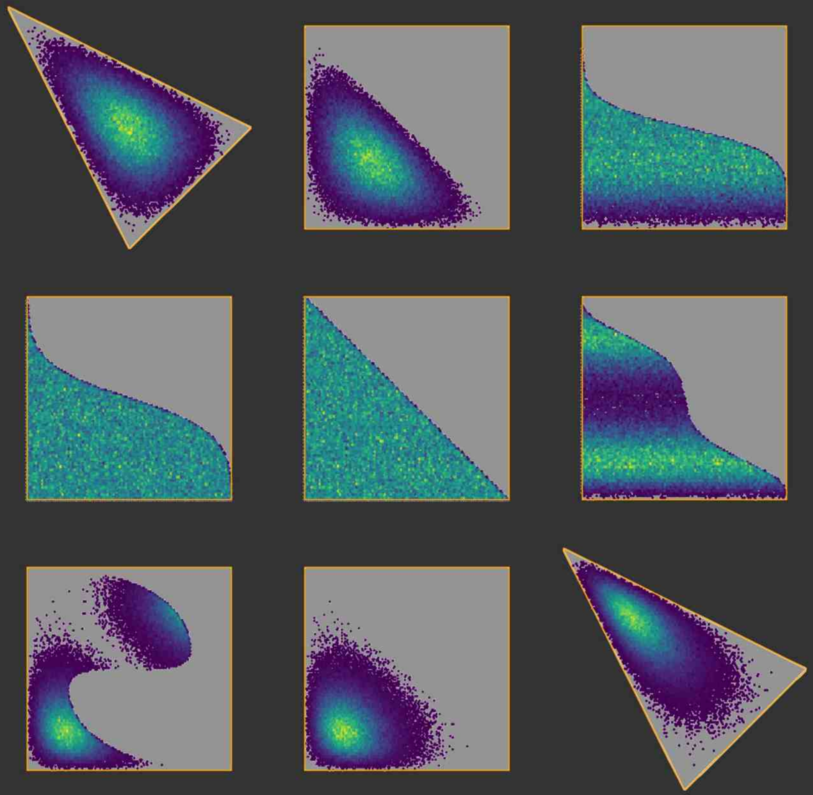
Properties and uses of approximate trivializing maps in lattice QCD



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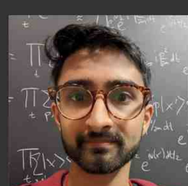

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Basic concepts

- Change of variables $Z = \int \mathrm{d}U\, e^{-S} = \int \mathrm{d}V\, e^{-S + \log|J|}$
- Trivializing map condition $-S + \log|J| = 0$ minimizes relative entropy (Kullback-Leibler divergence) w.r.t. Haar measure $\longrightarrow$ full thermodynamic integration
- Less ambitious: $-S + \log|J| = -S'$ $\longrightarrow$ partial thermodynamic integration
  - $S' \equiv S_{\text{defect}}$ $\longrightarrow$ restoration of topological ergodicity
  - $S' \equiv S_{\Lambda}$ $\longrightarrow$ renormalization group interpretation
  - $\ldots$

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.

Renormalization group interpretation

Weinberg, *Why The Renormalization Group Is A Good Thing* (1983)

What would be the short-distance or the high-energy behavior of such a theory? Well, suppose we make a graph in coupling-constant space showing the trajectory of the coupling constants G, f, f', h, etc., as we vary the renormalization scale. The renormalization group applies here; a theory doesn't have to be renormalizable for us to apply the renormalization-group method to it. These trajectories simply describe how all the couplings change as you go from one renormalization scale to another. Now many of those trajectories—in fact, perhaps most of them—go off to infinity as you go to short-distance renormalization scales. However, it may be that there's a fixed point somewhere in coupling-constant space. A fixed point, remember, is defined by the condition that if you put the coupling constant at that point it stays there as you vary the renormalization scale. Now, it is a fairly general phenomenon that for each fixed

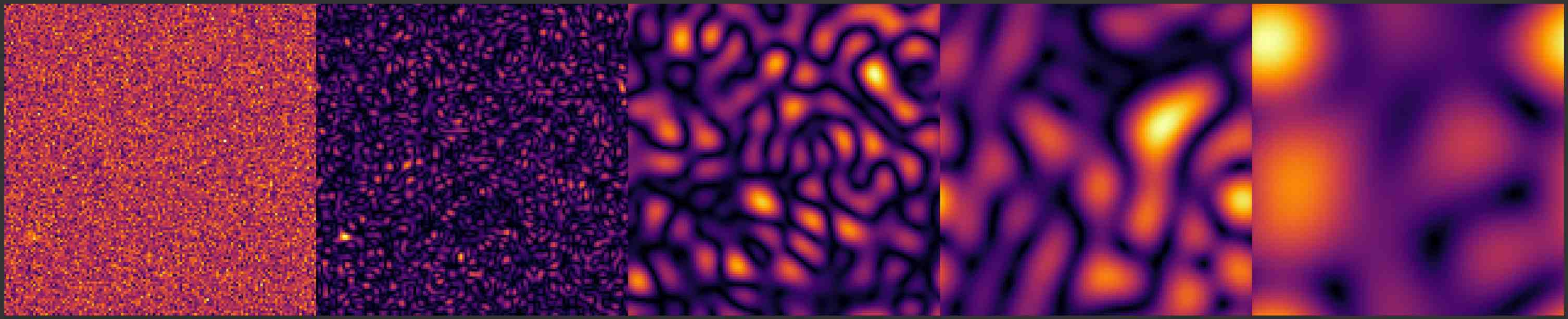
Wilsonian RG interpretation (smoothing)

- 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

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

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*

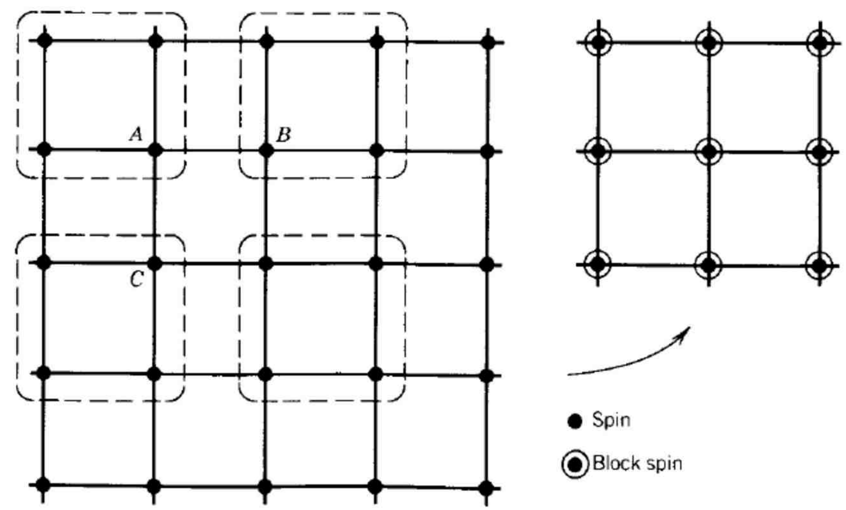
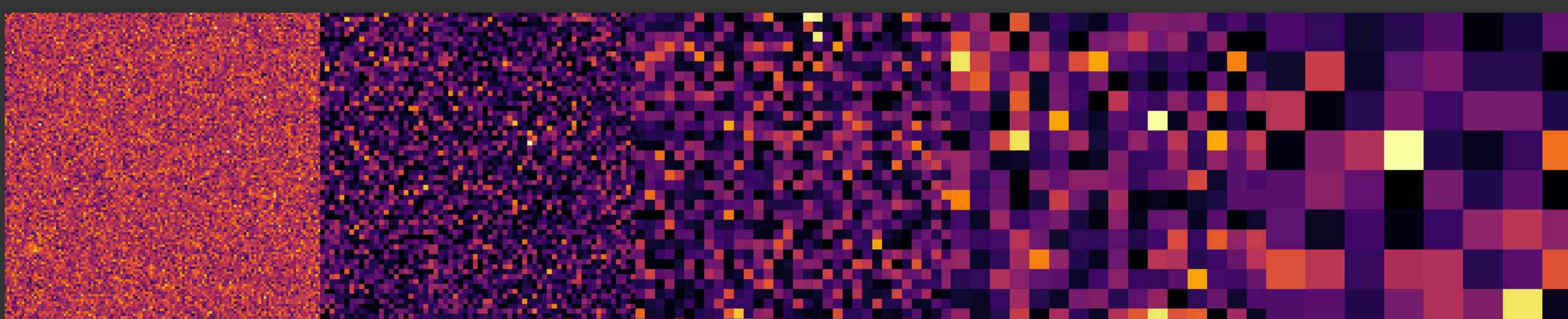
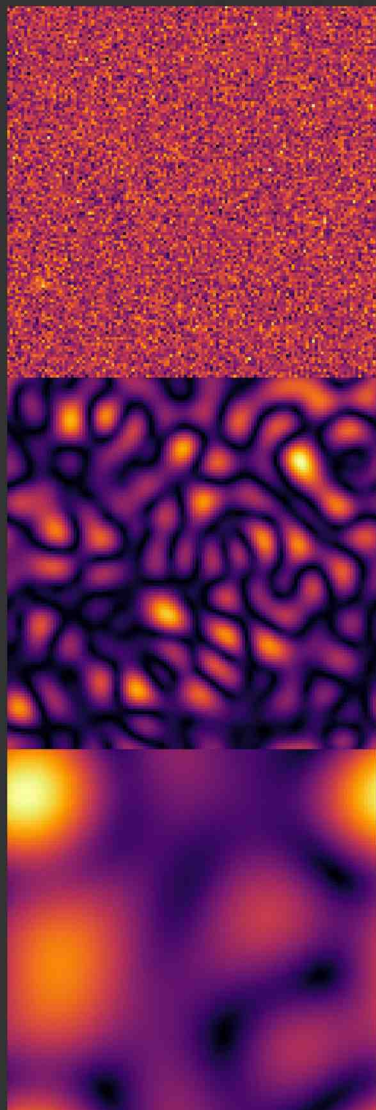


Fig. 18.1 Block-spin transformation: averaging the spins in a block, and then rescaling the lattice to the original size. In more than one dimension, the indirect interaction between B and C gives rise to next-to-nearest-neighbor interactions of the block spins.



Wilson vs Kadanoff

Huang, *Statistical Mechanics*



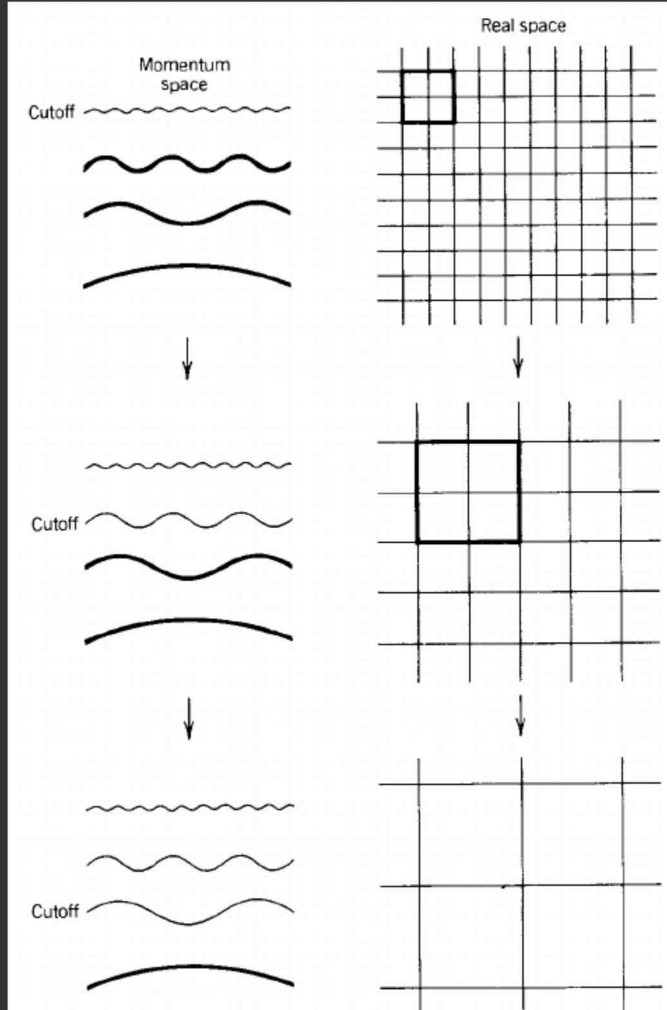
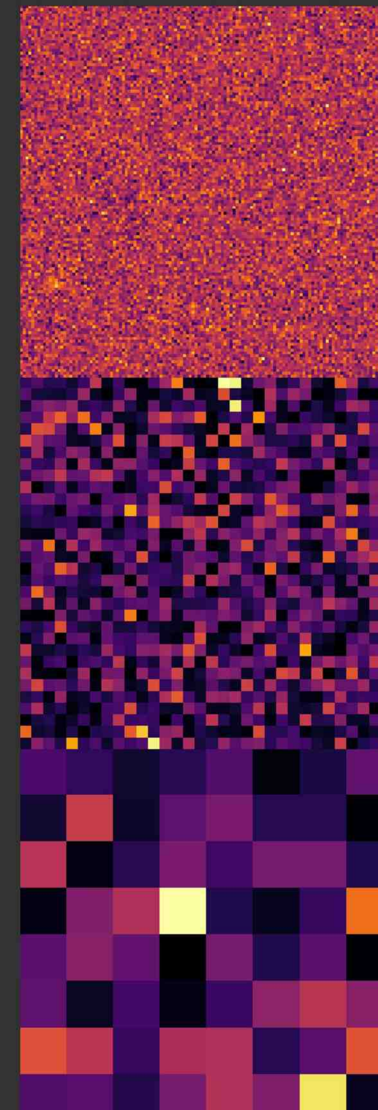
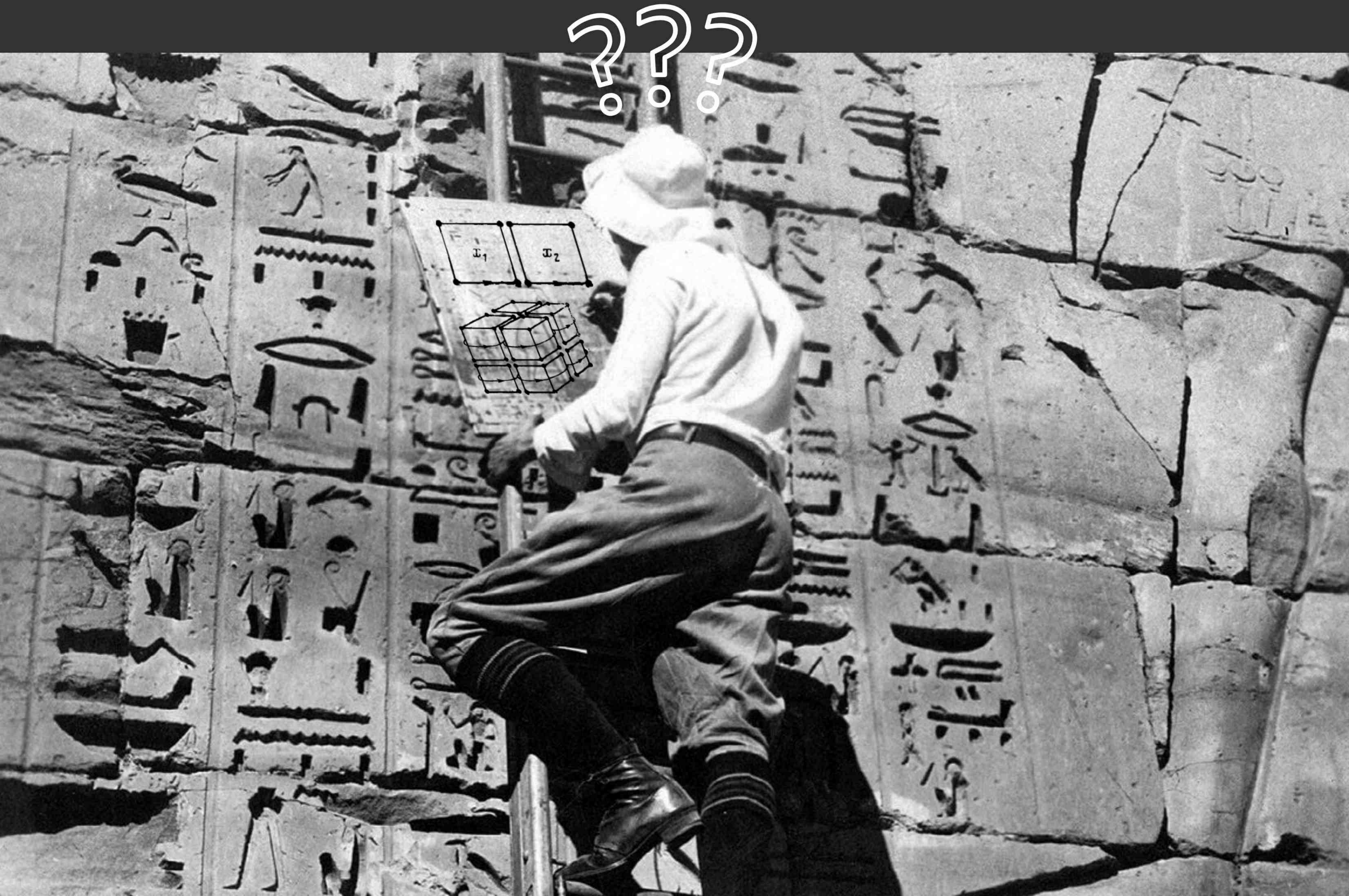


Fig. 18.5 Coarse-graining in momentum space and in real space. In the former, one effectively lowers the cutoff. In the latter, one blots out finer details, enlarging the effective lattice spacing.



