Flow-based models for lattice ensemble generation

Gurtej Kanwar
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Based on …

… flow-based sampling for lattice QFT:

[Albergo, GK, Shanahan **PRD100 (2019) 034515**]
[Albergo, Boyda, Hackett, GK, Cranmer, Racanière, Rezende, Shanahan **2101.08176**]
[Albergo, GK, Racanière, Rezende, Urban, Boyda, Cranmer, Hackett, Shanahan **2106.05934**]
[Hackett, Hsieh, Albergo, Boyda, Chen, Chen, Cranmer, GK, Shanahan **2107.00734**]

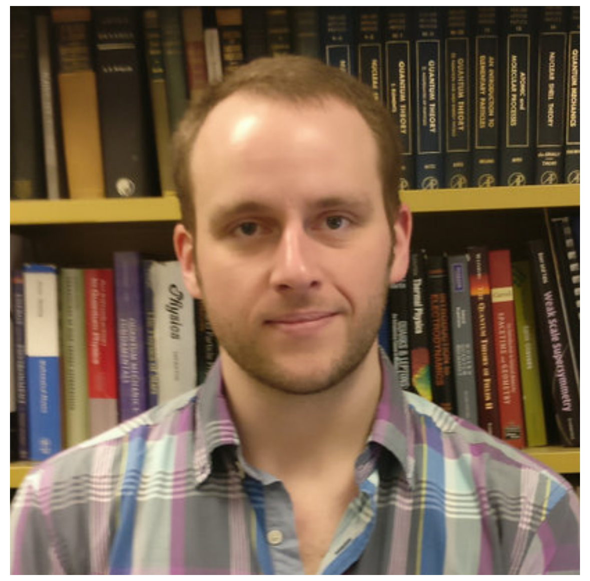
… flows for compact vars & lattice gauge theories:

[GK, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan **PRL125 (2020) 121601**]
[Rezende, Papamakarios, Racanière, Albergo, GK, Shanahan, Cranmer **ICML (2020) 2002.02428**]
[Boyda, GK, Racanière, Rezende, Albergo, Cranmer, Hackett, Shanahan **PRD103 (2021) 074504**]

ML for HEP, on and off the lattice | ECT* Trento | Sept 29, 2021

Massachusetts Institute of Technology

Phiala Shanahan



Dan Hackett

Denis Boyda

DeepMind

Sébastien Racanière

Danilo Rezende

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Julian Urban

NEW YORK UNIVERSITY

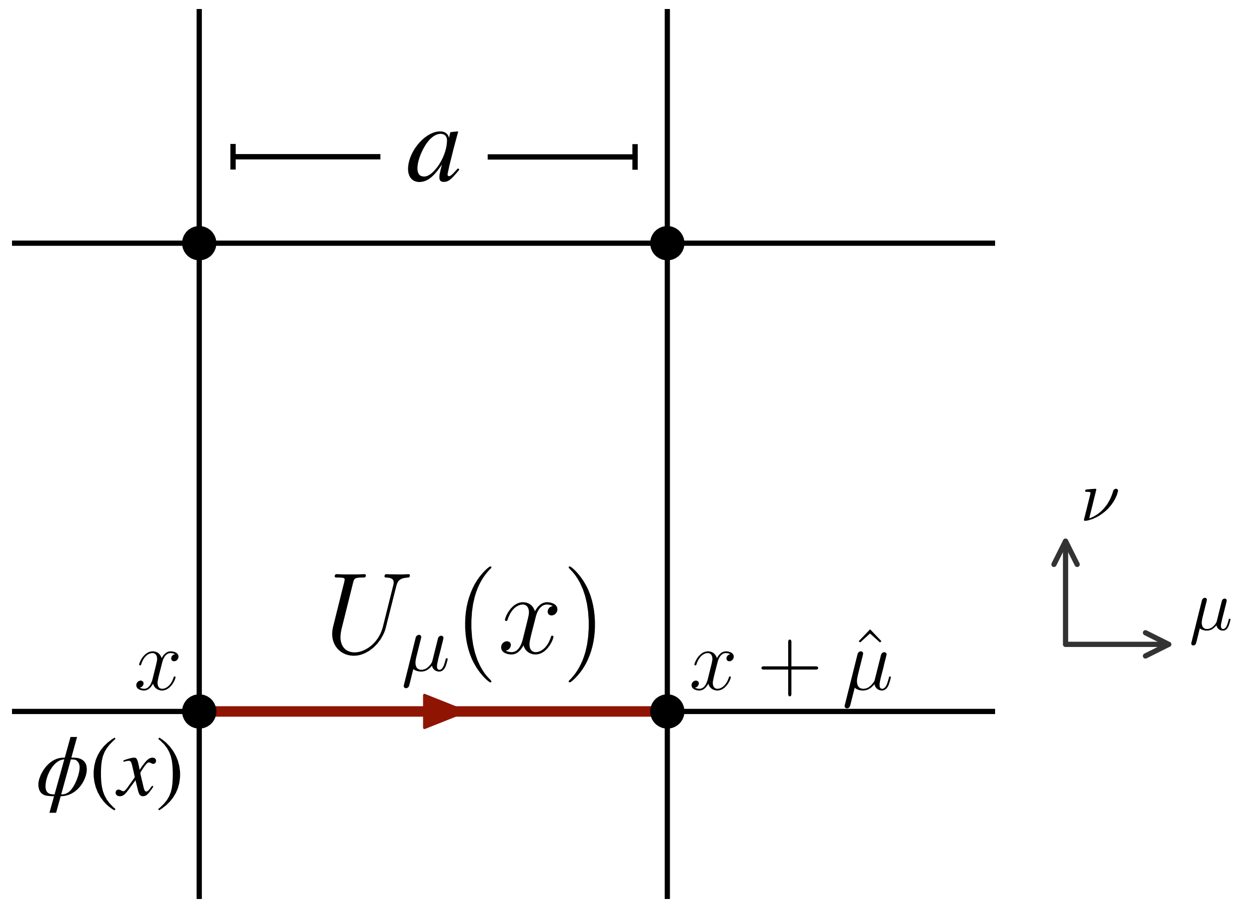
Kyle Cranmer

Michael Albergo

30 second Lattice QFT primer

Lattice discretization:

- Gauge field discretized on links $U_\mu(x) \in G$ [e.g. $\mathrm{SU}(3)$]
- Other fields $\phi(x)$ discretized to live on sites x

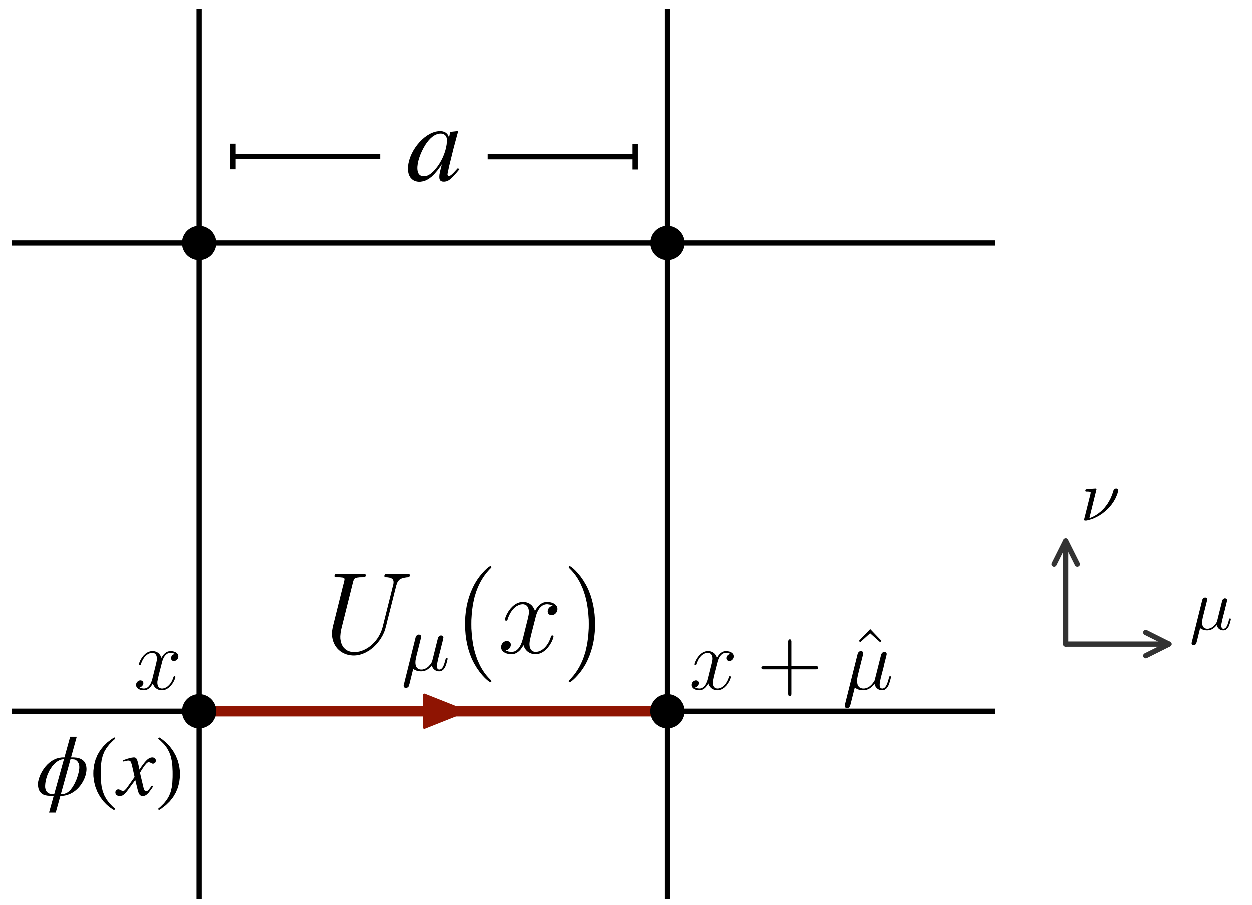


Lattice path integral → observables

Caveats:

- Euclidean spacetime $t \to i\tau$
- Discretization effects (must take $a \to 0$)

30 second Lattice QFT primer



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Vaccum/thermal expt. value of quantum operator

✓ In principle tractable integral

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

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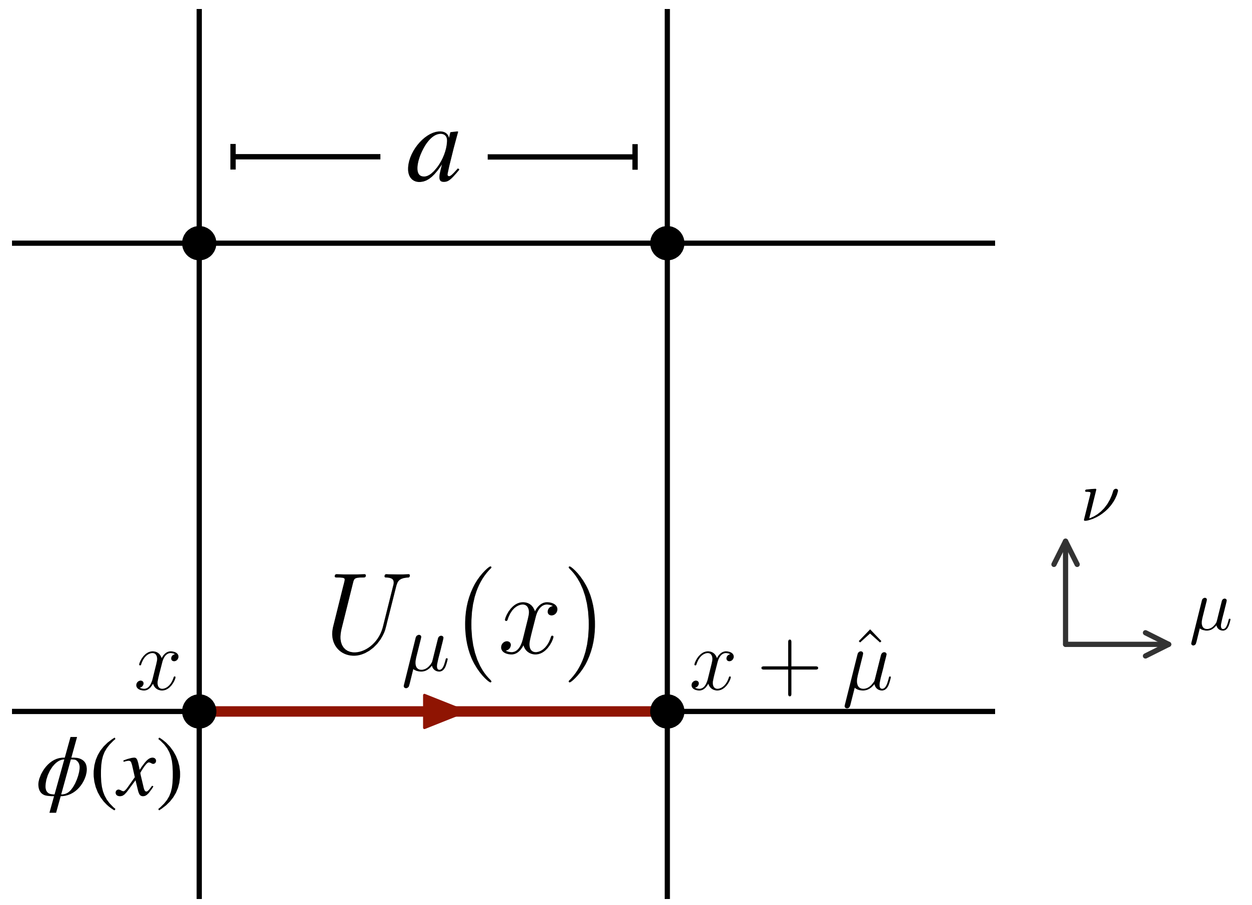

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$$Z = \int \mathcal{D}U \, e^{-S(U)}, \qquad \int \mathcal{D}U = \prod_{x,\mu} \int dU_\mu(x)$$

Normalizing constant

Path integral measure

Caveats:

- Euclidean spacetime $t \to i\tau$
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Importance sampling: the workhorse of LQFT

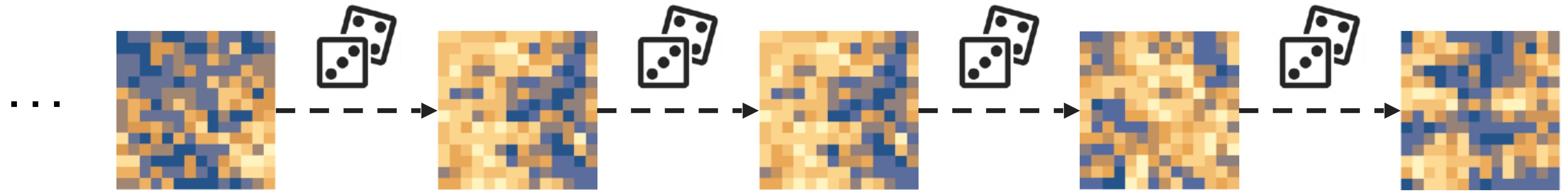
Monte Carlo sampled ensembles allow estimates of (many) QFT observables

Desired continuum QFT quantity

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

Target distribution

Markov chain Monte Carlo (MCMC)



Example: MCMC for scalar field configurations

- **Asymptotically** converges to distribution p
- However: States of the chain are “autocorrelated”
- Skip thermalization steps, ensemble “thinned” to a subset

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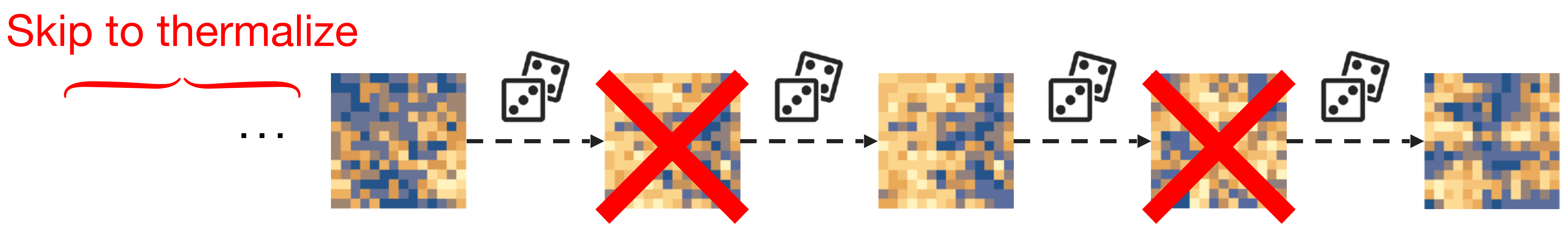

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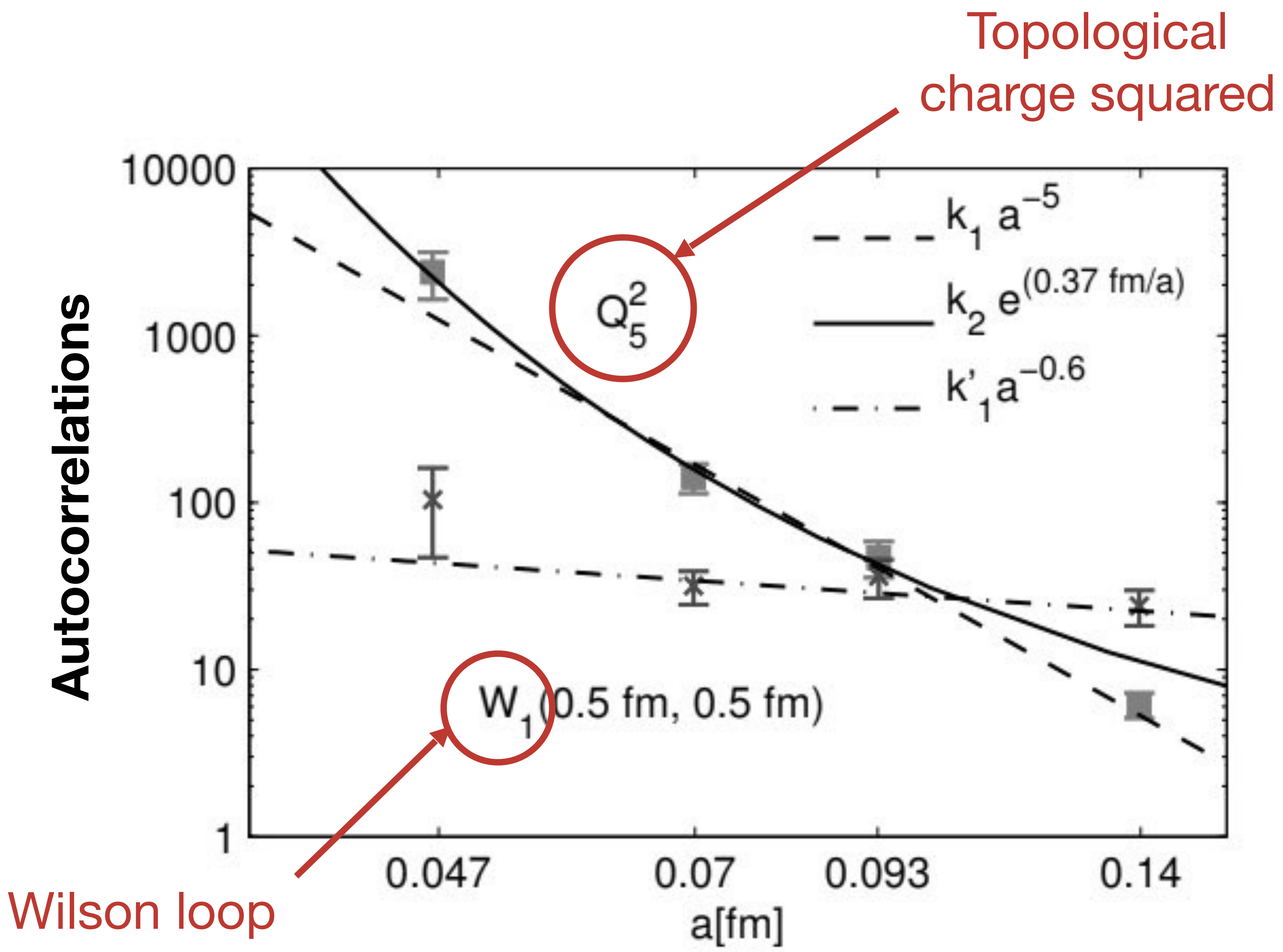
Critical slowing down (CSD)

Local/diffusive Markov chains inefficient as $a \to 0$

- Correlation length grows in lattice units, but information transfer is local
- Rare to update entire field coherently



[Schaefer et al. / ALPHA collaboration **NPB845 (2011) 93**]

Critical slowing down: diverging autocorrelations due to local mixing

Topological freezing: Markov chain gets “stuck” in topological sectors

CSD also affects a number of other models:

- CP^{N-1} [Flynn, et al. **1504.06292**]
- O(N) [Frick, et al. **PRL63 (1989) 2613**]
- ϕ^4 [Vierhaus; Thesis, **doi:10.18452/14138**]
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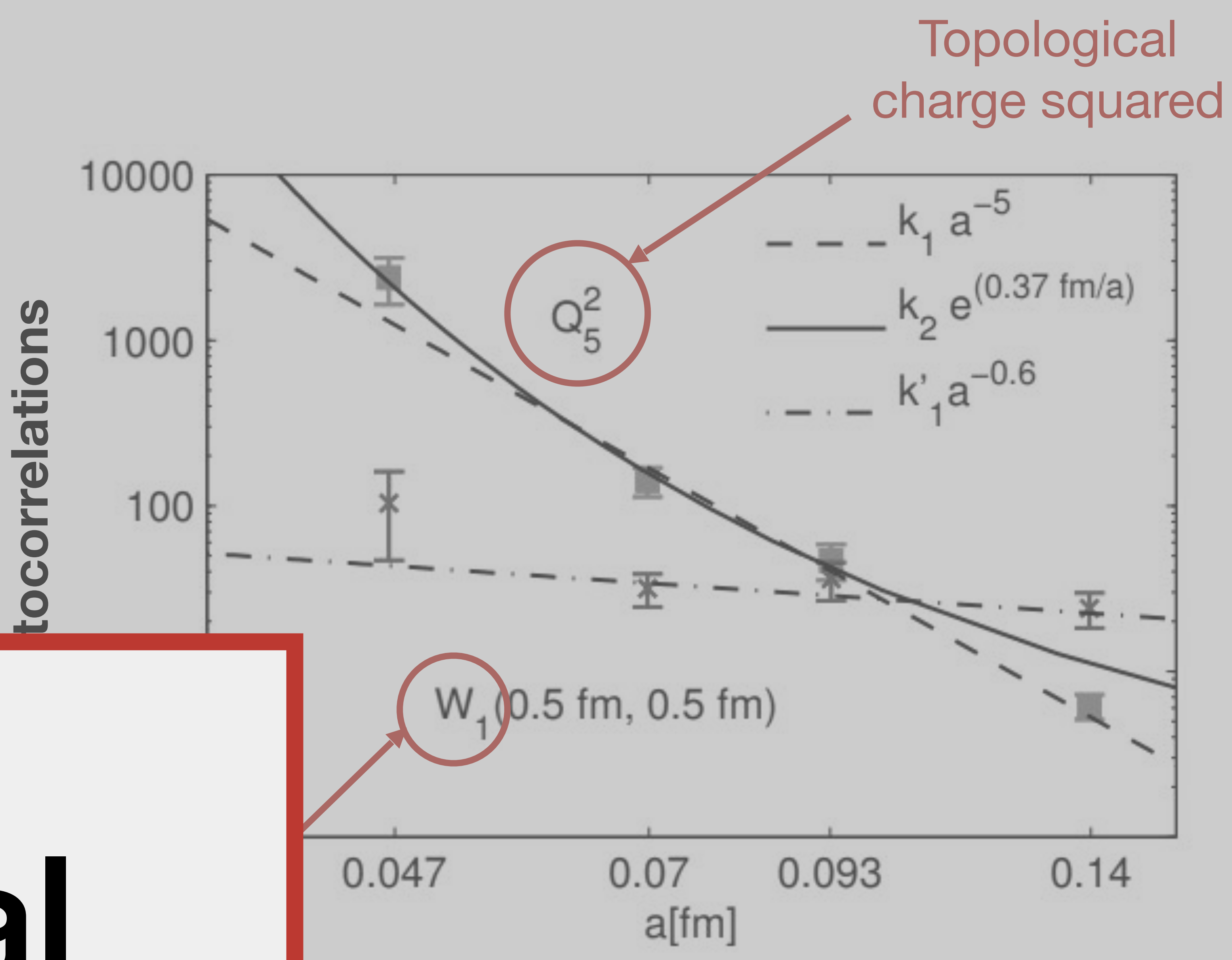
CSD & Topological freezing:

Significant obstacles to continuum limit



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Circumventing CSD?

Avoid diffusive/local Markov chain updates.

Proposal: Sample from generative ML models.

Caveats:

⚠️ We require **exactness**

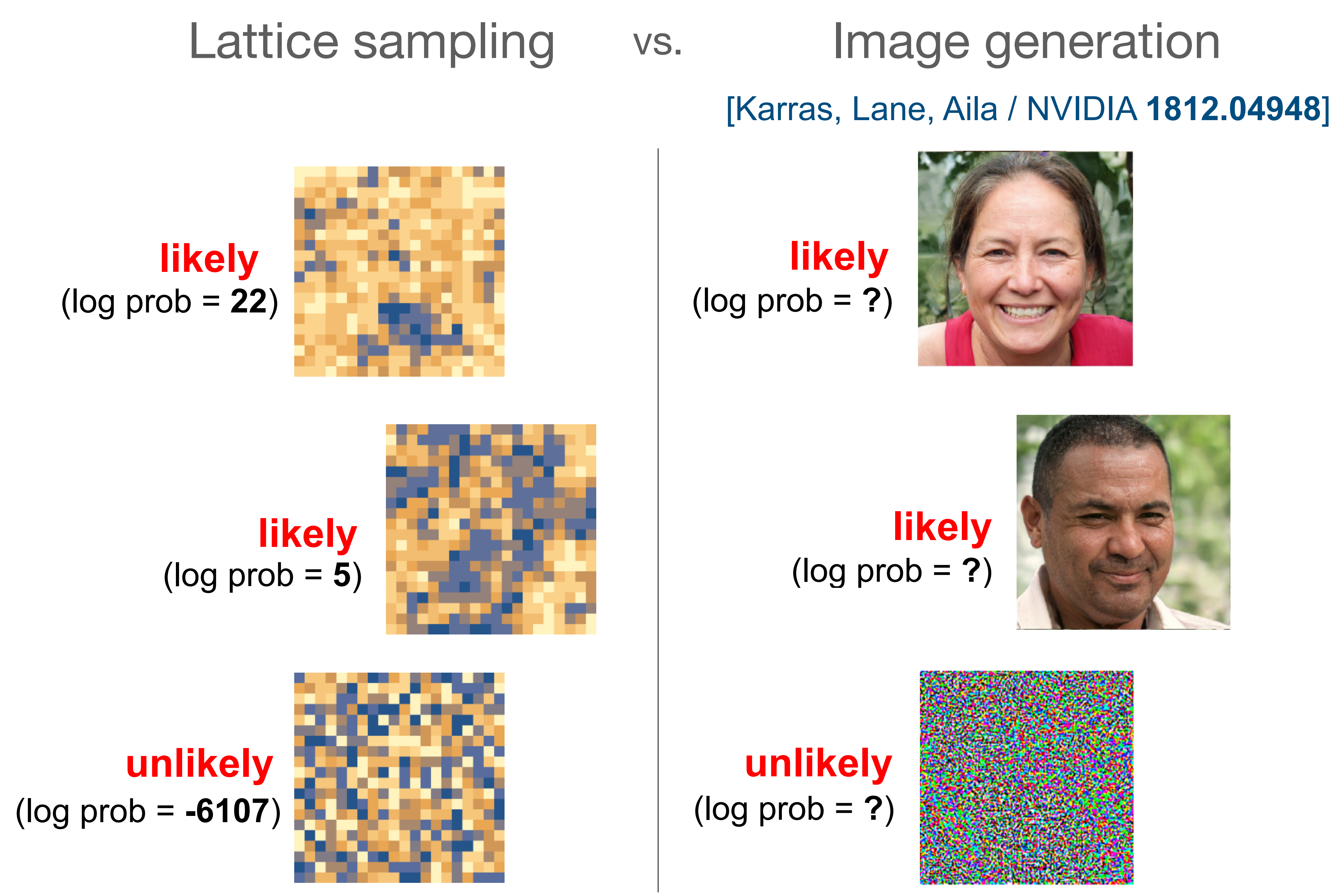
⚠️ Inverted data hierarchy
… $\sim 10^9 - 10^{10}$ DoFs in a config
… $\sim 10^3$ configs

✓ Target probability density $e^{-S(U)}/Z$

✓ Physical symmetries = “flat directions”

We choose **flow-based models.**

AKA ‘normalizing flows’



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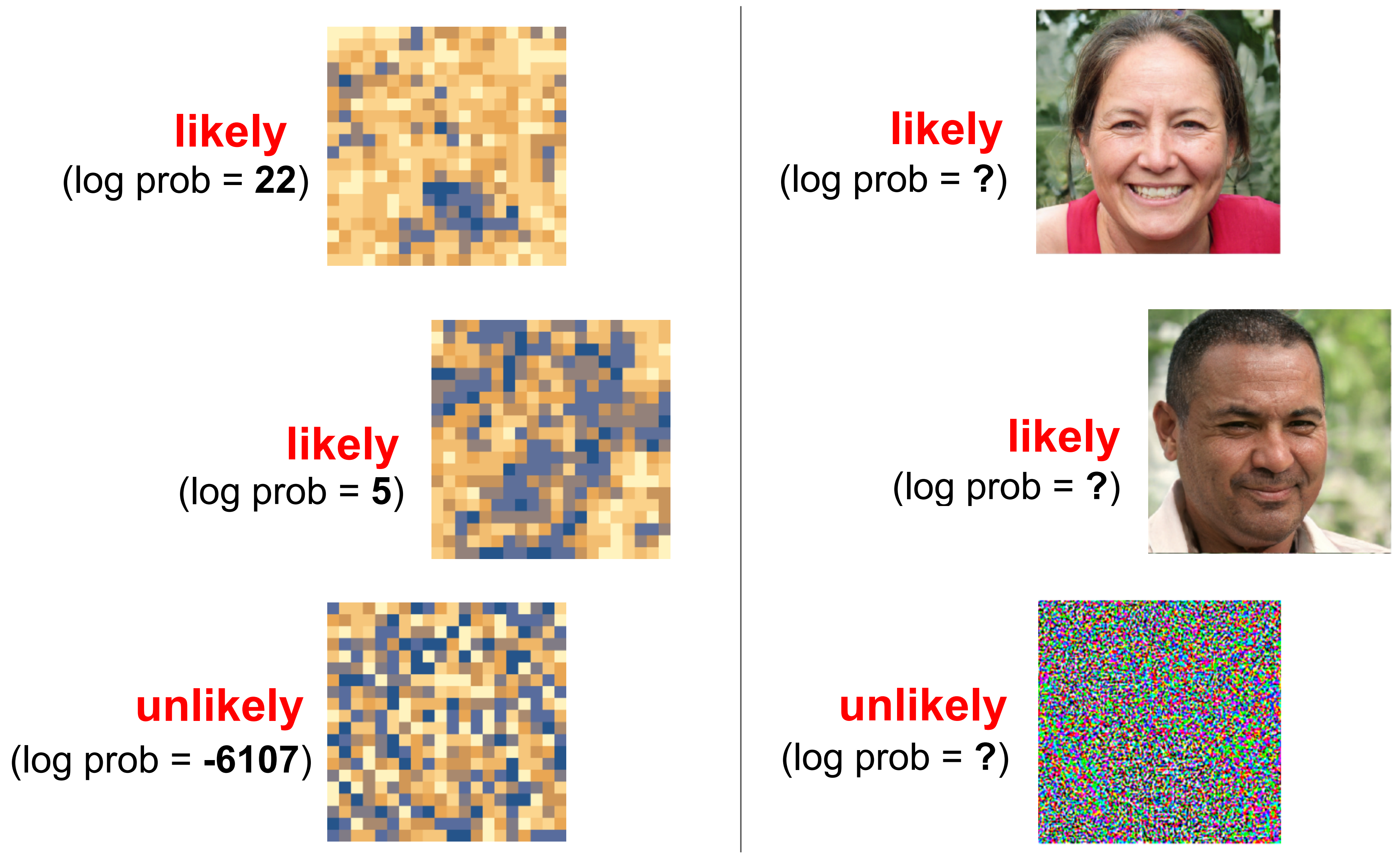
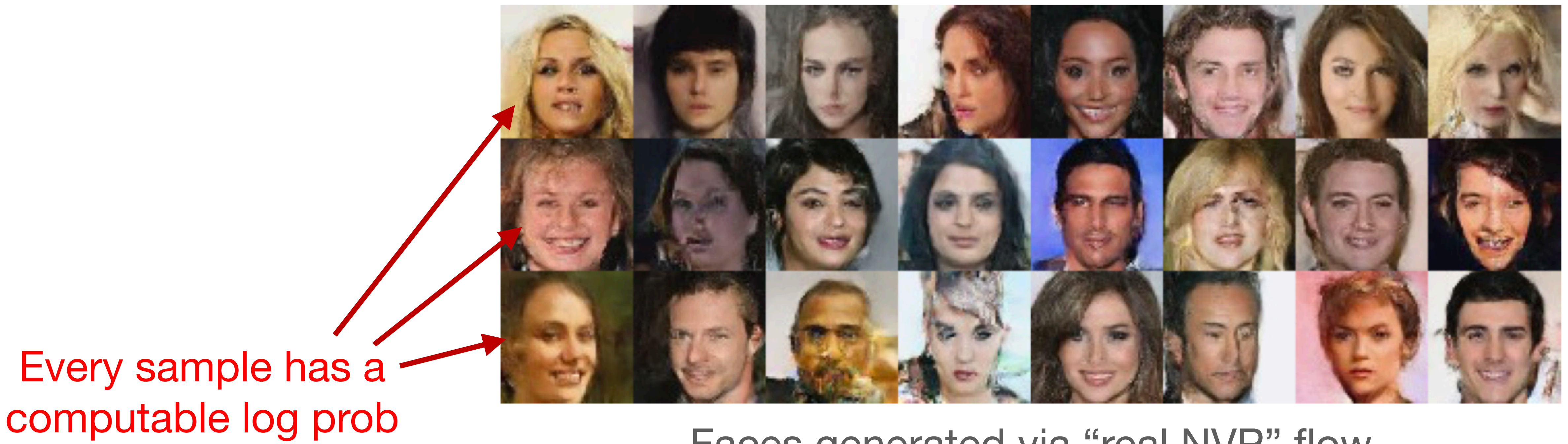
Lattice sampling vs. Image generation

