Ensemble generation for lattice QFT using machine learning

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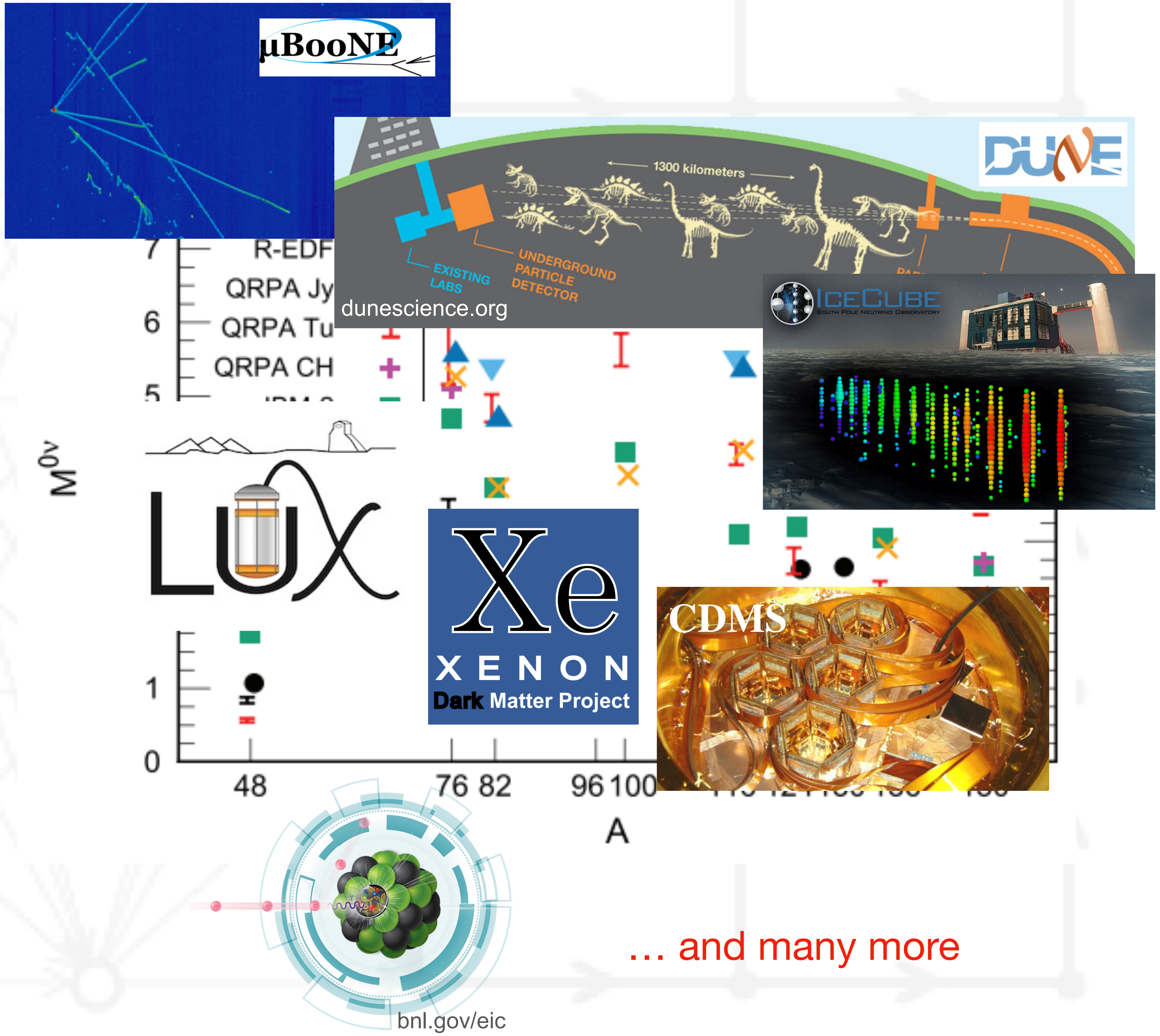
(Just one) Motivation for an ab initio approach

- Many experiments for new physics rely on nuclear targets / samples

- Need to know SM predictions for nuclear matrix elements, structure functions

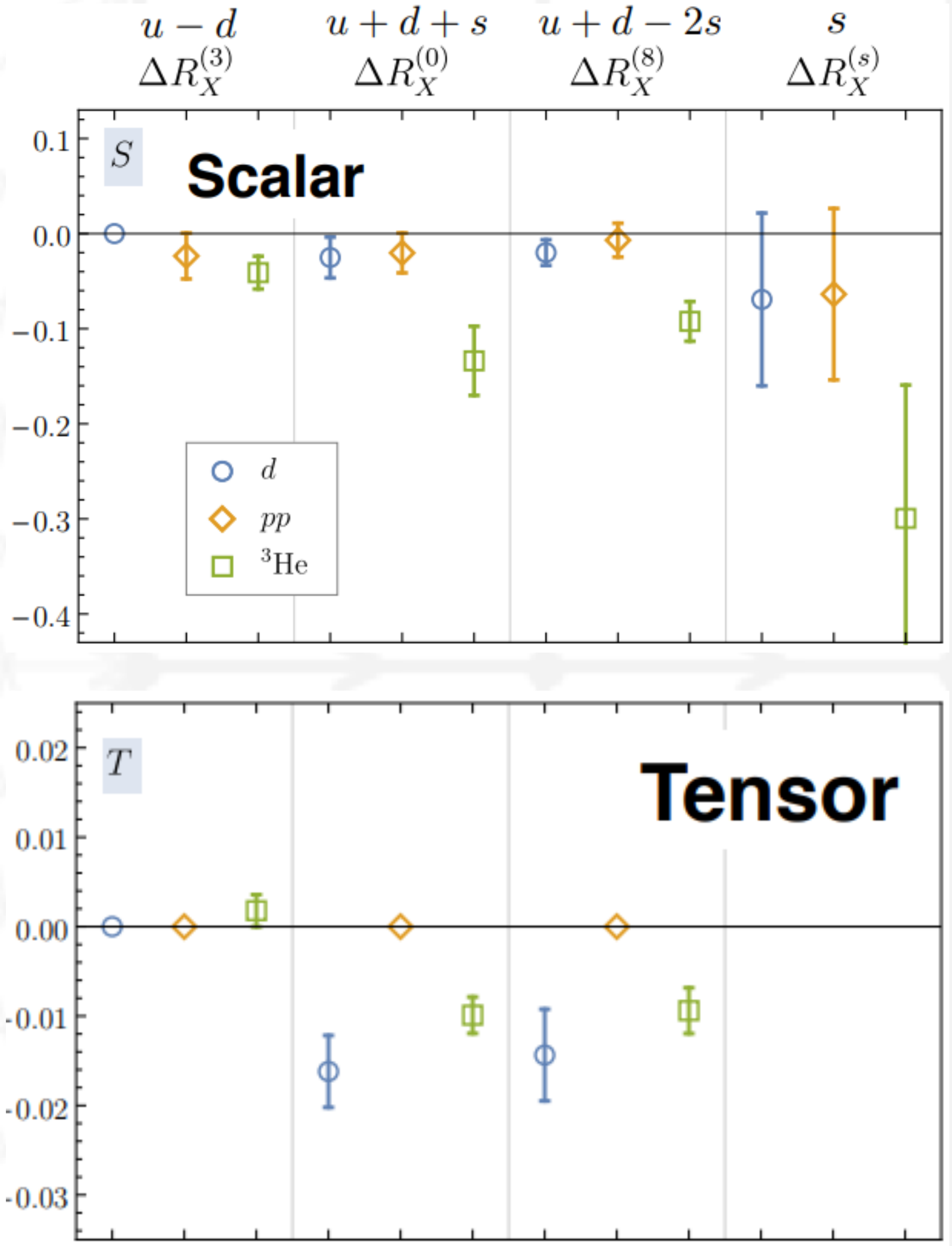
- Models disagree: **ab initio is key!**



… and many more

Ab initio nuclear physics

- **Lattice QCD** gives theoretical input in non-perturbative regime
- Nuclear matrix elements from theory → LECs for EFT methods
- Complementary to experiment



[Chang et al, PRL120 (2018) 152002]
[Shanahan, INT-18-70]

Outline

- Background:
  - Lattice gauge theories
  - Efficient ensemble generation
- Normalizing flows:
  - “Flow-based” MCMC sampler
  - Imposing symmetries (e.g. gauge, translational, …)
- Applications:
  - Scalar theory and U(1) + SU(N) gauge theory in 2D

[Albergo, **GK**, Shanahan PRD100 (2019) 034515]

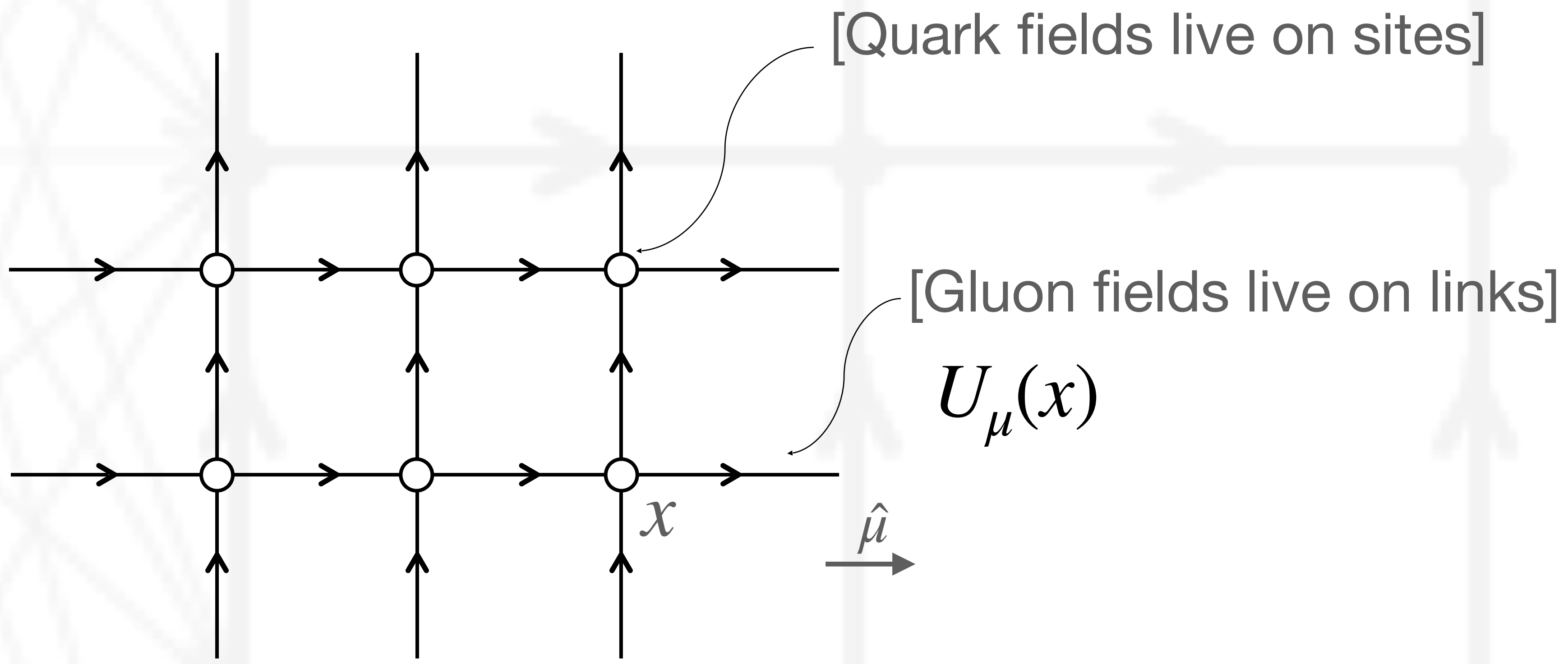
[**GK**, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan 2003.06413, PRL in production]
[Boyda, **GK**, Racanière, Rezende, Albergo, Cranmer, Hackett, Shanahan 2008.05456]

Background

Lattice gauge theory

- Non-perturbative regularization for gauge theories
    - Low-energy limit of QCD
    - Strongly-coupled composite dark matter [Kribs, Neil 1604.04627]
- Discretized (Euclidean) spacetime
    - Lattice spacing acts to cut off momenta
    - Exact gauge invariance
- Regularized path integral to compute observables

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \, \mathcal{O}[U] e^{-S[U]}$$



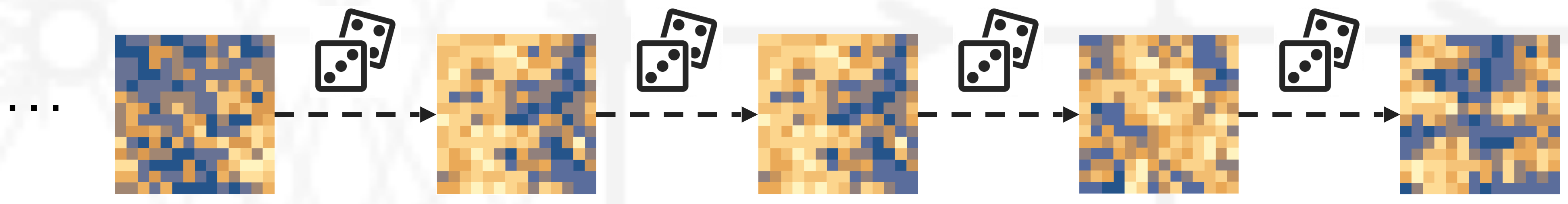
Discretization of QCD on a lattice
[Image credit: Dan Hackett]

Importance sampling

- Sampling histories in path integral enables efficient estimation of (many) observables

$$\langle \mathcal{O} \rangle \approx \frac{1}{n} \sum_{i=1}^{n} \mathcal{O}[U_i] \qquad\qquad U_i \sim p(U) = e^{-S(U)}/Z$$

- Markov chain Monte Carlo (MCMC)



Example: MCMC to generate ensembles for scalar field theory

- Performance limitations of local MCMC
  - Information transfer limited by local updates
  - Rare to update entire field coherently

⚠ **critical slowing down** ⚠

⚠ **topological freezing** ⚠

Better importance sampling?

- Ideal world: independently draw samples directly from your distribution
  - E.g. sampling Gaussian variables via the Box-Muller transform

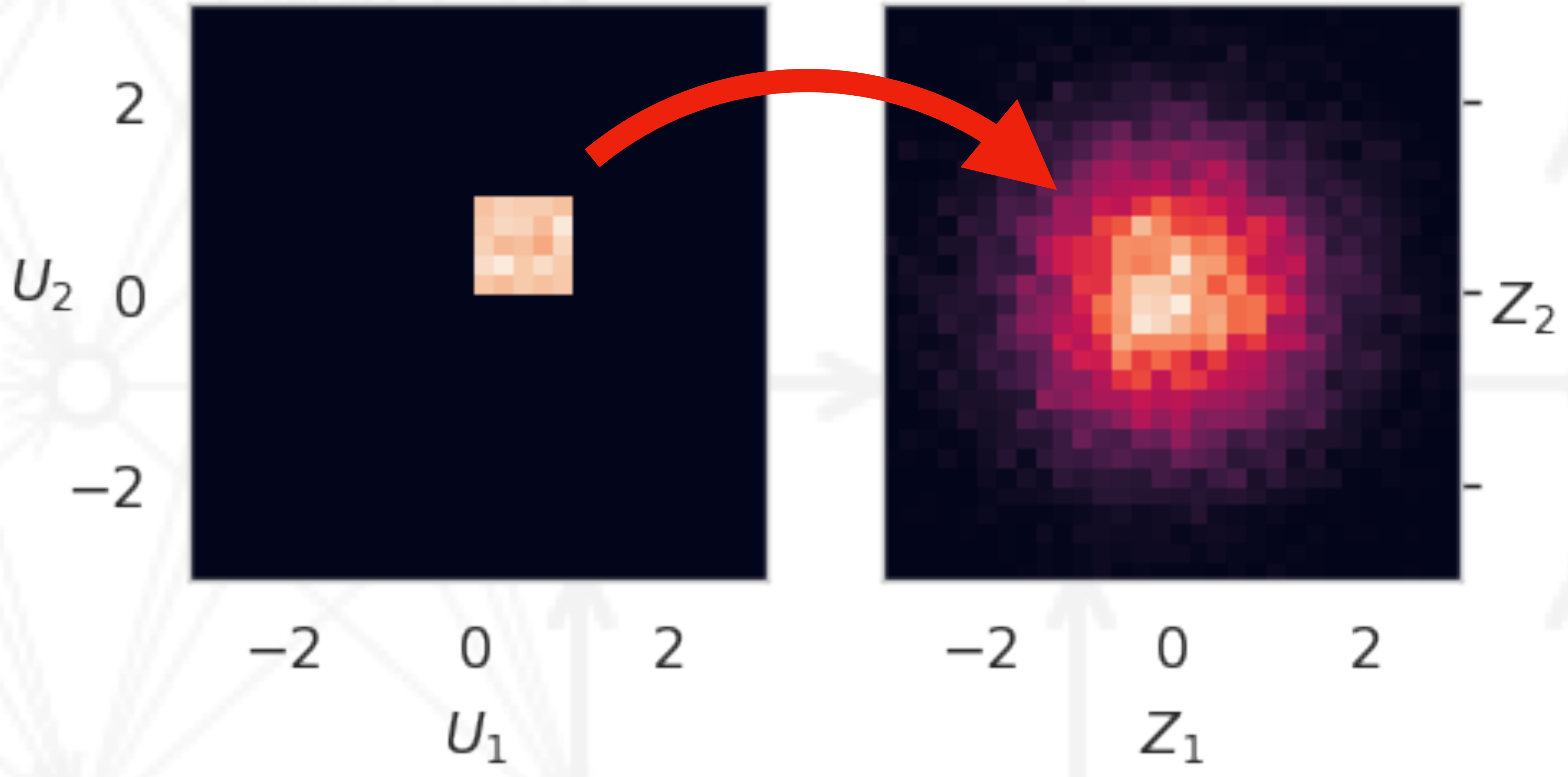
1. Draw samples $U_1, U_2 \in [0,1]^2$ from (uncorrelated) uniform distribution r

2. Change variables

$$Z_1 = \sqrt{-2\log U_1}\cos 2\pi U_2$$
$$Z_2 = \sqrt{-2\log U_1}\sin 2\pi U_2$$

3. Know $r\left(U_1, U_2\right) = 1$

$$p(Z_1, Z_2) = r(U_1, U_2)\left|\det_{kl}\frac{\partial Z_k}{\partial U_l}\right|^{-1}$$
$$= \frac{1}{2\pi}e^{-(Z_1^2+Z_2^2)/2}$$



Density is affected by the change of measure!

Better importance sampling?