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*

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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

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Received 23 October 1980

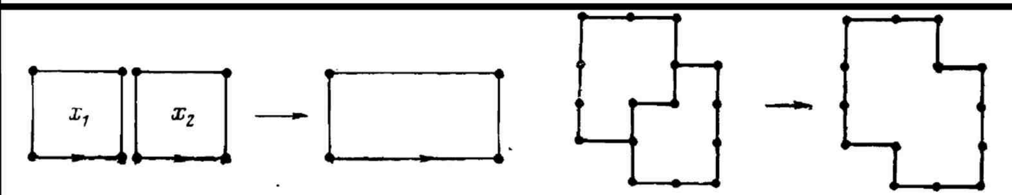
We study the Migdal recursion relations and the reformulation due to Kadanoff for SU(2) and SU(3) lattice gauge theory, using analytic approximations for large and small couplings and numerical methods for all couplings. In SU(2) we obtain the beta function and the expectation value of the plaquette, 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

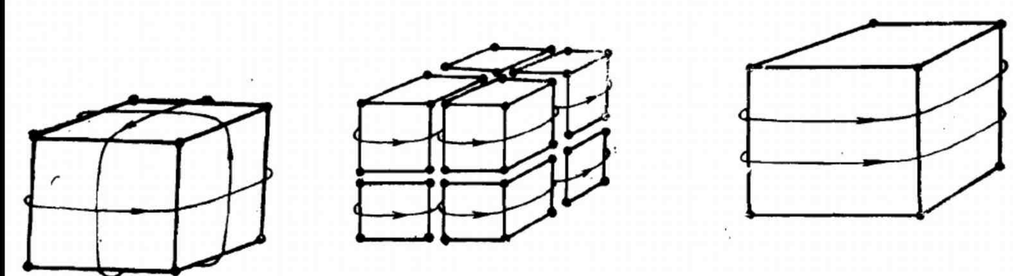
L. D. Landau Theoretical Physics Institute, USSR Academy of Sciences
(Submitted June 11, 1975)
Zh. Eksp. Teor. Fiz. **69**, 1457–1465 (October 1975)

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*

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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

Ref.TH.2974-CERN

ON INVARIANT GROUP INTEGRALS IN LATTICE QCD

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A B S T R A C T

3. N = 3 INTEGRALS

In evaluating the SU(3) one-link integral, we have found it very useful to parametrize[8)] the SU(3) group manifold in terms of two normalized, complex three-vectors $\underline{u}$ and $\underline{v}$. Each g in SU(3) can then be written in the form

$$g = \begin{pmatrix} u_1^* & u_2^* & u_3^* \\ v_1^* & v_2^* & v_3^* \\ w_1 & w_2 & w_3 \end{pmatrix} \quad (8)$$

where $w_i = \varepsilon_{ijk} u_j v_k$ and $\underline{u}^* \cdot \underline{v} = 0$, which leads to eight independent variables. An integration over SU(3) can be re-expressed in terms of the $\underline{u},\underline{v}$ variables in (8). For the case G = SU(3) in (1) we obtain

$$\int_{SU(3)} dg\, e^{Tr(gm^\dagger + g^\dagger m)} = \frac{1}{2\pi^2}\int_{-\infty}^{\infty} ds\, e^{is}\int_{-\infty}^{\infty} dt\, e^{it} \cdot \int d^2z \int d^6u \int d^6v\; e^{-i(s\,\underline{u}^*\cdot\underline{u} + t\,\underline{v}^*\cdot\underline{v})}\, e^{iz(\underline{u}^*\cdot\underline{v} + \underline{v}^*\cdot\underline{u})} \cdot e^{Tr(gm^\dagger + g^\dagger m)} \quad (9)$$

Volume 102B, number 2,3 PHYSICS LETTERS 11 June 1981

SU(N) ONE-LINK INTEGRAL BY RECURSION

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Received 24 February 1981

The SU(3) one-link integral is calculated by solving recursion relations by computer. The method is applicable to SU(N) for small N.

In order to obtain the generating functional of Green's functions in lattice gauge theory it is useful to determine the one-link integral over the group space:

$$Z[A,\bar{A}] = \int_G d\mu(U)\exp[\mathrm{tr}(\bar{A}U + U^\dagger A)] \quad (1)$$

where $d\mu$ denotes the Haar-measure on G. The sources A and $\bar{A}$ represent sources for the gauge field on the link or pairs of Dirac fields coming from the covariant derivative term in a theory with fermions. In case one starts from the euclidean formulation of field theory the complex matrices A and $\bar{A}$ are unrelated. In case one starts from minkowskian field theory $\bar{A}$ is the hermitean conjugate $A^\dagger$ of A.

N and consists of the derivation of equations for Z and solving them by a power series in terms of invariants. The equations are found by differentiating (1) and then use the group relations. The unitarity relation $U^\dagger U = \mathbf{1}$ leads to

$$\delta^2 Z/\delta A^a{}_p \delta \bar{A}^p{}_b = Z\delta^b_a, \quad (2)$$

det $(U^\dagger) = 1$ leads to:

$$\epsilon^{a_1 \ldots a_N}\epsilon_{b_1 \ldots b_N}\delta^N Z/(\delta A^{a_1}{}_{b_1} \ldots \delta A^{a_N}{}_{b_N}) = N!\,Z, \quad (3)$$

and an analogous relation is obtained from det $U = 1$. Because the left-invariant Haar-measure is also right-invariant on the compact group SU(N) the functional $Z[A,\bar{A}]$ is invariant under the transformation

M	$i\,j\,k\,l$	$\tilde{d}_{ijkl}$	$\tilde{c}_{ijkl}$
0:	0 0 0 0	1	0
2:	0 0 1 0	1	1
3:	0 1 0 0	1	1
4:	0 0 0 1	−1	−1
4:	0 0 2 0	9/8	1/8
5:	0 1 1 0	3/4	−1/4
6:	0 0 1 1	−3/5	2/5
6:	0 0 3 0	9/8	−1/4
6:	0 2 0 0	1/2	−1/2
6:	1 1 0 0	3/5	−2/5
7:	0 1 0 1	−2/5	3/5
7:	0 1 2 0	3/5	−1/40
8:	0 0 0 2	4/15	−11/15
8:	0 0 2 1	−2/5	−3/40
8:	0 0 4 0	81/80	69/320
8:	0 2 1 0	3/10	3/10
8:	1 1 1 0	7/20	1/4
9:	0 1 1 1	−1/5	−9/20
9:	0 1 3 0	9/20	39/160
9:	0 3 0 0	3/20	13/20
9:	1 2 0 0	1/5	1/2
10:	0 0 1 2	4/35	68/105
10:	0 0 3 1	−9/35	−9/35
10:	0 0 5 0	459/560	39/560
10:	0 2 0 1	−1/10	−4/5
10:	0 2 2 0	3/16	−1/20
10:	1 1 0 1	−4/35	−5/7
10:	1 1 2 0	3/14	−1/28
11:	0 1 0 2	2/35	104/105
11:	0 1 2 1	−3/28	27/140
11:	0 1 4 0	351/1120	−213/560
11:	0 3 1 0	3/40	−3/5
11:	1 2 1 0	27/280	67/140

get $Z[A,\bar{A}]$ from $Z[A,A^\dagger]$, by replacing $A^\dagger$ everywhere by $\bar{A}$. So we can use as set of basic invariants:

$$\mu = \det A, \quad \bar{\mu} = \det \bar{A},$$
$$\kappa = \mathrm{tr}(A\bar{A}), \quad \lambda = \mathrm{tr}((A\bar{A})^2). \quad (6)$$

Substitution of the series expansion

$$Z = \sum_{i,j,k,l=0}^{\infty} d_{ijkl}\,\mu^i\bar{\mu}^j\kappa^k\lambda^l \quad (7)$$

in (2) and (3) leads to recursion relations for d_{ijkl} which can be solved by computer. Terms up to order 30 have been calculated, where the order of a term in the expansion is defined to be the number of source-fields (A or $\bar{A}$) in it. In table 1 the values of d's which belong to terms of order up till 12 are given, and also the values of c's from the analogous expansion of log(Z). For ease of representation a factor has been taken out:

$$d(c)_{ijkl} = \tilde{d}(\tilde{c})_{ijkl}/i!j!k!l!(3!)^{i+j+k}(48)^l. \quad (8)$$

The values for Z are consistent with those derived in ref. [5]. [Note: one must use their Y as defined by their eq. (11) and not by their expression (12).]

I would like to thank Jan Smit for suggesting the problem and helpful discussions, and I am indebted to NIKHEF for use of their computer facilities.

Trivializing maps, the Wilson flow and the HMC algorithm

Martin Lüscher

LeapfrogLayers: A Trainable Framework for Effective Topological Sampling

Sam Foreman,[a,*] Xiao-Yong Jin[a,b] and James C. Osborn[a,b]

HMC with Normalizing Flows

Sam Foreman,[a,*] Taku Izubuchi,[b,c] Luchang Jin,[d] Xiao-Yong Jin,[a] James C. Osborn[a] and Akio Tomiya[b]

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]

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

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

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]

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

Jacob Finkenrath[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]

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]

Learning Trivializing Gradient Flows for Lattice Gauge Theories

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

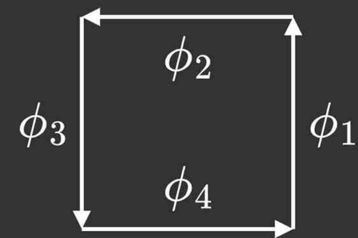
Normalizing flows for lattice gauge theory in arbitrary space-time dimension

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

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



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

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

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

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

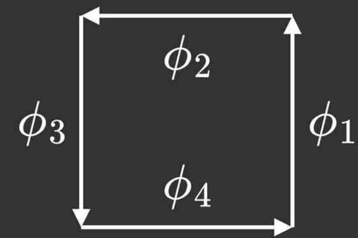
$$\longrightarrow\ Z = \int_0^{2\pi} \mathrm{d}\chi' \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4 \ \left|\frac{\partial \chi'}{\partial \chi}\right|^{-1} \exp\left(\beta \cos(\chi)\right) = \frac{\mathcal{I}(2\pi)}{2\pi} \int_0^{2\pi} \mathrm{d}\chi' \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4$$

- Change of variables: $\phi_1'(\chi') = \chi' - \sum_{k=2}^{4} \phi_k \in \left[-\sum_{k=2}^{4} \phi_k, 2\pi - \sum_{k=2}^{4} \phi_k\right) \equiv [\underline{\phi}_1', \overline{\phi}_1') \longrightarrow \frac{\partial \phi_1'}{\partial \chi'} = 1$

$$\longrightarrow\ Z = \frac{\mathcal{I}(2\pi)}{2\pi} \int_{\underline{\phi}_1'}^{\overline{\phi}_1'} \mathrm{d}\phi_1' \int_0^{2\pi} \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4 \equiv \frac{\mathcal{I}(2\pi)}{2\pi} \int_0^{2\pi} \mathrm{d}\phi_1' \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4$$

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

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



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

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

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

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

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

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

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

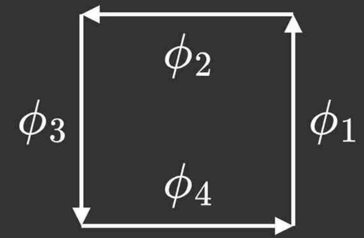
- Change of variables: $\phi_1'(\chi') = \chi' - \sum_{k=2}^{4}\phi_k \in \left[-\sum_{k=2}^{4}\phi_k, 2\pi - \sum_{k=2}^{4}\phi_k\right) \equiv [\underline{\phi}_1', \overline{\phi}_1') \longrightarrow \frac{\partial \phi_1'}{\partial \chi'} = 1$

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

$$\longrightarrow Z = \frac{\mathcal{I}(2\pi)}{2\pi}\int_{\underline{\phi}_1'}^{\overline{\phi}_1'} \mathrm{d}\phi_1' \int_0^{2\pi} \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4 \equiv \frac{\mathcal{I}(2\pi)}{2\pi}\int_0^{2\pi} \mathrm{d}\phi_1' \mathrm{d}\phi_2 \mathrm{d}\phi_3 \mathrm{d}\phi_4$$

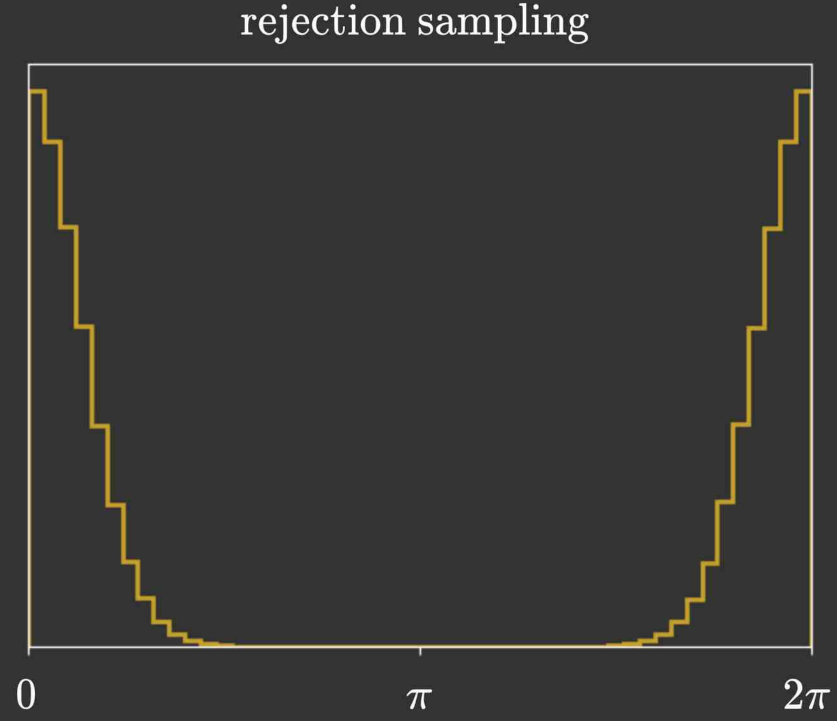
(Un-)trivializing (1+1)d U(1) LGT

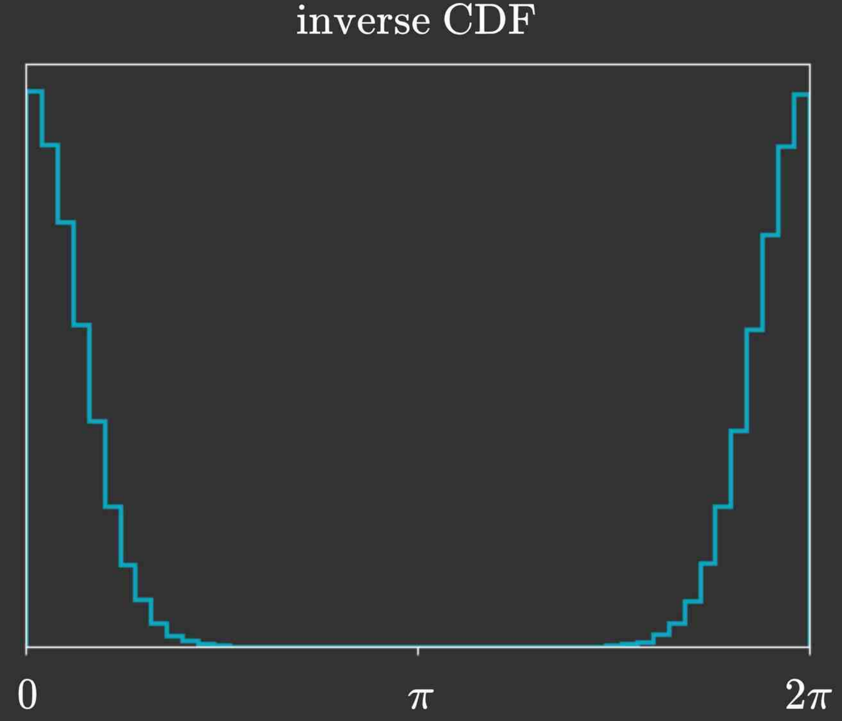
$$\phi_k \in [0, 2\pi), \;\; S = -\beta \cos\Big(\sum_{k=1}^{4} \phi_k\Big)$$



