Flow-based sampling for lattice gauge theories

Fernando Romero-López

BNL

February 17th

Massachusetts Institute of Technology

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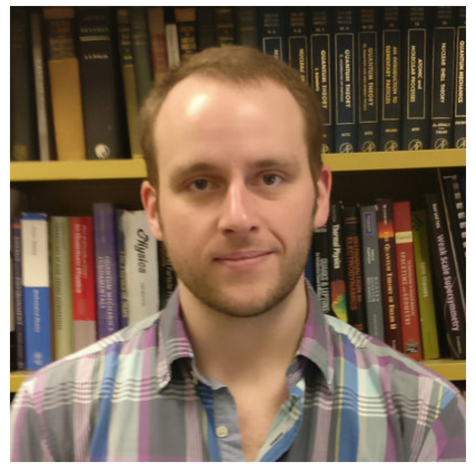
Collaboration (non-exhaustive)

Massachusetts Institute of Technology

- Phiala Shanahan



- Dan Hackett

- Fernando Romero-Lopez

- Ryan Abbot

- Julian Urban

- Denis Boyda

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- Kyle Cranmer

WISCONSIN UNIVERSITY OF WISCONSIN–MADISON

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- Michael Albergo

u^b

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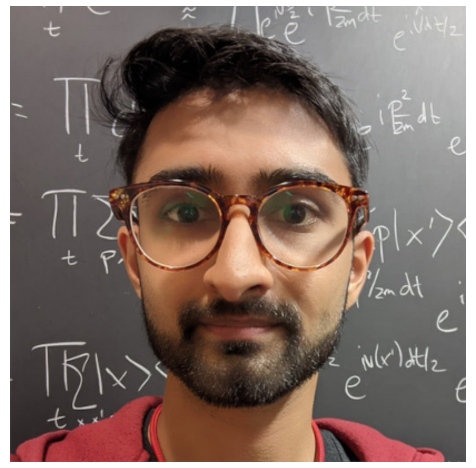

- Gurtej Kanwar

DeepMind

- Sébastien Racanière

- Danilo Rezende

- Ali Razavi

- Aleksandar Botev

- Alex Matthews

Outline

1. Introduction to Lattice QCD
2. Critical slowing down in Lattice QCD
3. Flow-based sampling for Lattice Field Theory
4. Flow-based sampling for gauge theories
5. Flows for fermionic gauge theories

Introduction to Lattice QCD

Quantum Chromodynamics

> Quantum chromodynamics is conceptually simple. Its realization in nature, however, is usually very complex.
>
> Frank Wilczek

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$$\mathscr{L}_{QCD} = \sum_i^{N_f} \bar{q}_i \left(D_\mu \gamma^\mu + m_i \right) q_i + \frac{1}{4 g_s^2} G^a_{\mu\nu} G_a^{\mu\nu}$$

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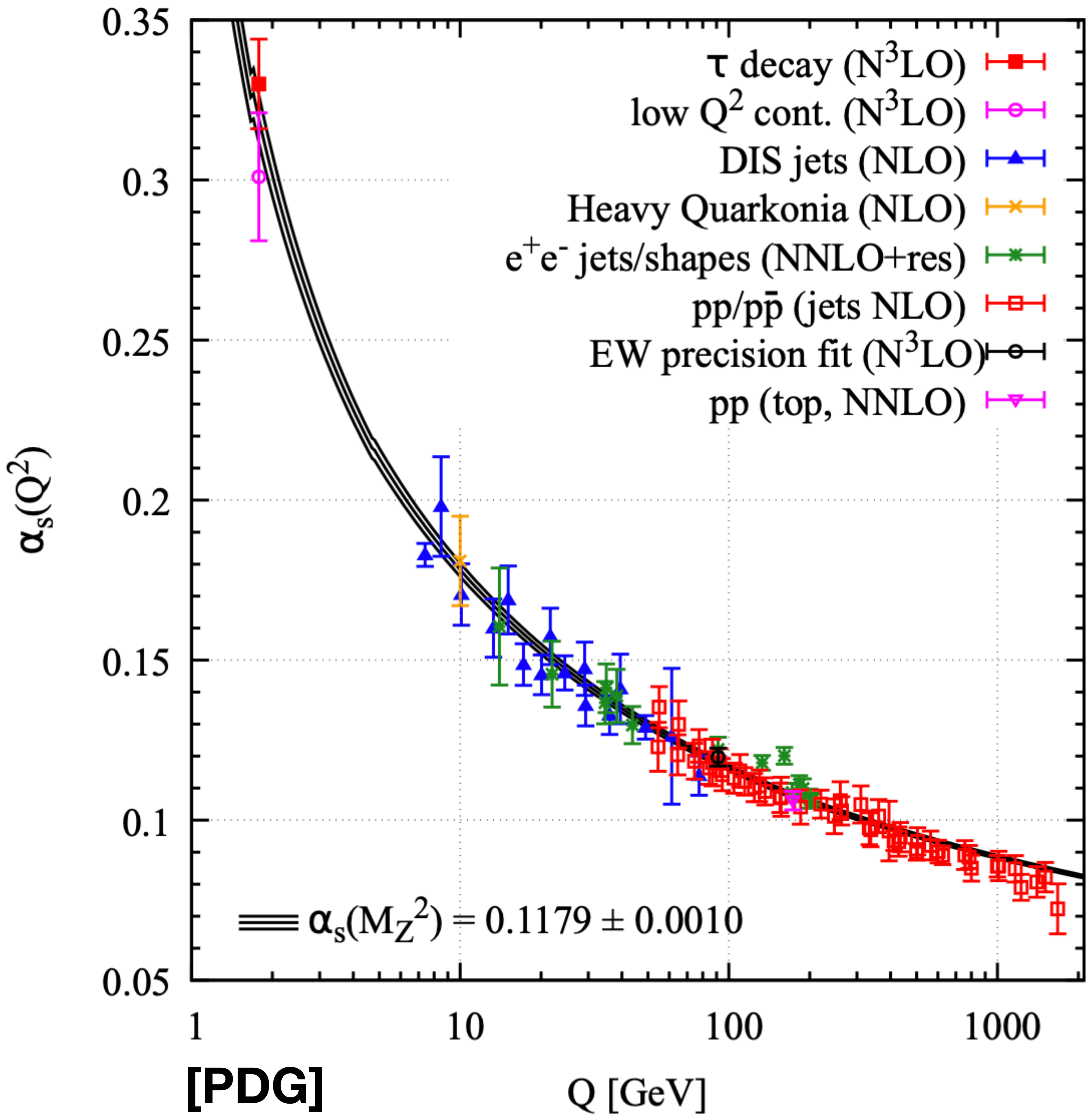
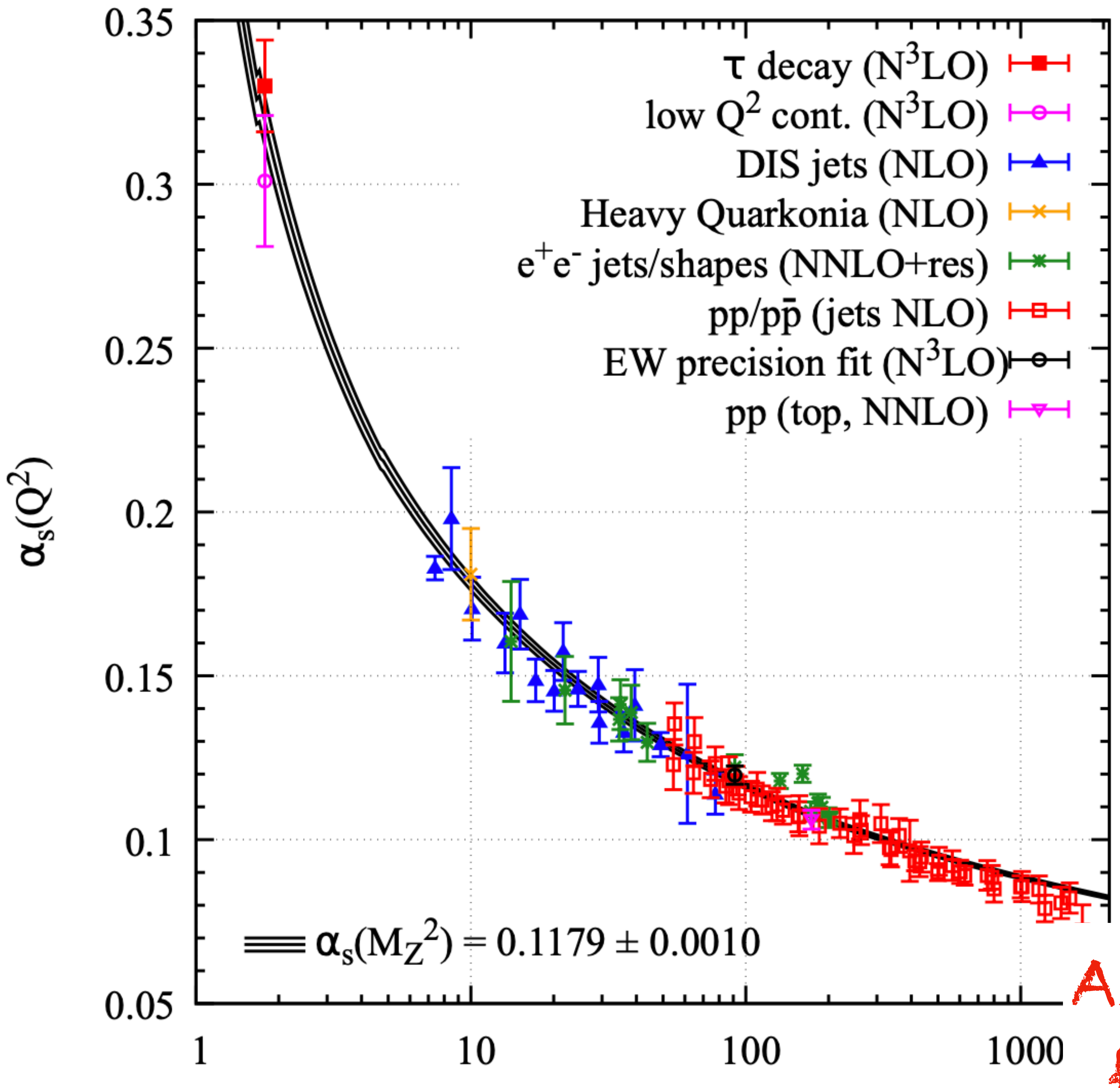
Quantum Chromodynamics



[PDG]

Quantum Chromodynamics



[PDG]

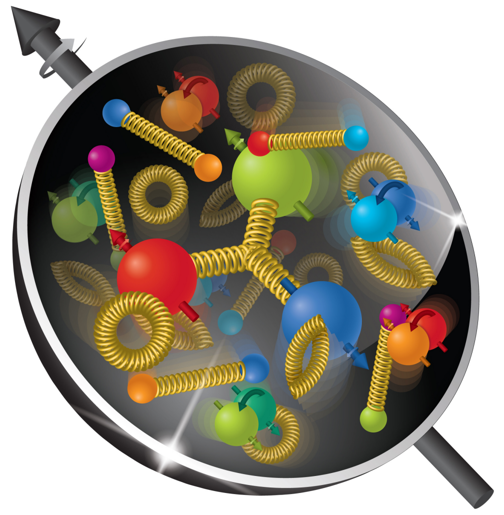
Asymptotic freedom

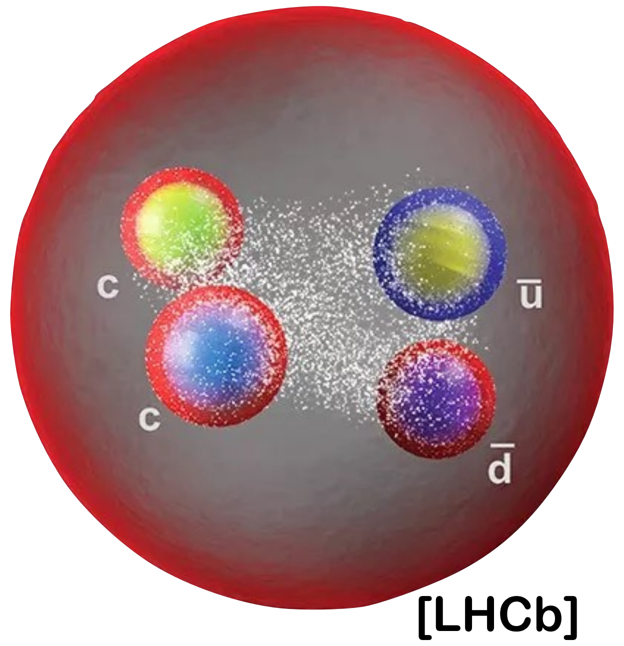
Perturbation theory:

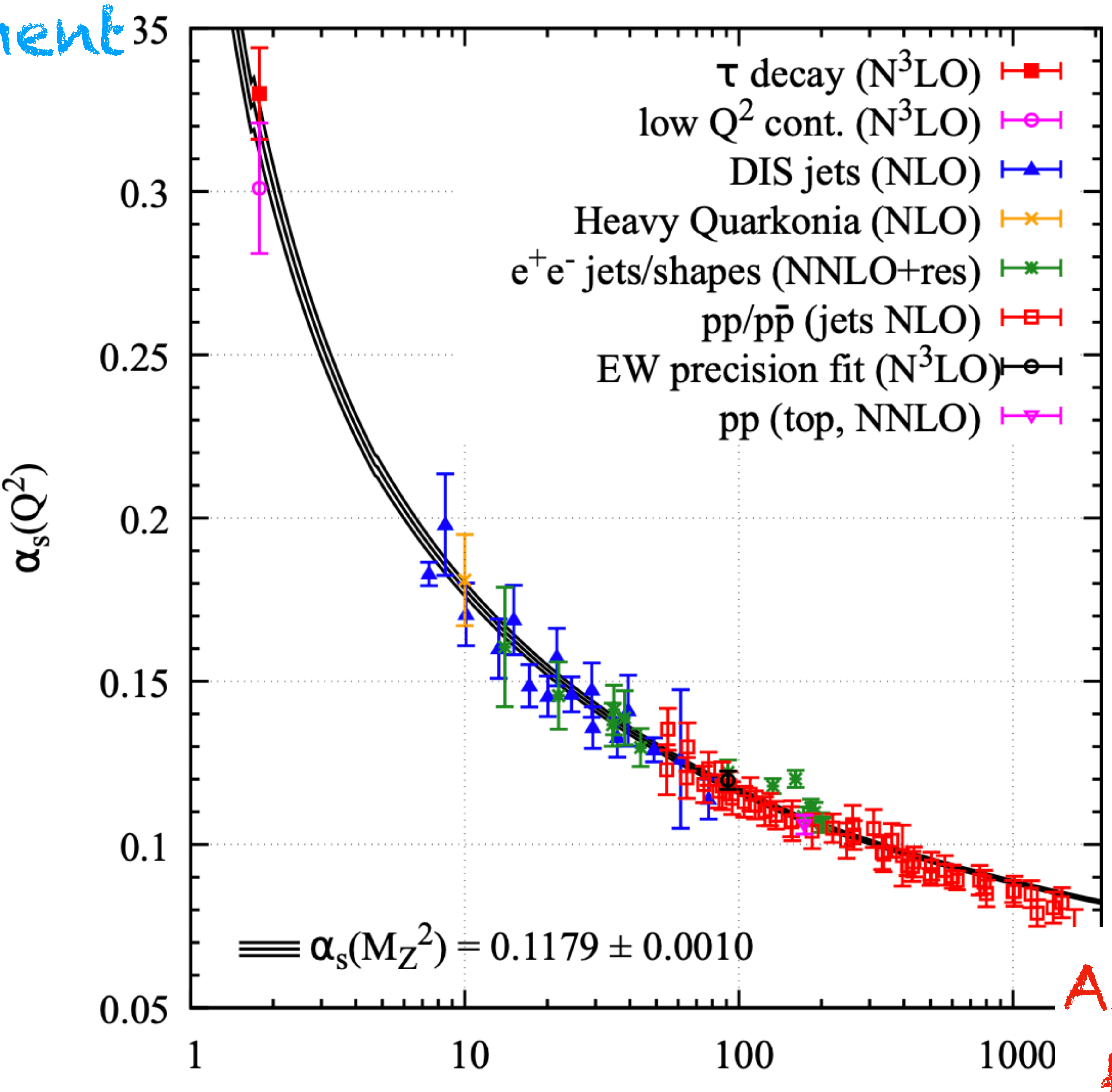
$$\mathcal{O} = \mathcal{O}_0 + \alpha_s \mathcal{O}_1 + \alpha_s^2 \mathcal{O}_2 + \ldots$$

Quantum Chromodynamics

Confinement







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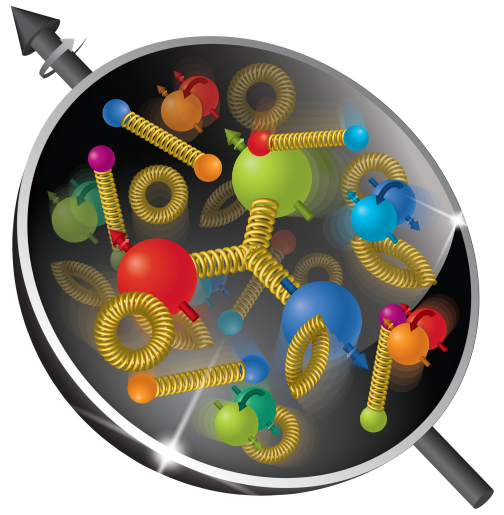
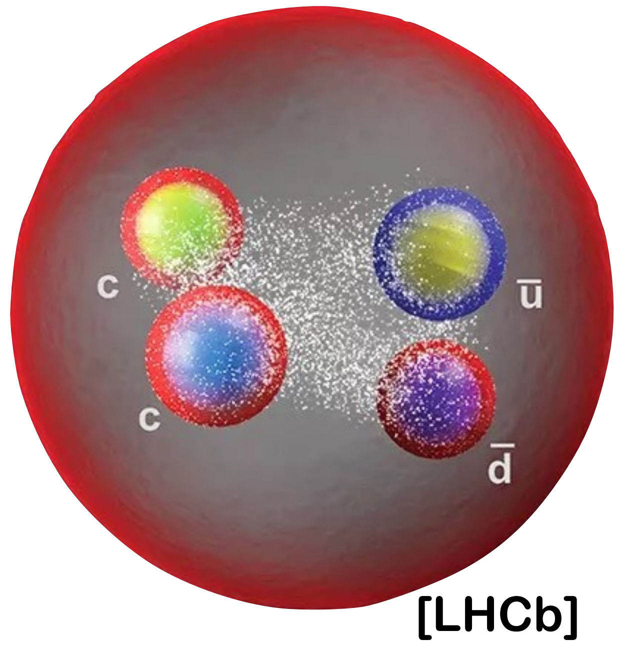
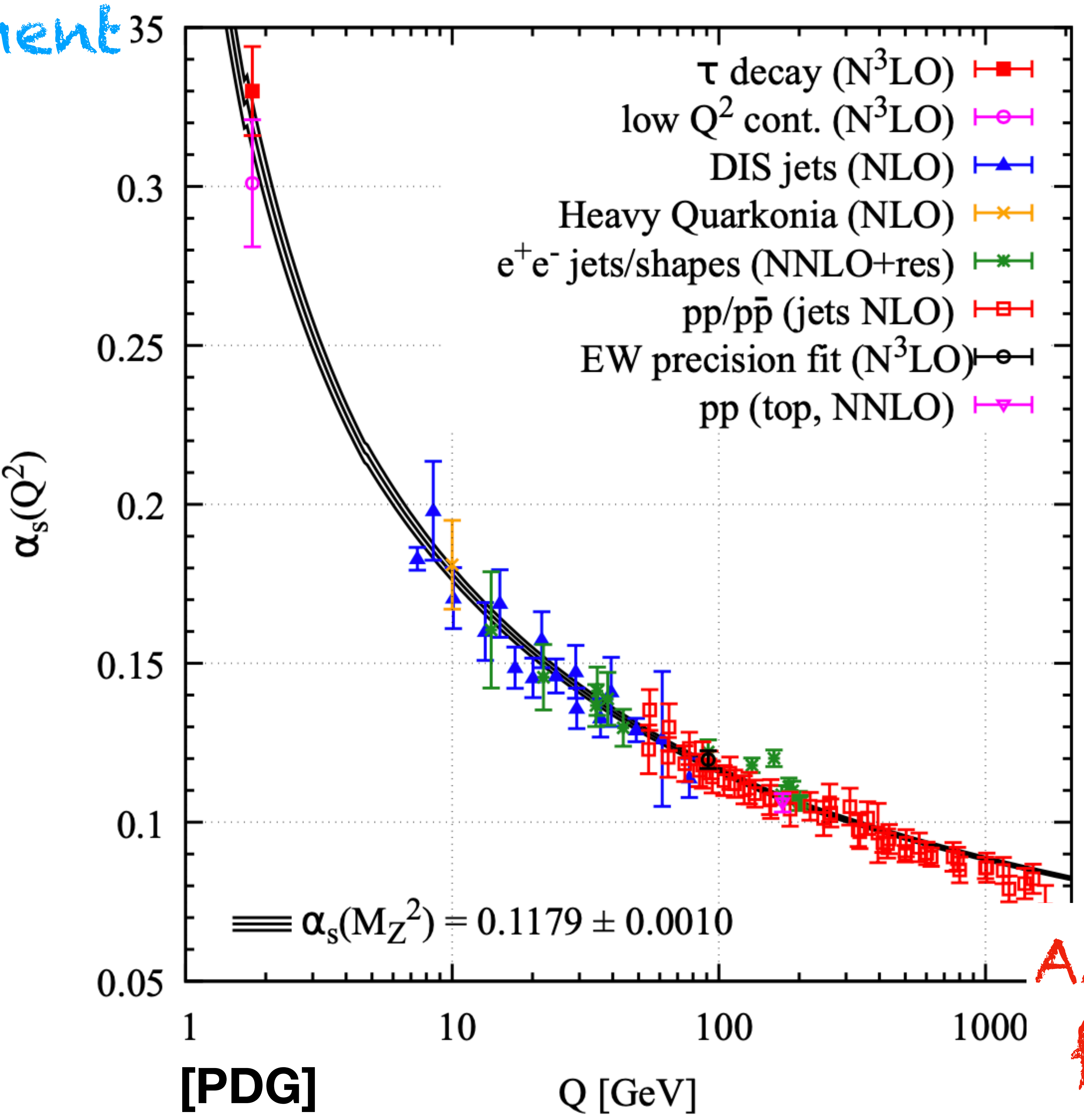