[Karras, Lane, Aila / NVIDIA **1812.04948**]





Faces generated via "real NVP" flow
[Dinh, Sohl-Dickstein, Bengio **1605.08803**]

A story of symmetries & generative models

(In three parts)

1. Flow-based generative models

2. Gauge symmetry & translational symmetry

3. Fermions & translational symmetry

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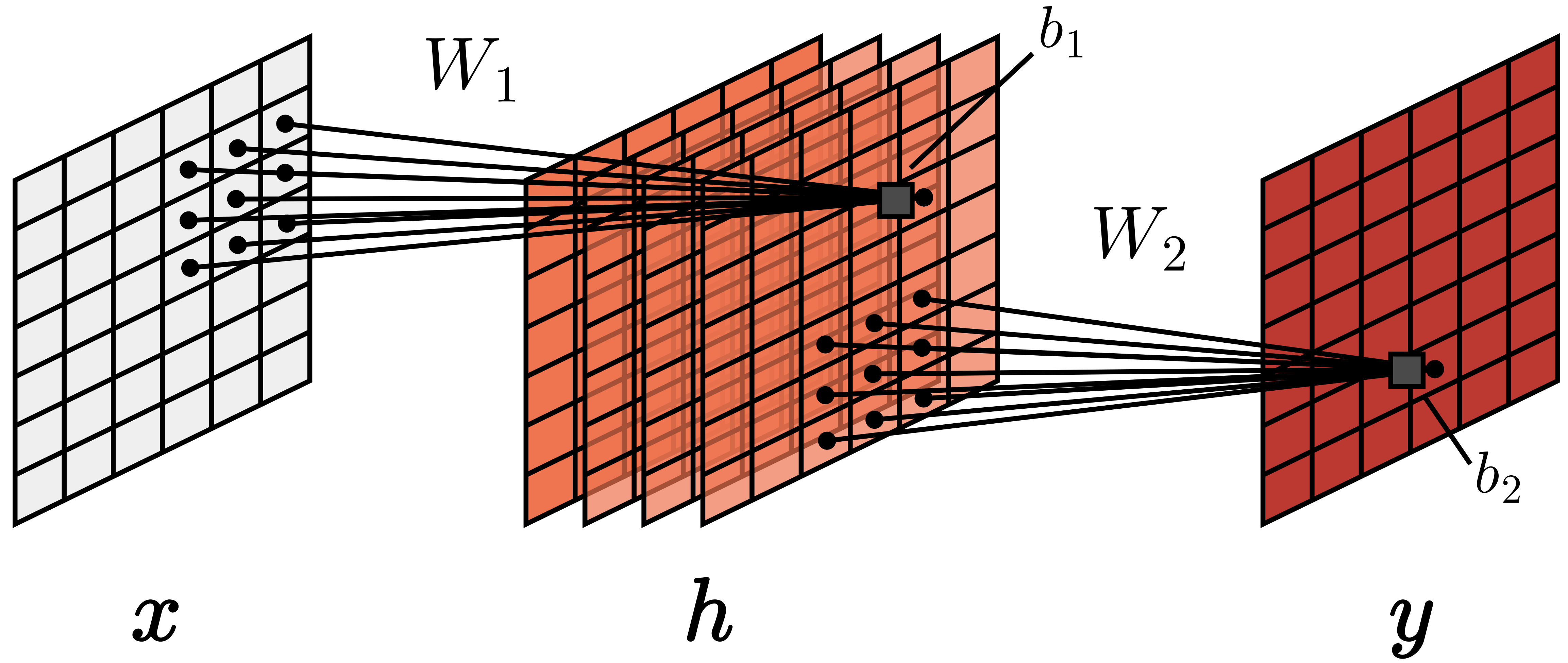
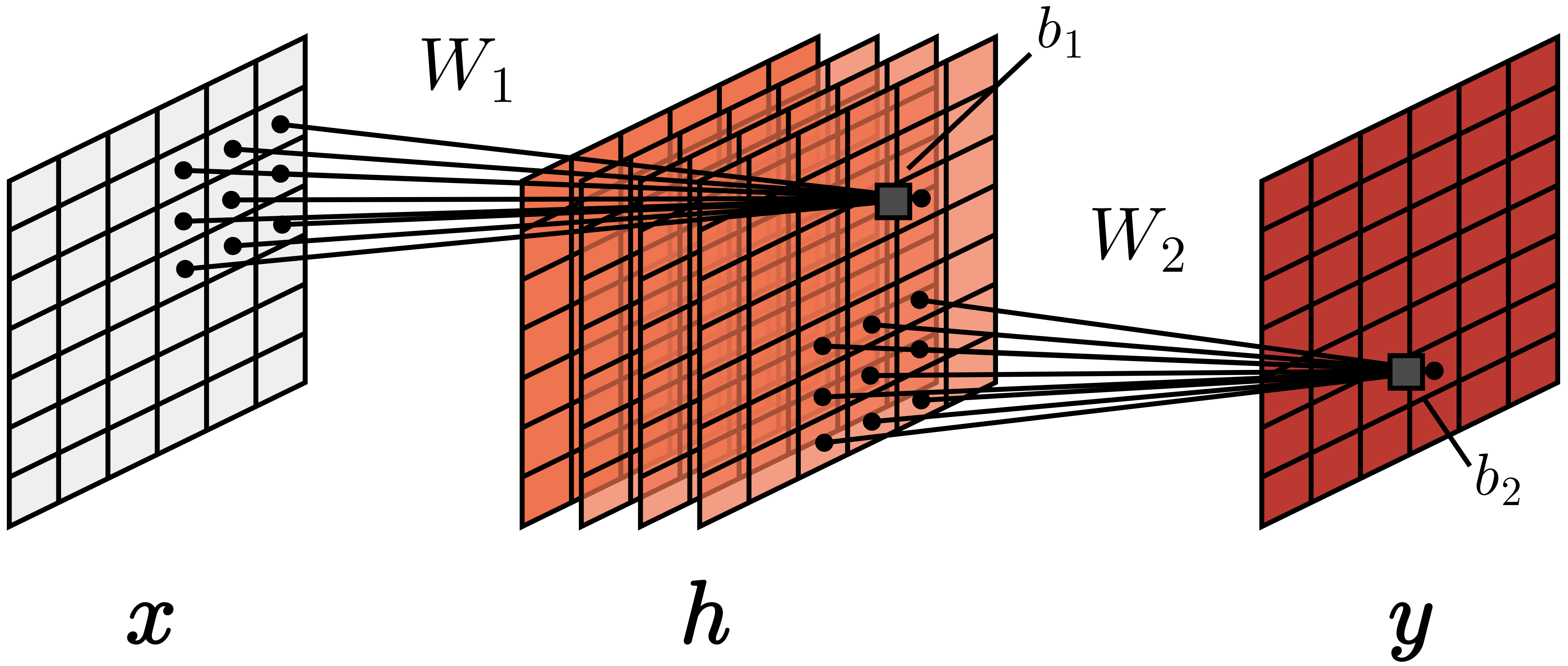
Flow-based sampling: Overview



Flow-based sampling: Overview

(Convolutional) neural networks: Black-box (local) function approximators



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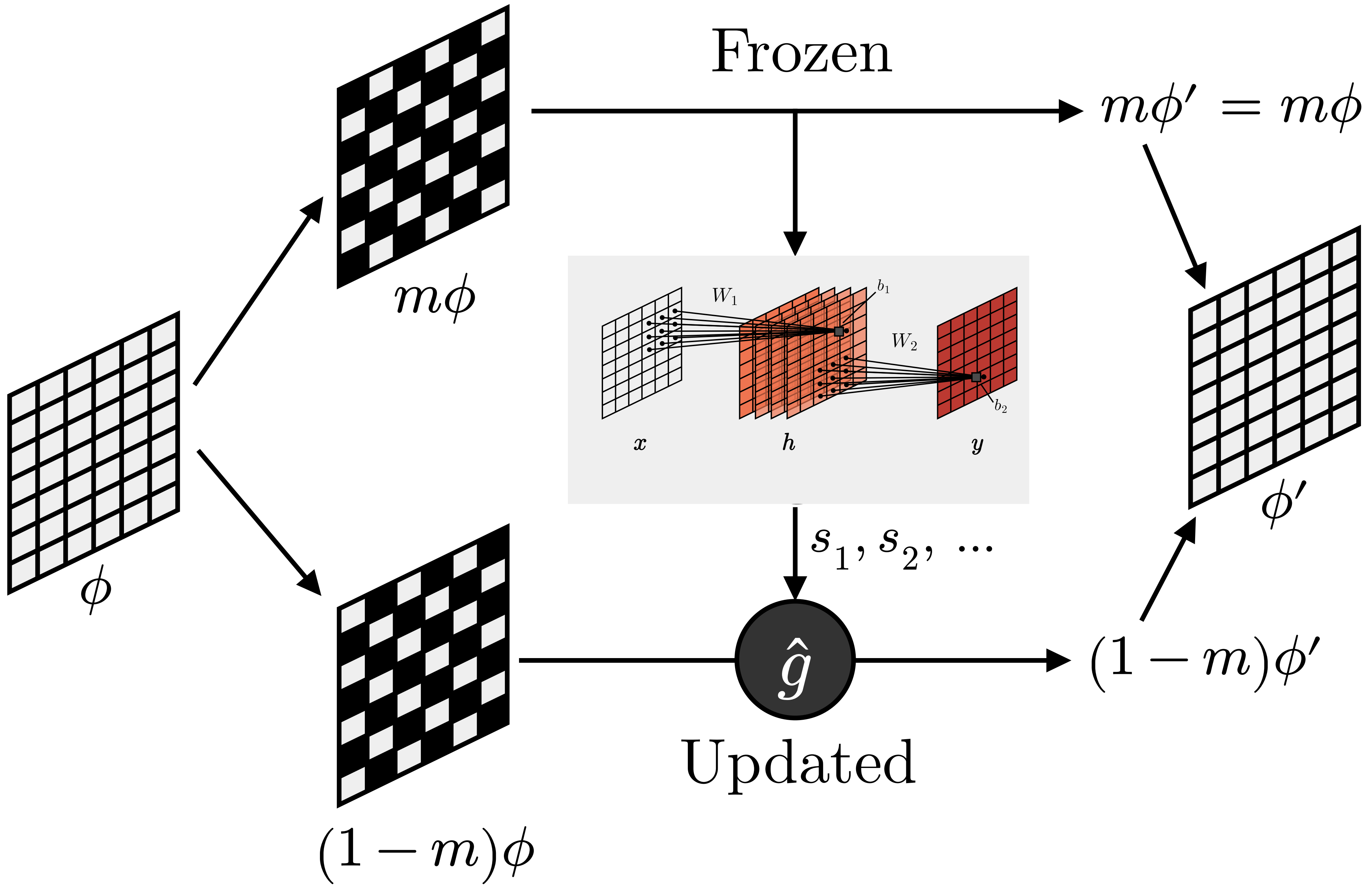
Coupling layers: Invertible transformations, tractable Jacobian



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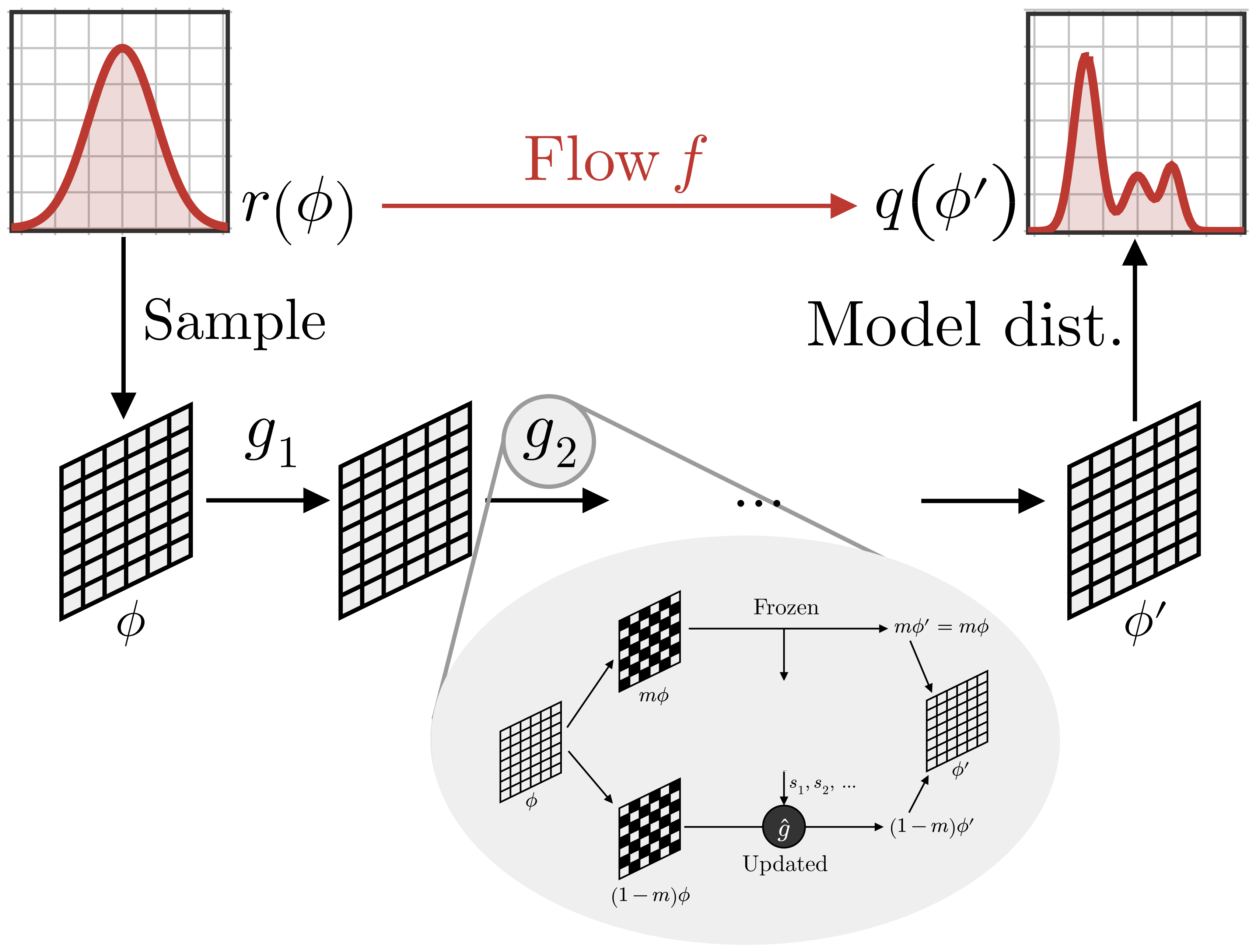
Flow model: Prior density + flow = **sampleable + computable** output density



$$q(\phi') = r(\phi) \left| \det_{ij} \frac{\partial [f(\phi)]_i}{\partial \phi_j} \right|^{-1}$$

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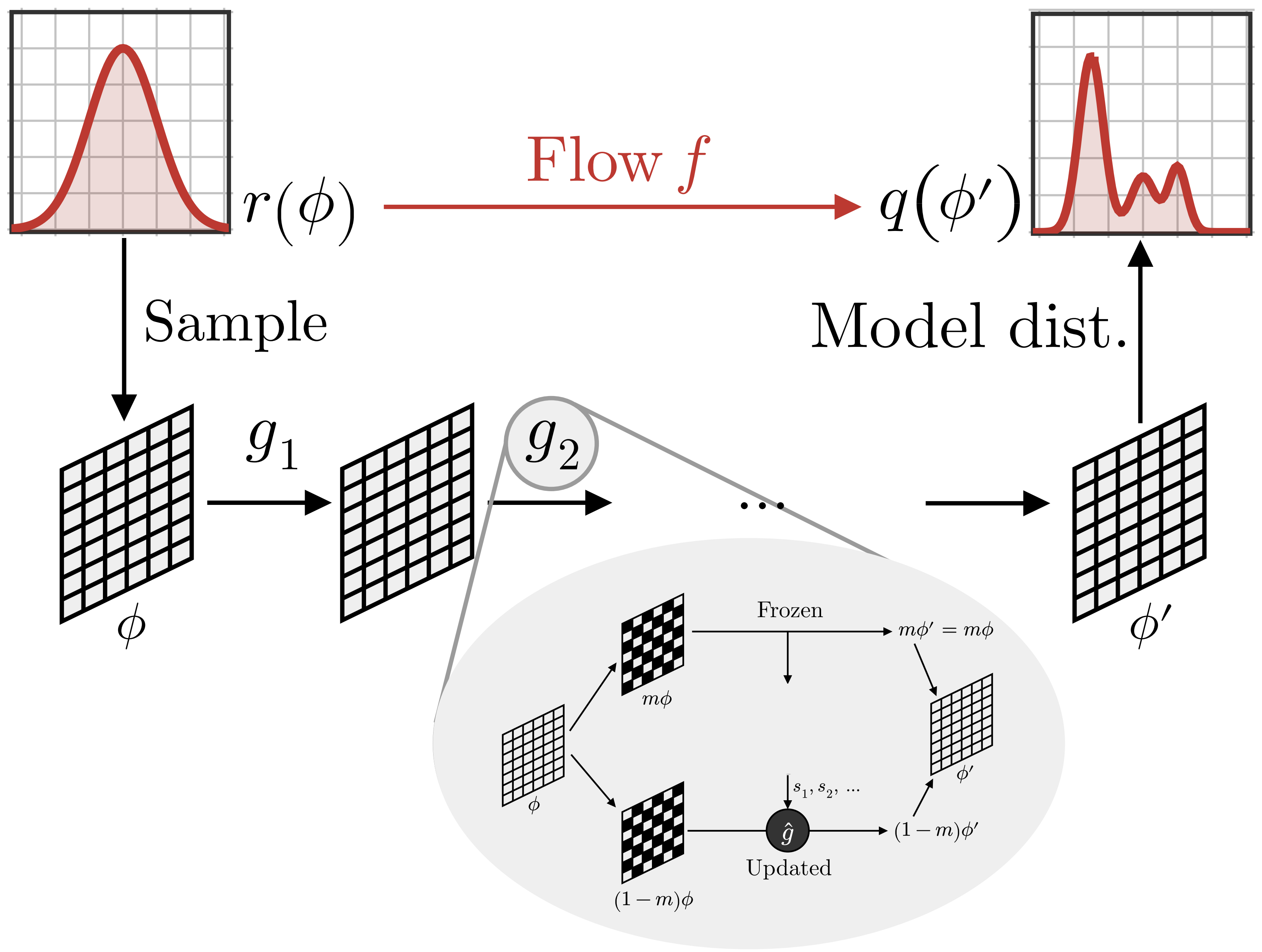
- Measure KL divergence
- Apply gradient-based opt



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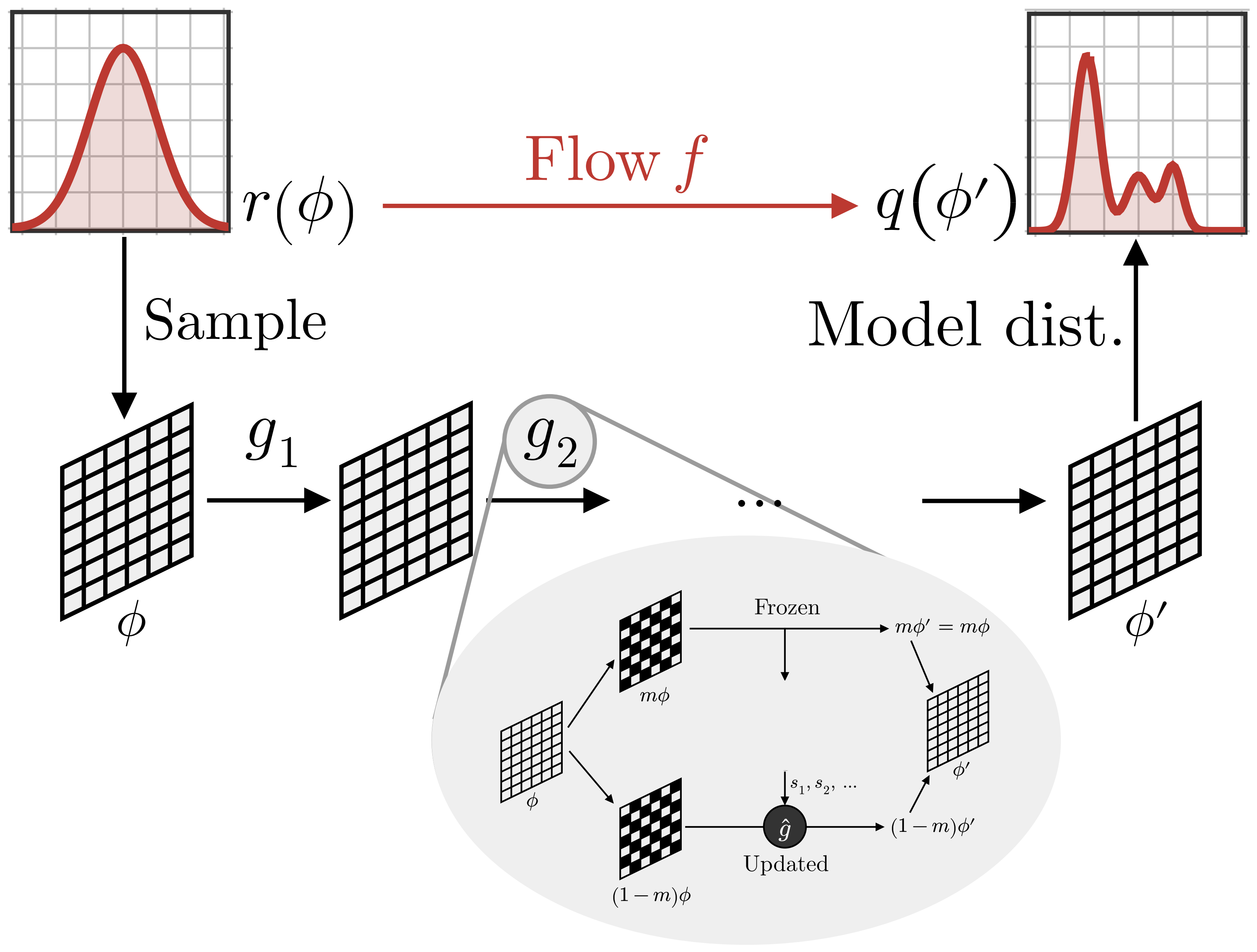
Exactness:

- Use $q(\phi')$ and $p(\phi')$to correct approximation



$$q(\phi') = r(\phi) \left| \det_{ij} \frac{\partial [f(\phi)]_i}{\partial \phi_j} \right|^{-1}$$

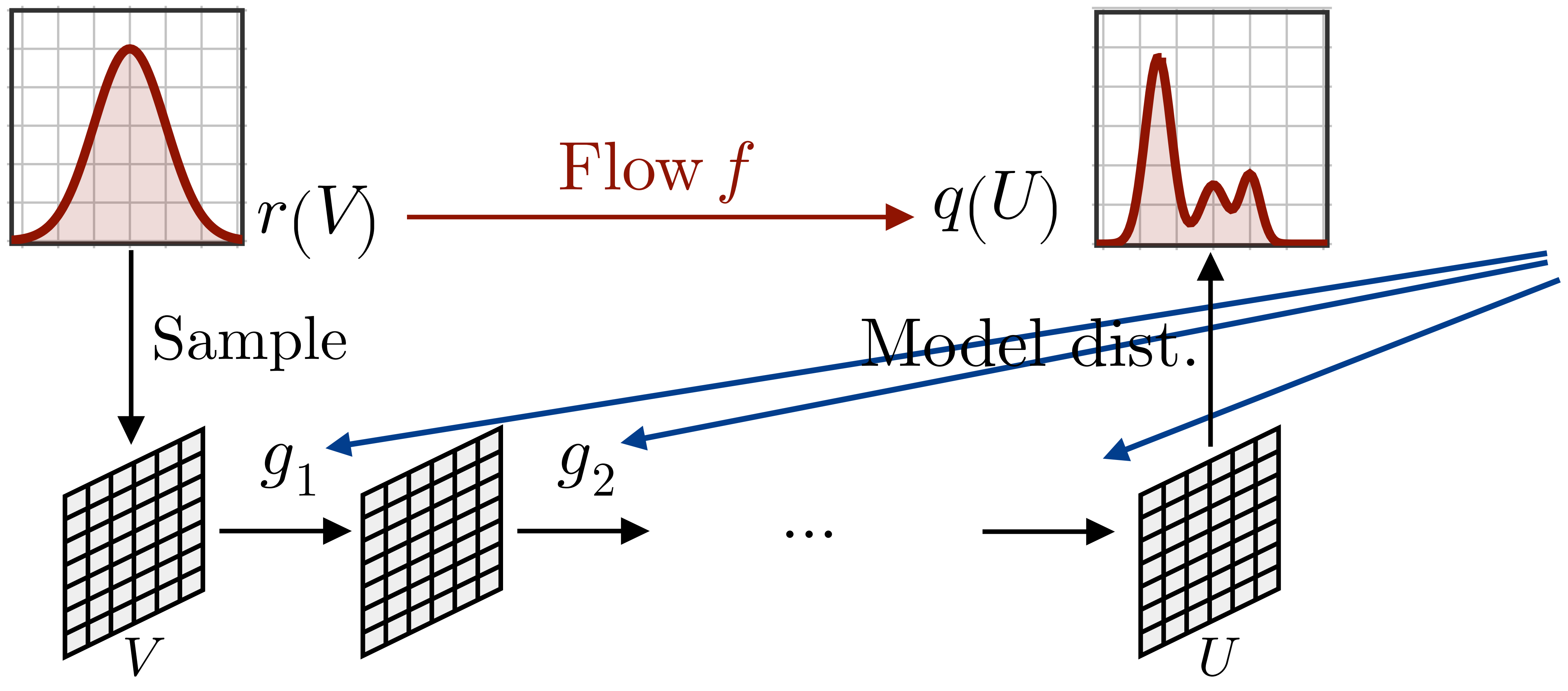
$$q(U) = r(V)\left|\det_{ij}\frac{\partial[f(V)]_i}{\partial V_j}\right|^{-1}$$

Defining the flow function

The "flow" f must be **invertible** and have **tractable Jacobian determinant**

- For LQFT, don't know what f needs to be *a priori*
- Construct expressive parameterized ansatz and optimize it

Key to expressivity — **Use composition.**



Each layer is **invertible**, has **tractable Jac.**

Simple individual layers combine to give complex transformations.

Coupling layers

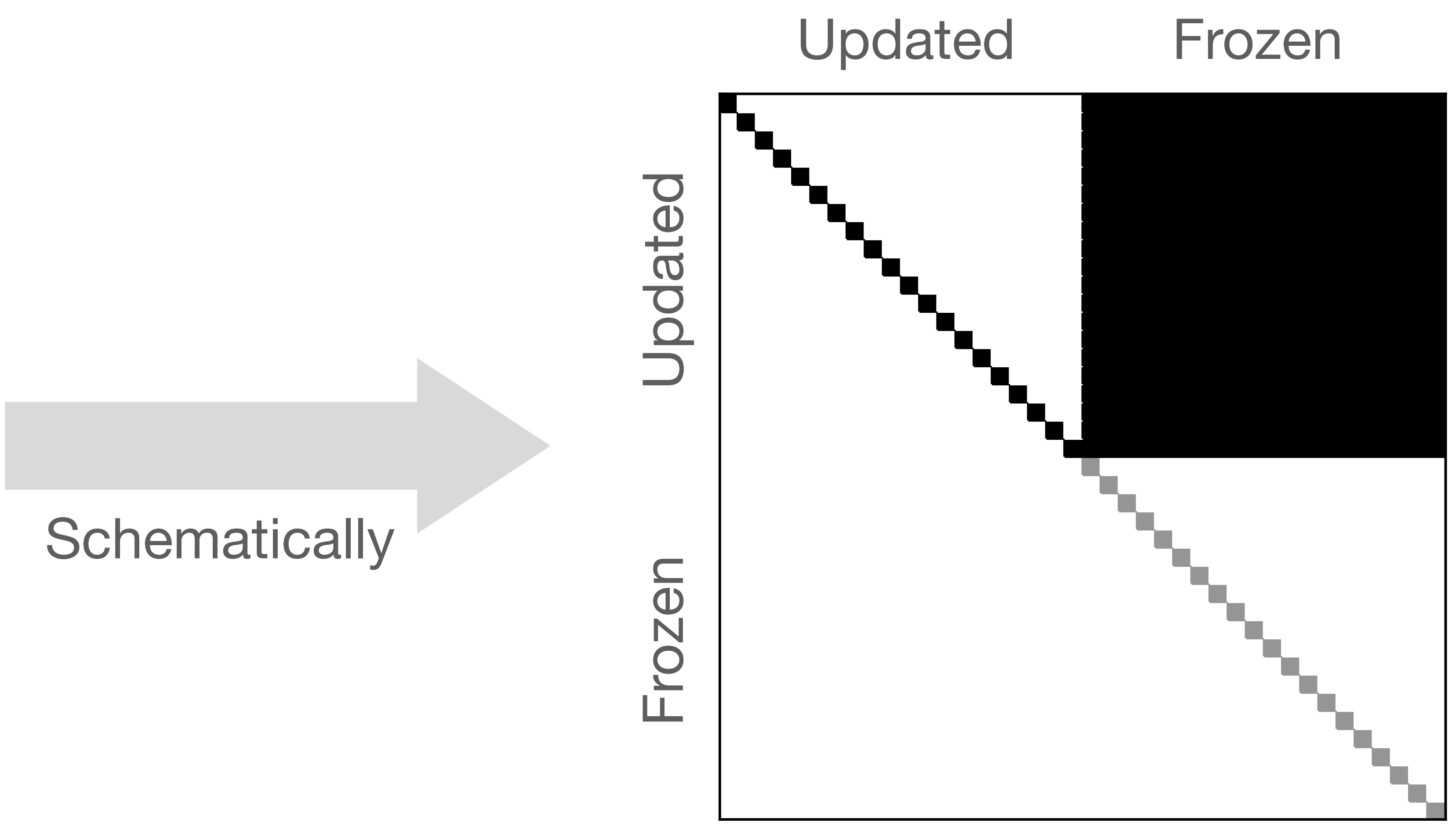
Similar to leapfrog integrator

Idea: Construct each g to act on a **subset** of components, conditioned only on the complimentary subset. “Masking pattern” m defines subsets.

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

“Updated” i ($m_i = 0$) “Frozen” i ($m_i = 1$)

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



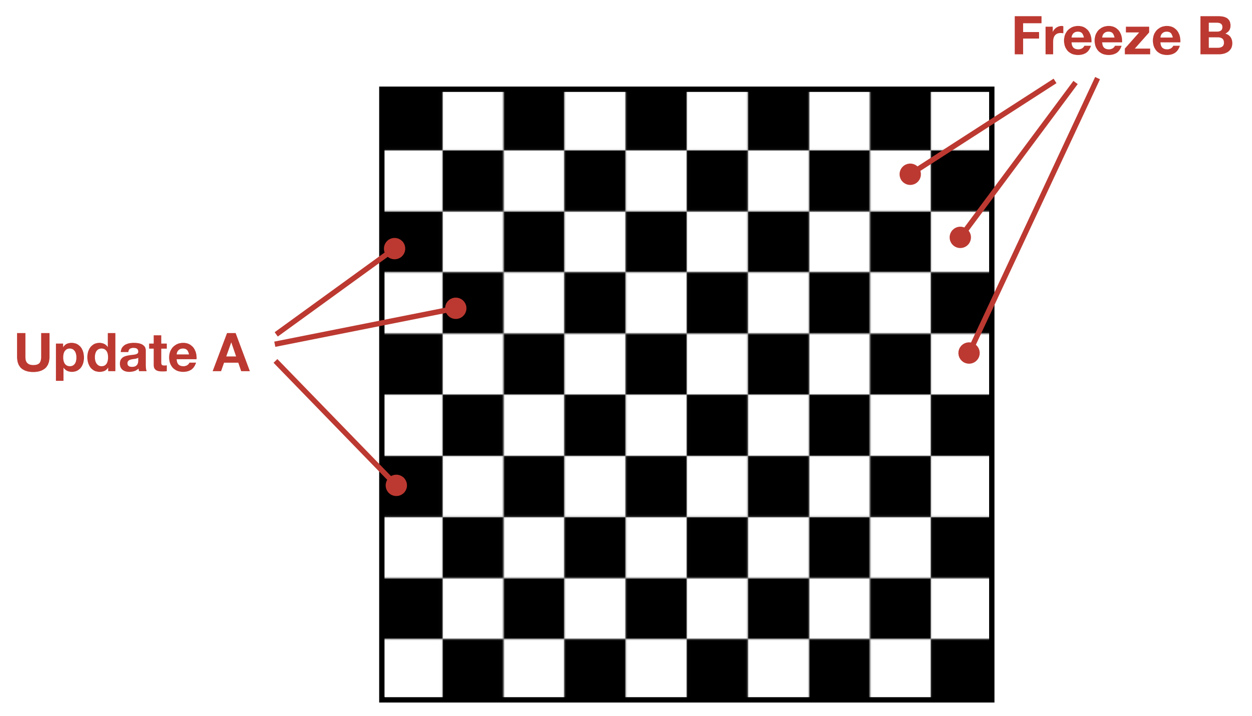
→ Invertible if each diag component invertible, $\partial[g(V)]_i/\partial V_i \neq 0$.