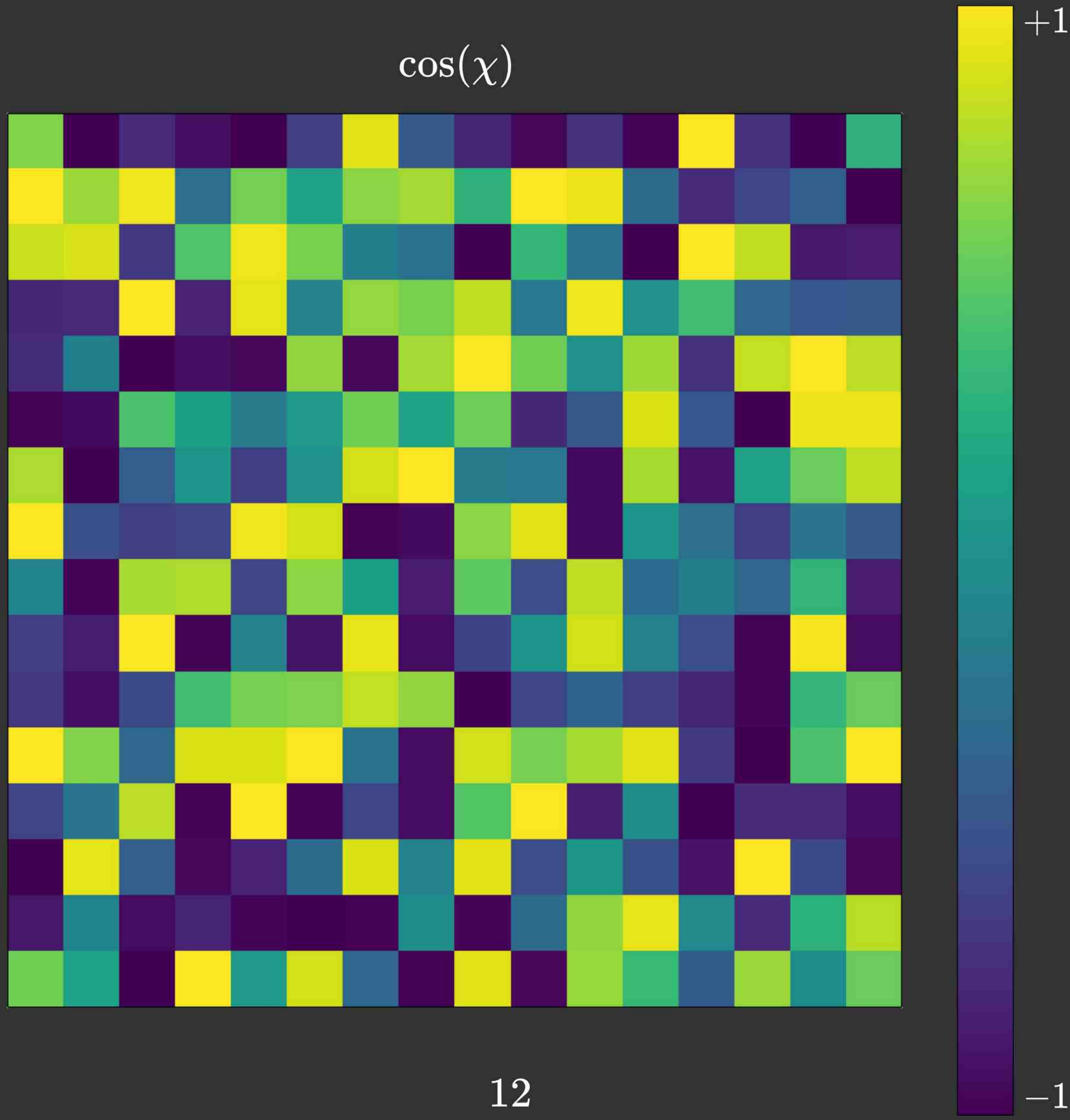
$$Z = \prod_{k=1}^{4} \Big(\int_0^{2\pi} \mathrm{d}\phi_k\Big) \exp\Big(-S\Big(\sum_{k=1}^{4} \phi_k\Big)\Big)$$

