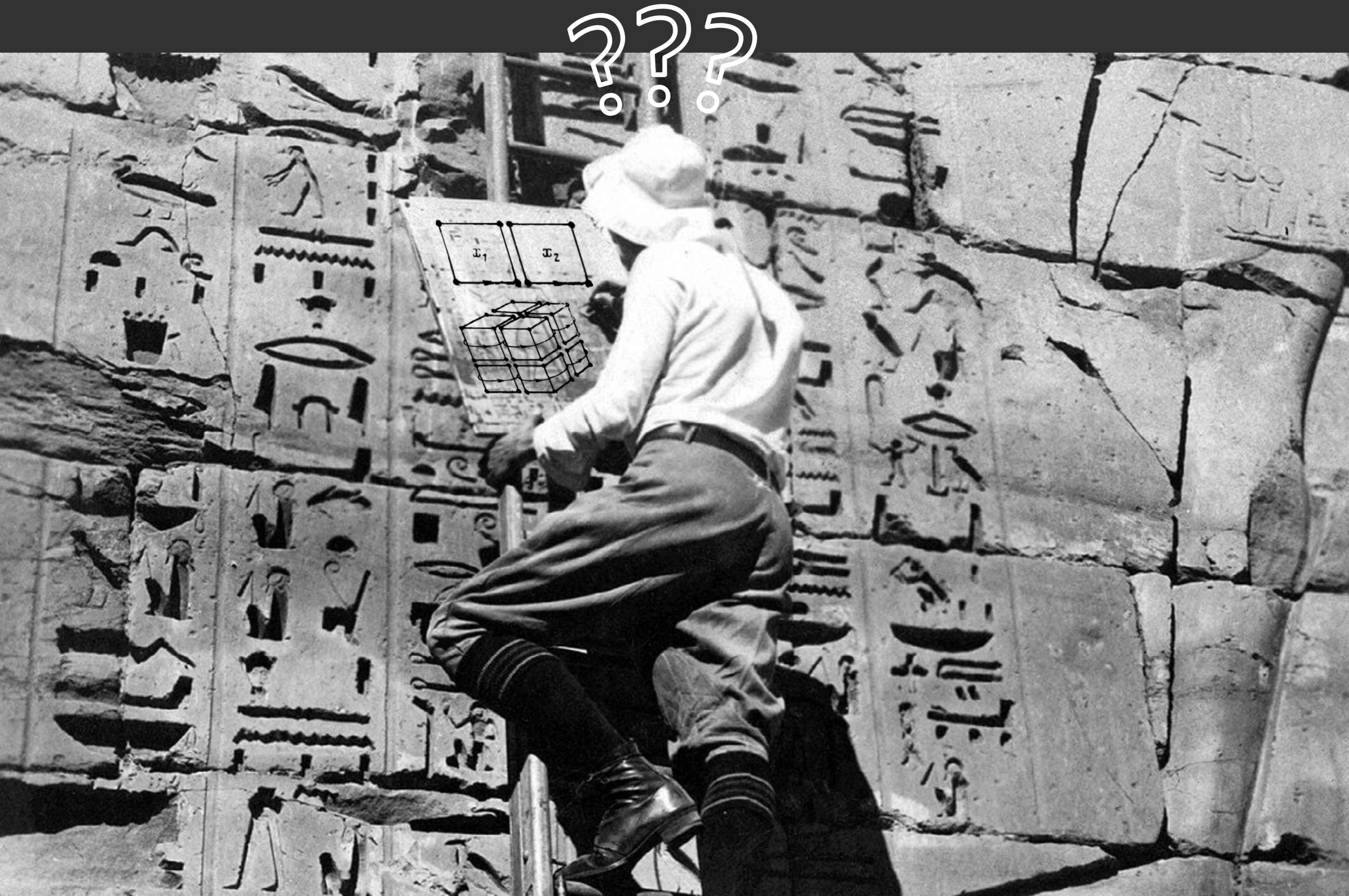


Fig. 18.5 Coarse-graining in momentum space and in real space. In the former, one effectively lowers the cutoff. In the latter, one blots out finer details, enlarging the effective lattice spacing.



Archeological survey of trivializing maps for LGT



Recursion equations in gauge field theories

A. A. Migdal

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences
(Submitted April 28, 1975)
Zh. Eksp. Teor. Fiz. **69**, 810–822 (September 1975)

An approximate recursion equation is formulated, describing the scale transformation of the effective action of a gauge field. In two-dimensional space-time the equation becomes exact. In four-dimensional theories it reproduces asymptotic freedom to an accuracy of 30% in the coefficients of the β-function. In the strong-coupling region the β-function remains negative and this results in an asymptotic prison in the infrared region. Possible generalizations and applications to the quark-gluon gauge theory are discussed.

PACS numbers: 11.10.Np

Notes on Migdal's Recursion Formulas*

LEO P. KADANOFF[†]

The James Franck Institute, The University of Chicago, Chicago, Illinois 60637

Received March 24, 1976

A set of renormalization group recursion formulas which were proposed by Migdal are rederived, reinterpreted, and critically analyzed. The new derivation shows the connection between these formulas and previous work on renormalization via decimation

MIGDAL-KADANOFF RECURSION RELATIONS IN SU(2) AND SU(3) GAUGE THEORIES

Michael NAUENBERG

Physics Department, University of California, Santa Cruz, California 95060 and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA

Doug TOUSSAINT

Physics Department and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA

Received 23 October 1980

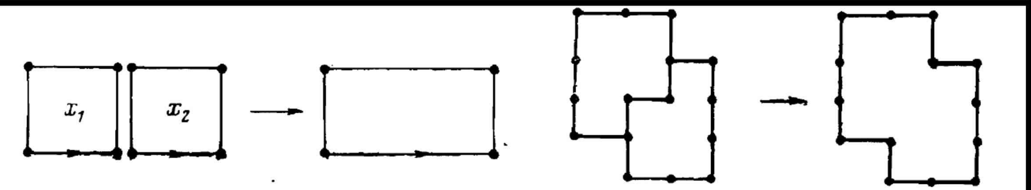
We study the Migdal recursion relations and the reformulation due to Kadanoff for SU(2) and SU(3) lattice gauge theory, using analytic approximations for large and small couplings and numerical methods for all couplings. In SU(2) we obtain the beta function and the expectation value of the plaquette, which is compared with recent Monte Carlo results. In analogy to U(1), we find that a Villain form (periodic gaussian) for the exponential of the plaquette action is a good approximation to the result of the Migdal renormalization transformation. We also perform some calculations in SU(3) and find that its behavior is similar to SU(2).

Phase transitions in gauge and spin-lattice systems

A. A. Migdal

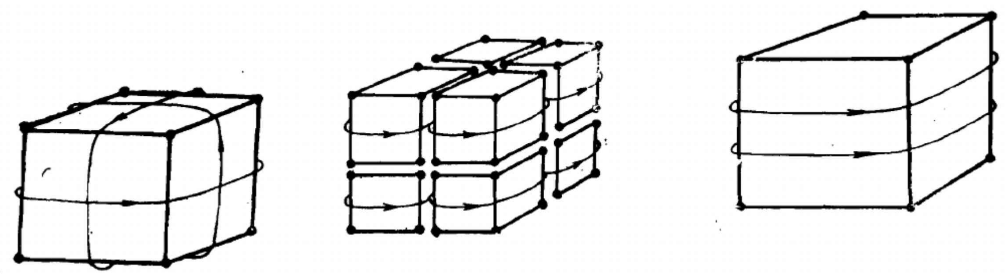
L. D. Landau Theoretical Physics Institute, USSR Academy of Sciences
(Submitted June 11, 1975)
Zh. Eksp. Teor. Fiz. **69**, 1457–1465 (October 1975)

A simple recursion equation giving an approximate description of critical phenomena in lattice systems is proposed. The equations for a d-dimensional spin system and a $2d$-dimensional gauge system coincide. An interesting consequence is the zero transition temperature in the two-dimensional Heisenberg model and four-dimensional Yang-Mills model; this corresponds to asymptotic freedom in field theory.



As above, the integration is carried out independently in each plane, and joining 2^D L-cubes into one 2L-cube, we obtain

$$Z_{2L} = \prod_{\mu<\nu}\prod_{x_\perp,i}\sum_{p} F_p^4(L)\, d_p \chi_p(v_{\mu\nu}(x_\perp)), \tag{38}$$



GROUP INTEGRATION FOR LATTICE GAUGE THEORY AT LARGE *N* AND AT SMALL COUPLING*

Richard C. BROWER and Michael NAUENBERG

Physics Department, University of California, Santa Cruz, California 94064, USA

Received 15 July 1980

We consider the fundamental SU(N) invariant integrals encountered in Wilson's lattice QCD with an eye to analytical results for $N \to \infty$ and approximations for small g^2 at fixed N. We develop a new semiclassical technique starting from the Schwinger-Dyson equations cast in differential form to give an exact solution to the *single*-link integral for $N \to \infty$. The third-order phase transition discovered by Gross and Witten for two-dimensional QCD occurs here for any

Contemporary survey of trivializing maps for LGT

Trivializing maps, the Wilson flow and the HMC algorithm

Martin Lüscher

Tackling critical slowing down using global correction steps with equivariant flows: the case of the Schwinger model

Jacob Finkenrath[1]

hi

Use of Schwinger-Dyson equation in constructing an approximate trivializing map

Decimation Map in 2D for accelerating HMC

Monday, 16:00

Peter Boyle,[a,b] Taku Izubuchi,[b,c] Luchang Jin,[d] Chulwoo Jung,[b] Christoph Lehner,[e] Nobuyuki Matsumoto[c] and Akio Tomiya[f]

Learning Trivializing Gradient Flows for Lattice Gauge Theories

Simone Bacchio,[1] Pan Kessel,[2,3] Stefan Schaefer,[4] and Lorenz Vaitl[2]

Equivariant flow-based sampling for lattice gauge theory

Gurtej Kanwar,[1] Michael S. Albergo,[2] Denis Boyda,[1] Kyle Cranmer,[2] Daniel C. Hackett,[1] Sébastien Racanière,[3] Danilo Jimenez Rezende,[3] and Phiala E. Shanahan[1]

Sampling using SU(N) gauge equivariant flows

Denis Boyda,[1,*] Gurtej Kanwar,[1,†] Sébastien Racanière,[2,‡] Danilo Jimenez Rezende,[2,§] Michael S. Albergo,[3] Kyle Cranmer,[3] Daniel C. Hackett,[1] and Phiala E. Shanahan[1]

Flow-based sampling in the lattice Schwinger model at criticality

Michael S. Albergo,[1] Denis Boyda,[2,3,4] Kyle Cranmer,[1] Daniel C. Hackett,[3,4] Gurtej Kanwar,[5,3,4] Sébastien Racanière,[6] Danilo J. Rezende,[6] Fernando Romero-López,[3,4] Phiala E. Shanahan,[3,4] and Julian M. Urban[7]

Gauge-equivariant flow models for sampling in lattice field theories with pseudofermions

Ryan Abbott,[1,2] Michael S. Albergo,[3] Denis Boyda,[4,1,2] Kyle Cranmer,[3] Daniel C. Hackett,[1,2] Gurtej Kanwar,[5,1,2] Sébastien Racanière,[6] Danilo J. Rezende,[6] Fernando Romero-López,[1,2] Phiala E. Shanahan,[1,2] Betsy Tian,[1] and Julian M. Urban[7]

Sampling QCD field configurations with gauge-equivariant flow models

Ryan Abbott,[a,b] Michael S. Albergo,[c] Aleksandar Botev,[g] Denis Boyda,[a,b,d] Kyle Cranmer,[c,e] Daniel C. Hackett,[a,b] Gurtej Kanwar,[a,b,f] Alexander G. D. G. Matthews,[g] Sébastien Racanière,[g] Ali Razavi,[g] Danilo J. Rezende,[g] Fernando Romero-López,[a,b] Phiala E. Shanahan[a,b,*] and Julian M. Urban[a,b,h]

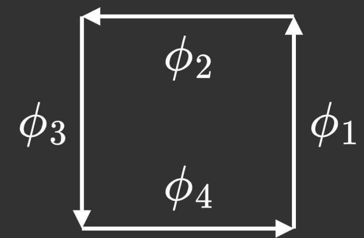
Normalizing flows for lattice gauge theory in arbitrary space-time dimension

Ryan Abbott,[1,2] Michael S. Albergo,[3] Aleksandar Botev,[4] Denis Boyda,[1,2] Kyle Cranmer,[5] Daniel C. Hackett,[1,2] Gurtej Kanwar,[6,1,2] Alexander G.D.G. Matthews,[4] Sébastien Racanière,[4] Ali Razavi,[4] Danilo J. Rezende,[4] Fernando Romero-López,[1,2] Phiala E. Shanahan,[1,2] and Julian M. Urban[1,2]

To be continued ...