- ~~Ideal world~~: independently draw samples directly from your distribution

- Do not know how to exactly sample lattice gauge theory distributions

- Can we use an approximate independent sampler (without introducing bias)?
  - Yes, but we need to know **prob. density** $q(U)$ **being sampled**
  - Reweighting or Independence Metropolis MCMC give unbiased estimates

$$\boxed{\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}U\, q(U) \left[\mathcal{O}(U) \frac{p(U)}{q(U)} \right]}{\int \mathcal{D}U\, q(U) \left[\frac{p(U)}{q(U)} \right]}}$$

Sample $q(U)$ as proposals in a Metropolis-Hasting Markov chain (more later)

Approximate sampling

- Machine learning techniques are effective for doing things approximately

i.e., “variational techniques”

- Normalizing flow models (rest of the talk) learn distributions, and can both:
  1. **Sample** $U \sim q(U)$
  2. **Measure** $q(U)$ given U

We can use Reweighting or Independence Metropolis for unbiased estimates

Normalizing flows for sampling

Normalizing flows

We already saw a normalizing flow: Box-Muller transform to draw Gaussian vars.

ML method to construct samplers for complicated probability distributions; originally for image generation

Faces generated via “real NVP” flow from uncorrelated noise
[Dinh, Sohl-Dickstein, Bengio 1605.08803]

1. Start with a prior distribution r in which

   …it is **easy to draw samples** V

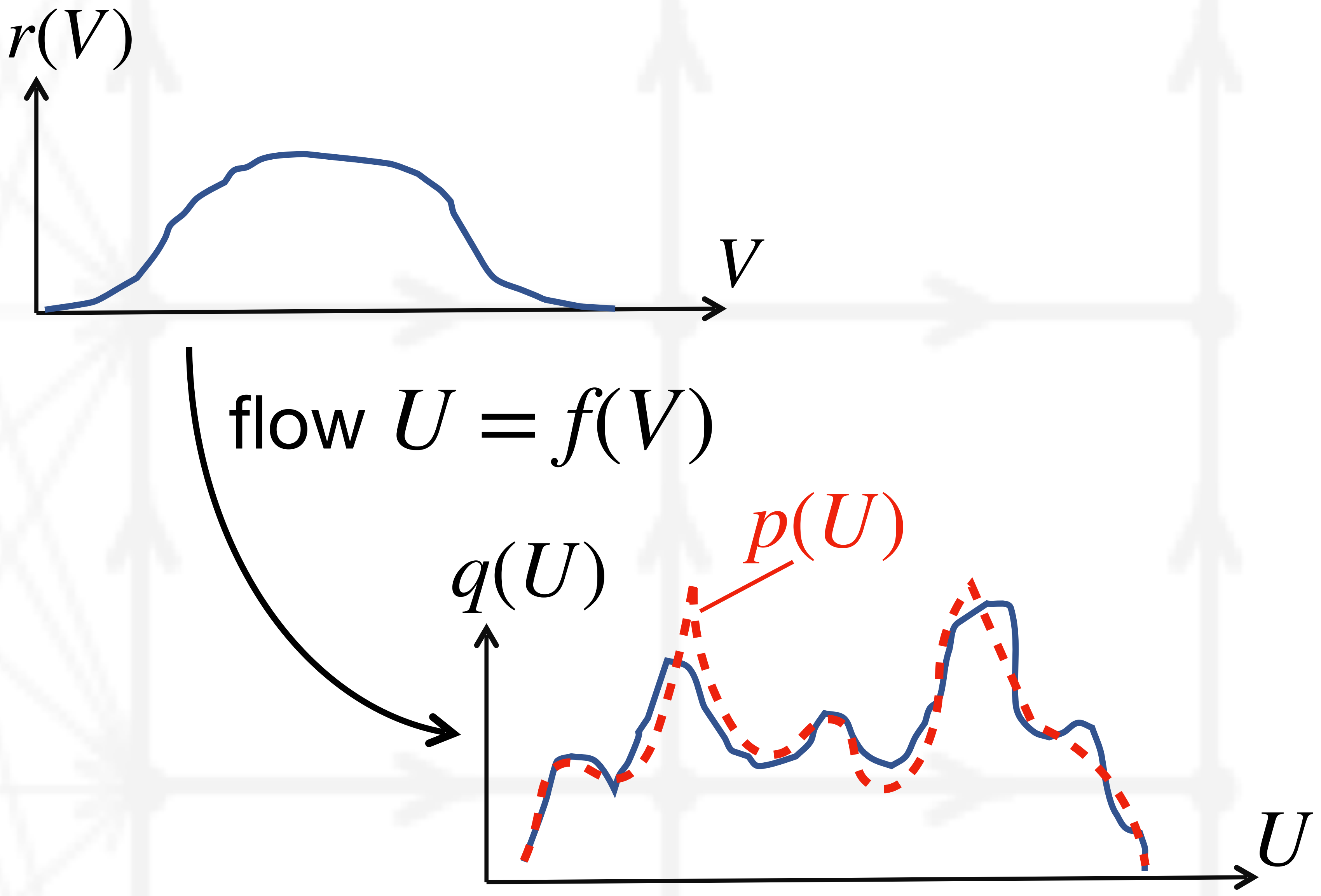
   …you **can compute** $r(V)$ for each V

   Ex: uncorrelated uniform, Gaussian, …

2. “Flow” to distribution q (approximating the target p) using a parametrized change of vars f that

   …is **invertible**

   …has a (tractably) **computable log-det-Jacobian**



$$\boxed{q(U) = r(V) \left| \det_{ij} \frac{\partial [f(V)]_i}{\partial V_j} \right|^{-1}}$$

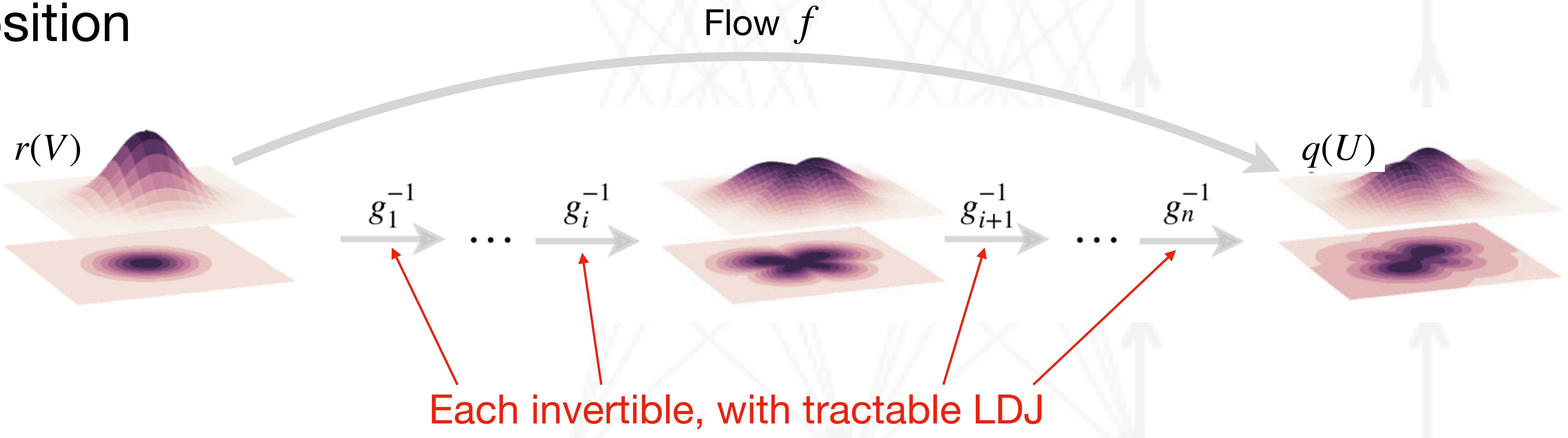
Approach: Construct flow as a variational ansatz for p, optimize so that $q \approx p$

[Slide credit: Dan Hackett]

Defining the flow function

$$q(U) = r(V) \left| \det_{ij} \frac{\partial [f(V)]_i}{\partial V_j} \right|^{-1}$$

- The "flow" f must be **invertible** and have **tractable log-det-Jacobian (LDJ)**
  - In Box-Muller transform, f is precisely constructed to produce the Gaussian dist
  - For LQFT, don't know what f needs to be; instead, construct parametrized ansatz and optimize it
- Composition



Coupling layers

Idea: Construct each g to act on a **subset** of components, conditioned only on the complimentary subset.

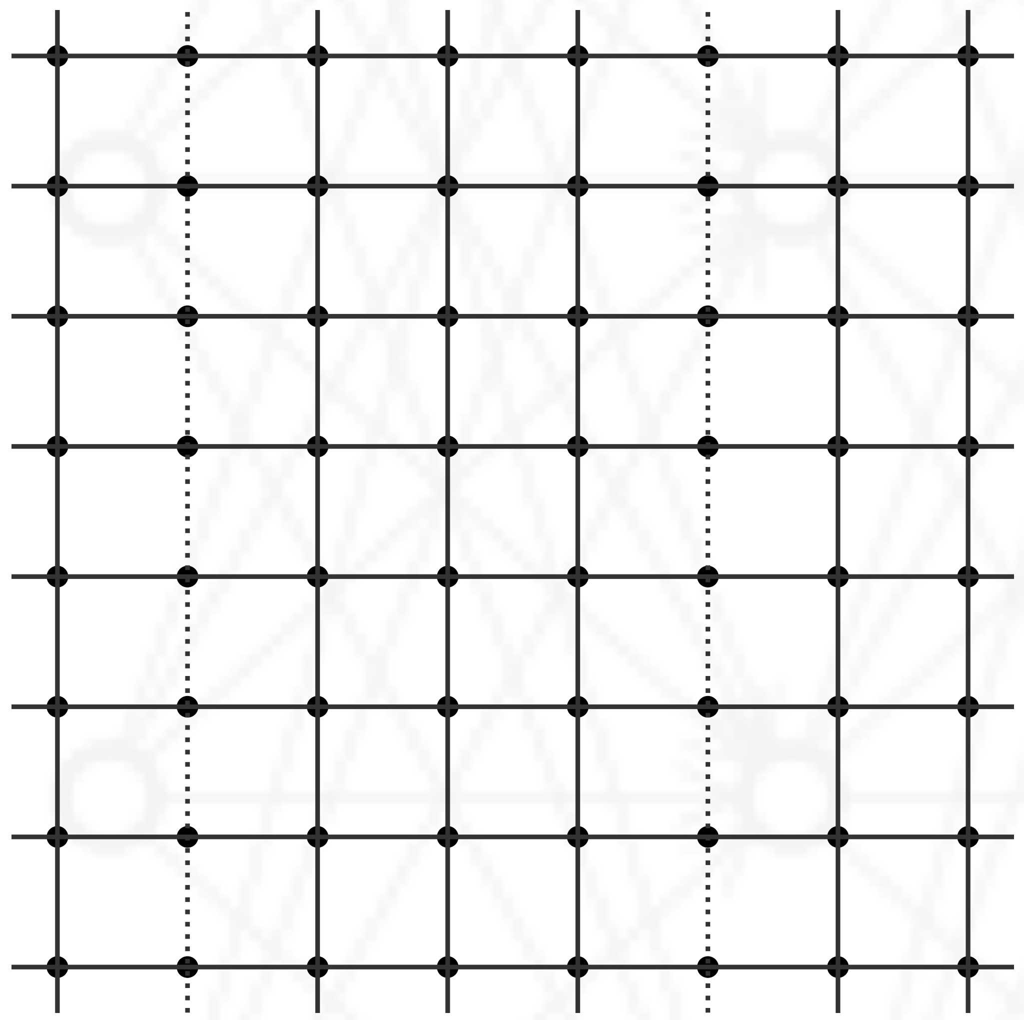
→ Jacobian is explicitly upper-triangular (get LDJ from diag elts)

$$\frac{\partial[g(V)]_i}{\partial V_j} = \left(\begin{array}{ccc|ccc} \frac{\partial[g(V)]_1}{\partial V_1} & & & & & \\ & \frac{\partial[g(V)]_2}{\partial V_2} & & & \text{(nonzero)} & \\ & & \ddots & & & \\ \hline & & & 1 & & \\ & 0 & & & 1 & \\ & & & & & \ddots \end{array}\right)$$

→ Invertible if each diag component invertible, $\dfrac{\partial[g(V)]_i}{\partial V_i} \neq 0.$

Ex: coupling layer for gauge theory

- **Masking pattern:** define which links to freeze and condition on
  - Idea: leave enough frozen context so transform can build correlations between DOFs
  - E.g. freeze all but specific columns (or rows) of links



- Ex: left-multiplication by group-valued function on unfrozen links

$$U'_\mu(x) = \boxed{\exp\left(iW_\xi(\text{frozen neighbors}) \cdot \lambda\right)} U_\mu(x)$$

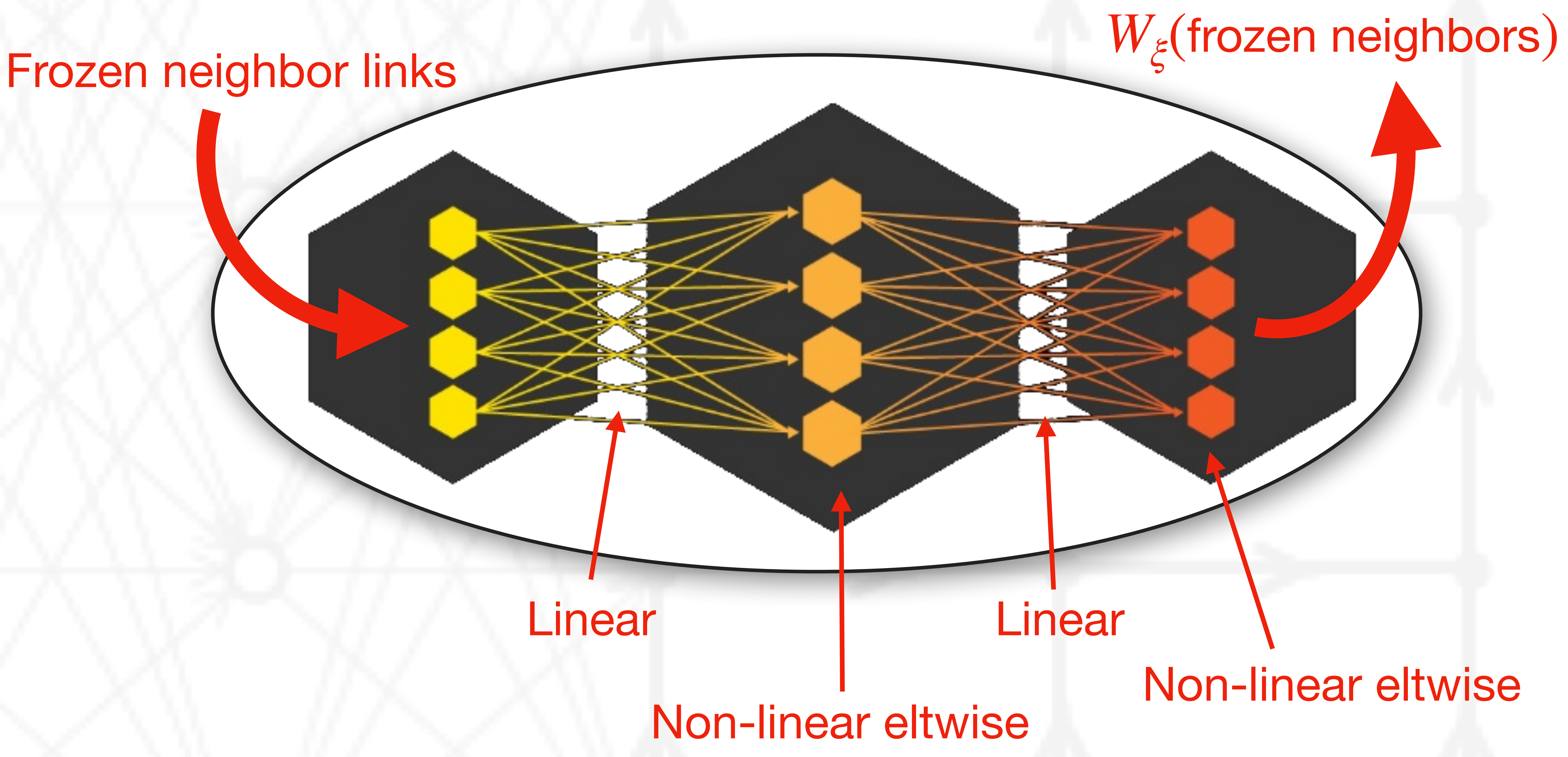
“What is W_ξ?”

Any parametrized function accepting a collection of $SU(N)$ variables as input.

Our terminology: “*context function*”.

Neural networks: compose parametrized linear transforms with non-linear elementwise functions.

→ Universal function approximators



Matrices of weights define linear transforms. Altogether, these weights compose the model parameters ξ.

Optimizing via “self-training”

Optimization by comparing model likelihood $q(U)$ vs true likelihood $p(U)$ on sample configurations U.

- Must not require a large number of samples from real distribution to optimize!
- **Self-training:** take samples from the model, not true distribution
- Kullback-Leibler (KL) divergence between q and p given samples

Flow-based MCMC

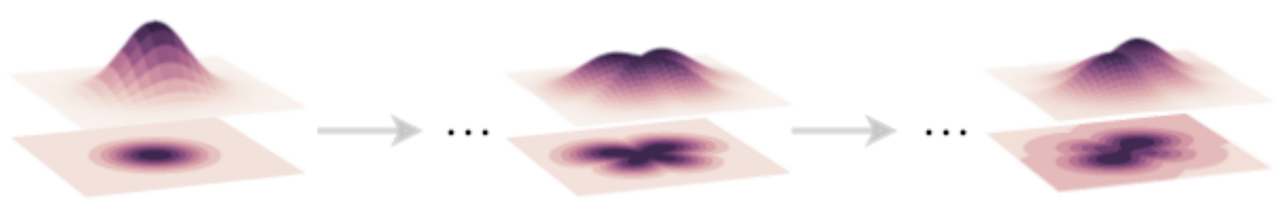
Markov chain constructed using Independence Metropolis accept/reject on model proposals.