$\longrightarrow$ inverse transform sampling the von Mises distribution

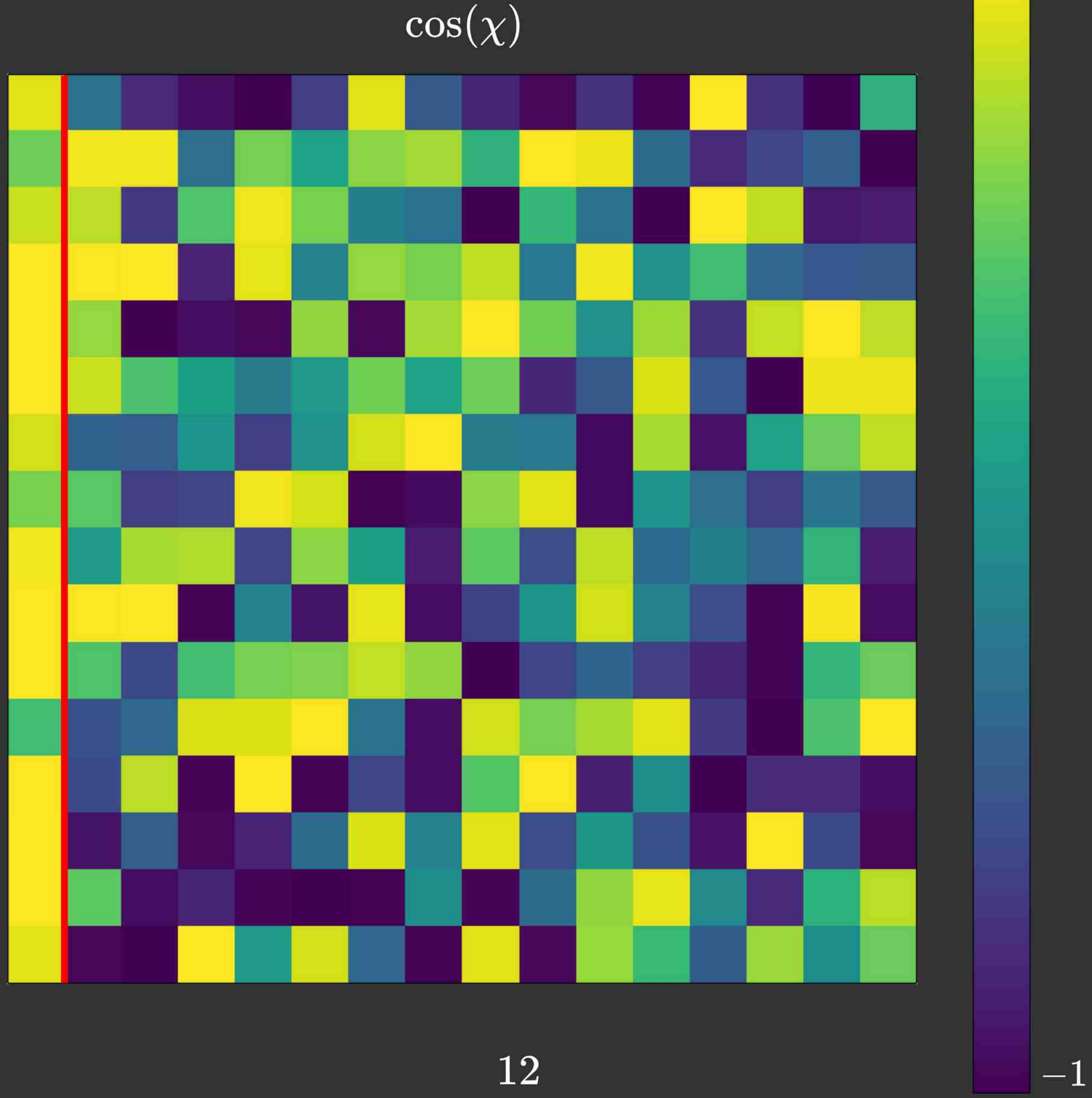




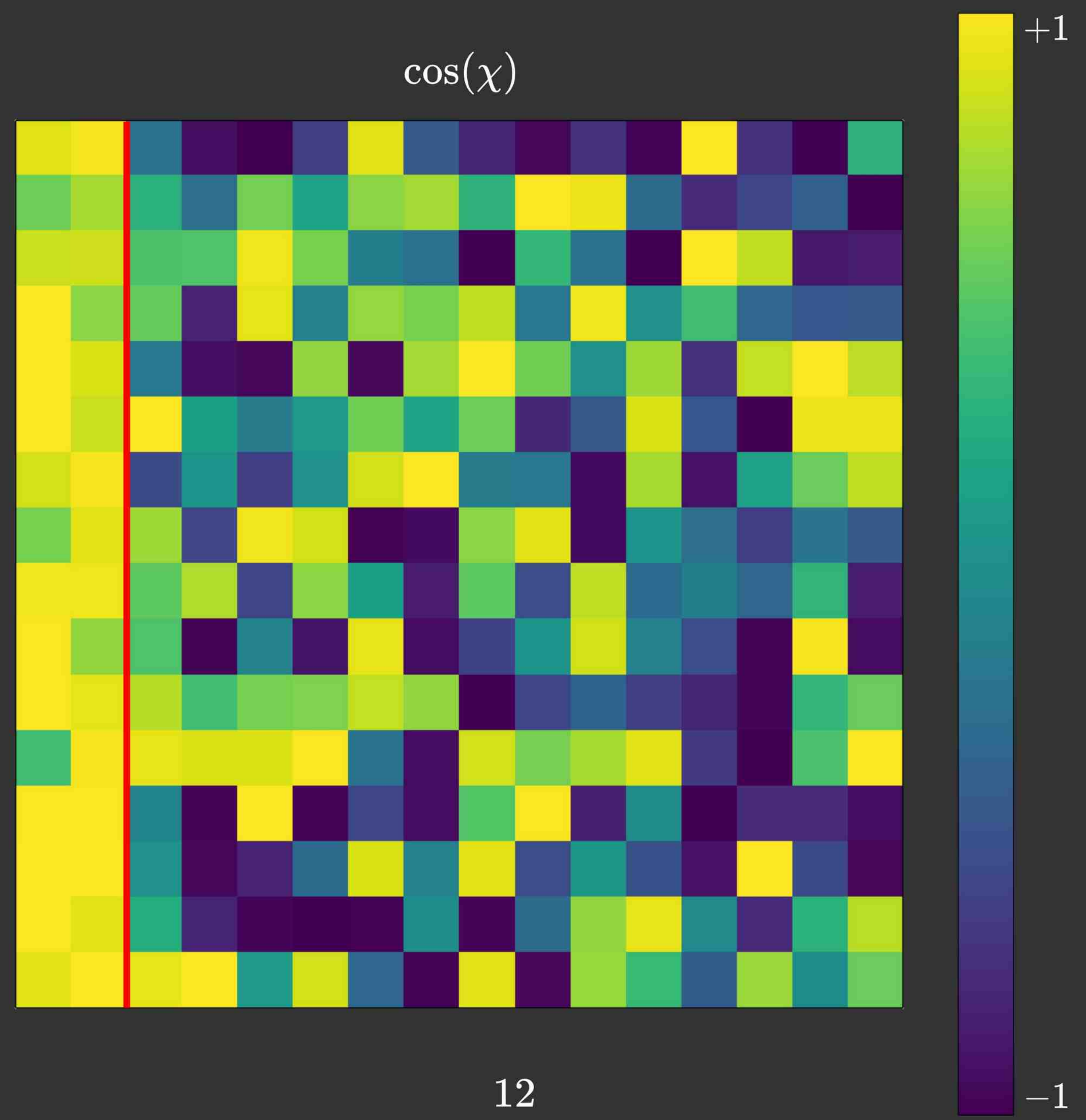
(Un-)trivializing (1+1)d U(1) LGT



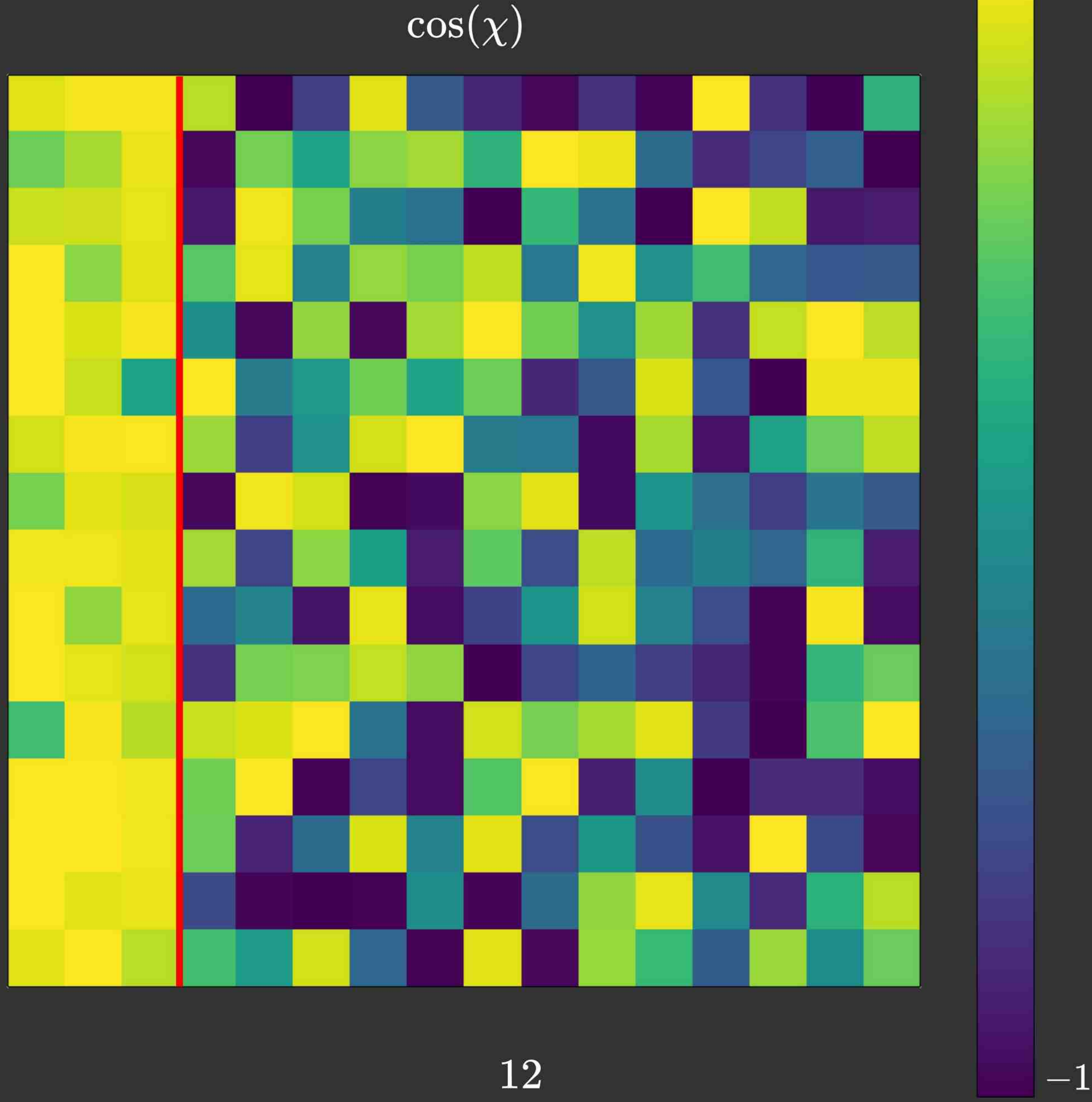
(Un-)trivializing (1+1)d U(1) LGT



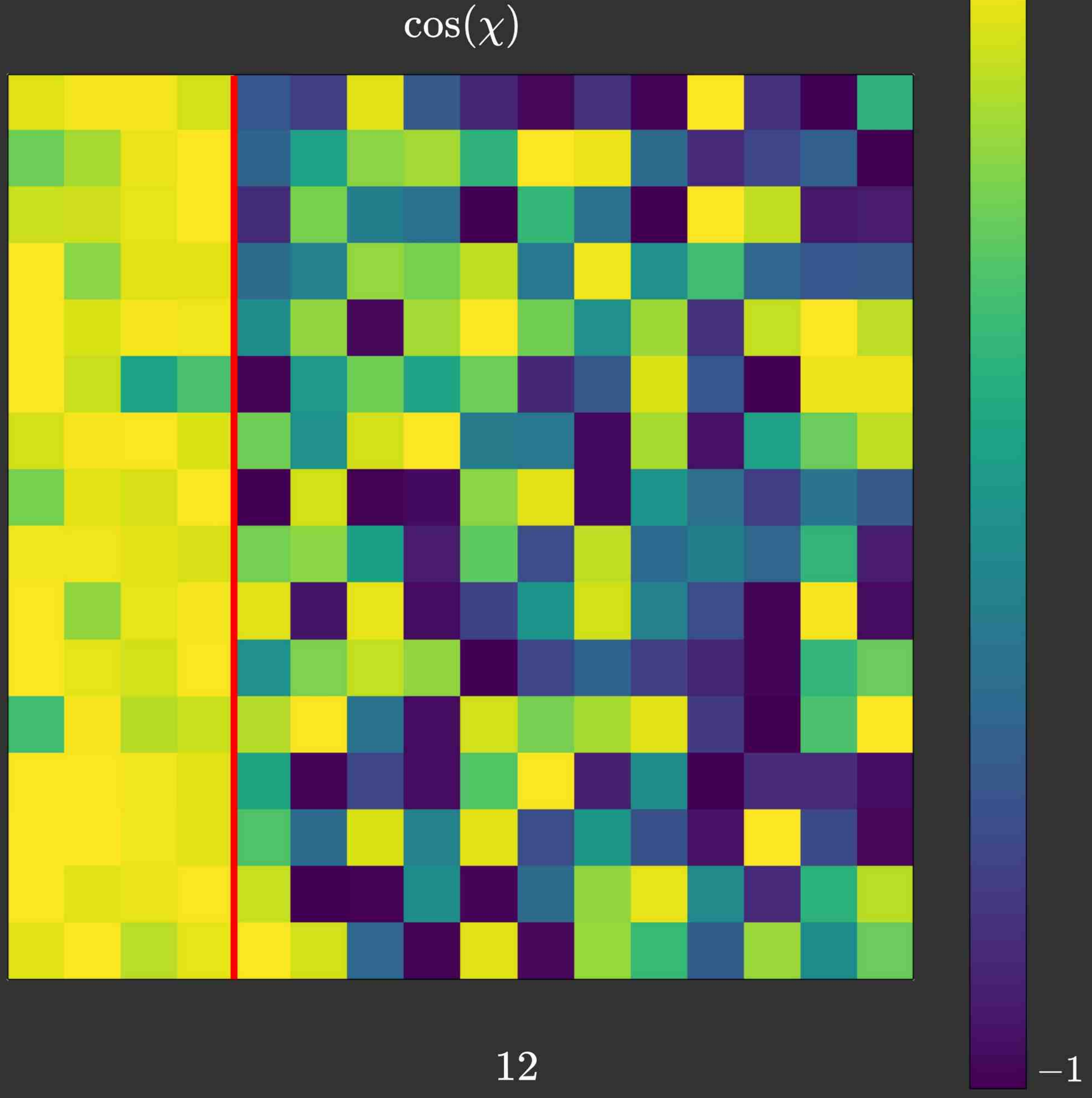
(Un-)trivializing (1+1)d U(1) LGT



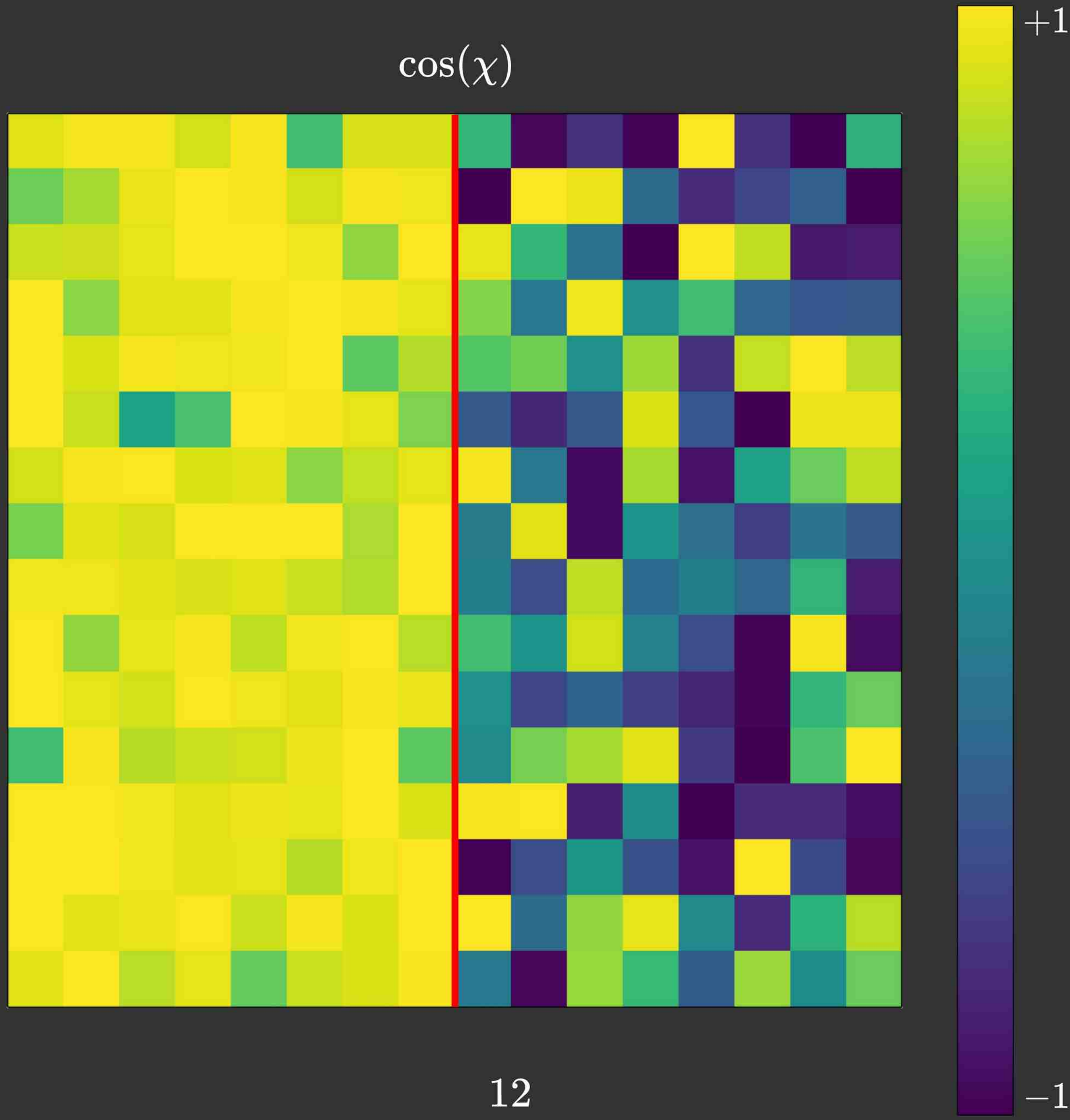
(Un-)trivializing (1+1)d U(1) LGT



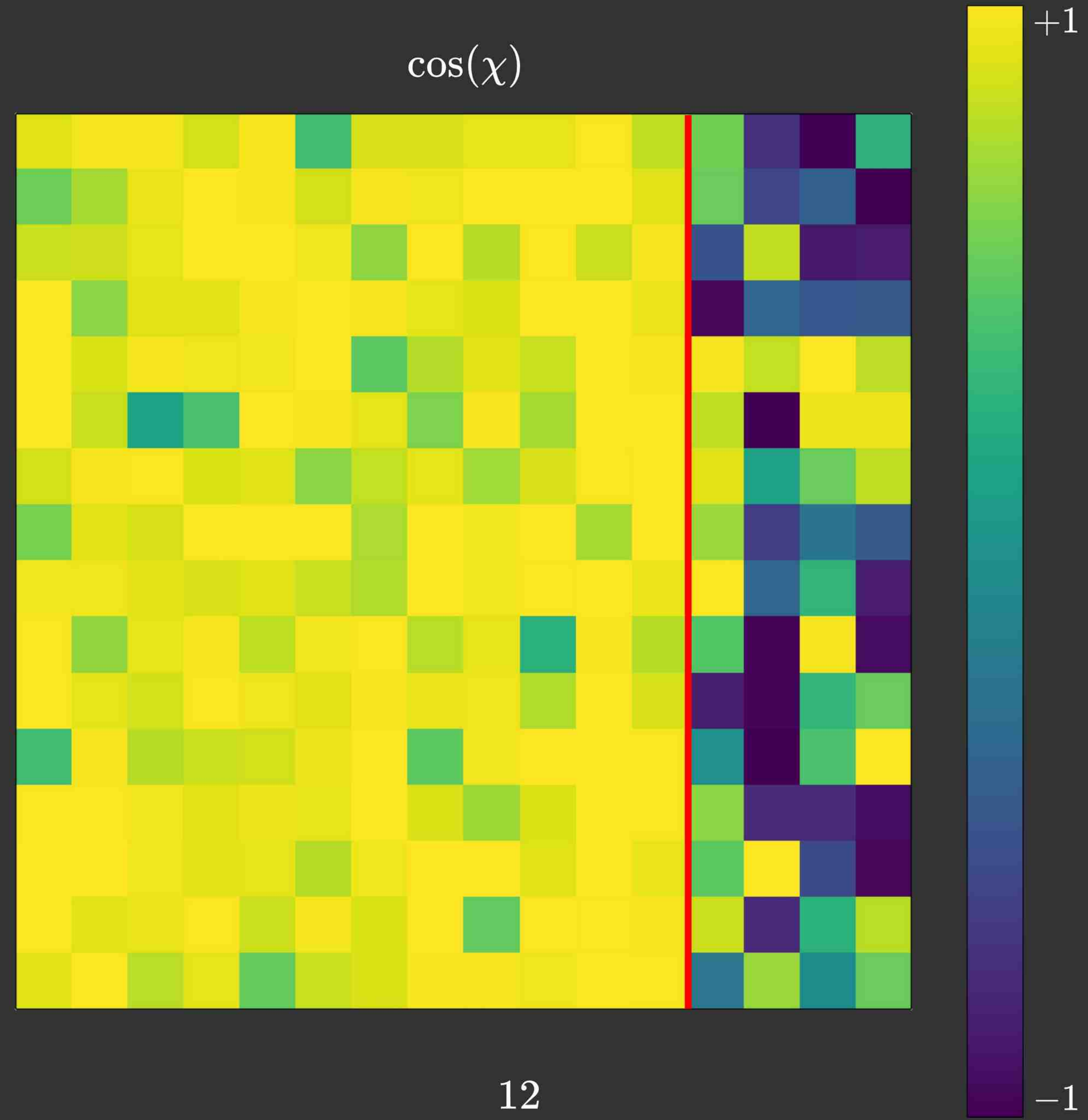
(Un-)trivializing (1+1)d U(1) LGT



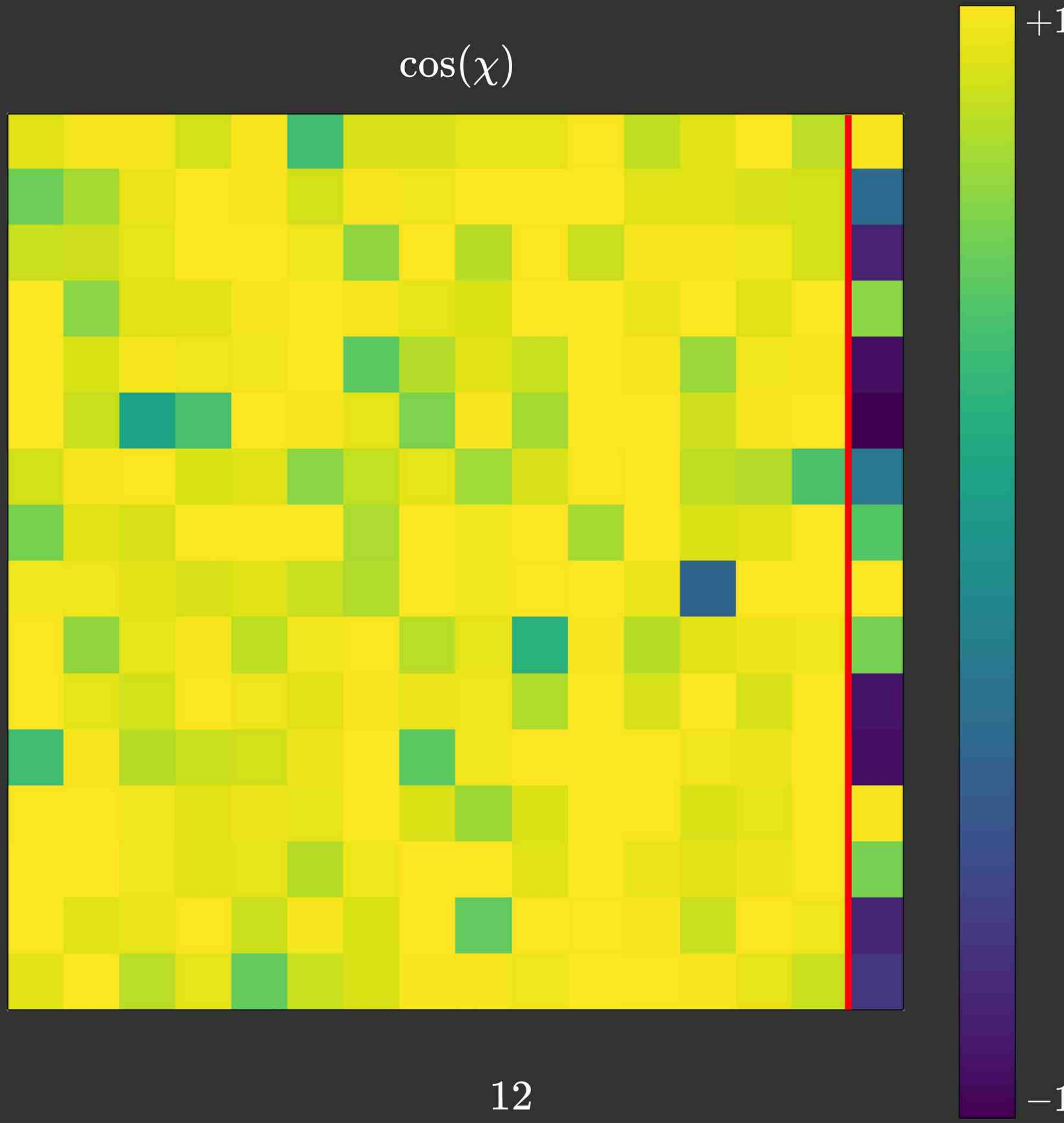