Example: RNVP for scalar fields

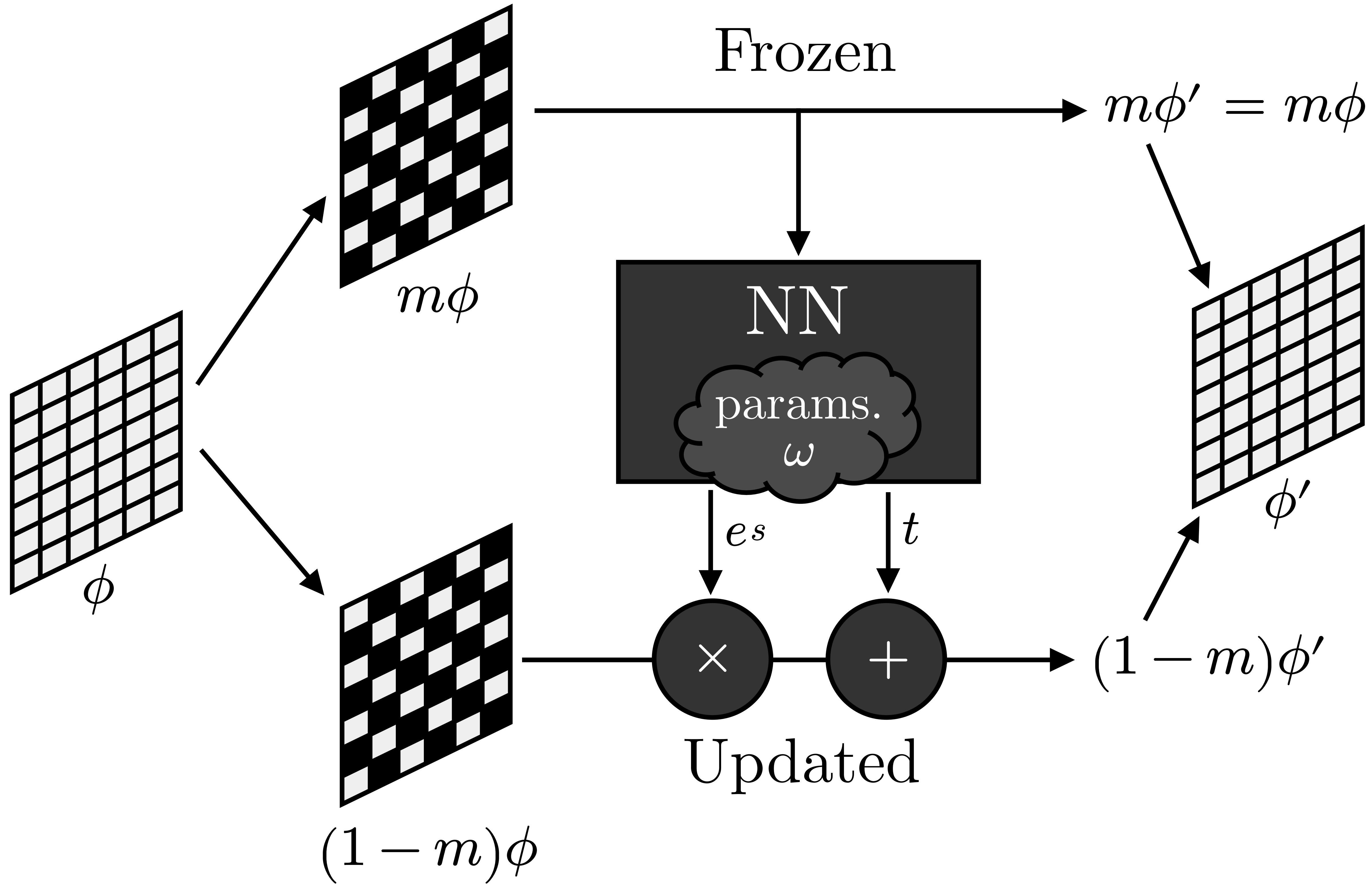
Scalar field $\phi(x) \in \mathbb{R}$ $\approx$ grayscale image

Real NVP coupling layer:

[Dinh, Sohl-Dickstein, Bengio **1605.08803**]



Checkerboard masking pattern m



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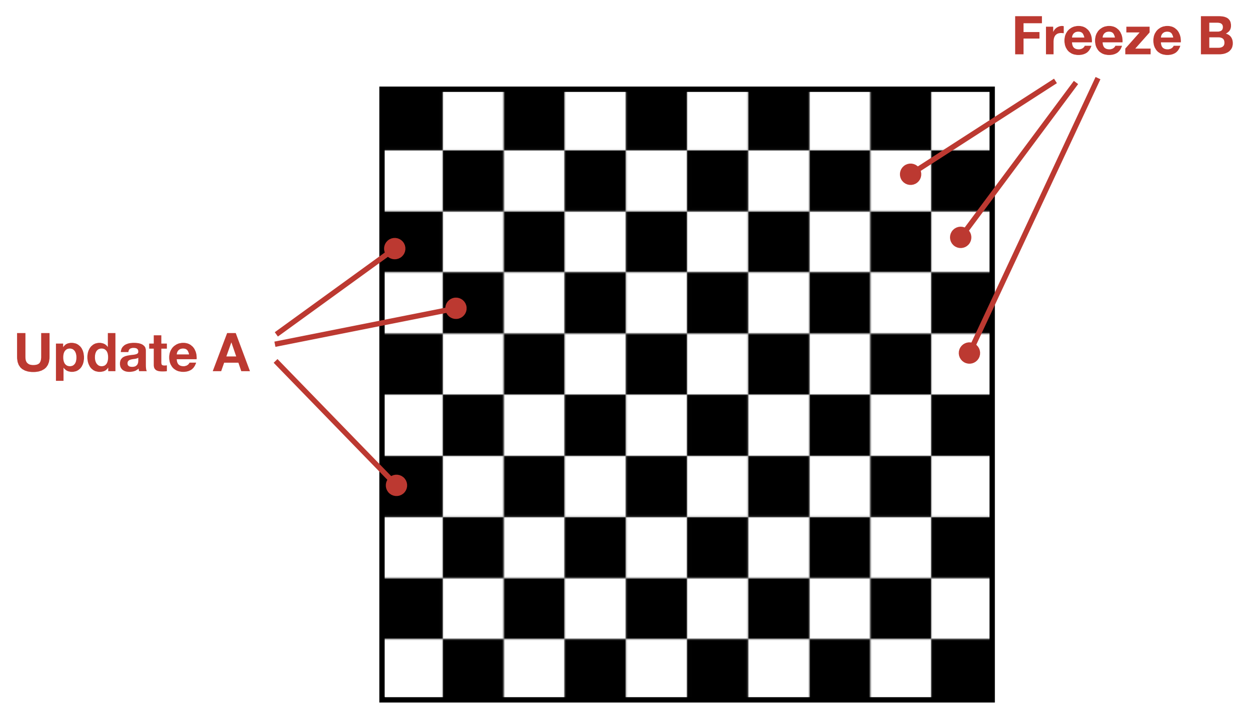

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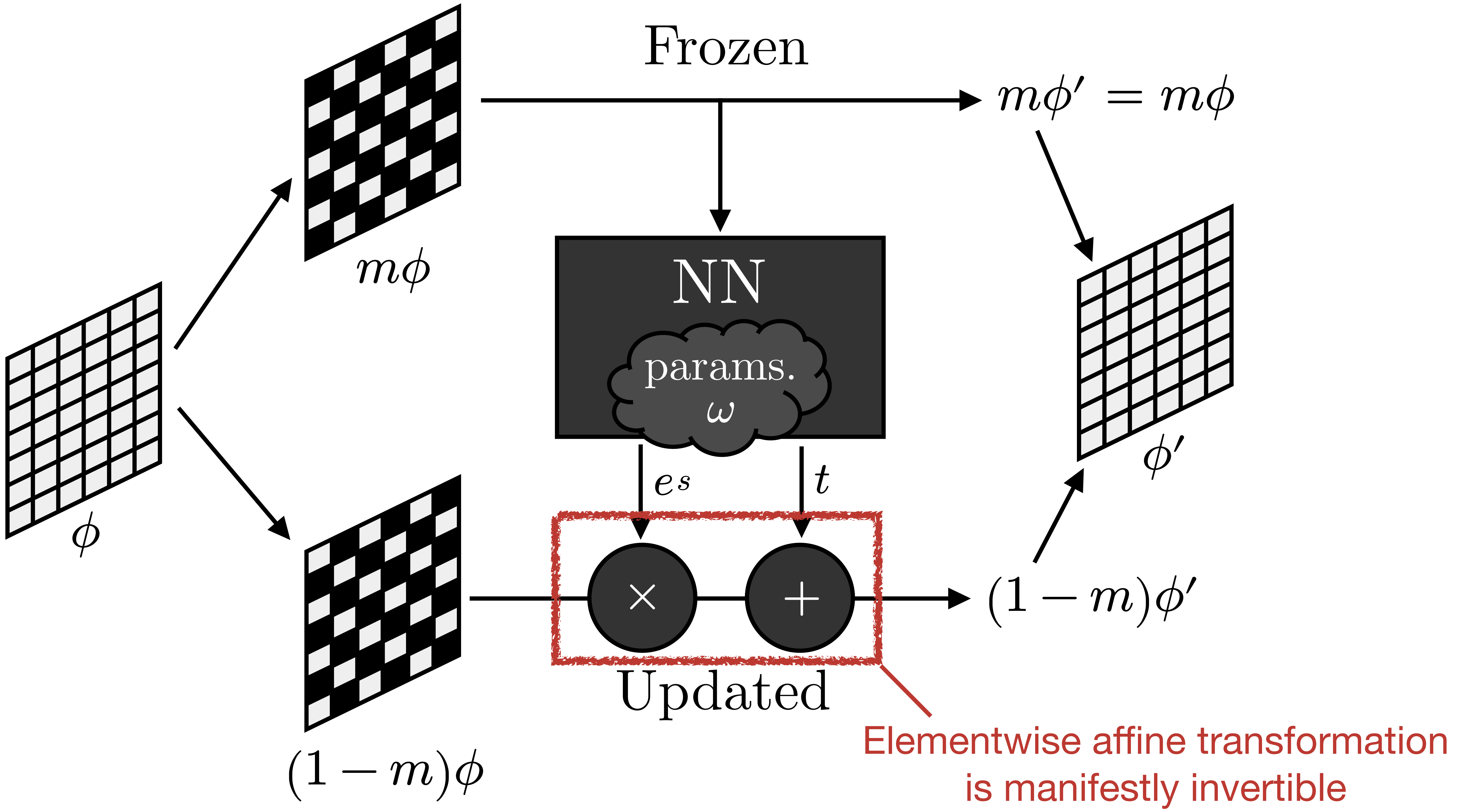

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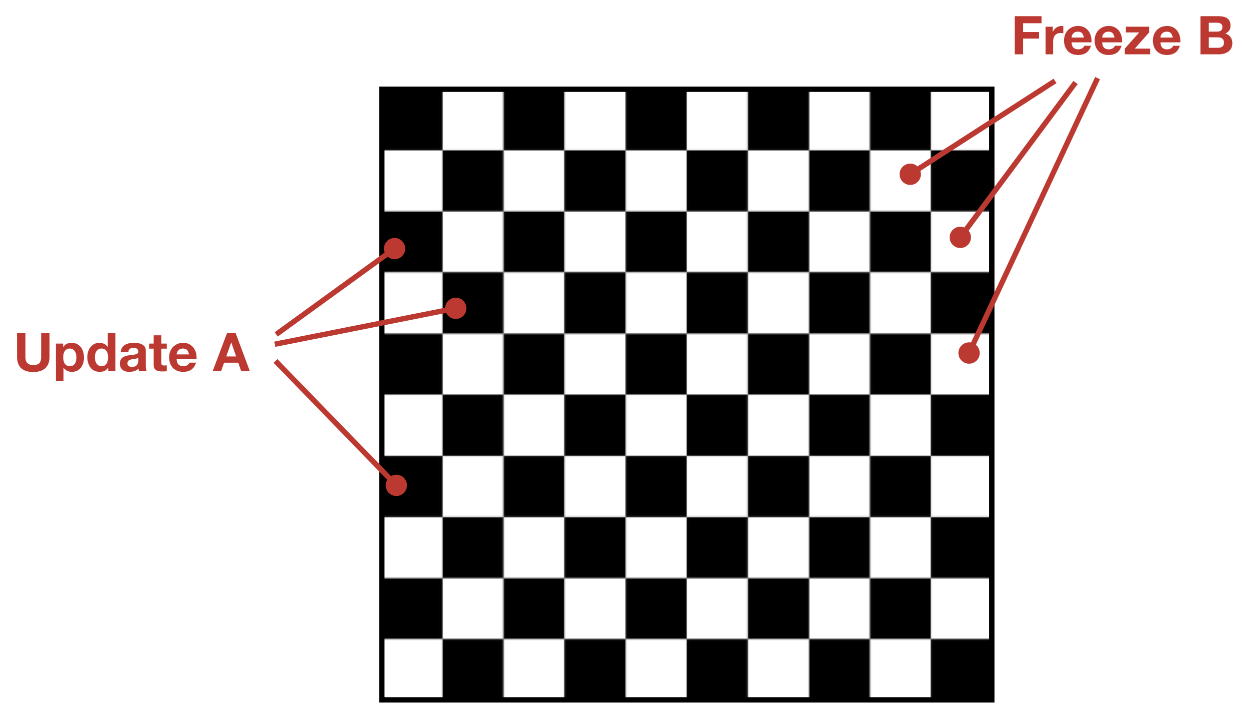

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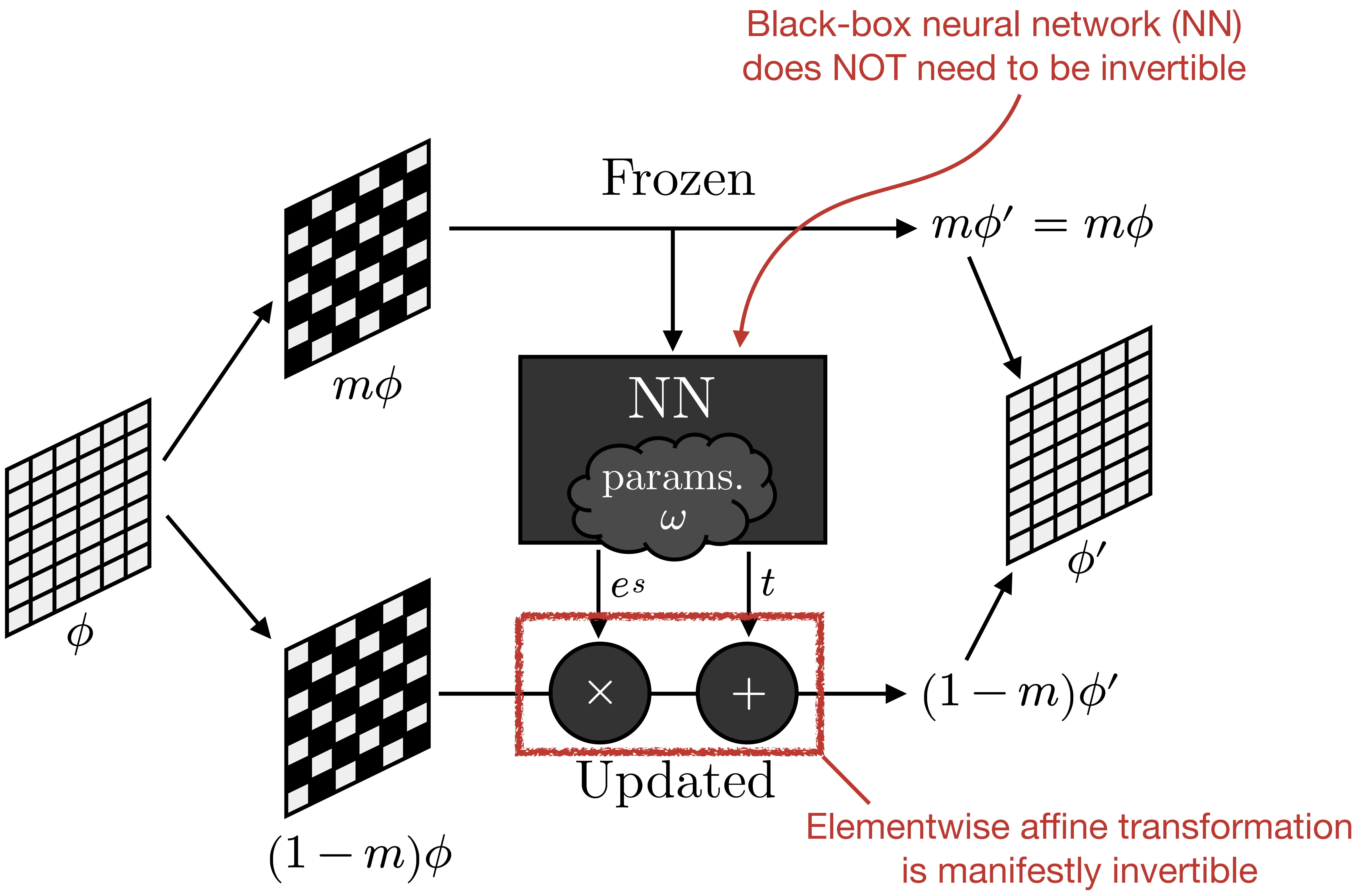


Symmetries in flows

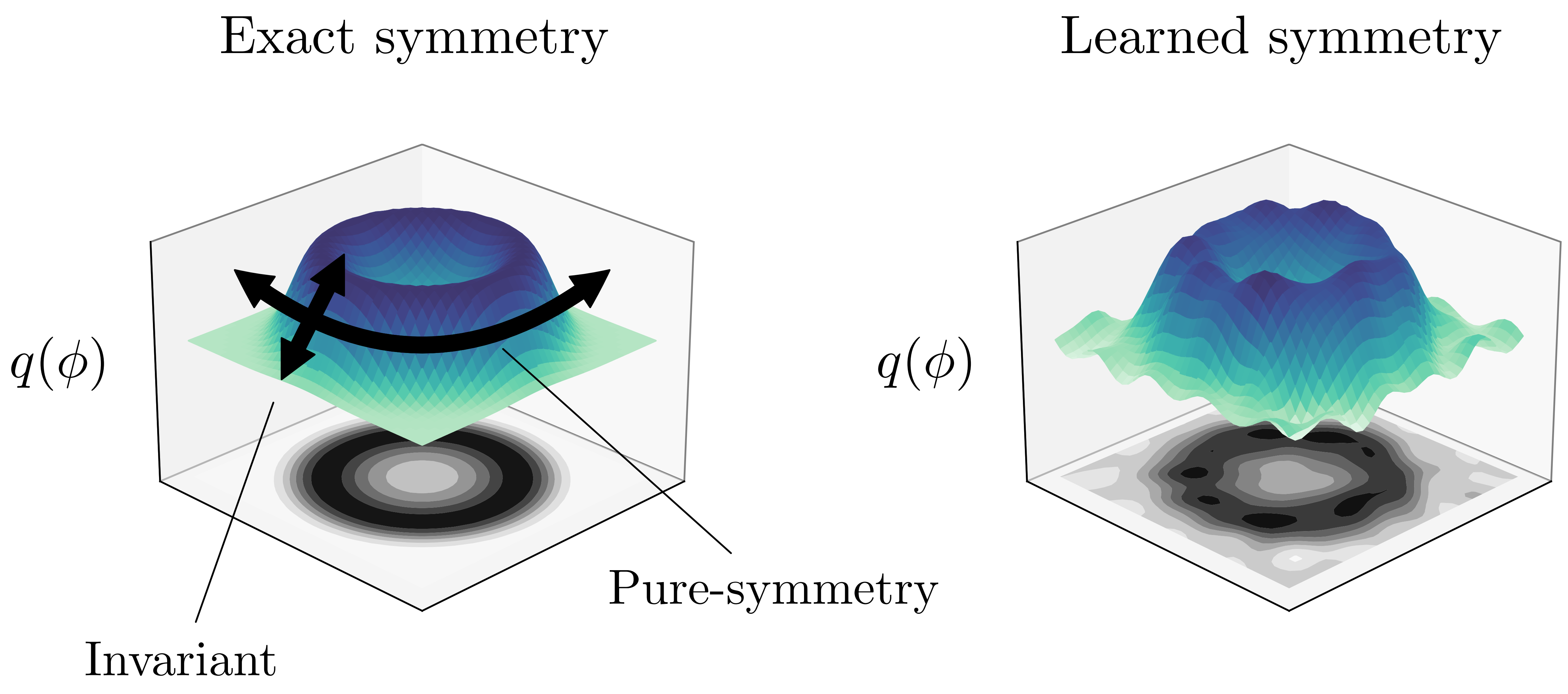
Motivation: Target $p(\phi)$ is often invariant under symmetries. Make $q(\phi)$ automatically invariant too?

Invariant prior + **equivariant** flow = symmetric model [Cohen, Welling 1602.07576]

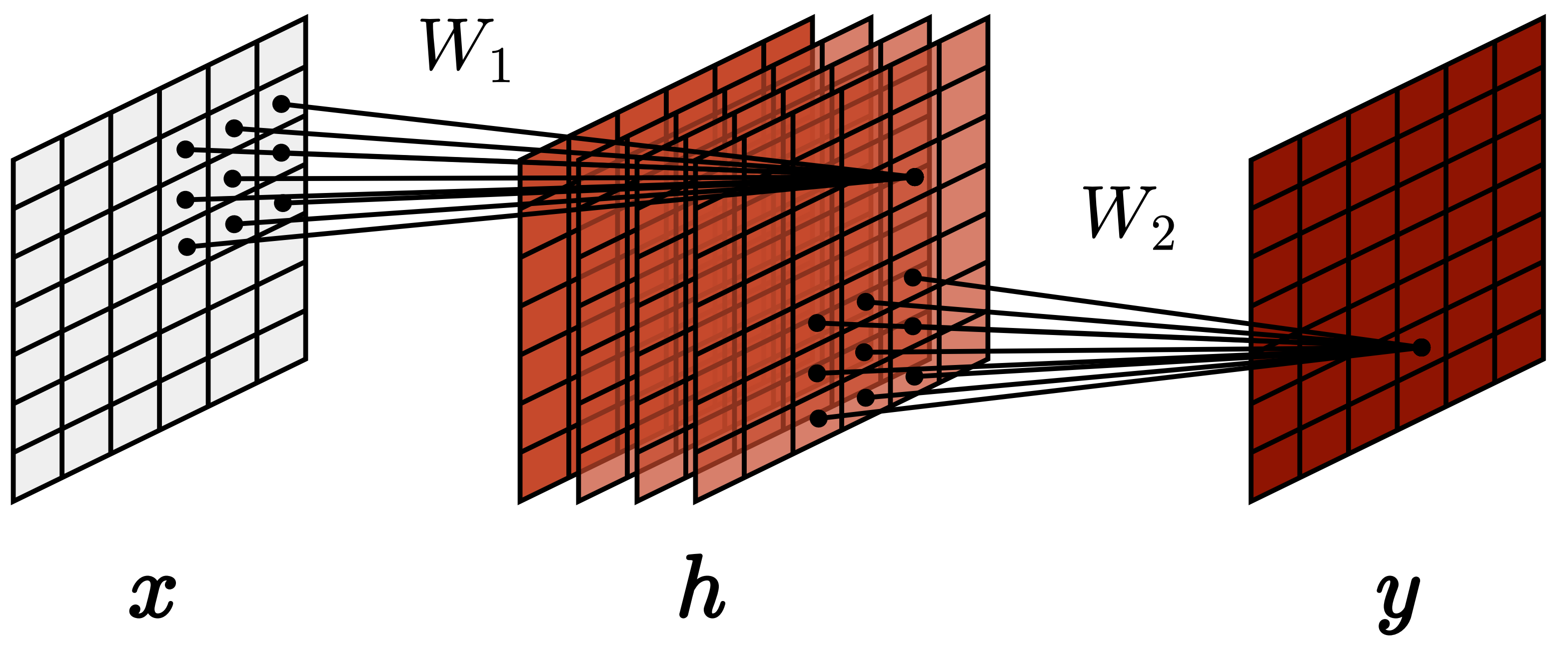
$r(t \cdot U) = r(U)$ $f(t \cdot U) = t \cdot f(U)$

Symmetries…

- ✓ Reduce data complexity of training
- ✓ Reduce model parameter count
- ✓ May make "loss landscape" easier



Translational equivariance



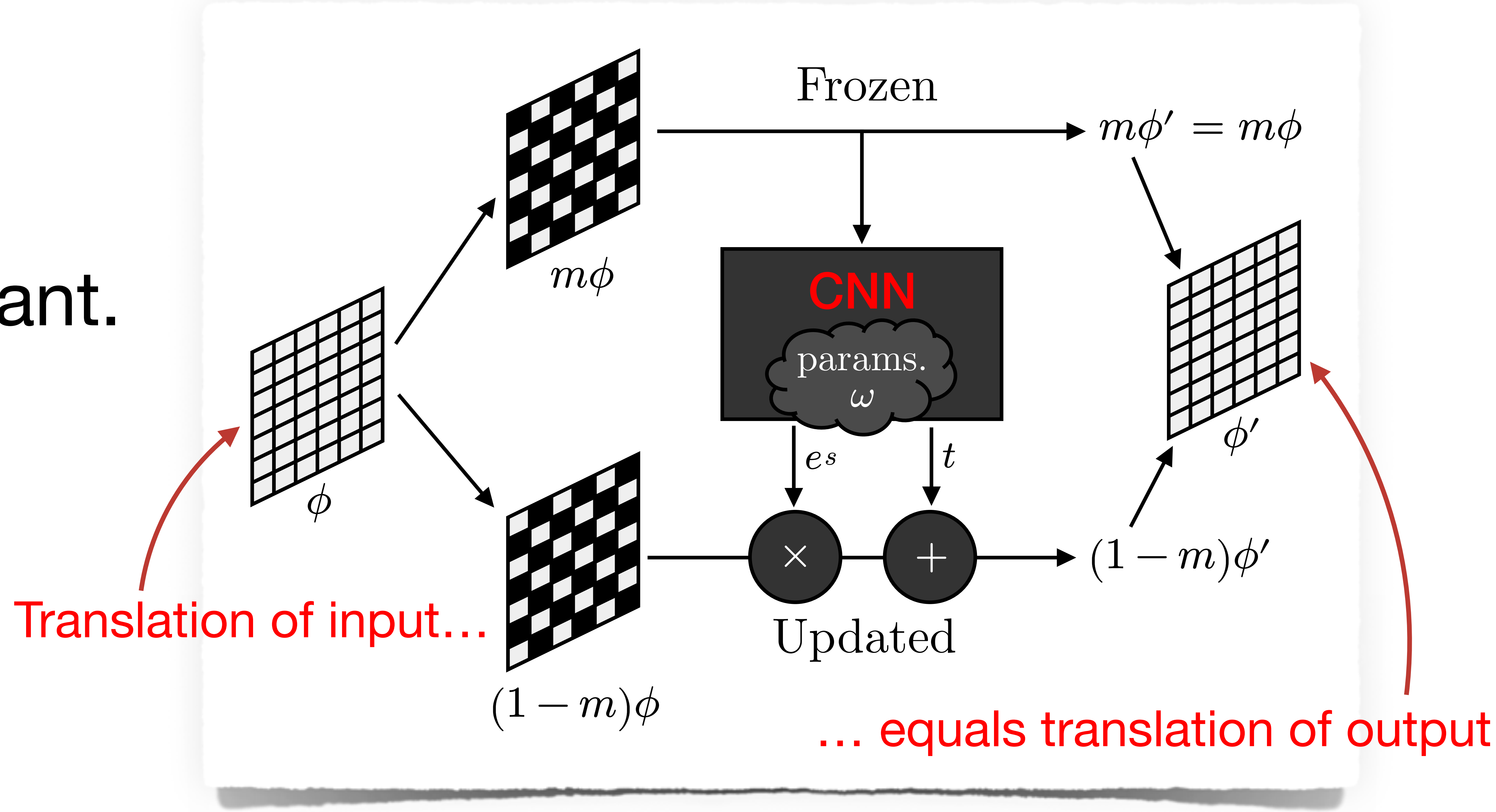
1. Use **Convolutional Neural Nets (CNNs).**

- Output values (e.g. $e^{s(x)}$ and $t(x)$) for each site are local functions of frozen DoFs

- CNNs are equivariant under translations

2. Make masking pattern (mostly) invariant.

- E.g. checkerboard



See also Self-Learning Monte Carlo (SLMC) methods:
[Huang, Wang **PRB95 (2017) 035105**;
Liu, et al. **PRB95 (2017) 041101**;
… and many more …]

Optimizing the model

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

Self-training:

1. Loss function = modified **Kullback-Leibler (KL)** divergence

$$D_{KL}(q\,||\,p) := \int \mathcal{D}U\, q(U)\left[\log q(U) - \log p(U)\right] \geq 0$$

Constant shift removes unknown normalization

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

(Using $p(U) = e^{-S(U)}/Z$)

2. Stochastic estimate: draw samples U_i **from the model**, then measure

$$\frac{1}{M}\sum_{i=1}^{M}\left[\log q(U_i) + S(U_i)\right]$$

Exactness

Samples from **model** are from biased distribution $q(\phi) \neq p(\phi)$, but…

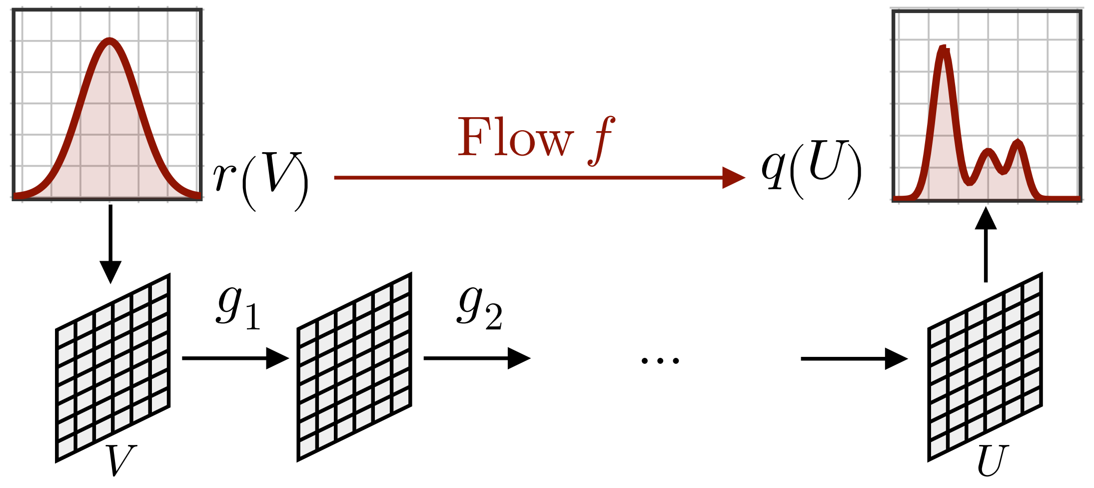
For each ϕ_i drawn from the model, we know $q(\phi_i)$ and $p(\phi_i)$

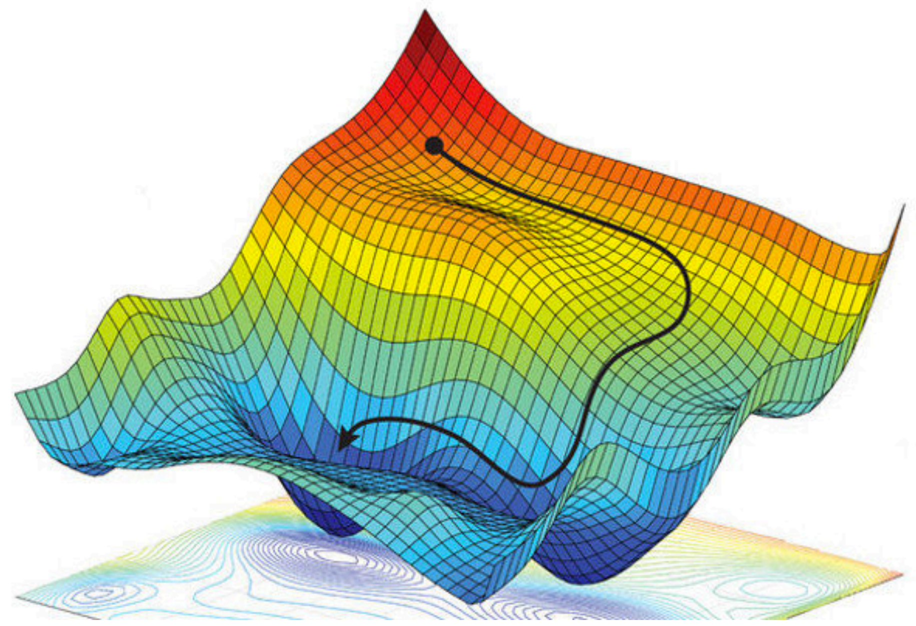
→

Exact bias correction possible
(e.g. "flow-based MCMC" or reweighting)

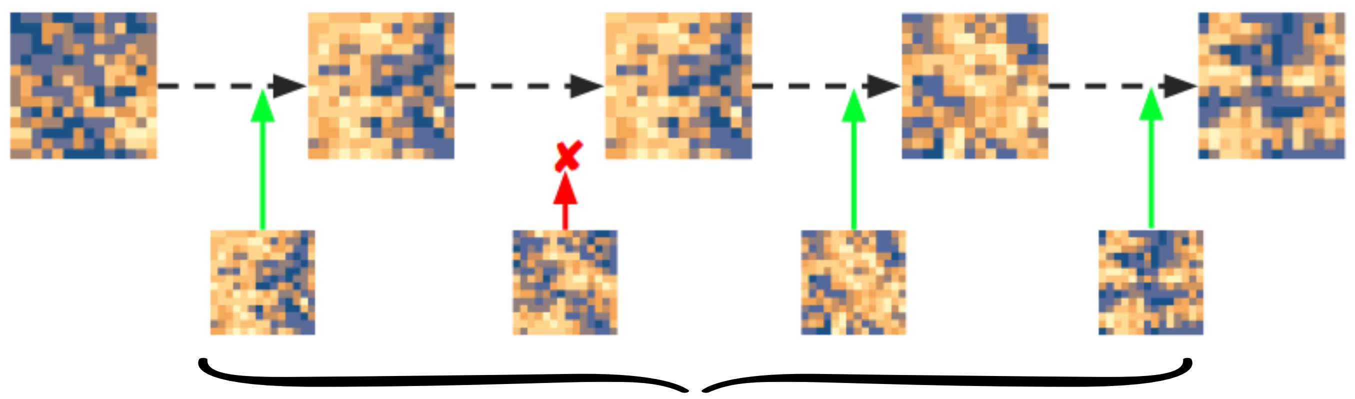
Note: Efficiency of bias correction depends on how close q and p are.