[LHCb]

Non-perturbative at low energies

Lattice QCD



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Fernando Romero-López, MIT

Lattice Field Theory

- LFT is the first-principles treatment of the generic QFT

  - Path integral

$$\mathcal{Z} = \int D\phi \, e^{-iS(\phi)}$$

Lattice Field Theory

- LFT is the first-principles treatment of the generic QFT

  - Path integral in Euclidean or imaginary time: statistical meaning

$$\mathcal{Z} = \int D\phi \, e^{-S_E(\phi)} \quad \text{, where} \quad S_E(\phi) = \int d^4x \, \mathscr{L}_E(\phi)$$

Boltzmann factor

Euclidean action

Lattice Field Theory

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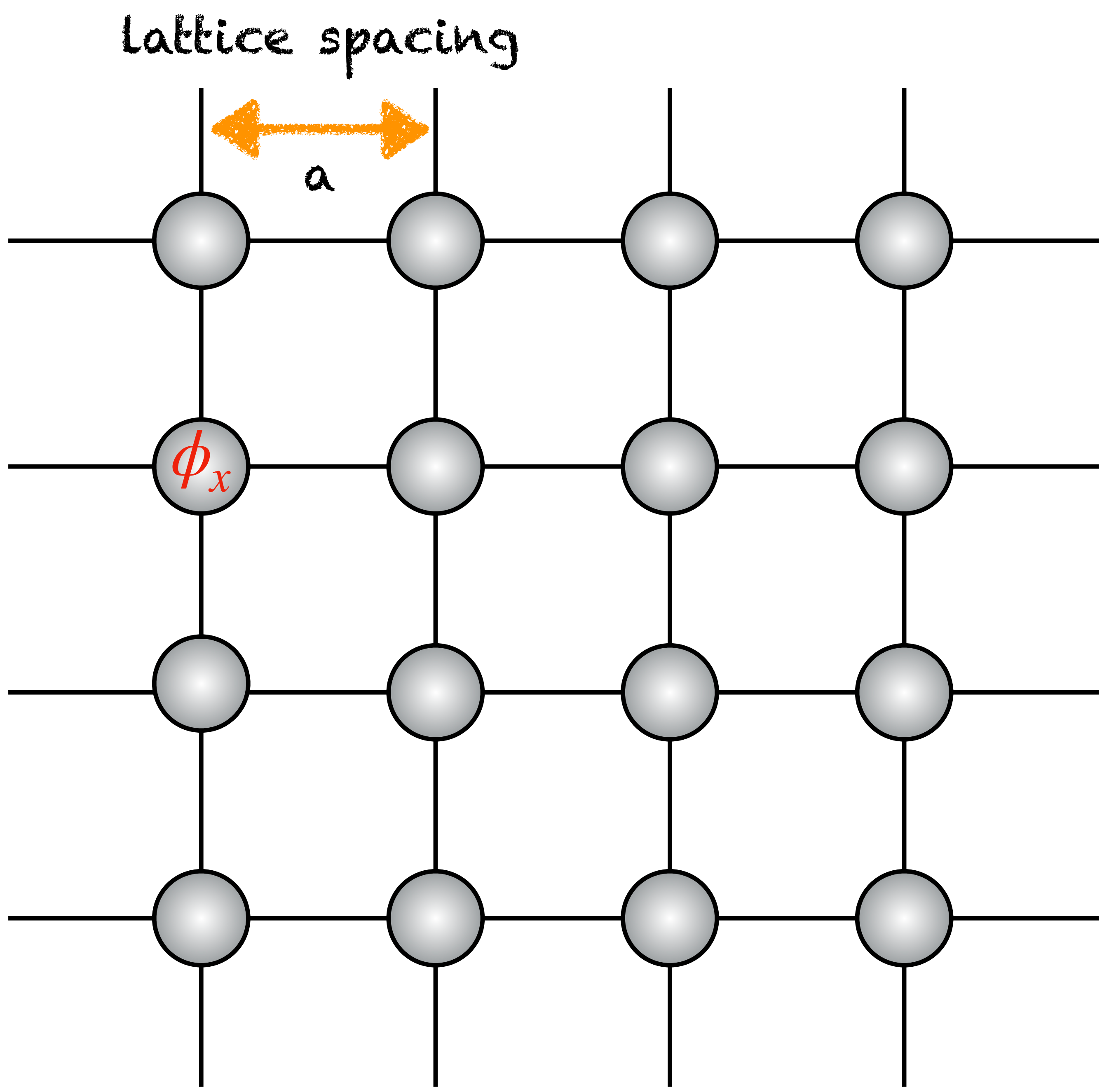
Euclidean action

  - Discretize quantum fields (real scalars):

Continuum: $$S_E = \int d^4x \left[\frac{1}{2} \partial_\mu \phi(x)^2 + \frac{m^2}{2} \phi(x)^2 + \lambda \phi(x)^4 \right]$$

Lattice: $$S_E = a^4 \sum_x \frac{1}{2a^2} (\phi_{x+\mu} - \phi_x)^2 + \frac{m^2}{2} \phi_x^2 + \lambda \phi_x^4$$



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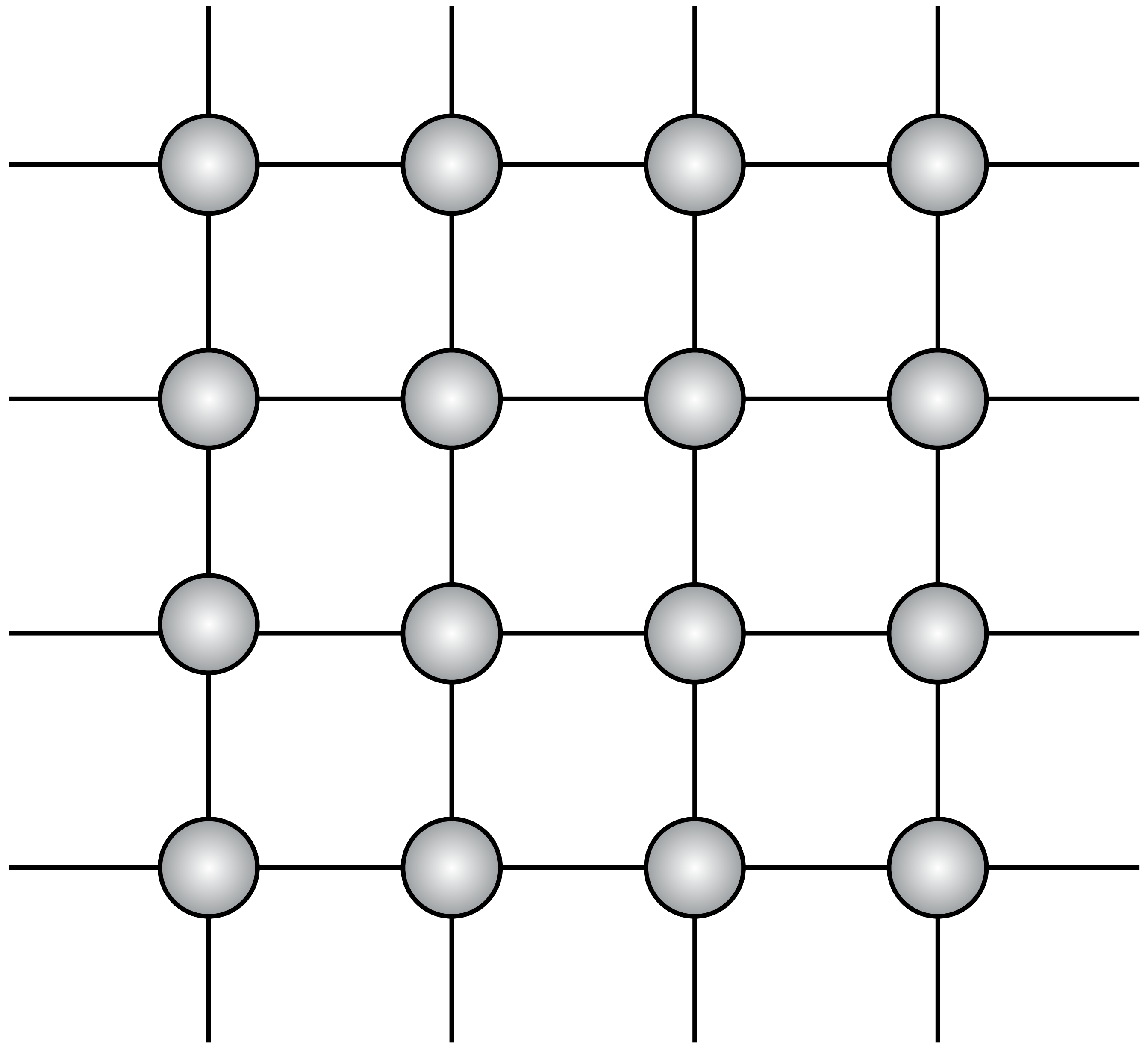
Lattice QCD

- **LFT applied to QCD can be used to solve the dynamics of the strong interaction at hadronic energies**

  - **Lattice QCD partition function**

$$\mathcal{Z} = \int D\psi D\bar{\psi} DA e^{-S_E(\psi,\bar{\psi},A_\mu)}$$

Boltzmann factor



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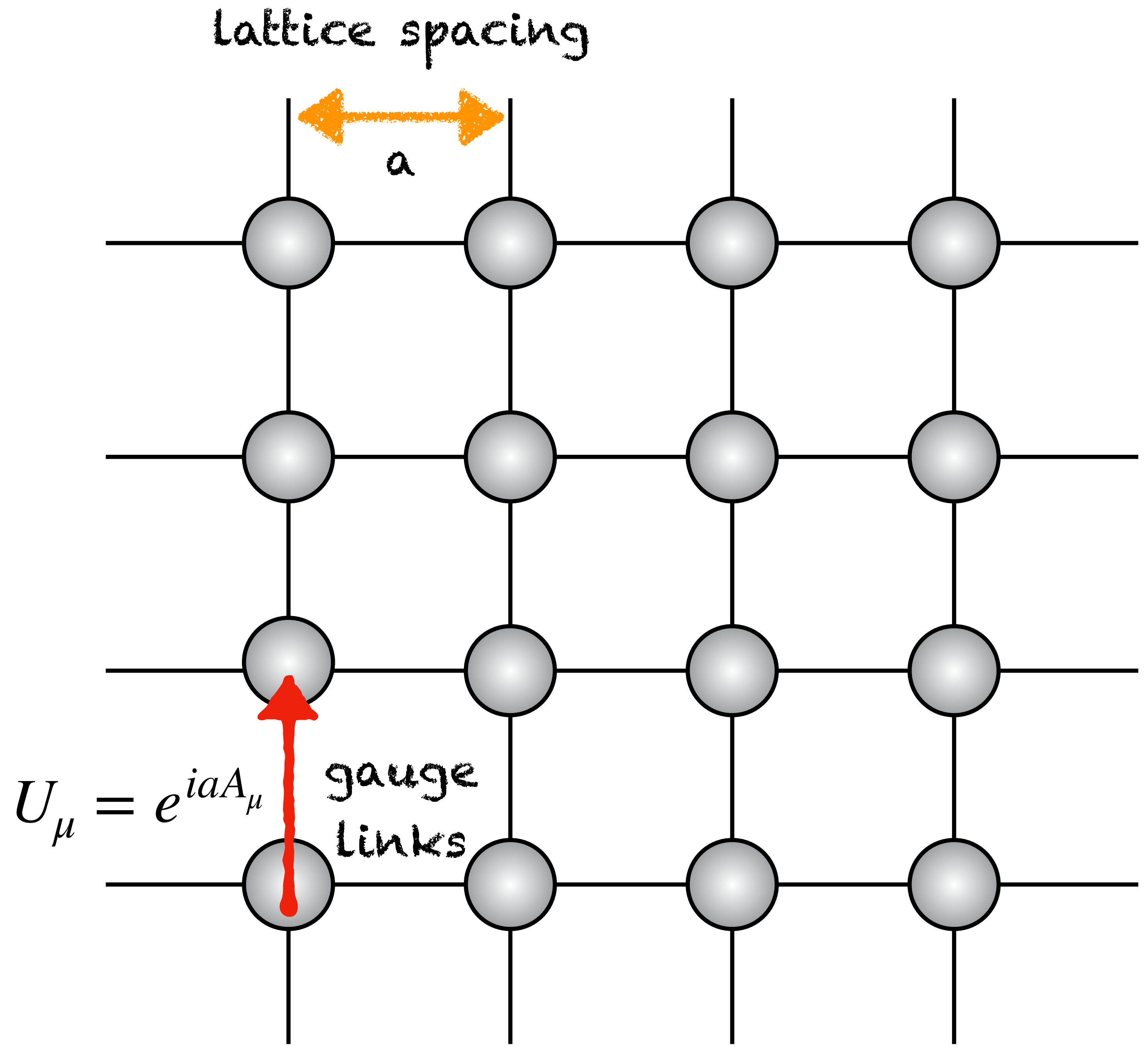
  - Discretize gauge fields and fermion fields:

    →Under control but technical

    →Need continuum limit



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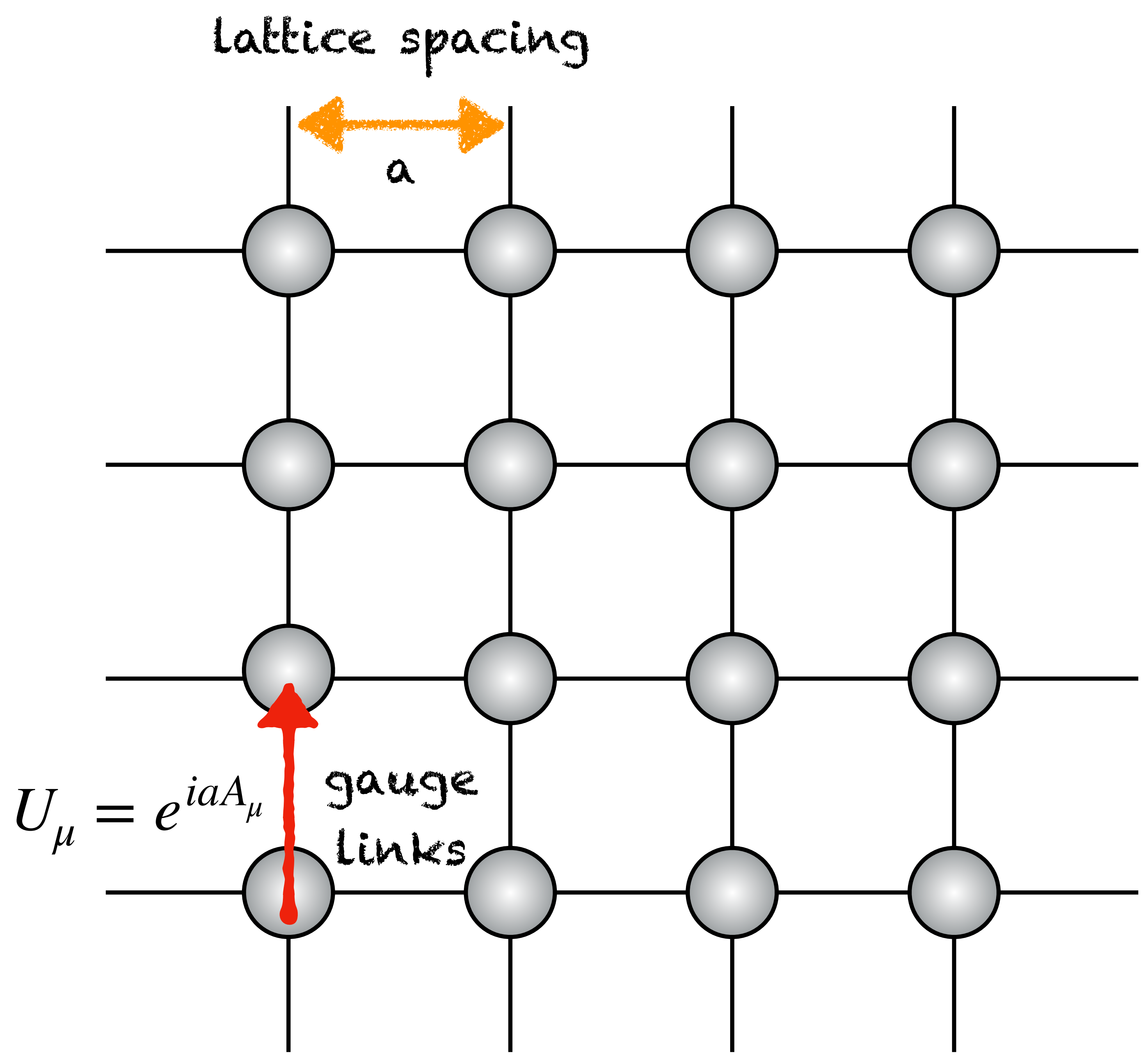
Boltzmann factor

- **Discretize gauge fields and fermion fields:**
  - →Under control but technical
  - →Need continuum limit

- **Compute observables as expectation values**

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int D\psi D\bar{\psi} DA\, \mathcal{O}\, e^{-S(\psi,\bar{\psi},A_\mu)}$$



An integral over many variables:
$2 \times 3^2 \times 4 \times L^4 \simeq 10^{10}$

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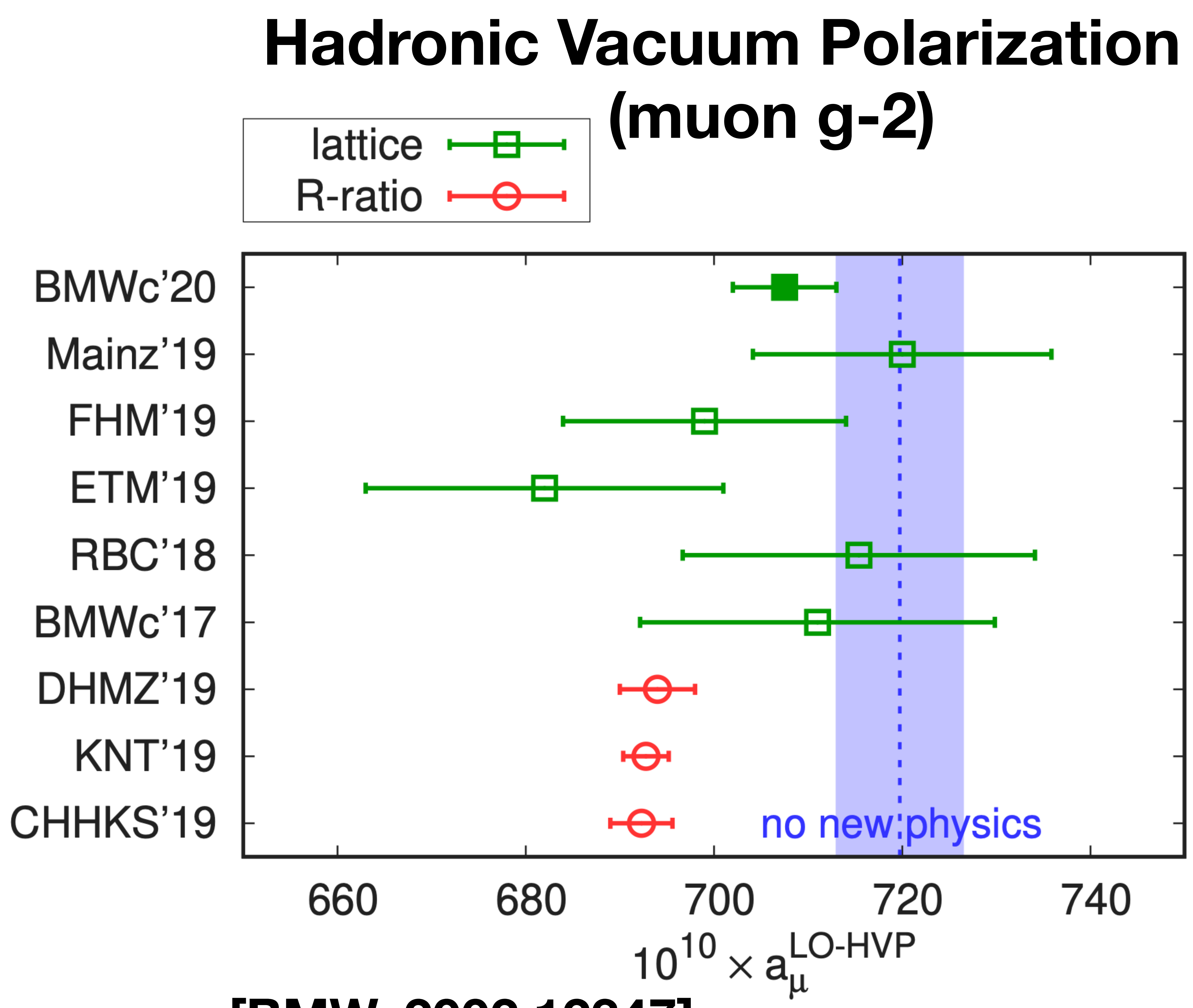
Many different applications