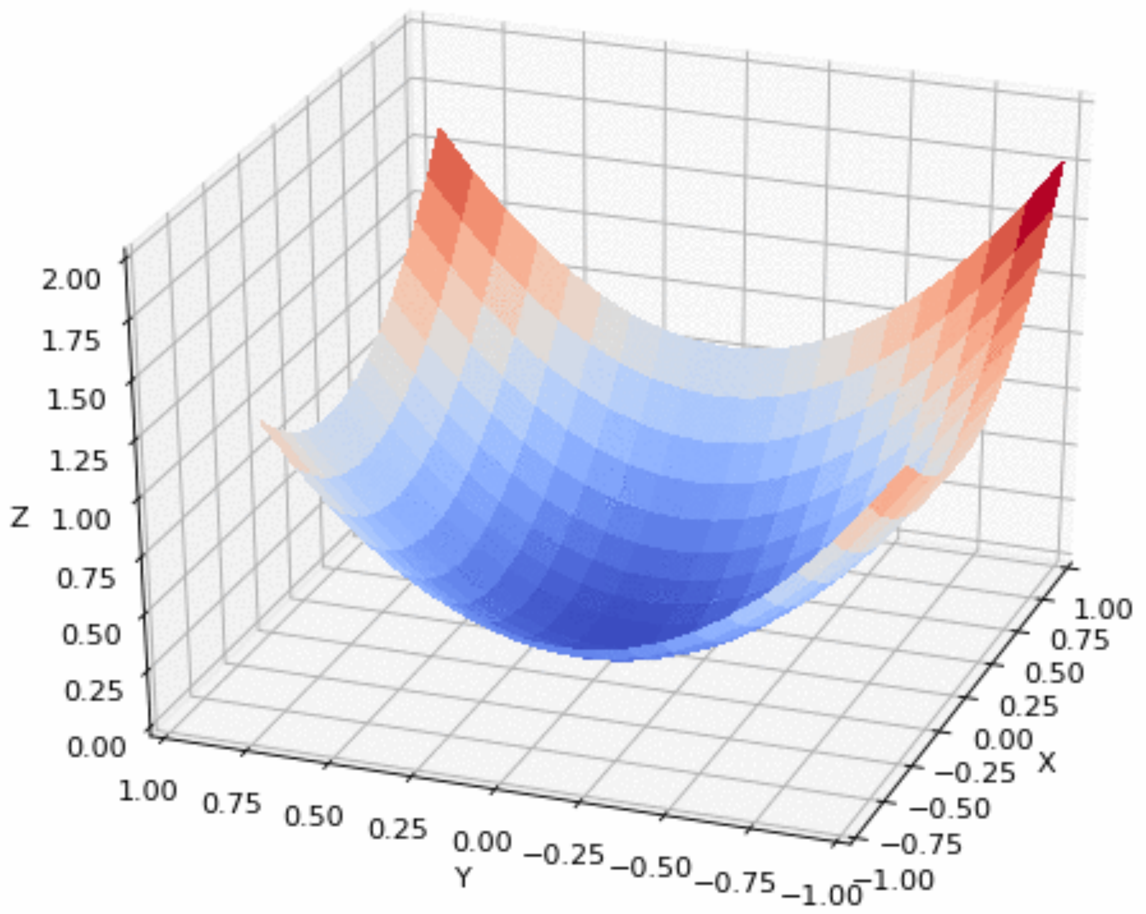
- **Independent** proposals U' from model distribution q
- **Accept** proposal U', making it next elt of Markov chain, with probability

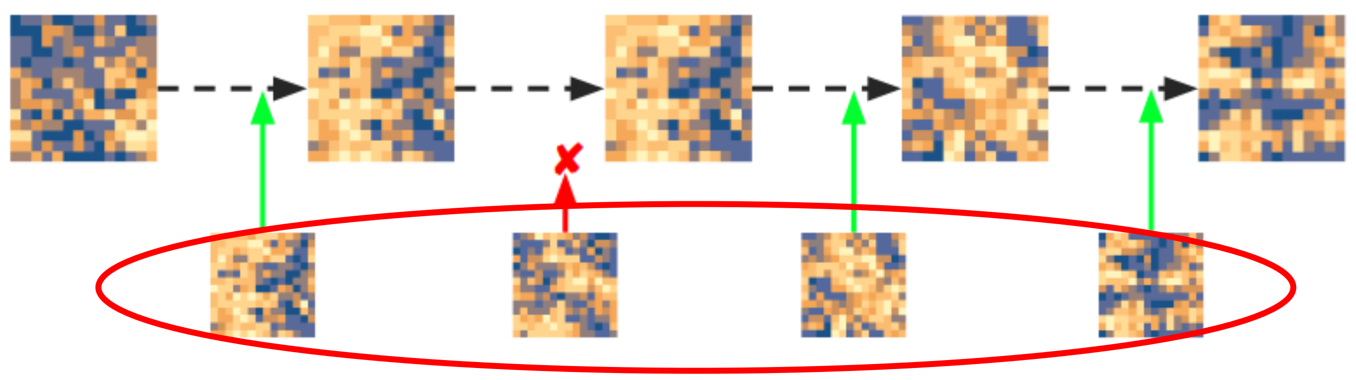
$$p_{\text{acc}}(U \to U') = \min\left(1, \frac{p(U')}{q(U')}\frac{q(U)}{p(U)}\right).$$

- If **rejected**, duplicate previous elt of Markov chain
  - Only need to compute observables on duplicated elts once!

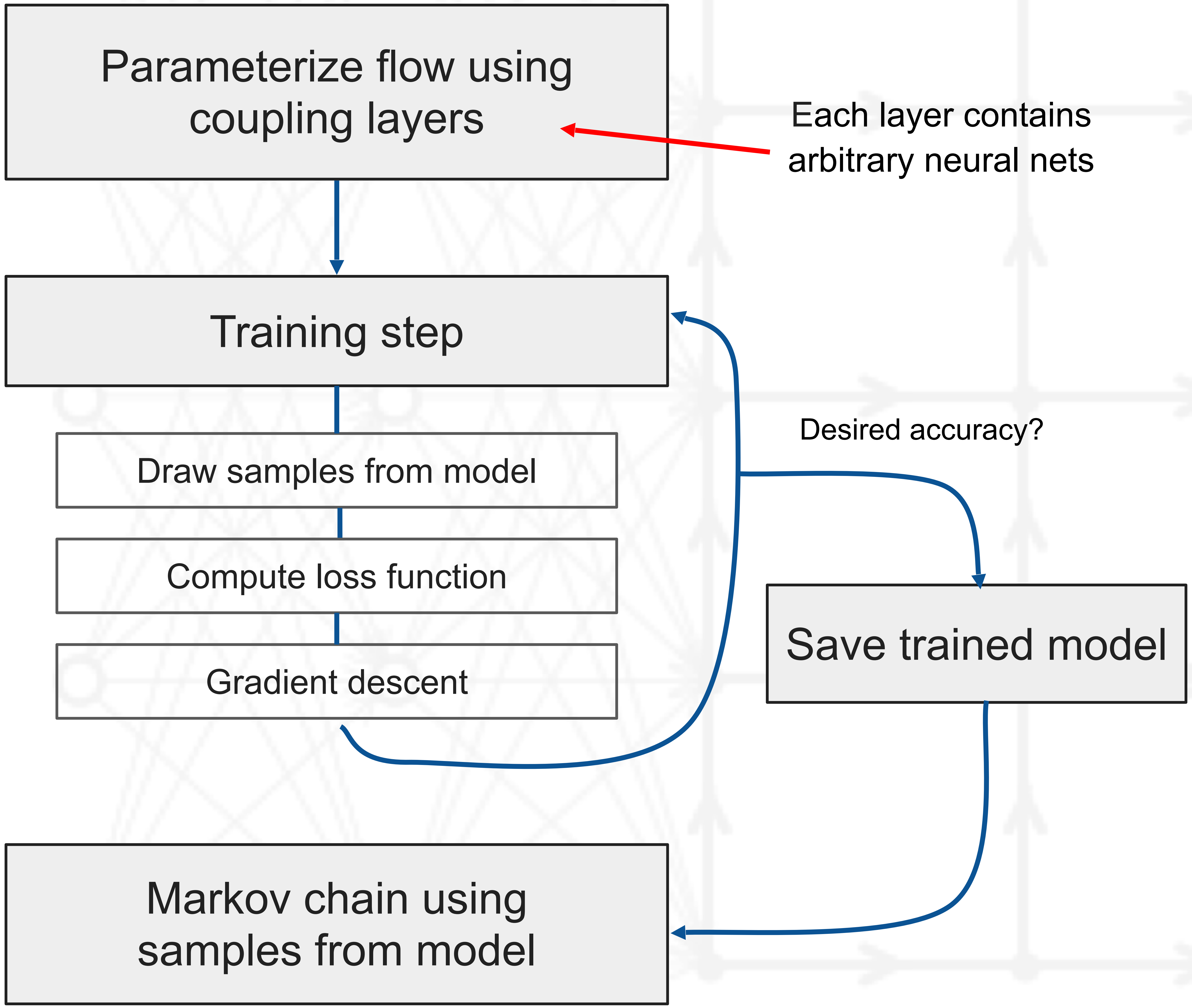
Birds-eye view







generating samples is "embarrassingly parallel"



Symmetries

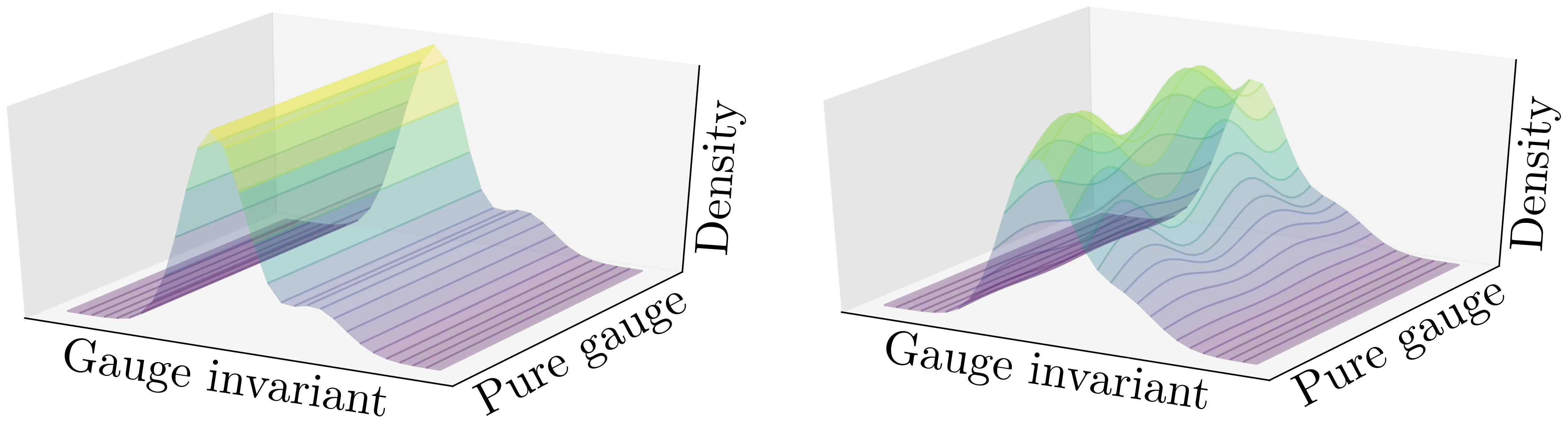
Typical lattice gauge theories are symmetric under

1. (Discrete) translational symmetry
2. Hypercubic symmetry
3. Gauge symmetry

   Elements defined by group-valued fields $\Omega(x)$ that transform the gauge field as

$$(\Omega \cdot U)_\mu(x) = \Omega(x) U_\mu(x) \Omega^\dagger(x+\hat{\mu})$$

Symmetries **factor** distribution into uniform component along symmetry direction, and non-uniform component along invariant direction. Ex for gauge symmetry (schematically):



Learning symmetries

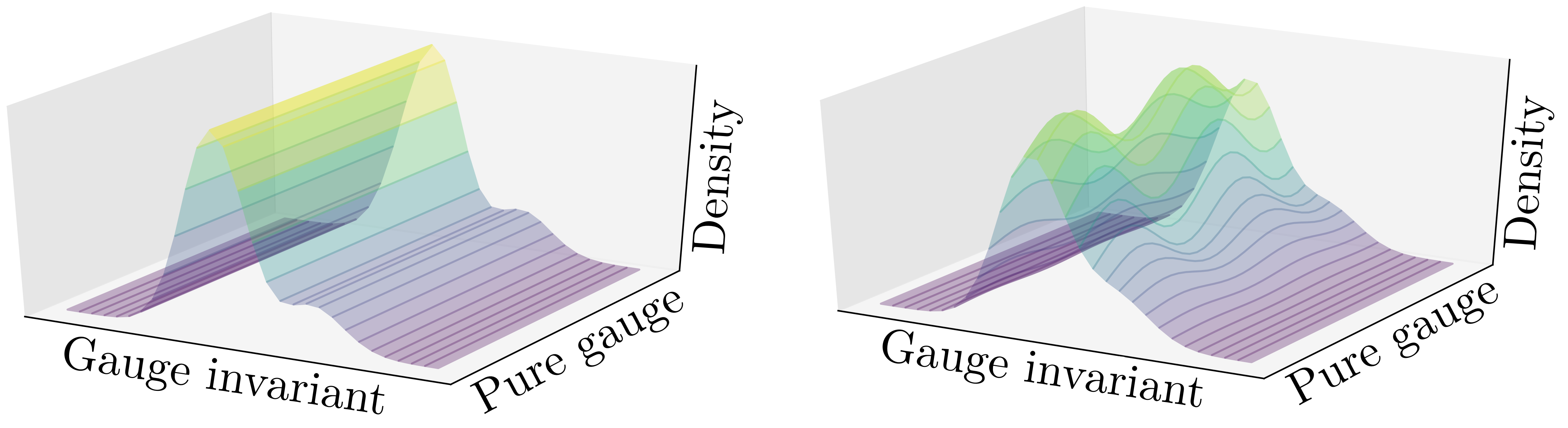
Models will learn any symmetries of the action **approximately**.

- Always made exact after reweighting / flow-based MCMC

Some symmetry groups quite large. We can do better by **encoding them explicitly** in model structure!

- Variational ansatz is restricted to only explore distributions like the left one

Symmetries **factor** distribution into uniform component along symmetry direction, and non-uniform component along invariant direction. Ex for gauge symmetry (schematically):



Symmetries in normalizing flows

Can be imposed on the model by ensuring

1. Prior is **invariant** under the symmetry

Uniform prior distribution is invariant under all symmetries of interest in lattice gauge theory.

2. Flow f is **equivariant** under the symmetry

[Cohen, Welling 1602.07576]

Must construct flow to satisfy equivariance!

Equivariance: symmetry operations commute with application of f

- Translational equivariance achieved by using (1) Convolutional Neural Networks in context functions and (2) symmetric masking patterns.
- Our recent contribution: gauge equivariance

Applications: 1+1D lattice theories

Proof-of-principle at low computational cost,
no theoretical obstacle to higher dims

Scalar theory on a 2D lattice

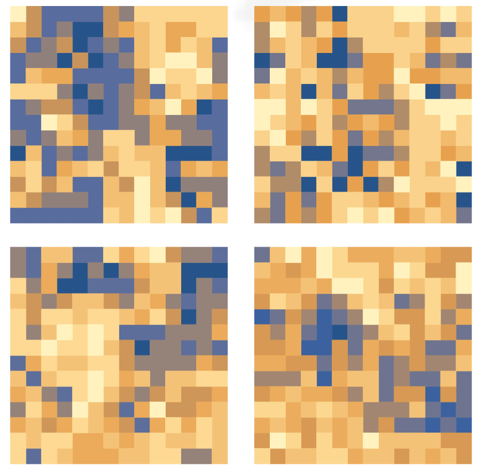
$$S_E(\phi) = \sum_x \left(\sum_y \phi(x) \Box(x,y) \phi(y) + m^2 \phi(x)^2 + \lambda \phi(x)^4 \right)$$

- Real DoF per lattice site, $\phi(x) \in \mathbb{R}$
- 6×6 through 14×14 lattices studied
- Scalar particle mass tuned to give correlation length ~ $L/4$
- Affine coupling layers for flow models:

$$\phi'(x) = e^s \phi(x) + t$$

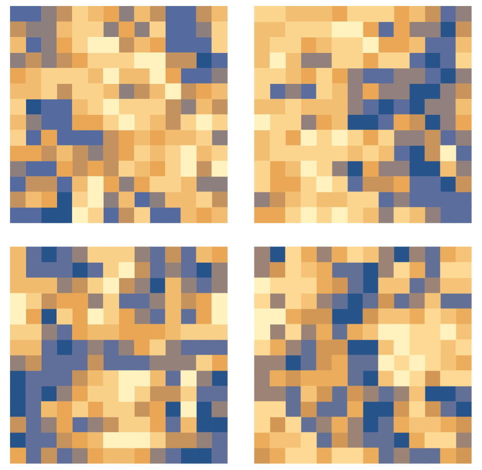
Context functions, implemented using NNs acting on frozen sites (checkerboard pattern)

Flow model samples

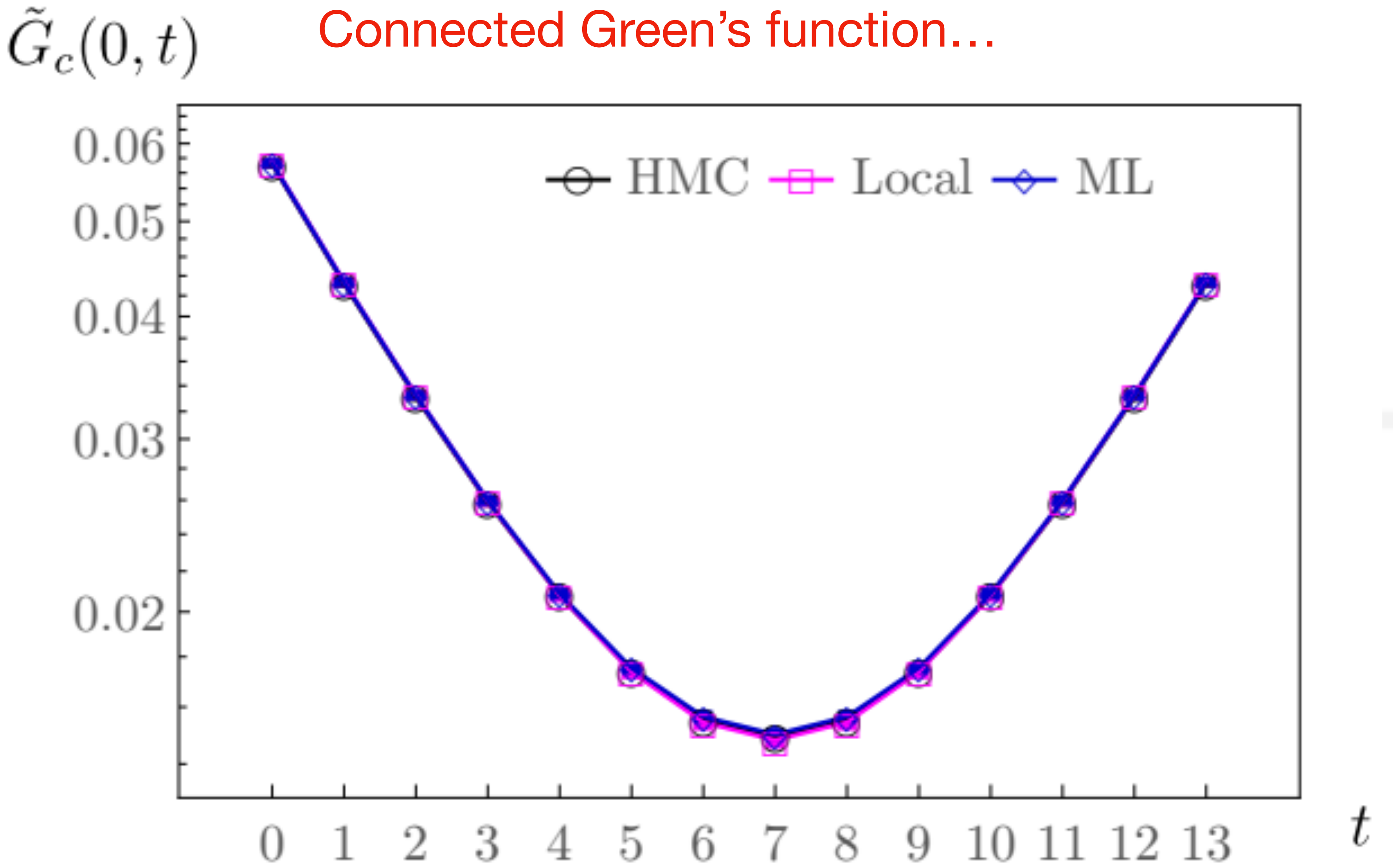


~ vs ~

HMC samples



Connected Green's function…



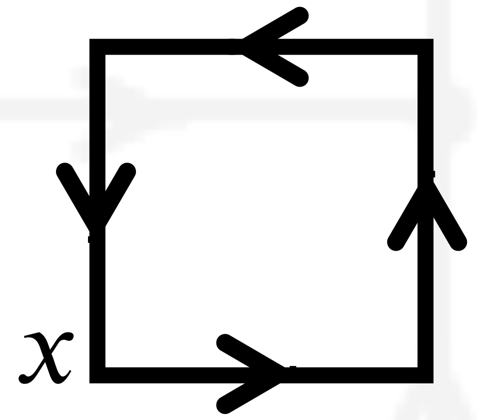
… and several other observables all consistent

Lattice gauge theory in 2D

- Wilson gauge action, $SU(N)$:

$$S(U) = -\frac{\beta}{N}\sum_x \mathrm{Re}\,\mathrm{tr}\left[P_{01}(x)\right]$$

$$P_{\mu\nu}(x) = U_\mu(x)U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu^\dagger(x)$$



untraced!