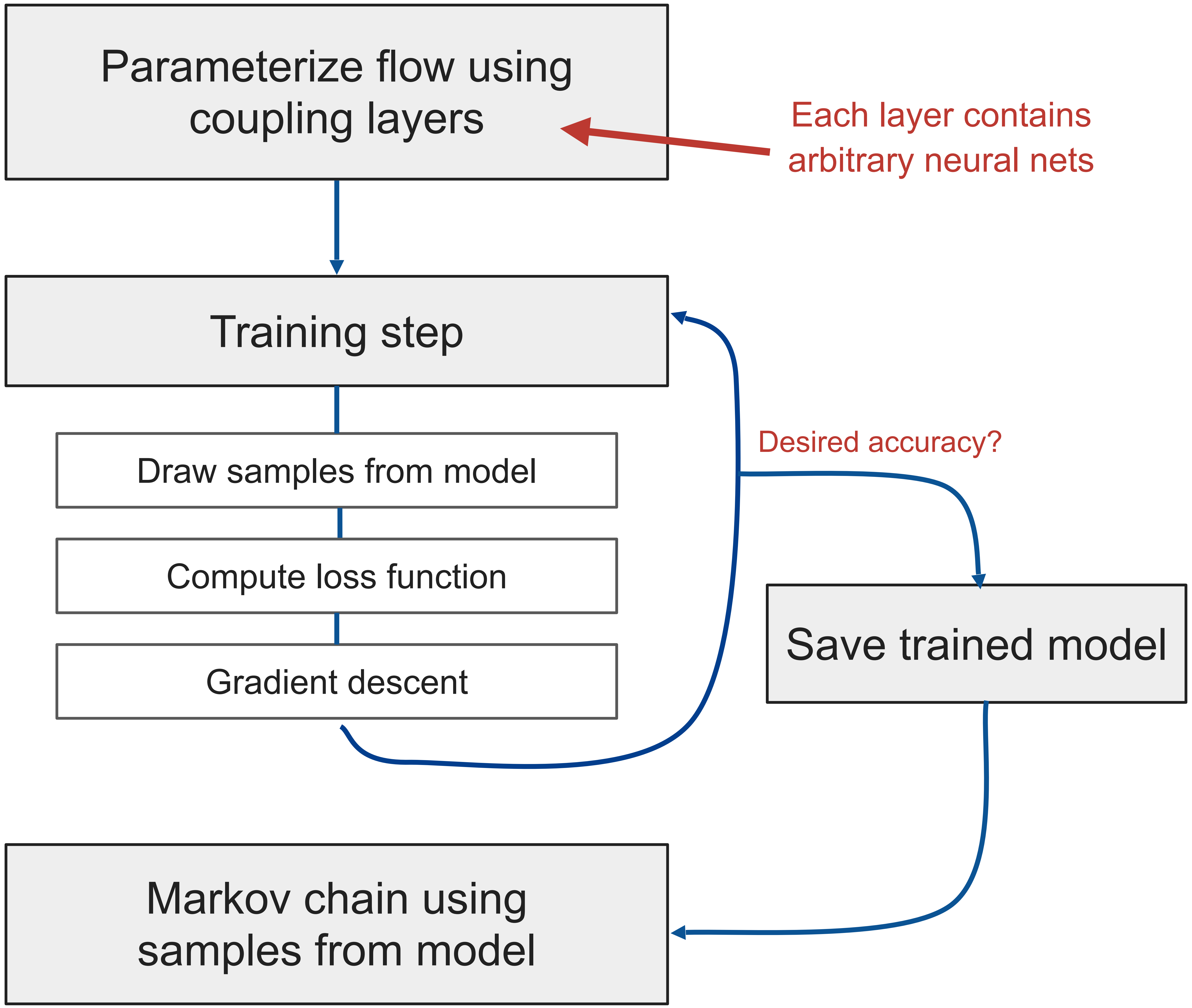
Birds-eye view





[Image credit: 1805.04829]





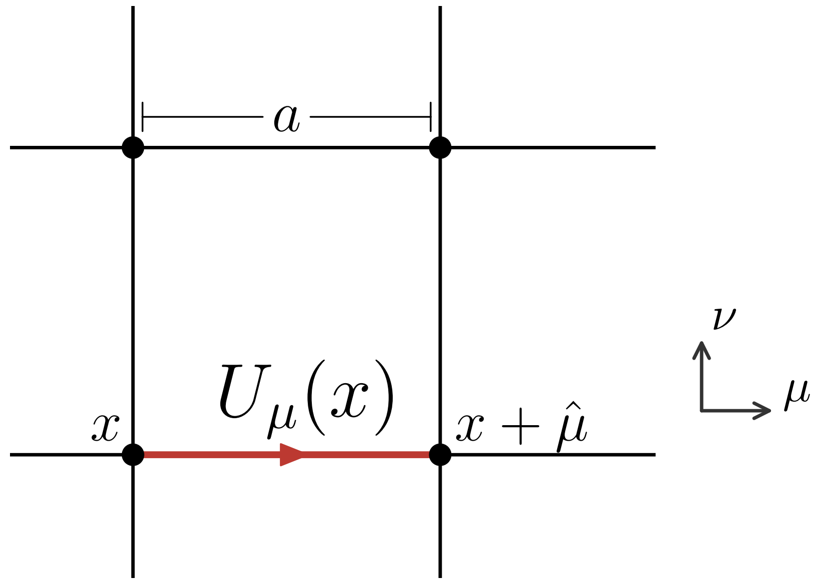
A story of symmetries & generative models

(In three parts)

1. Flow-based generative models
2. **Gauge symmetry & translational symmetry**
3. Fermions & translational symmetry

Lattice gauge theory & Symmetries

Gauge field **discretized** in terms of parallel transporters (links) $U_\mu(x)$.

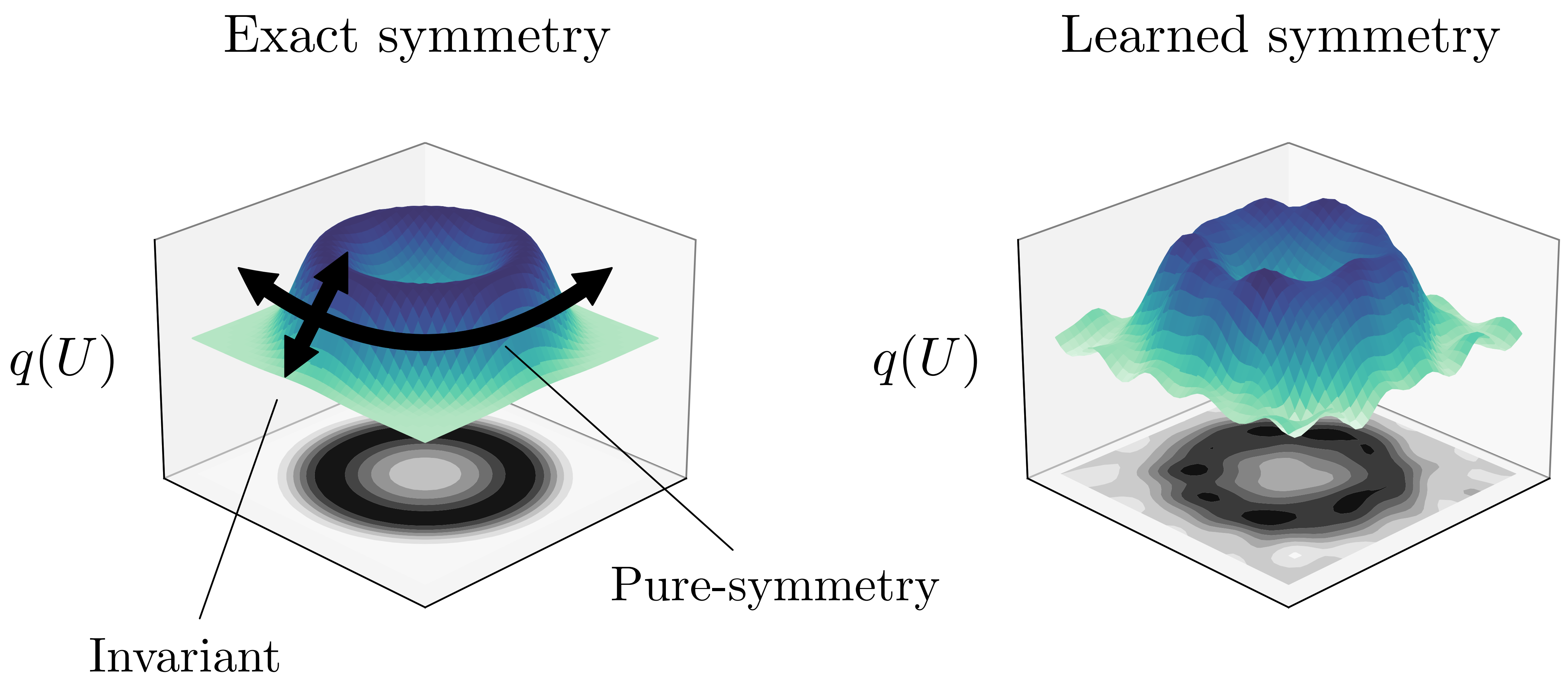


Lattice gauge theory actions (typically) **satisfy symmetries**:

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

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

Symmetries **factor** distribution into uniform component along symmetry direction, and non-uniform component along invariant direction. Schematically:



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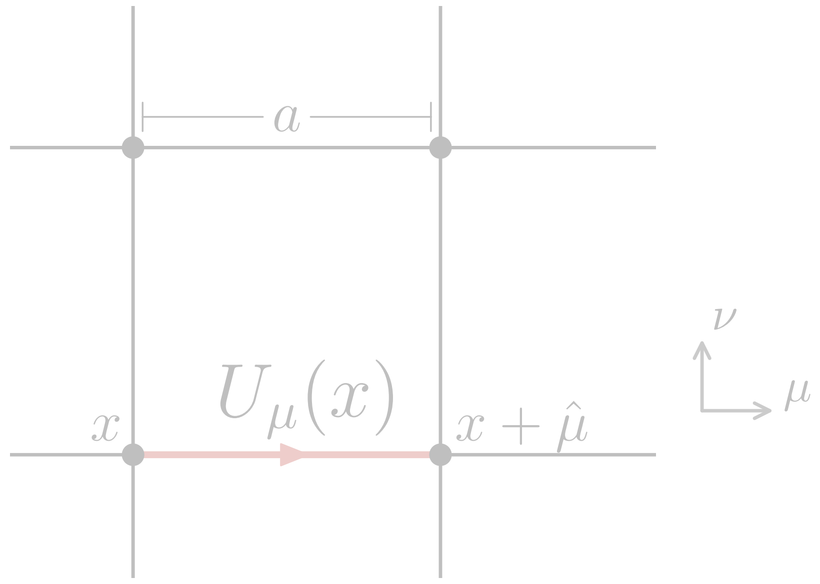

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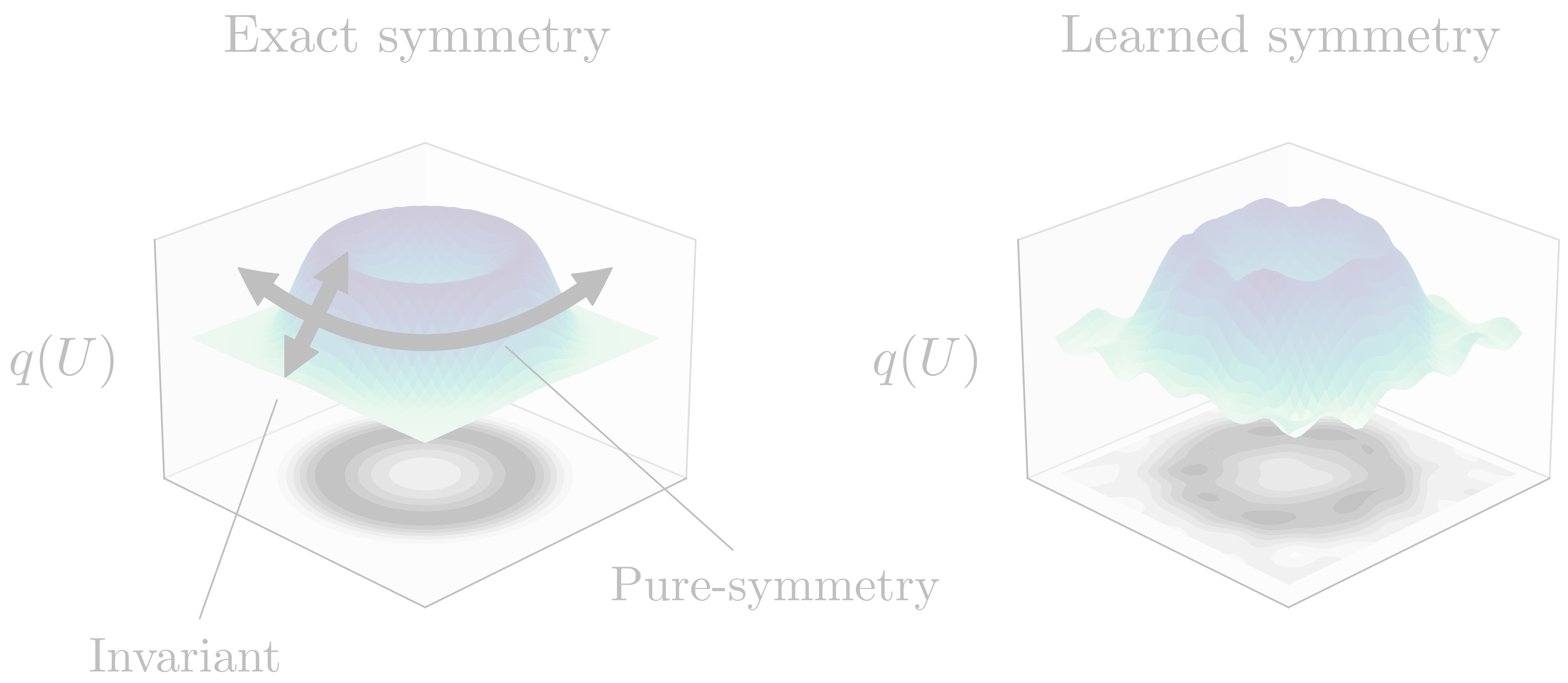

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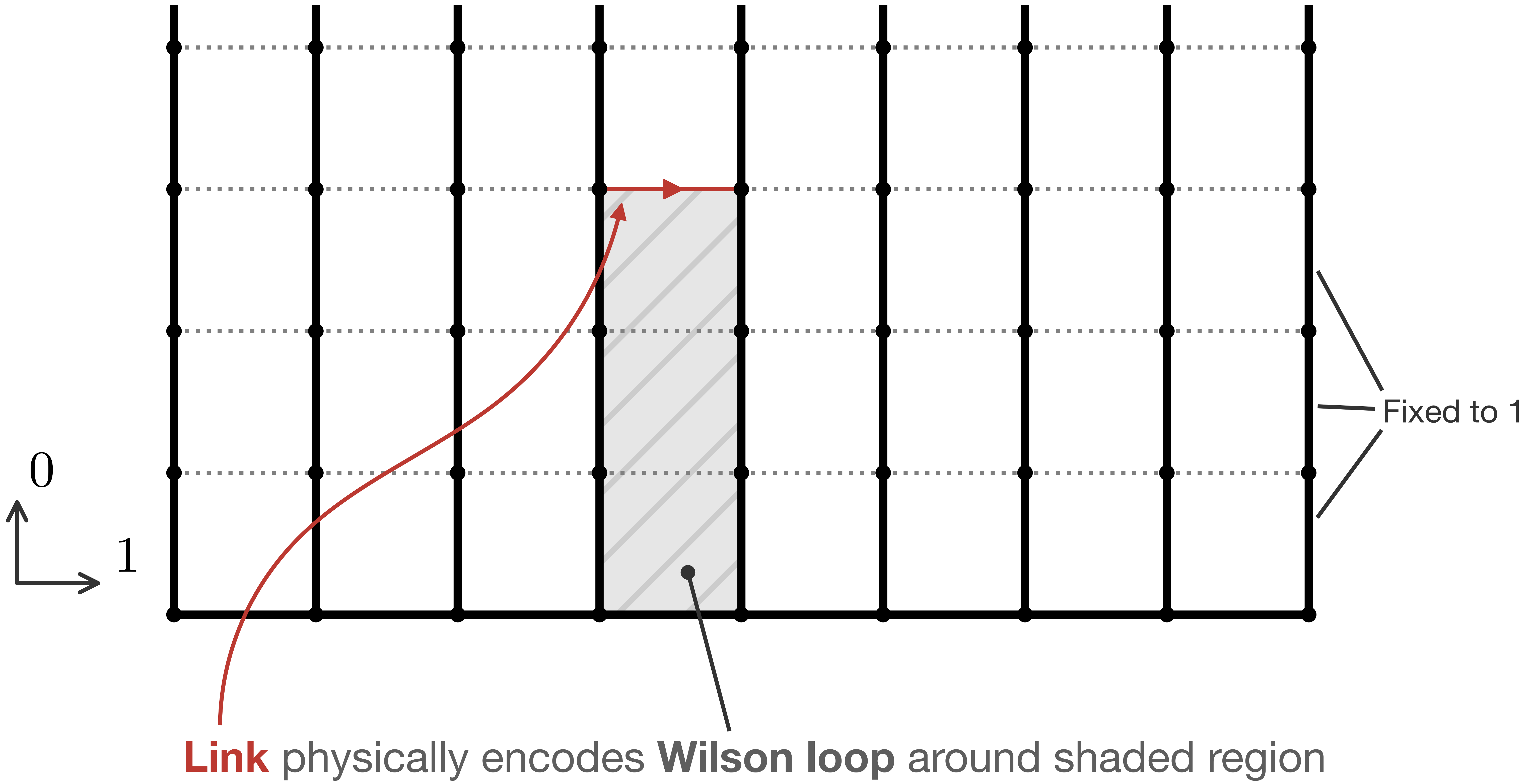
Gauge symmetry via gauge fixing?

Where gauge DoFs are explicitly factored out, e.g. maximal tree

Explicit gauge fixing is at odds with **translational symmetry** + **locality**



Gauge symmetry via gauge fixing?

Where gauge DoFs are fixed by solving a constraint, e.g. Landau gauge

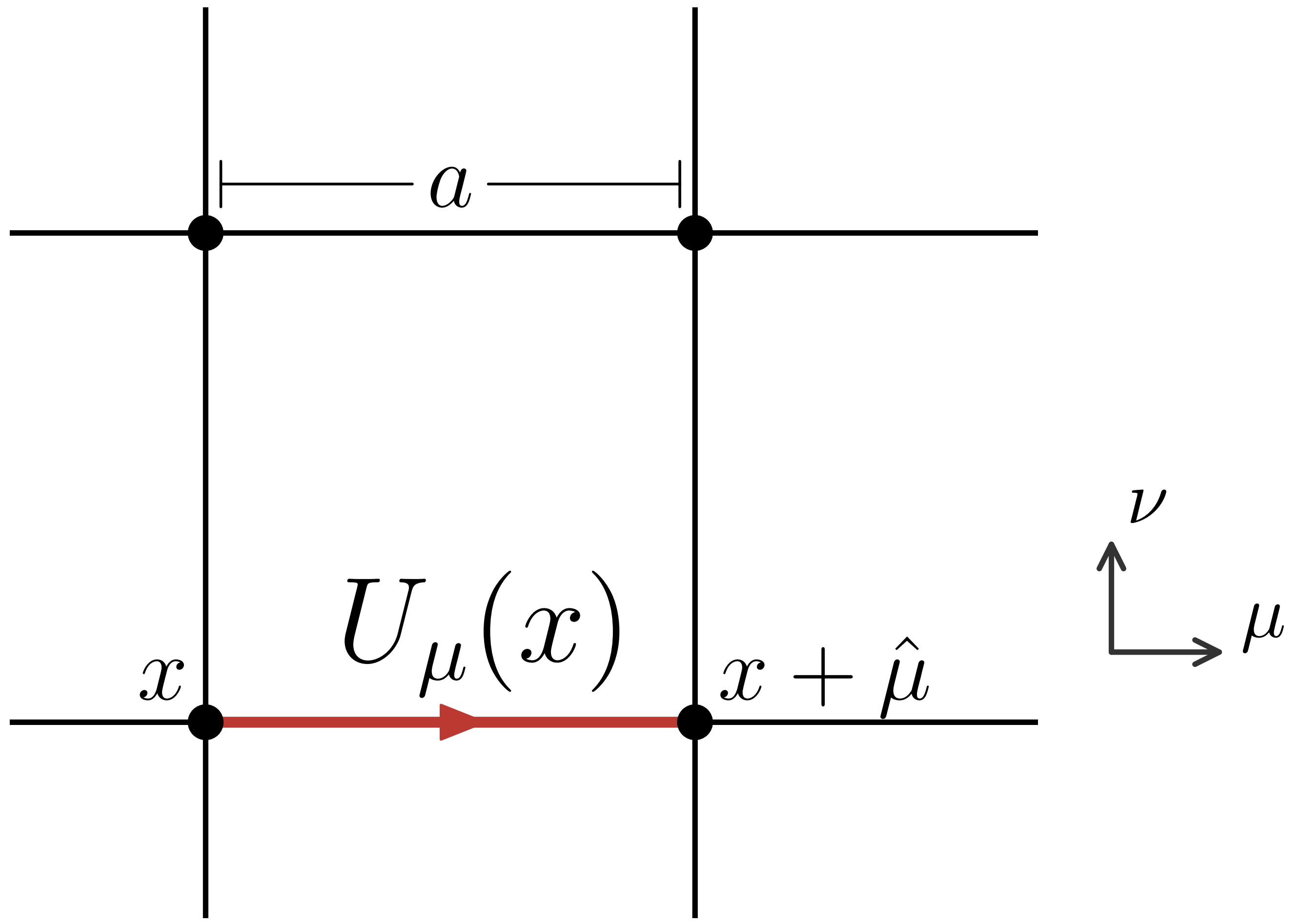
Implicit gauge fixing difficult to act on via **flow-based models**

Landau gauge: $$U_\mu^{\mathrm{fix}}(x) = \mathrm{argmin}_{U^\Omega} \sum_x \sum_{\mu=1}^{N_d} \mathrm{ReTr}[U_\mu^\Omega(x)]$$

Coulomb gauge: $$U_\mu^{\mathrm{fix}}(x) = \mathrm{argmin}_{U^\Omega} \sum_x \sum_{\mu=1}^{N_d-1} \mathrm{ReTr}[U_\mu^\Omega(x)]$$

Unclear how to invertibly transform $U_\mu^{\mathrm{fix}}(x)$.

Gauge symmetries in flows



Choose to act on the un-fixed link representation $U_\mu(x)$.

Carefully construct architecture to enforce…

Gauge-invariant prior:

Not very difficult!
Uniform distribution works.

With respect to Haar measure

$$r(U) = 1$$

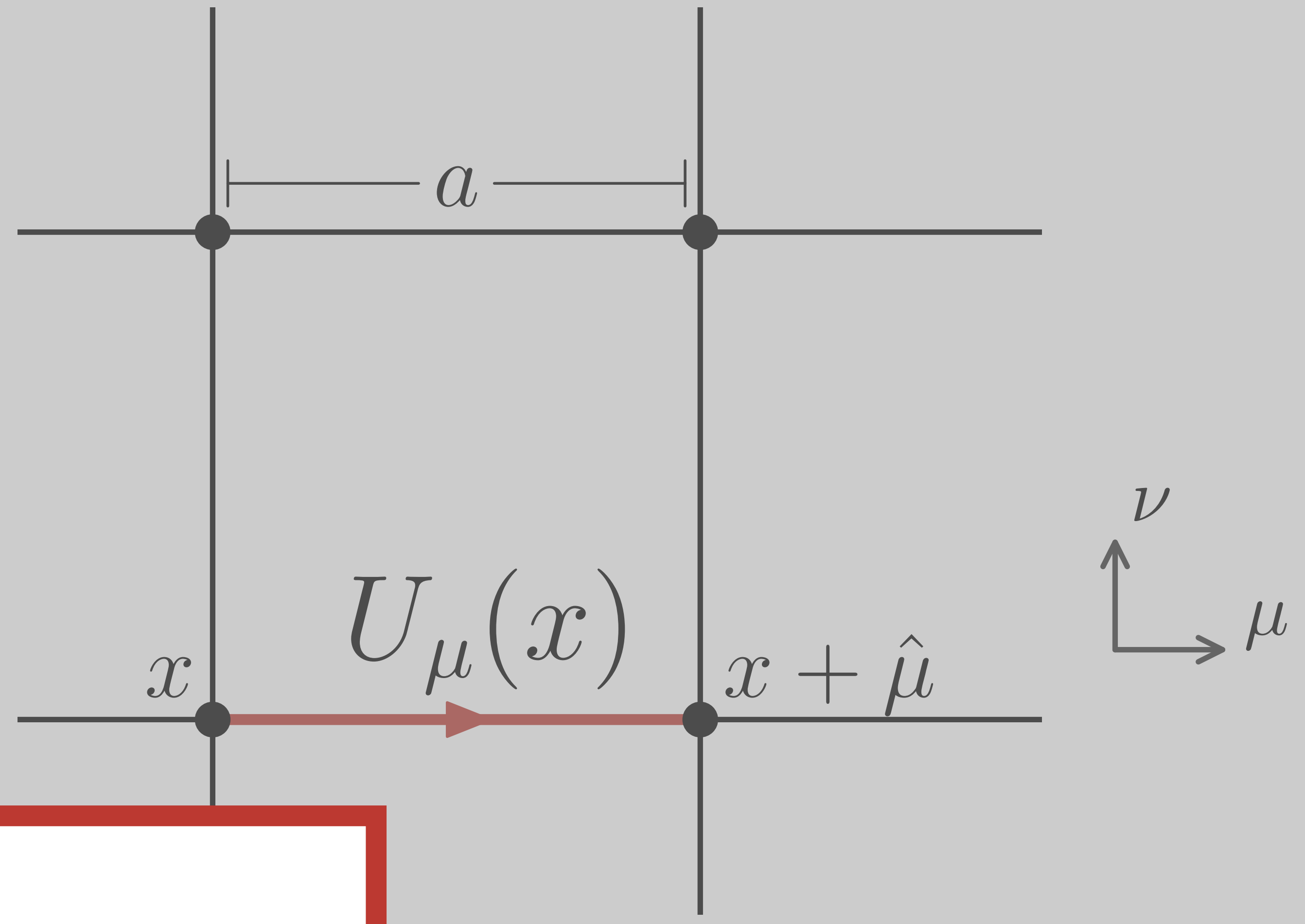
Gauge-equivariant flow:

Coupling layers acting on (untraced) Wilson loops.

Loop transformation easier to satisfy.

Gauge symmetries in flows

Choose to act on the un-fixed link representation $U_\mu(x)$.

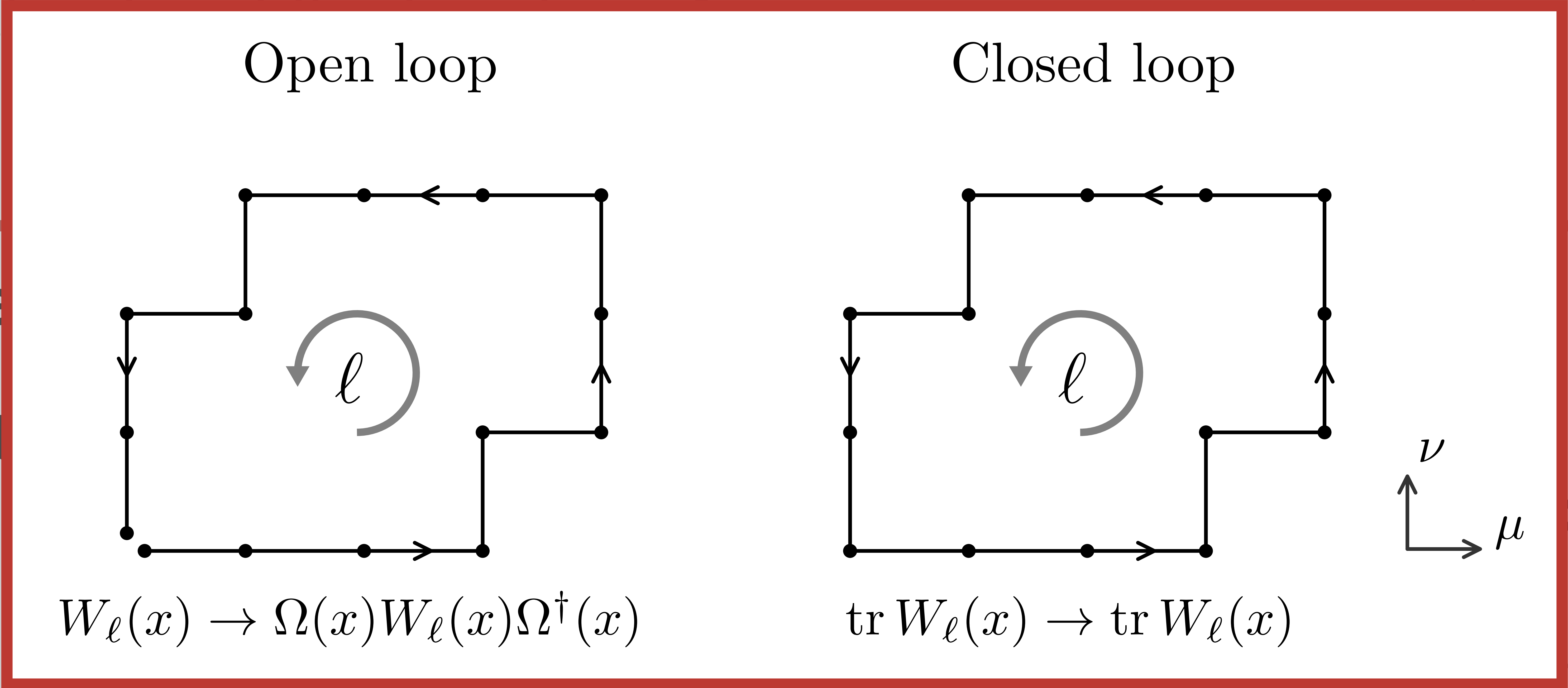


Carefully cons

Gauge

Not
Uniform

With respect to Haar measure



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Gauge-equivariant coupling layer

Compute a **field of Wilson loops** $W_\ell(x)$.

Inner coupling layer [function of $W_\ell(x)$]

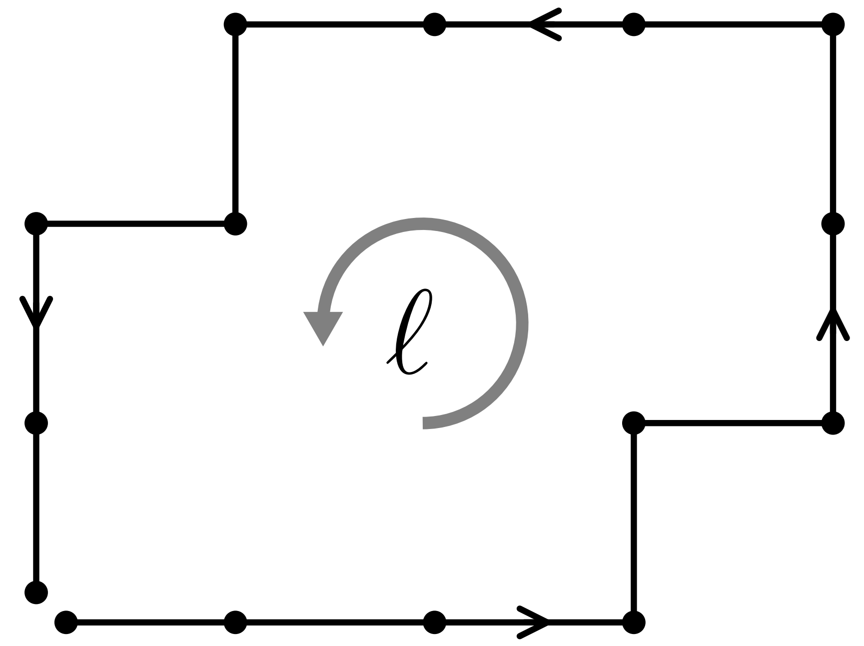
- "Actively" update a subset of loops.*
- Condition on "frozen" closed loops.

Gauge invariant!