(Un-)trivializing (1+1)d U(1) LGT



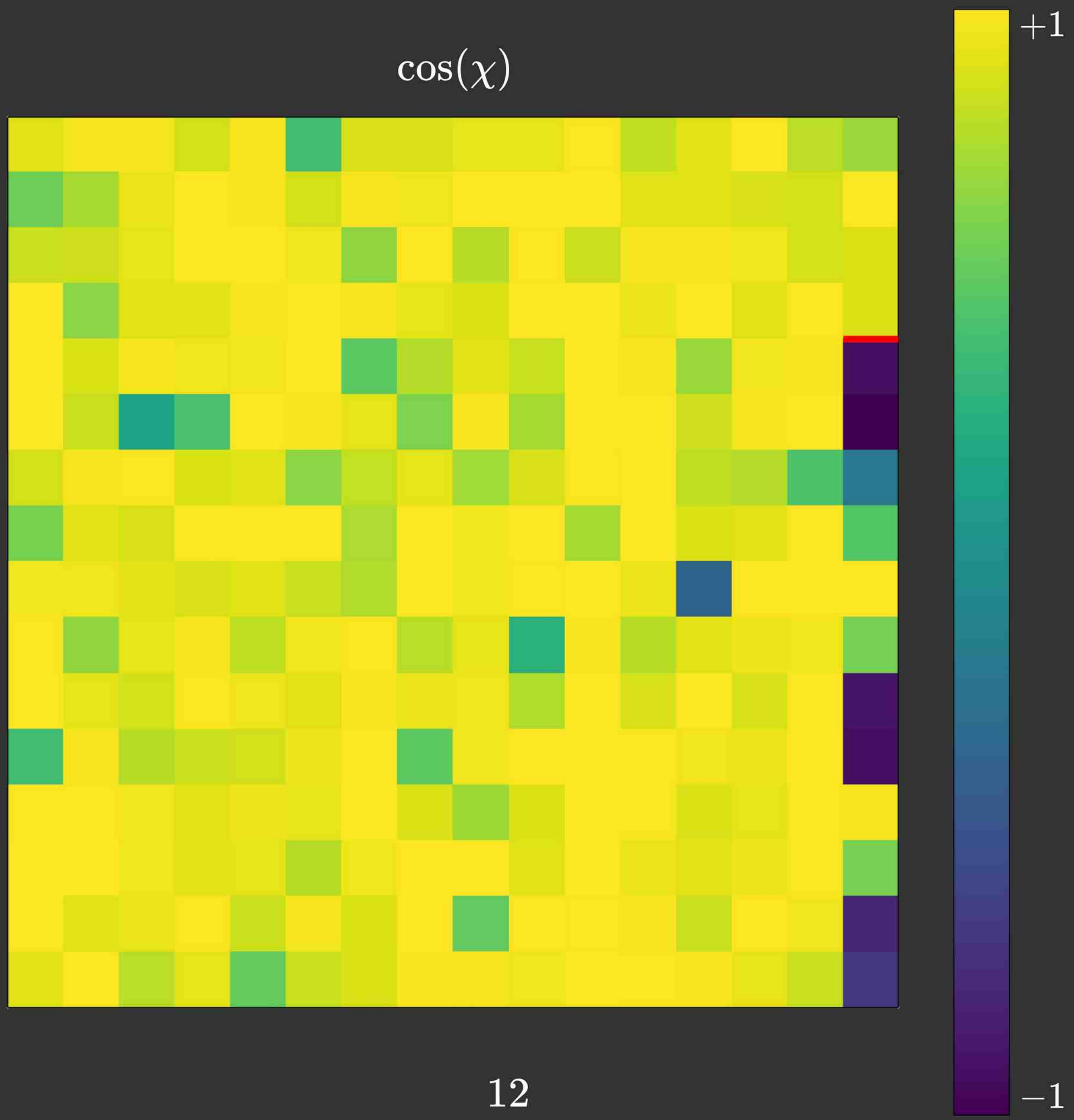
(Un-)trivializing (1+1)d U(1) LGT



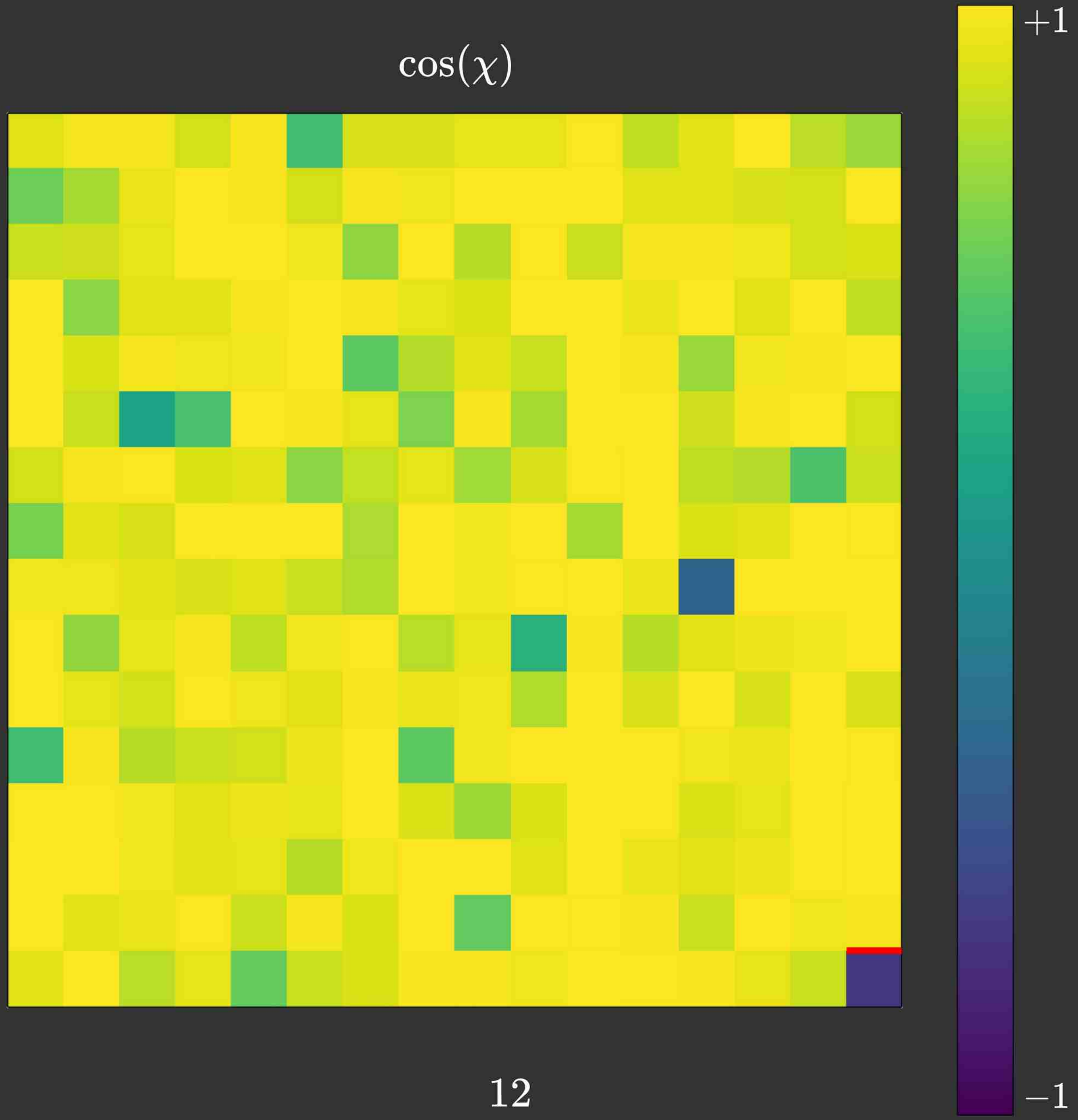
(Un-)trivializing (1+1)d U(1) LGT



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



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



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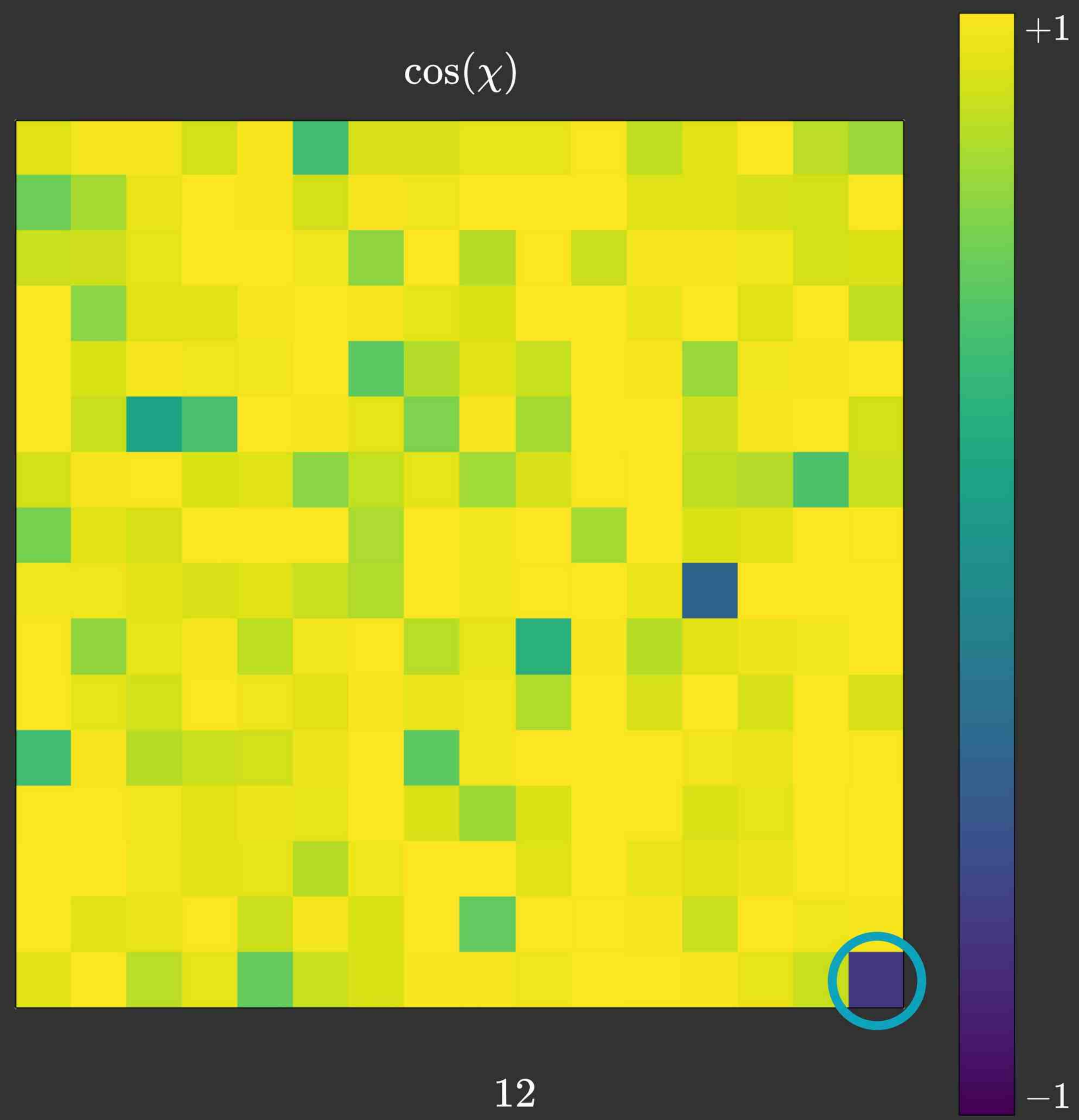
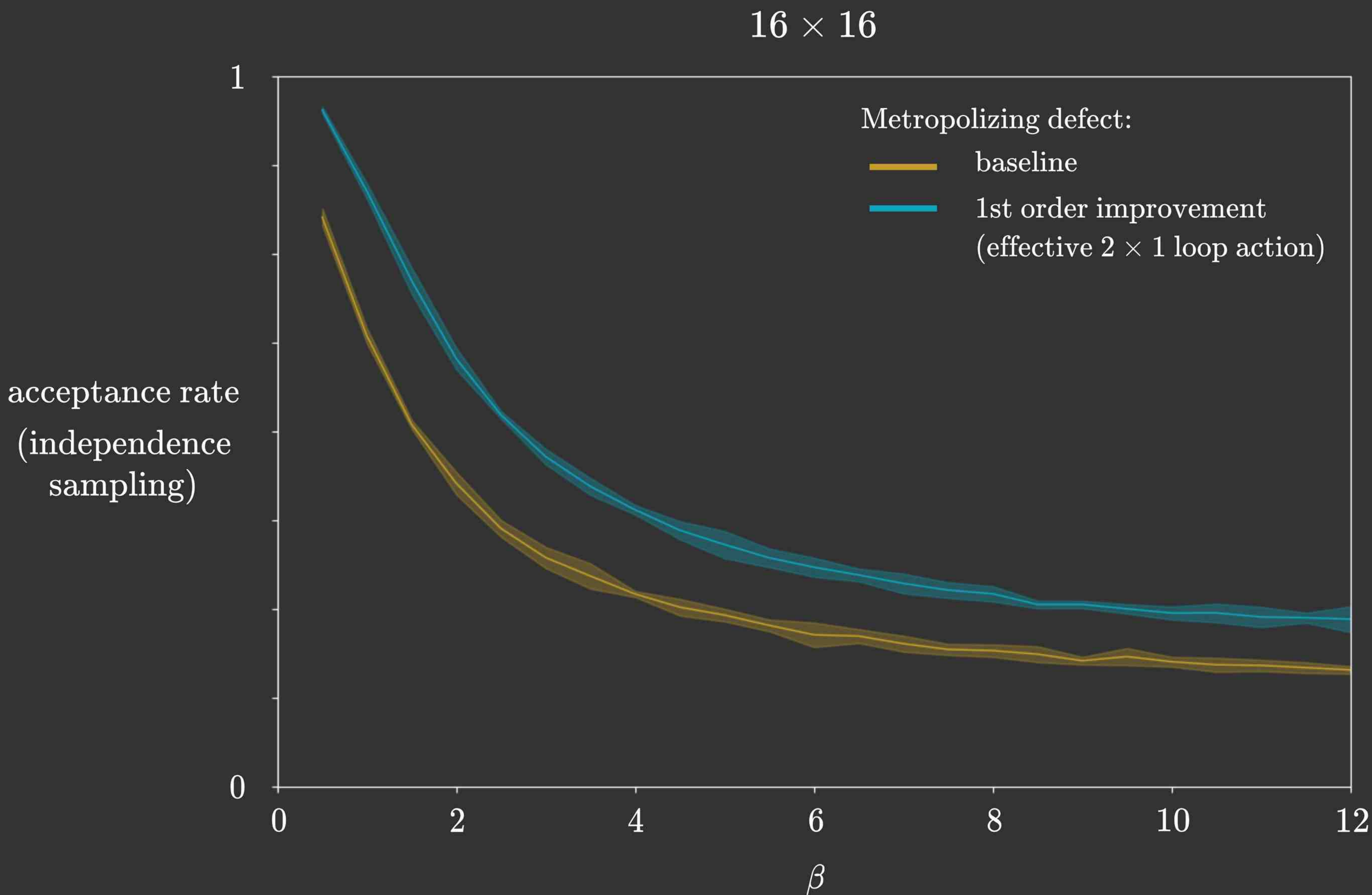
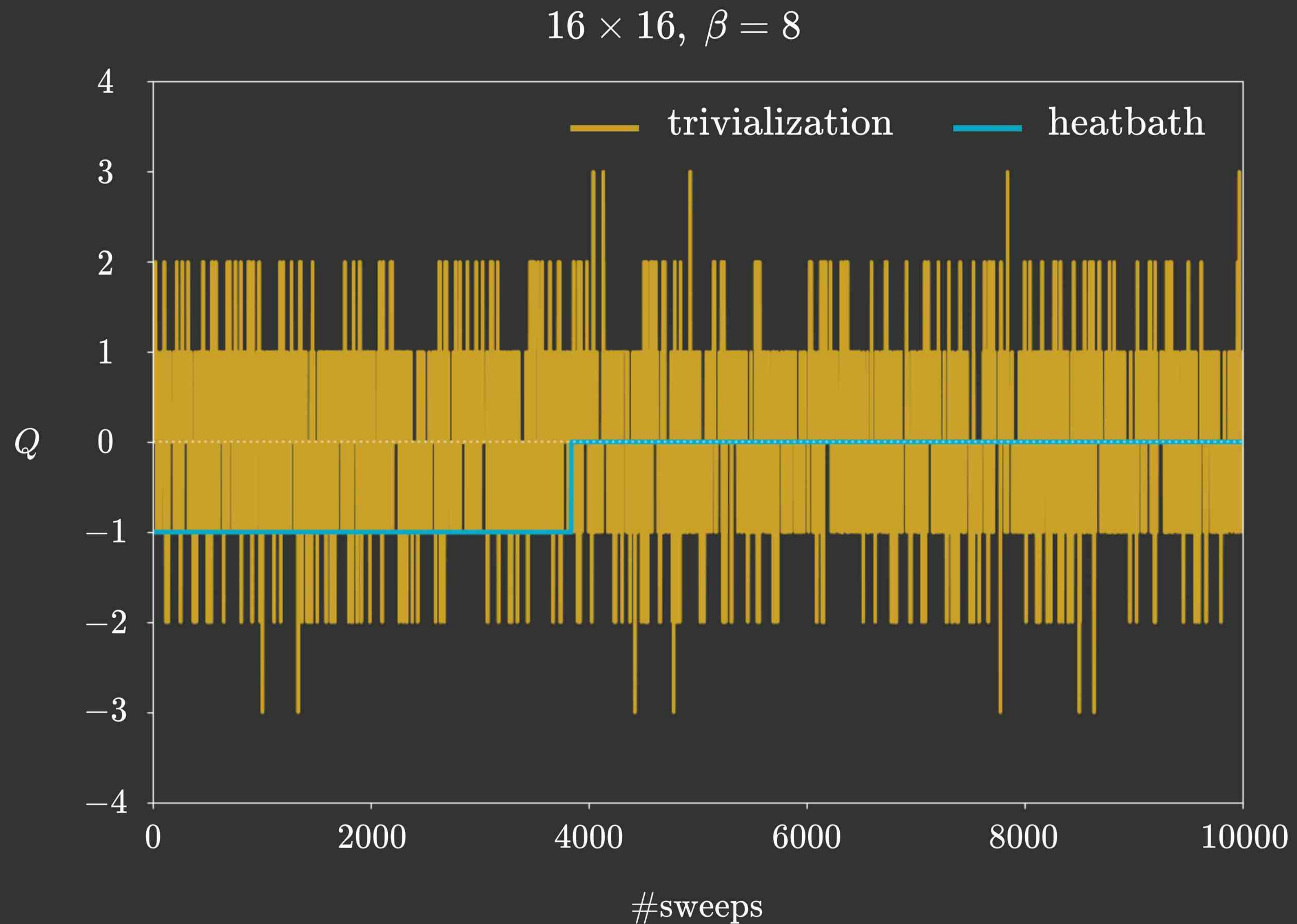
(Un-)trivializing (1+1)d U(1) LGT