[BMW, 2002.12347]

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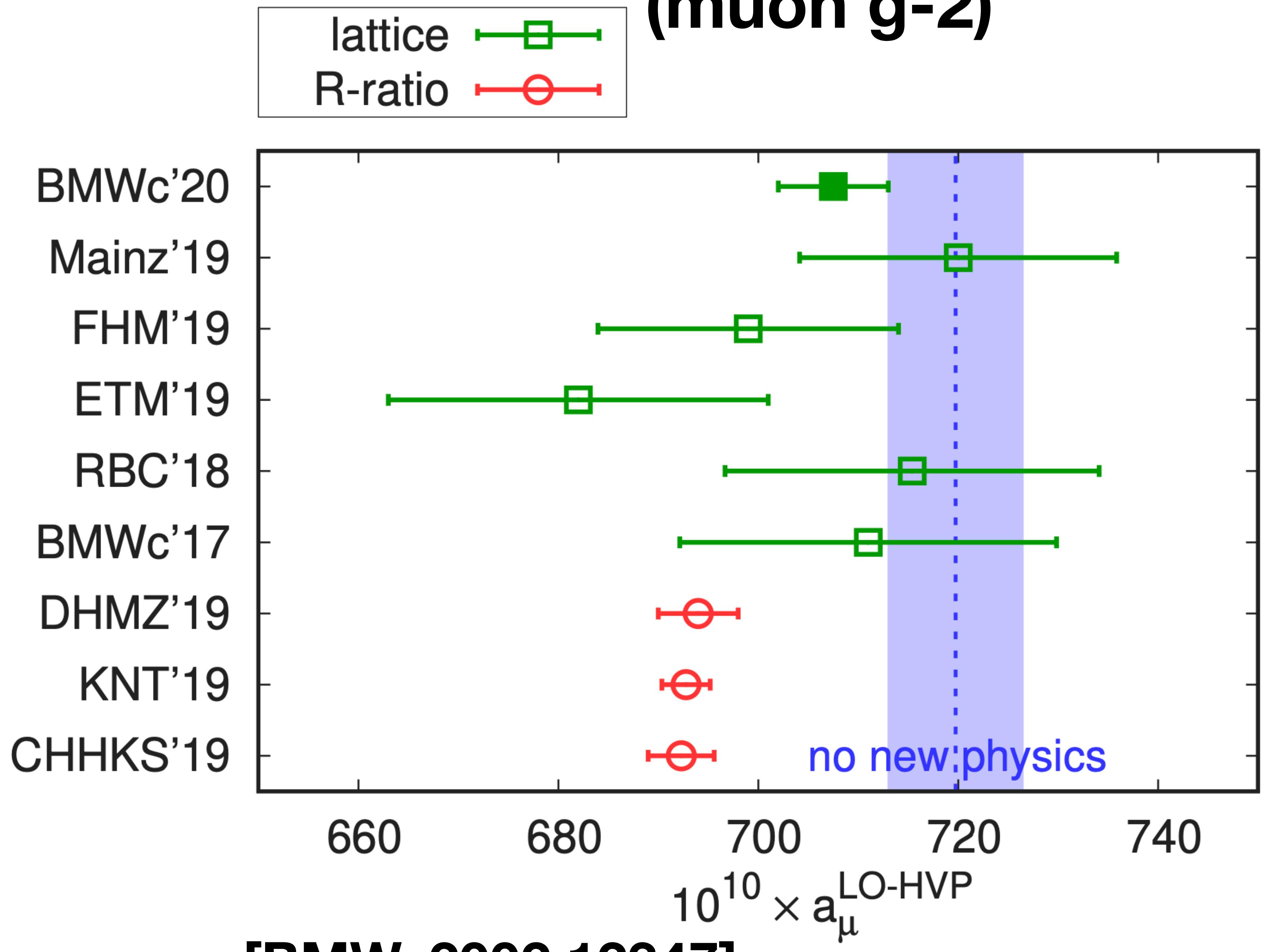
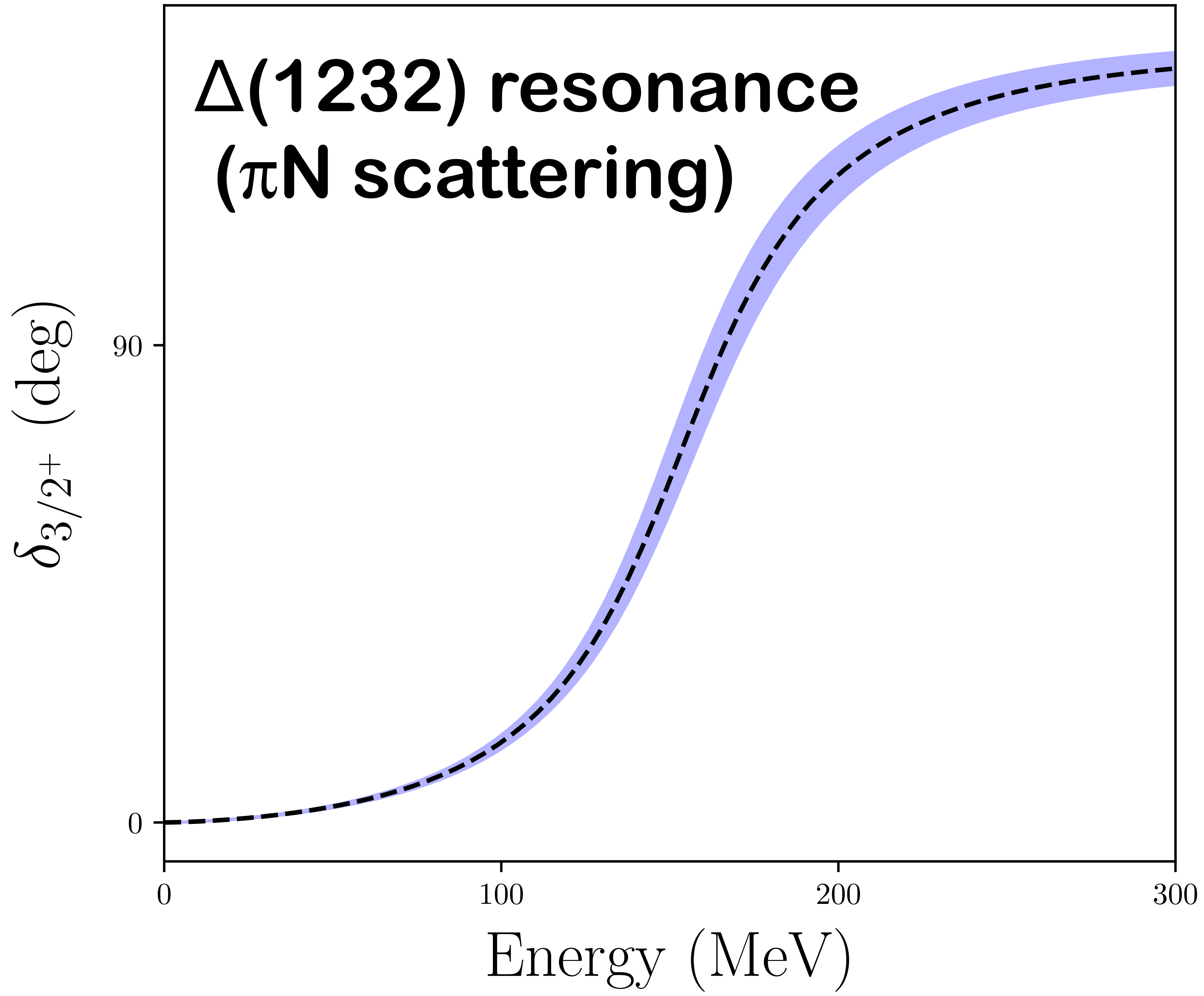
Many different applications

Hadronic Vacuum Polarization (muon g-2)



[BMW, 2002.12347]

Scattering properties of hadrons



[Bulava, Hanlon, Hörz, Morningstar, Nicholson, FRL, Skinner, Vranas, Walker-Loud, 2208.03867]

Critical slowing down in Lattice QCD

Markov Chain Monte Carlo

Lattice QCD is sampling problem over a very large number of variables

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Lattice QCD is sampling problem over a very large number of variables

→Generate field configurations: $$\{U_i\} \sim p(U) = \frac{e^{-S_E(U)}}{\mathcal{Z}}$$

→Compute observables: $$\langle \mathcal{O} \rangle \simeq \sum_{i=0}^{N_{conf}} O(U_i)$$

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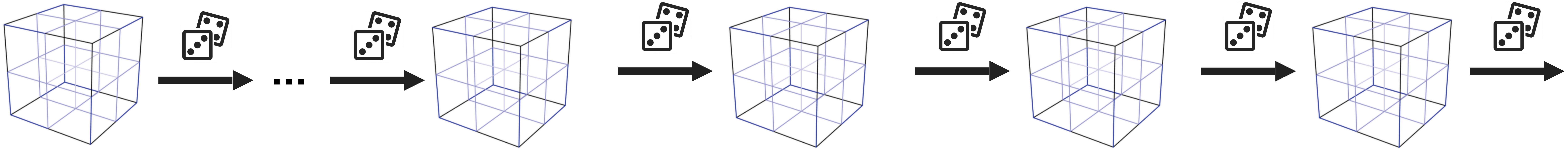

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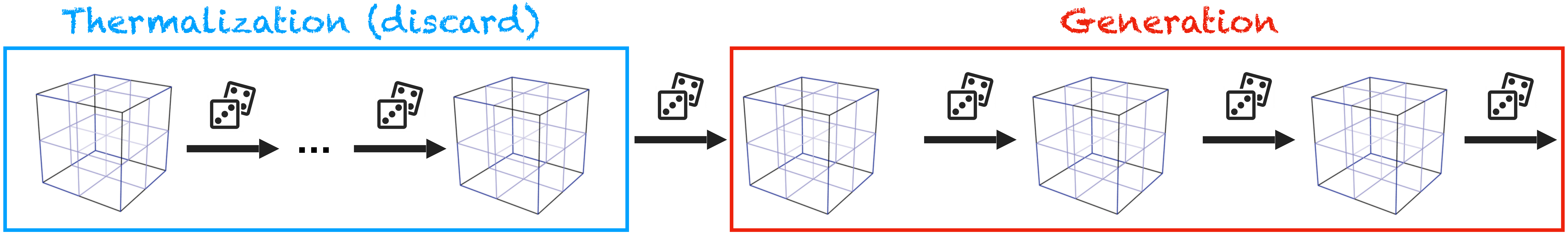

Fernando Romero-López, MIT

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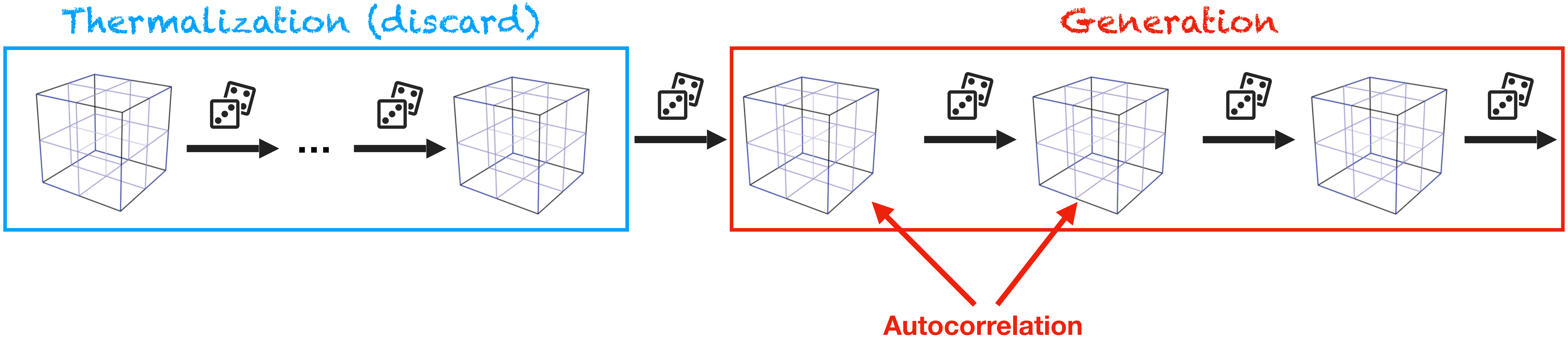

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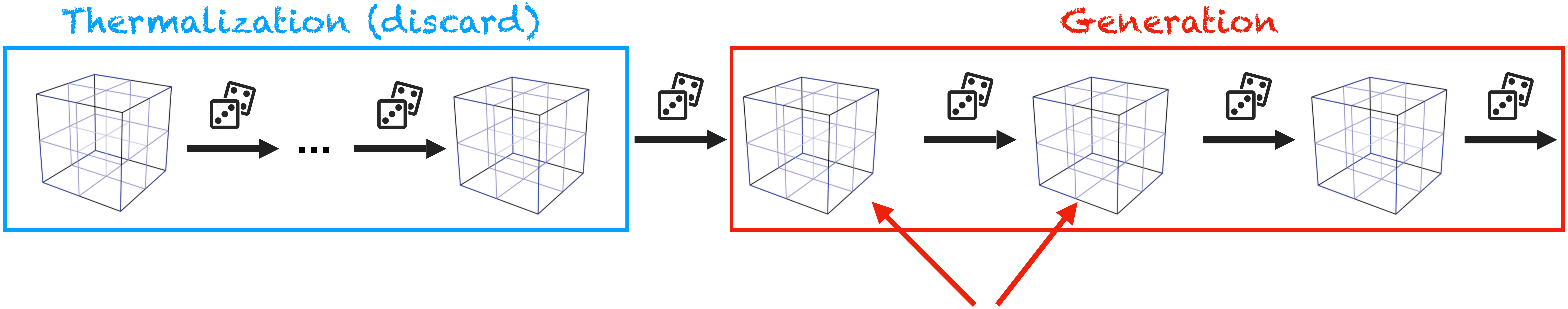

Autocorrelation $\equiv$ **Computational cost**

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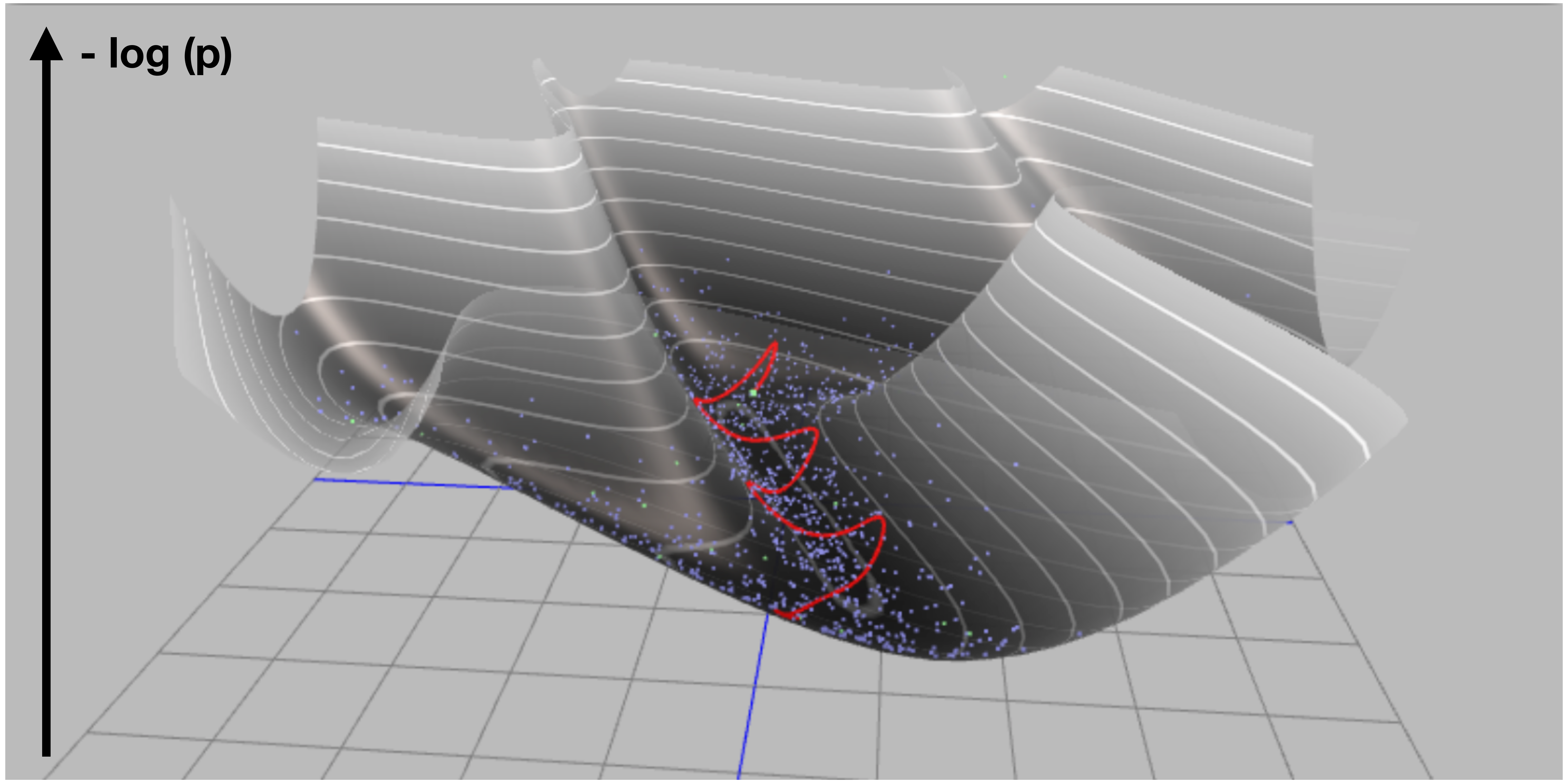
Generation of gauge configs

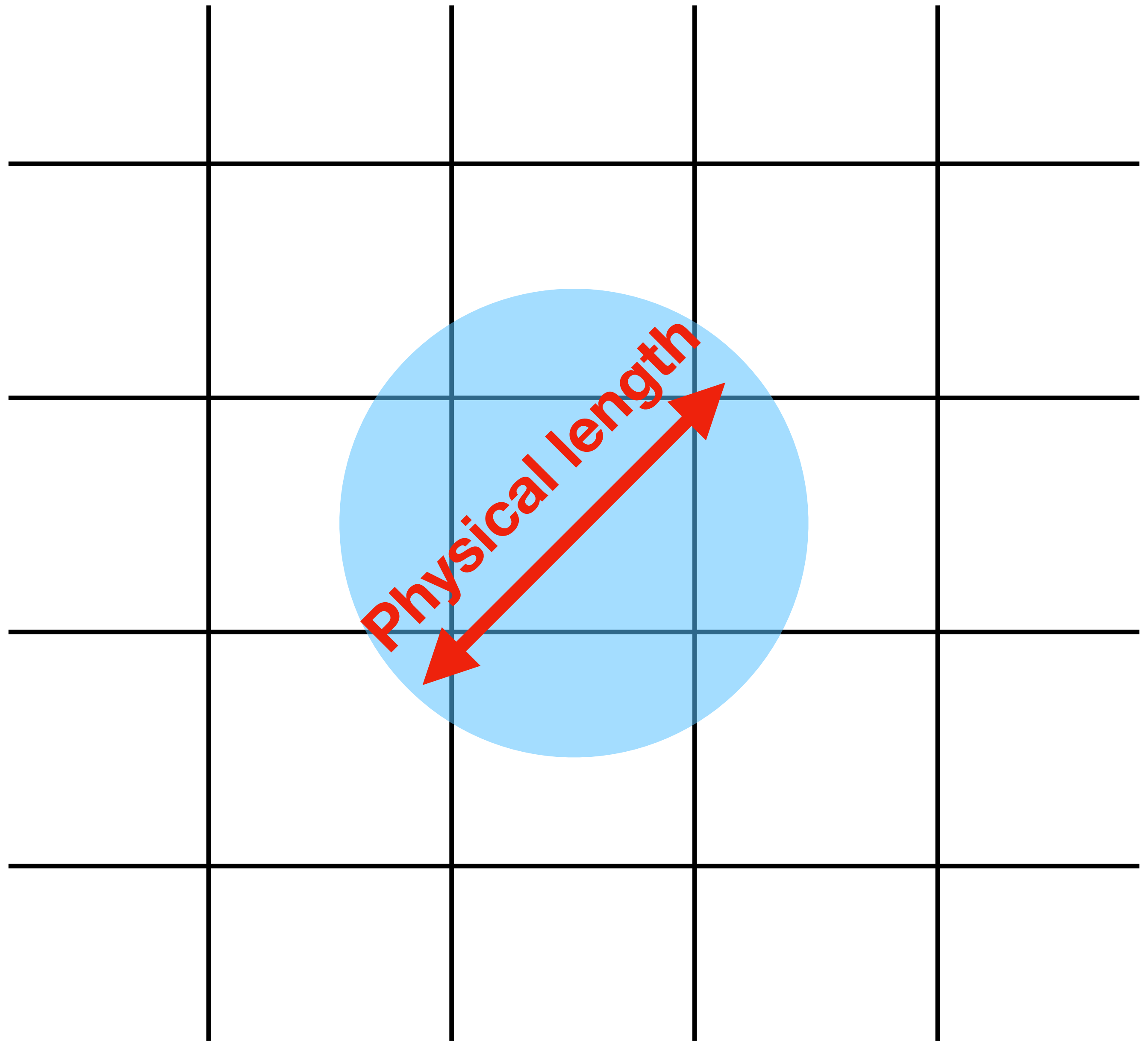
Hybrid/Hamiltonian Monte Carlo (HMC)

Molecular dynamics + Markov Chain Monte Carlo



The challenging continuum limit

- Remove discretization effects by taking the continuum limit.