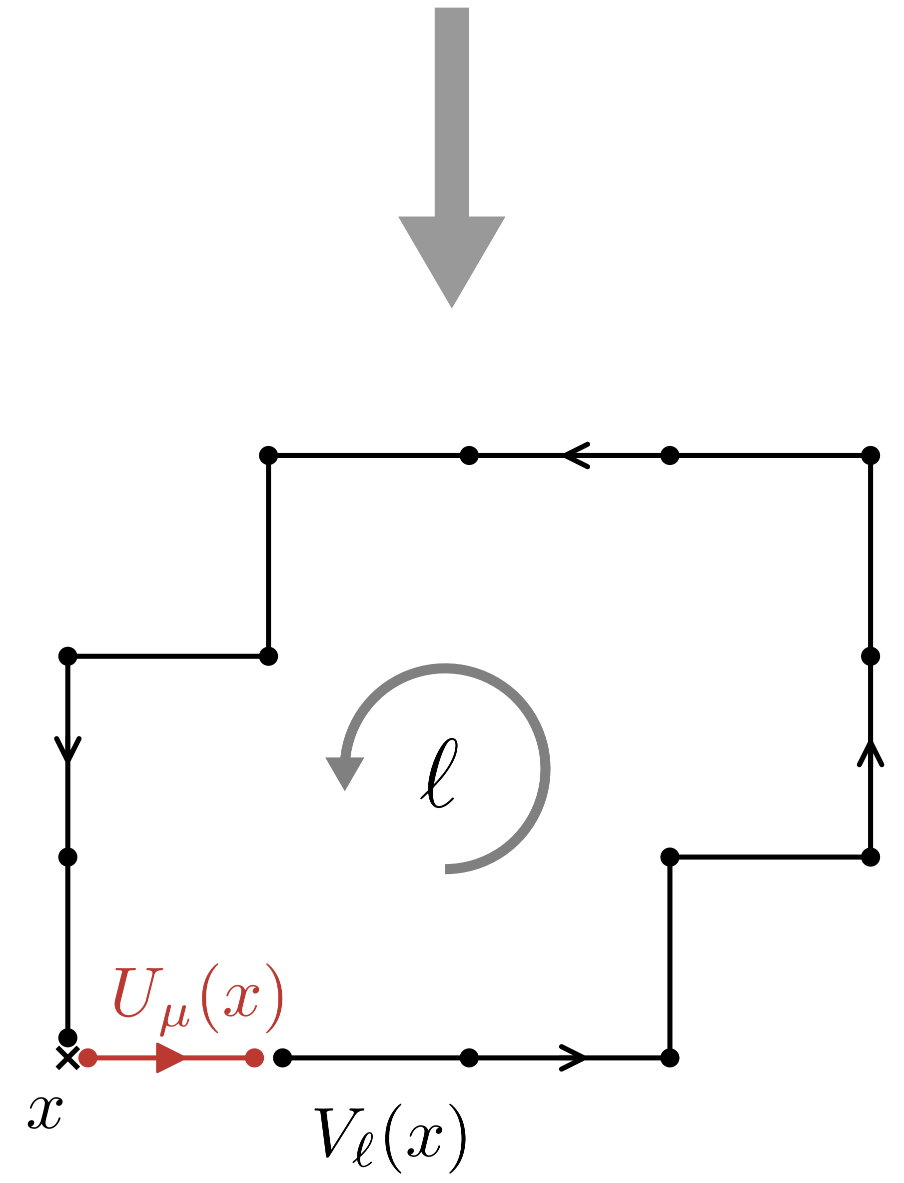
Outer coupling layer [function of $U_\mu(x)$]

- Solve for link update to satisfy actively updated loops.
- Other loops in $W_\ell(x)$ may "passively" update.

Open loop



$$W_\ell(x) \xrightarrow{\text{Flow}} W'_\ell(x)$$



$$U'_\mu(x) = W'_\ell(x)\, V^\dagger_\ell(x)$$

[GK, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan **PRL125 (2020) 121601**]
[Boyda, GK, Racanière, Rezende, Albergo, Cranmer, Hackett, Shanahan **PRD103 (2021) 074504**]

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Inner coupling layer [function of $W_\ell(x)$]

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Gauge invariant!

> * This **"kernel"** must satisfy:
>
> $$h(W_\ell^\Omega(x)) = h^\Omega(W_\ell(x))$$

Outer coupling layer [function of $U_\mu(x)$]

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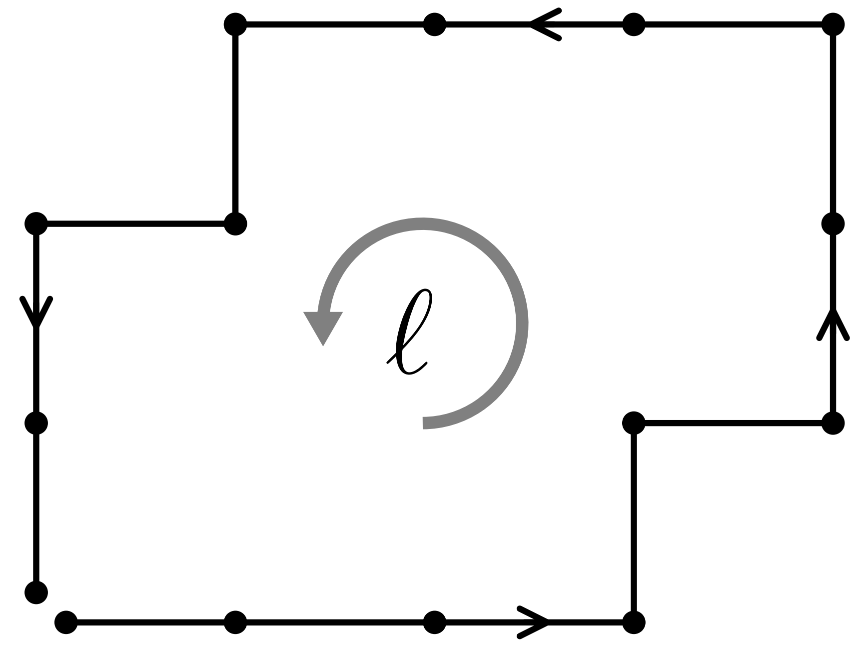

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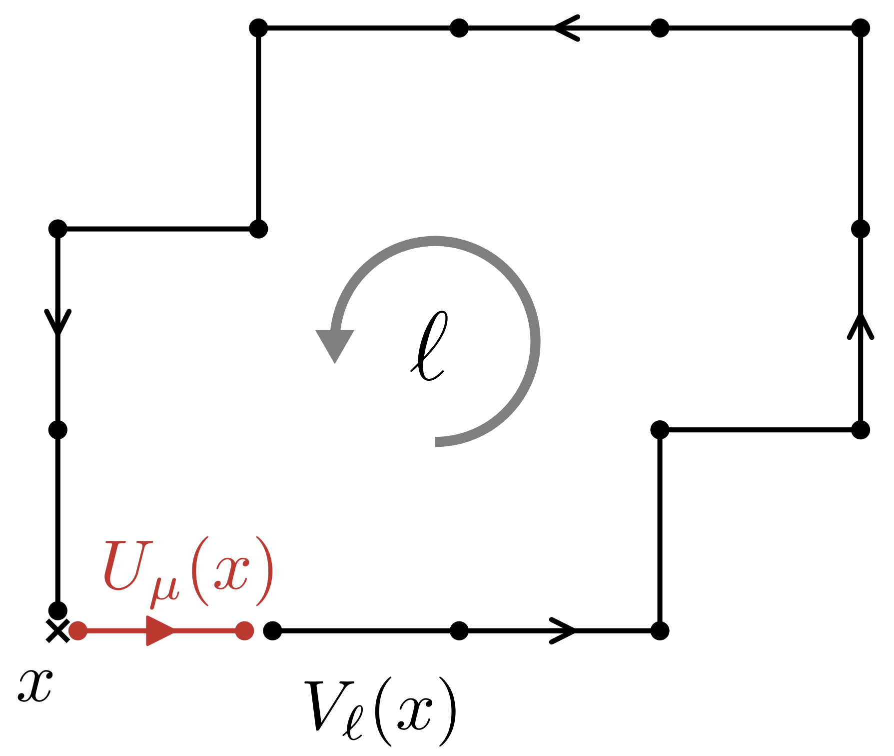

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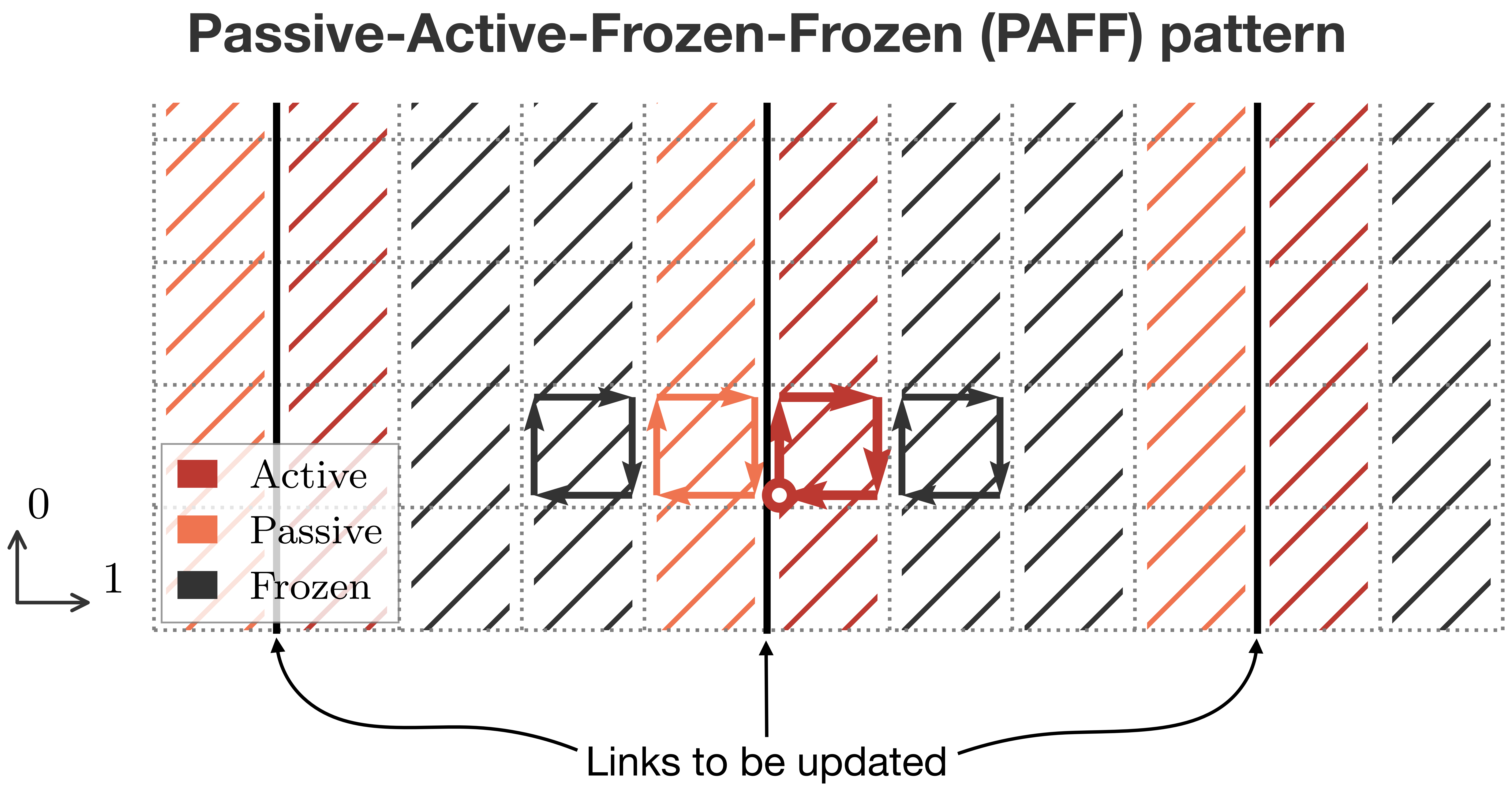
Active, passive, and frozen loops



Kernels

Coupling layers required **kernels** satisfying **conjugation equivariance**:

$$h(\Omega W \Omega^\dagger) = \Omega h(W) \Omega^\dagger$$

U(1): Trivially satisfied because $h(\Omega W \Omega^\dagger) = h(W) = \Omega h(W) \Omega^\dagger$.

However, invertible transforms on the compact domain required.

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

SU(N): Non-trivial constraint requiring some **fun mathematical engineering**…

SU(N) kernels: strategy

SU(N) matrix-conj. equivariance is **non-trivial**.

$$h(\Omega W \Omega^\dagger) = \Omega h(W) \Omega^\dagger$$

Useful observations:

- Conjugation only rotates eigenvectors.
- Spectrum is invariant.
- Wilson loop spectrum encodes gauge-invariant physics → **This is what we want to transform.**

Strategy: Invertibly transform only the spectrum of W via a "spectral map".

Or, "spectral flow".

[Boyda, GK, Racanière, Rezende, Albergo, Cranmer, Hackett, Shanahan **PRD103 (2021) 074504**]

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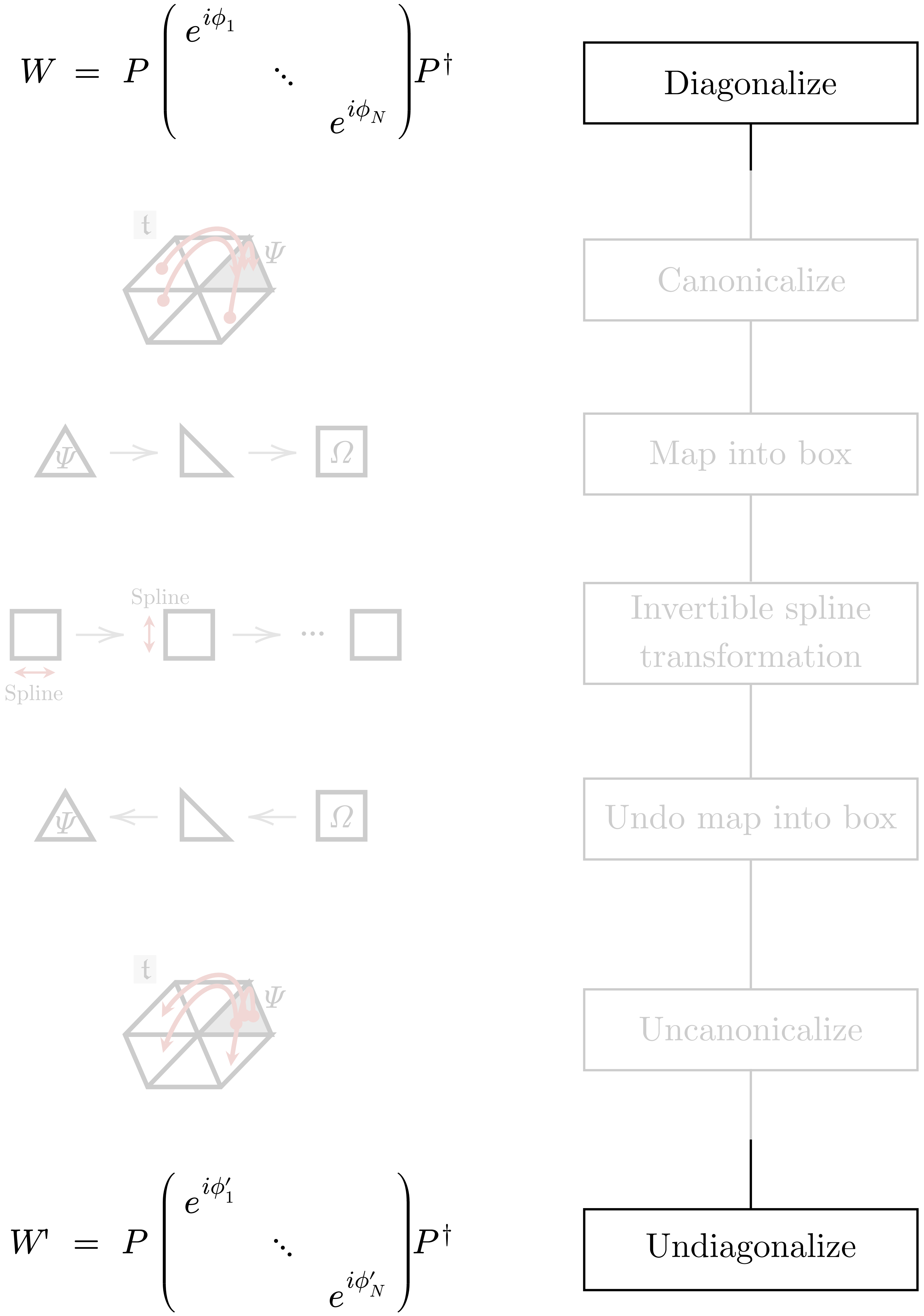
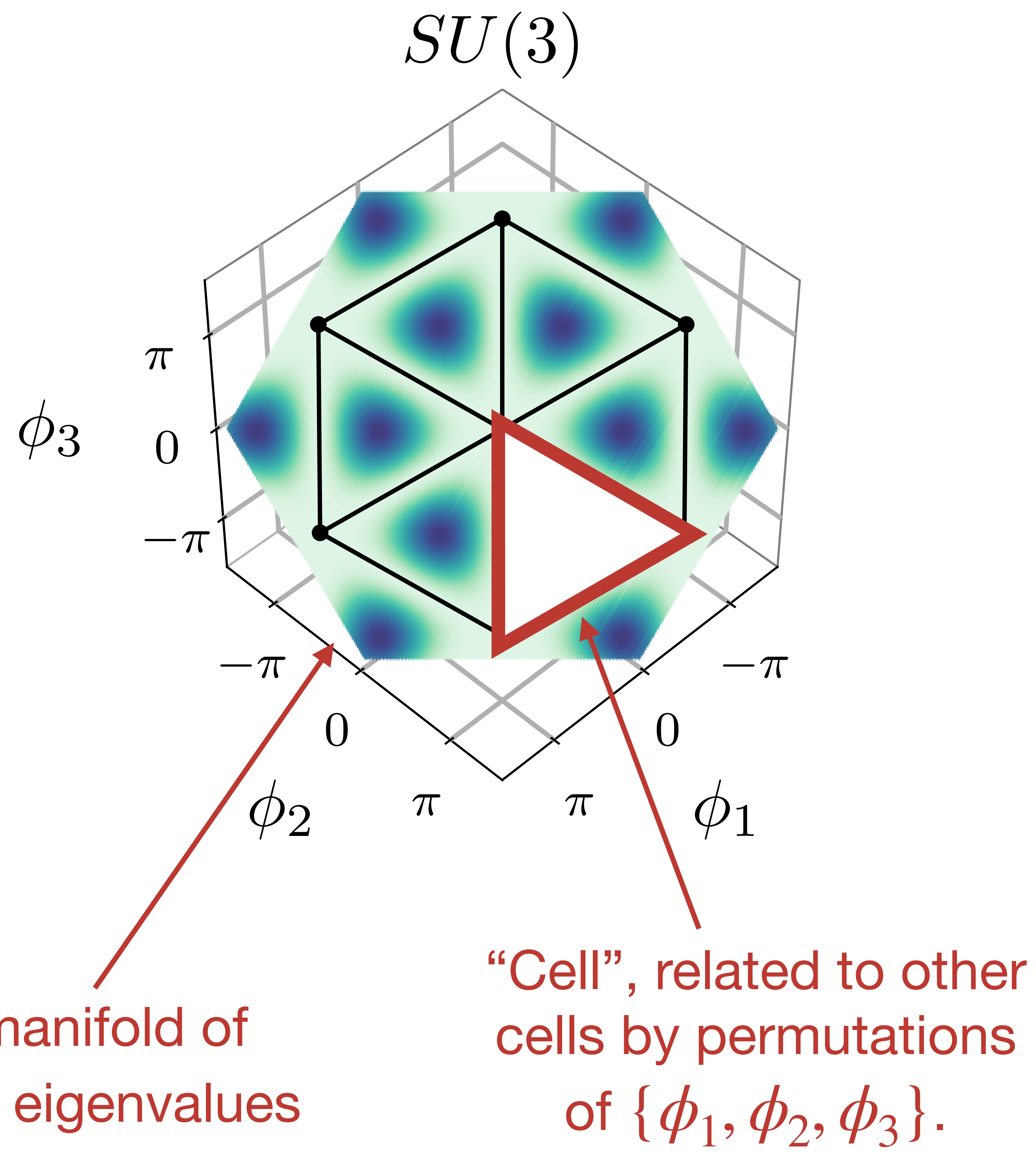
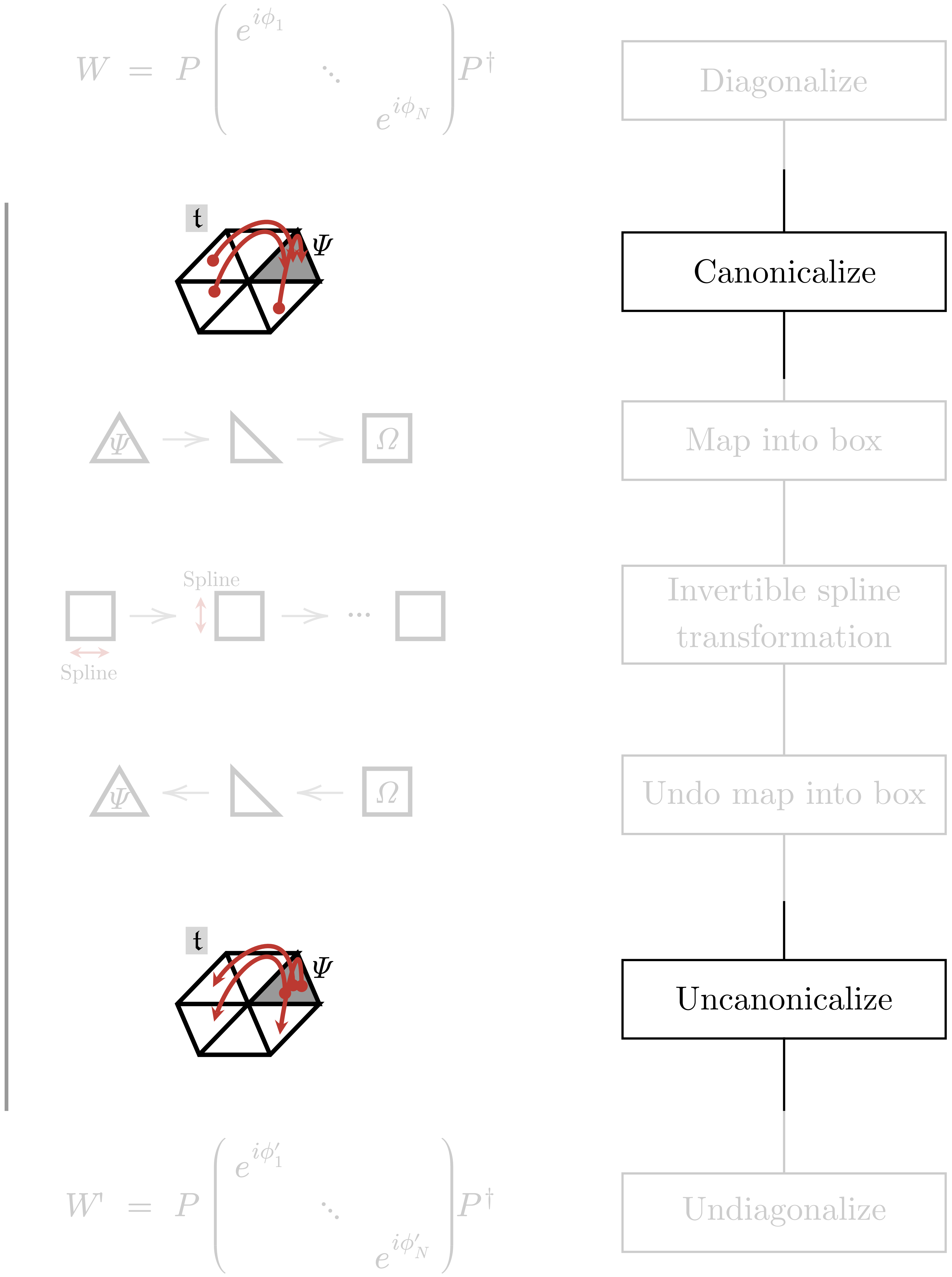


[Boyda, GK, Racanière, Rezende, Albergo, Cranmer, Hackett, Shanahan **PRD103 (2021) 074504**]

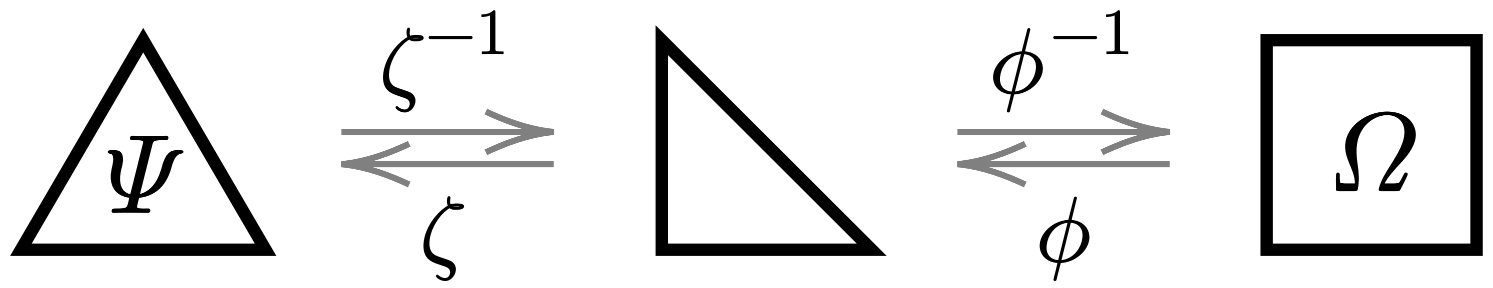
SU(N) kernels:
Permutation equivariance





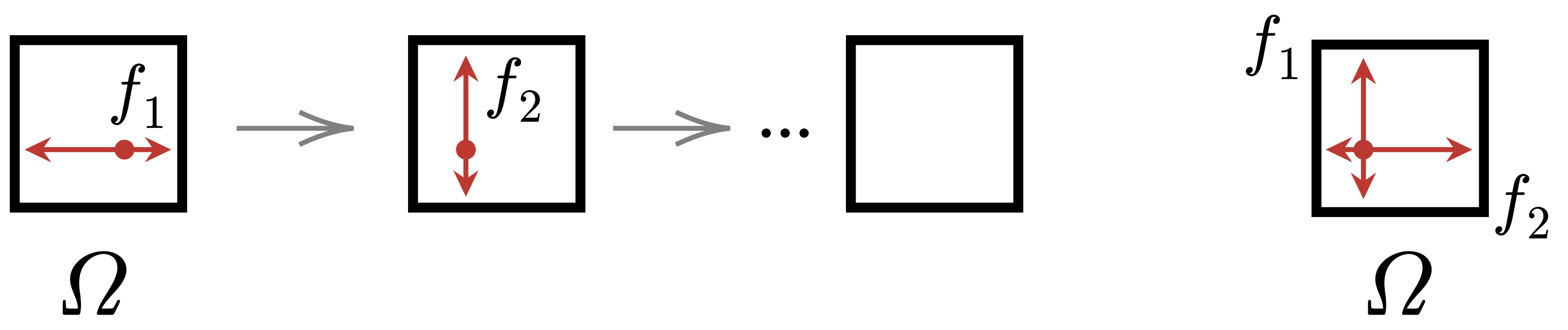
SU(N) kernels:
Transform the canonical cell

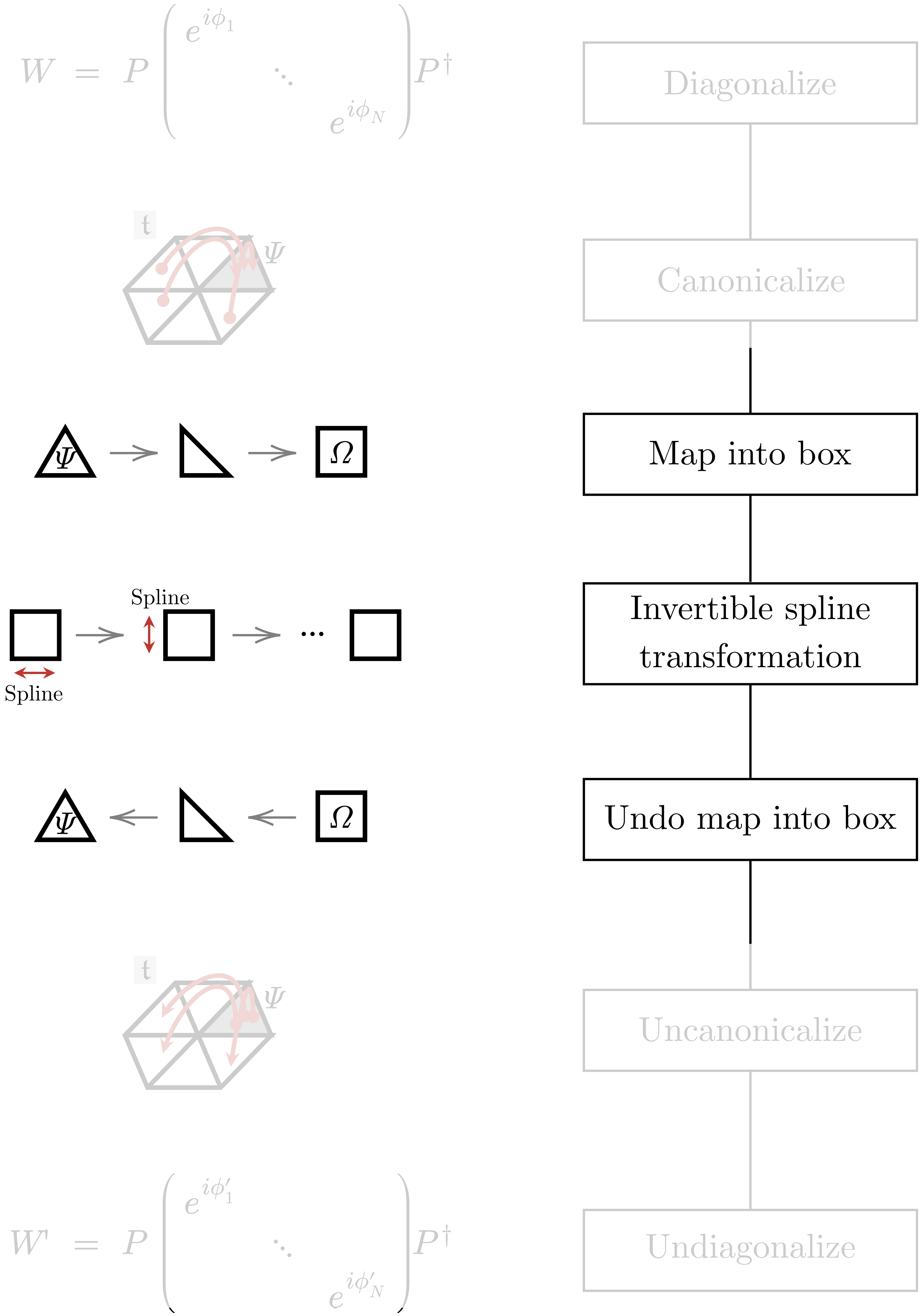
Change variables to rectilinear box Ω



Transform by acting on coords of box Ω, either…

Autoregressive … or … Independent



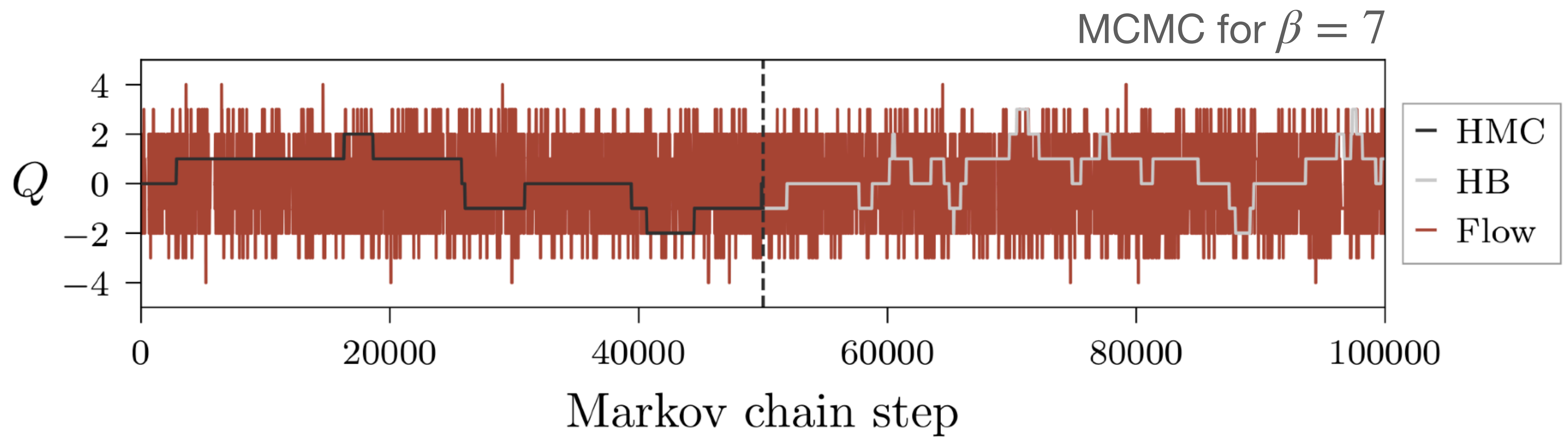


U(1) gauge theory in 1+1D

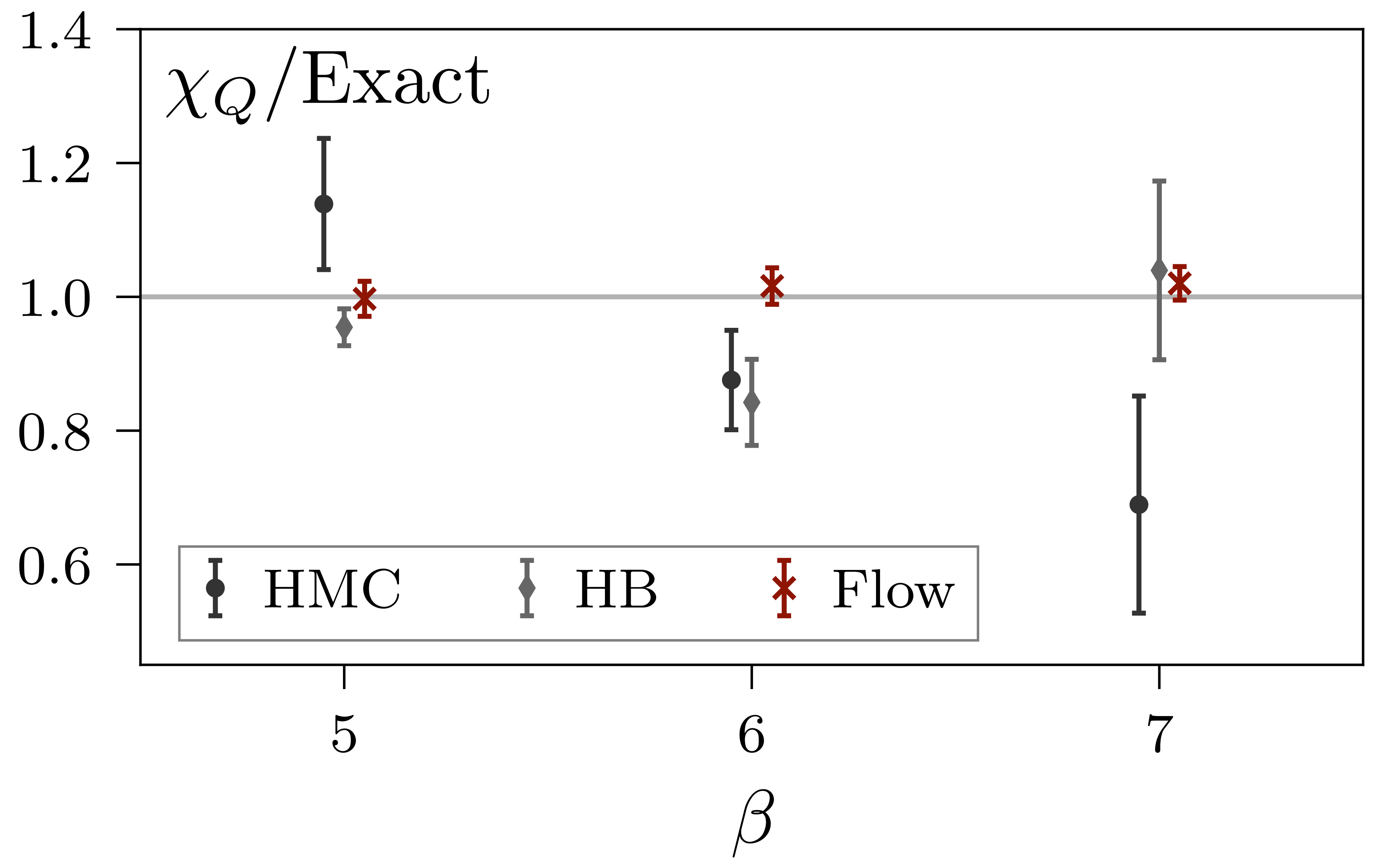
$$S(U) = -\beta \sum_x \sum_{\mu<\nu} \mathrm{Re}\, P_{\mu\nu}(x)$$
$$P_{\mu\nu}(x) = U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)$$

There is exact lattice topology in 2D.