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

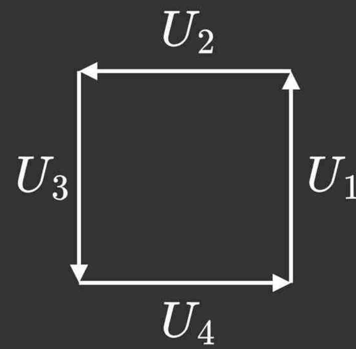


(Un-)trivializing (1+1)d U(1) LGT



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

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



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

- Change of variables: $P(U_1) = U_1 \prod_{k=2}^{4} U_k \longrightarrow Z = \int \mathrm{d}P\mathrm{d}U_2\mathrm{d}U_3\mathrm{d}U_4\ \exp(-S(P))$

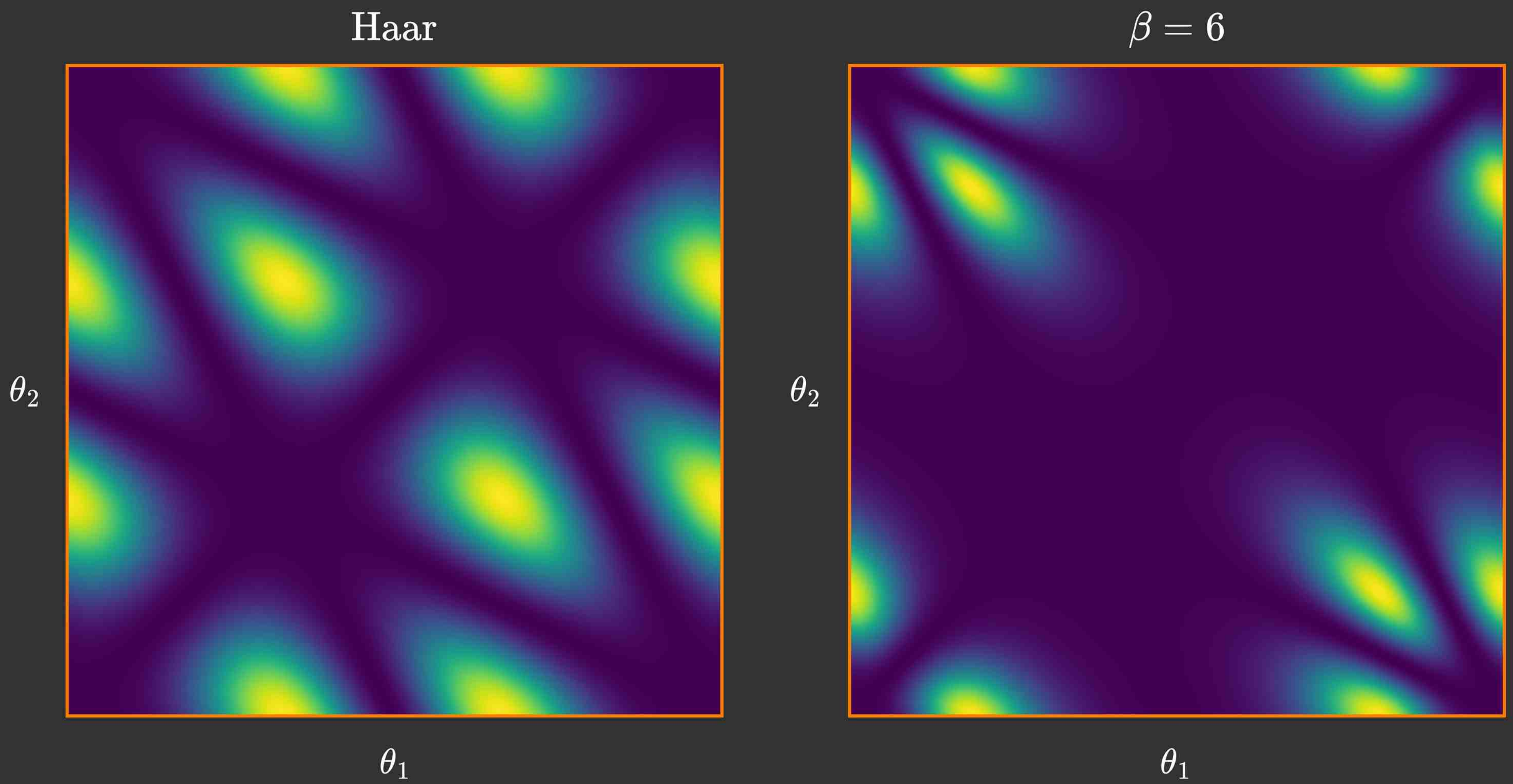
- Weyl integration formula for compact connected Lie group G in terms of a maximal torus T :

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

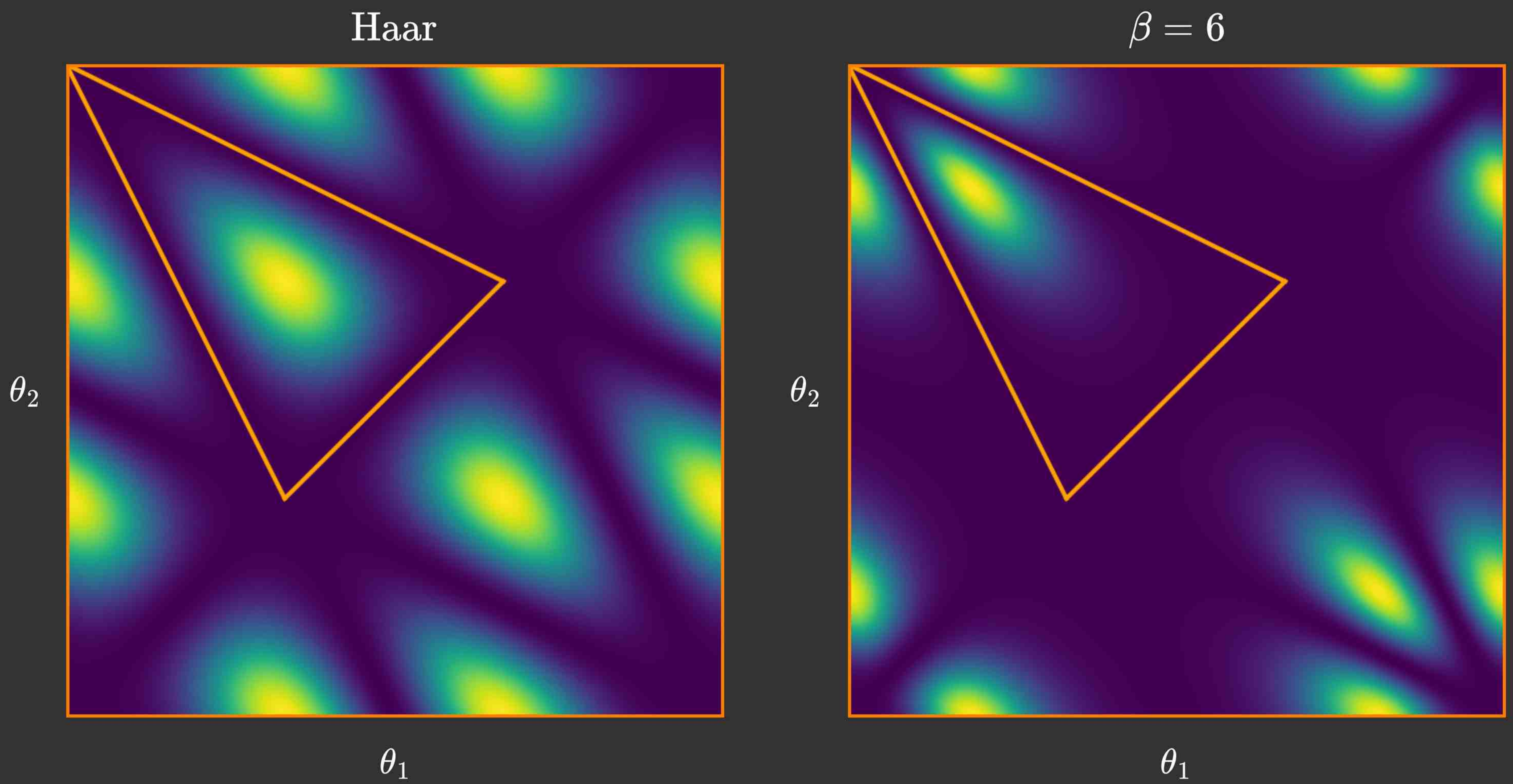
where f is a class function, i.e. $f(U) = f(\Omega U \Omega^\dagger)$ (conjugation-invariant),
and $e^{\mathrm{i}\theta_k}$ are unique eigenvalues ($N-1$ for $\mathrm{SU}(N)$).

$\longrightarrow$ 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

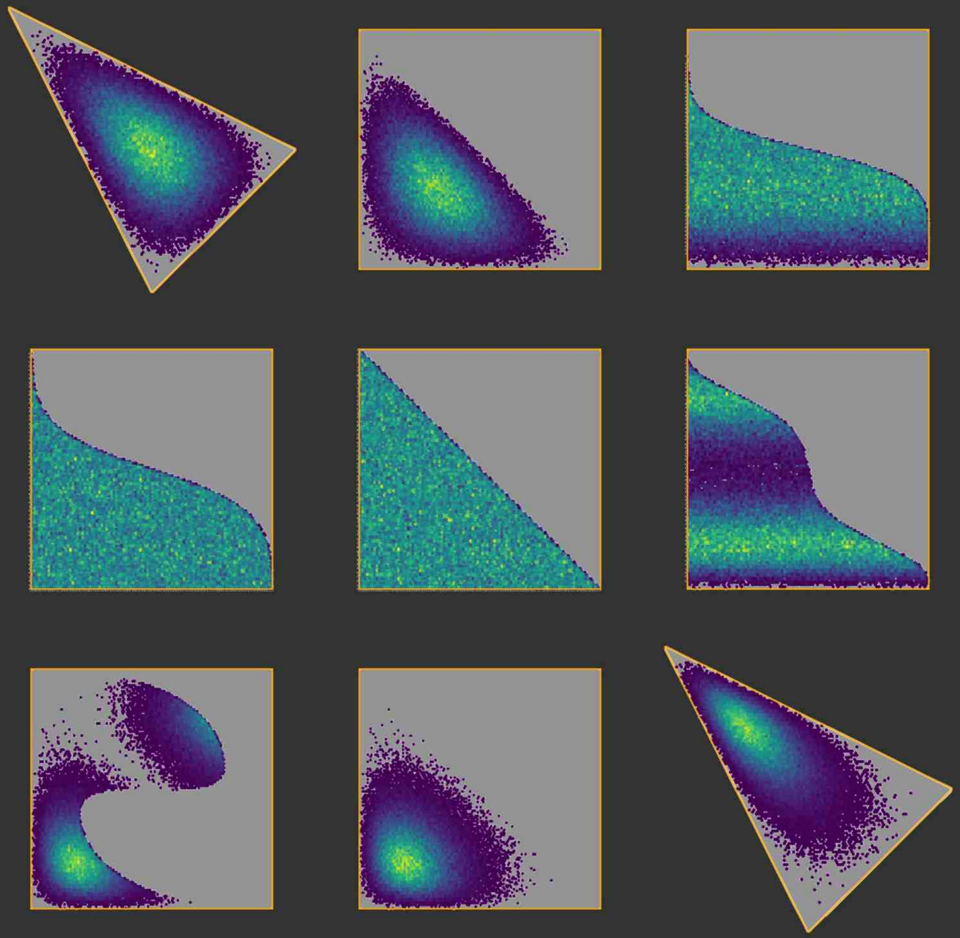


(Un-)trivializing (1+1)d SU(3) LGT



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

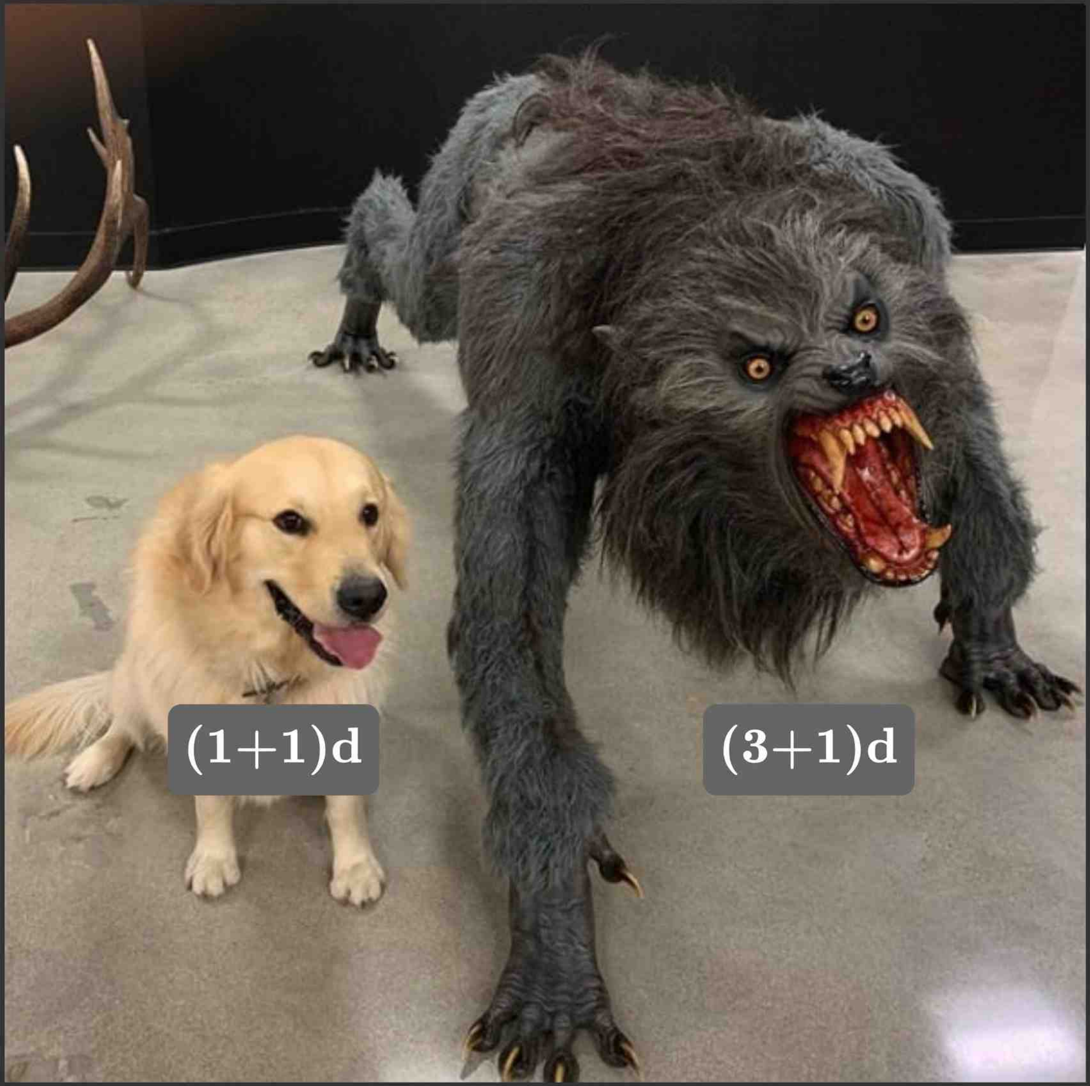
- Approximate solution with tractable Jacobian using differentiable quadrature:



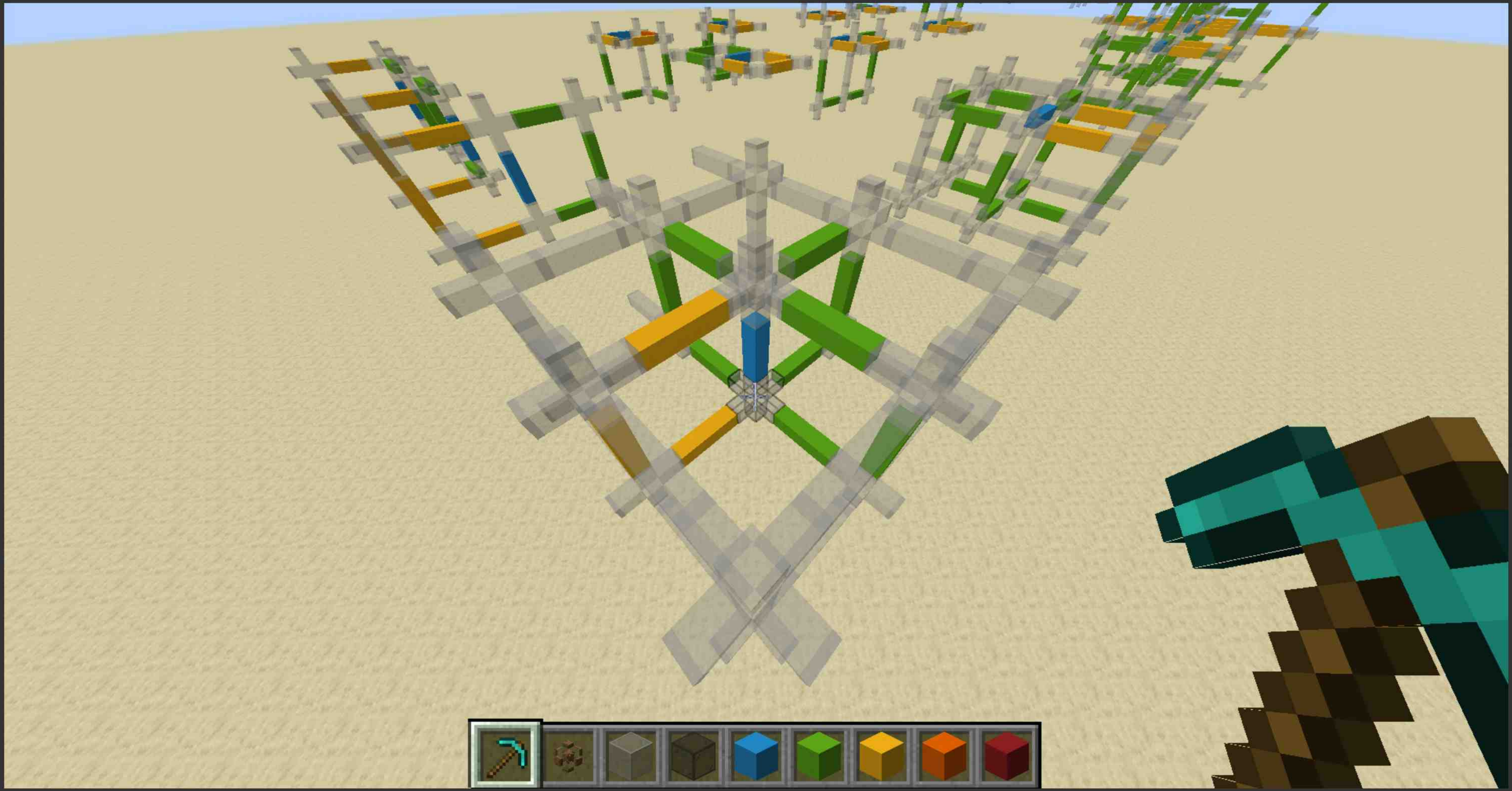
(further details will be provided in Lattice2023 PoS)

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

Higher dimensions?

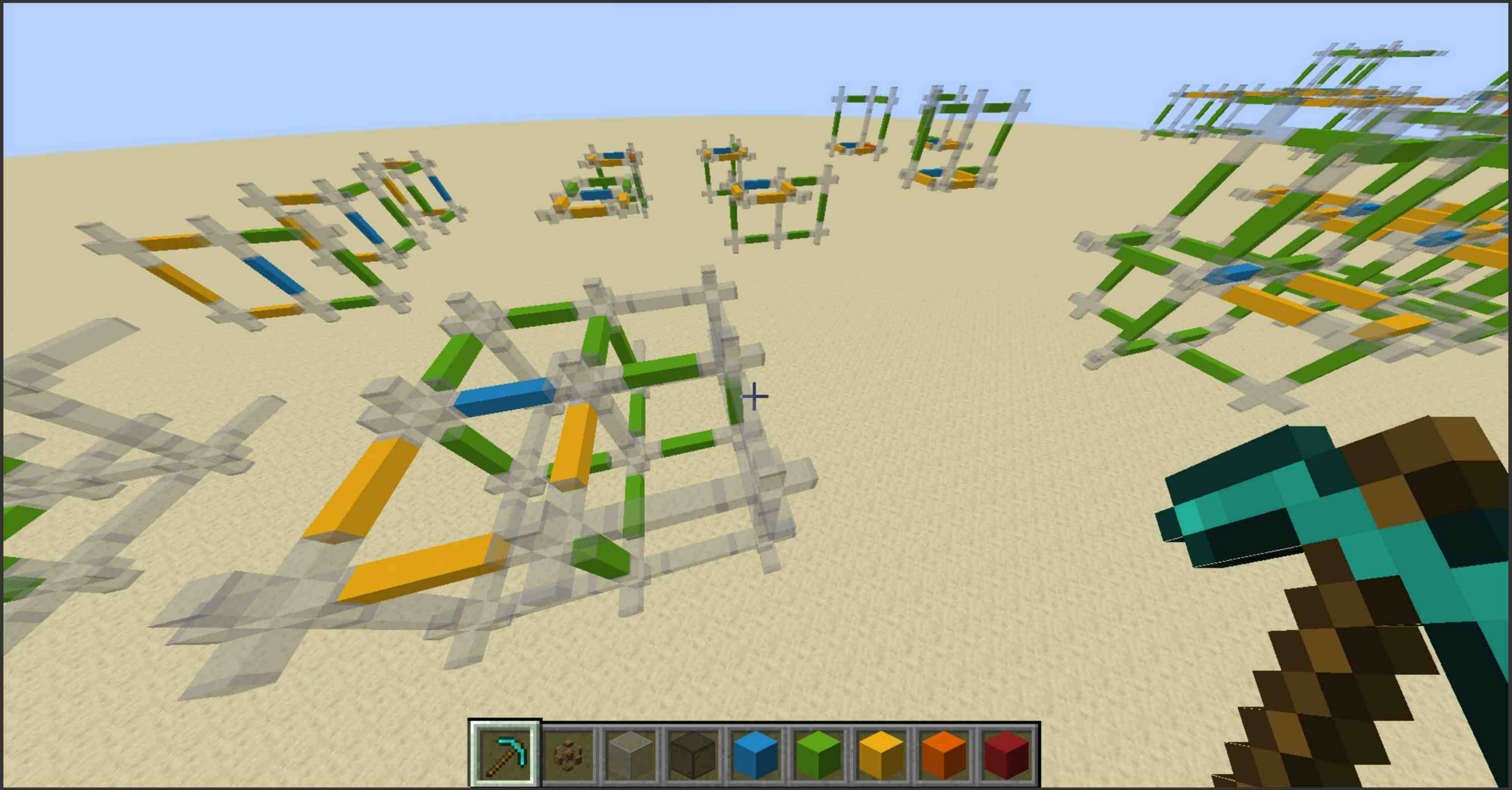


Higher dimensions?

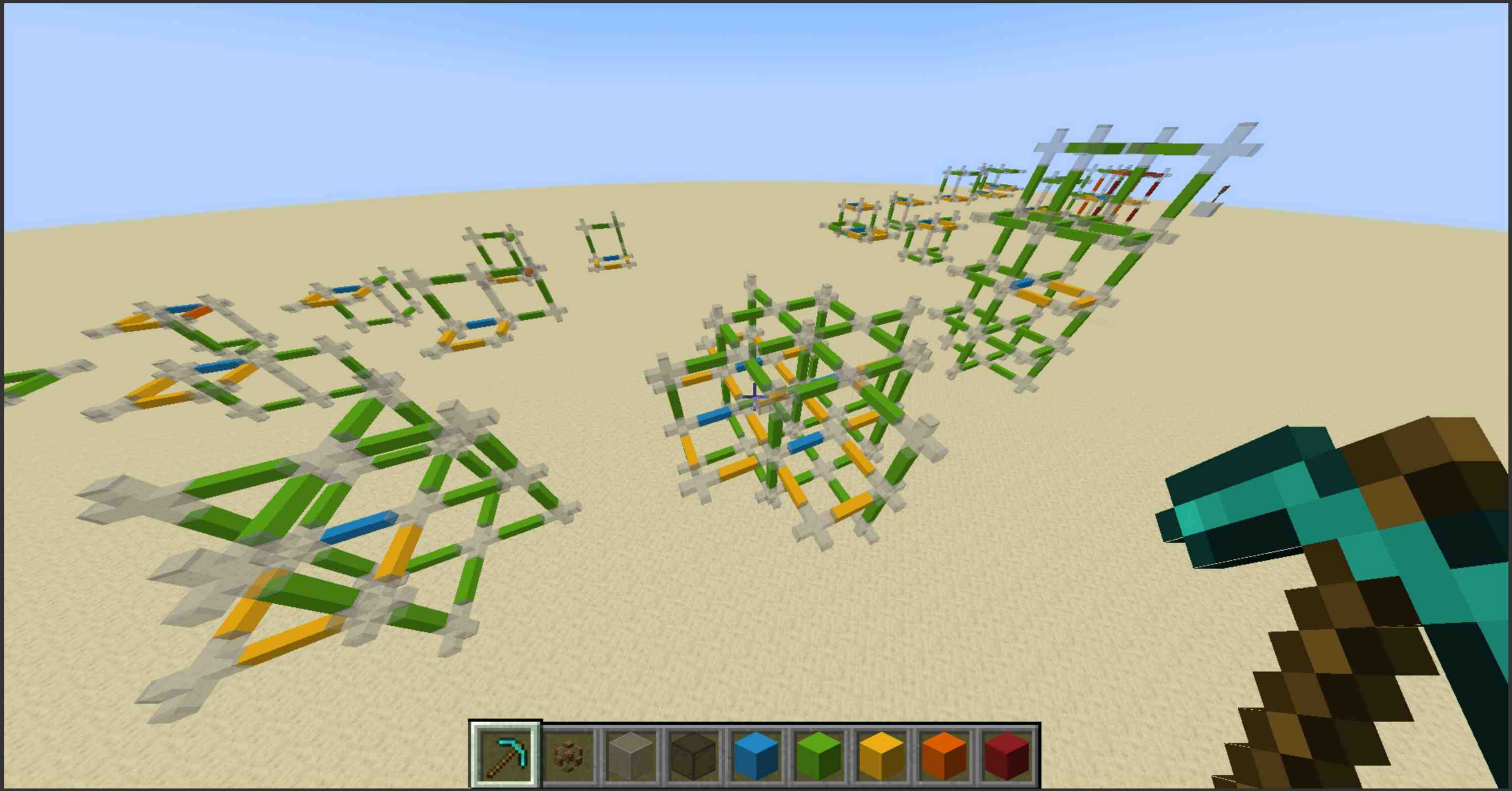


Higher dimensions?

Higher dimensions?



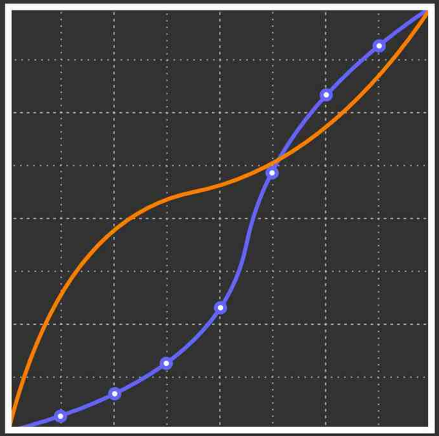
Higher dimensions?



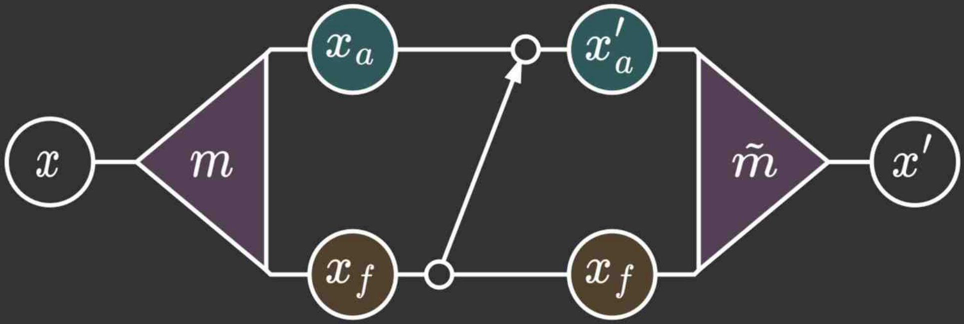
(Un-)trivializing (n+1)d SU(3) LGT with ML

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



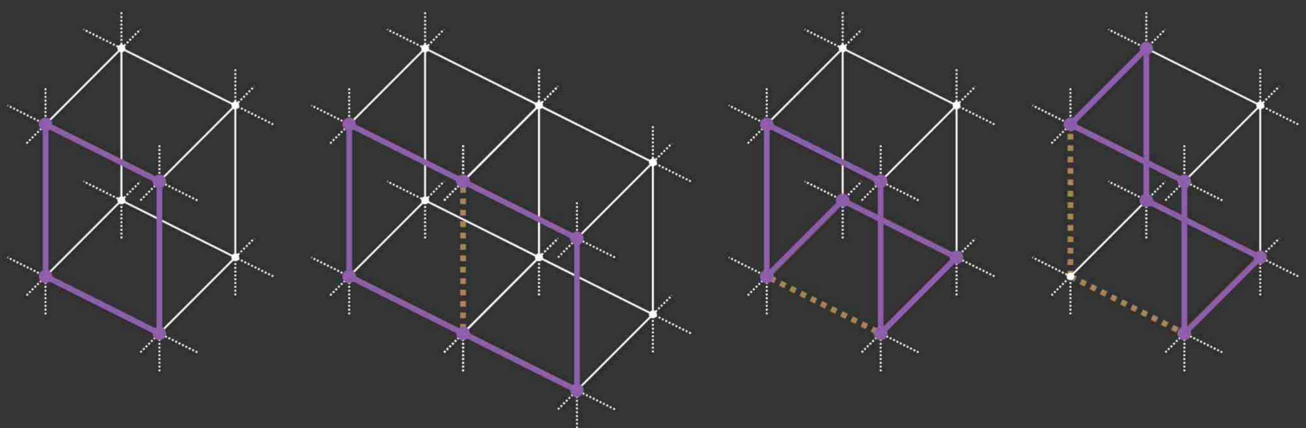
- Locally compute spline parameters from surrounding features using neural networks
- Global invertibility from alternating masking patterns $\longrightarrow$ coupling layers