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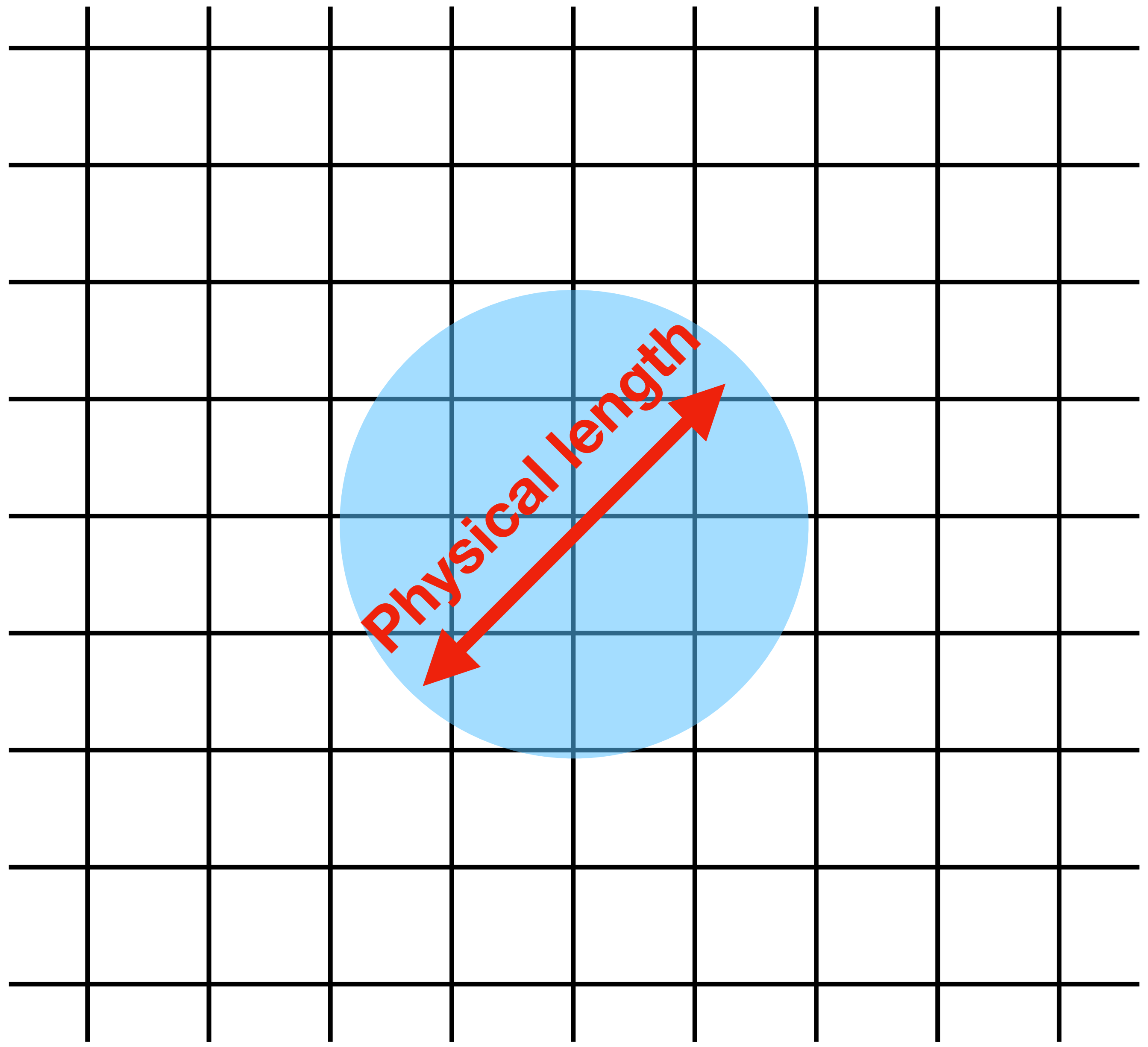

Lattice spacing ⟶ 0

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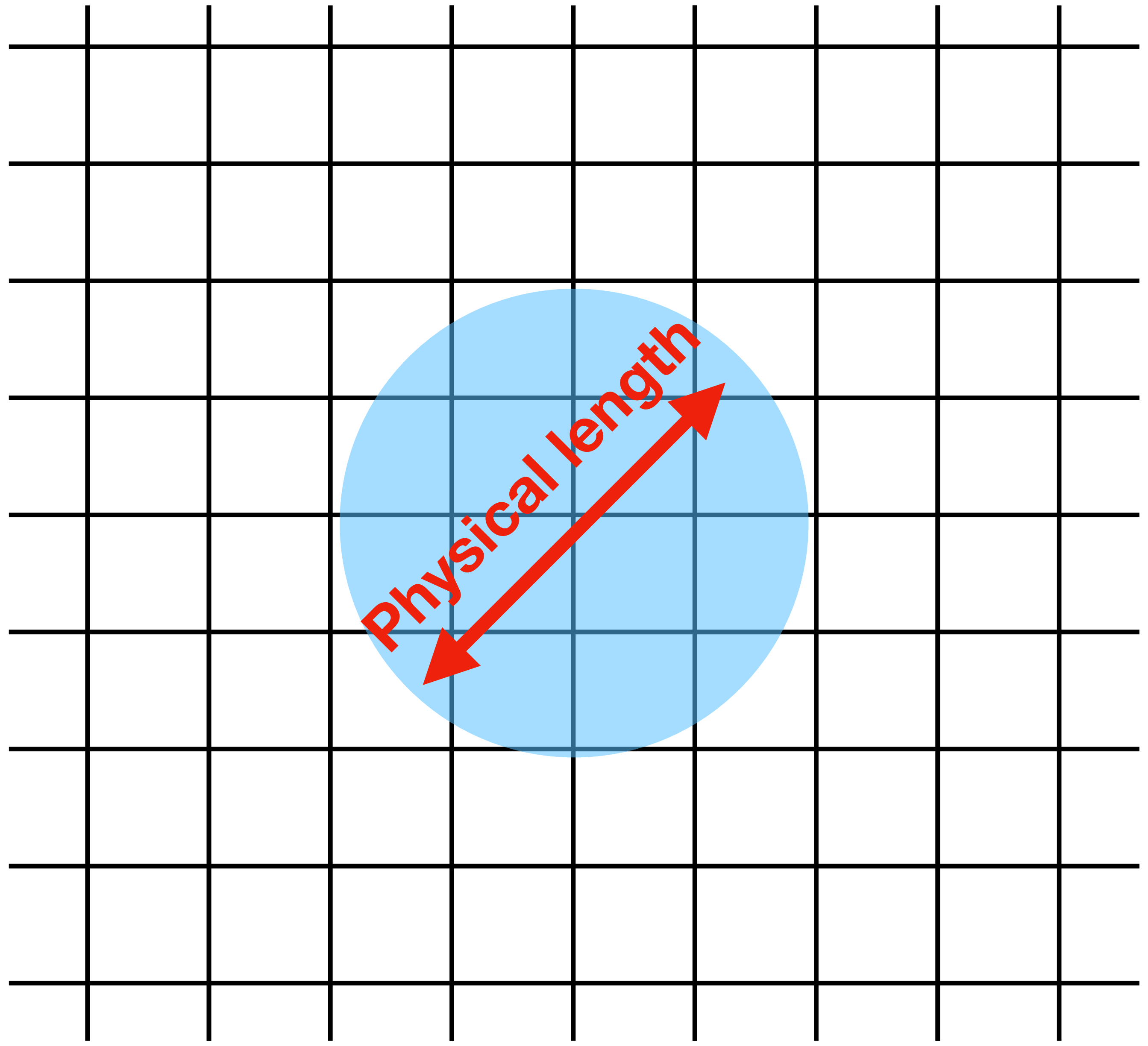

Lattice spacing $\longrightarrow 0$

Number of updates to change fixed physical length scale $\longrightarrow \infty$

Fernando Romero-López, MIT

The challenging continuum limit

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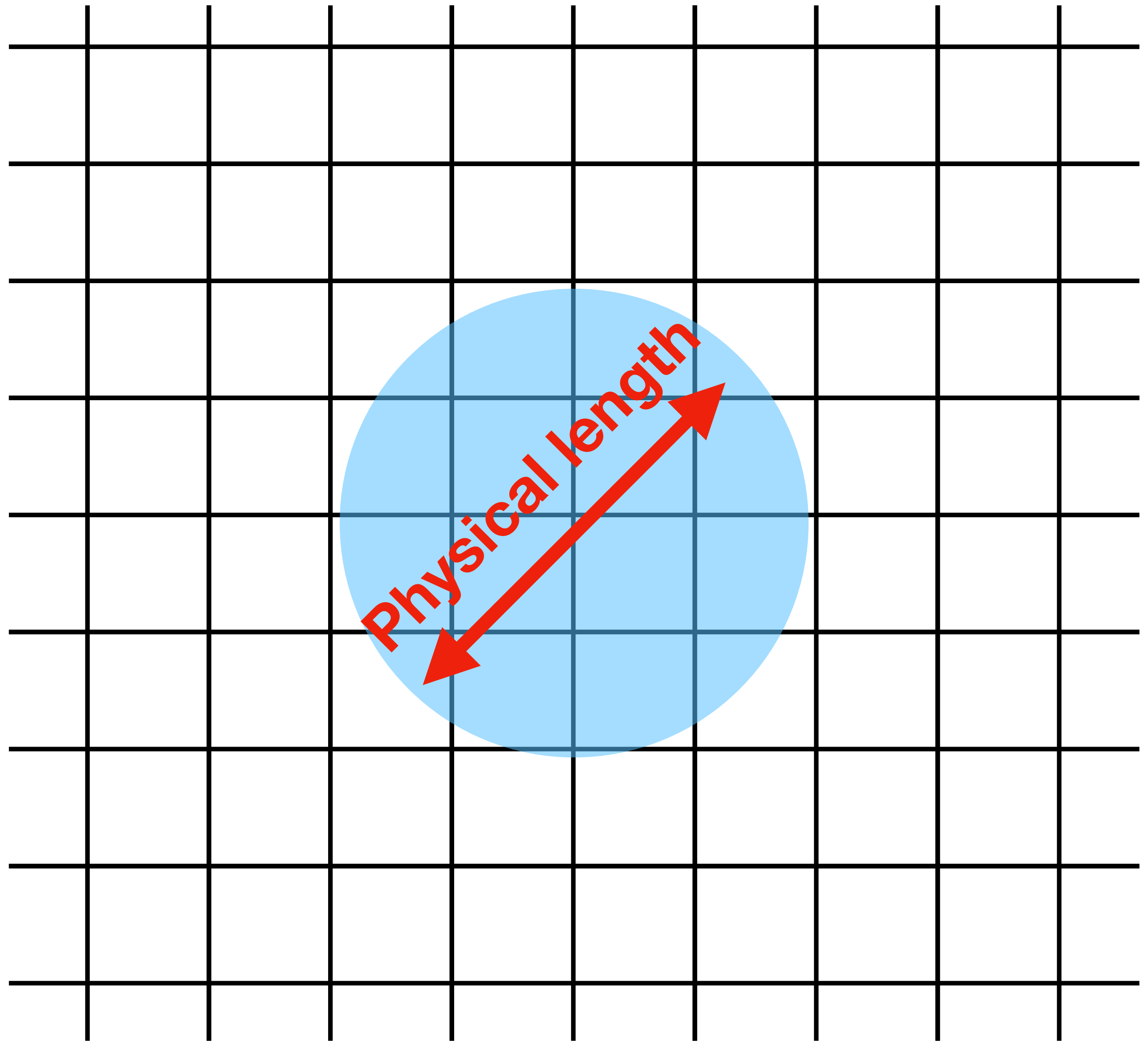


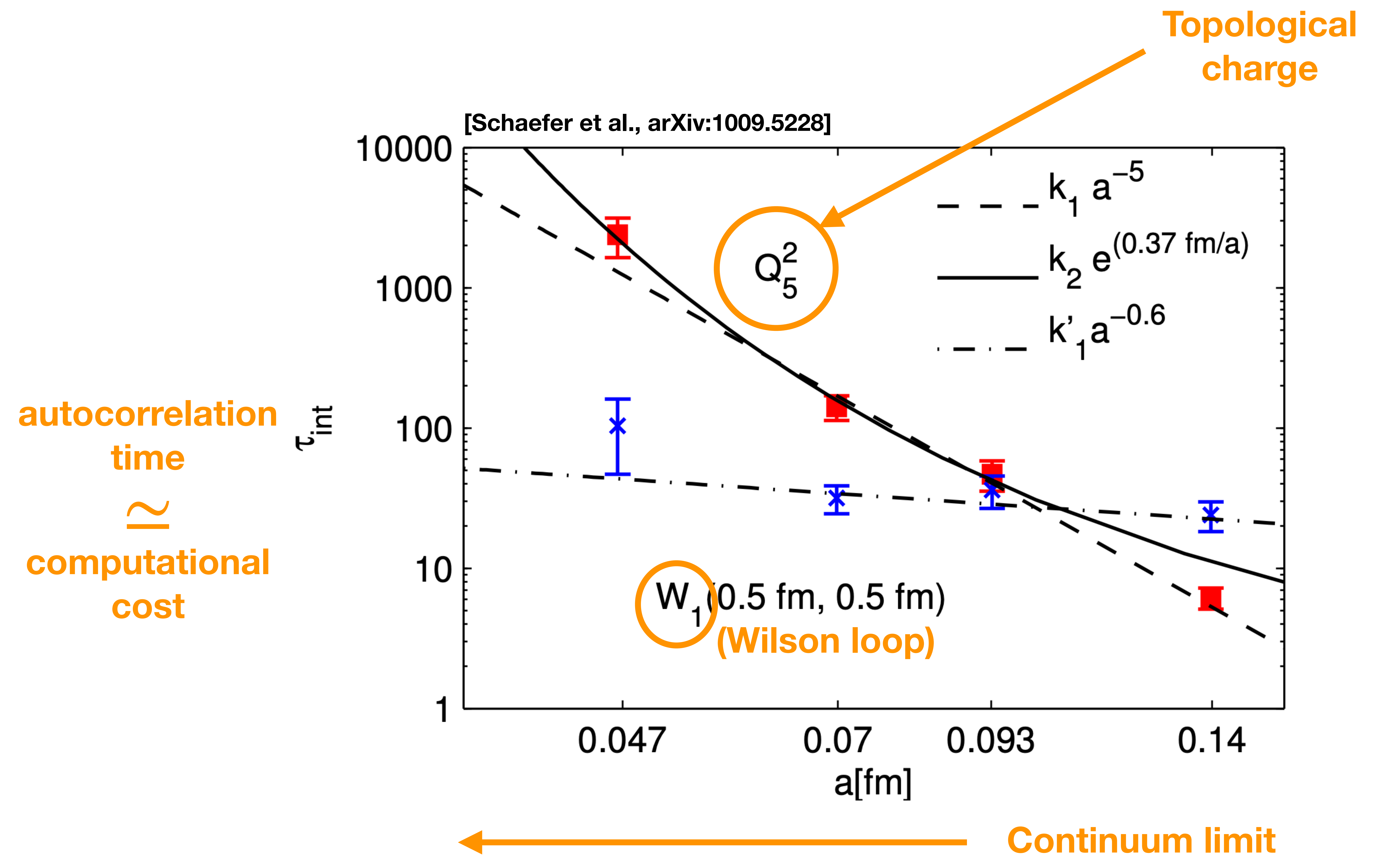
Lattice spacing $\longrightarrow$ 0

Number of updates to change fixed physical length scale $\longrightarrow$ ∞

> **"Critical slowing-down"**
> of generation of uncorrelated samples

Fernando Romero-López, MIT

Critical slowing down



CSD is a well-know obstacle to extend the reach of state-of-the-art lattice QCD calculations

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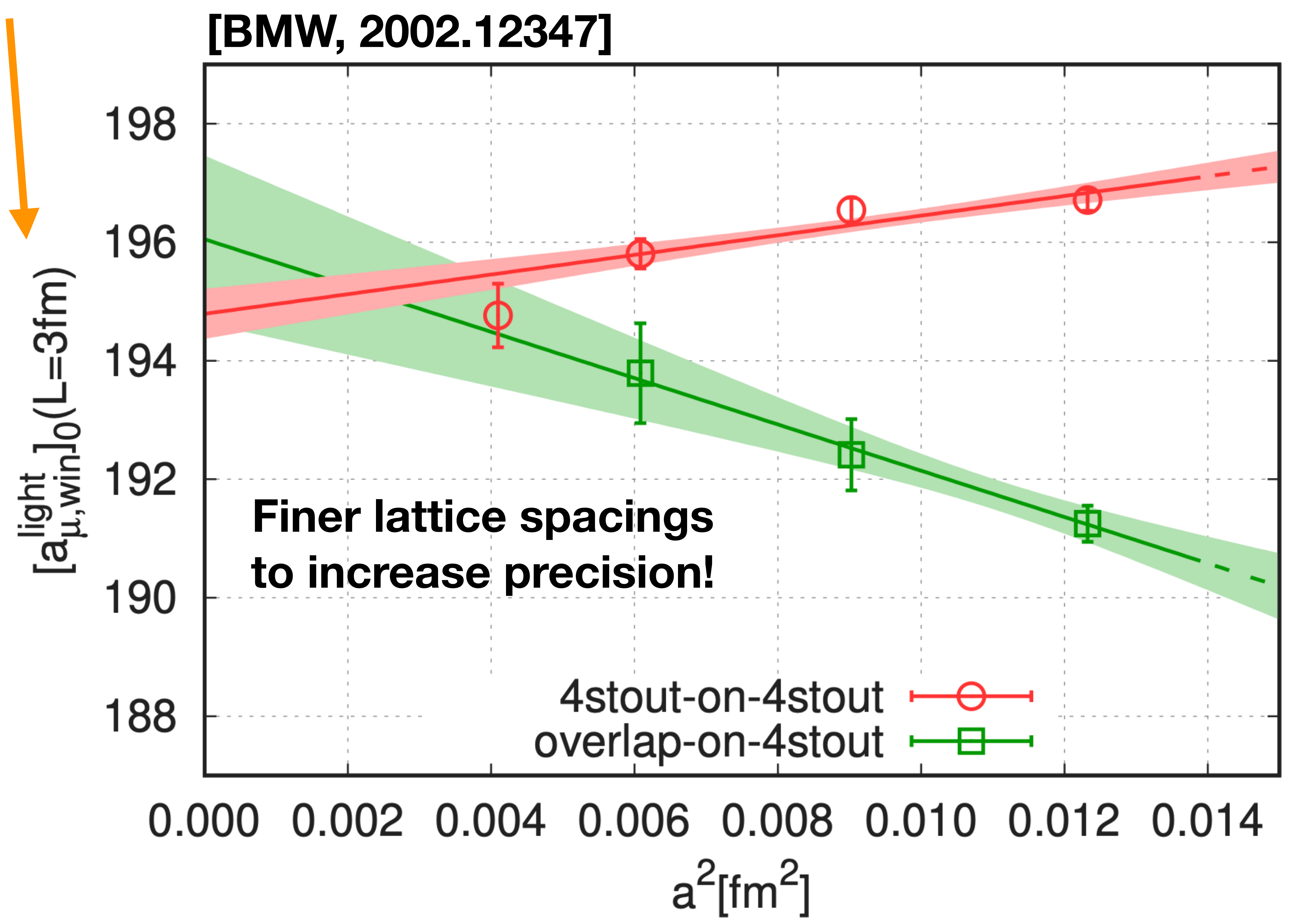
Critical slowing down