(Un-)trivializing (1+1)d U(1) LGT

$$\phi_k \in [0, 2\pi),\ S = -\beta \cos\left(\sum_{k=1}^{4} \phi_k\right)$$



$$Z = \prod_{k=1}^{4} \left(\int_0^{2\pi} \mathrm{d}\phi_k\right) \exp(-S\left(\sum_{k=1}^{4} \phi_k\right))$$

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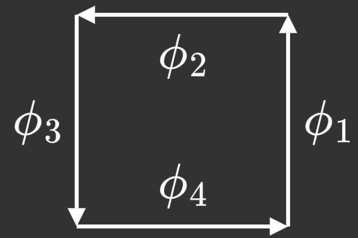

$Z = \prod_{k=1}^{4} \Big(\int_0^{2\pi} \mathrm{d}\phi_k\Big) \exp(-S\Big(\sum_{k=1}^{4} \phi_k\Big))$

- Change of variables: $\chi(\phi_1) = \phi_1 + \sum_{k=2}^{4} \phi_k \in \Big[\sum_{k=2}^{4} \phi_k, 2\pi + \sum_{k=2}^{4} \phi_k\Big) \equiv [\underline{\chi}, \overline{\chi}) \longrightarrow \frac{\partial \chi}{\partial \phi_1} = 1$

$$\longrightarrow\ Z = \int_{\underline{\chi}}^{\overline{\chi}} \mathrm{d}\chi \int_0^{2\pi} \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4 \exp\big(\beta \cos(\chi)\big) \equiv \int_0^{2\pi} \mathrm{d}\chi \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4 \exp\big(\beta \cos(\chi)\big)$$

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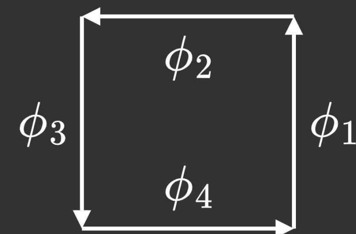

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- Trivialization: $\mathcal{I}(\eta) = \int_0^{\eta} \mathrm{d}x \exp\big(\beta \cos(x)\big),\ \chi' = 2\pi \dfrac{\mathcal{I}(\chi)}{\mathcal{I}(2\pi)} \longrightarrow \dfrac{\partial \chi'}{\partial \chi} = \dfrac{2\pi}{\mathcal{I}(2\pi)} \exp\big(\beta \cos(\chi)\big)$

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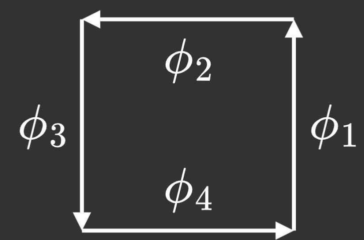

$$Z = \prod_{k=1}^{4} \Big(\int_0^{2\pi} \mathrm{d}\phi_k\Big) \exp\Big(-S\Big(\sum_{k=1}^{4}\phi_k\Big)\Big)$$

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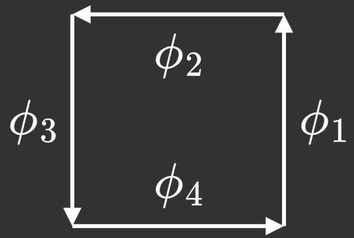

$Z = \prod_{k=1}^{4}\left(\int_0^{2\pi} \mathrm{d}\phi_k\right) \exp(-S\left(\sum_{k=1}^{4}\phi_k\right))$

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change of variables: gauge fields (links) $\longleftrightarrow$ invariants (plaquettes)

$$\longrightarrow Z = \int_{\underline{\chi}}^{\overline{\chi}} \mathrm{d}\chi \int_0^{2\pi} \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4 \exp\left(\beta\cos(\chi)\right) \equiv \int_0^{2\pi} \mathrm{d}\chi \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4 \exp\left(\beta\cos(\chi)\right)$$

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(un-)trivialization via (inverse) cumulative distribution function

$$\longrightarrow Z = \int_0^{2\pi} \mathrm{d}\chi' \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4 \left|\frac{\partial \chi'}{\partial \chi}\right|^{-1} \exp\left(\beta\cos(\chi)\right) = \frac{\mathcal{I}(2\pi)}{2\pi}\int_0^{2\pi} \mathrm{d}\chi' \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4$$

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(Un-)trivializing (1+1)d U(1) LGT

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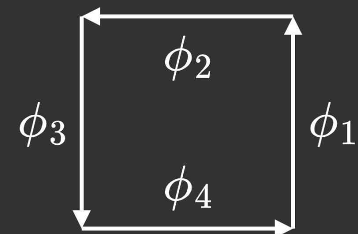
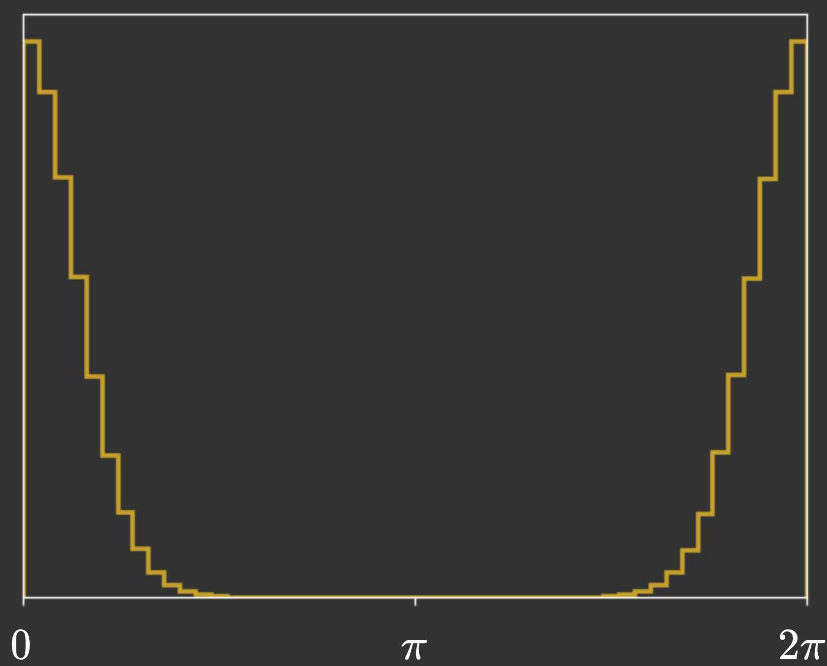


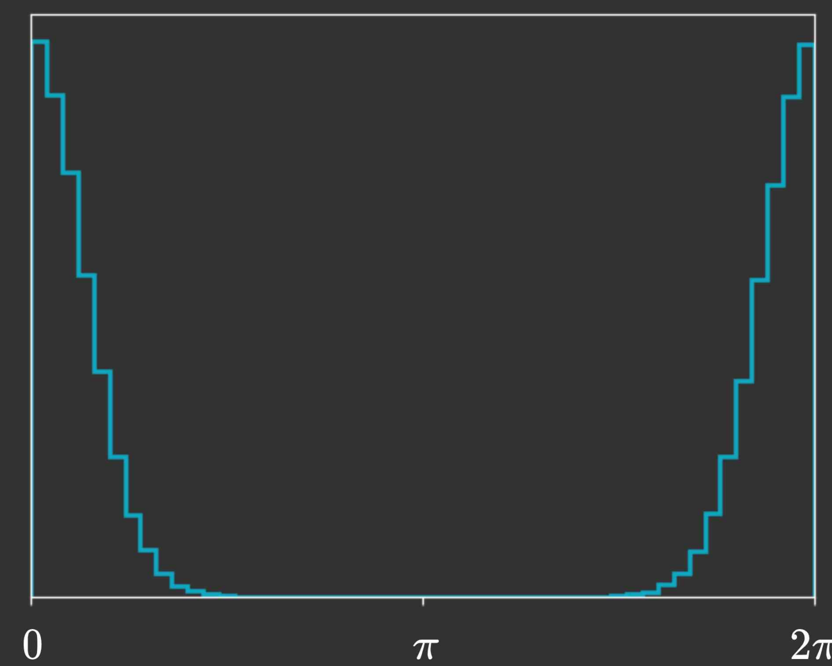
$$Z = \prod_{k=1}^{4} \left(\int_0^{2\pi} \mathrm{d}\phi_k\right) \exp\left(-S\left(\sum_{k=1}^{4} \phi_k\right)\right)$$

$\longrightarrow$ inverse transform sampling the von Mises distribution

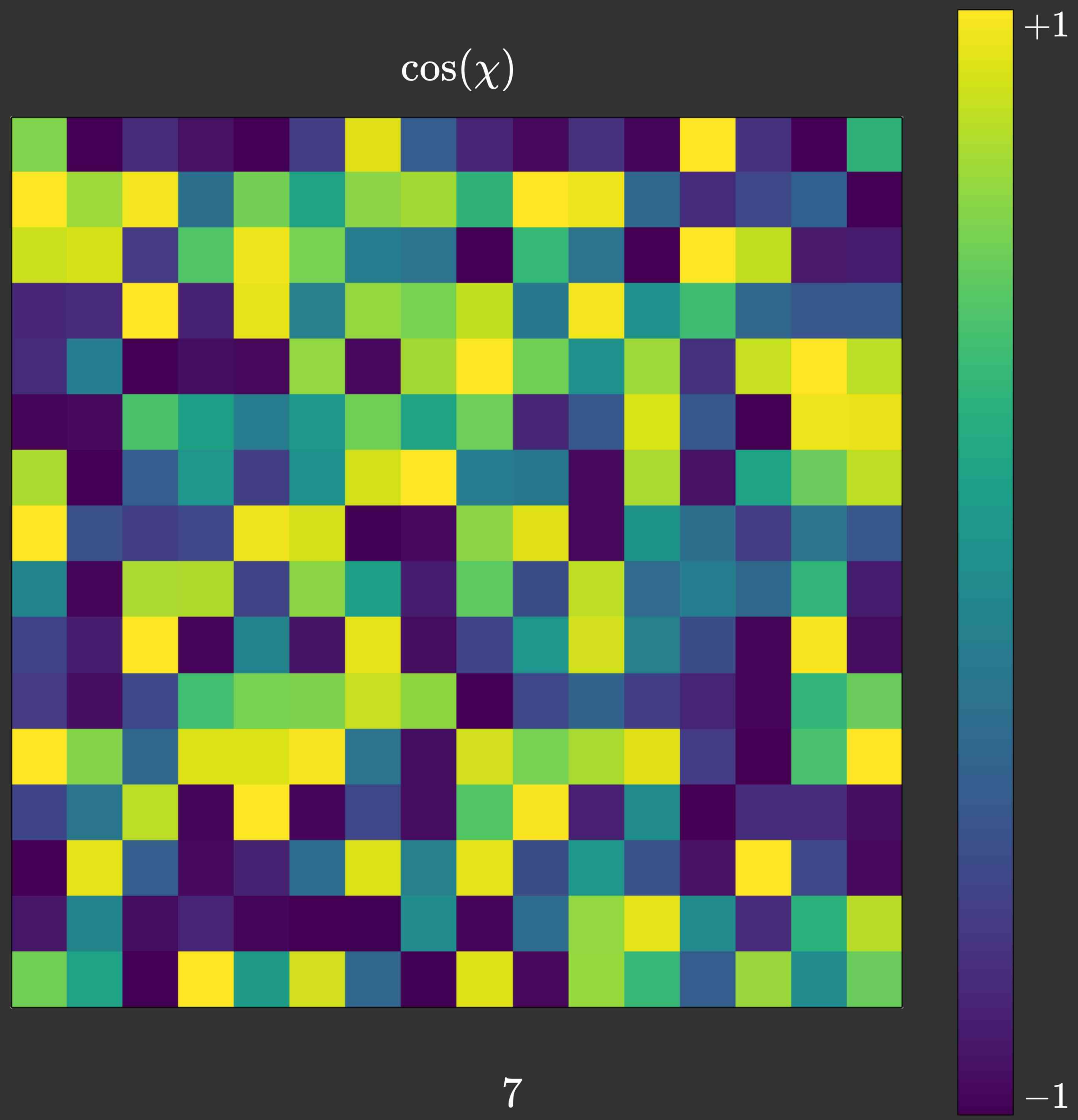
rejection sampling



inverse CDF



(Un-)trivializing (1+1)d U(1) LGT



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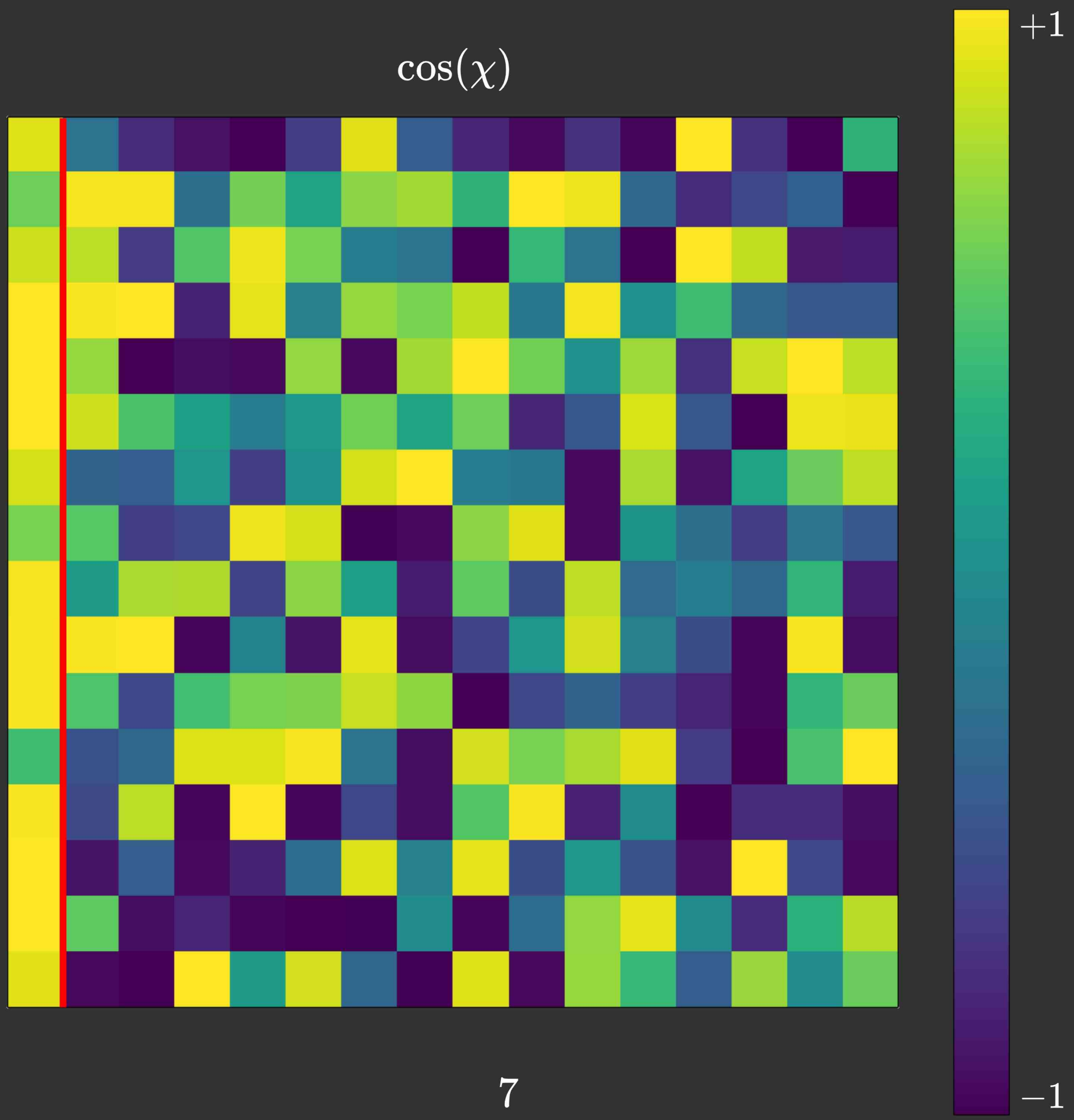