- Gauge transforms are a symmetry of the action:

$$(\Omega \cdot U)_\mu(x) = \Omega(x)U_\mu(x)\Omega^\dagger(x+\hat{\mu})$$

- Confinement, ultralocal dynamics

$$p(P_{01}(x)) \approx \exp\left(\frac{\beta}{N}\mathrm{Re}\,\mathrm{tr}P_{01}(x)\right)/Z$$

  - Each plaq has independent statistics, up to correlations that are a finite volume effect

Gauge equivariance

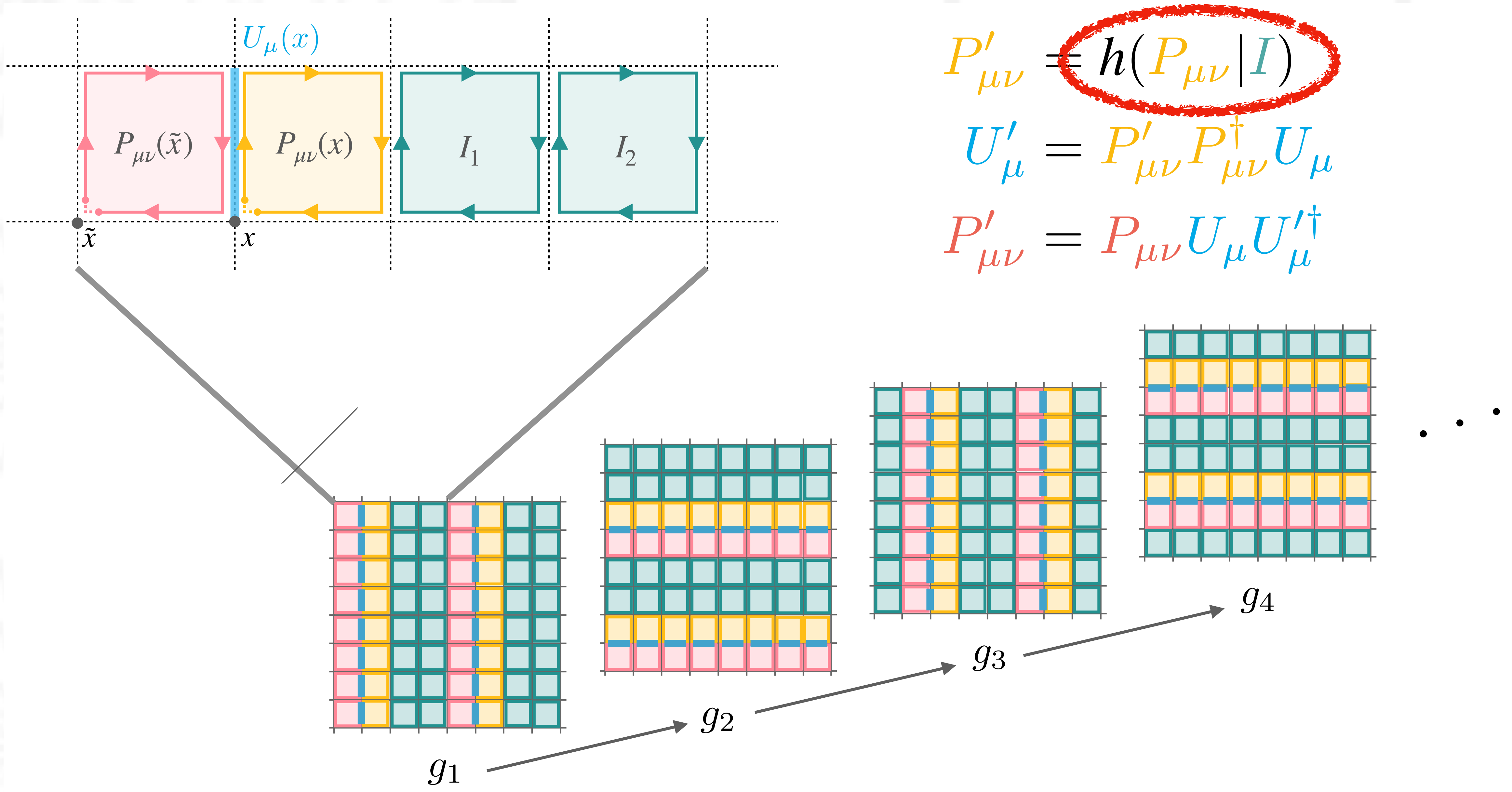
E.g. traced plaquettes, traced Wilson loops

Intuition: act on gauge-invariant quantities only

- Factorized action of coupling layer
- Issue: must remain invertible
- Issue: preserve trans. symmetry

× Gauge fixing with **explicit factorization** (e.g. maximal tree) does not preserve trans. symmetry!

× Gauge fixing with **implicit factorization** (e.g. Landau gauge) hard to preserve across coupling layer!



"kernel"

$$P'_{\mu\nu} = h(P_{\mu\nu}|I)$$
$$U'_\mu = P'_{\mu\nu}P^\dagger_{\mu\nu}U_\mu$$
$$P'_{\mu\nu} = P_{\mu\nu}U_\mu U'^\dagger_\mu$$

Solution: transform group-valued untraced Wilson loops, "absorb" update using link representation

“What is a kernel?”

The core of a gauge-equivariant coupling layer; acts on a selection of untraced Wilson loops (e.g. subset of untraced plaquettes)

Must satisfy:

1. Invertible and tractable log-det-Jacobian

2. Equivariant under matrix conjugation

$$h(XPX^{-1}) = X\,h(P)\,X^{-1}$$

3. Only conditioned on gauge-invariant frozen quantities

Guarantees **gauge equiv**: gauge transforms act on untraced loops via matrix conjugation

“Condition on”: pass as input to context functions used in defining h

[Image credit: Dan Hackett]

Kernel for $U(1)$ gauge theory

- Variables are 1×1 matrices (i.e. scalars):

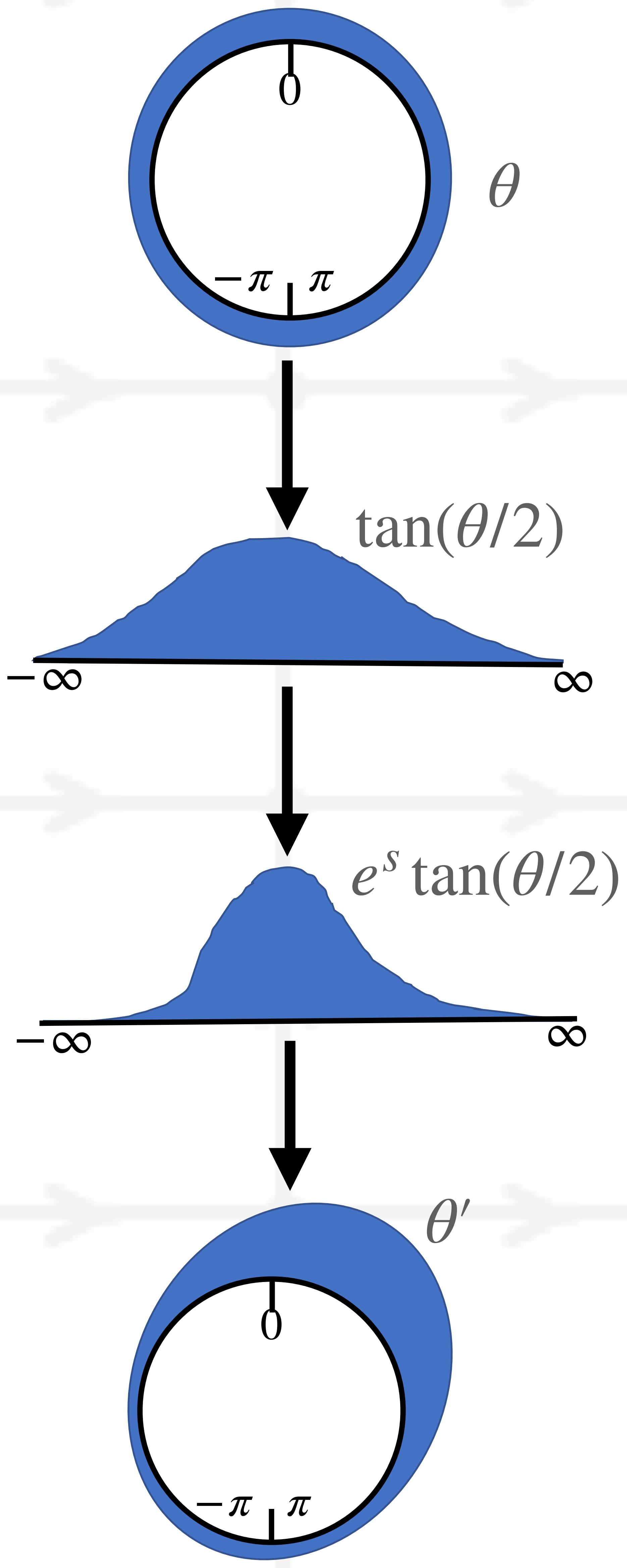
$$XPX^{-1} = P$$

- Required: invertible function suitable for $U(1)$ vars
  - Developed flows for compact variables (tori and spheres) in [†]
  - We choose a "non-compact projection" transform:

s, t = convolutional NNs

$$\theta' = 2\arctan\left(e^{s_\xi(I)}\tan(\theta/2)\right) + t_\xi(I)$$

ξ = model parameters $\quad$ I = nearby frozen plaquettes



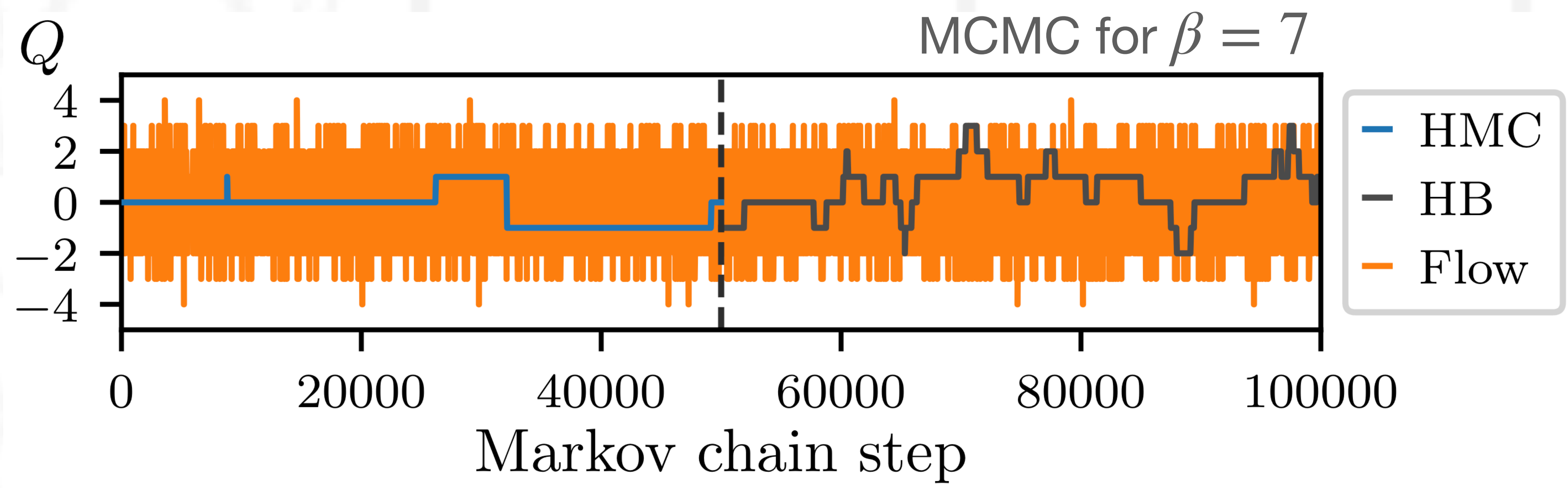
"Non-compact projection" for $U(1)$

[†] [Rezende, Papamakarios, Racanière, Albergo, **GK**, Shanahan, Cranmer ICML(2020) 2002.02428]

Results for $U(1)$ gauge theory

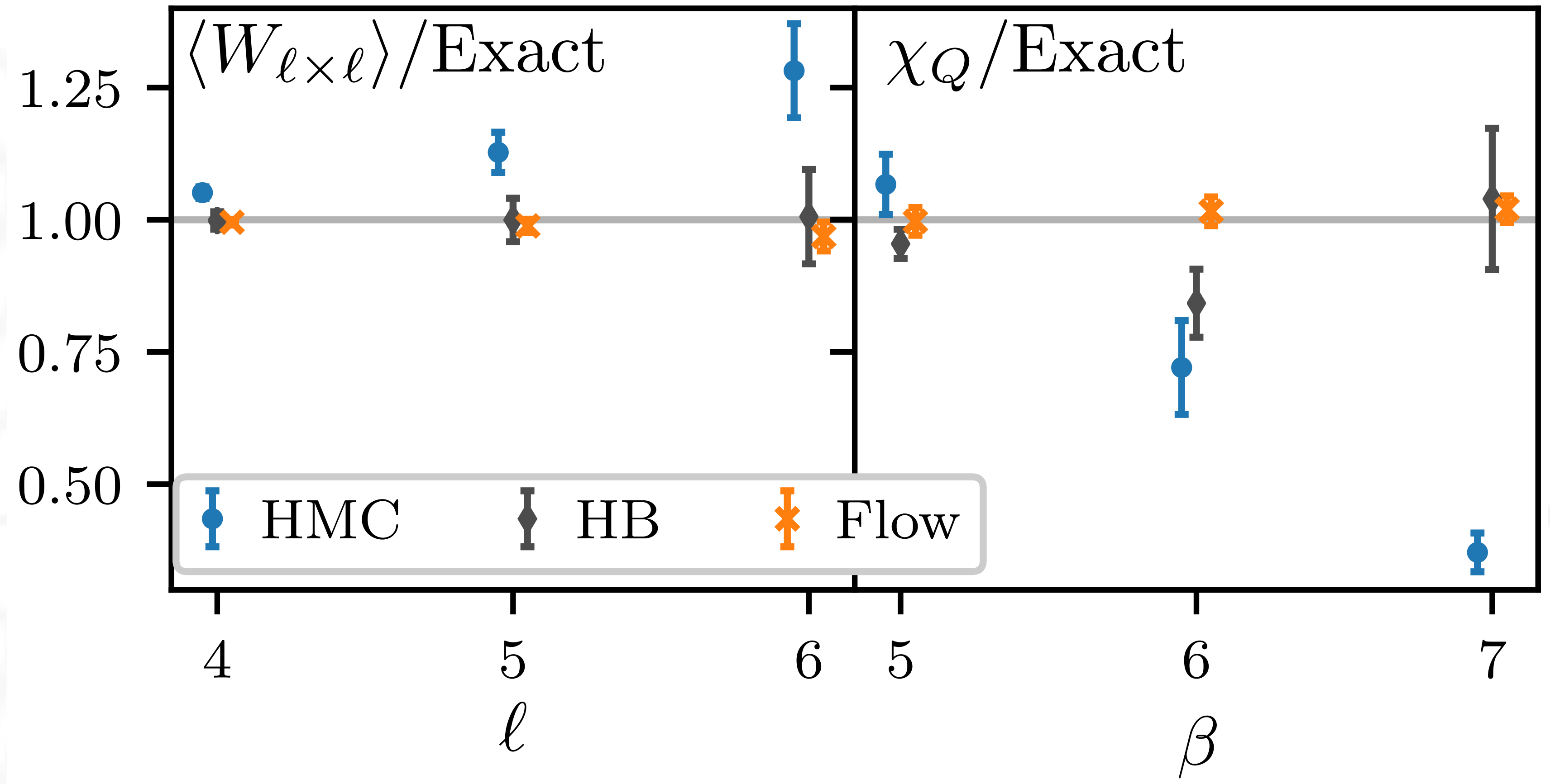
There is exact lattice topology in 2D.

$$Q = \frac{1}{2\pi} \sum_x \arg(P_{01}(x))$$



Comparison: flow, analytical, HMC, and heat bath on 16×16 lattices for $\beta = \{1, \ldots, 7\}$

- Topo freezing in HMC and heat bath
  - Direct sampling approaches known, but do not generalize
- Flow-based MCMC observables agree with analytical