HVP of muon
magnetic moment



Continuum limit

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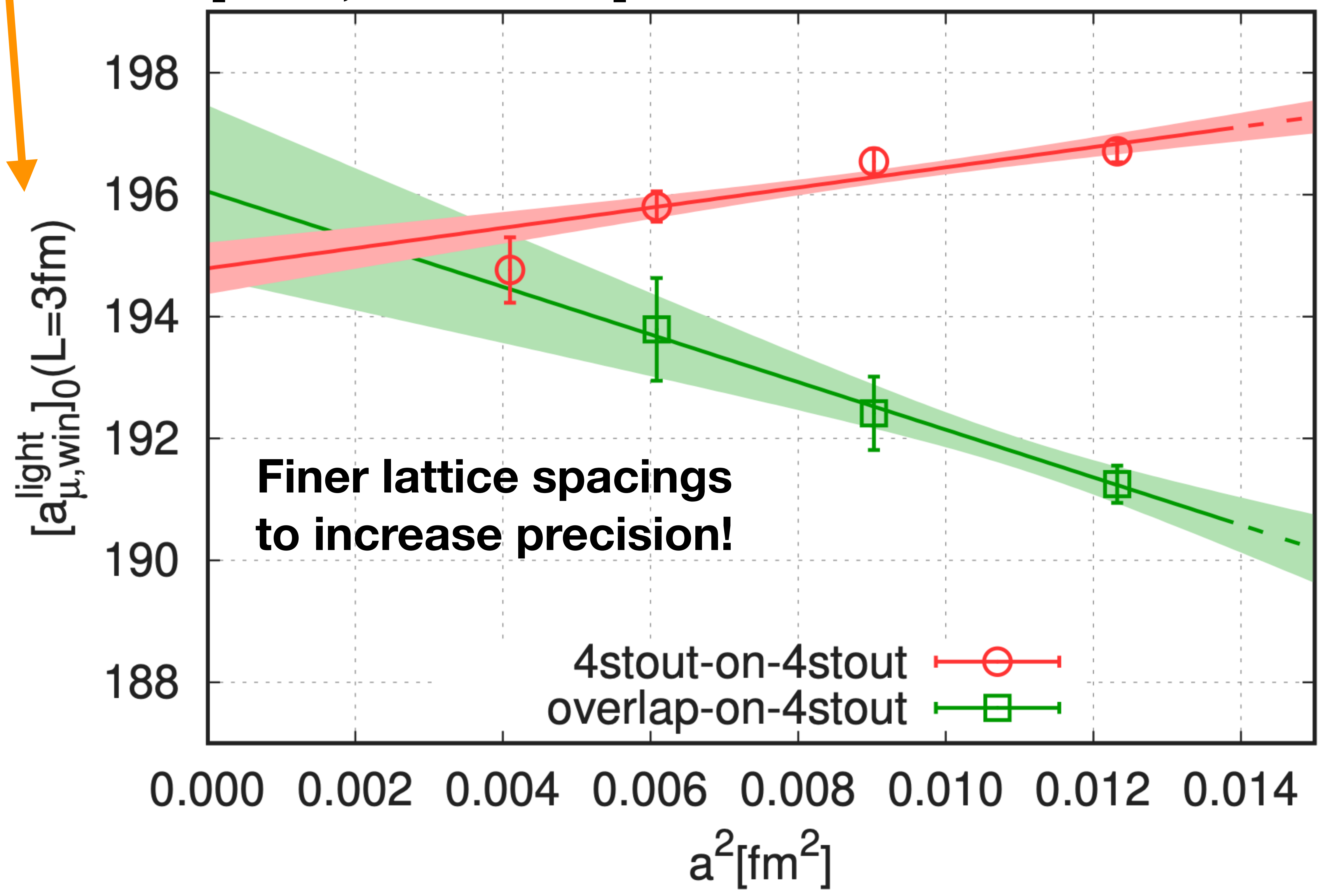
[BMW, 2002.12347]



Continuum limit

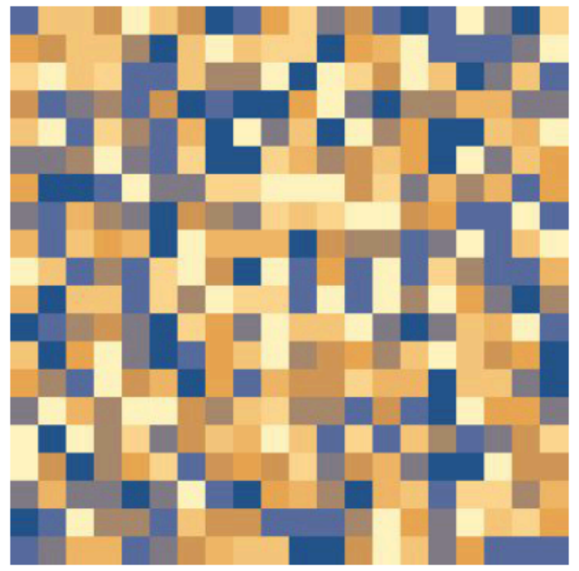
CSD is a well-know obstacle to extend the reach of state-of-the-art lattice QCD calculations

Can ML help?

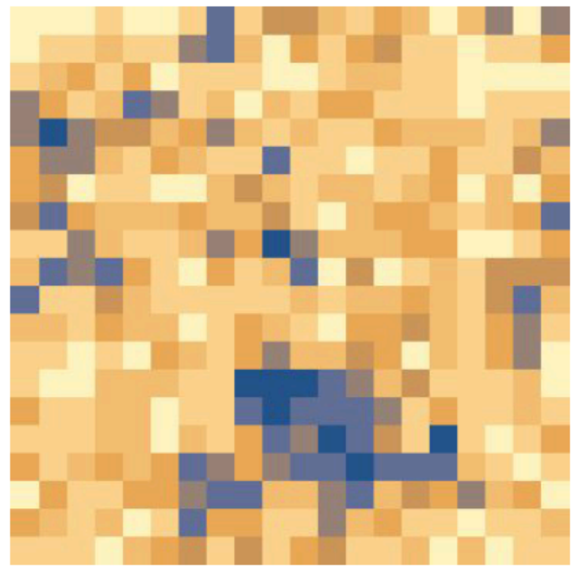
Flow-based sampling for Lattice Field Theories

Test case: scalar theory

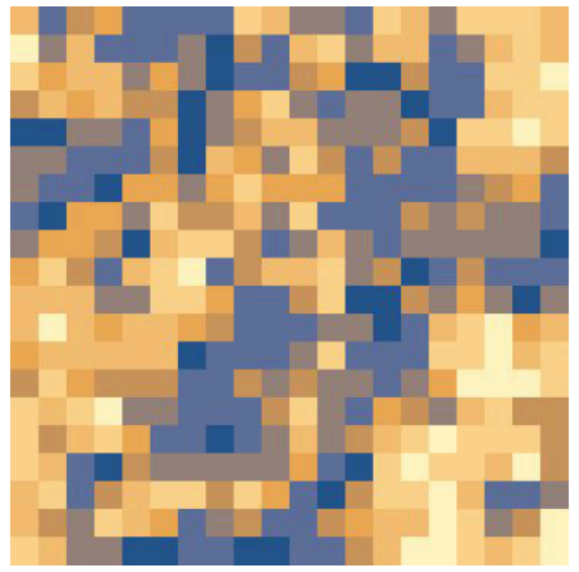
- A real scalar field per lattice site in a 2D lattice. $\phi(x) \in (-\infty, +\infty)$



unlikely
(log prob = -6107)



likely
(log prob = 22)



likely
(log prob = 5)

Field configurations with probability:

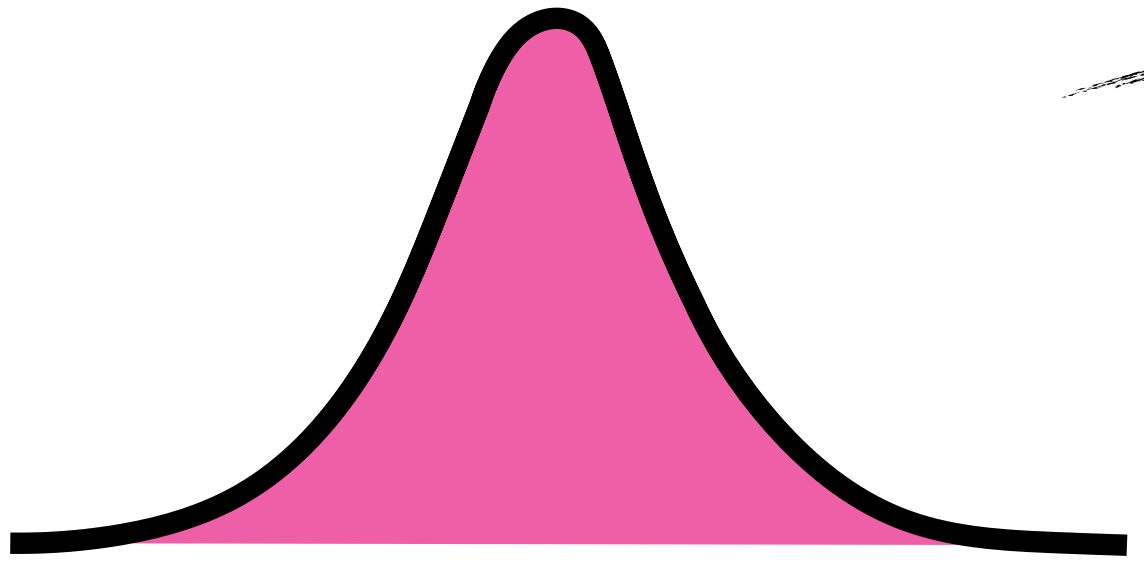
$$P[\phi(x)] \sim e^{-S[\phi(x)]}$$

- Lattice action: $$S = a^4 \sum_x \frac{1}{2a^2}(\phi_{x+\mu} - \phi_x)^2 + \frac{m^2}{2}\phi_x^2 + \lambda \phi_x^4$$

Generative flow models

[Rezende, Mohamed, 1505.05770]

$r(z)$

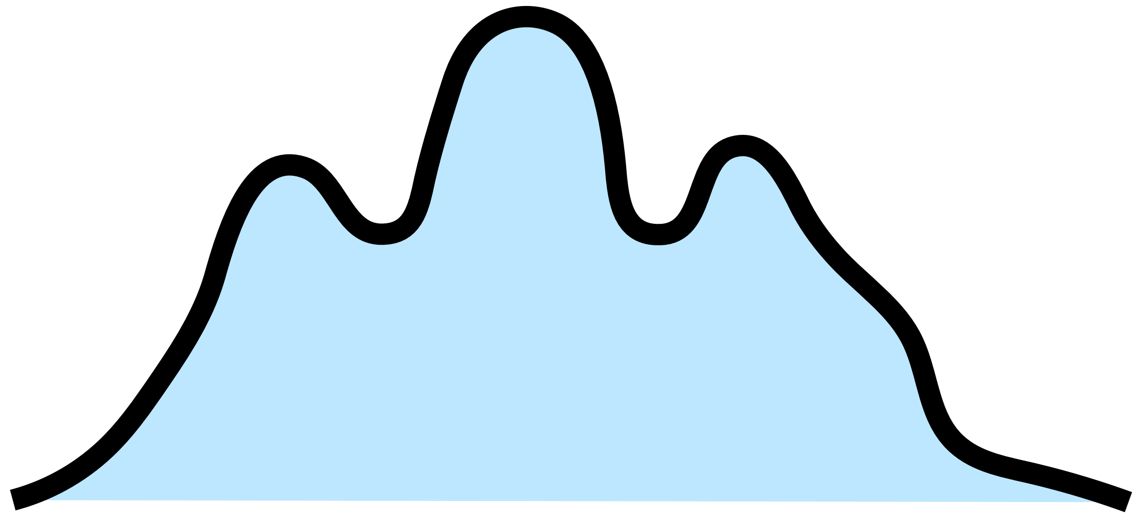


easily sampled
distribution
(prior)

$f(z)$

tractable Jacobian
&
invertible

$q(\phi) \simeq p(\phi)$



approximates
target distribution
(model)

“Trainable change of variables”

Model probability

$$q(\phi) = r(z) \left| \det \frac{\partial f(z)}{\partial z} \right|^{-1}$$

Generative flow models

[Rezende, Mohamed, 1505.05770]

$r(z)$ $f(z)$ $q(\phi) \simeq p(\phi)$

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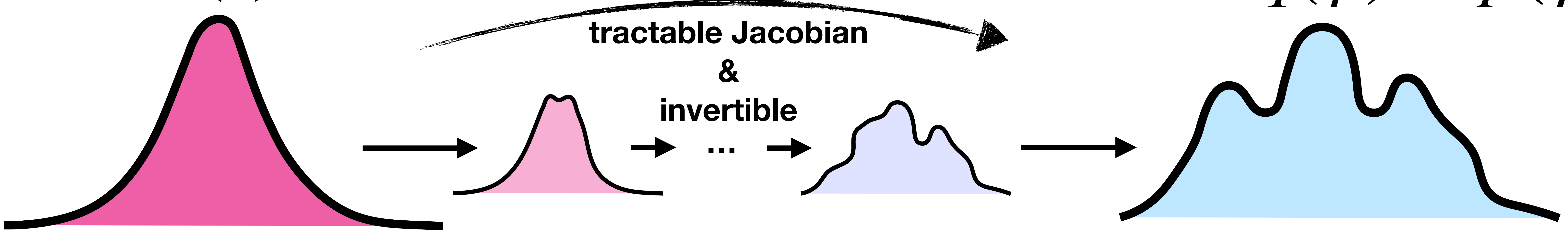

easily sampled
distribution
(prior)

approximates
target distribution
(model)

parametrized by neural networks
(trainable and expressive)

composed of
many simple layers

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Generative flow models

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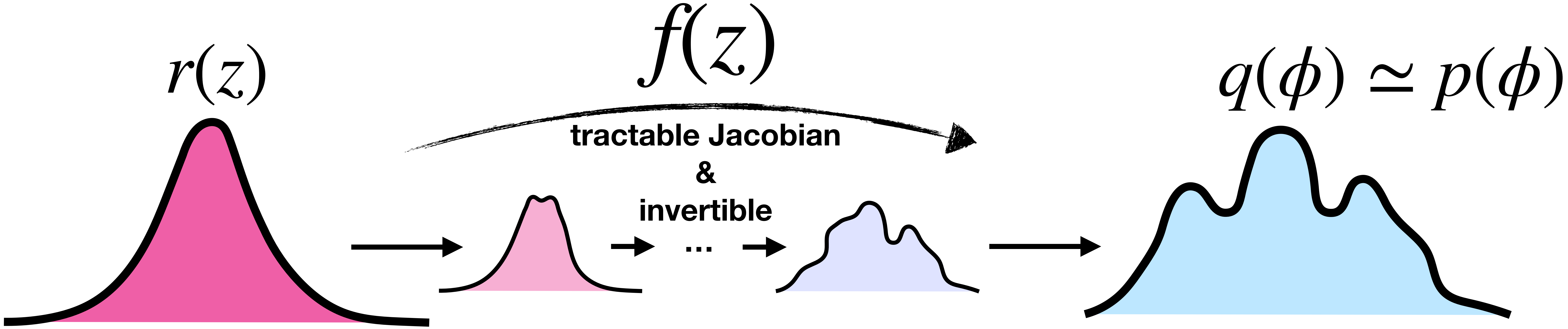

easily sampled distribution (prior)

approximates target distribution (model)

parametrized by neural networks (trainable and expressive) → composed of many simple layers

❗ Trained models are not perfect.

☑ But exact sampling can be recovered via Markov Chain

"Trainable change of variables"

Model probability

$$q(\phi) = r(z) \left| \det \frac{\partial f(z)}{\partial z} \right|^{-1}$$

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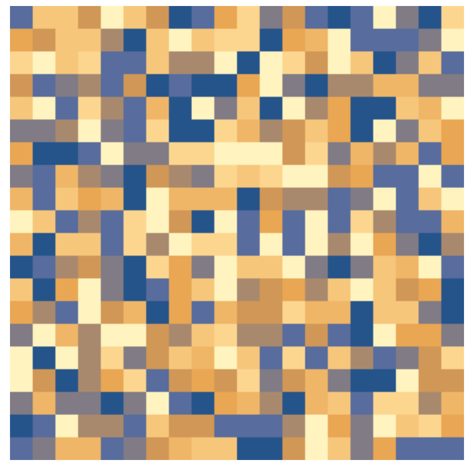
Implementing flows for scalar theory

$\phi(x) \in (-\infty, +\infty)$



→**Efficient flow models need tractable Jacobians.**

Idea: Each layer acts on a subset of components, conditioned only on the complimentary subset.

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Implementing flows for scalar theory

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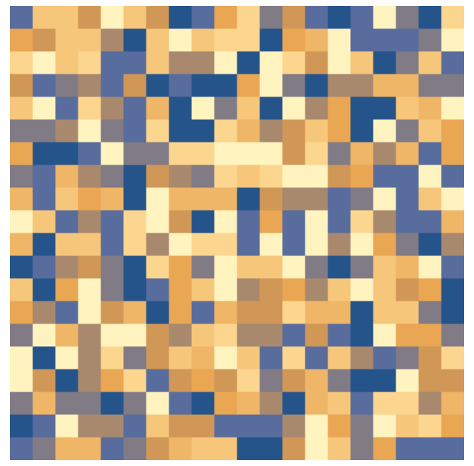

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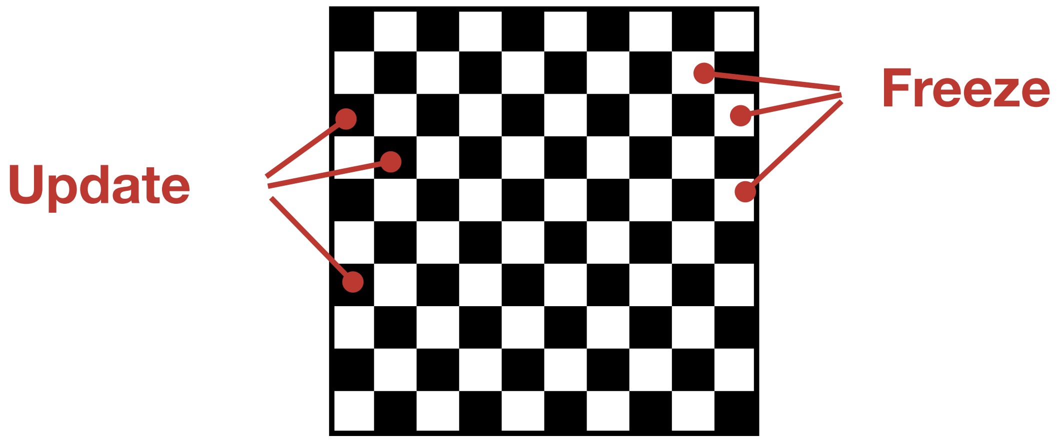
Idea: Each layer acts on a subset of components, conditioned only on the complimentary subset.

"Masking pattern" m defines subsets.



$$\phi' = \begin{cases} \phi'_{\text{frozen}} = \phi_{\text{frozen}} \\ \phi'_{\text{active}} = h(\phi_{\text{frozen}}) \times \phi_{\text{active}} + t \end{cases}$$

conditioning

Implementing flows for scalar theory

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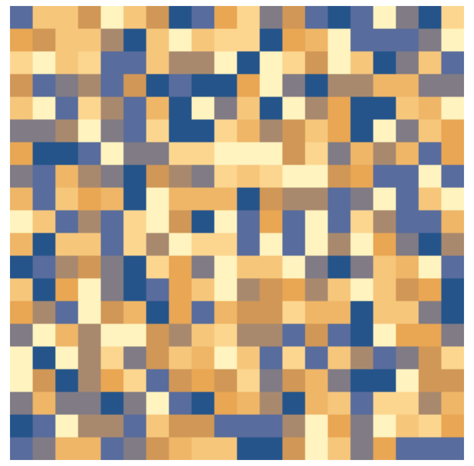

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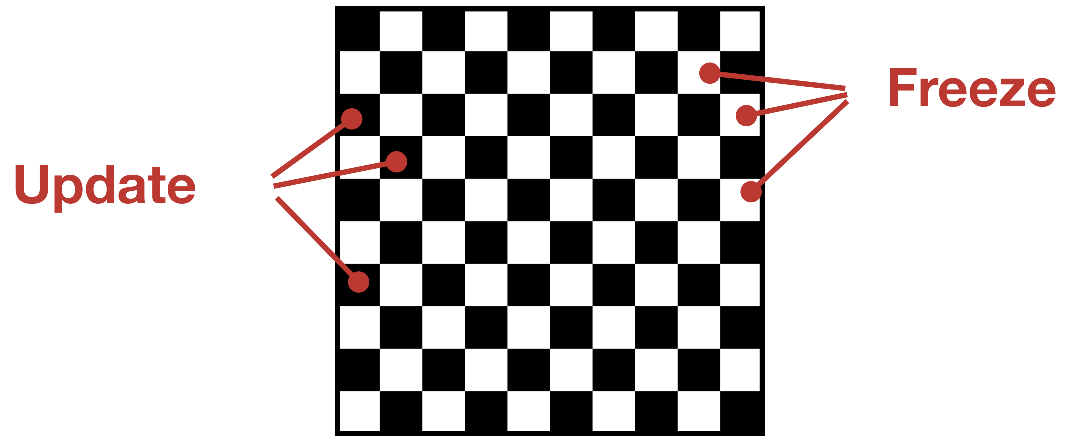