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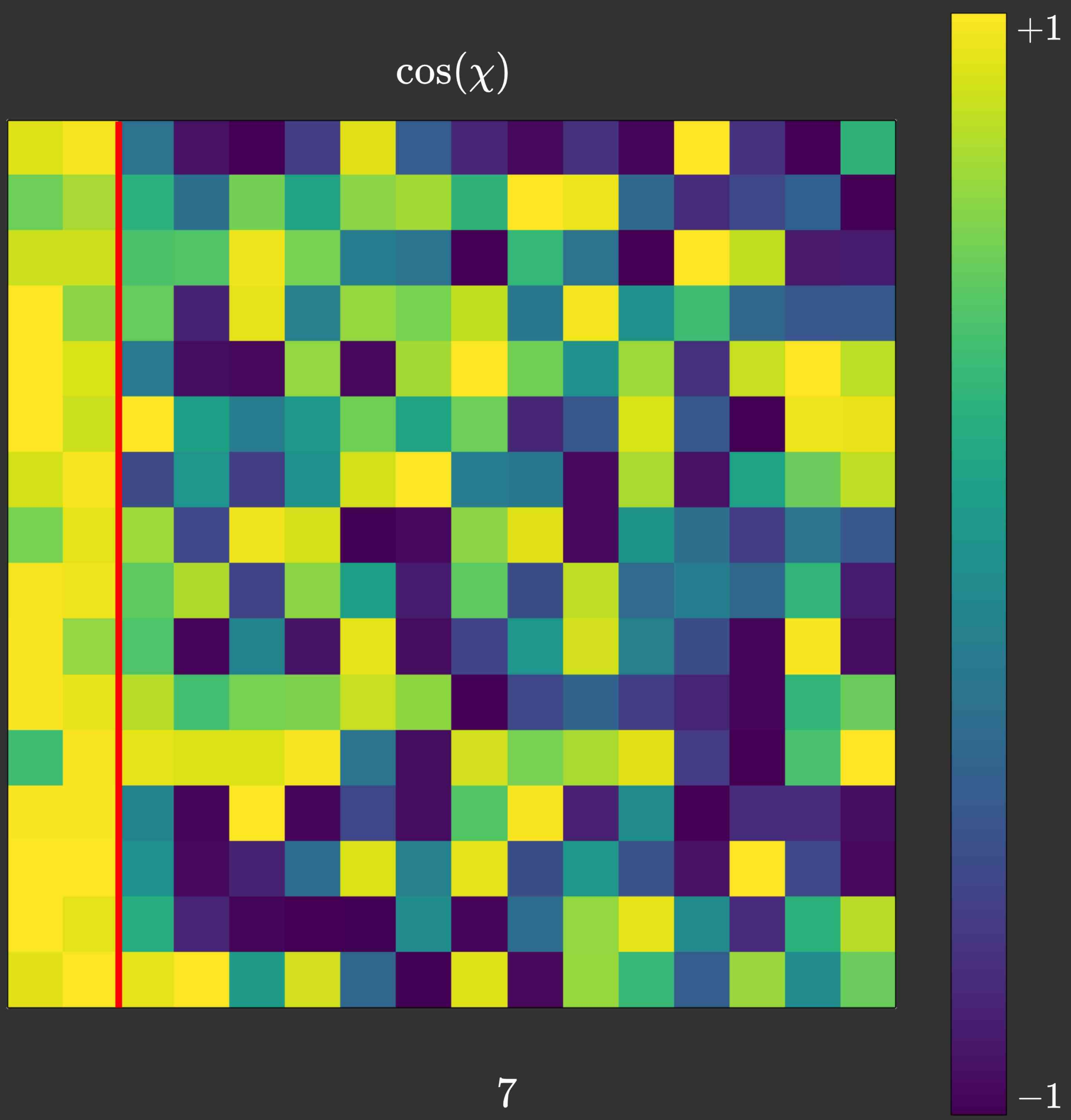

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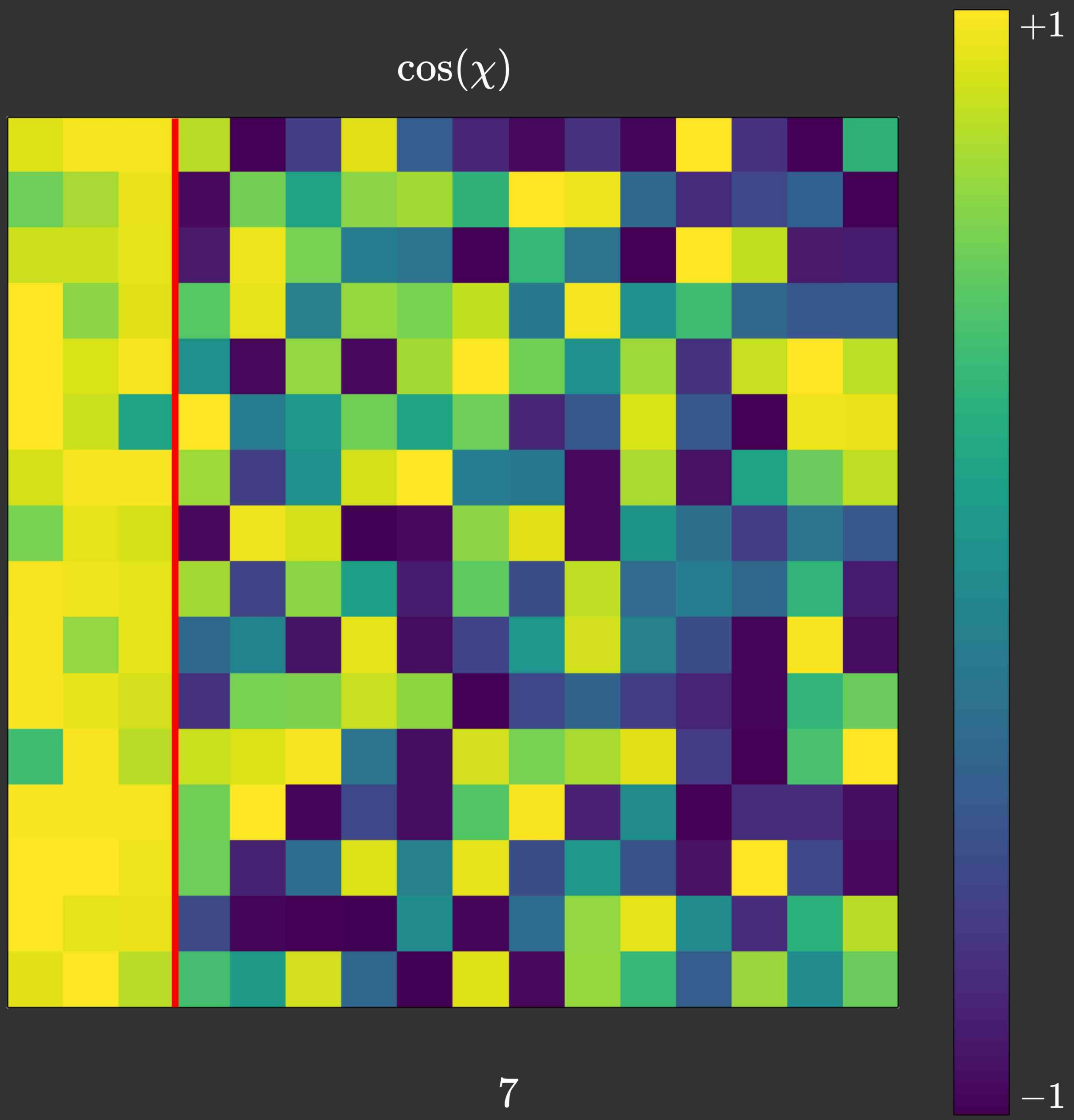
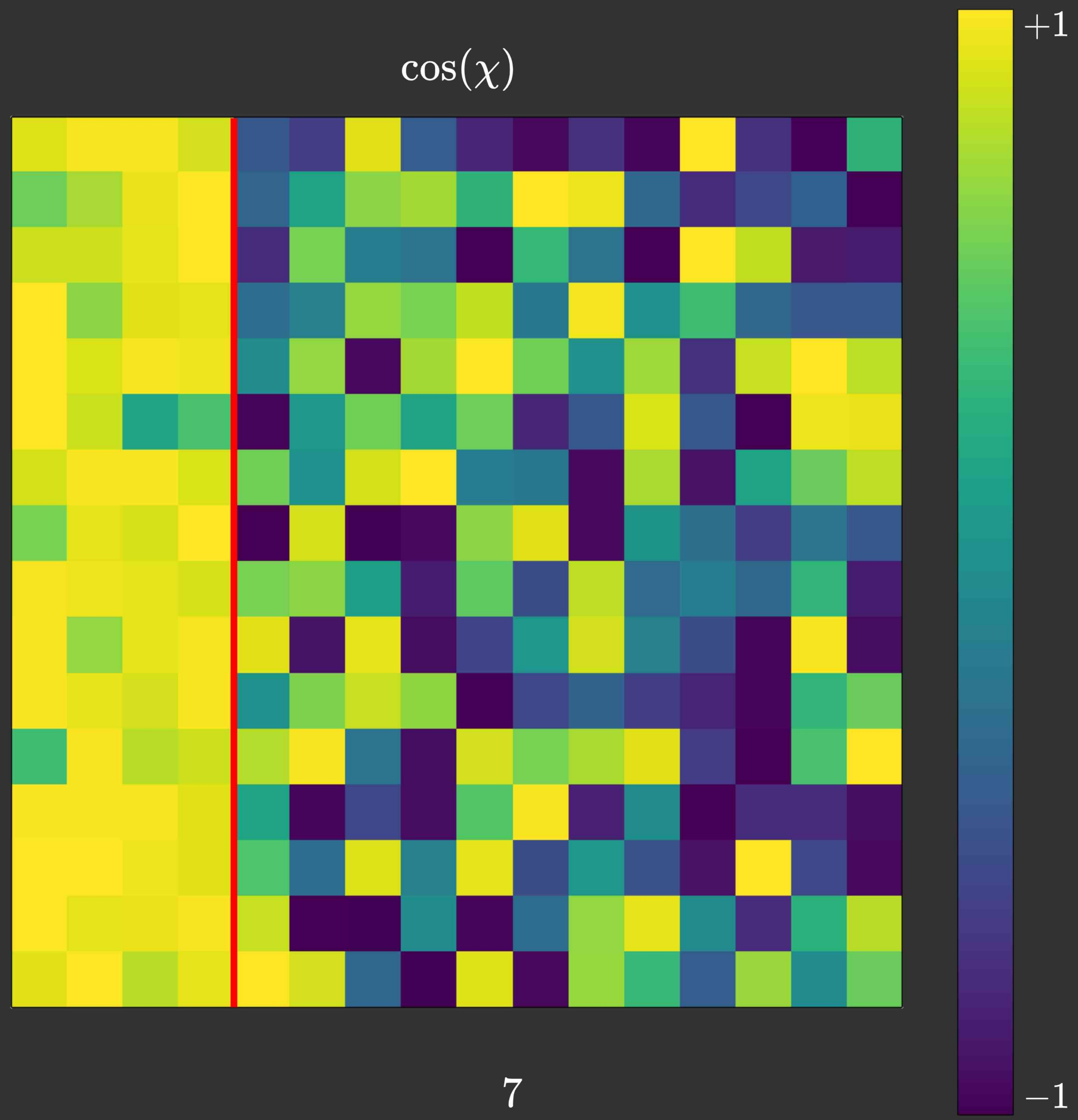
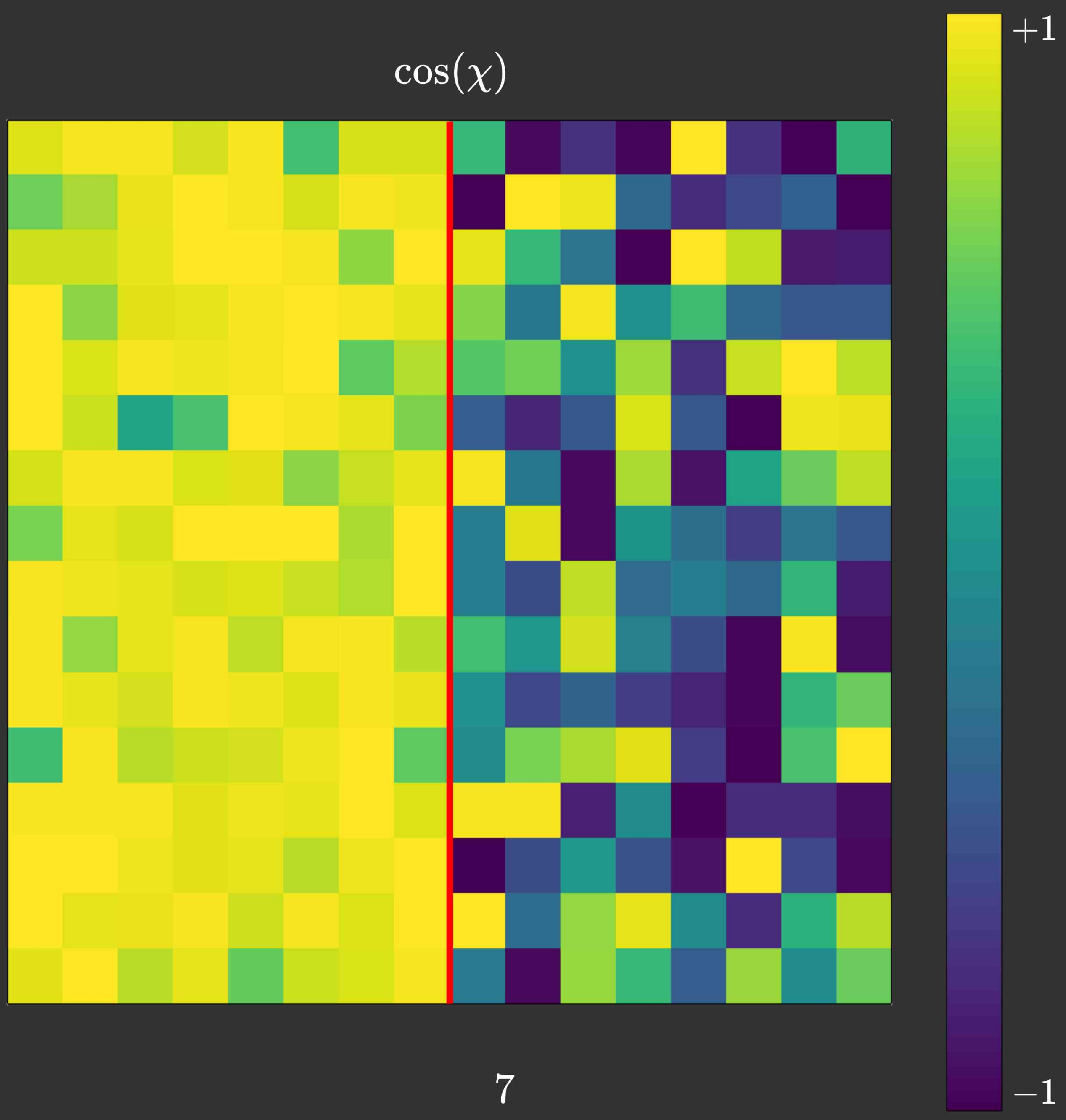