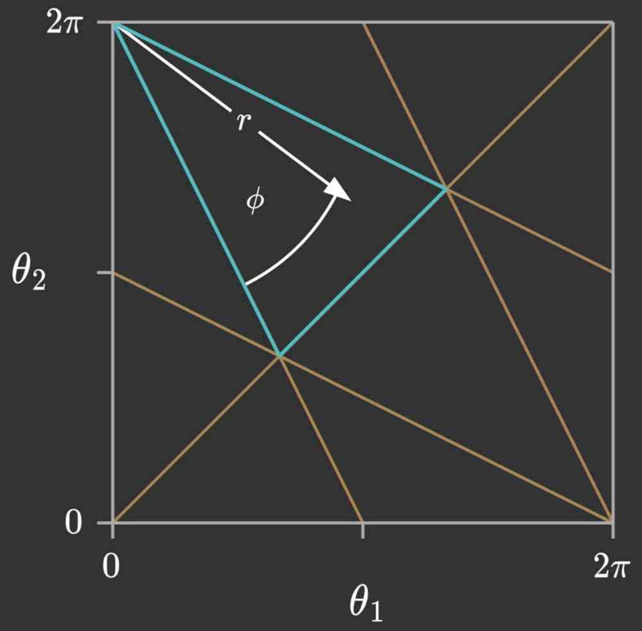


- Variational optimization by minimizing reverse Kullback-Leibler divergence

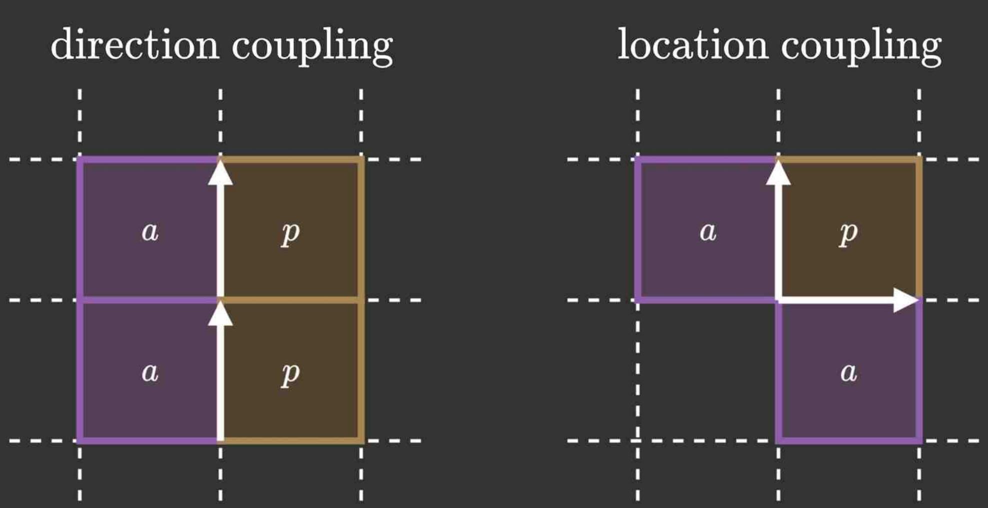
Neural RQS eigenvalue flow

- 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:

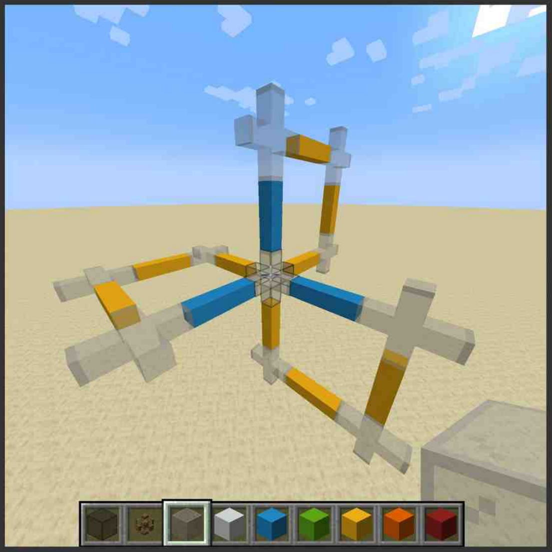




- Choose local coupling geometry, e.g.



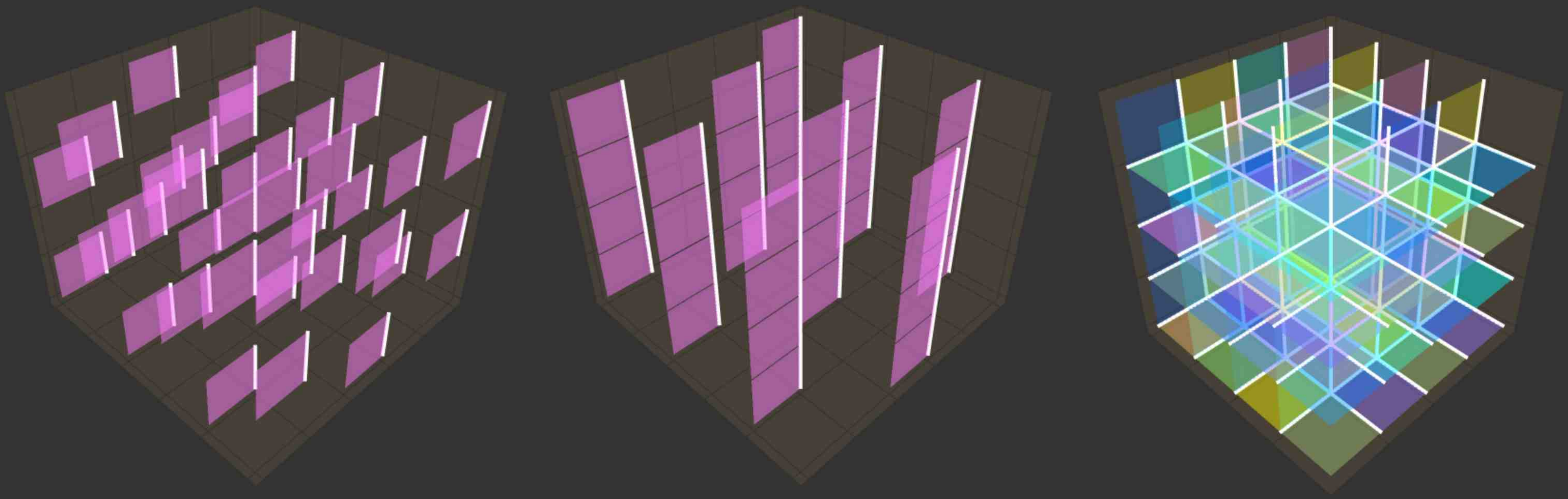
location coupling in (2+1)d



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

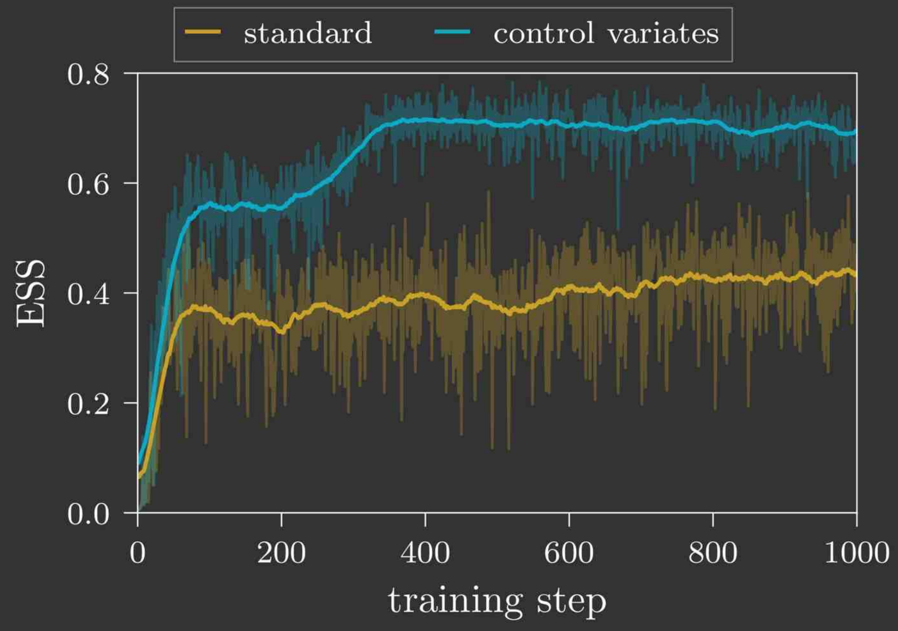
- Variance reduction in gradient estimates using path gradients + control variates

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
flow	residual	0.09	0.18

Practical applications (cf. Dan Hackett)

App 1: Correlated ensembles

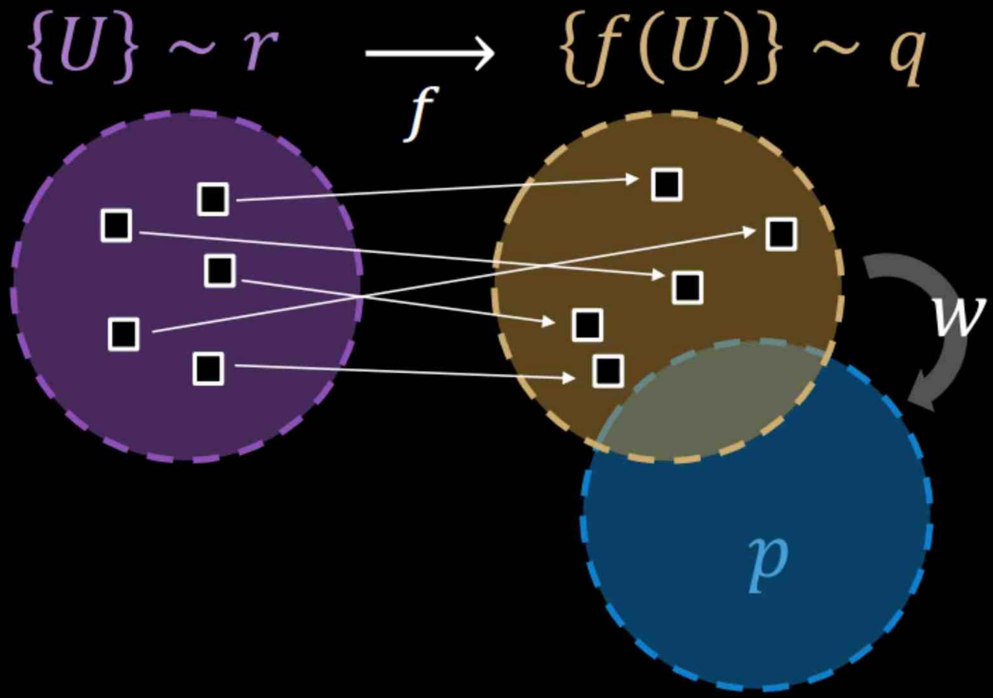
Flow an ensemble

→ $\{U\}$ and $\{f(U)\}$ are correlated

This is useful!

e.g. for noise cancellation in differences

$$\langle O\rangle_p - \langle O\rangle_r$$
$$= \langle wO\rangle_q - \langle O\rangle_r$$
$$= \langle w(f(U))\, O(f(U)) - O(U)\rangle_{U\sim r}$$



Application: Feynman-Hellmann $\quad S \to S + \lambda\, O \quad \left.\frac{\partial E_h}{\partial \lambda}\right|_{\lambda=0} \sim \langle h|O|h\rangle$

(Complication: involves fits for E_h, but same idea)

See also [Bacchio 2305.07932]

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Practical applications (cf. Dan Hackett)

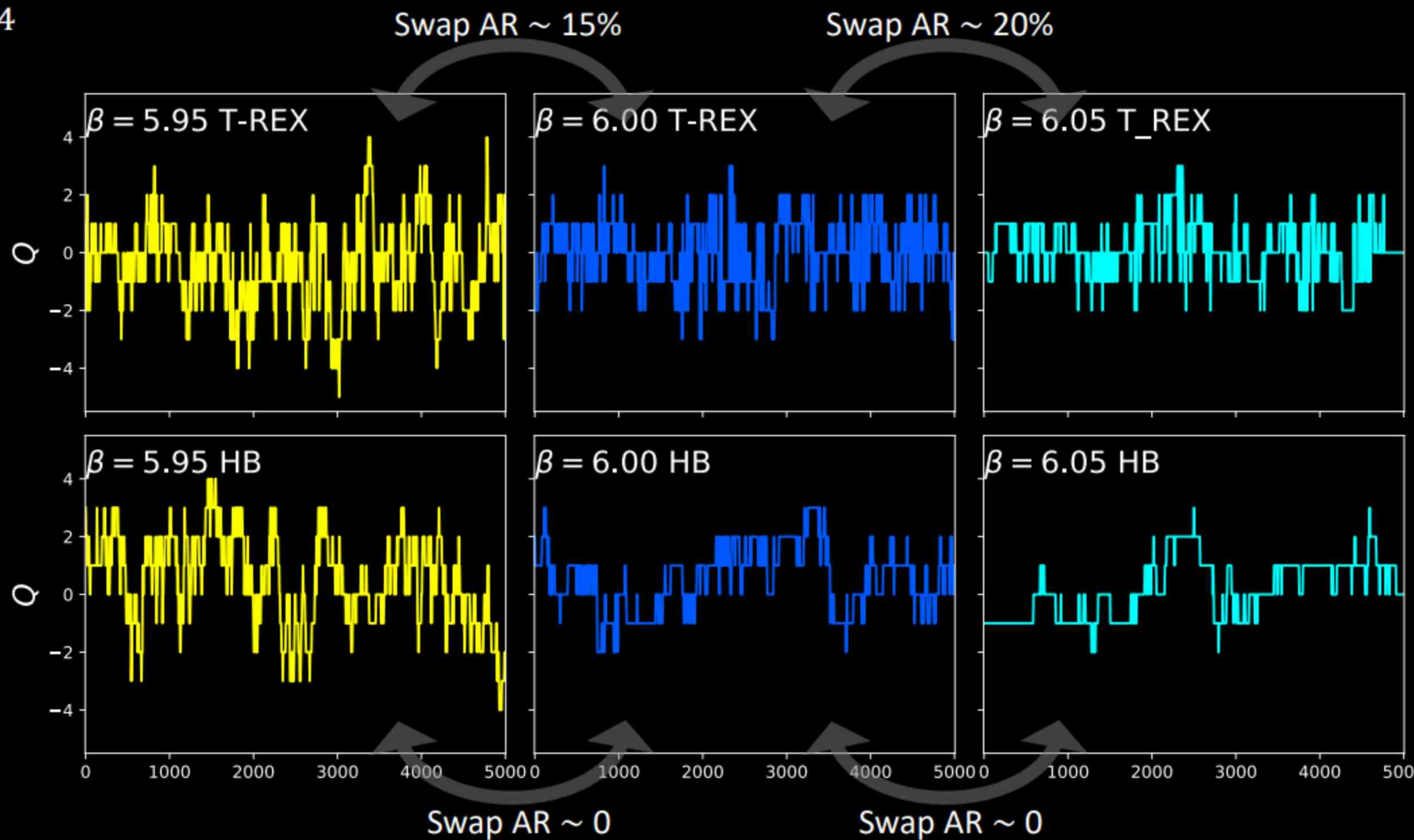
App 2: T-REX Results

Three target βs on 12^4

Two different flows

$5.95 \leftrightarrow 6$

$6 \leftrightarrow 6.05$



1 step = 5 HB + 2 OR, propose swaps every 5 steps

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, analytic trivialization attempts suggest missing information

  $\longrightarrow$ need covariant features 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 trivialization / thermodynamic integration on small volumes

  $\longrightarrow$ practical applications are within reach (correlated ensembles, parallel tempering)

Thanks!