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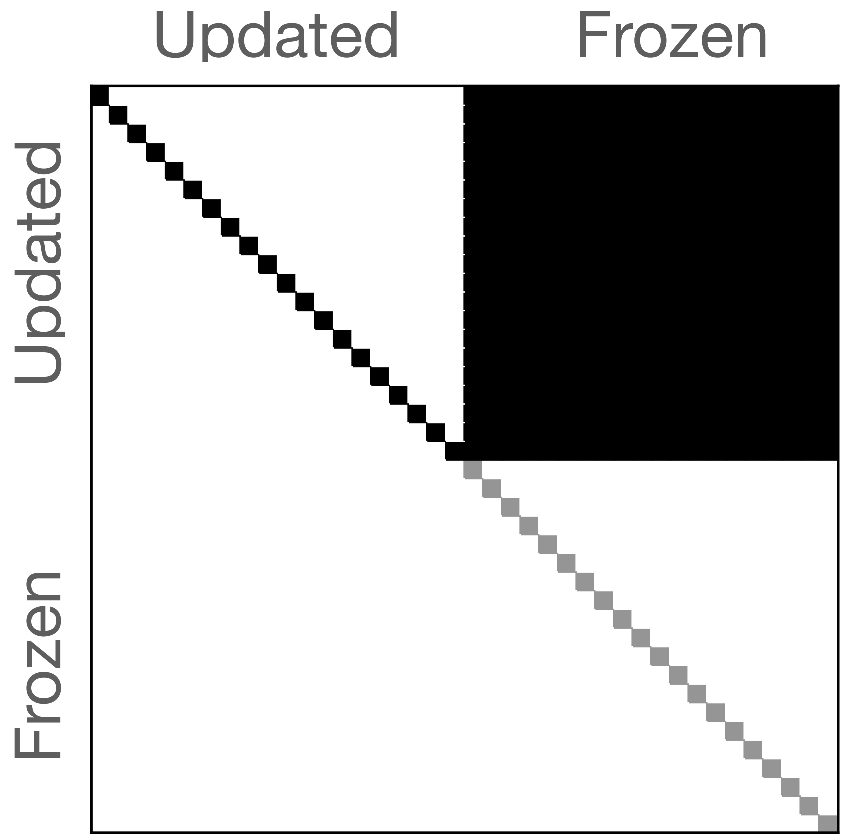
conditioning

Jacobian $= \dfrac{\partial \phi'}{\partial \phi} =$



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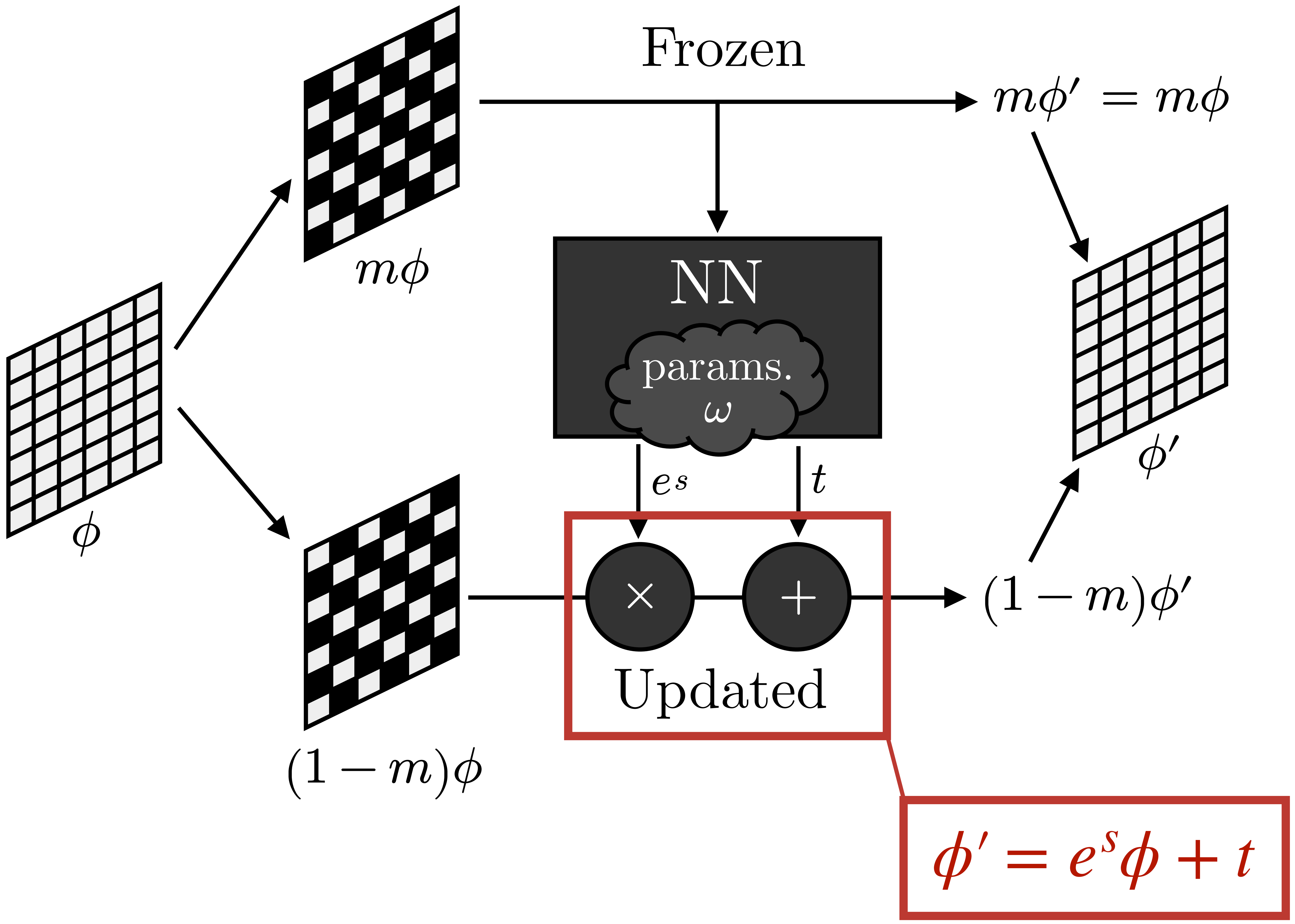
Implementing flows for scalar theory

Non-volume preserving coupling layer:

[Dinh, Sohl-Dickstein, Bengio 1605.08803]



Training the models

- **Target distribution know up to a constant:**

$$p[\phi(x)] \sim e^{-S[\phi(x)]}$$

- **Train to minimize Kullback-Leibler divergence:**

$$D_{\mathrm{KL}}(q\|p) = \sum_{\text{samples}} \log[q(\phi)/p(\phi)]$$

Measures deviation between model and target

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Measures deviation between model and target

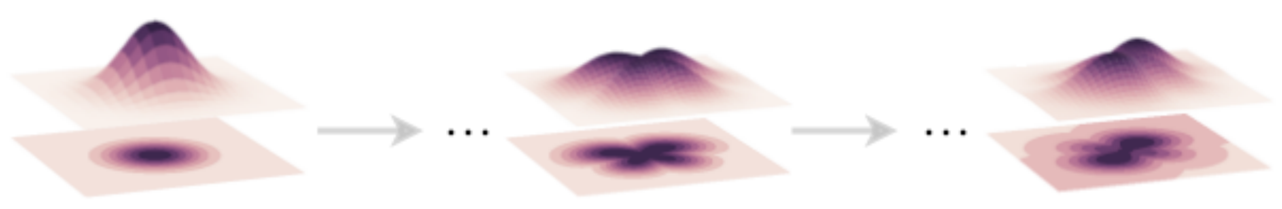
- Self-training:

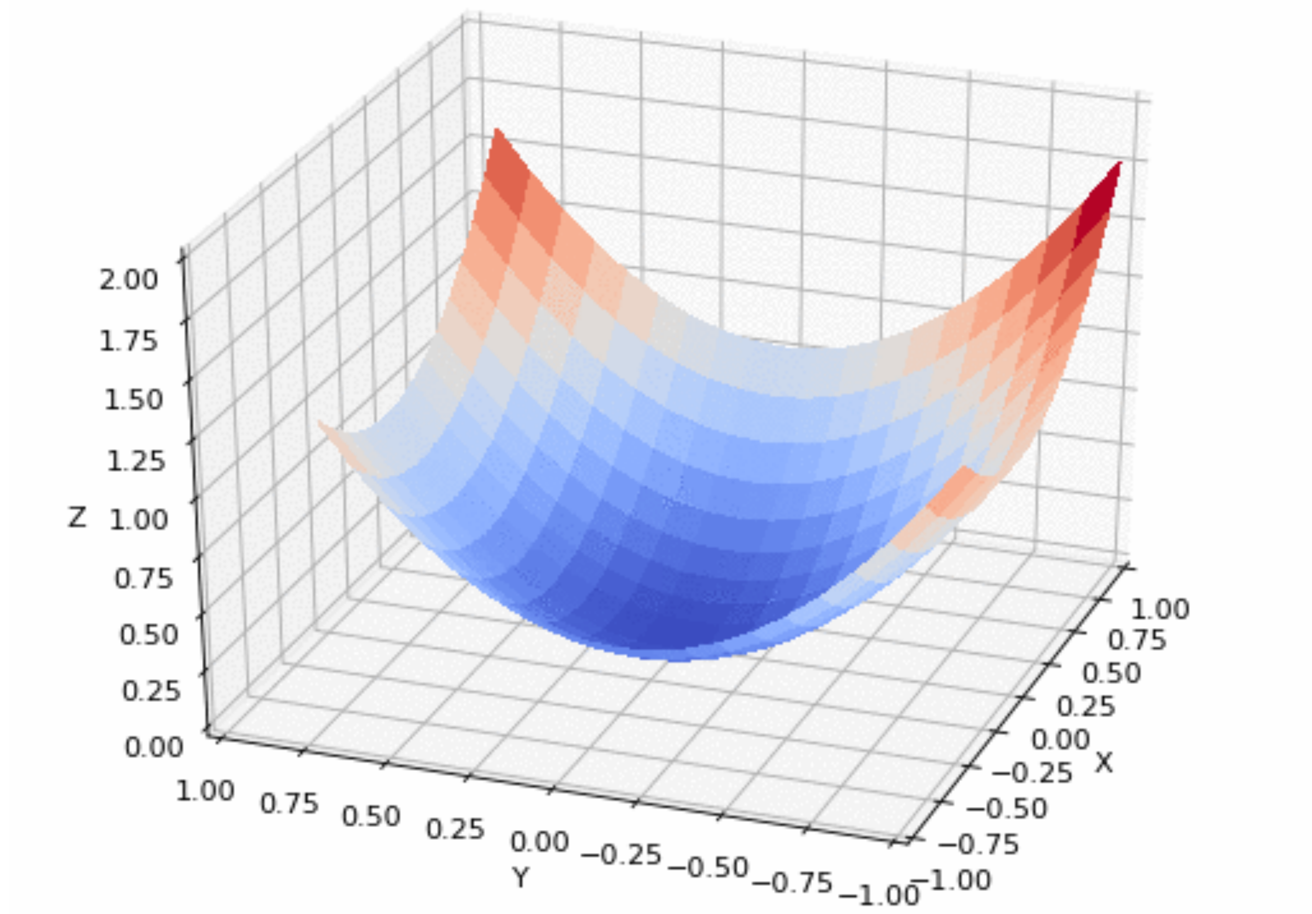
    1. Draw samples from the model to measure sample mean of $\log[q(\phi)/p(\phi)]$

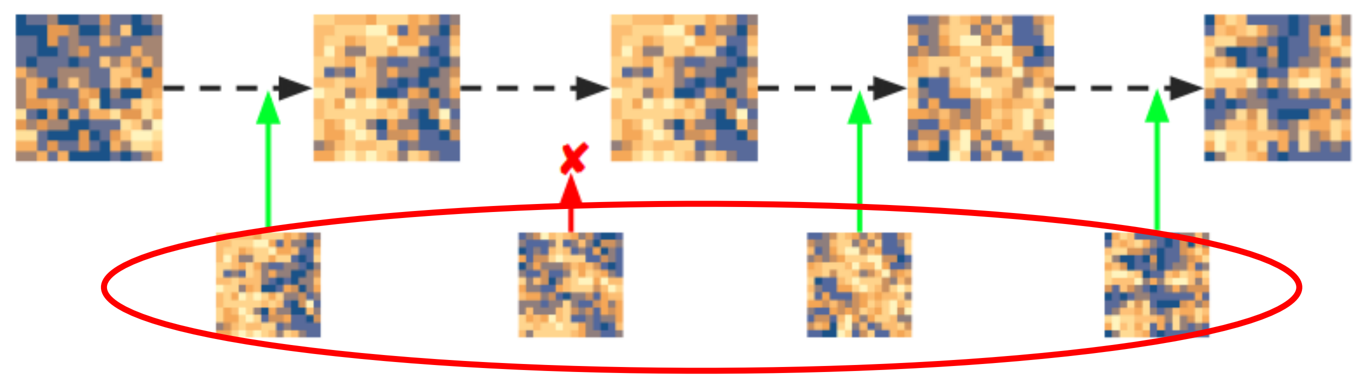
    2. Gradient-based methods to optimize model parameters (e.g. Adam optimizer)

[Kingma, Ba, arXiv:1412.6980]

Lattice QFT via flow models







generating samples is
"embarrassingly parallel"

Parameterize flow using coupling layers

Each layer contains arbitrary neural nets

Training step

Draw samples from model

Compute loss function

Gradient descent

Desired accuracy?

Save trained model

Markov chain using samples from model

[credits: G. Kanwar]

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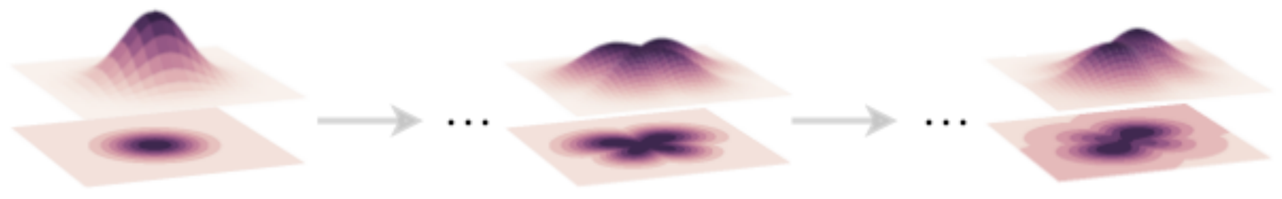
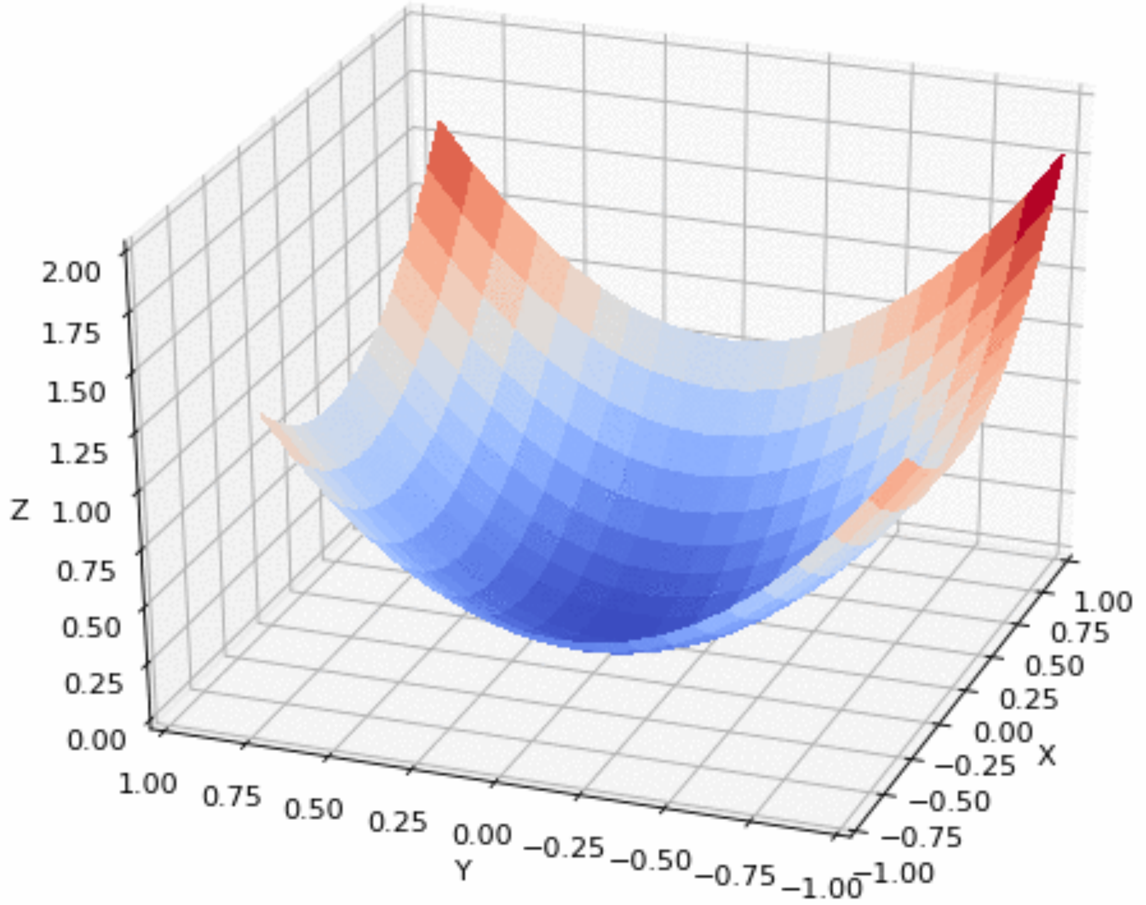
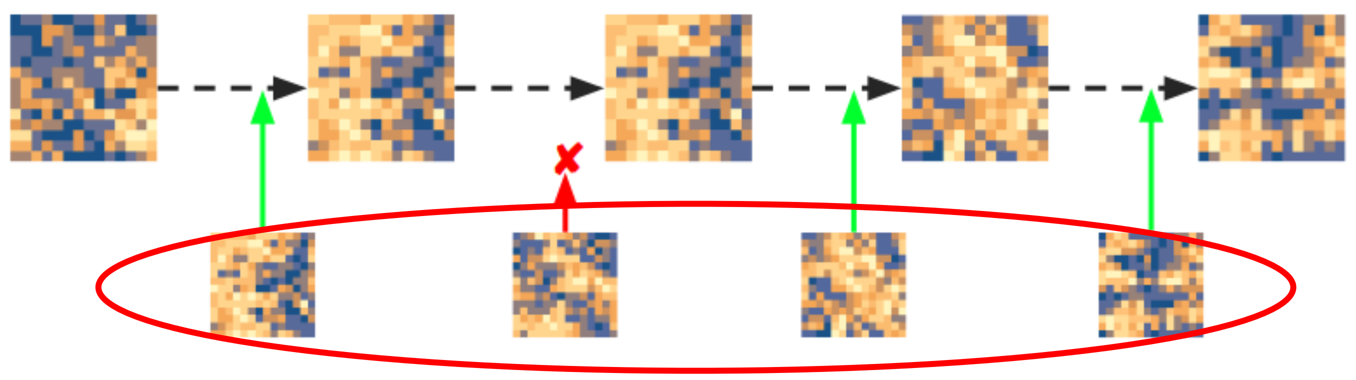
Lattice QFT via flow models







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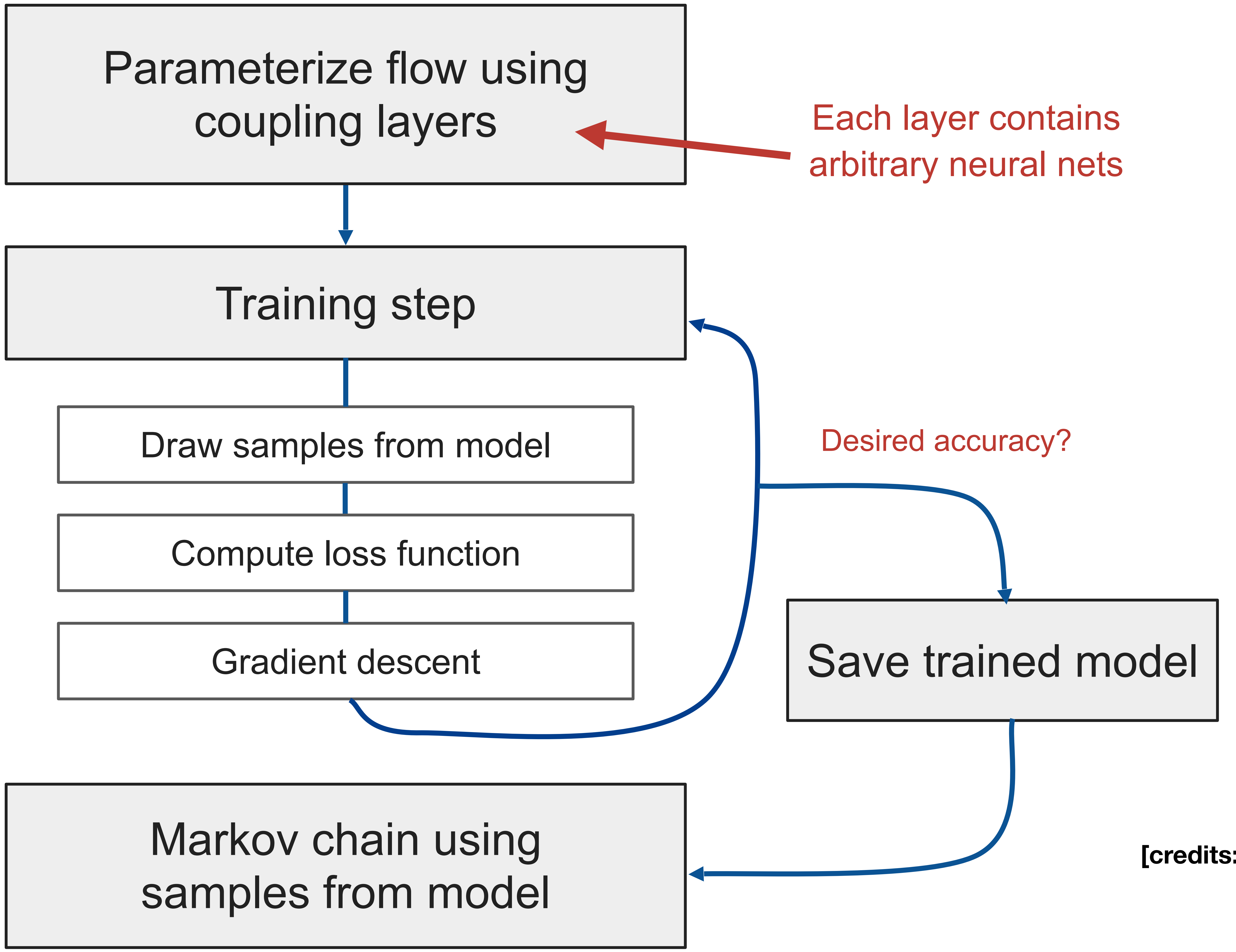