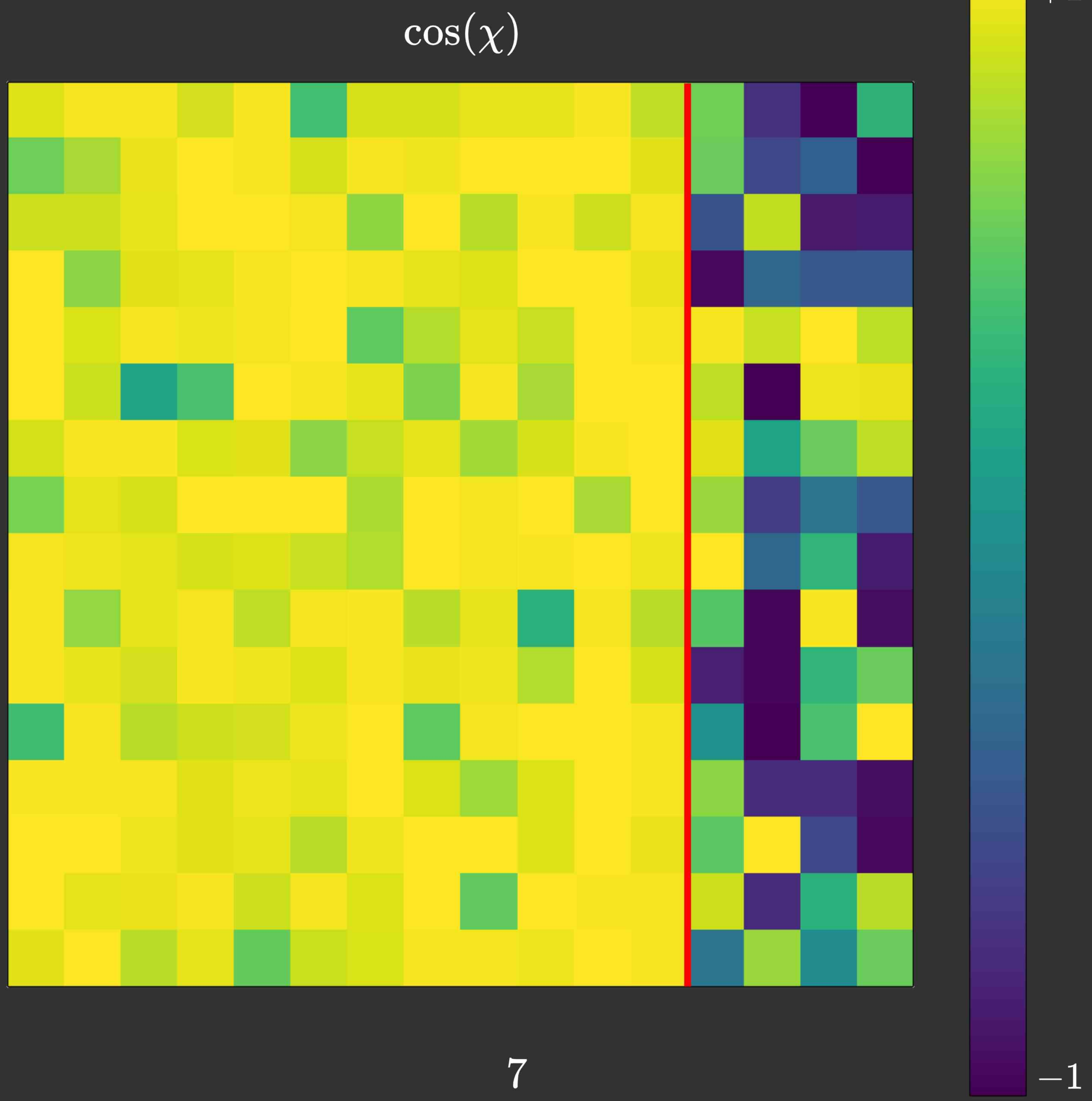
(Un-)trivializing (1+1)d U(1) LGT



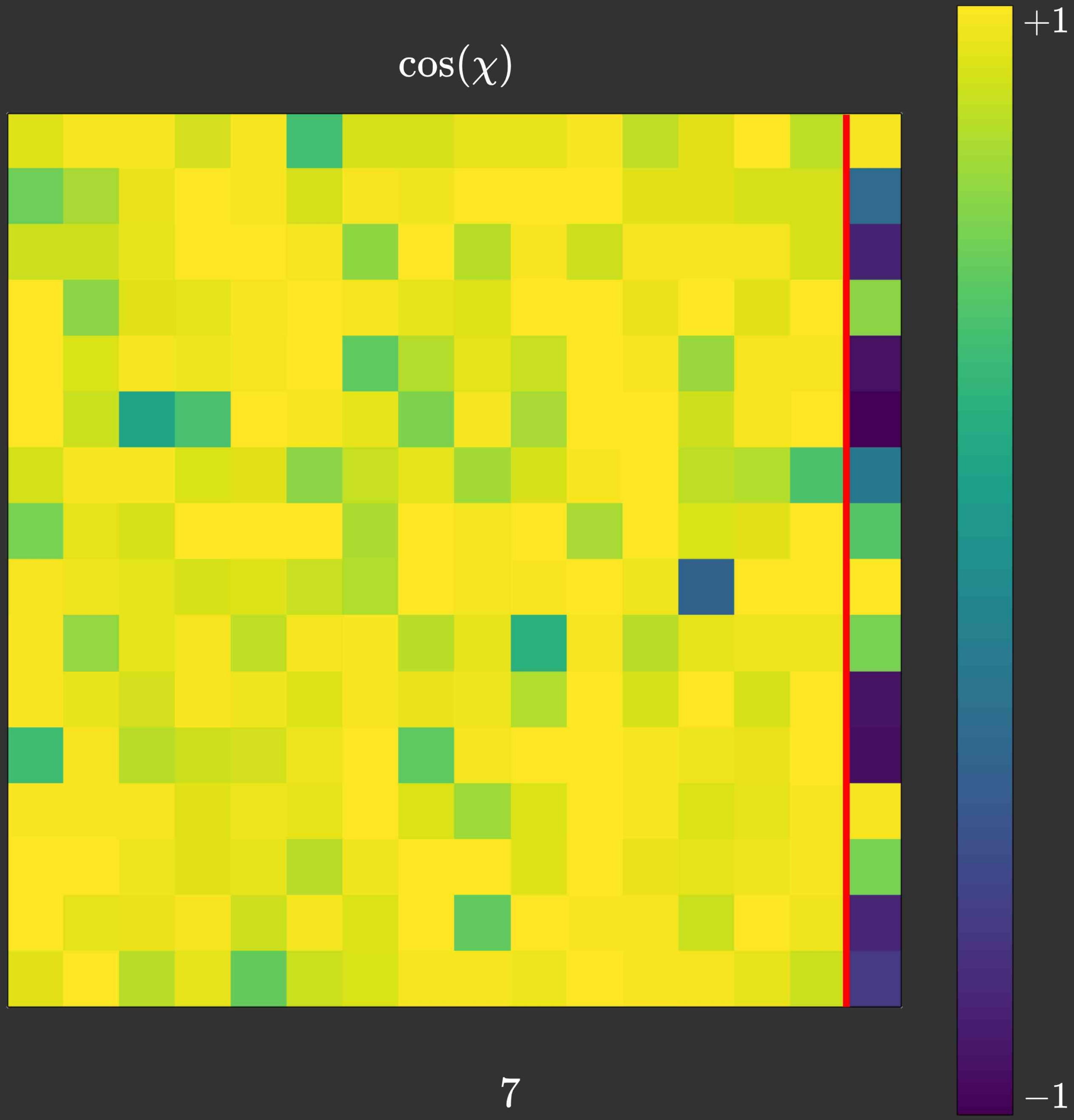
(Un-)trivializing (1+1)d U(1) LGT



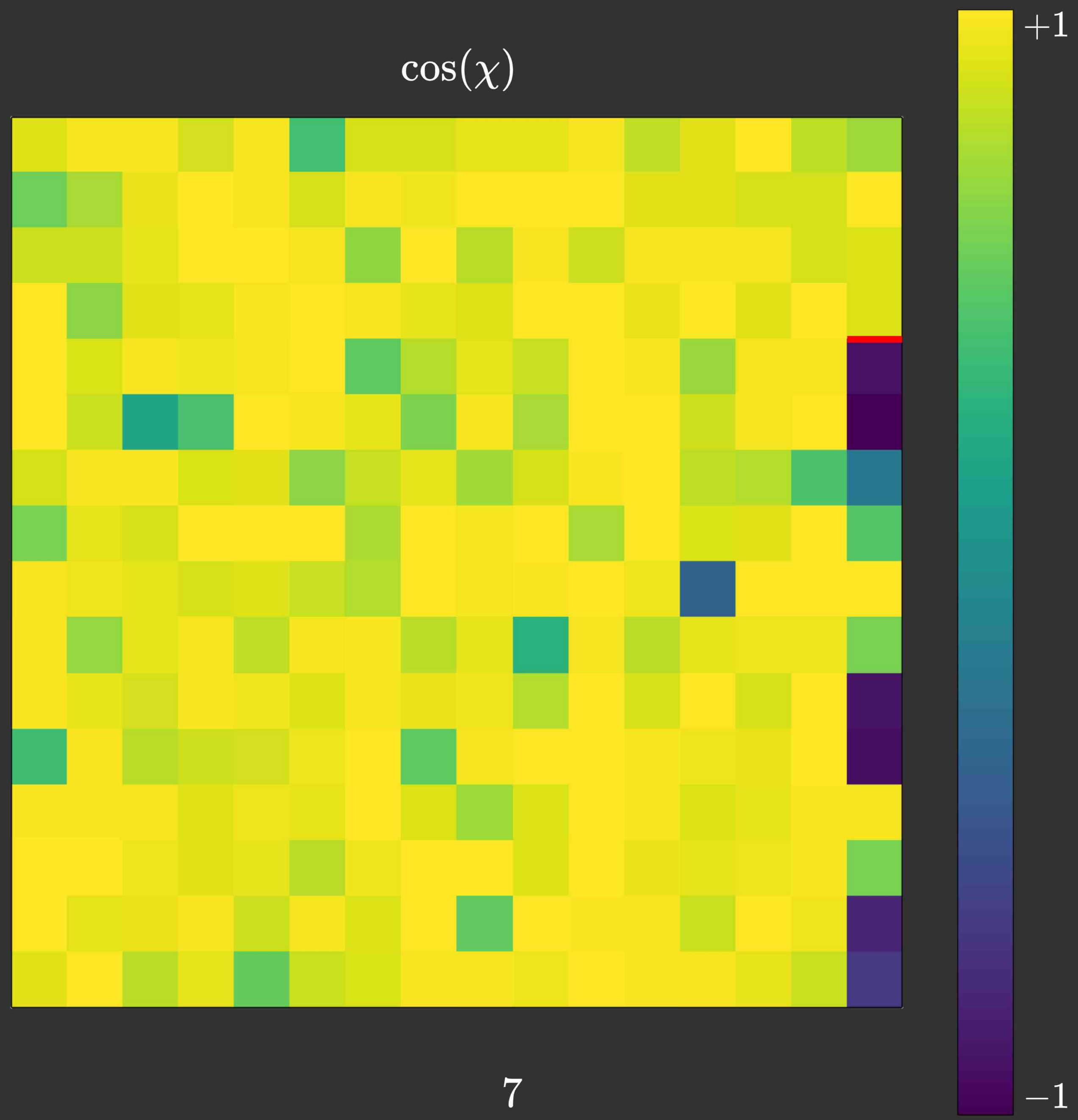
(Un-)trivializing (1+1)d U(1) LGT



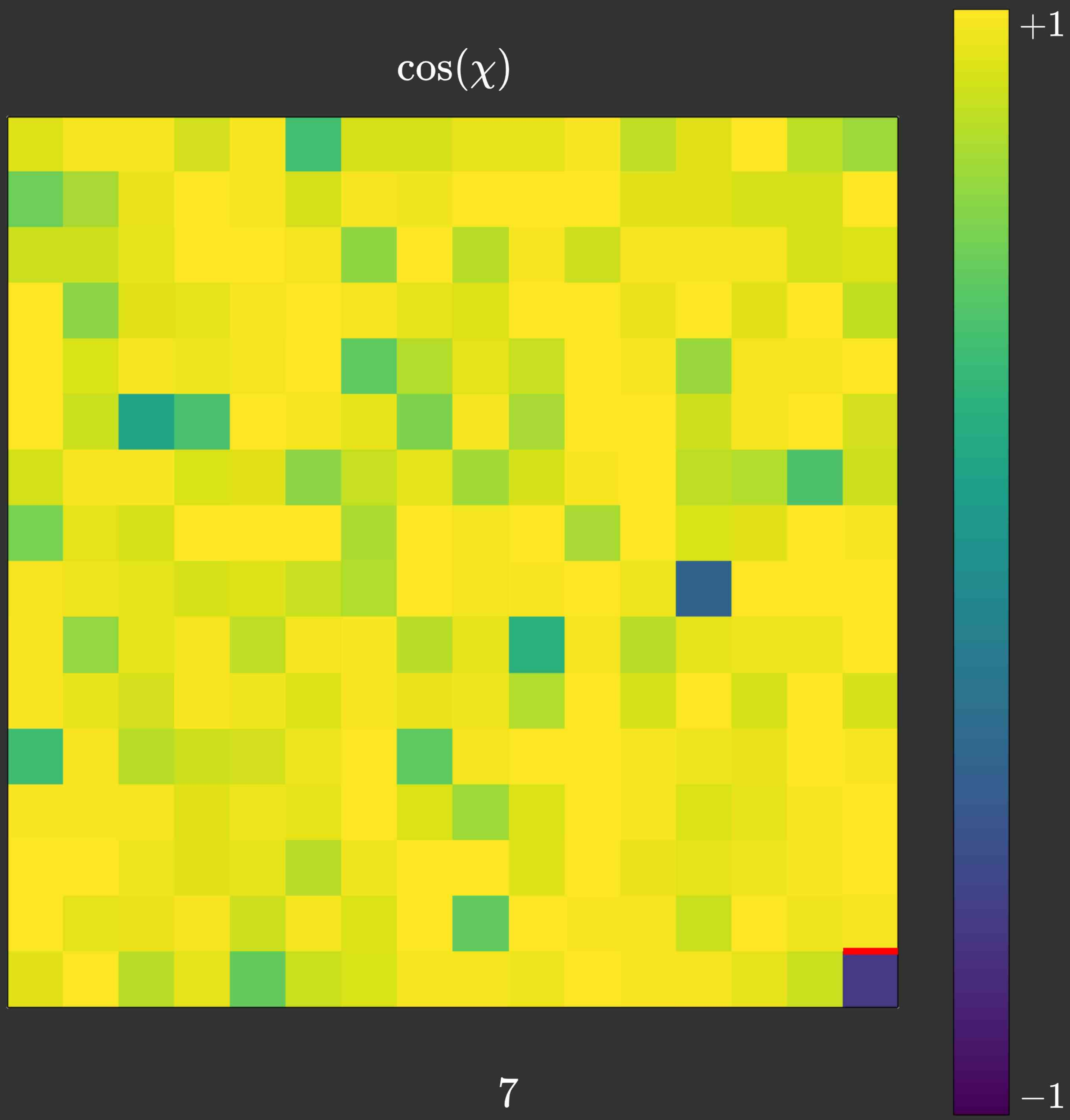
(Un-)trivializing (1+1)d U(1) LGT



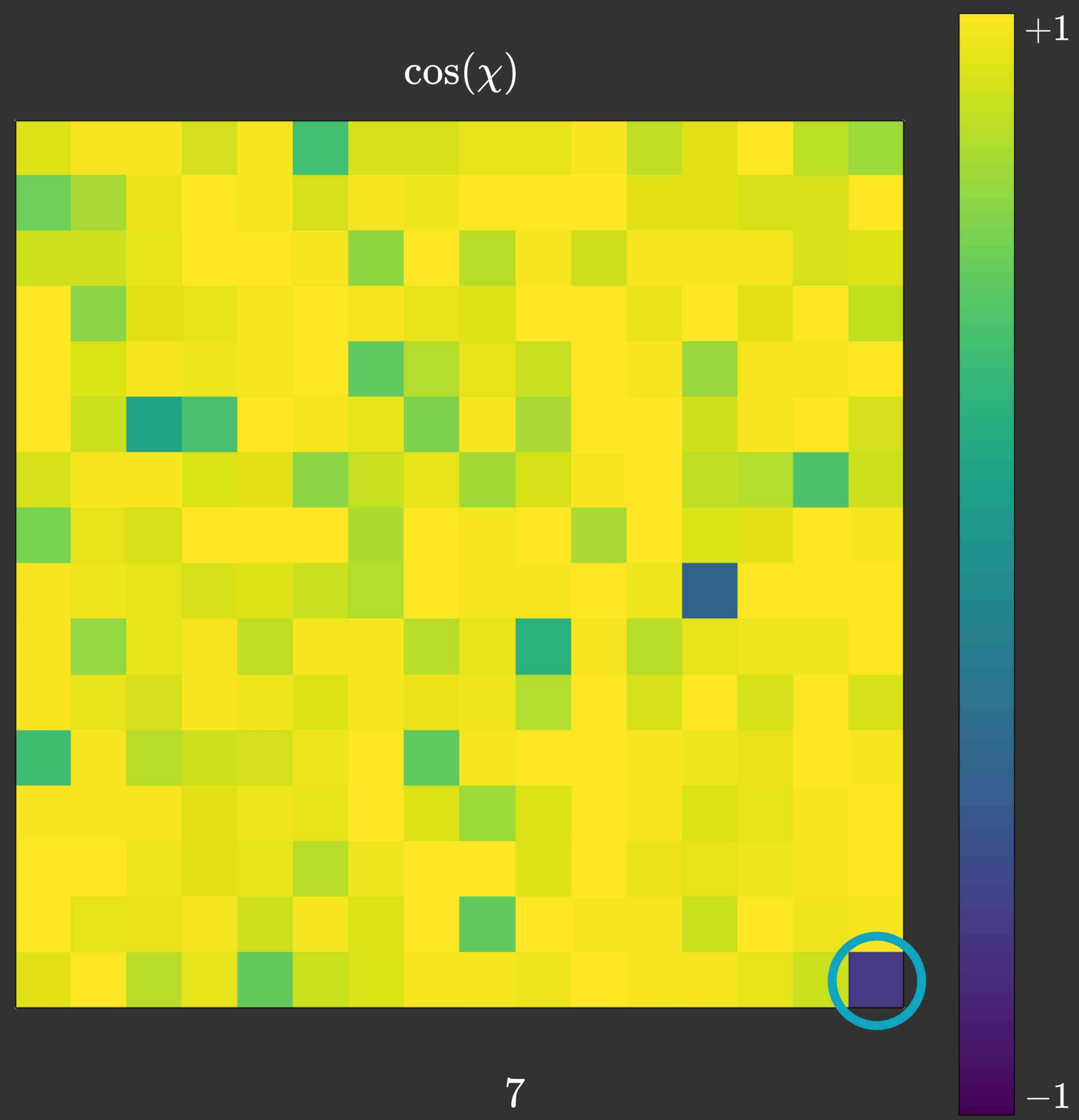
(Un-)trivializing (1+1)d U(1) LGT



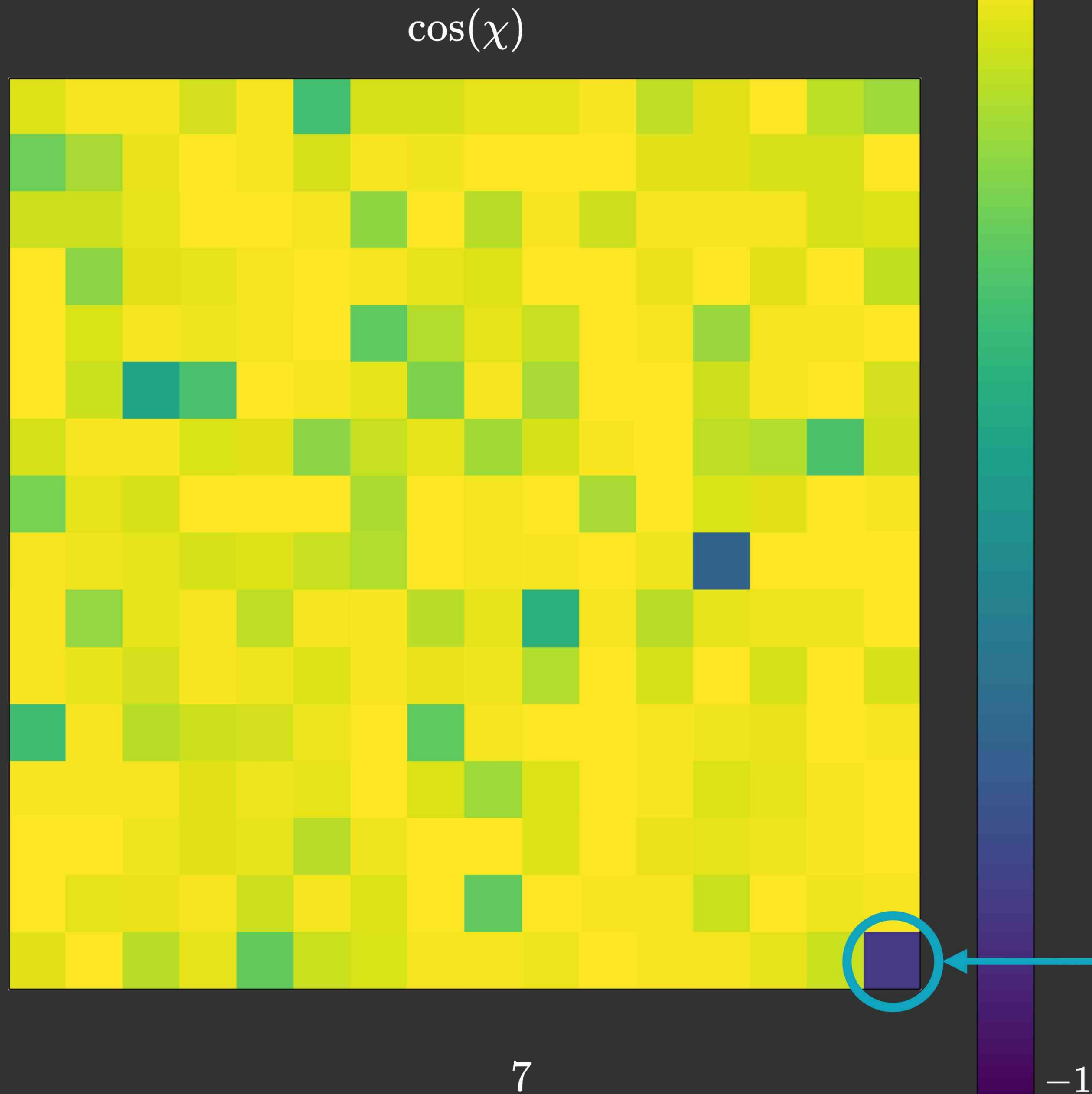
(Un-)trivializing (1+1)d U(1) LGT



(Un-)trivializing (1+1)d U(1) LGT