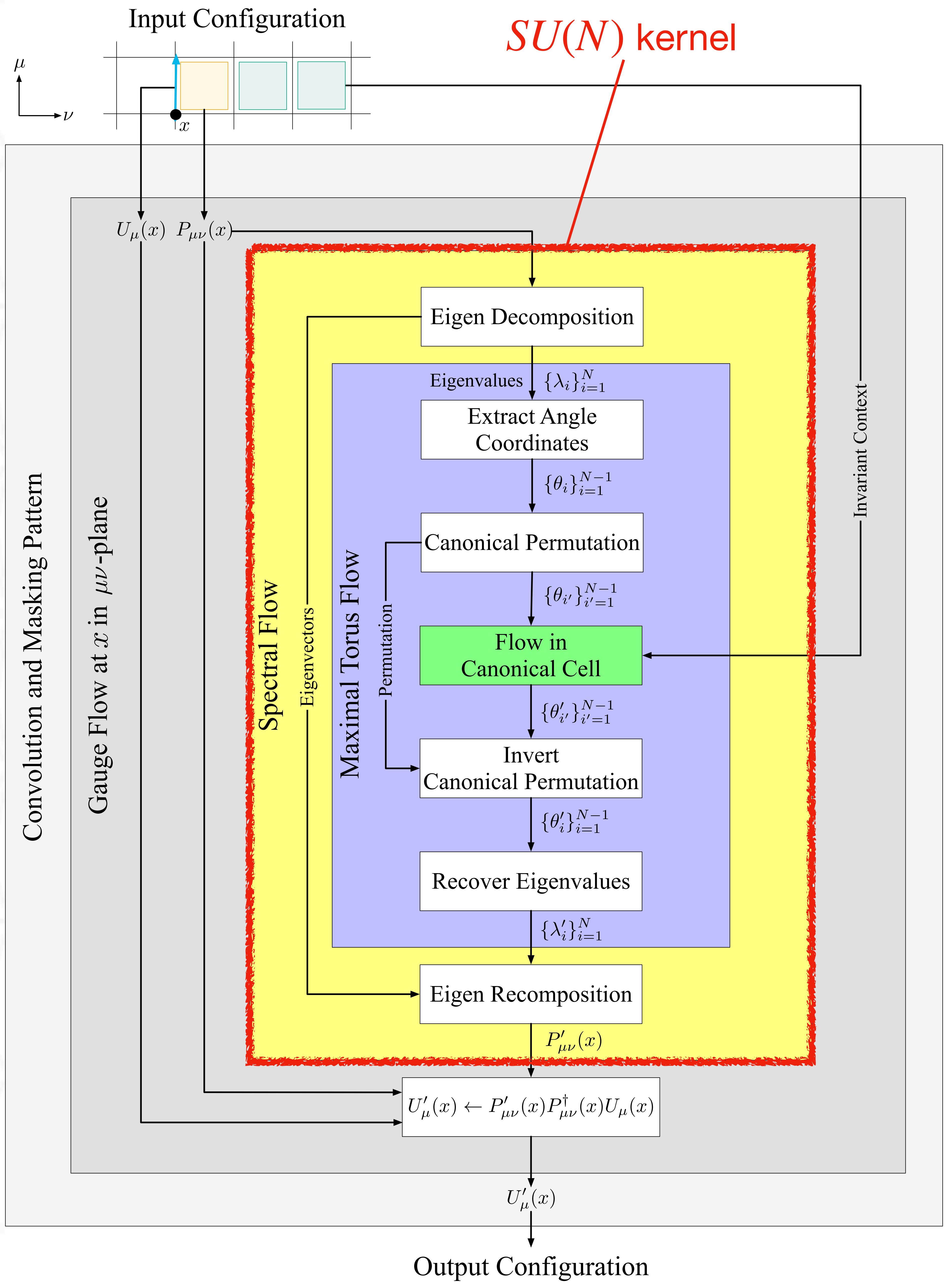
$$W_{\ell \times \ell} = \prod_{x \in \ell \times \ell} P_{01}(x) \qquad \chi_Q = \langle Q^2 / V \rangle$$

Kernel for $SU(N)$ theories

Intuition: should move points between conjugacy classes, without moving around within CCs

Conjugacy classes for $SU(N)$ described by **spectrum** of the matrix: unordered set of eigenvalues. Kernel should transform spectrum!

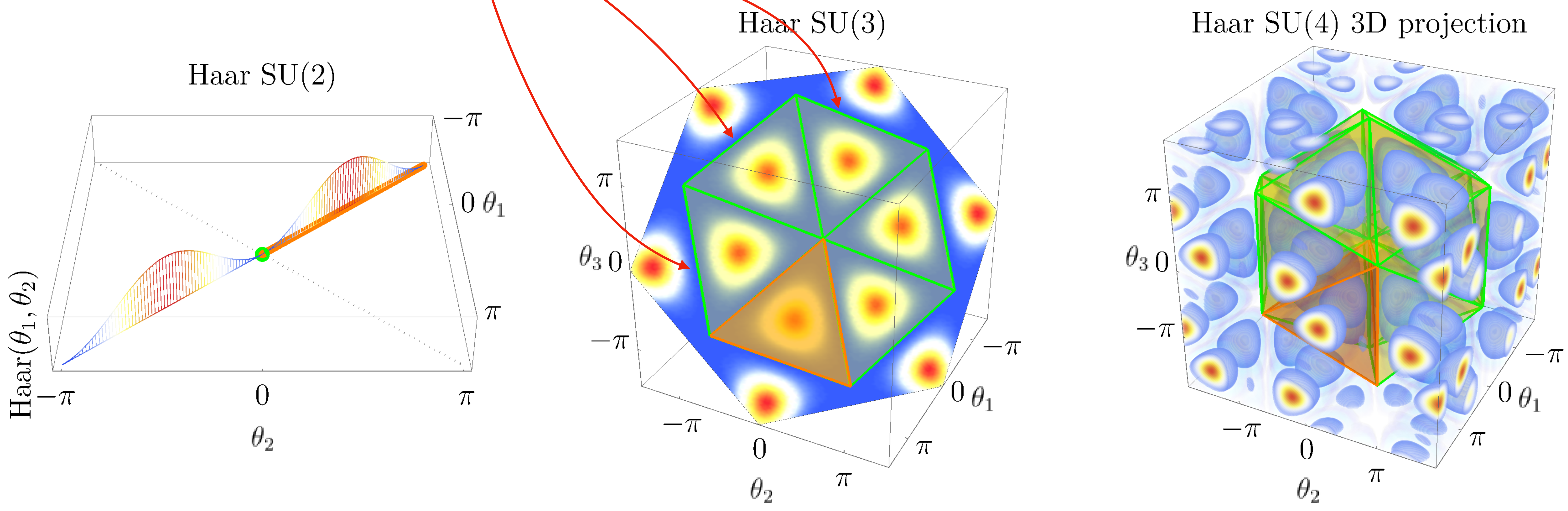
- Act on list of eigenvalues
- Equivariant under permutations



Permutations on $SU(N)$ eigenvalues

Eigenvalues satisfy $\prod_k \lambda_k = 1 \;\rightarrow\; \boxed{\sum_k \theta_k = 0 \pmod{2\pi}}$ maximal torus of $SU(N)$

Permutations exchange **cells** in the space of $\{\theta_k\}$



Approach: map input to a “canonical” cell, transform within cell, undo canonical map

Learning $SU(N)$ plaquette distributions

Tested kernel in isolation by learning distributions on a single $SU(N)$ variable

- Representative of marginal distribution on untraced plaquette
- Conjugation-invariant action with several choices of coefficients

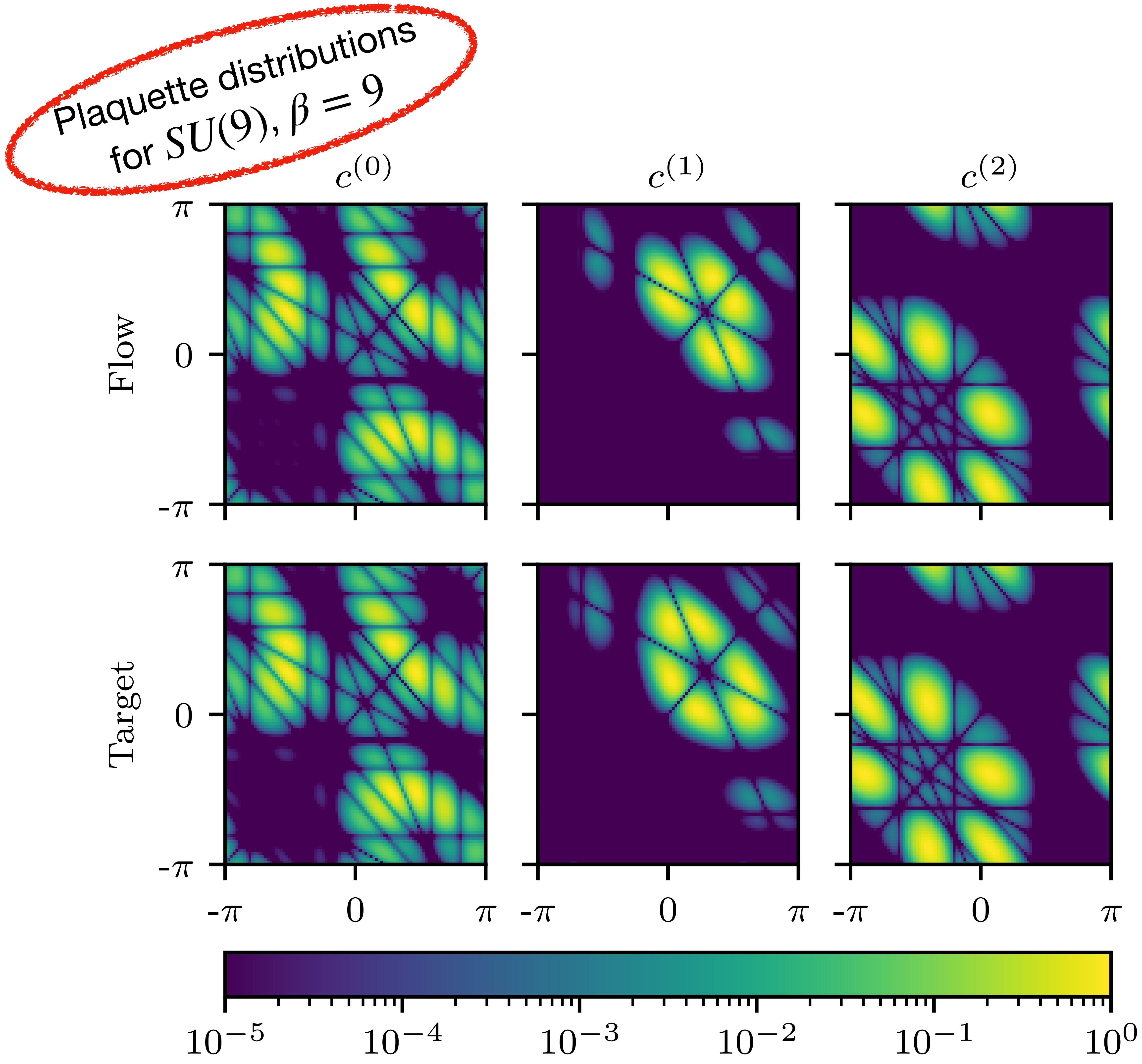
$$S_i(U) := -\frac{\beta}{N}\mathrm{Re}\,\mathrm{tr}\left[\sum_n c_n^{(i)} U^n\right]$$

set i	$c_1^{(i)}$	$c_2^{(i)}$	$c_3^{(i)}$
0	1	0	0
1	0.17	-0.65	1.22
2	0.98	-0.63	-0.21

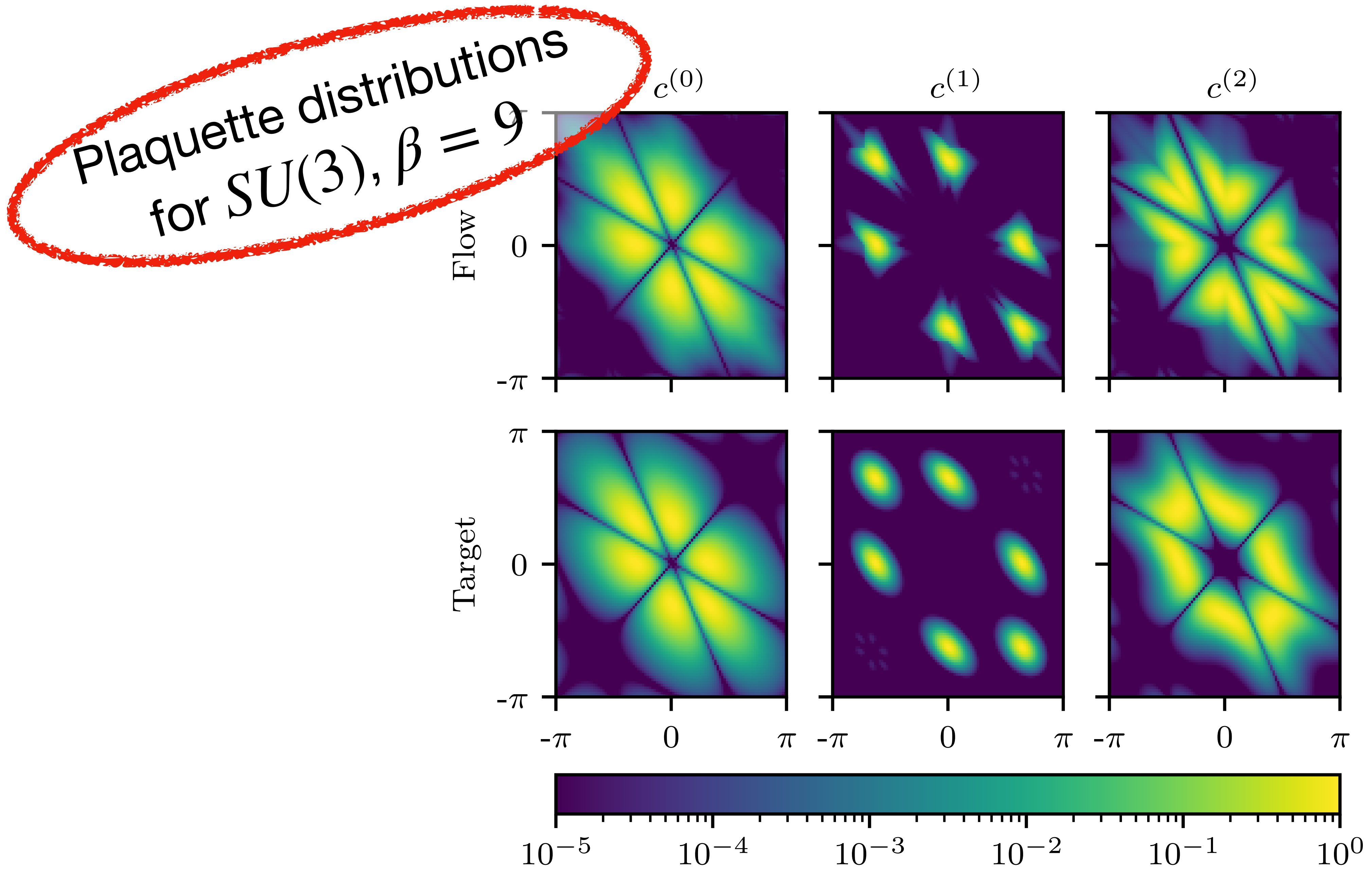
Exact marginal distribution on plaquettes

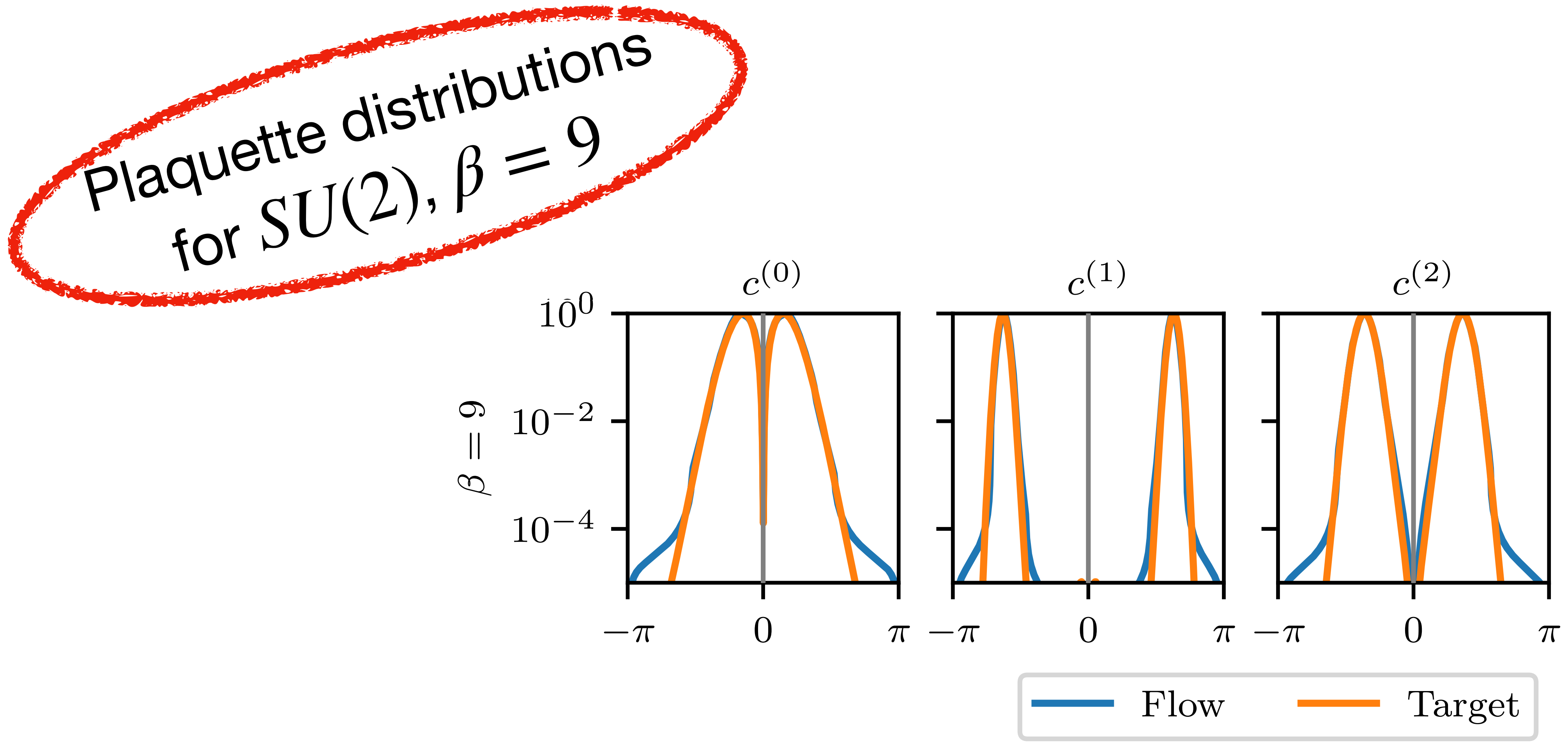
Randomly sampled coeffs with 1 mode

- Special case implementations tested for $SU(2)$ and $SU(3)$
- Unoptimized generic implementation learns $c^{(0)}$ for $SU(4), \ldots, SU(100)$



Density has zeros on vertical, horizontal, and
diagonal lines where the slice crosses walls of cells





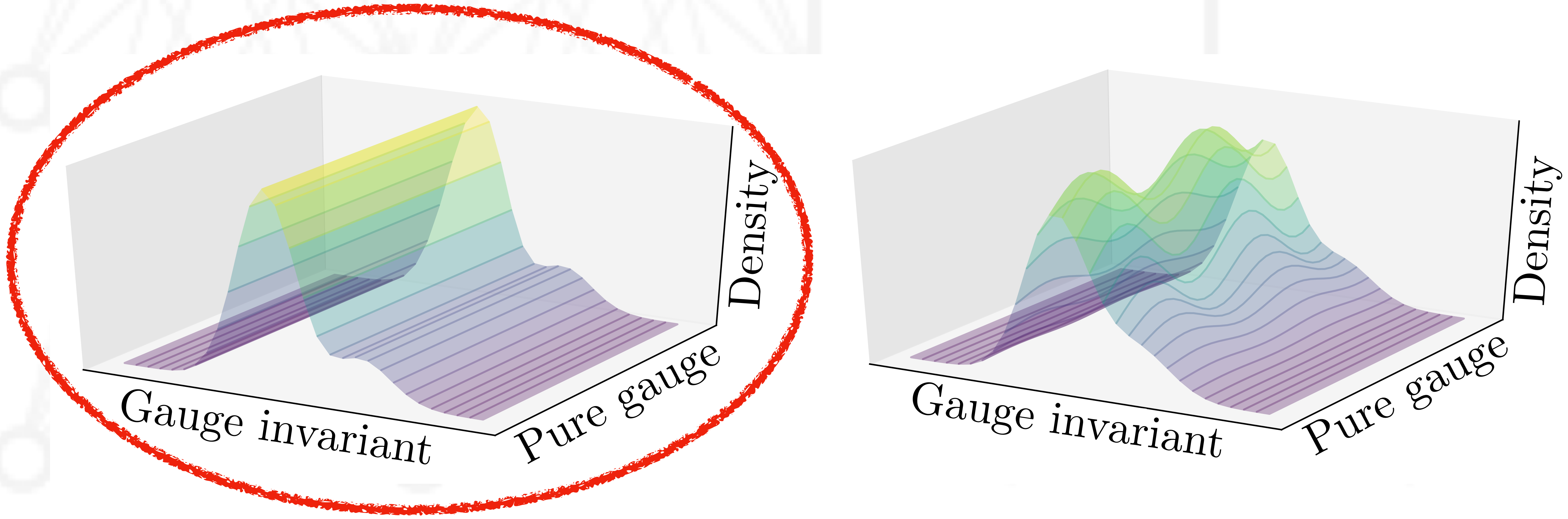
Learning $SU(2)$ and $SU(3)$ gauge theory

Normalizing flows trained for 2D lattice gauge theory on 16×16 lattices.