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



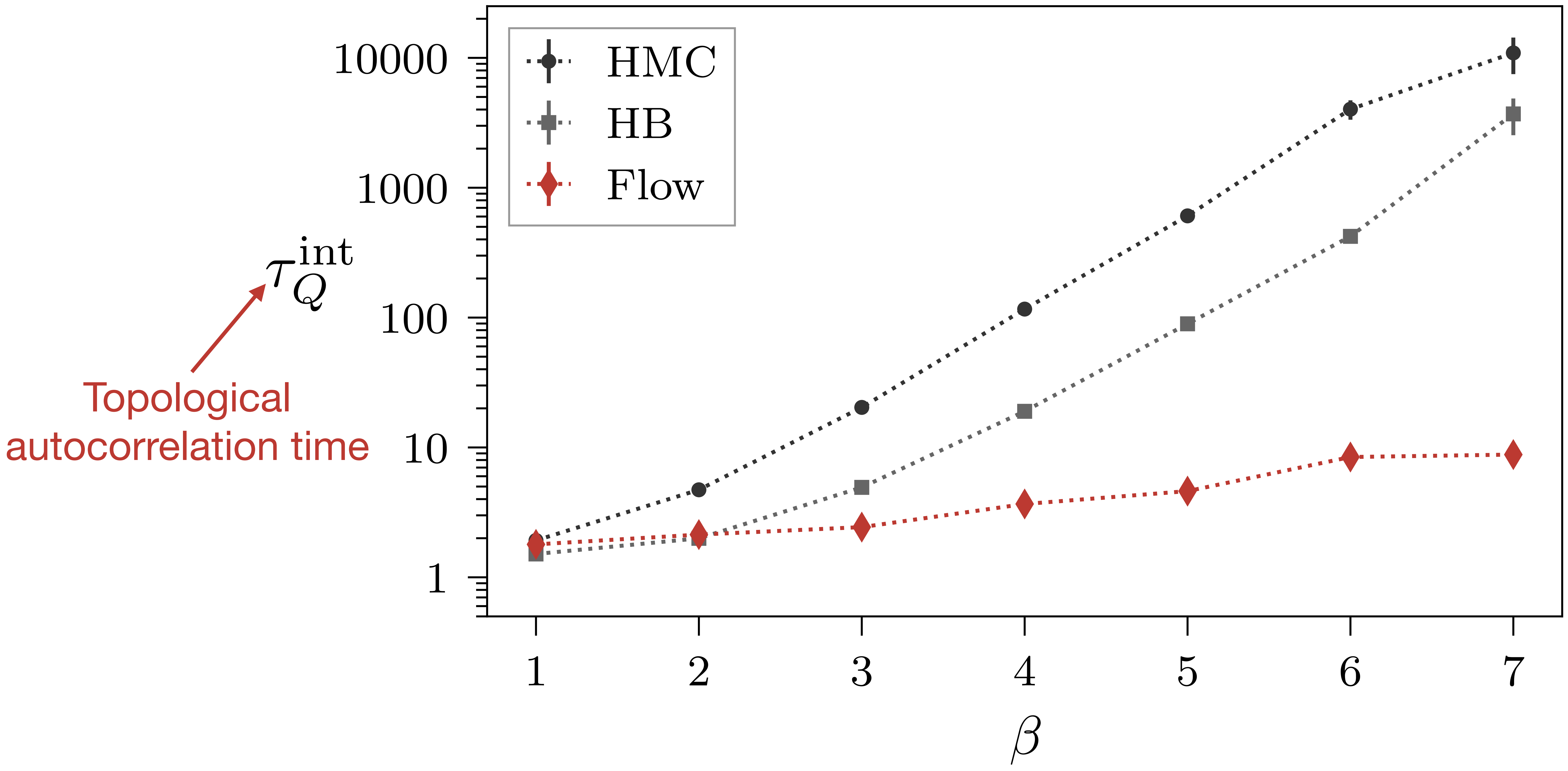
- Compared **flow, analytical, HMC**, and **heat bath** on 16×16 lattices for $\beta = \{1,\ldots,7\}$
- Topo freezing in HMC and heat bath
- Gauge-equiv flow-based model at each β
- Flow-based MCMC observables agree



Topological susceptibility $\chi_Q = \langle Q^2/V \rangle$

[GK, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan **PRL125 (2020) 121601**]

U(1) topological freezing mitigated



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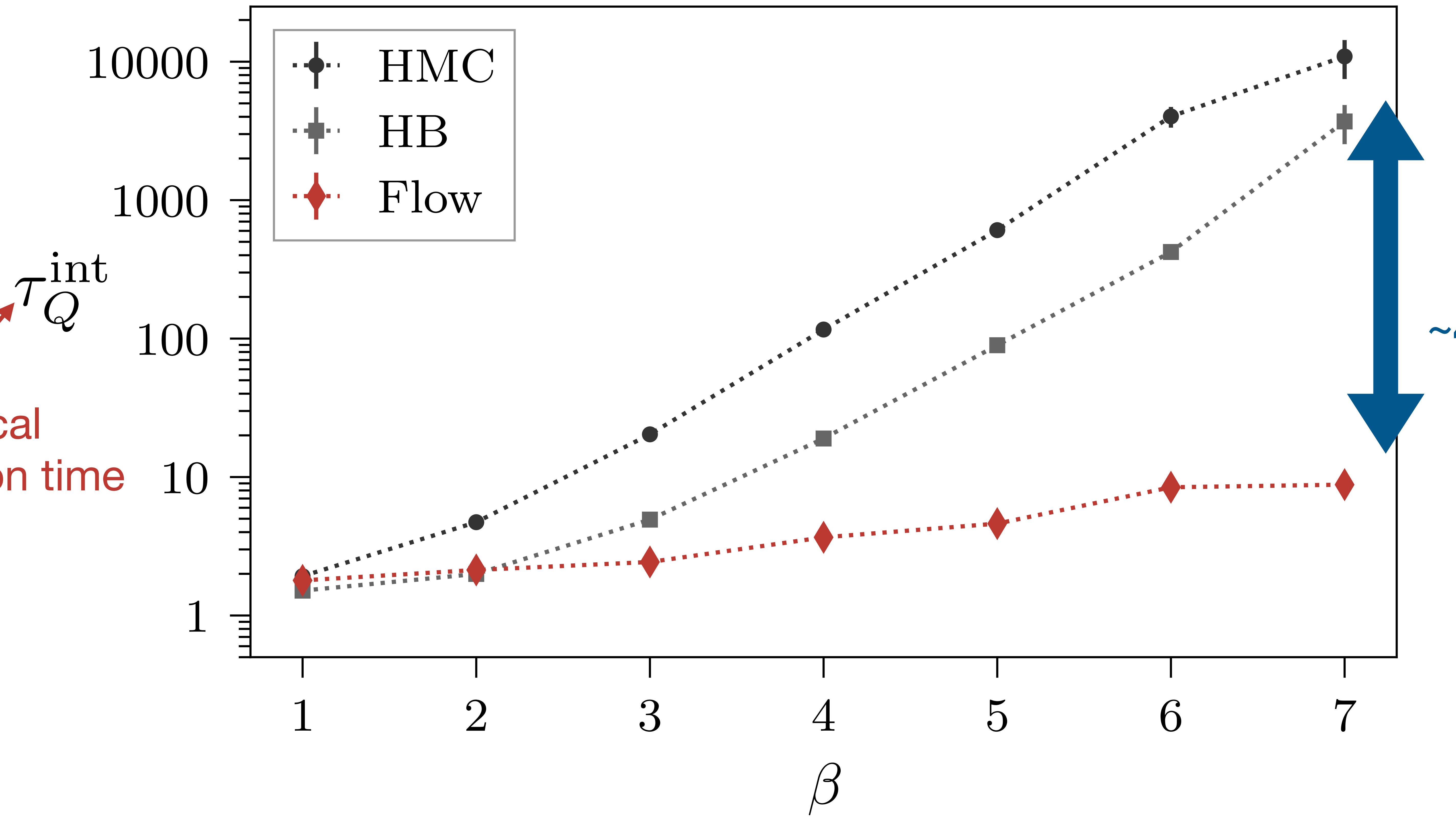


Topological autocorrelation time

Autocorrelation time reduced by **~4 orders of magnitude!**

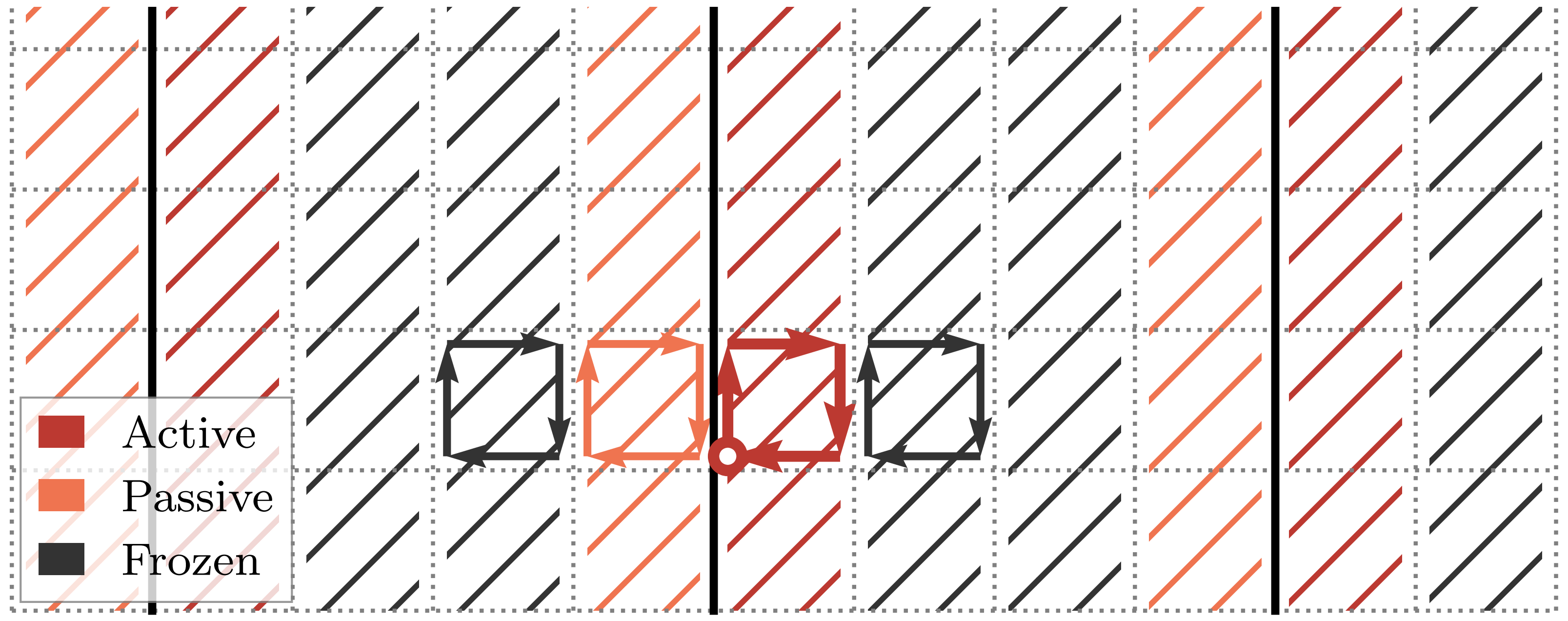
SU(N) gauge theory in 1+1D

$$S(U) = -\frac{\beta}{N}\sum_x \sum_{\mu<\nu} \mathrm{ReTr}\, P_{\mu\nu}(x)$$

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

Gauge-equiv flow models for 2D lattice gauge theory on 16×16 lattices.

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



- 48 **PAFF coupling layers**, links updated 6 times each

- No equivalent to $U(1)$ topological freezing, studied **absolute model quality**

[Boyda, GK, Racanière, Rezende, Albergo, Cranmer, Hackett, Shanahan **PRD103 (2021) 074504**]

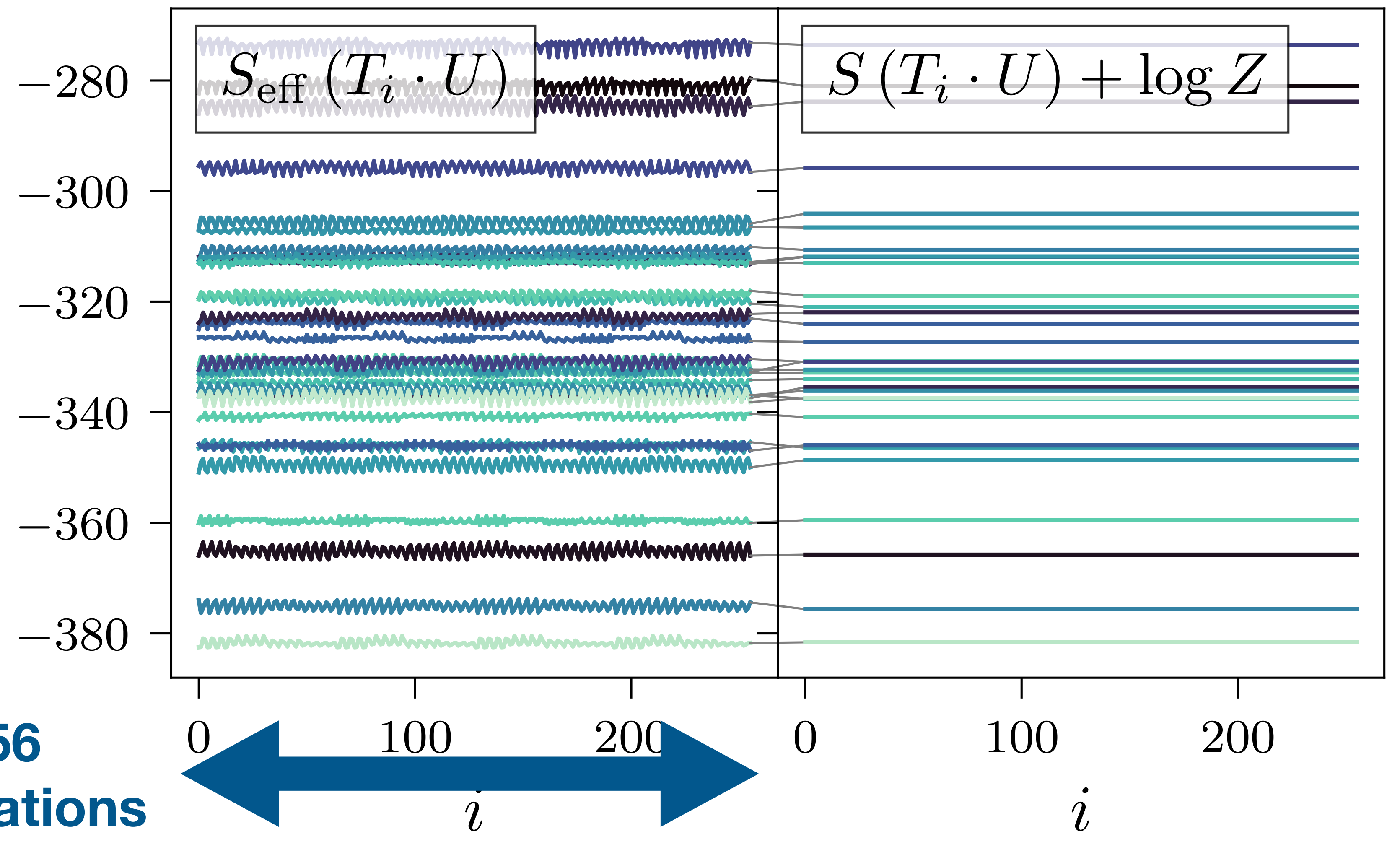
Results for SU(2) and SU(3) gauge theory

- Flow-based MCMC observables agree with analytical
- **High-quality models:** autocorrelation time in flow-based Markov chain τ_{int} = 1—4

	SU(2)			SU(3)		
β	1.8	2.2	2.7	4.0	5.0	6.0
ESS(%)	91	80	56	88	75	48

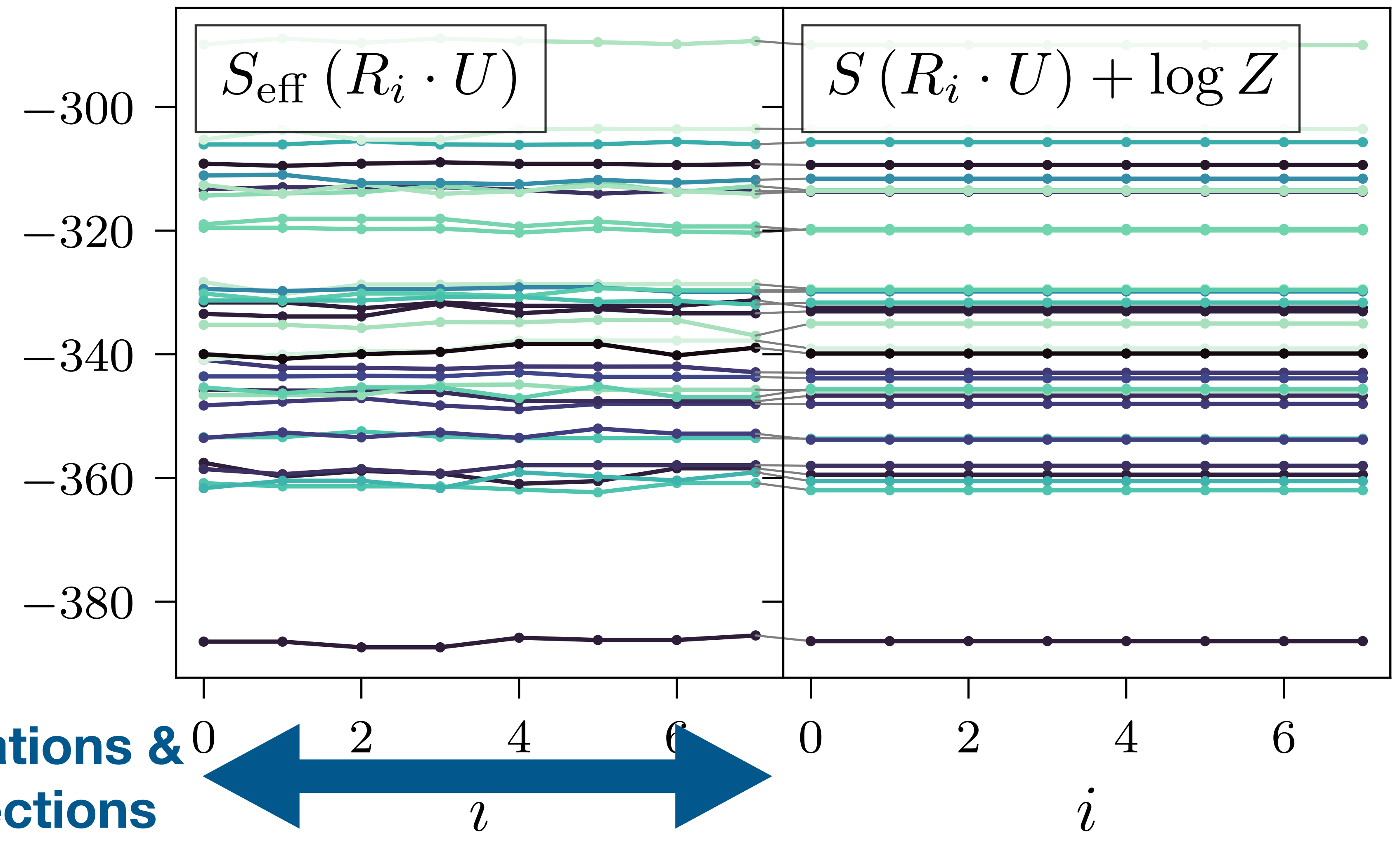
✓ “Effective Sample Sizes” indicating model overlap onto target are all larger than ~50% (100% = perfect model)

Exact translational subgroup; residual learned



256 translations

Rotation and reflection symmetry learned



8 rotations & reflections

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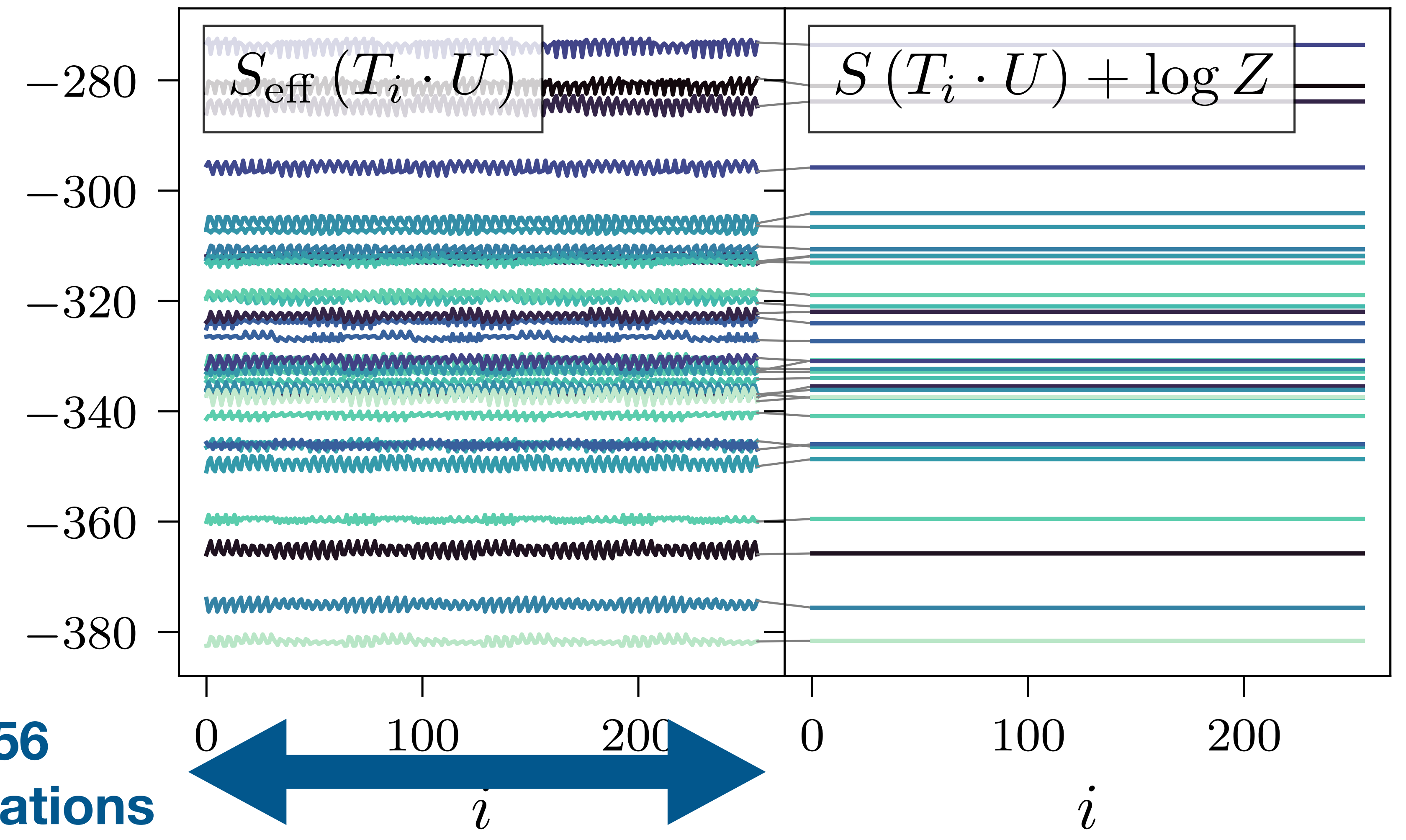

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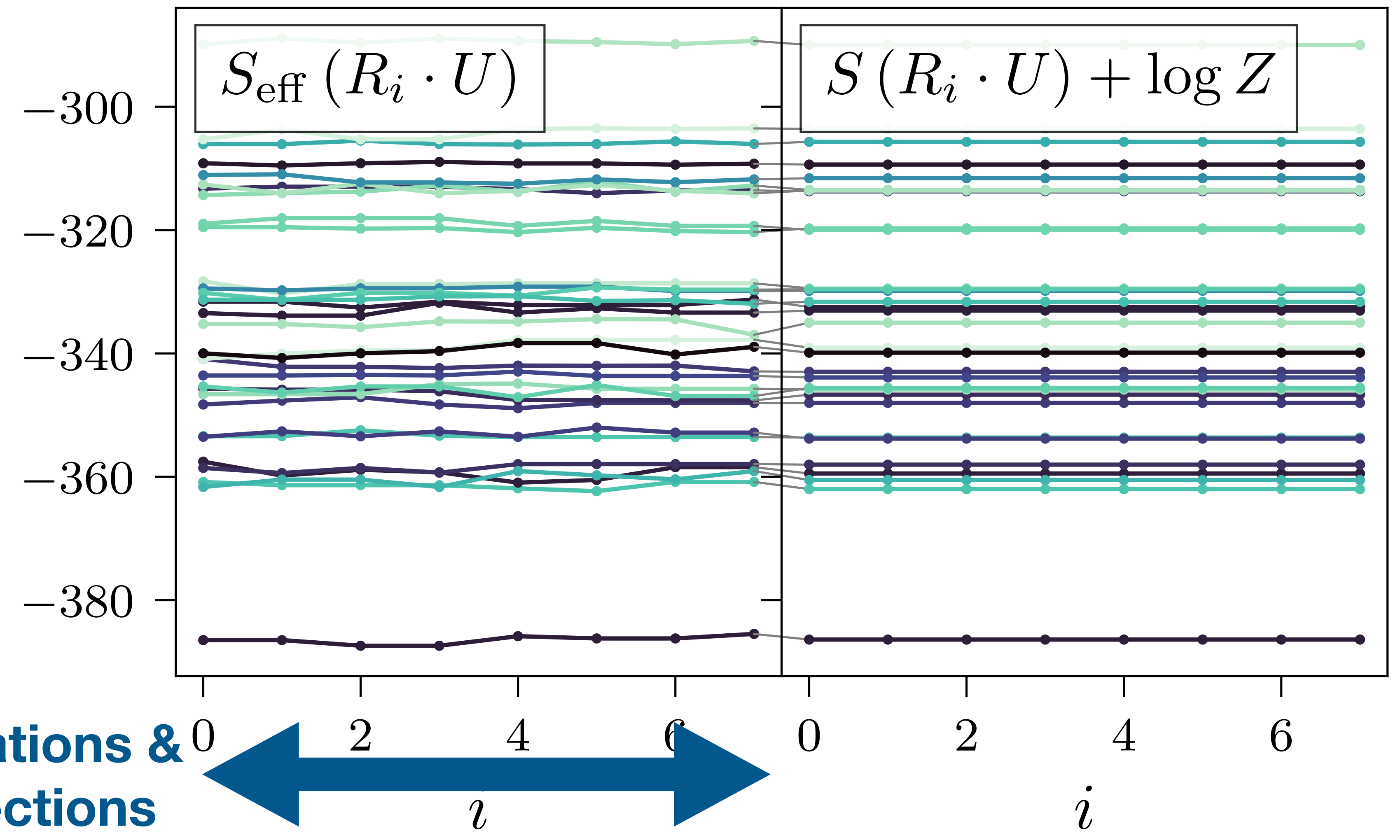


8 rotations & reflections

Promising early results. No theoretical obstacle to scaling to 4D $SU(N)$ lattice gauge theory.

A story of symmetries & generative models

(In three parts)

1. Flow-based generative models

2. Gauge symmetry & translational symmetry

3. **Fermions & translational symmetry**

Fermions in field theory

Grassmann representation in path integral means…

… we cannot sample fermion fields

… integrating out fermions results in costly fermion determinants

$$\int \mathcal{D}\psi \mathcal{D}\bar{\psi} \prod_f e^{-\bar{\psi}_f D_f \psi_f} = \prod_f \det D_f$$

Pseudofermions used in standard MCMC for theories with dynamical fermions.

$$\int \mathcal{D}\psi \mathcal{D}\bar{\psi} \prod_f e^{-\bar{\psi}_f D_f \psi_f} \propto \int \mathcal{D}\varphi \mathcal{D}\varphi^\dagger \prod_k e^{-\varphi_k^\dagger \mathcal{M}_k^{-1} \varphi_k}$$

Starting point for flow-based sampling

[Albergo, GK, Racanière, Rezende, Urban, Boyda, Cranmer, Hackett, Shanahan **2106.05934**]

5 ways to marginalize

Any could in principle be learned by flow-based models.

Below: Bosonic part of action written generically as $S_B(\phi)$

Name	Probability density
Joint[A]	$p(\phi, \varphi) = \frac{1}{Z} \exp(-S_B(\phi) - \varphi^\dagger [\mathcal{M}(\phi)]^{-1} \varphi)$
ϕ-marginal	$p(\phi) = \frac{Z_\mathcal{N}}{Z} \exp(-S_B(\phi)) \det \mathcal{M}(\phi)$
φ-conditional[A,B]	$p(\varphi \vert \phi) = \frac{1}{Z_\mathcal{N} \det \mathcal{M}(\phi)} \exp(-\varphi^\dagger [\mathcal{M}(\phi)]^{-1} \varphi)$
φ-marginal[C]	$p(\varphi) = \frac{1}{Z} \int d\phi \, \exp(-S_B(\phi) - \varphi^\dagger [\mathcal{M}(\phi)]^{-1} \varphi)$
ϕ-conditional[A]	$p(\phi \vert \varphi) = \frac{\exp(-S_B(\phi) - \varphi^\dagger [\mathcal{M}(\phi)]^{-1} \varphi)}{\int d\phi \, \exp(-S_B(\phi) - \varphi^\dagger [\mathcal{M}(\phi)]^{-1} \varphi)}$

Expensive to evaluate det exactly

Can actually be sampled directly (e.g. pseudofermion refresh in HMC)

Intractable density (even unnormalized)

Translational invariance

Pseudofermion fields $\varphi(x)$ satisfy **antiperiodic BCs** in the time direction.

Marginalizations with PFs should address this for translational equivariance.