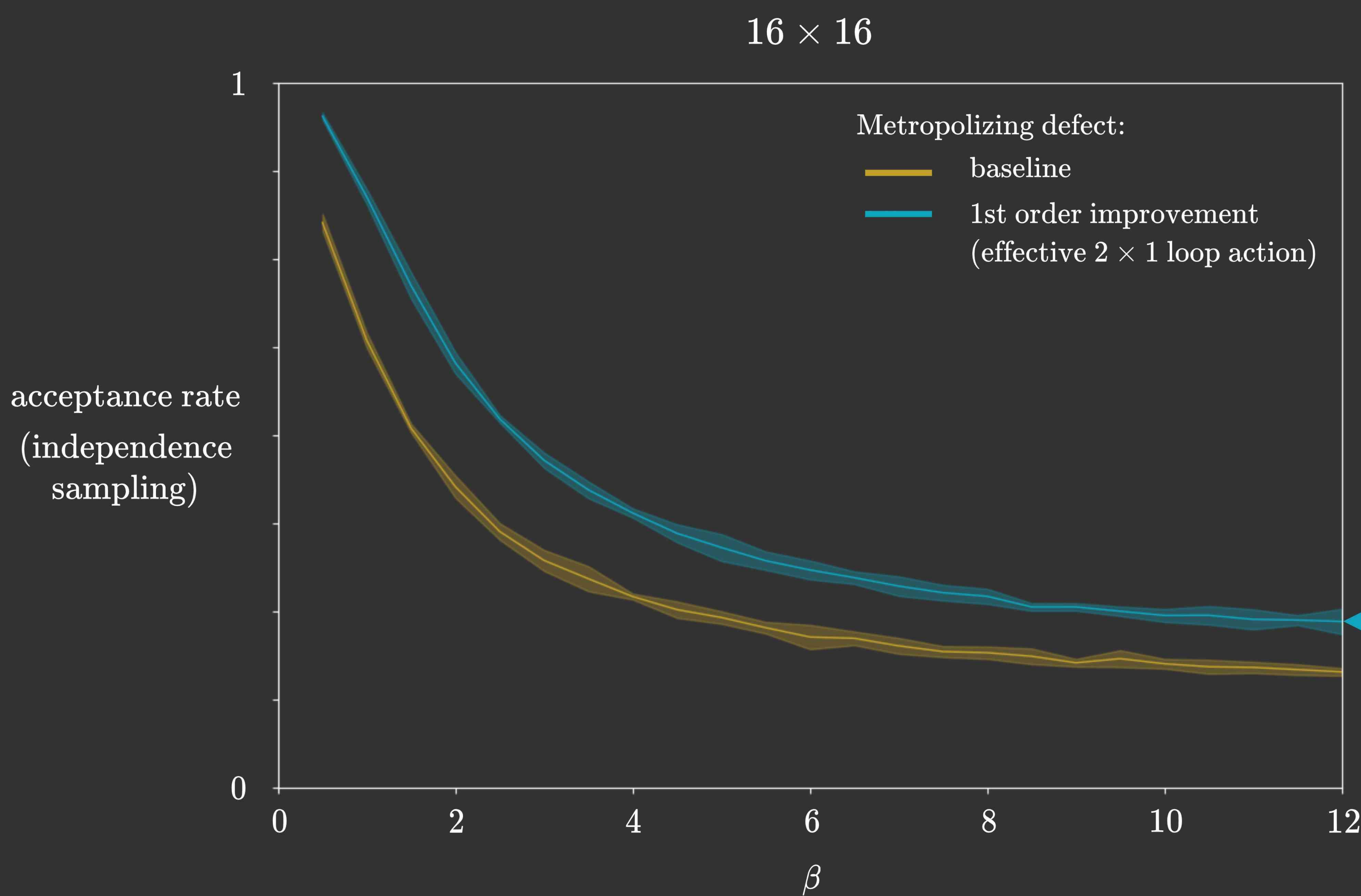
(Un-)trivializing (1+1)d U(1) LGT



Denis Boyda

Thursday, 14:50

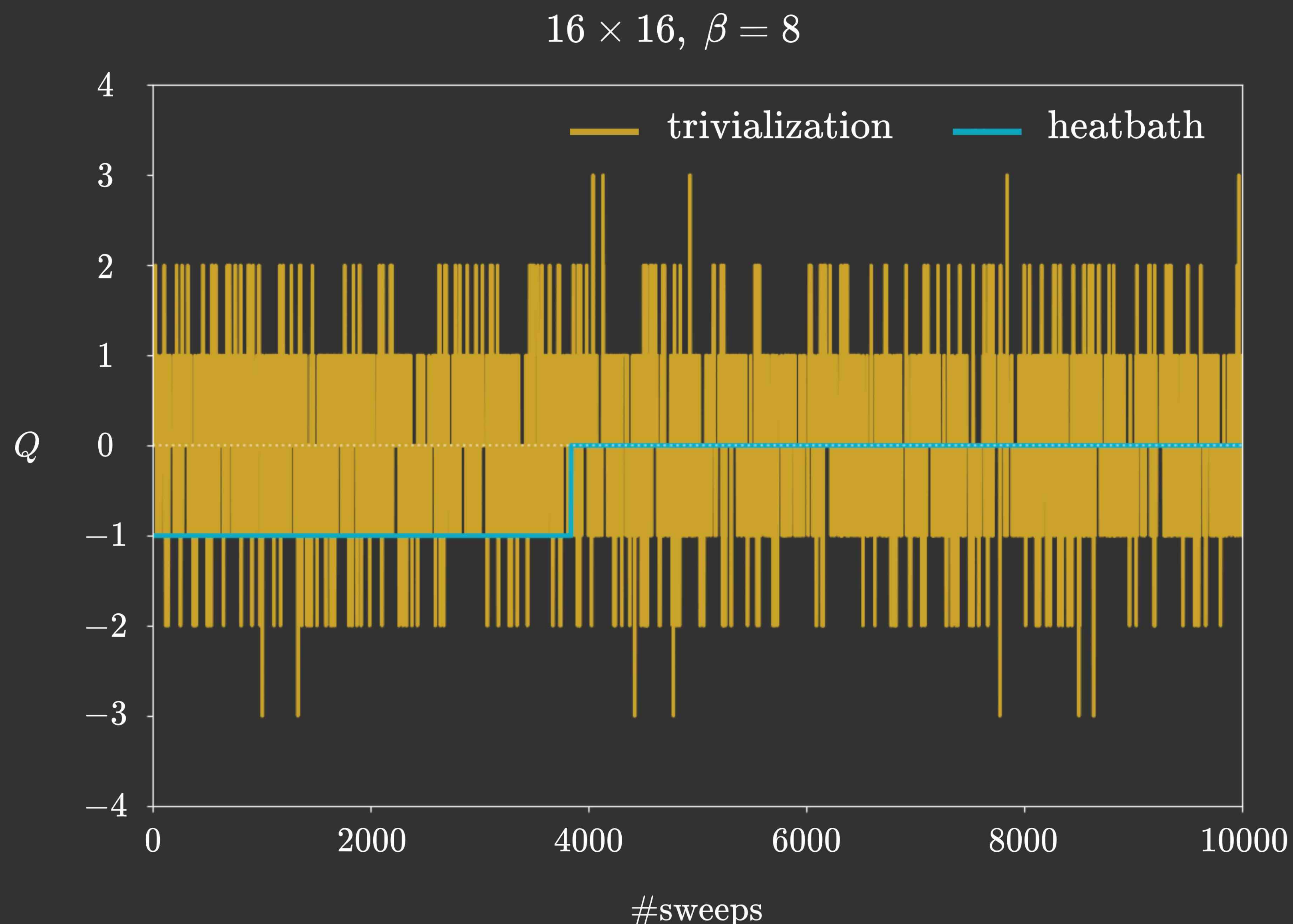
(Un-)trivializing (1+1)d U(1) LGT



Denis Boyda

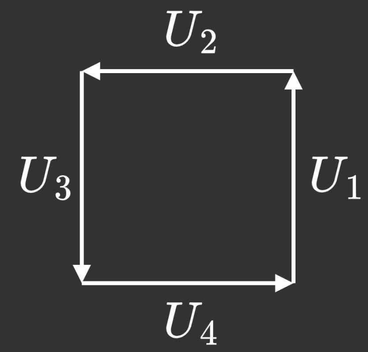
Thursday, 14:50

(Un-)trivializing (1+1)d U(1) LGT



(Un-)trivializing (1+1)d SU(3) LGT

$U_k \in \mathrm{SU}(3),\; S = -\frac{\beta}{3}\mathrm{Re\,Tr}\Big(\prod_{k=1}^{4} U_k\Big)$



$Z = \prod_{k=1}^{4}\Big(\int \mathrm{d}U_k\Big)\exp\big(-S\big(\prod_{k=1}^{4} U_k\big)\big)$