- Approx equal 't Hooft couplings:
  $\beta = \{1.8, 2.2, 2.7\}$ for $SU(2)$ and
  $\beta = \{4.0, 5.0, 6.0\}$ for $SU(3)$

- 48 coupling layers, update all links 6 times

- Kernels suitable for $SU(N)$ for **exact gauge invariance**



Symmetries in $SU(2)$ and $SU(3)$ models

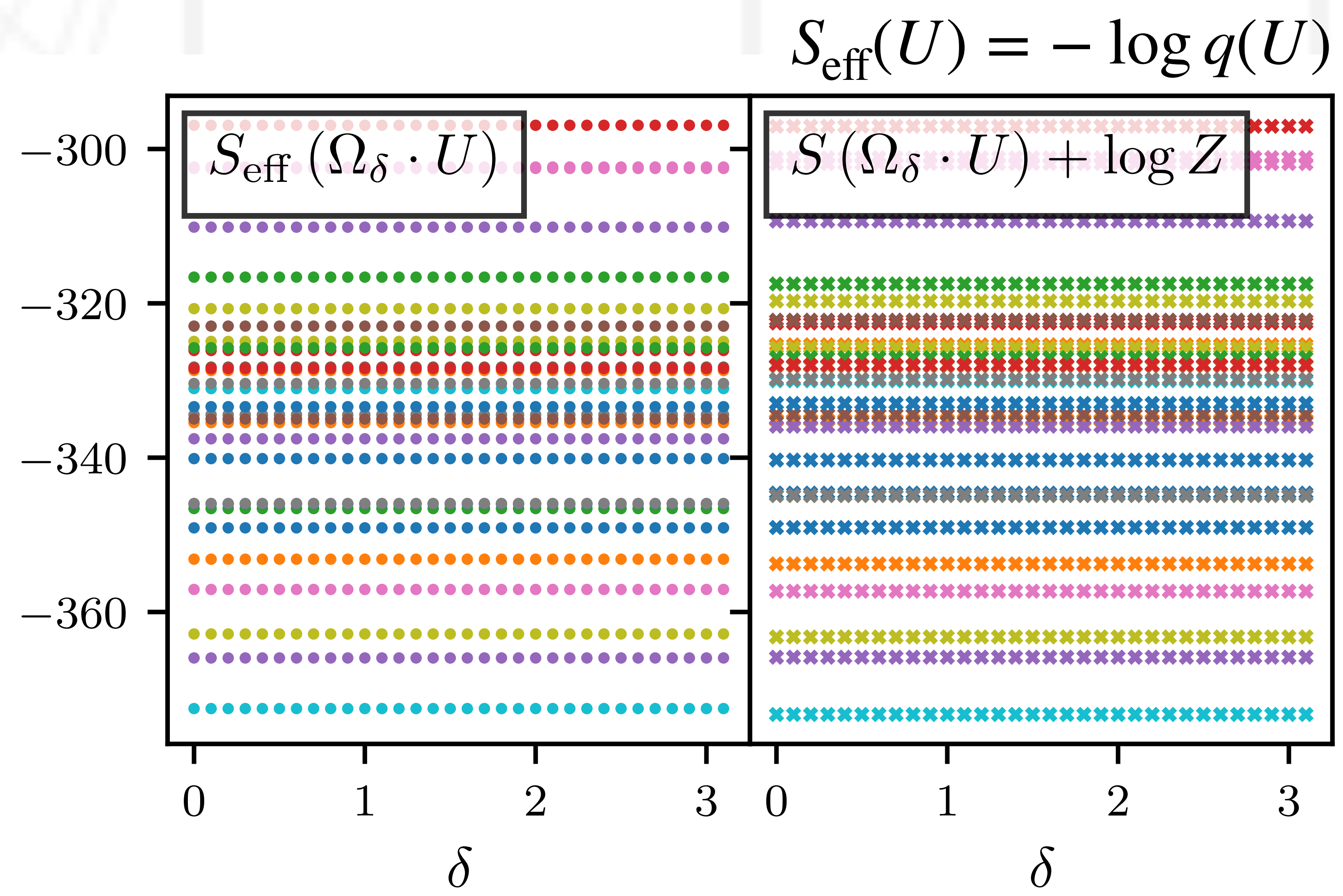
Exact **gauge symmetry** by construction.

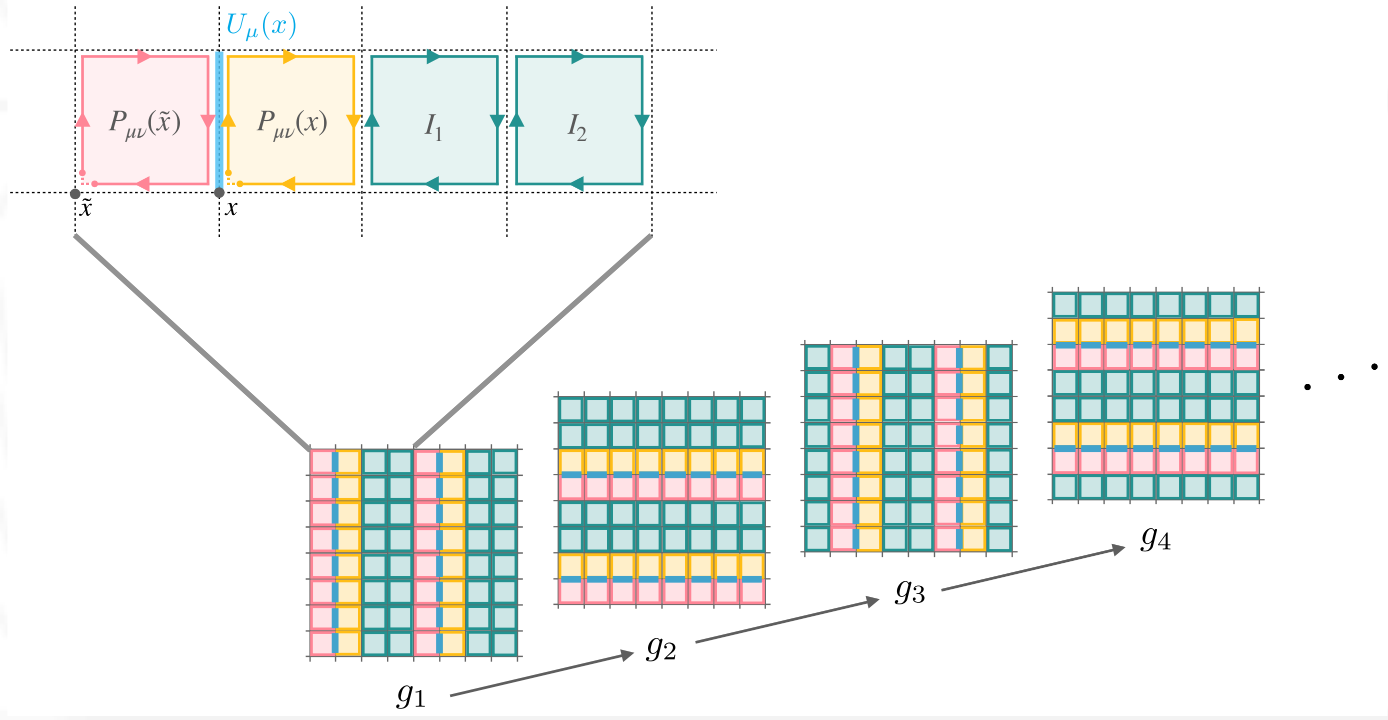
Exact **center symmetry** due to choice of loops:

- Plaquettes invariant under center symm
- Should include Polyakov loops if center symmetry explicitly broken in theory

Large subgroup of **translational symmetry**

- $\mathbb{Z}_4 \times \mathbb{Z}_4$ breaking due to 4-site spacing in masking pattern
- 16-elt residual group to be learned, independent of volume

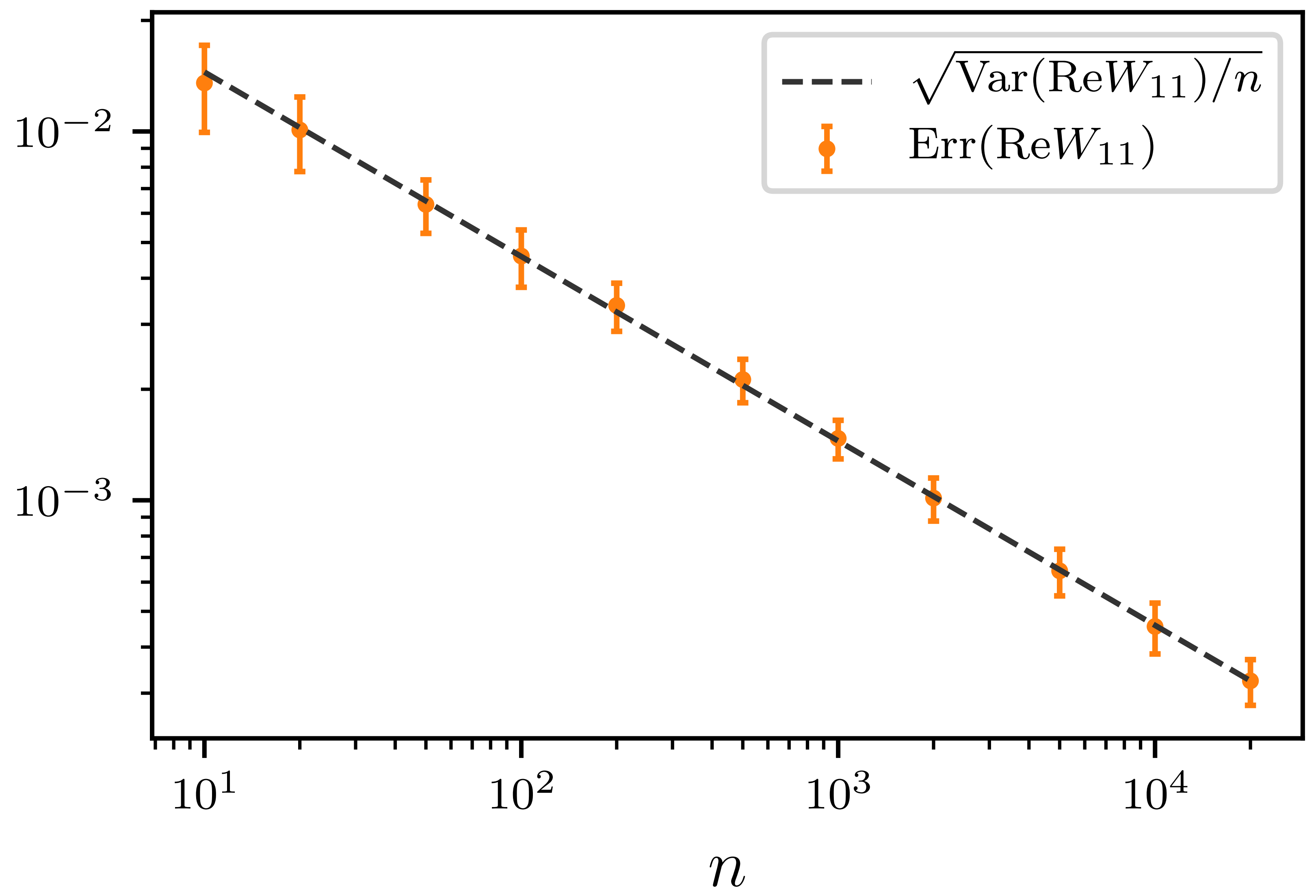


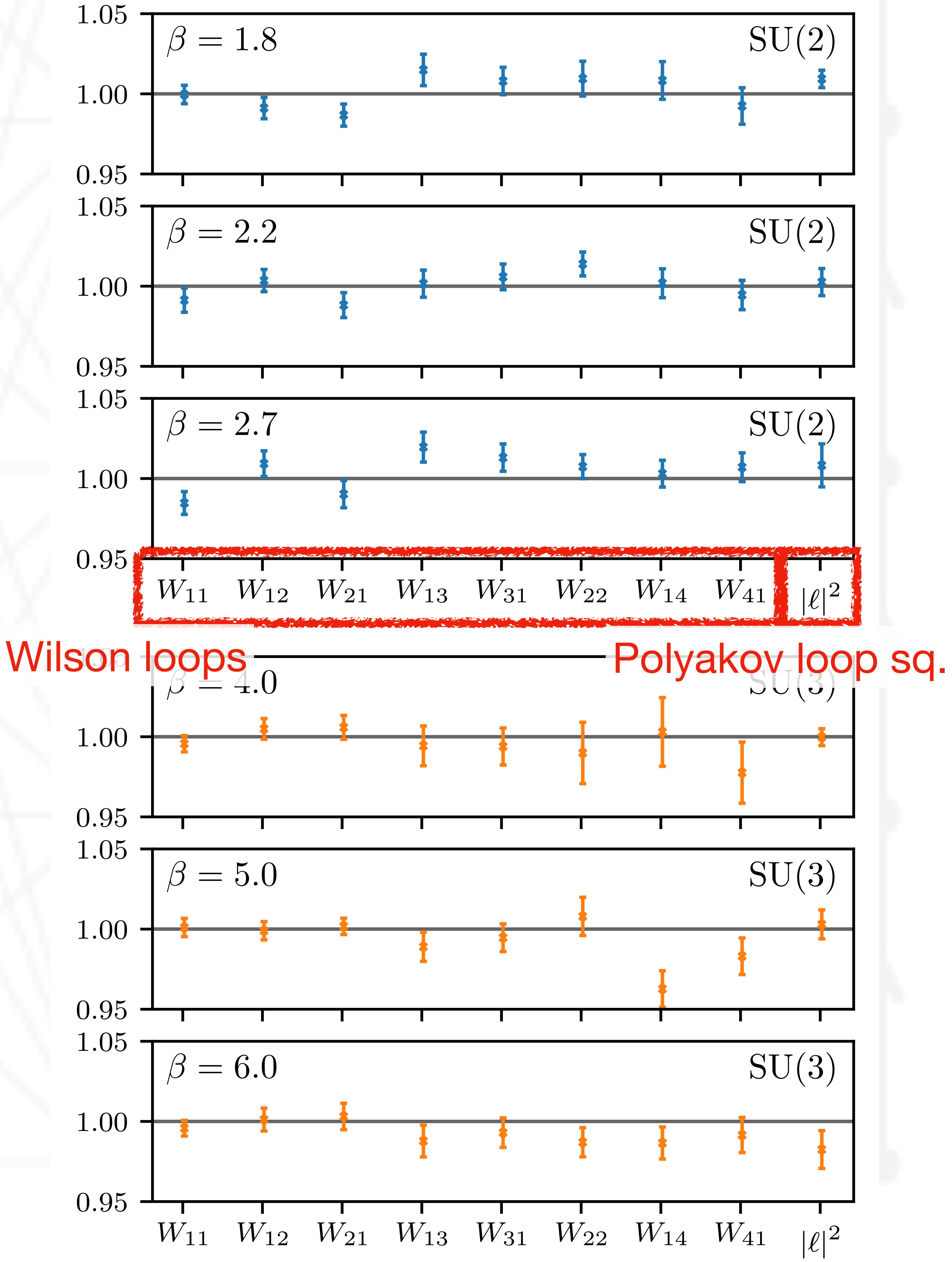


Results for $SU(2)$ and $SU(3)$ gauge theory

- Flow-based MCMC observables agree with analytical
- High-quality model: autocorrelation time in flow-based Markov chain τ_{int} = 1—4
- $1/\sqrt{n}$ scaling with number of samples n

thinned by τ_{int}!





Summary

- Flow-based MCMC gives exact results from approximate model proposals
  - Inaccuracies in the model = increased autocorrelation time
- Gauge symmetry can be incorporated without breaking (most of) translational symmetry
  - Gauge equivariant coupling layers
  - Kernels for $U(1)$ and $SU(N)$

And a simple alternative for $U(N)$ in our paper!