Building blocks:

Explicit averaging:

- CNN outputs averaged over time translations with correct BCs

Restricted CNNs:

- Channels either **antiperiodic (AP)** or **periodic (P)** in time
- Operations restricted for well-defined outputs (either P or AP)
- AP activations only odd fns

Invertible linear layers:

- Flow = composed linear operators $\mathscr{W}_n \circ \ldots \circ \mathscr{W}_1$
- Each $\mathscr{W}_i$ is a conv with fixed direction (and correct BCs)

$$\begin{bmatrix} a_1 & & & & \pm b_1 \\ b_2 & a_2 & & 0 & \\ & \cdots & \cdots & & \\ & 0 & & & \\ & & & b_L & a_L \end{bmatrix}$$

$$\det \mathscr{W}_i = \prod_k a_k \pm \prod_k b_k$$

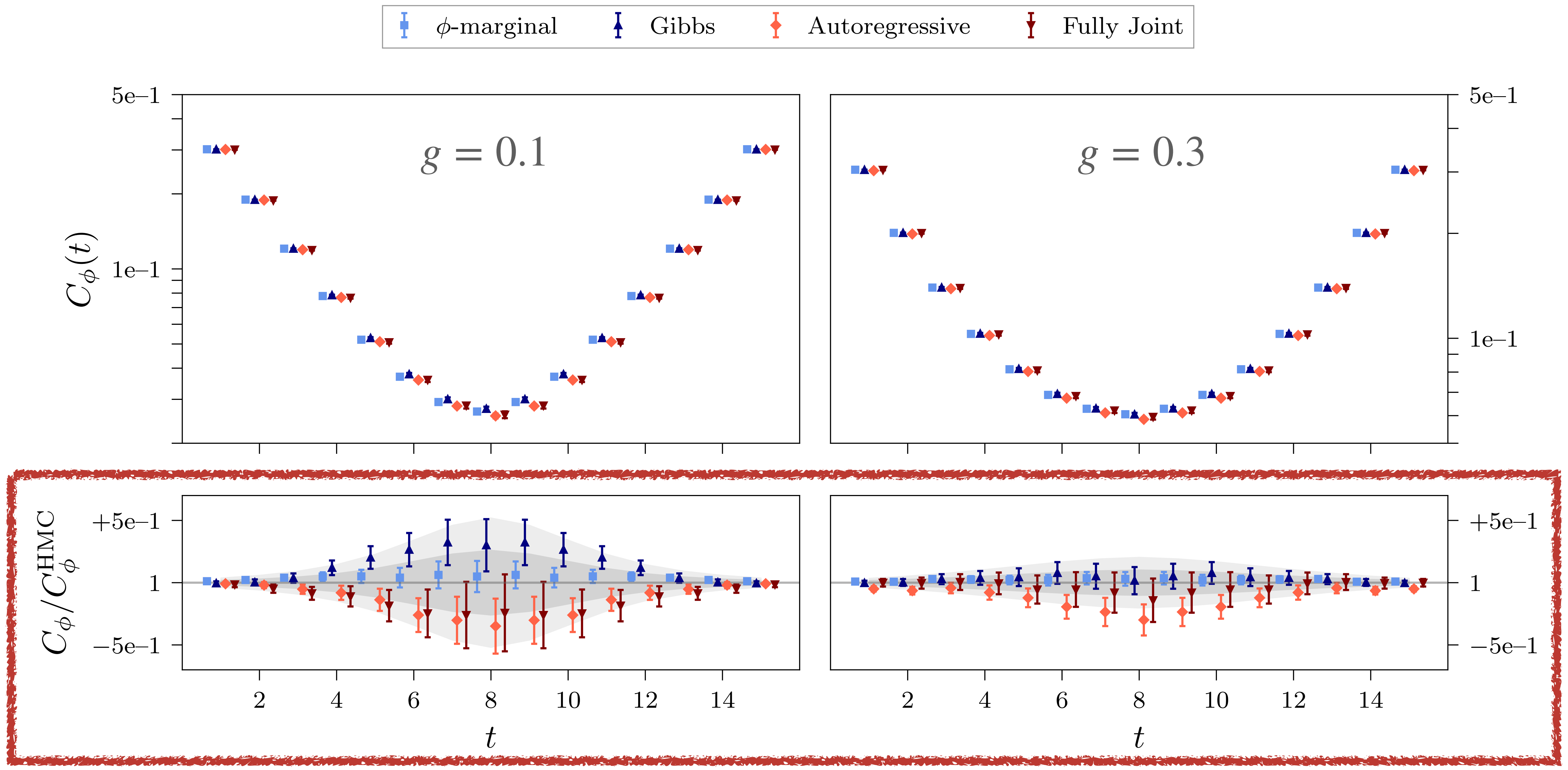
Results for Yukawa model

Staggered Dirac op with Yukawa coupling $g\phi\bar{\psi}\psi$ and mass term $M\bar{\psi}\psi$

Studied 2D ϕ^4 model coupled via Yukawa interaction to staggered ψ

$$S(\phi,\psi) = \sum_{x\in\Lambda}[-2\sum_{\mu=1}^{d}\phi(x)\phi(x+\hat{\mu}) + (m^2+2d)\phi(x)^2 + \lambda\phi(x)^4] + \sum_{f=1}^{N_f}\bar{\psi}_f D_f[\phi]\psi_f$$

- 16×16 lattices
- Two degenerate fermions ($N_f = 2$)
- Massless ($M = 0$)
- Variety of models, all 4 sampling schemes



✓ Correlation functions effectively reproduced

Summary and Outlook

Symmetries allow efficient & consistent training of flow-based models.

Gauge symmetry + **translational** symmetry addressed throughout.

Effective models produced for $U(1)$, $SU(2)$, $SU(3)$ lattice gauge theory and a ϕ^4 Yukawa model in 1+1D.

Future directions:

1. Higher spacetime dims
2. Tuning of training hyperparameters
3. Efficient model architectures at scale?

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See also:

Approaches to multimodal sampling and mixed HMC + flow-based sampling:

[Hackett, Hsieh, Albergo, Boyda, Chen, Chen, Cranmer, GK, Shanahan; **2107.00734**]

Jupyter notebook tutorial:

[Albergo, Boyda, Hackett, GK, Cranmer, Racanière, Rezende, Shanahan; **2101.08176**]

Backup Slides

Exactness: Flow-based MCMC

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

"Embarrassingly parallel" step!

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

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

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

Exactness: Reweighting

- Also possible to reweight independently drawn samples:

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

- May be preferable when observables $\mathcal{O}(U)$ are efficiently computed, and sampling is expensive.

- Observables $\mathcal{O}(U)$ are expensive in lattice QCD. We prefer resampling or MCMC approaches in these settings.

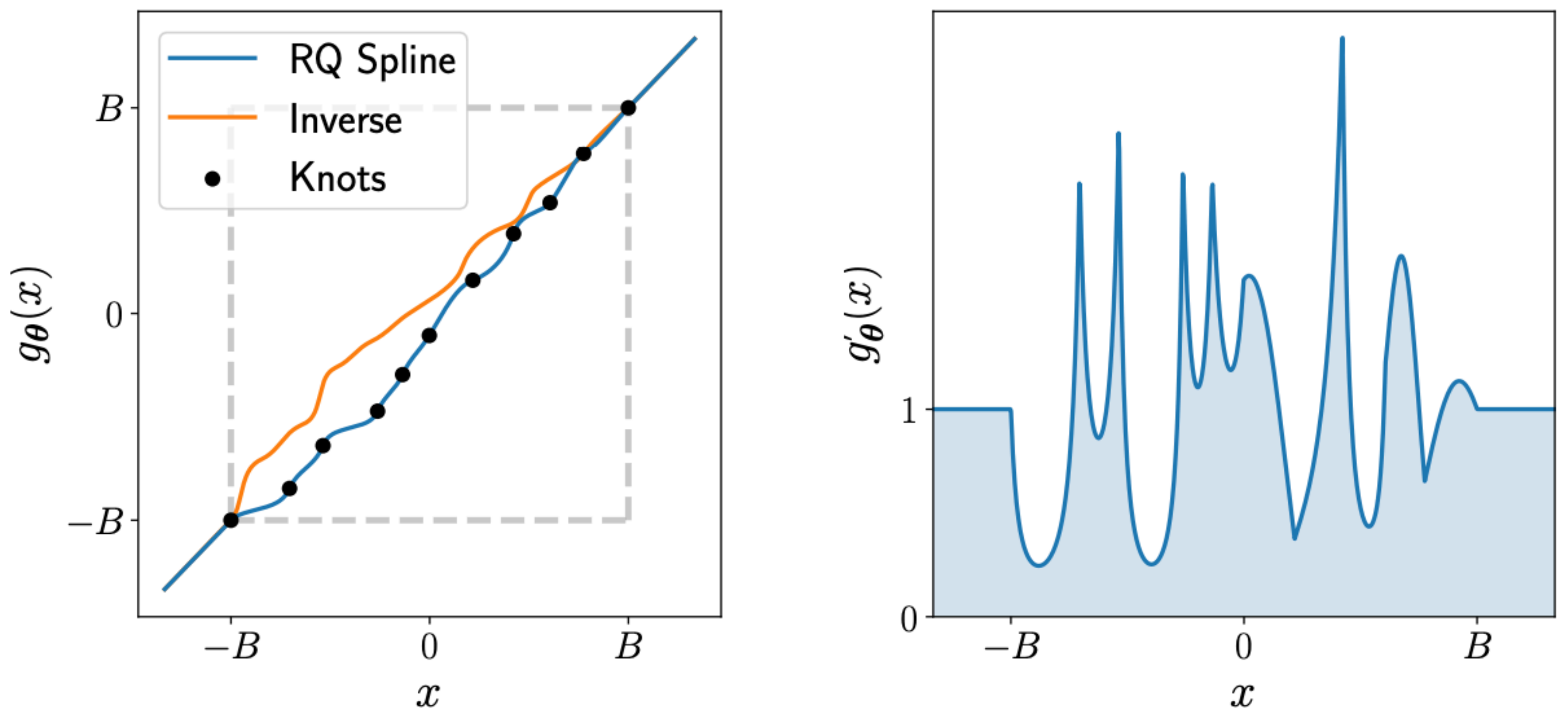
U(1) kernels

Conjugation equivariance trivially satisfied: $h(\Omega W \Omega^\dagger) = h(W) = \Omega h(W) \Omega^\dagger$.

Invertible maps on U(1) variables:

- **Periodic / compact domain** must be addressed.
- For details, see:
  [Rezende, Papamakarios, Racanière, Albergo, GK, Shanahan, Cranmer; **ICML (2020) 2002.02428**]

[Durkan, Bekasov, Murray, Papamakarios **1906.04032**]



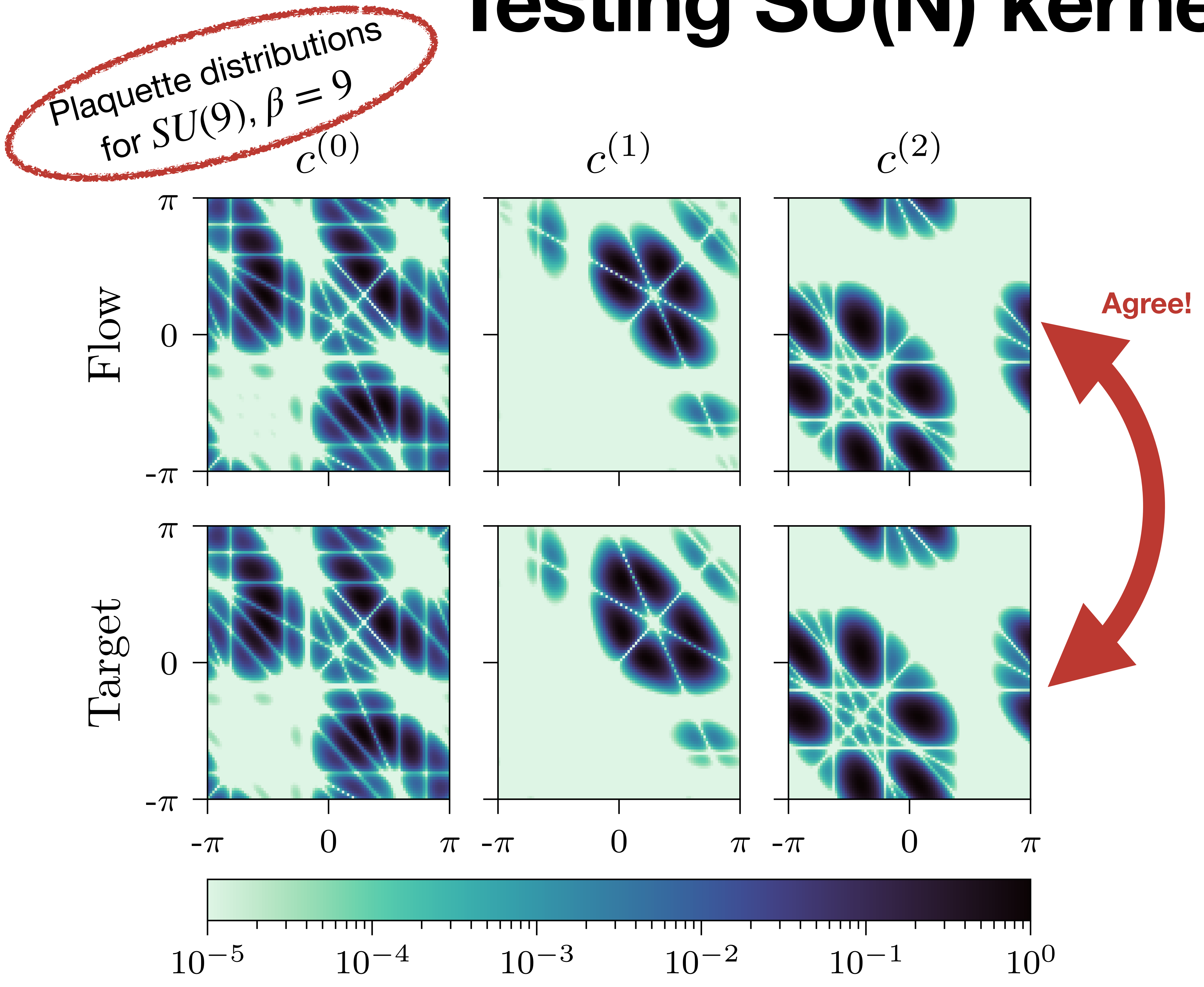
Non-compact projection:

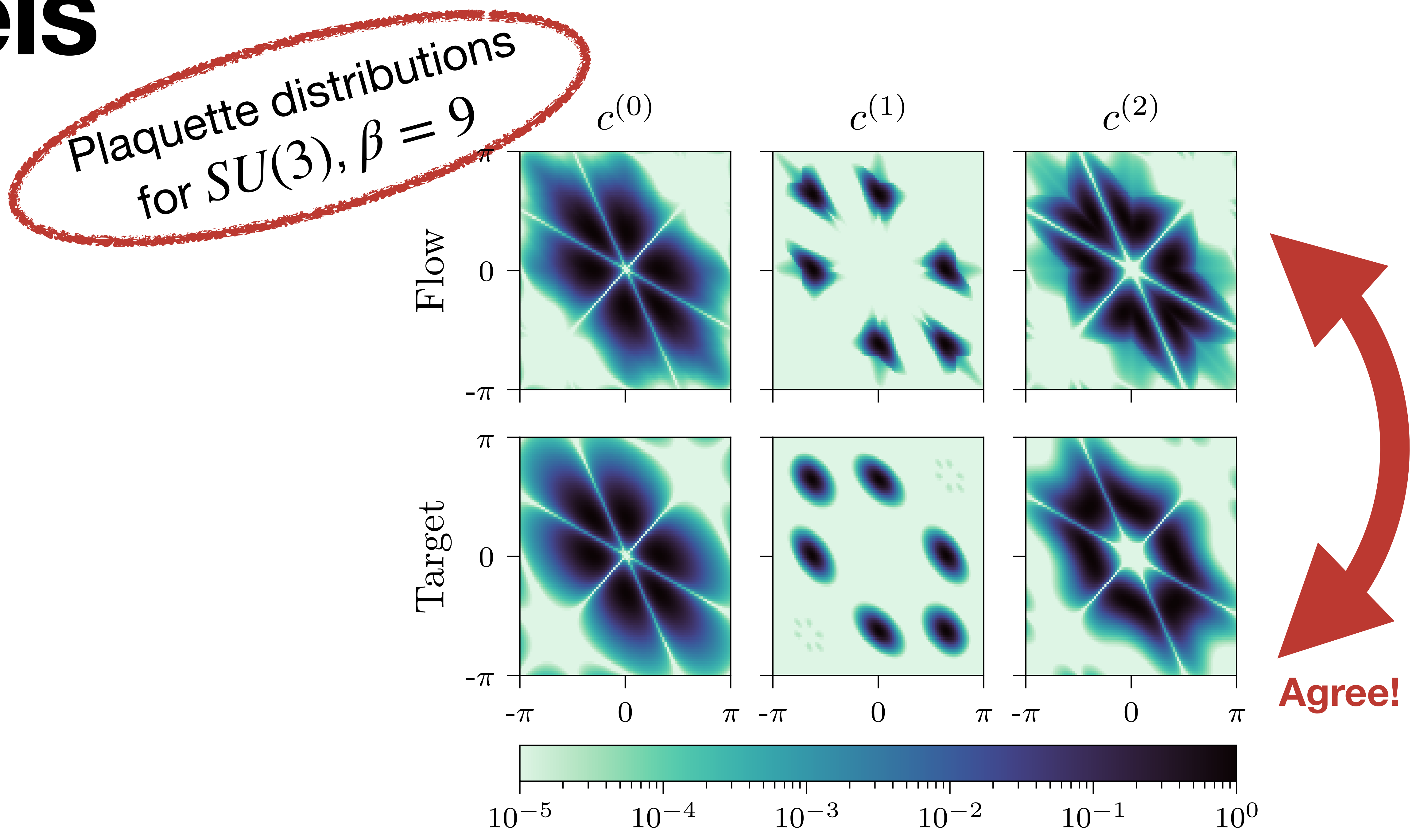
- Map $\theta \to x \in \mathbb{R}$, e.g. $\arctan(\theta/2)$
- Transform $x \to x'$ as usual
- Map $x' \to \theta' \in [-\pi, \pi]$

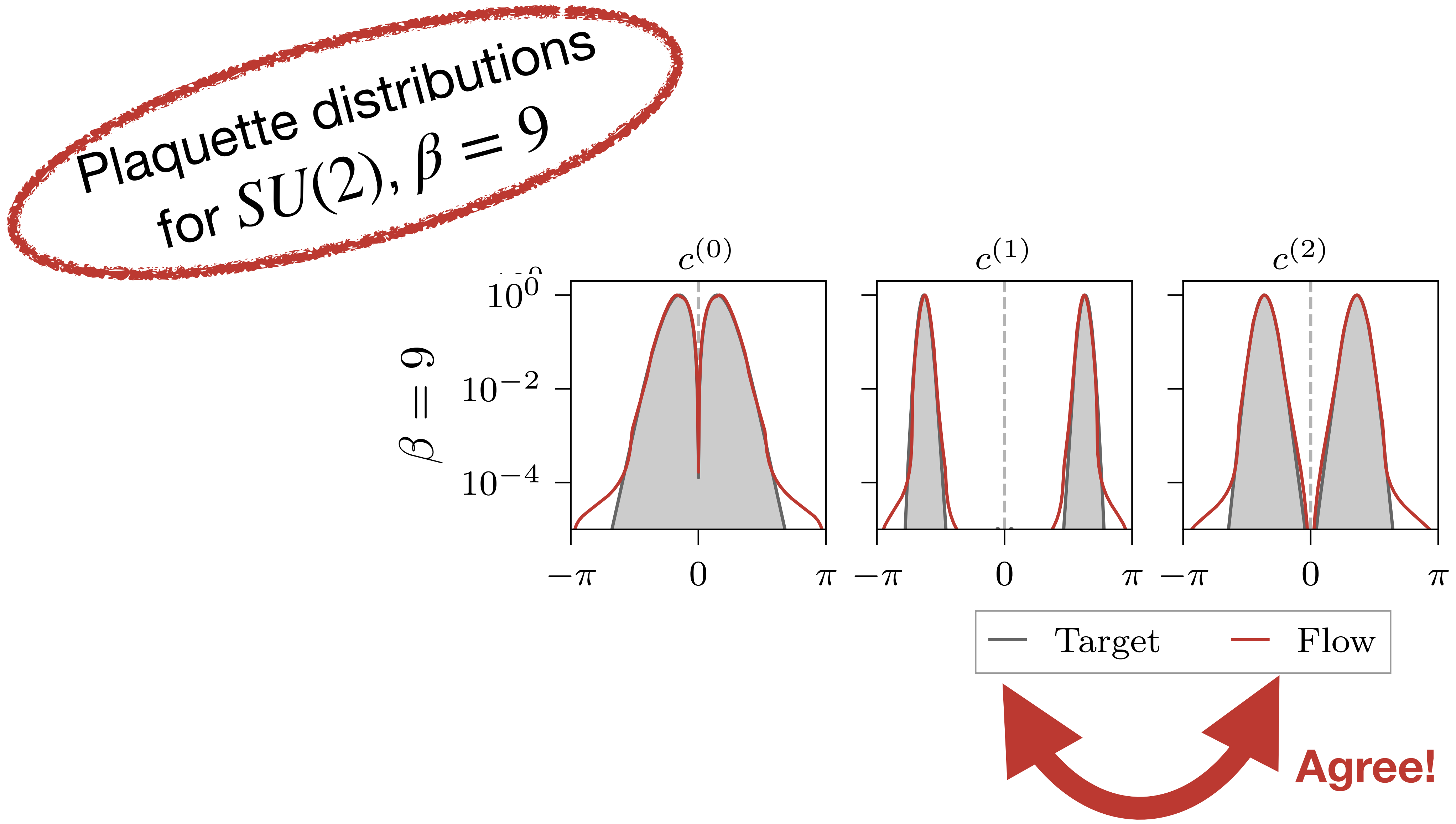
Circular invertible splines:

- Spline "knots" trainable fns
- Identify endpoints π and $-\pi$
- Number of knots $\leftrightarrow$ expressivity

Testing SU(N) kernels

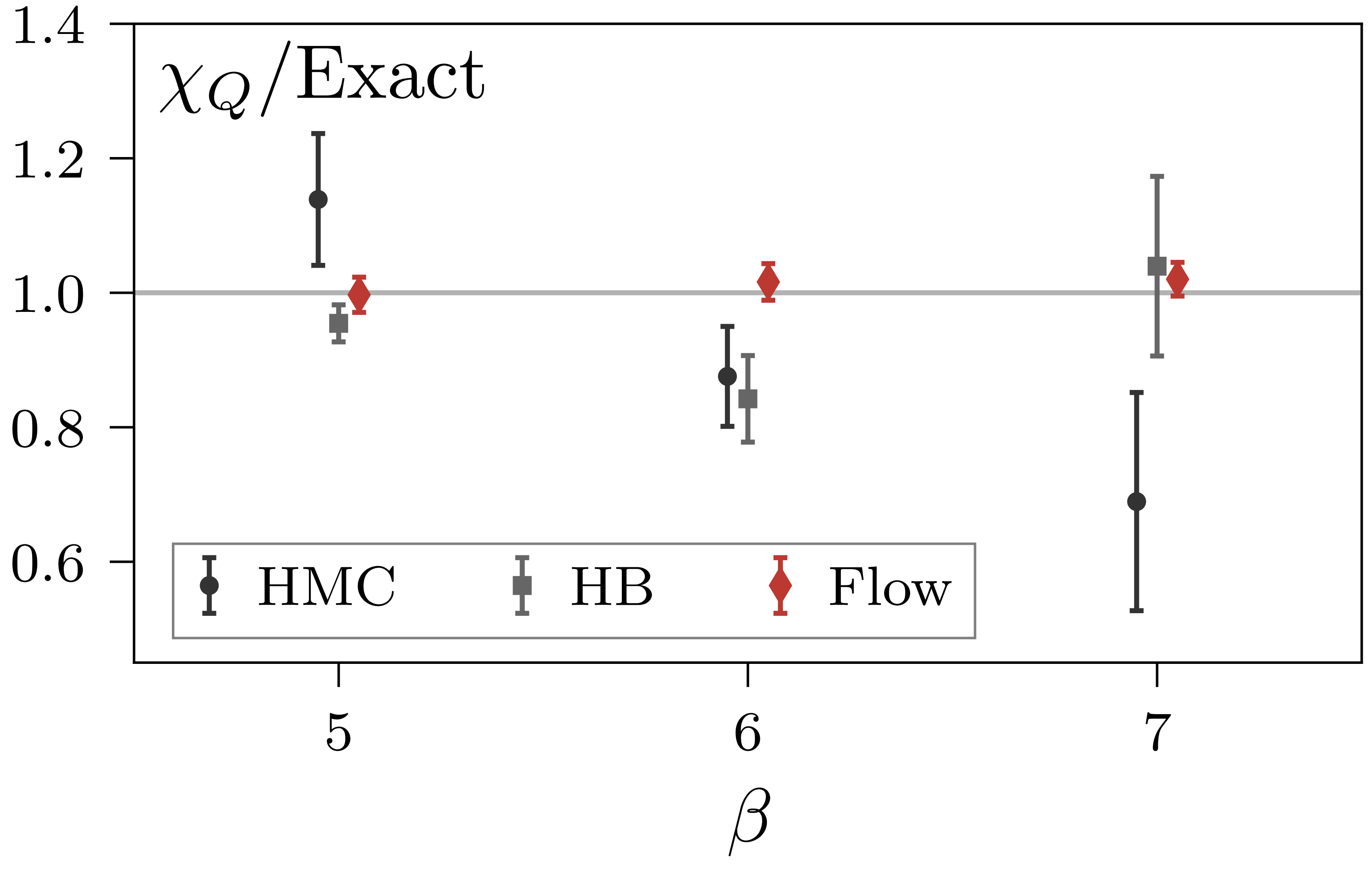


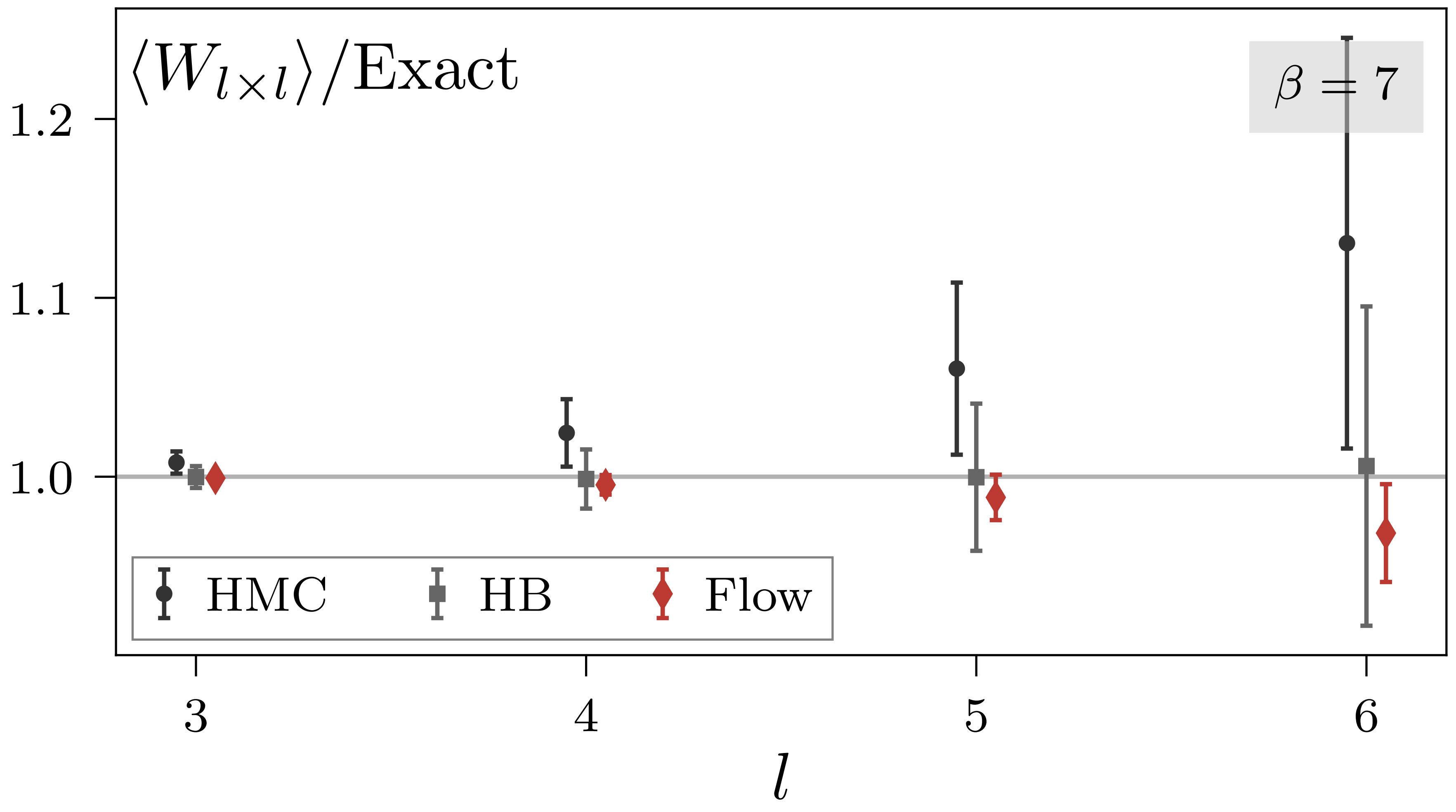


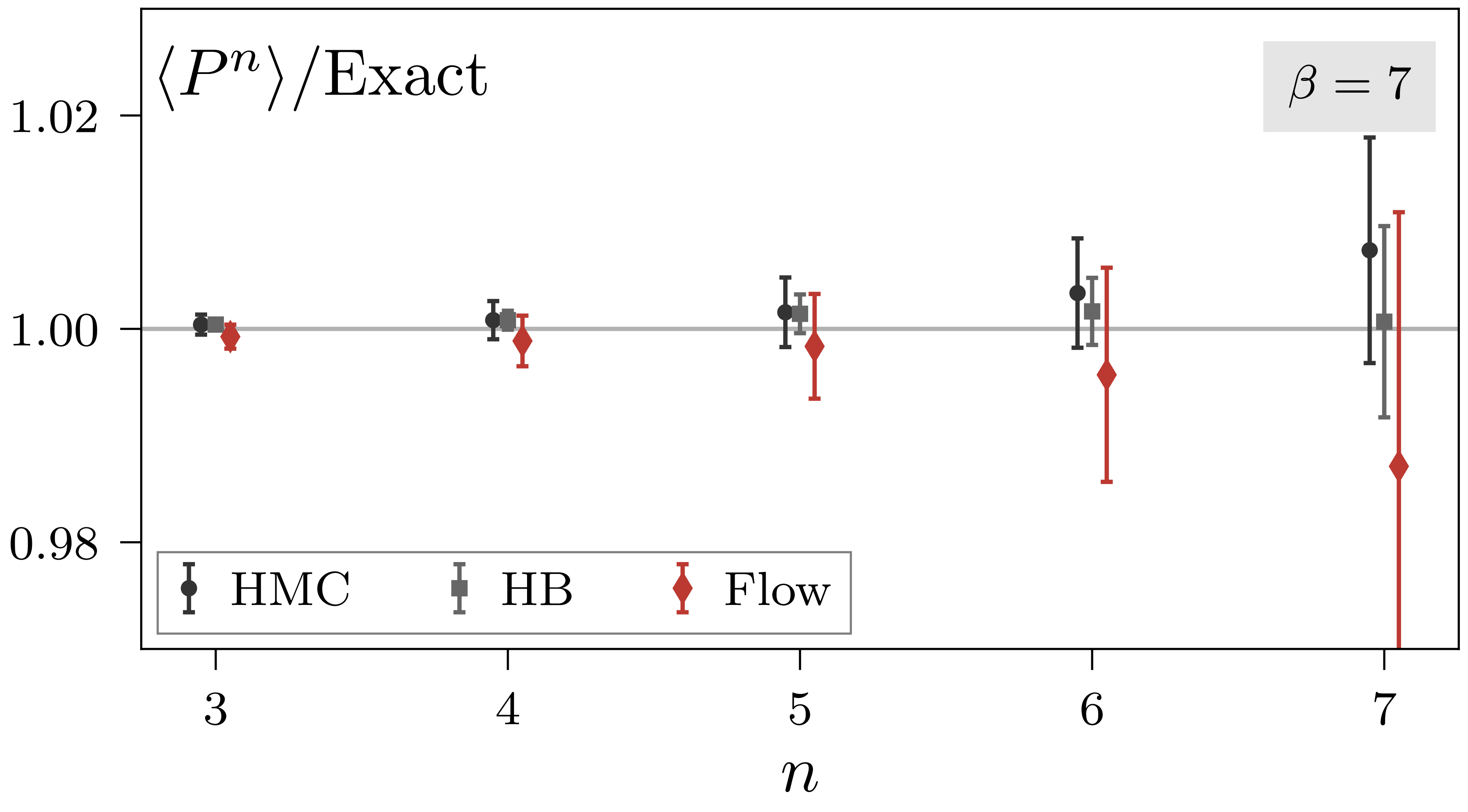


Density has zeros on vertical, horizontal, and diagonal lines where the slice crosses walls of cells