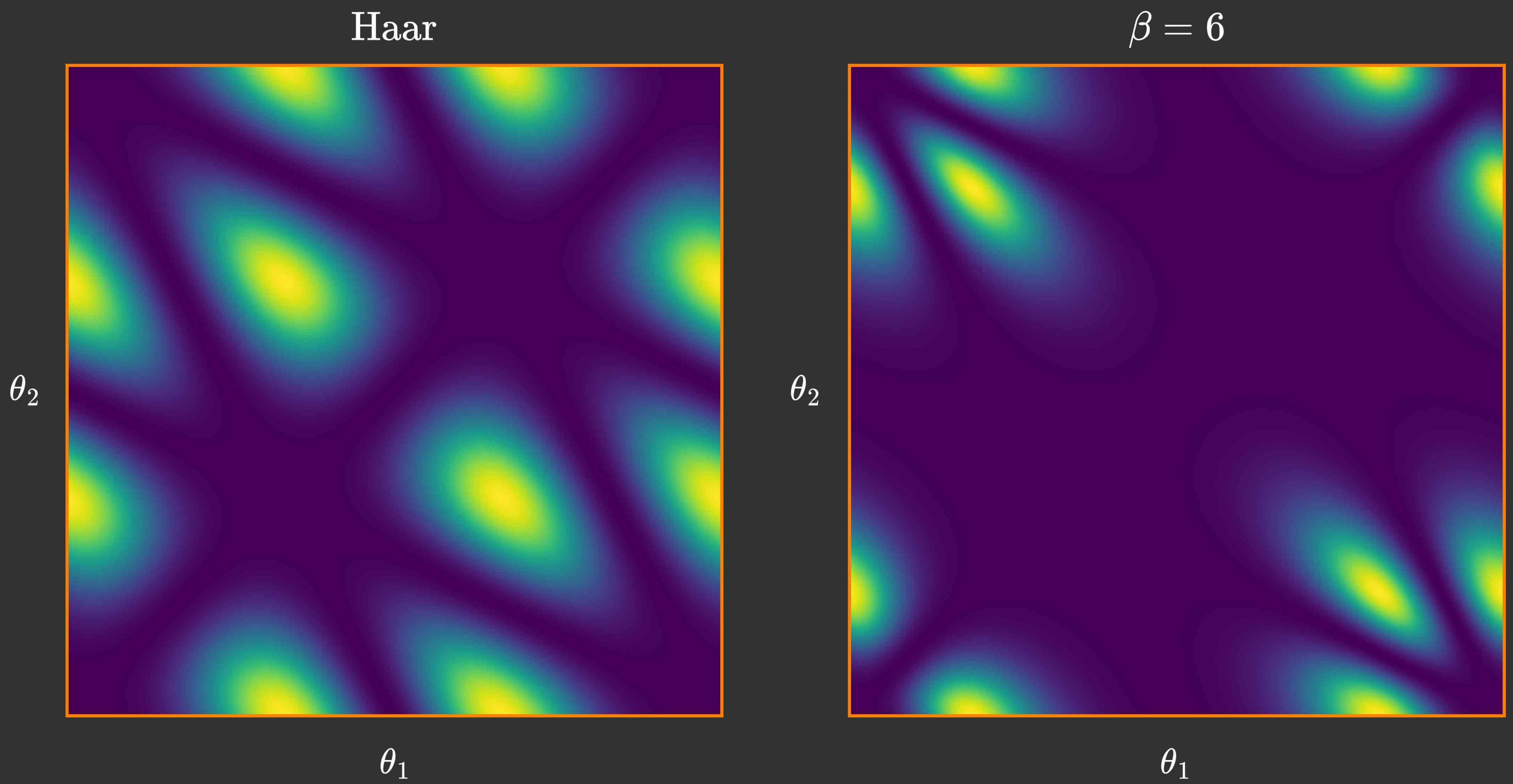
- Change of variables: $P(U_1) = U_1 \prod_{k=2}^{4} U_k \;\longrightarrow\; Z = \int \mathrm{d}P\mathrm{d}U_2\mathrm{d}U_3\mathrm{d}U_4\, \exp(-S(P))$
- Weyl integration formula for compact connected Lie group G in terms of a maximal torus T :

$$\int_G \mathrm{d}U\, f(U) = \int_T \mathrm{d}\mu(\theta)\, f(\theta) \;\text{ with }\; \mathrm{d}\mu(\theta) = \prod_{m>n}\left|e^{\mathrm{i}\theta_m} - e^{\mathrm{i}\theta_n}\right| \prod_k \mathrm{d}\theta_k\;,$$