- High-quality models produced for
  - Lattice scalar theory in 1+1D
  - $U(1)$, $SU(2)$, and $SU(3)$ lattice gauge theory in 1+1D

Outlook

Several directions for future work:

1. Choices of untraced loops to transform, gauge-inv loops as input
    - Higher degree of connectivity between loops and links in higher spacetime dims
2. Performance on multimodal distributions?
    - Relevant for broken symmetry regions of param space
3. Training hyperparameter tuning, different model arch for inner flows
4. Scaling of required model complexity in taking continuum limit?
    - Models with more params likely required as we scale, but how many more?
5. Incorporation of dynamical fermions

Outlook

If the method can be scaled to state-of-the-art calculations, ensemble generation could look like…

easily parallelized

… a single up-front cost to train a model

… more efficient parameter sweeps (retrain a model from nearby params)

easily parallelized

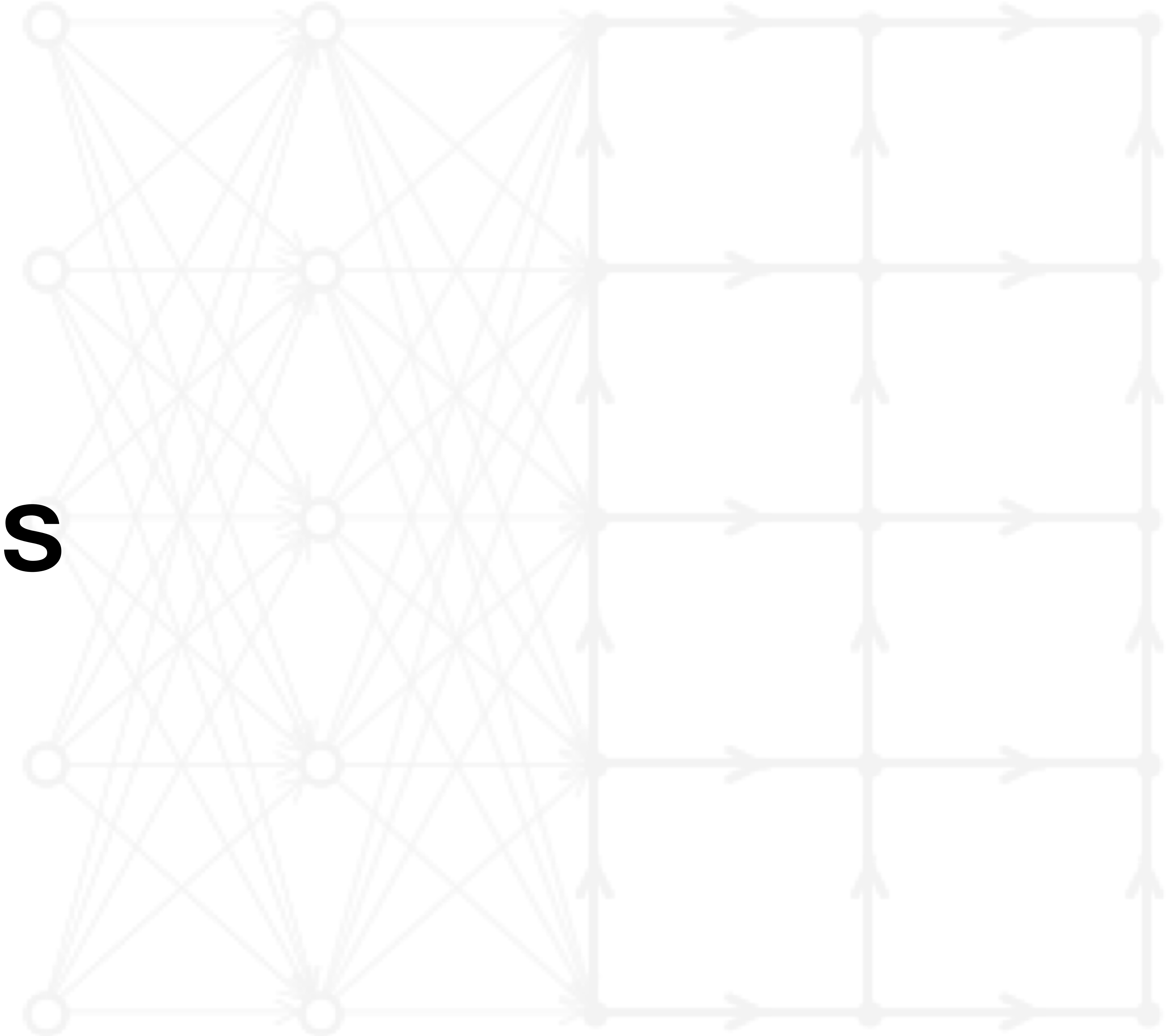
… cheap gauge field generation

… reduced storage costs (store/transfer the model, not configs!)

… or, no storage costs? (generate configs on the fly for measurements?)

In the upcoming exascale era, exploiting massively parallel resources will be key!

Backup slides



Related approaches

Generative Adversarial Networks (GANs):

- Highly expressive!
- Work in the direction of GANs for lattice

  [Urban, Pawlowski 1811.03533]

  [Zhou, Endrődi, Pang, Stöcker 1810.12879]

Variational AutoEncoders (VAEs):

- Can also learn meaningful directions in the prior variables

However: No access to $q(U)$… hard to make exact!

[Karras, Lane, Aila / NVIDIA 1812.04948]

These are machine learned faces!

[Shen & Liu 1612.05363]

These are machine learned faces!

Optimizing ("training") the model

Must not require a large number of samples from real distribution to optimize!

Self-training:

- Optimize model params using stochastic gradient descent on a loss function
- Loss function = modified Kullback-Leibler (KL) divergence

Measures difference between probability distributions

Constant shift removes unknown normalization

$$D_{\mathrm{KL}}(q\,||\,p) := \int \mathscr{D}U\, q(U)\big[\log q(U) - \log p(U)\big] \geq 0$$

$$D'_{\mathrm{KL}}(q\,||\,p) := \int \mathscr{D}U\, q(U)\big[\log q(U) + S(U)\big] \geq -\log Z$$

- To estimate loss for grad. descent, draw samples from the **model**, measure sample mean of $\big[\log q(U) + S(U)\big]$

Translational equivariance with CNNs

1. Make context functions Convolutional Neural Nets.

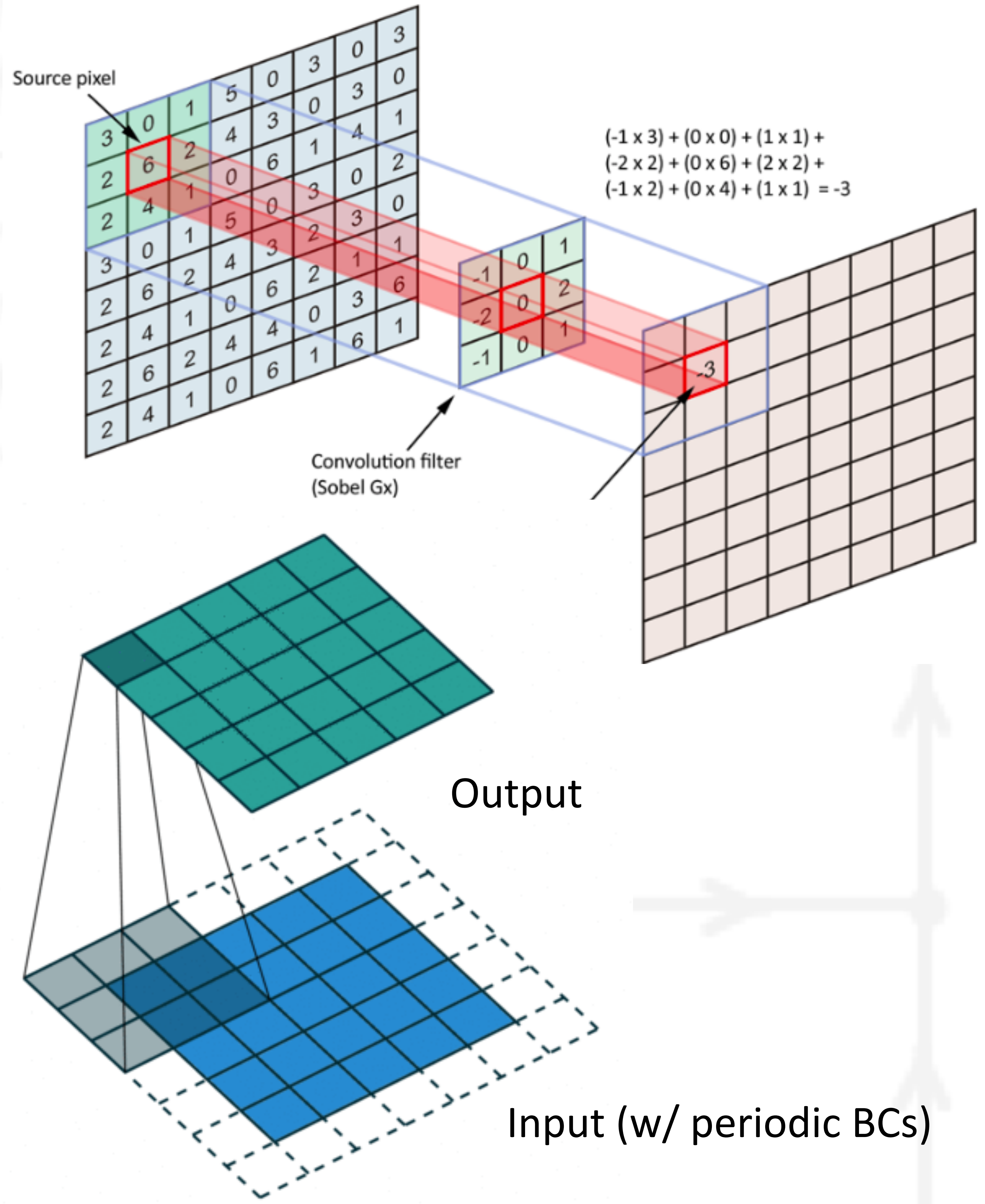
CNNs:

- Compute output value for each site from linear transform of nearby DOF only
- Reuse same weights, scanning kernel across the lattice

CNNs are equivariant under translations.

2. Make masking pattern (mostly) translationally invariant.

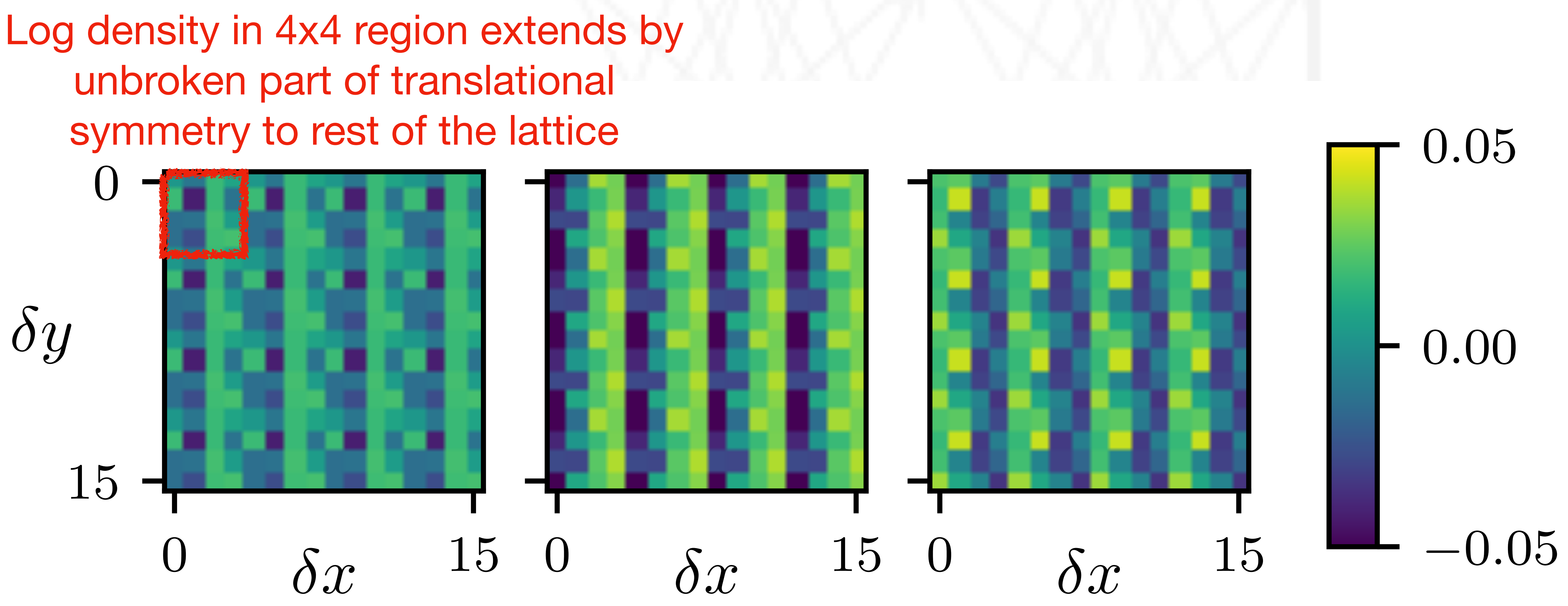
- Required to ensure whole coupling layer is equiv
- Our application: translational equiv modulo $\mathbb{Z}_4 \times \mathbb{Z}_4$



[Images from freecodecamp.org]

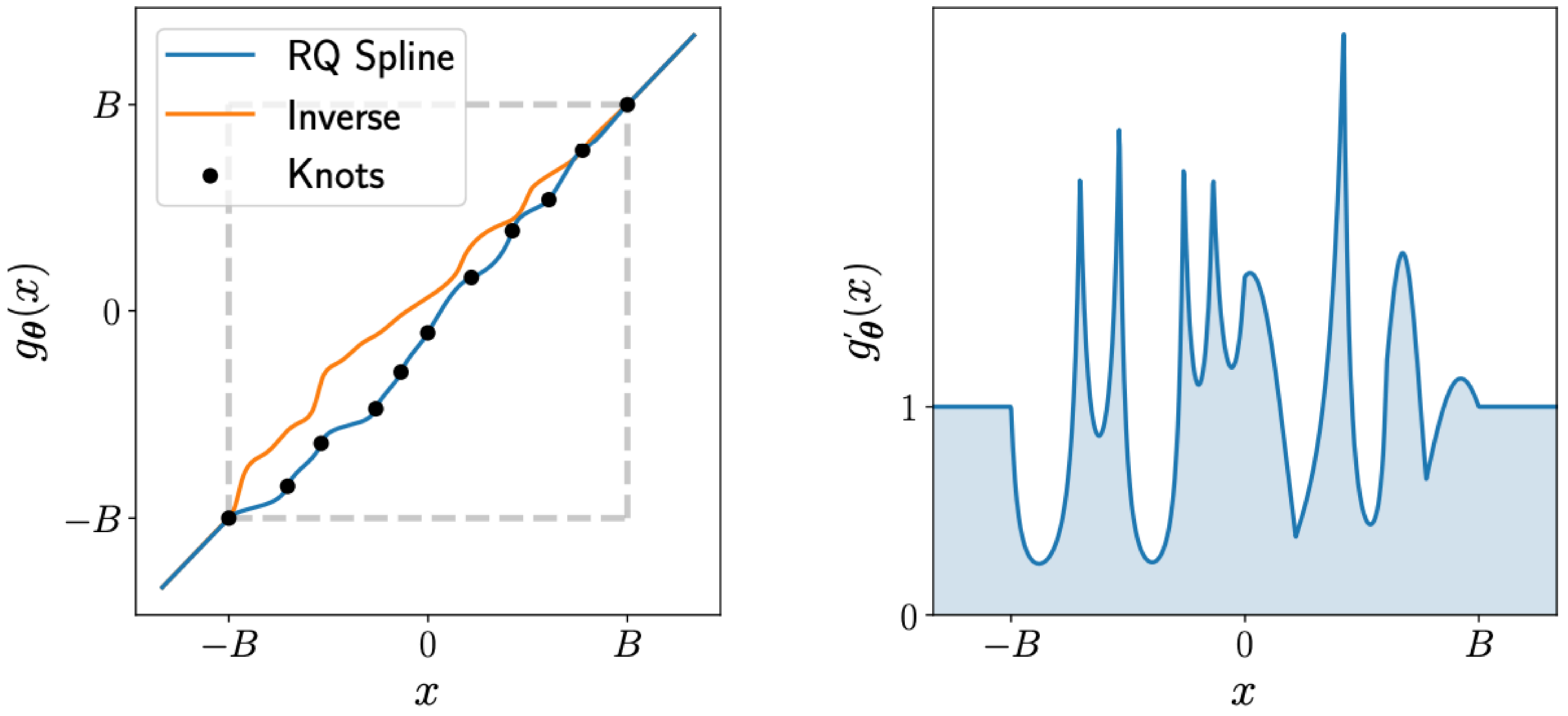
Translational symmetry breaking pattern

- Masking patten = repeating tile of size 1×4
- Rotate / translate the pattern between layers
- $\mathbb{Z}_4 \times \mathbb{Z}_4$ symmetry breaking



Details of $SU(2)$ models

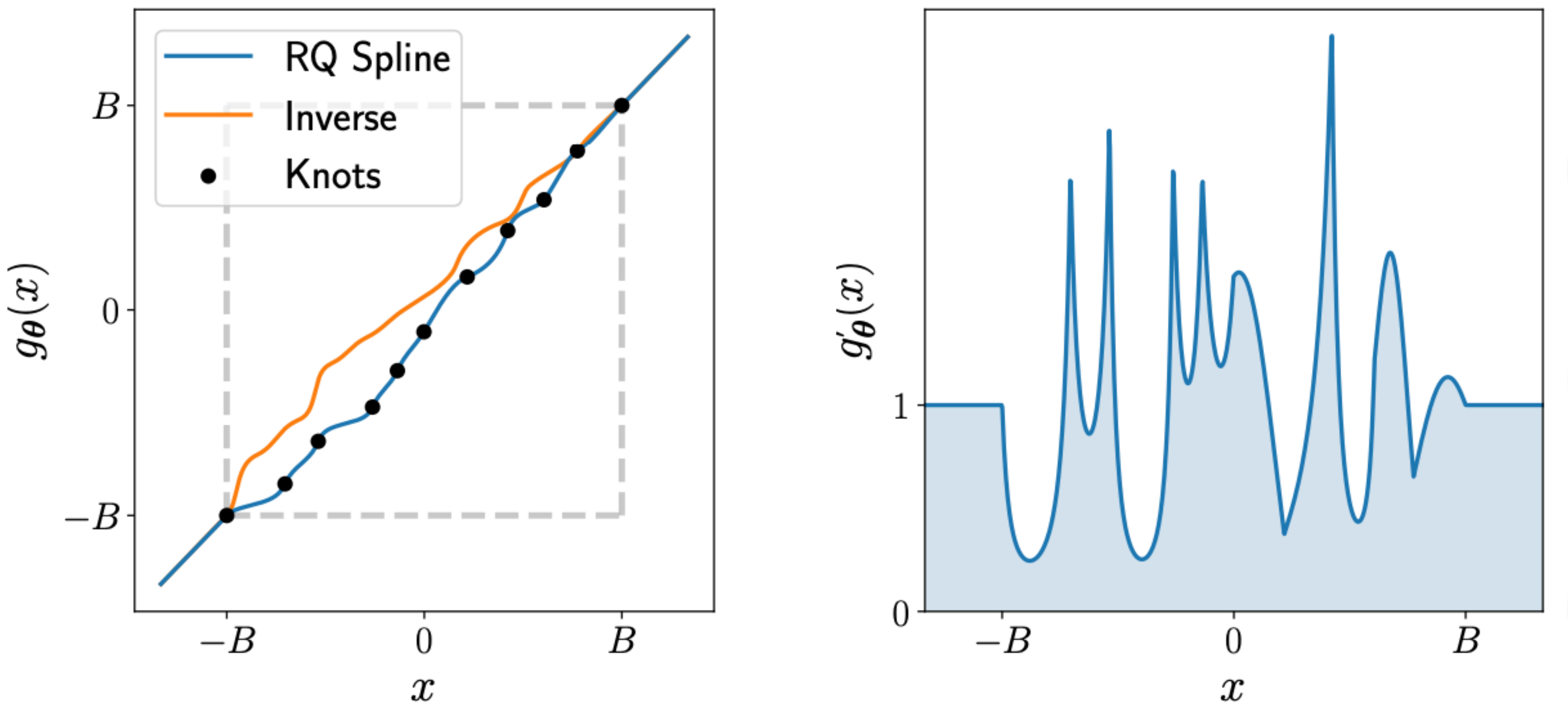
- Inner flow on open box Ω is a spline flow with **4 knots**
  - B and $-B$ boundaries align to 0 and 1 edges of the open box
- CNNs to compute the knot locations
  - 32 hidden channels
  - 2 hidden layers