[credits: G. Kanwar]

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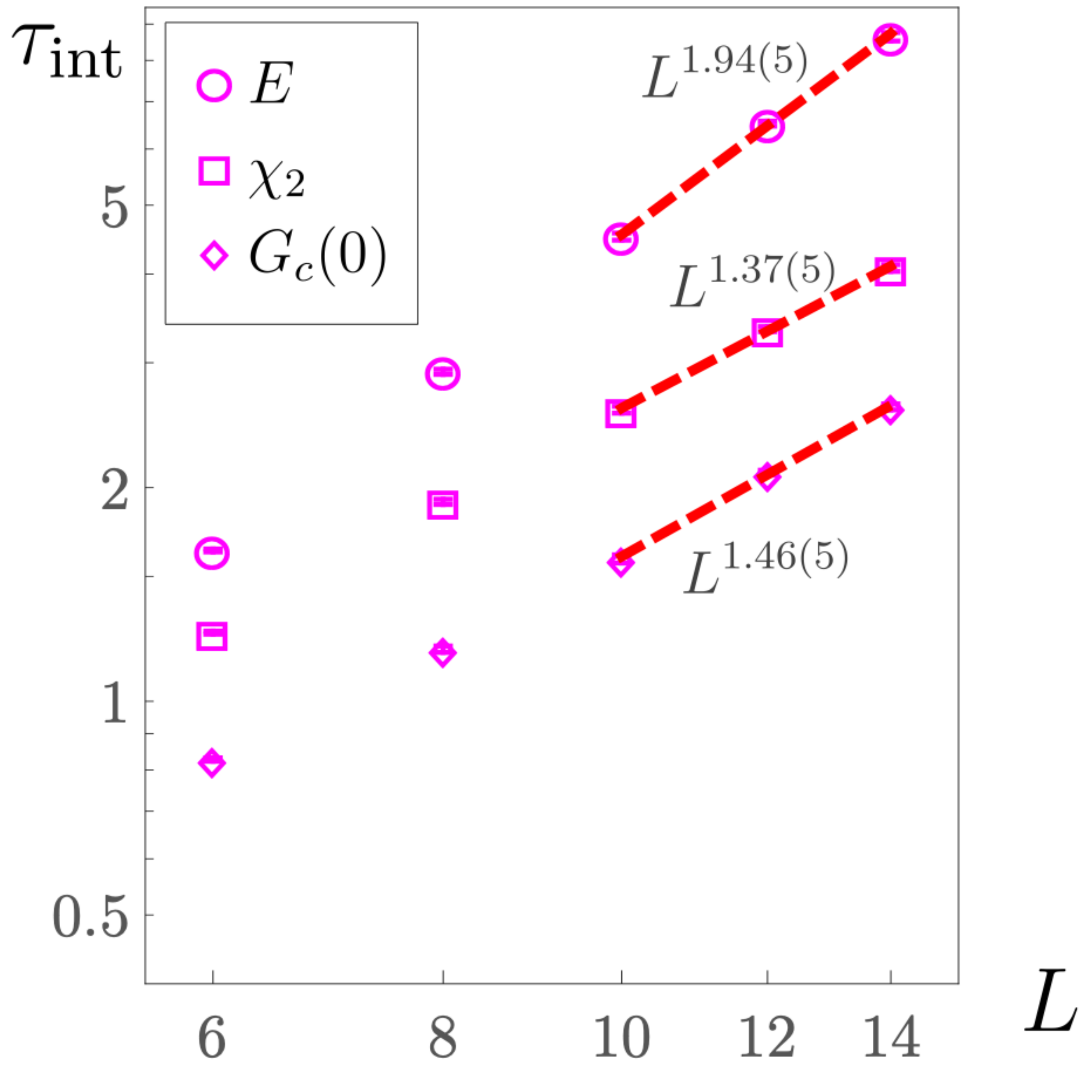
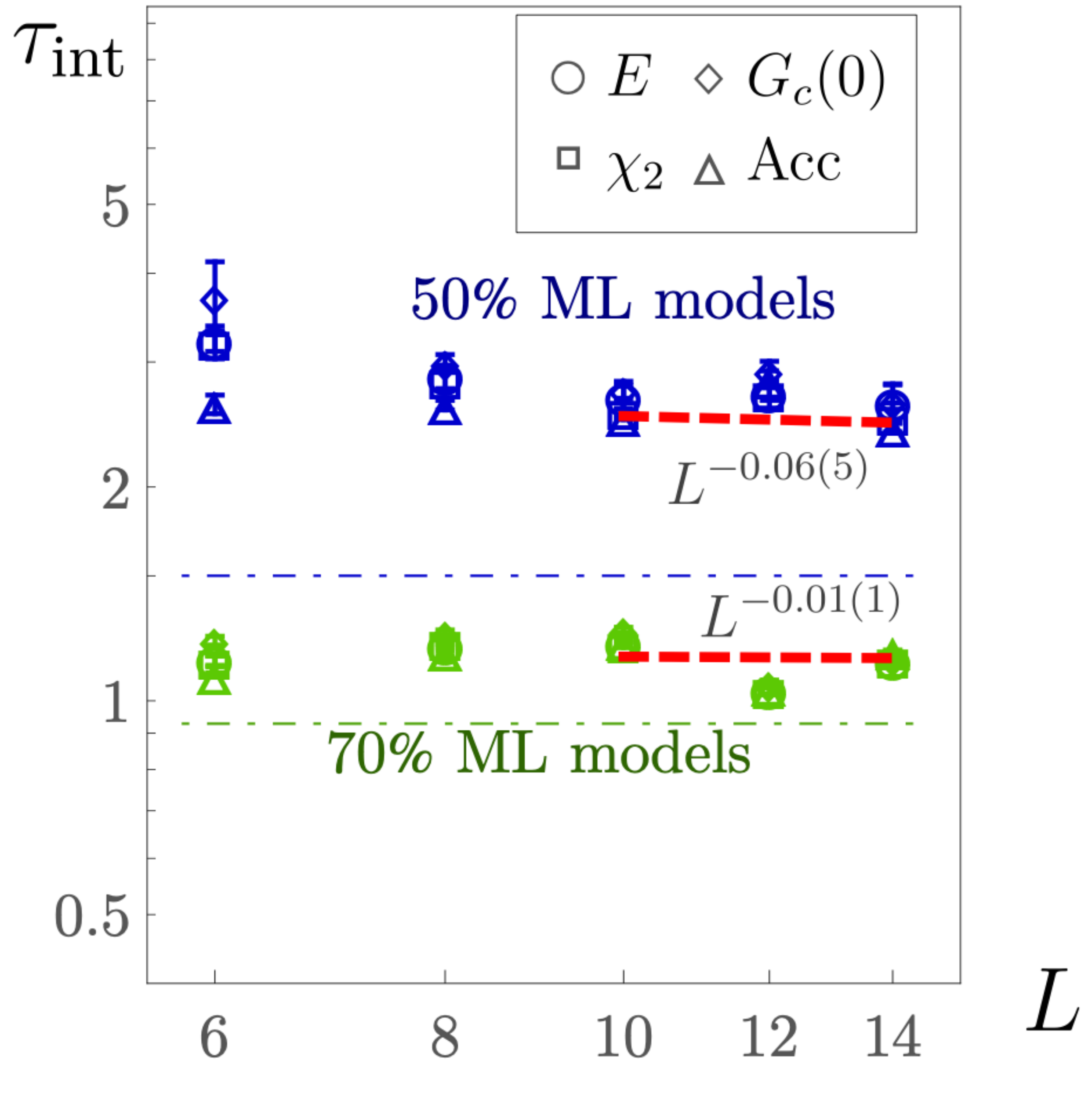
Scalar theory

No critical slowing down at the cost of up-front training



(b) Local Metropolis ensembles

Conventional approaches slow down



(c) Flow-based MCMC ensembles

No slow-down!

[Albergo, Kanwar, Shanahan 1904.12072]

Flow-based sampling for gauge theories

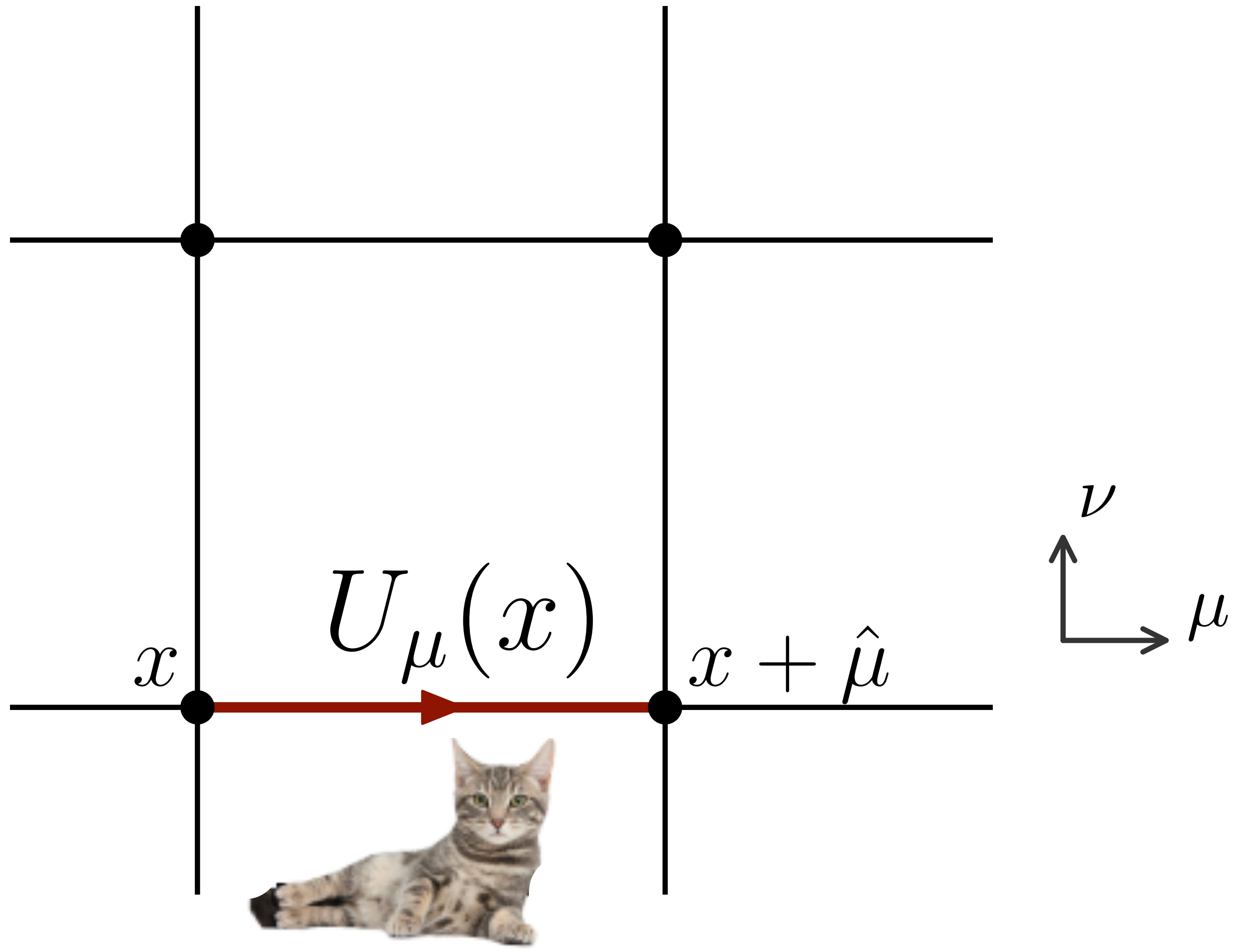
Lattice U(1) gauge symmetry

- Gauge variables are the gauge links

$$U_\mu(x) \in \mathrm{U}(1)$$

$$U_\mu(x) = e^{iagA_\mu(x)}$$

$$agA_\mu(x) \in [0, 2\pi)$$



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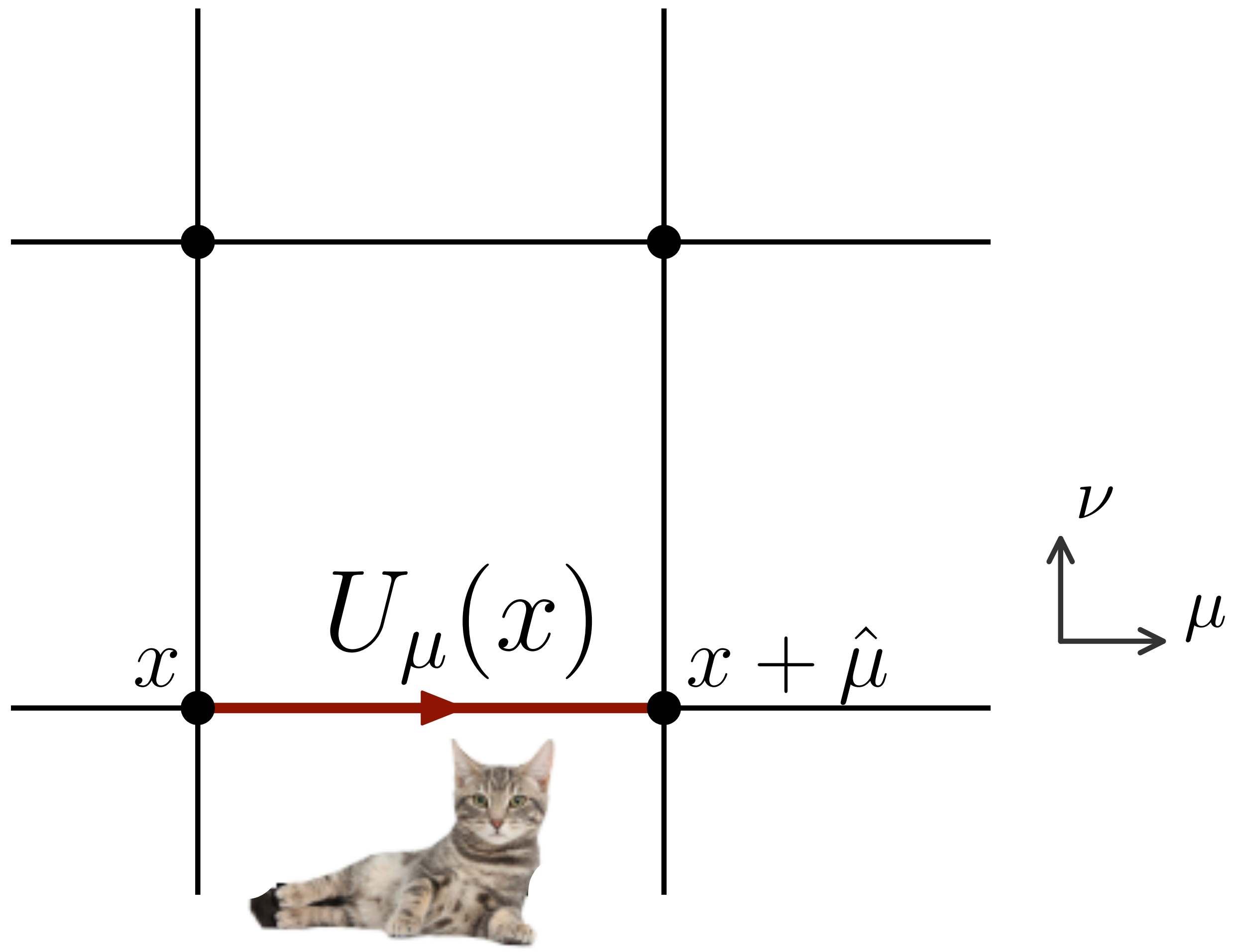
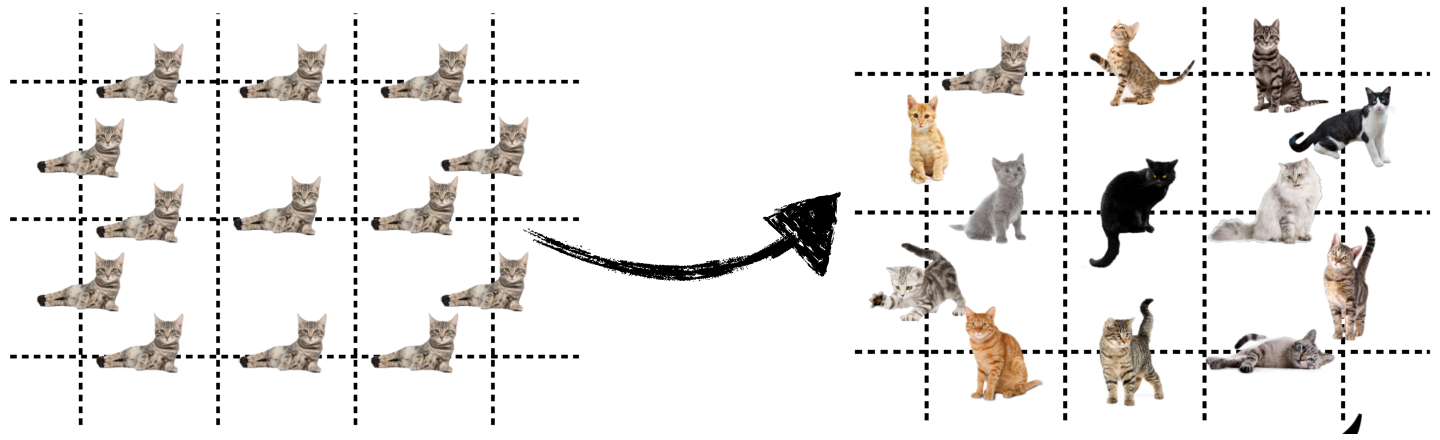


- A gauge transformation is:

$$U_\mu(x) \to \Omega(x) U_\mu(x) \Omega^\dagger(x+\hat{\mu})$$

$$\text{for all } \Omega(x) \in \mathrm{U}(1)$$



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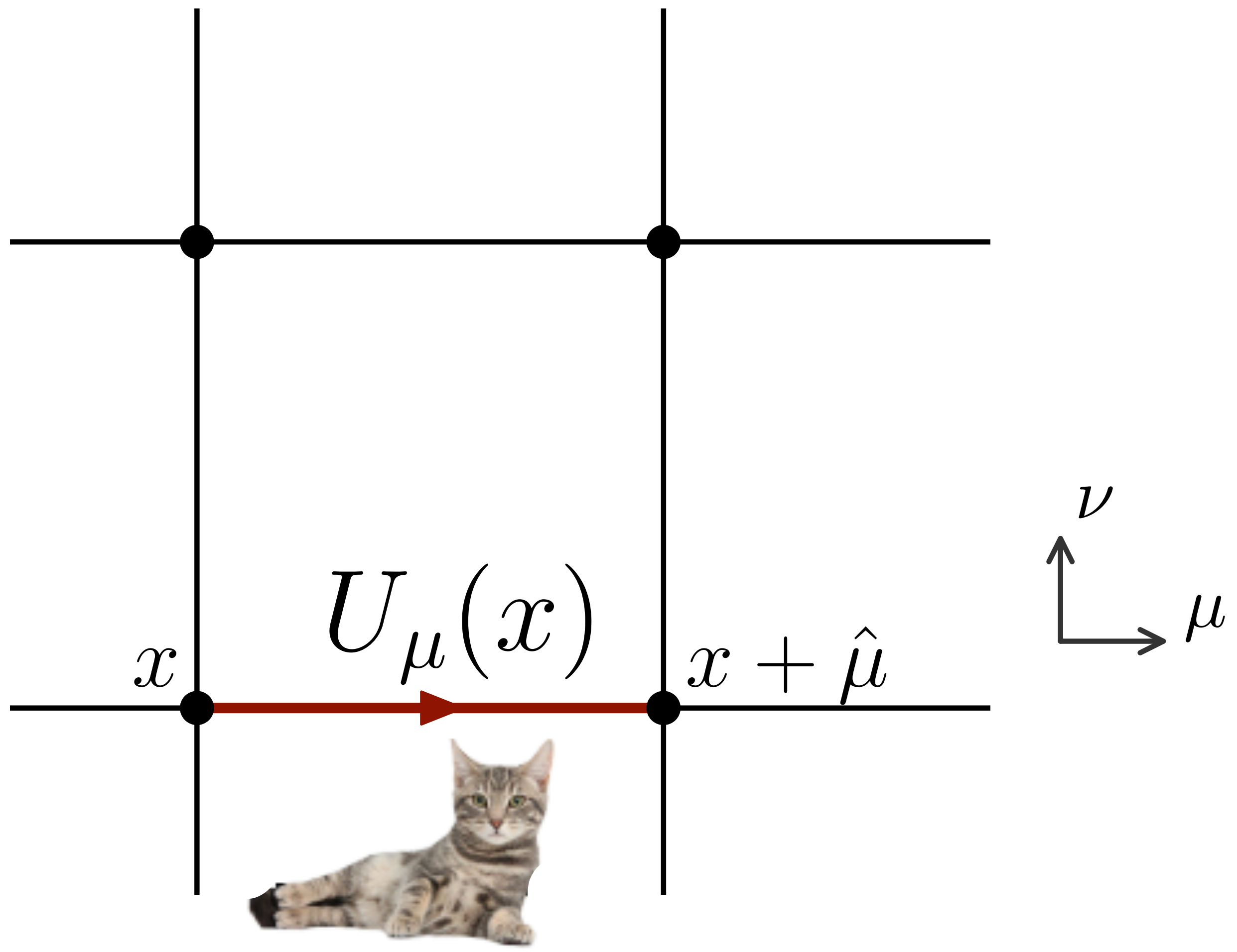