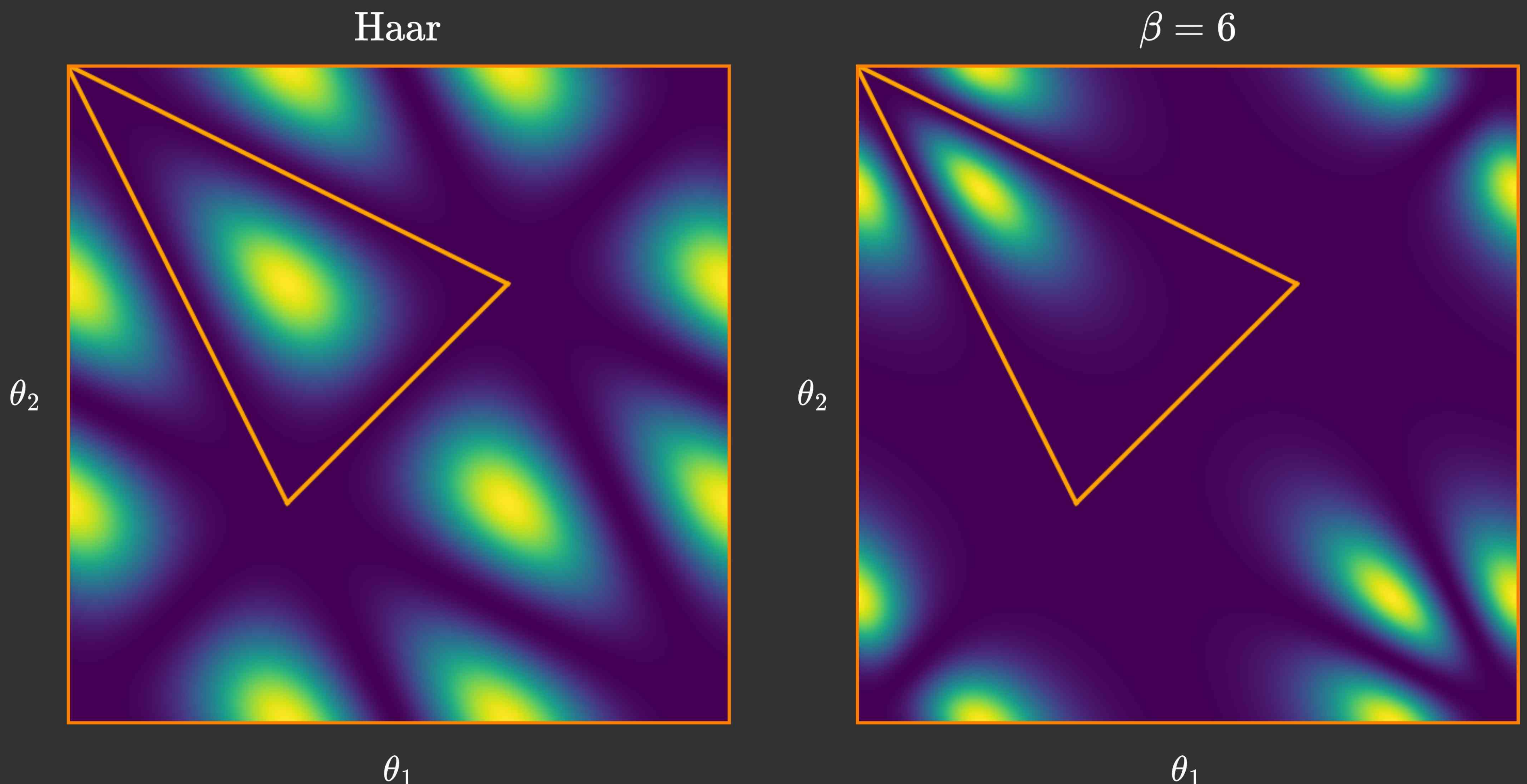
where f is a class function, i.e. $f(U) = f(\Omega U \Omega^\dagger)$ (conjugation-invariant),
and $e^{\mathrm{i}\theta_k}$ are unique eigenvalues ($N-1$ for $\mathrm{SU}(N)$).

$\longrightarrow$ reduces the eight-dim. map for the complete parameterization of SU(3) to a two-dim. map for the unique eigenvalue angles θ_k

(Un-)trivializing (1+1)d SU(3) LGT

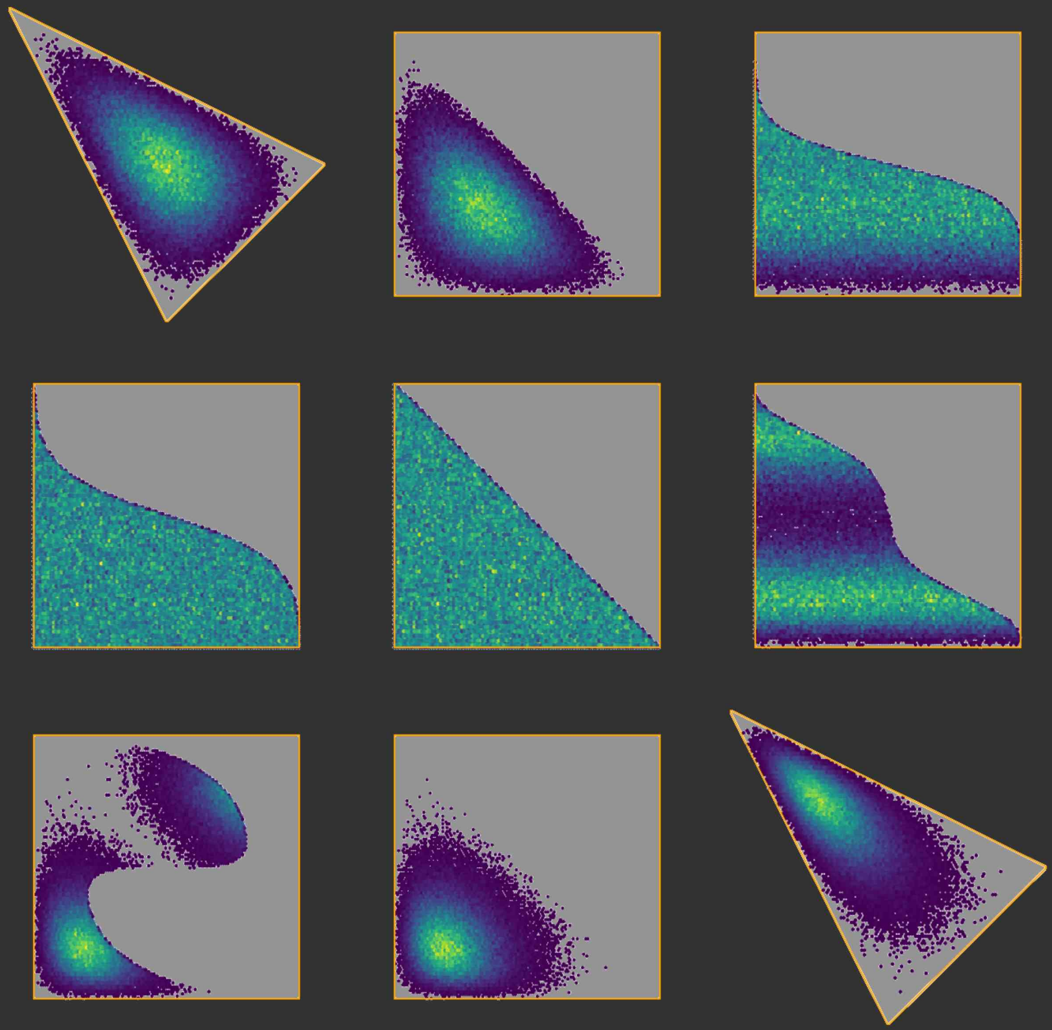


(Un-)trivializing (1+1)d SU(3) LGT



(Un-)trivializing (1+1)d SU(3) LGT

- Approximate solution with tractable Jacobian using differentiable quadrature:



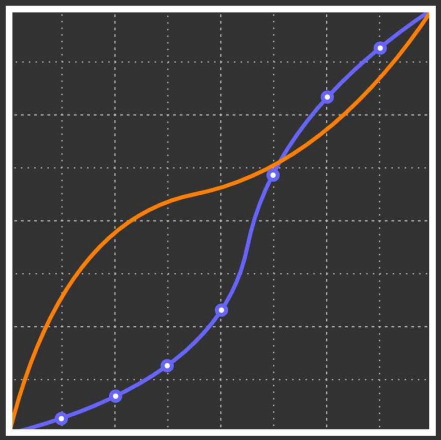
$\longrightarrow$ acceptance rate ~ 0.15 at $16 \times 16,\ \beta = 6$

Higher dimensions?

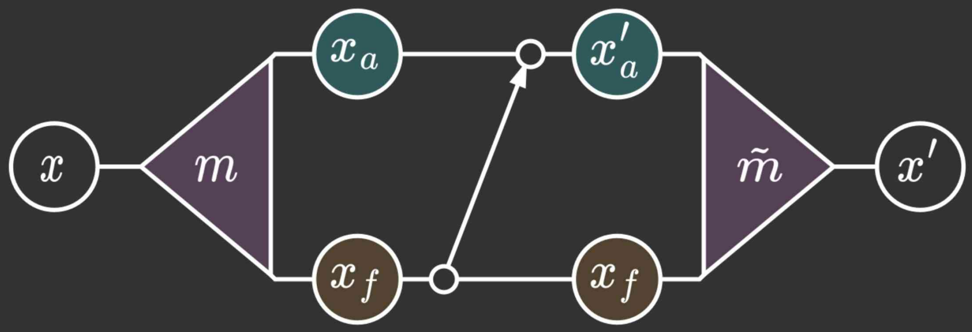
(Un-)trivializing (n+1)d SU(3) LGT with ML

Abbott et al [arXiv:2305.02402]

- Replace local conditional CDF with rational quadratic spline (RQS)
    - finite interval with fixed endpoints $\longrightarrow$ compactness
    - monotonicity $\longrightarrow$ invertibility
    - differentiability $\longrightarrow$ Jacobian
    - bounded derivative $\longrightarrow$ stability



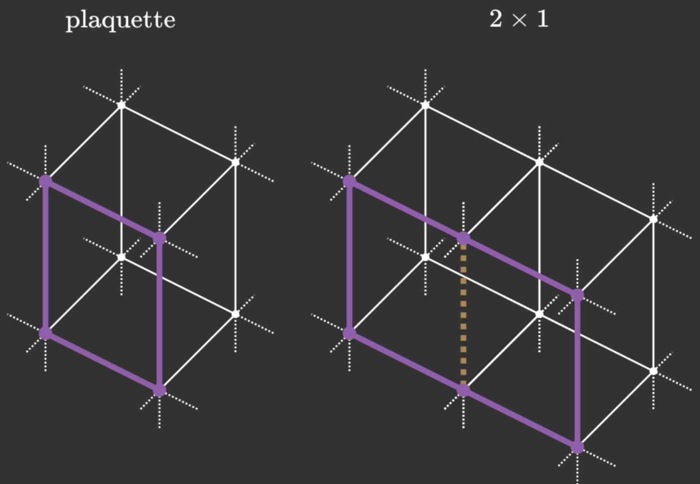
- Locally compute spline parameters from surrounding features using neural networks
- Global invertibility from alternating masking patterns $\longrightarrow$ coupling layers

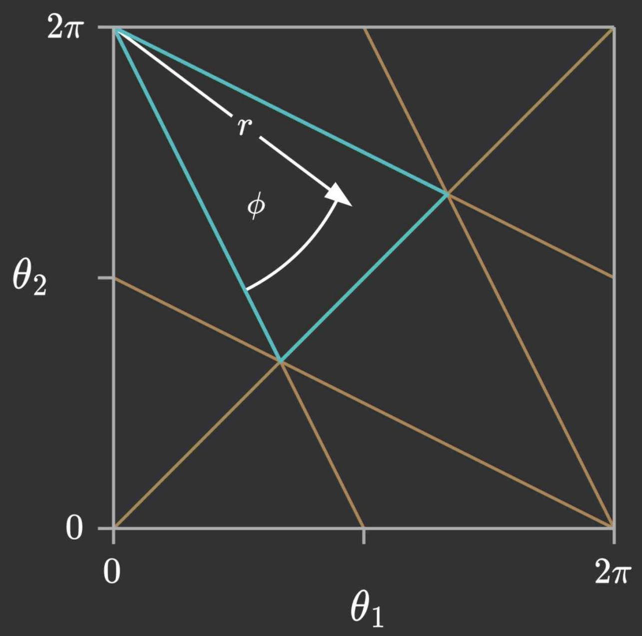


- Variational optimization by minimizing reverse Kullback-Leibler divergence

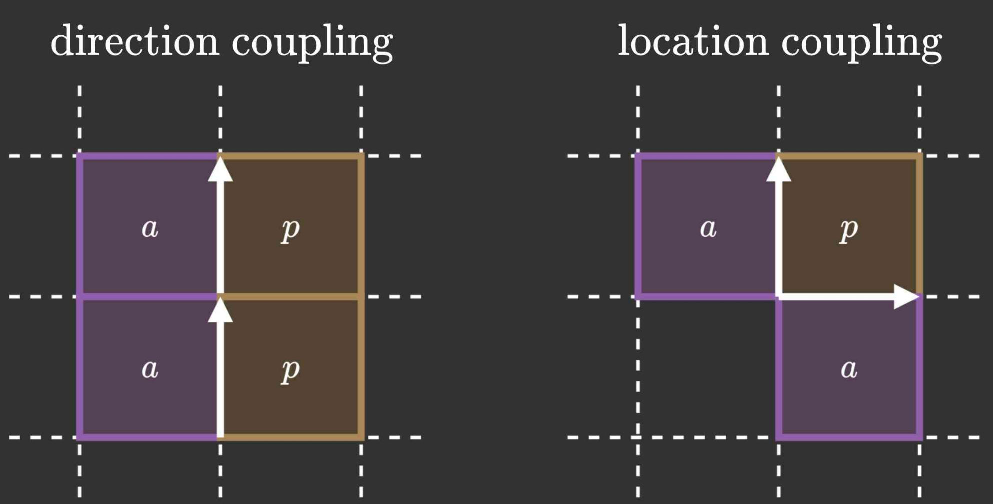
Neural RQS eigenvalue flow

- Choose suitable parameterization of canonical cell, e.g.
  polar coordinates $\longrightarrow$ best results so far
- Choose set of features preserving gauge covariance, e.g. loops:

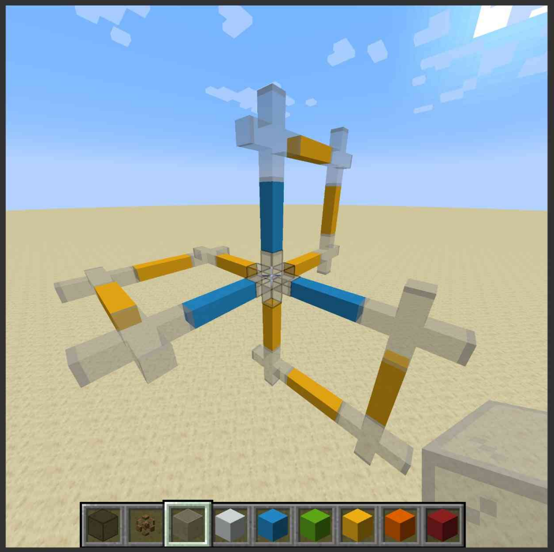




- Choose local coupling geometry, e.g.