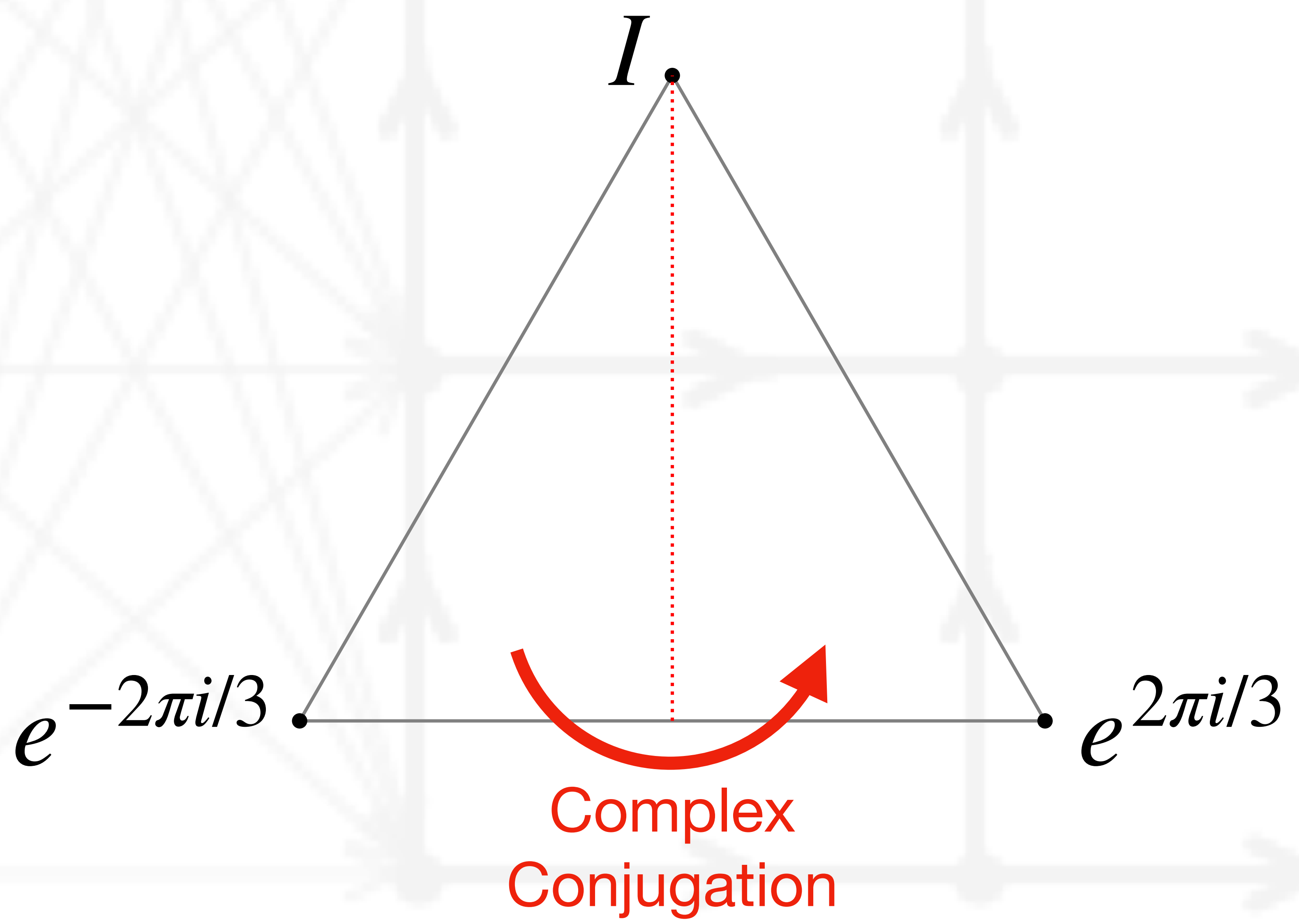
[Durkan, Bekasov, Murray, Papamakarios 1906.04032]

Details of $SU(3)$ models

- Inner flow on open box Ω is a spline flow with **16 knots**
  - B and $-B$ boundaries align to 0 and 1 edges of the open box
- CNNs to compute the knot locations
  - 32 hidden channels
  - 2 hidden layers
- Exact conjugation equivariance also imposed

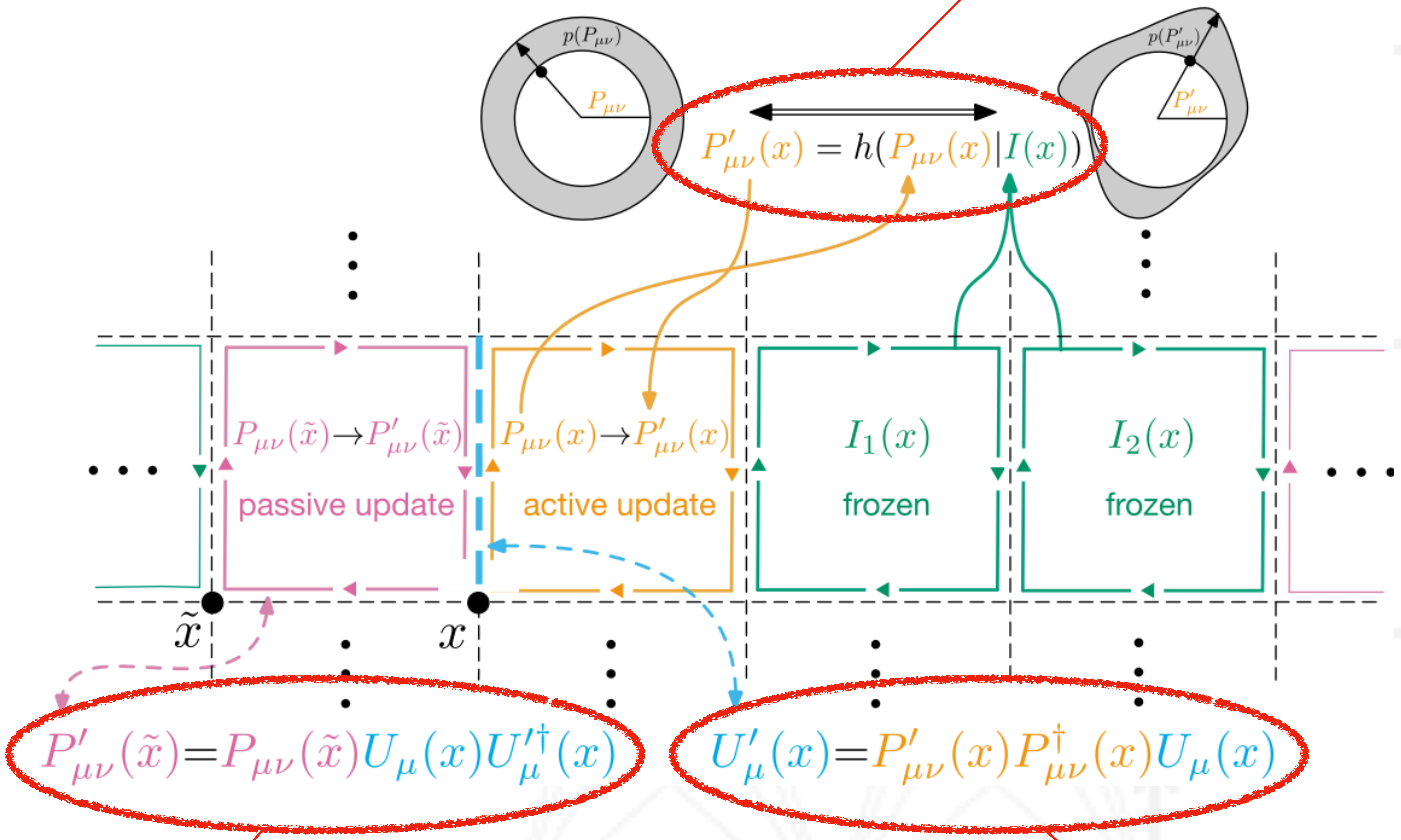


[Durkan, Bekasov, Murray, Papamakarios 1906.04032]



Gauge equivariance (details)

1. Kernel acts on subset of untraced plaquettes



3. Some plaquettes **passively** updated as a result of link changing

2. Link **absorbs** update via left-multiplication (invertible!)

Map into canonical cell

Want to permute eigenvalues into canonical order

- Sorting doesn't work directly: discontinuities when θ_k jumps across the $\pm\pi$ boundary
- Simply trying all $N!$ permutations is slow for large N
- Need to ensure permutation taking points in the same cell to canonical is the same

Short algorithm based on sorting works; Algorithm 1 of [‡]

[‡] [Boyda, **GK**, Racanière, Rezende, Albergo, Cranmer, Hackett, Shanahan 2008.05456]

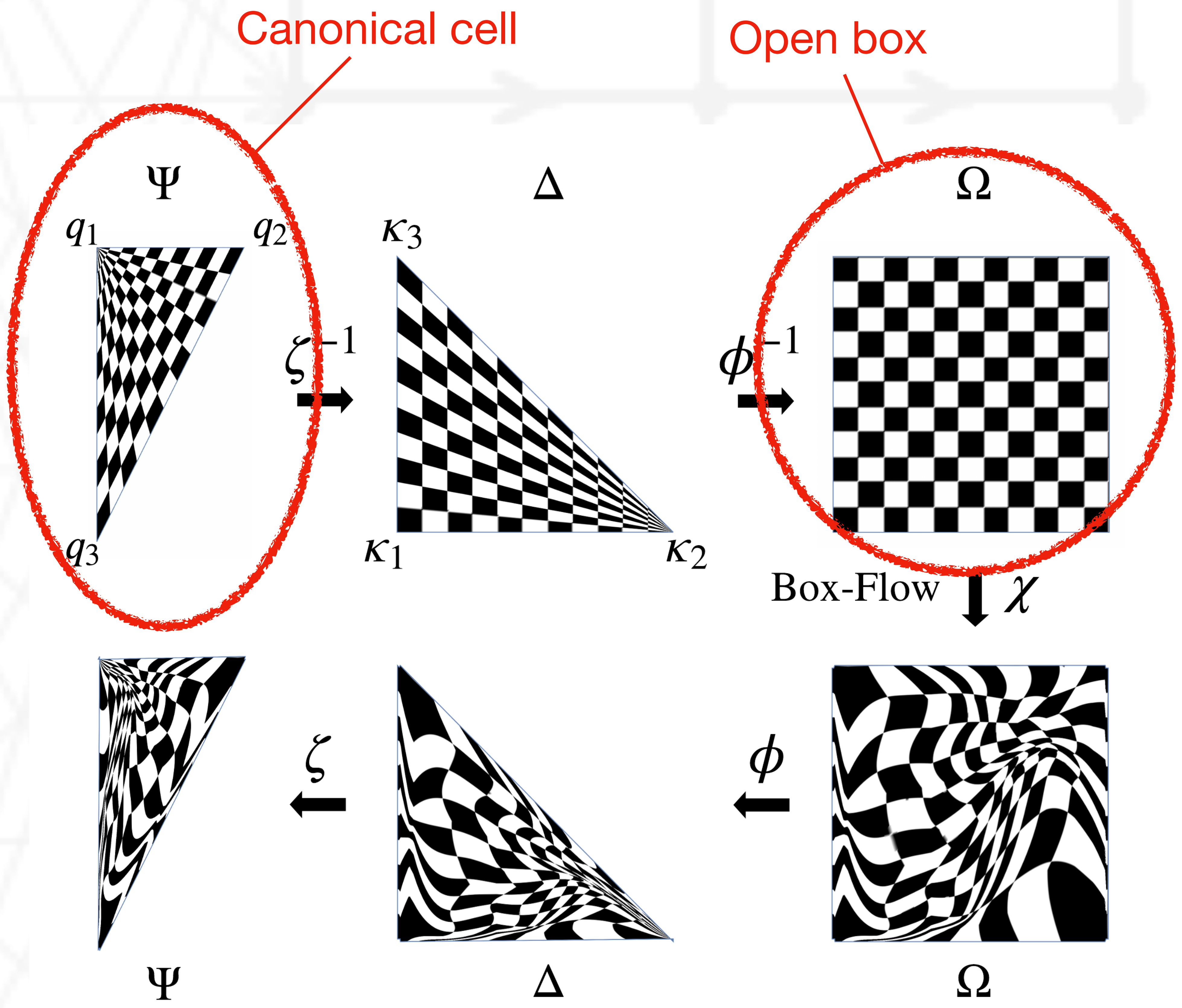
Transform within canonical cell

Require: boundary-preserving transformation within the cell

- Cell is a simplex bounded by vertices $\{y_k\}$,

$$[y_k]_j := 2\pi\left(\frac{k}{N} - \delta_{k\geq j}\right)$$

- Hard to transform directly, instead we first change coordinates to an open box $\Omega = (0,1)^N$



Composition of two maps, ζ and ϕ, give the change of coordinates

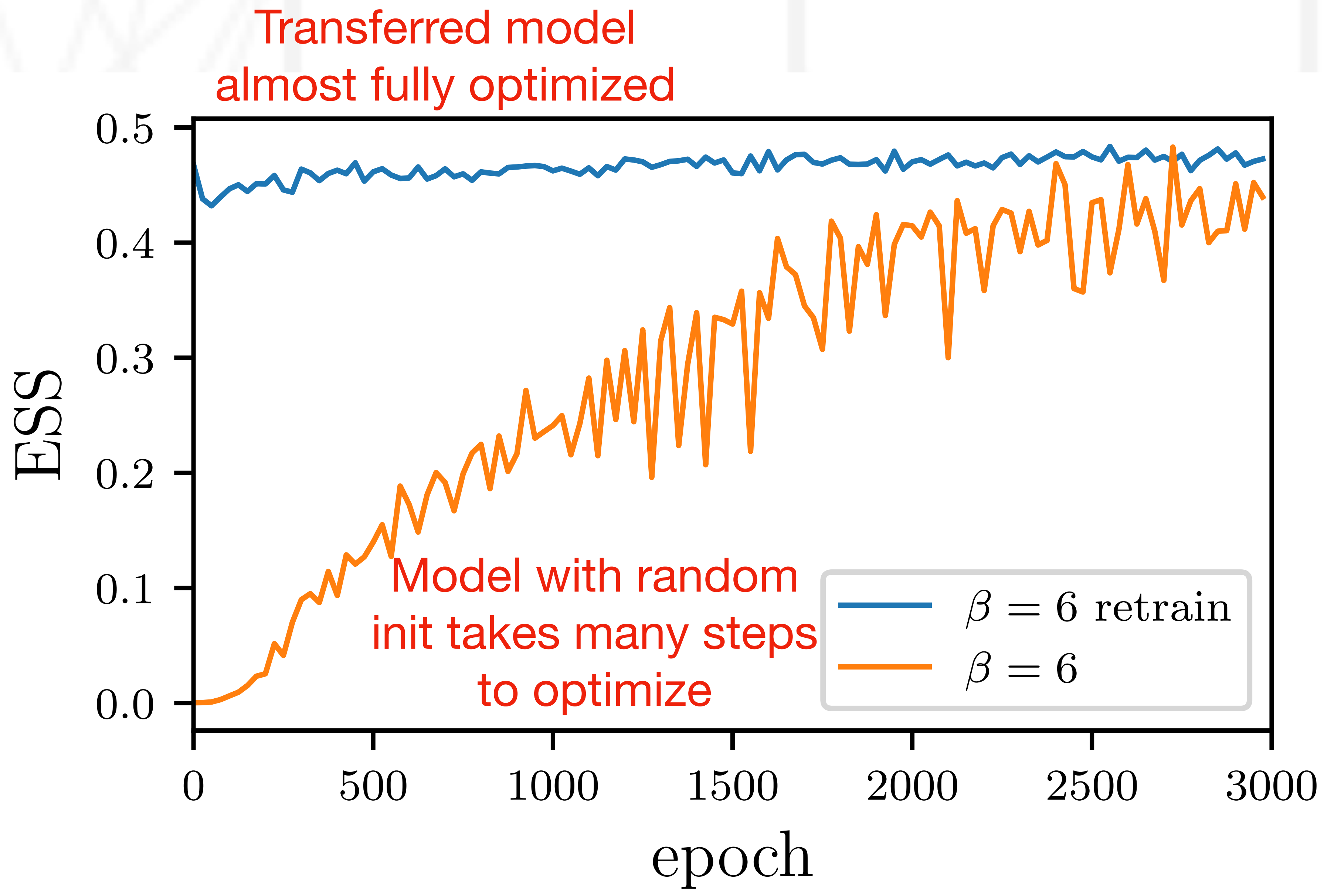
Boundary preserving map using **fixed-interval spline transformations** on each coordinate of Ω

Gauge theory model training

- Adam optimizer ~ stochastic grad. descent with momentum
  - Batches of size 3072 per gradient descent step
  - Monitored value of **effective sample size** (ESS)

$$\mathrm{ESS} = \frac{\left(\frac{1}{n}\sum_i w(U_i)\right)^2}{\frac{1}{n}\sum_i w(U_i)^2}, \quad U_i \sim q(U)$$

$w(U) = p(U)/q(U)$ "reweighting factors"



- Transfer learning: model trained first on 8×8 then used to initialize model for training on 16×16