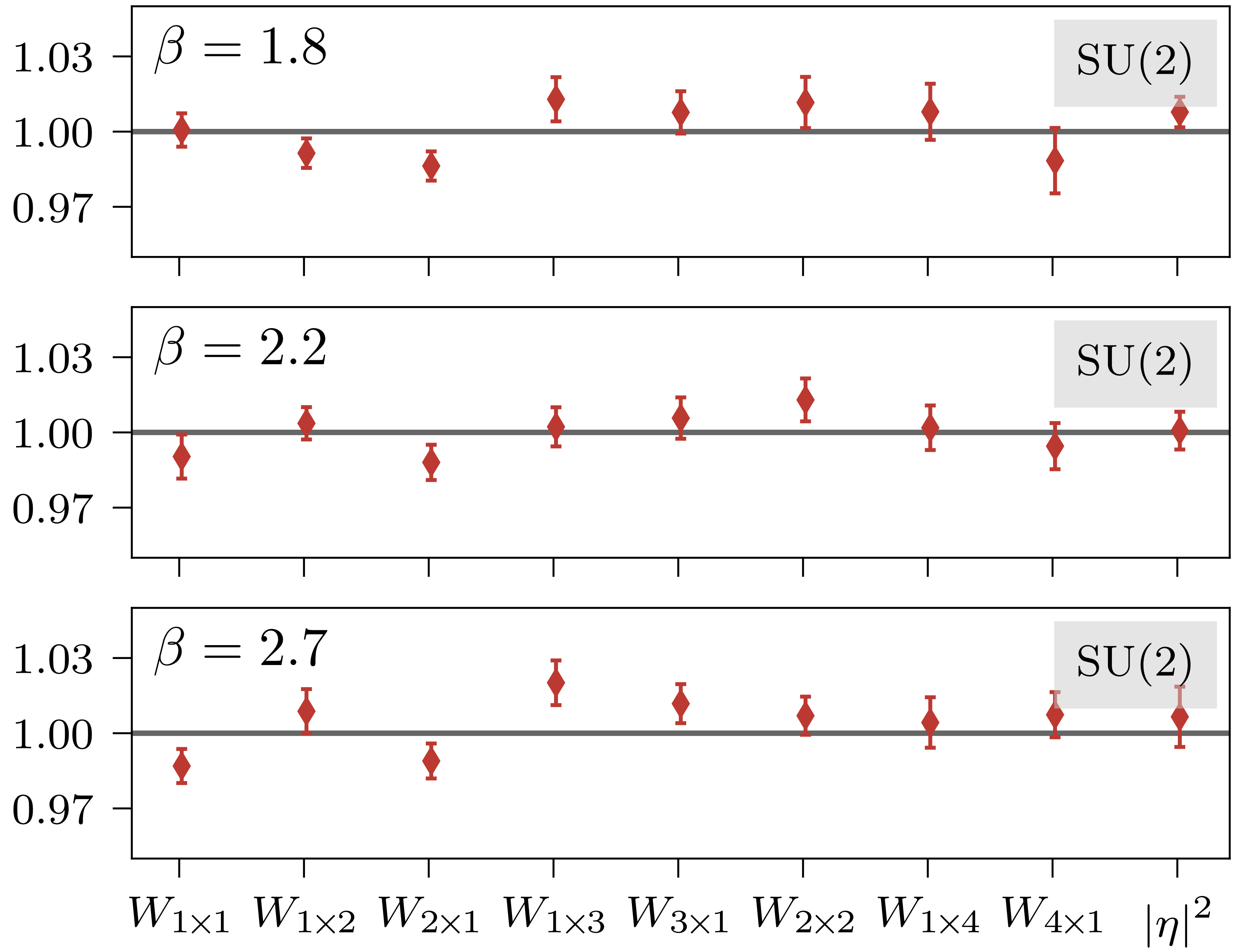
U(1) observables

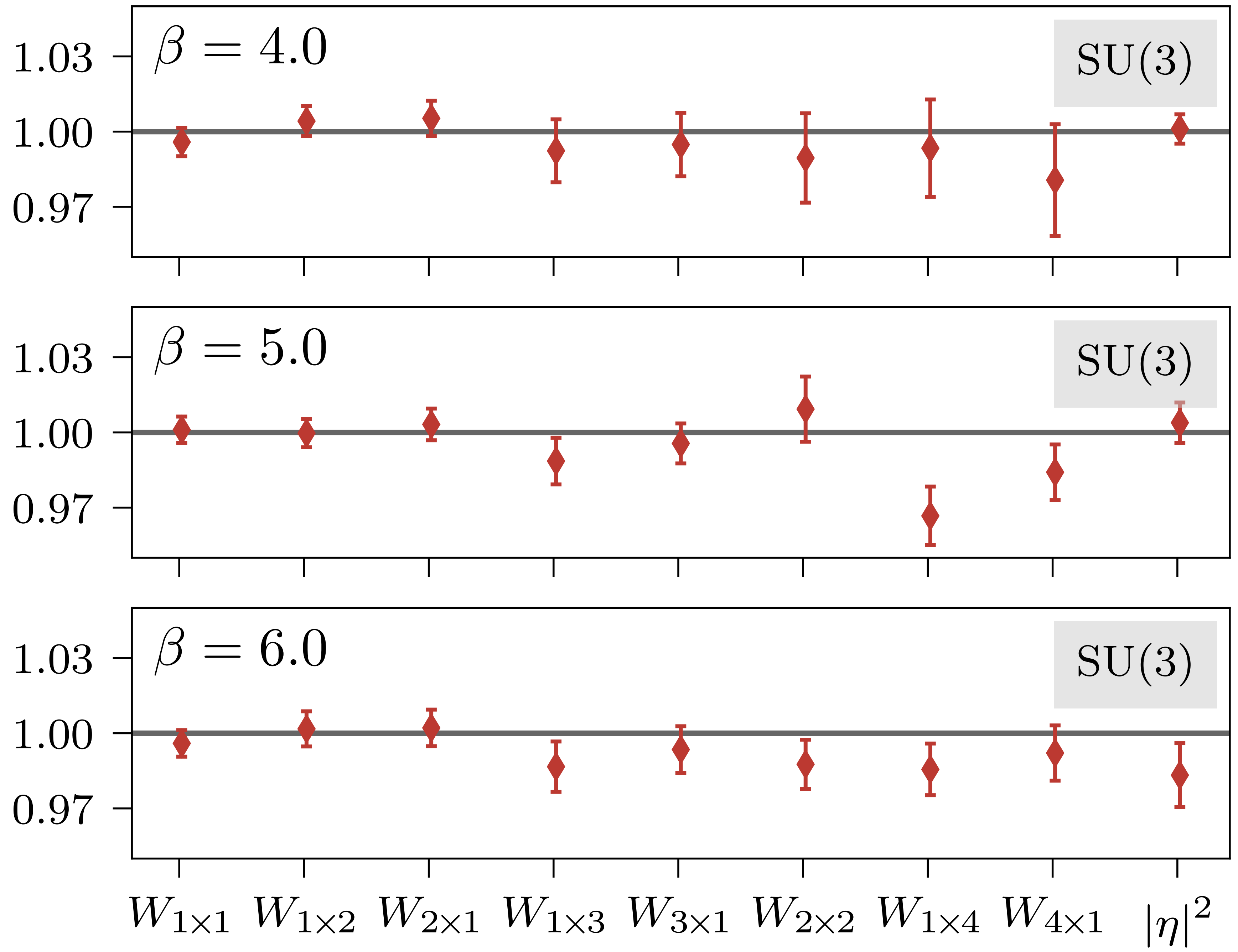






SU(N) observables



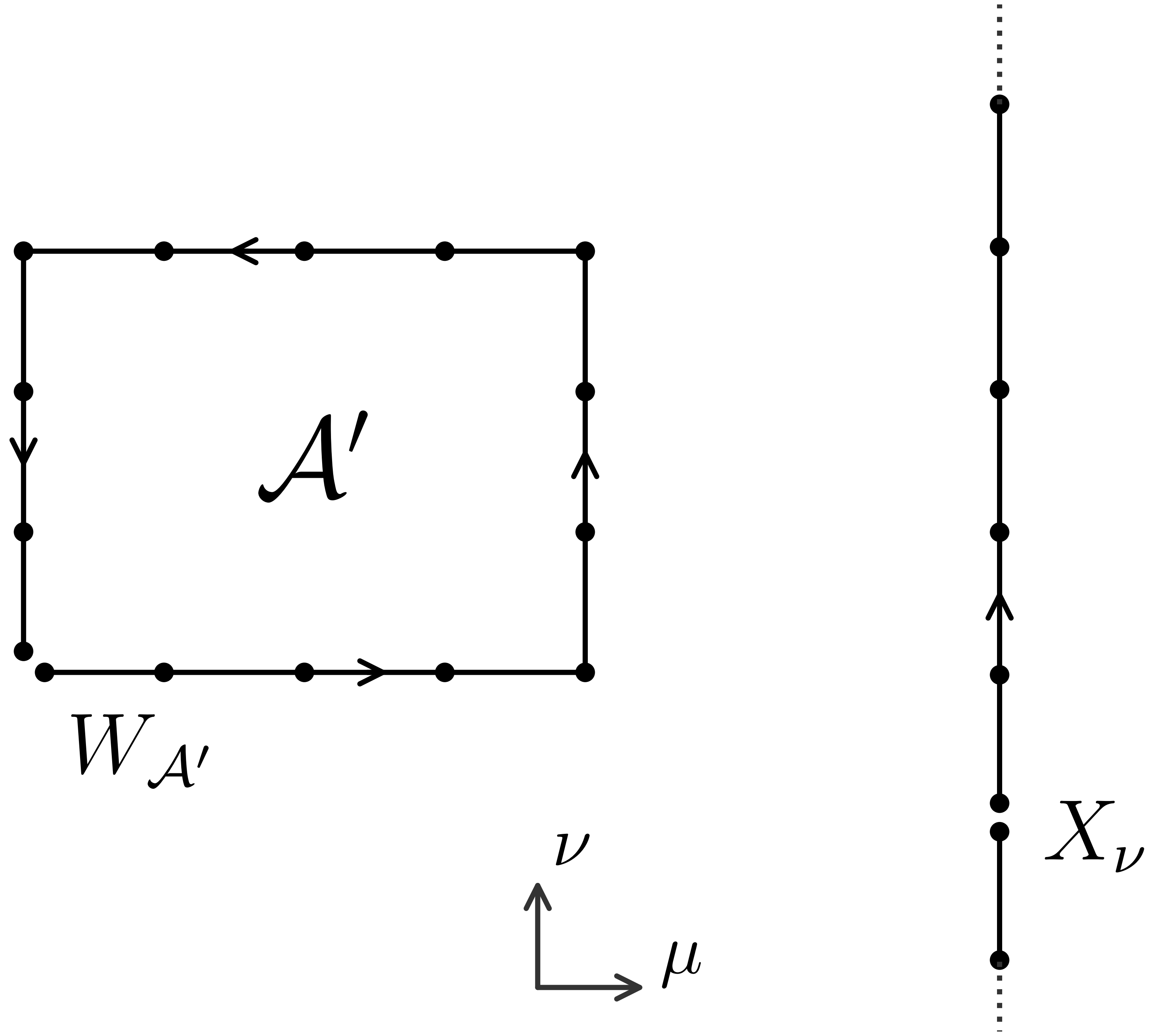


Center symmetry

Using **only contractible loops** in coupling layers enforces center symmetry.

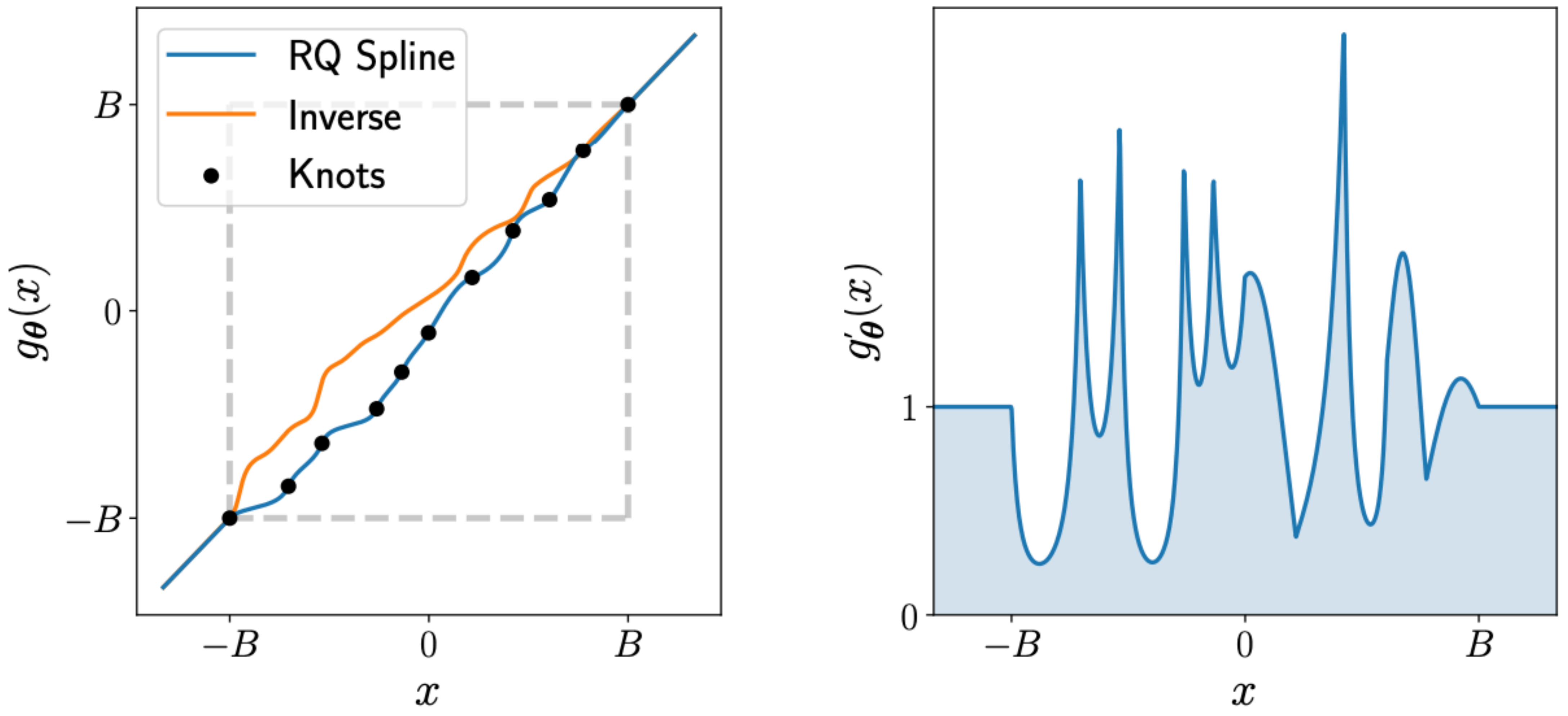
Fundamental fermions:

- Center symmetry explicitly broken
- Must include non-contractible loops (e.g. Polyakov) in the set of frozen and/or transformed loops



Details of $SU(2)$ models

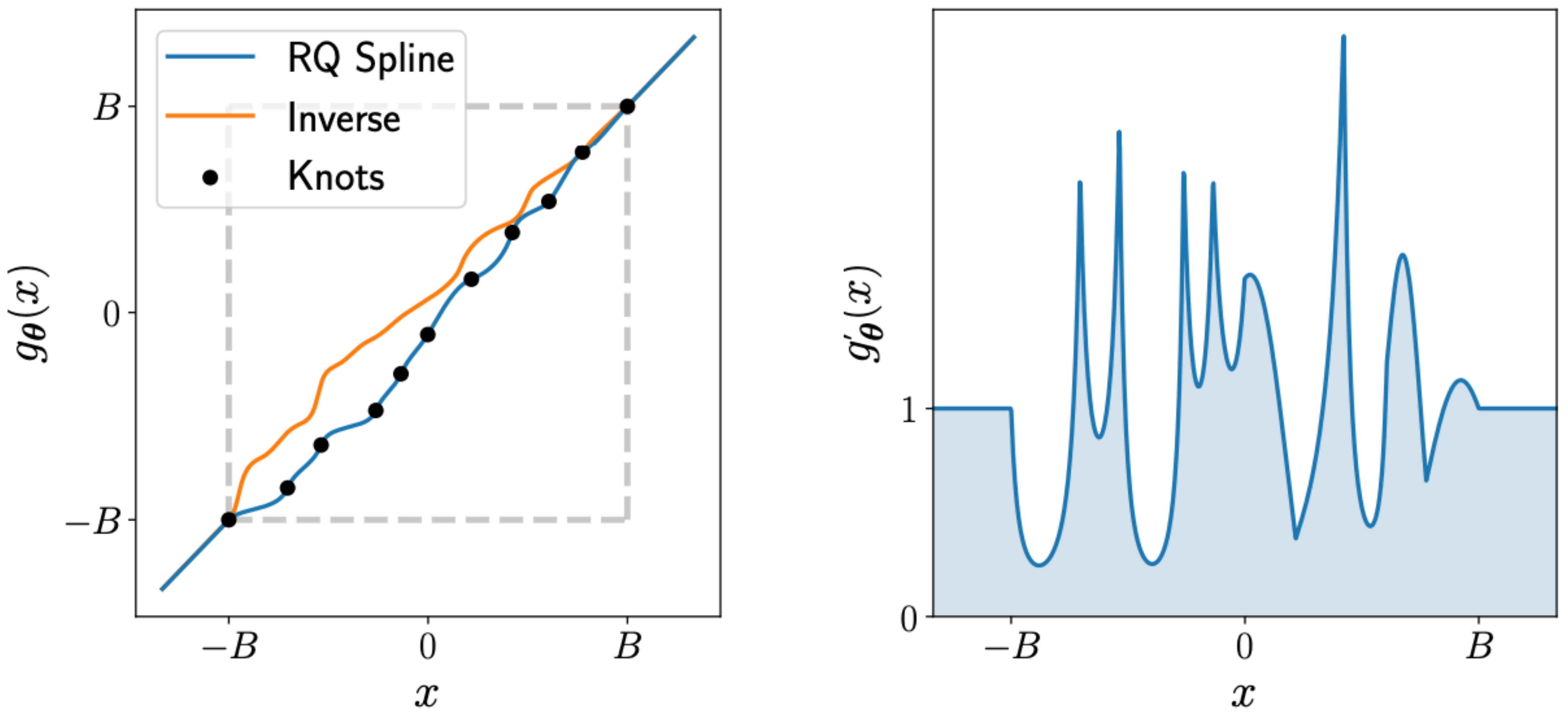
- Inner flow on open box Ω is a spline flow with **4 knots**
  - B and $-B$ boundaries align to 0 and 1 edges of the open box
- CNNs to compute the knot locations
  - 32 hidden channels
  - 2 hidden layers



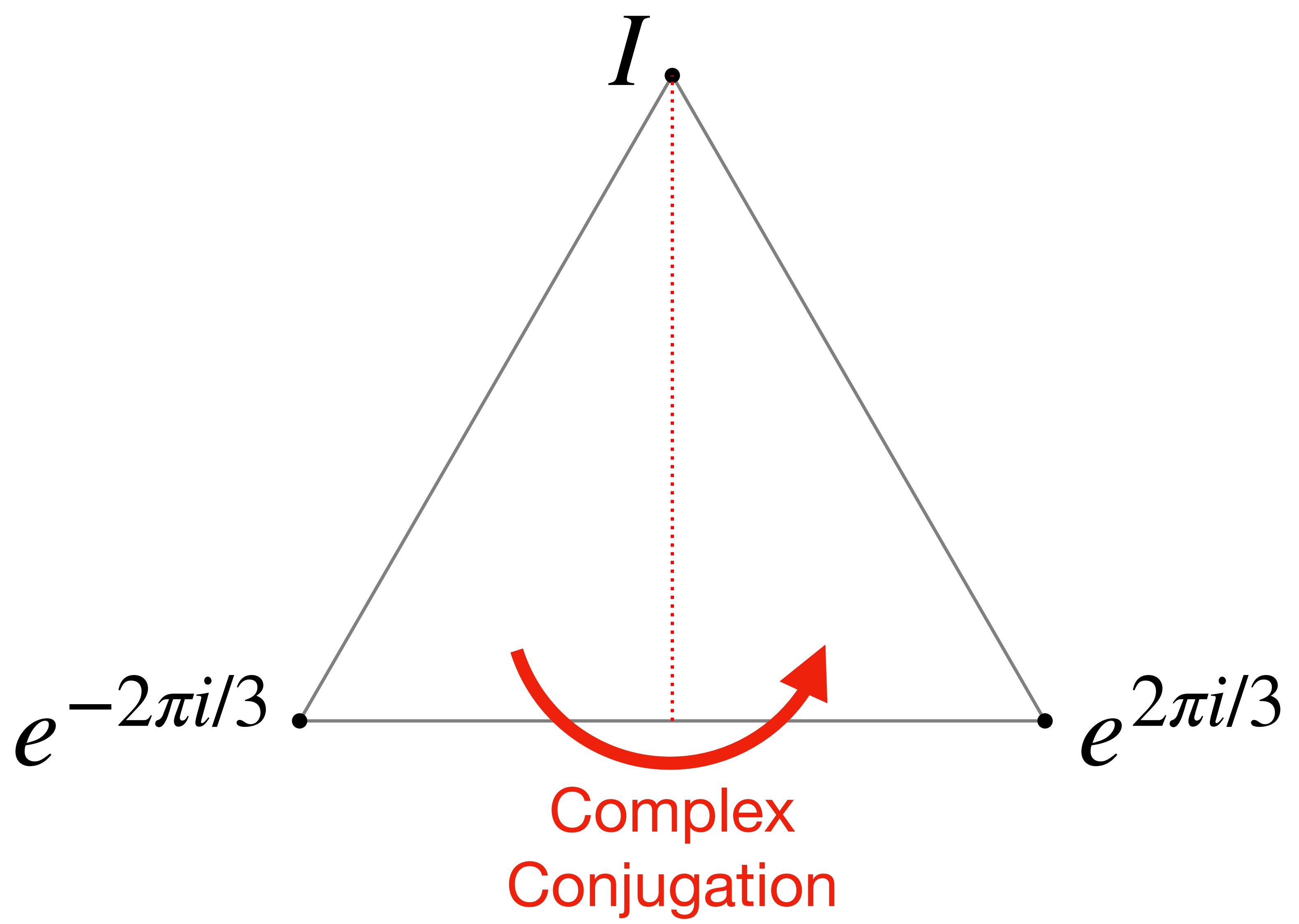
[Durkan, Bekasov, Murray, Papamakarios 1906.04032]

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]

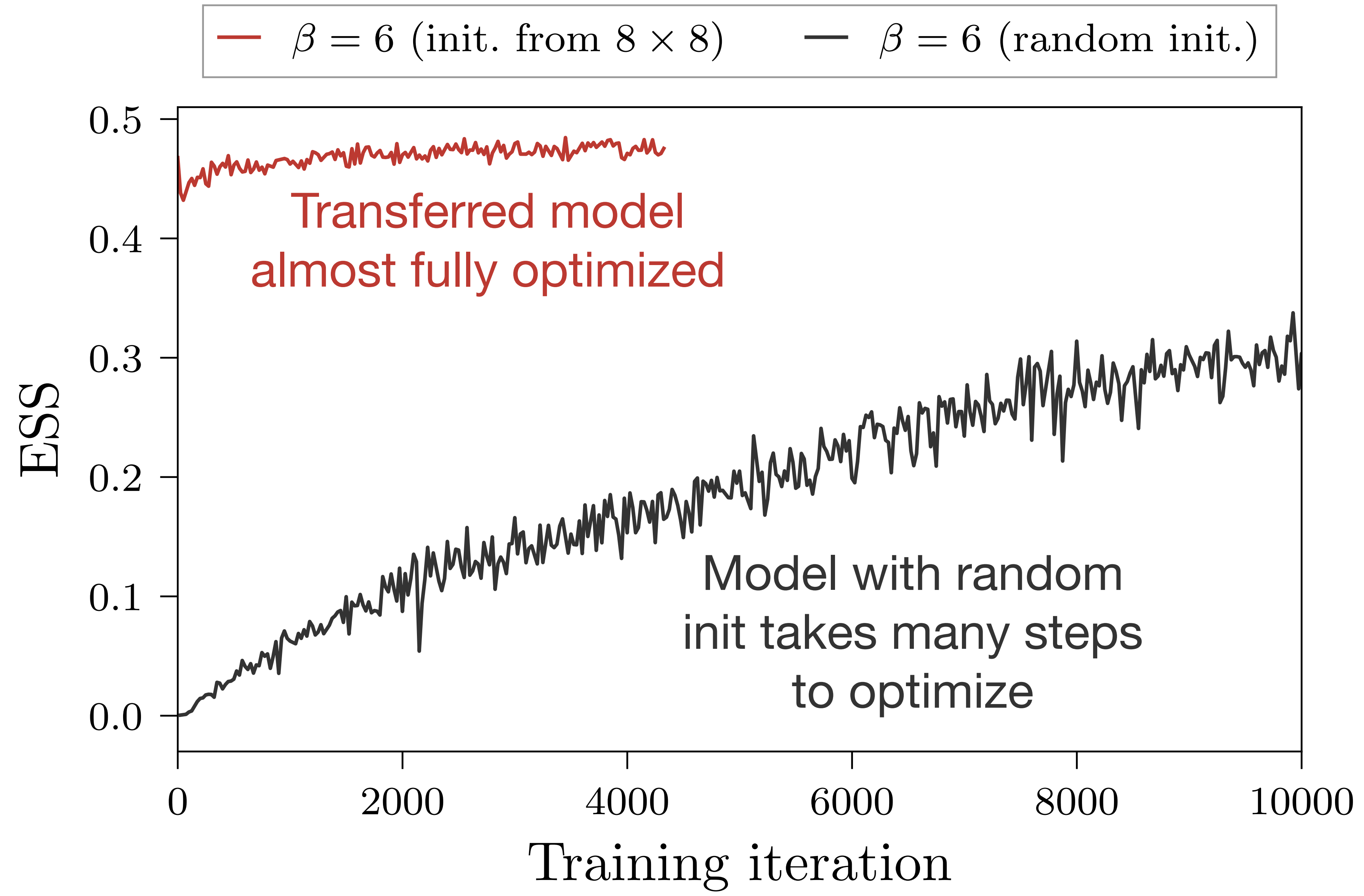


Gauge theory model training

- 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"



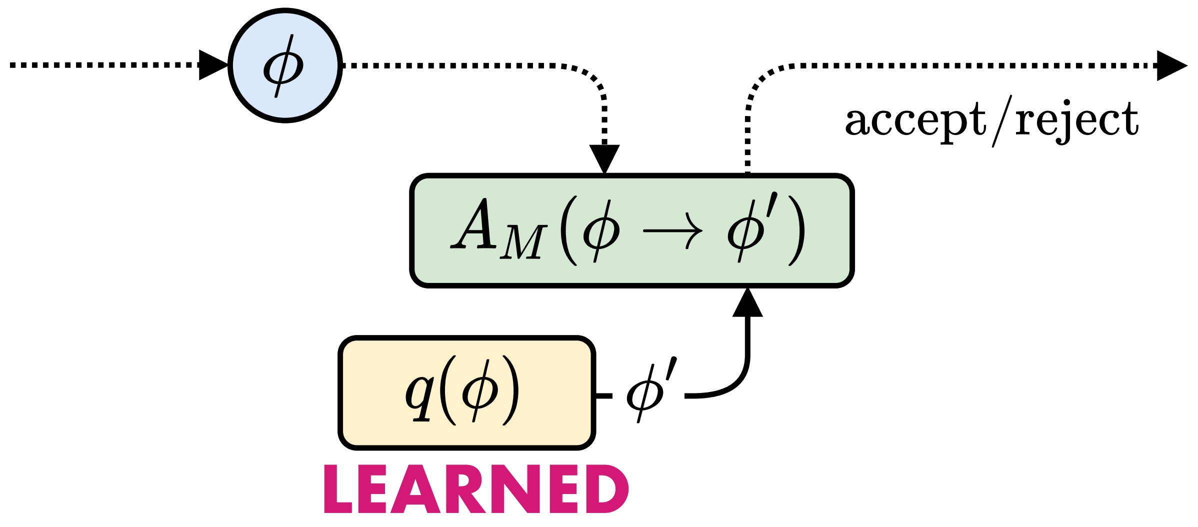
- **Transfer learning:** model trained first on 8×8 then used to initialize model for training on 16×16

[Albergo, GK, Racanière, Rezende, Urban, Boyda, Cranmer, Hackett, Shanahan **2106.05934**]

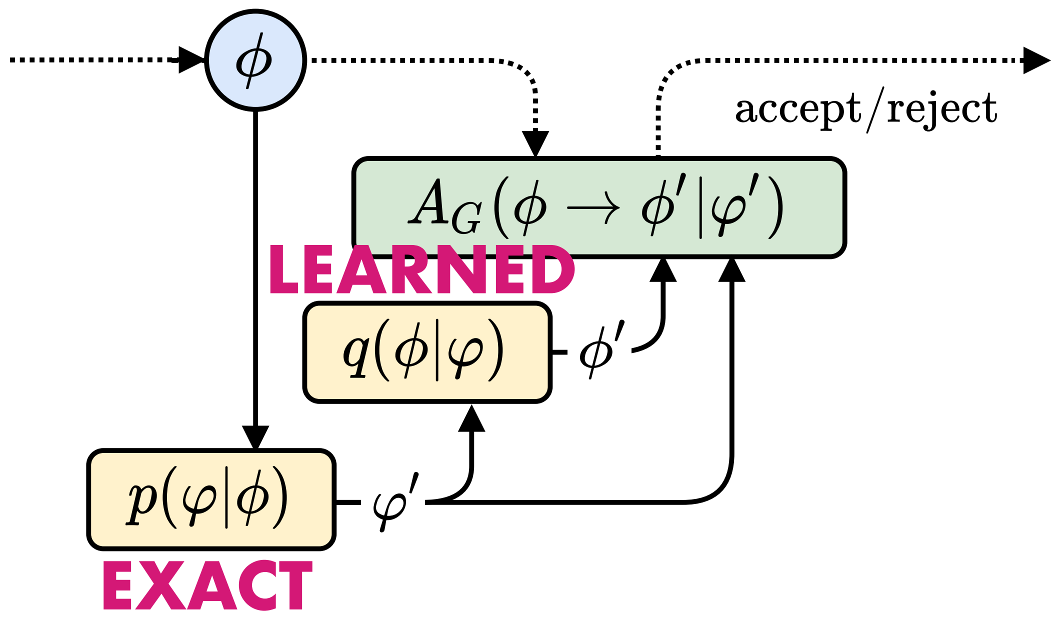
Proposed exact sampling schemes

Using a variety of learned densities $q(\ldots)$ — Best choice not yet clear!

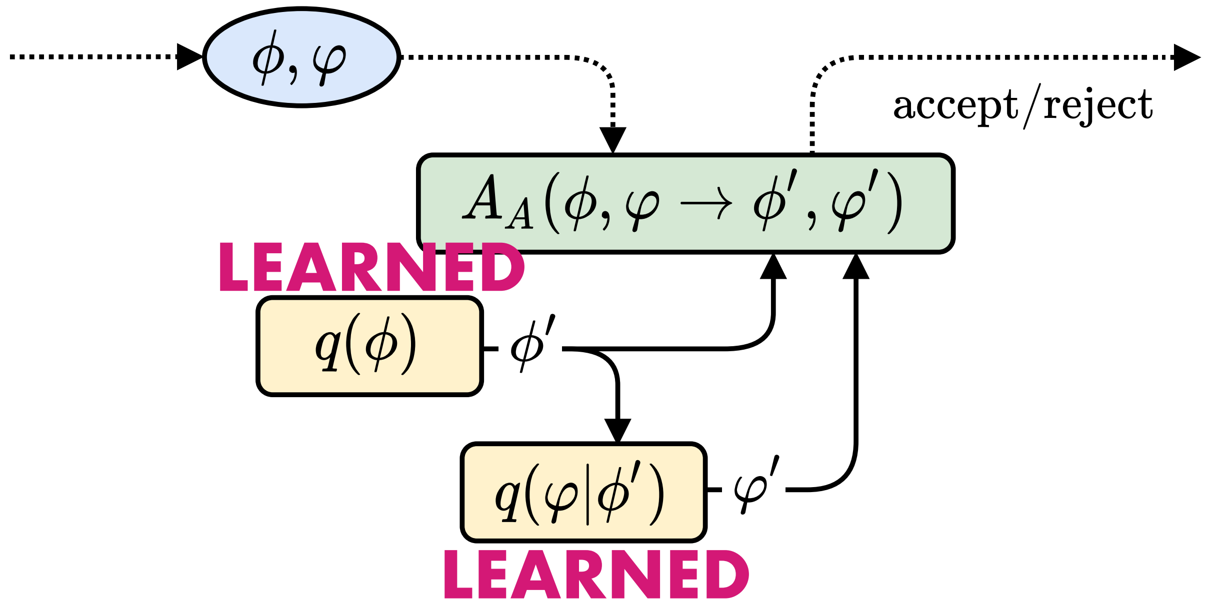
(1) ϕ-marginal



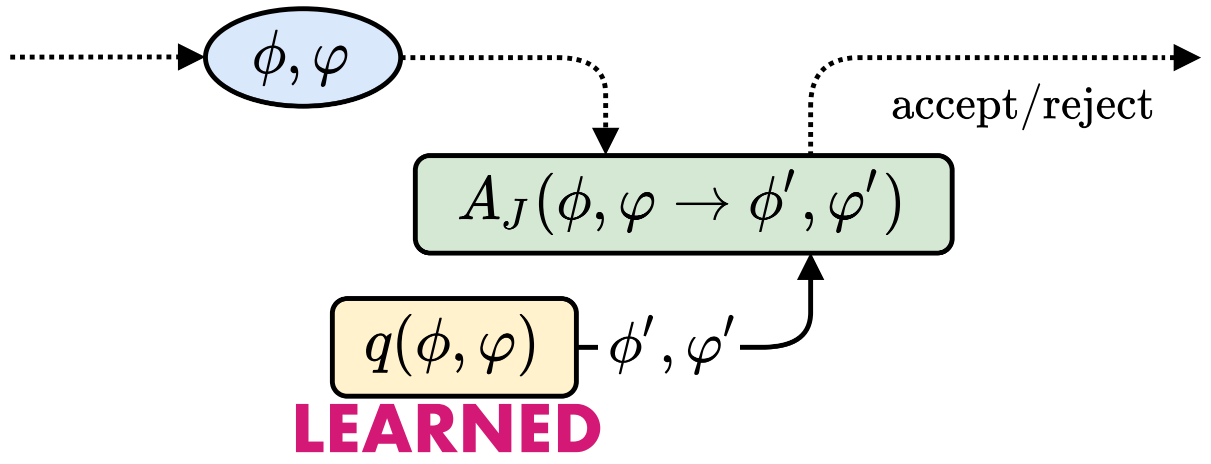
(2) Gibbs



(3) Autoregressive



(4) Joint



Key takeaways:

- **Exact** regardless of quality of modeled densities $q(\ldots)$
- Can define sampler over
  - … bosonic fields alone (ϕ) or
  - … bosonic + PF fields (ϕ, φ)
- For **Gibbs**, even a perfect model may have residual autocorrelations