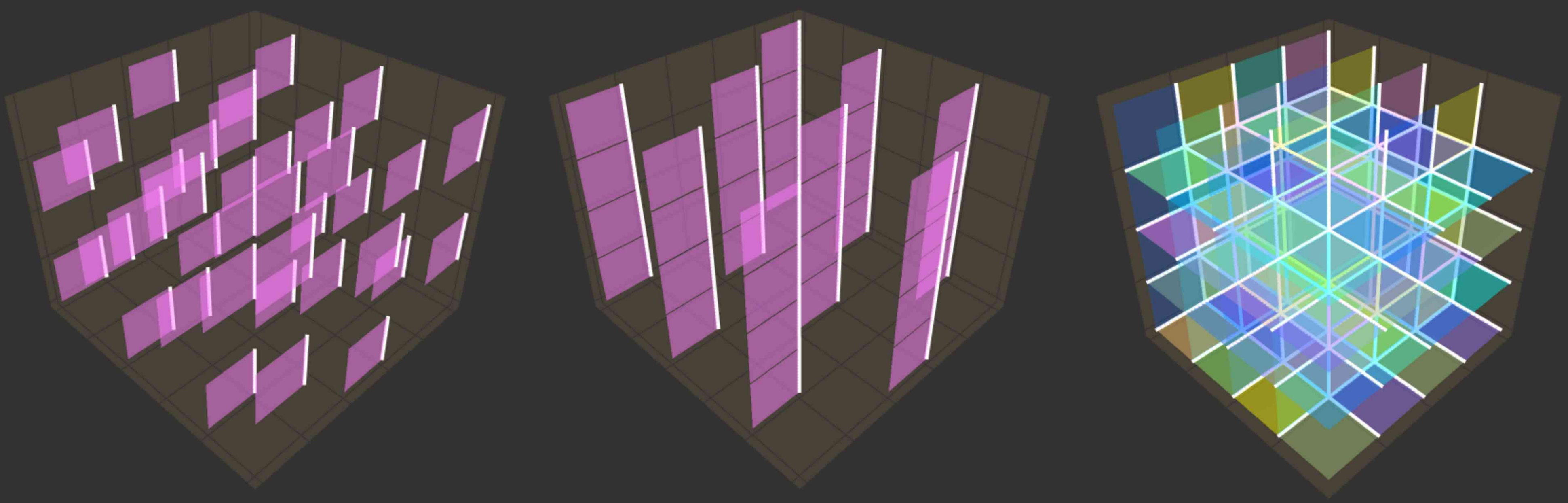


location coupling in (2+1)d



Masking pattern algorithm

- Flexible parameterization for automated construction of suitable masks in (n+1)d
- Simple alternation scheme via cyclic permutations of parameters
  $\longrightarrow$ cover all links in one cycle to avoid blind spots
- Iterate over loop orientations $\longrightarrow$ cover all plaquettes



- Full implementation and interactive visualizations in supplementary jupyter notebook

[arXiv:2305.02402]

Training and evaluation

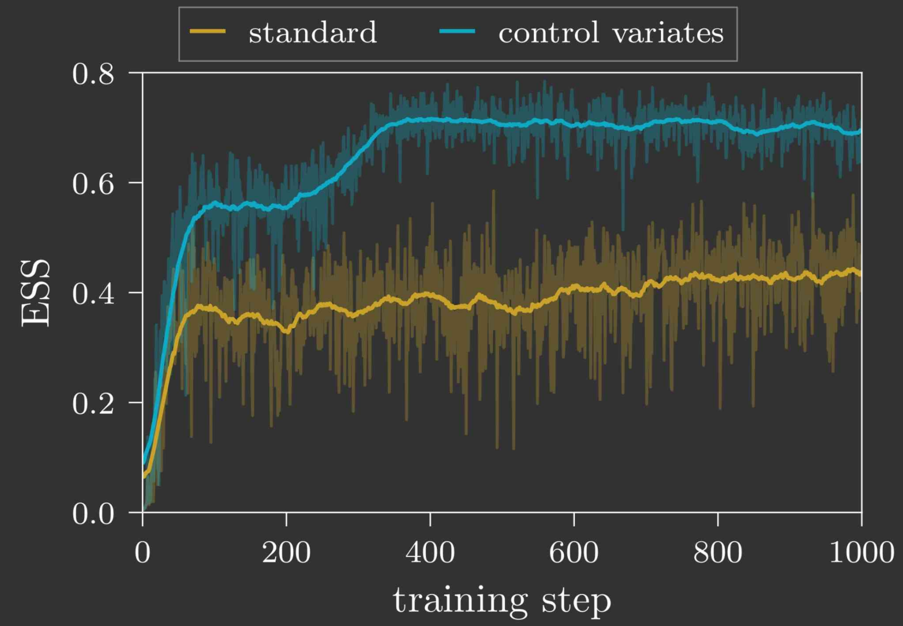
- Variance reduction in gradient estimates using path gradients + control variates

Estimated Sample Size (ESS)

$$\sim \frac{\left(\frac{1}{N}\sum_{k=1}^{N} w(U_k)\right)^2}{\frac{1}{N}\sum_{k=1}^{N} w(U_k)^2} \in \left[\frac{1}{N}, 1\right]$$

with N model samples $U_k \sim q(U_k)$

and $w(U_k) = \dfrac{\exp(-S(U_k))}{q(U_k)}$.



- Easy target (8^4, $\beta = 1$), testing heatbath prior with $0 < \beta_{\text{heatbath}} < \beta_{\text{target}}$

	ESS	prior $\beta = 0$	prior $\beta = 0.5$
flow	spectral	0.75	0.82
	residual	0.09	0.18

Summary

- (1+1)d LGT can be trivialized almost trivially with (semi-)analytic methods
- Proof-of-principle results for machine-learned maps applied to (3+1)d SU(3) LGT

Outlook

- Gauge invariants represent only the most basic data features from the perspective of geometric deep learning

  $\longrightarrow$ need covariant information to achieve expressivity

- Naive (un-)trivialization in (3+1)d leads to proliferation of defects due to the geometric properties of Wilson loop actions

  $\longrightarrow$ need hierarchical / multi-scale architectures

- Machine-learned maps are already capable of partial triviali-zation / thermodynamic integration on small volumes

  $\longrightarrow$ practical applications are within reach

Denis Boyda

Thursday, 14:50

Ryan Abbott

Monday, 16:20

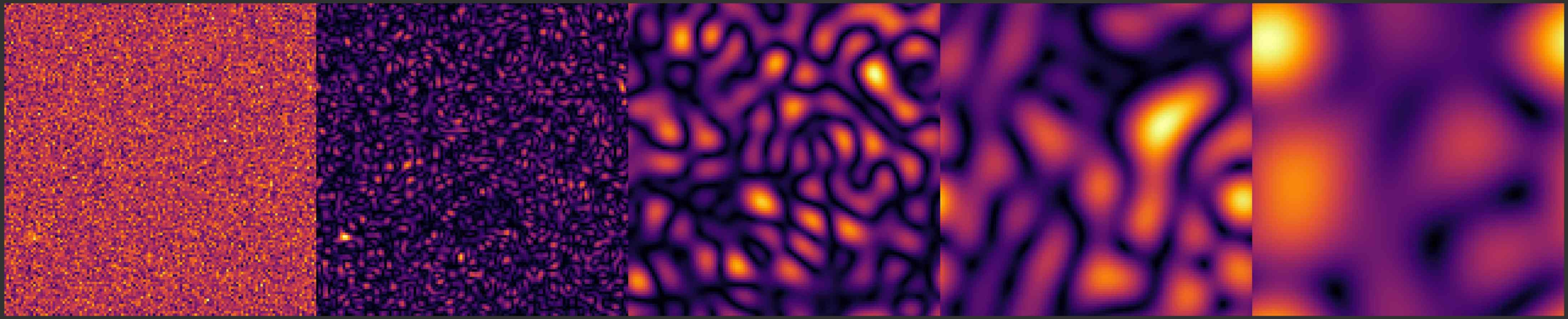
Daniel Hackett

Thursday, 15:10

Thanks!

Wilsonian RG interpretation (smoothing)

- Regularized stochastic quantization (Langevin equation): $\dfrac{\partial\phi}{\partial\tau} = -\dfrac{\delta S}{\delta\phi} + r_\Lambda(\Delta)\eta$
- Corresponding Fokker-Planck equation: $\dfrac{\partial p(\phi,\tau)}{\partial\tau} = \int \mathrm{d}^d x\, \dfrac{\delta}{\delta\phi}\left(\dfrac{\delta S}{\delta\phi} + r_\Lambda^2(\Delta)\dfrac{\delta}{\delta\phi}\right)p(\phi,\tau)$
- $\partial_\tau p = 0 \;\longrightarrow\; p_\Lambda(\phi) \propto \exp(-S - \Delta S_\Lambda)$ with $\Delta S_\Lambda = \dfrac{1}{2}\int \mathrm{d}^d p\, \phi(p)\Lambda^2\left(\dfrac{1}{r_\Lambda(p^2)} - 1\right)\phi(p)$
- Sharp cutoff: $r_\Lambda(p^2) = \theta(\Lambda^2 - p^2) \;\longrightarrow\; r_\Lambda(\Delta)\eta(x) = \dfrac{1}{(2\pi)^2}\int \mathrm{d}^d p\, e^{-\mathrm{i}px}\eta(p)\theta(\Lambda^2 - p^2)$



Pawlowski et al [arXiv:1705.06231]

Wilsonian RG interpretation (smoothing)

Gies [arXiv:hep-ph/0611146]

The functional RG combines this functional approach with the RG idea of treating the fluctuations not all at once but successively from scale to scale [9, 10]. Instead of studying correlation functions after having averaged over all fluctuations, only the *change* of the correlation functions as induced by an infinitesimal momentum shell of fluctuations is considered. From a structural viewpoint, this allows to transform the functional-integral structure of standard field theory formulations into a functional differential structure [11, 12, 13, 14]. This goes along not only with a better analytical and numerical accessibility and stability, but also with a great flexibility of devising approximations adapted to a specific physical system. In addition, structural investigations of field theories from first principles such as proofs of renormalizability can more elegantly and efficiently be performed with this strategy [13, 15, 16, 17].

Cotler et al [arXiv:2202.11737]

One of our main results is that Polchinski's equation can be written as

$$-\Lambda \frac{d}{d\Lambda} P_\Lambda[\phi] = -\nabla_{\mathcal{W}_2} S(P_\Lambda[\phi] \,\|\, Q_\Lambda[\phi]) \qquad (1.2)$$

where $\nabla_{\mathcal{W}_2}$ is a gradient with respect to a functional generalization of the Wasserstein-2 metric, $S(P \,\|\, Q) := \int [d\phi] P[\phi] \log(P[\phi]/Q[\phi])$ is a functional version of the relative entropy, and $Q_\Lambda[\phi]$ is a background probability functional which essentially defines our RG scheme. We emphasize that

Kadanoffian RG interpretation (blocking)

Huang, *Statistical Mechanics*

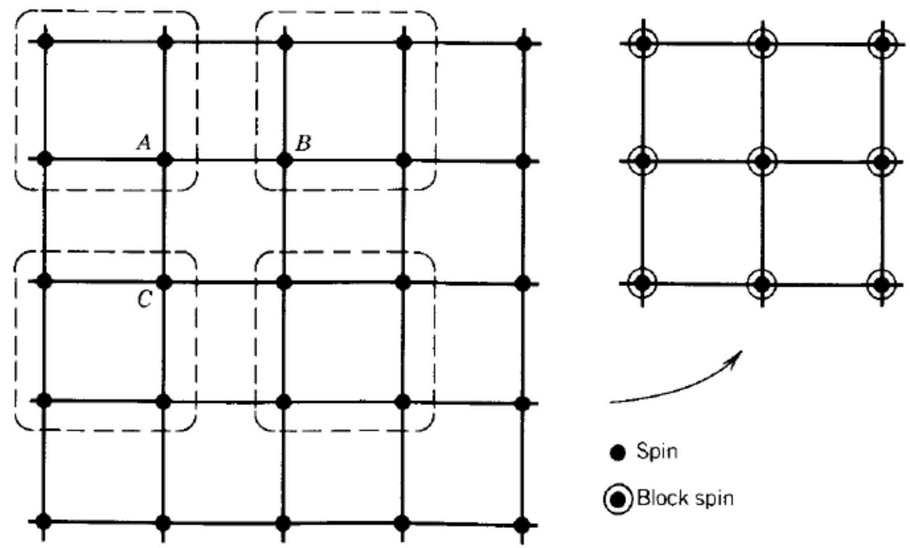


Fig. 18.1 Block-spin transformation: averaging the spins in a block, and then rescaling the lattice to the original size. In more than one dimension, the indirect interaction between B and C gives rise to next-to-nearest-neighbor interactions of the block spins.