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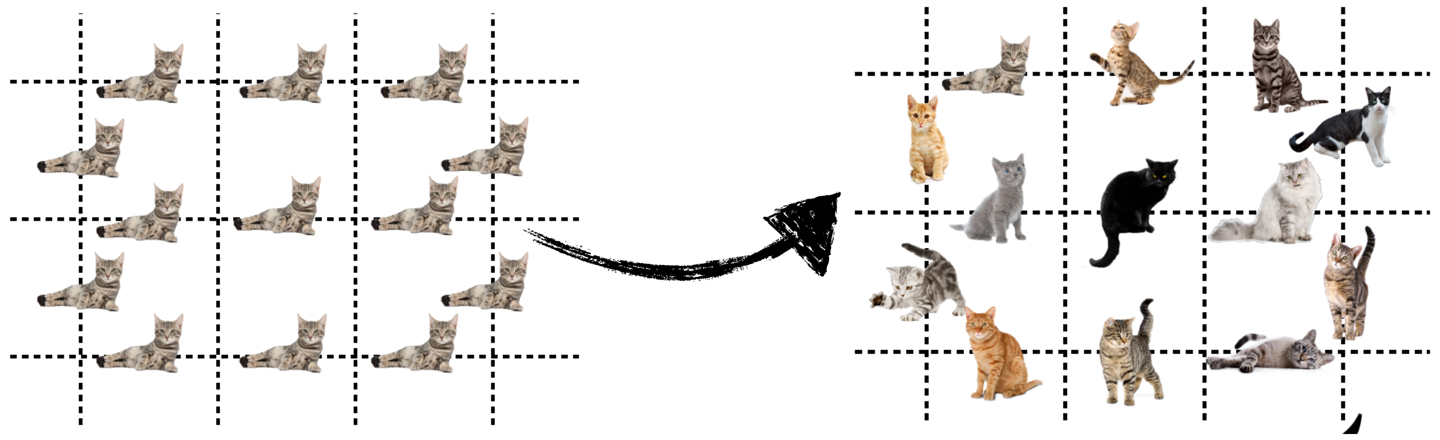
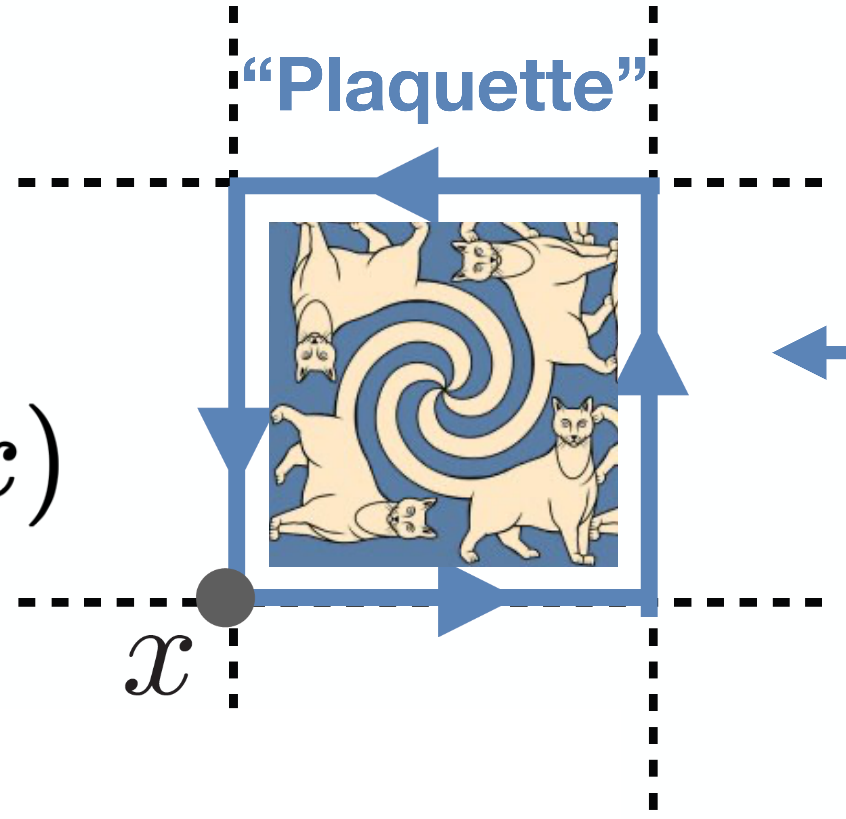


- Pure gauge lattice action:

$$S_E(U) = -\beta \sum_x \mathrm{Re}\, P_{\mu\nu}(x)$$

inverse gauge coupling



Gauge invariant
$P_{\mu\nu} \in U(1)$

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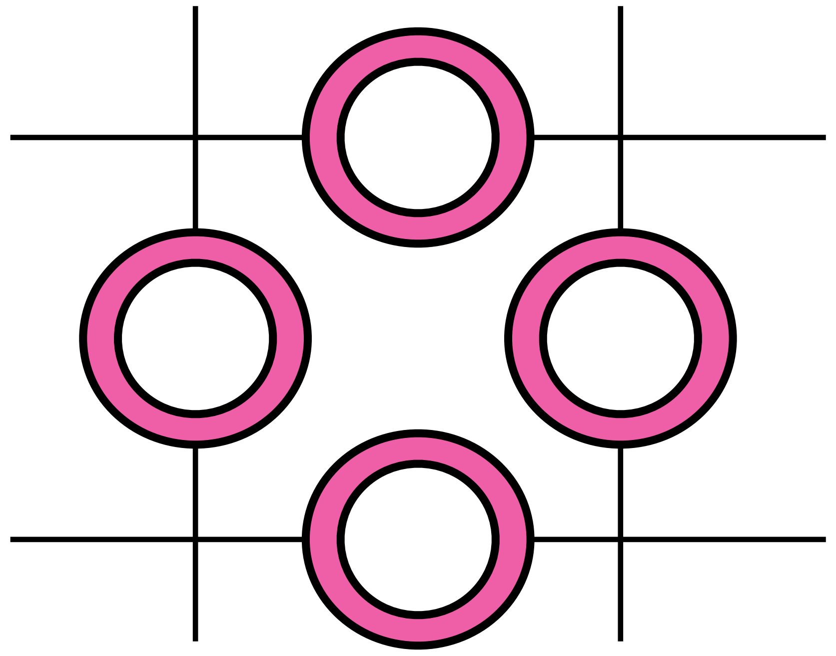
Flows for gauge theories

$r(z)$

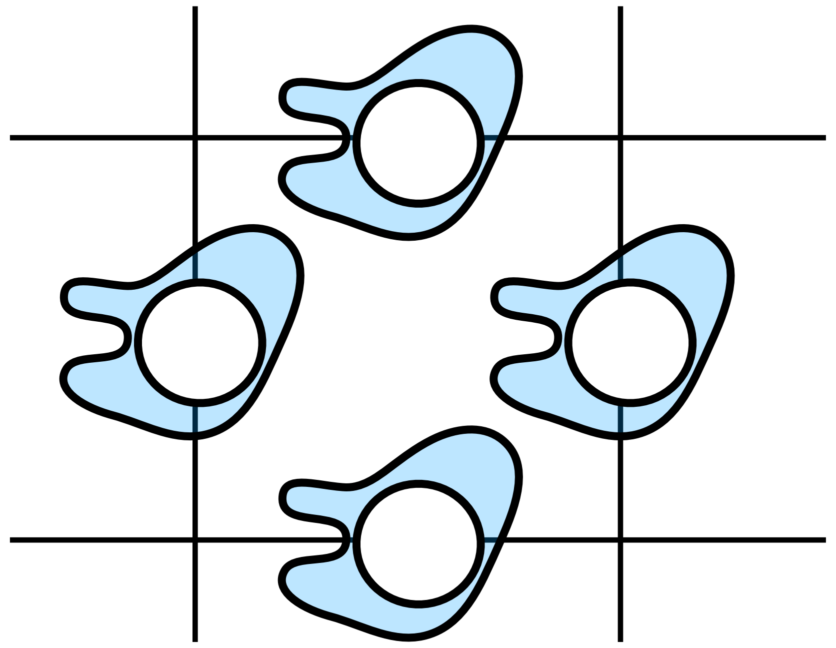


easily sampled distribution (prior)

$f(z)$

tractable Jacobian
&
invertible

$q(U) \simeq p = \frac{1}{\mathcal{Z}} e^{-S_E[U]}$



approximates target distribution (model)

- Gauge variables on compact connected manifolds
- Gauge symmetry should be included

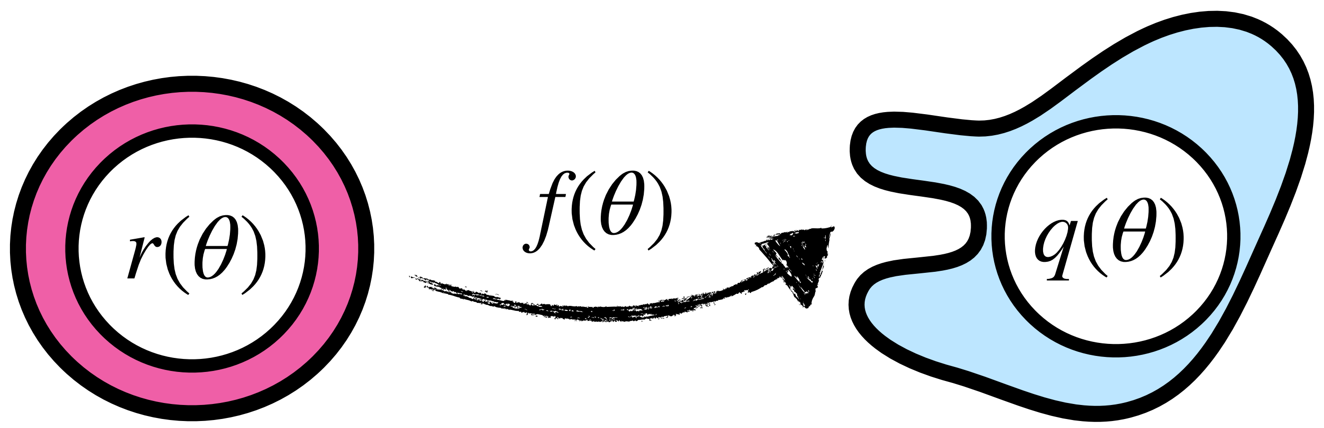
Model probability

$$q(U) = r(z) \left| \det \frac{\partial f(z)}{\partial z} \right|^{-1}$$

Flows on compact variables

- **Flows on compact connected manifolds:**

$$U_\mu(x) = \exp(i\theta) \in \mathrm{U}(1)$$



[Rezende, Papamakarios, Racanière , Albergo, Kanwar, Shanahan, Cranmer 2002.02428]

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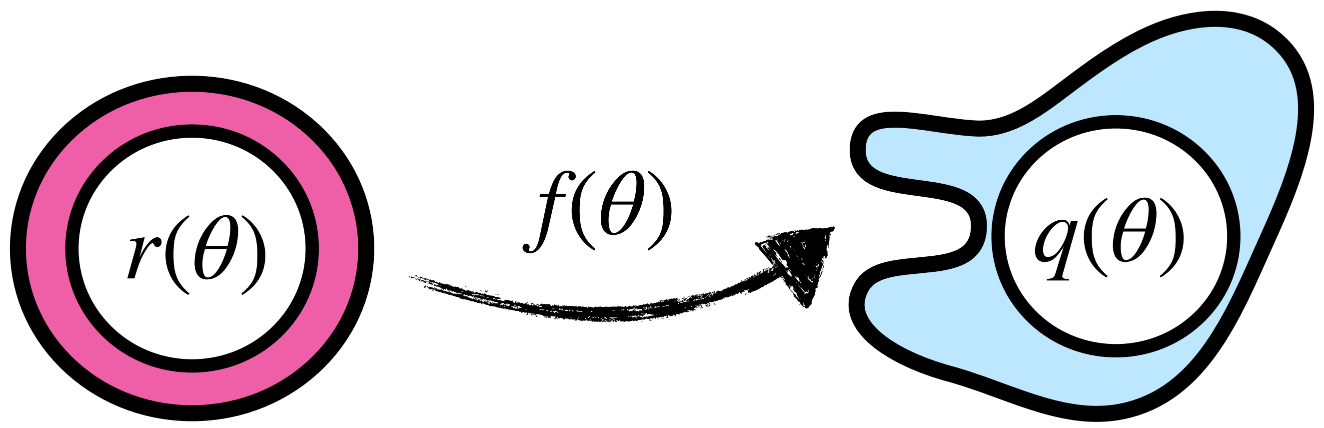

[Rezende, Papamakarios, Racanière , Albergo, Kanwar, Shanahan, Cranmer 2002.02428]

Diffeomorphism if:

$$\begin{aligned} f(0) &= 0, \\ f(2\pi) &= 2\pi, \\ \nabla f(\theta) &> 0, \\ \nabla f(\theta)|_{\theta=0} &= \nabla f(\theta)|_{\theta=2\pi} \end{aligned}$$

monotonic, invertible

Fernando Romero-López, MIT

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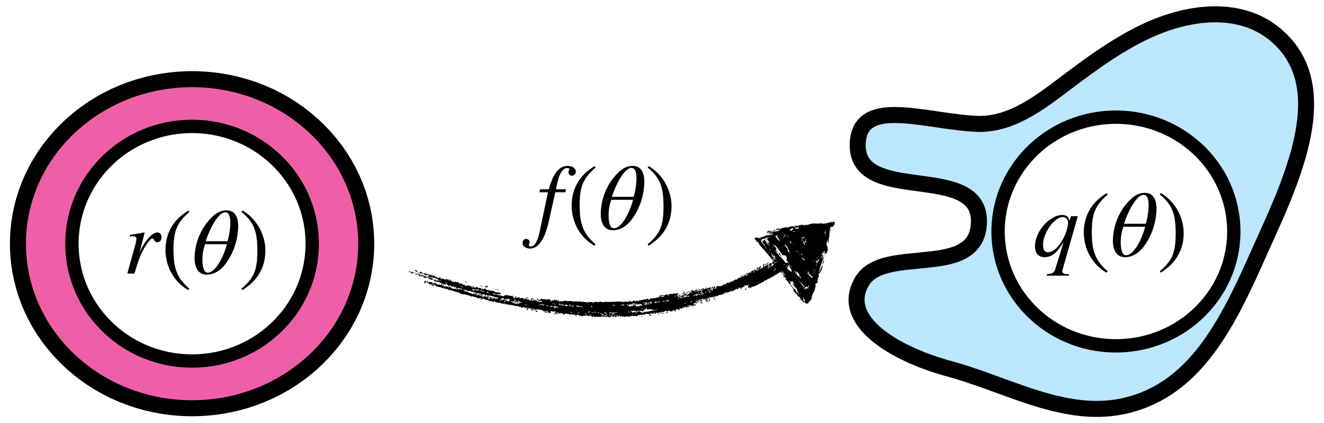

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$$\nabla f(\theta) > 0,$$
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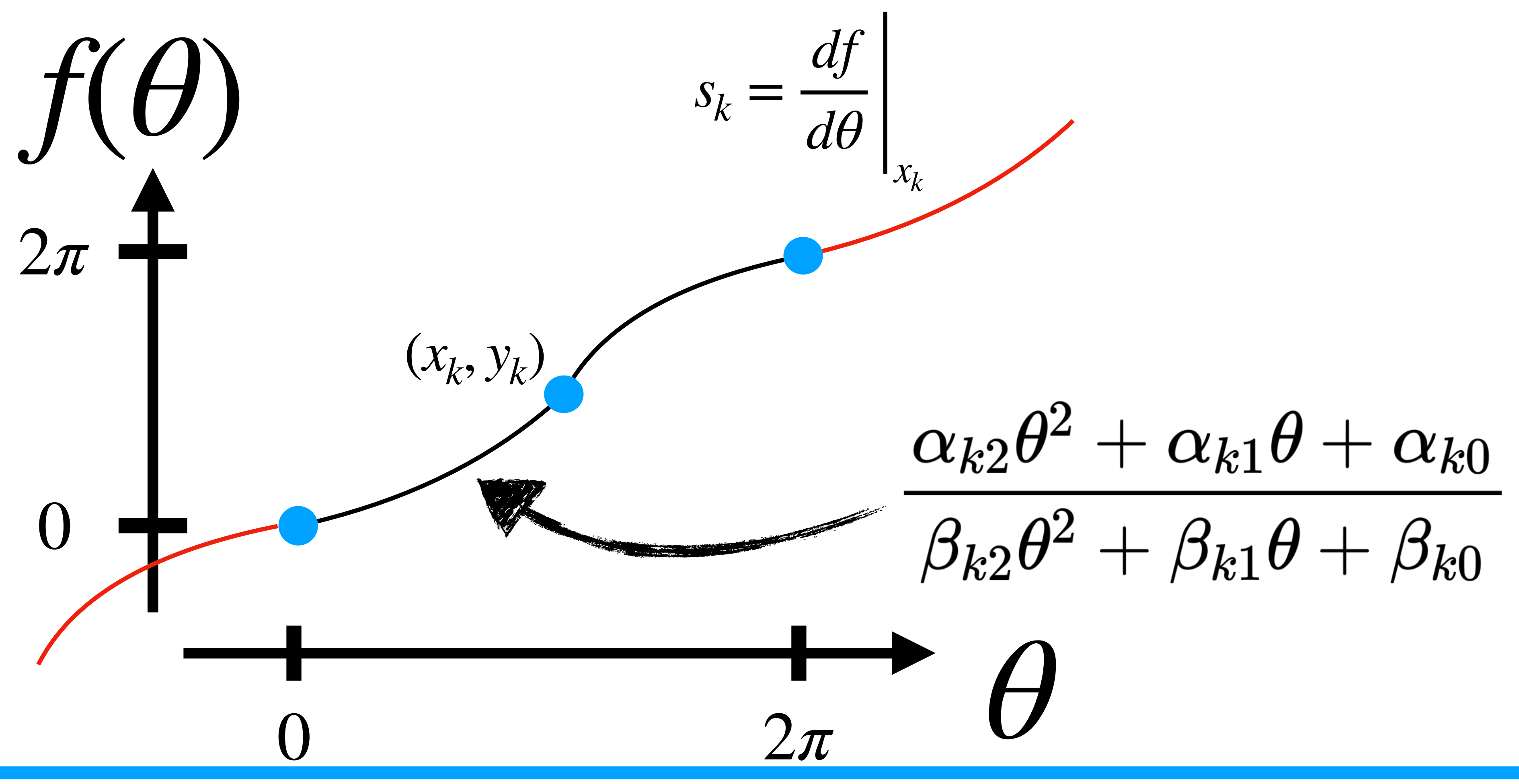
monotonic, invertible

Circular splines:



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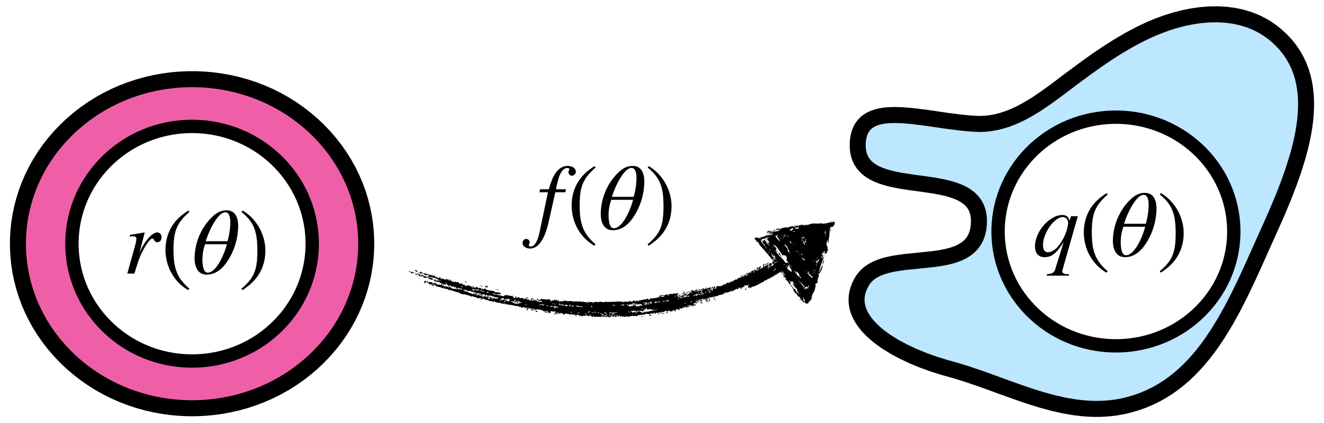

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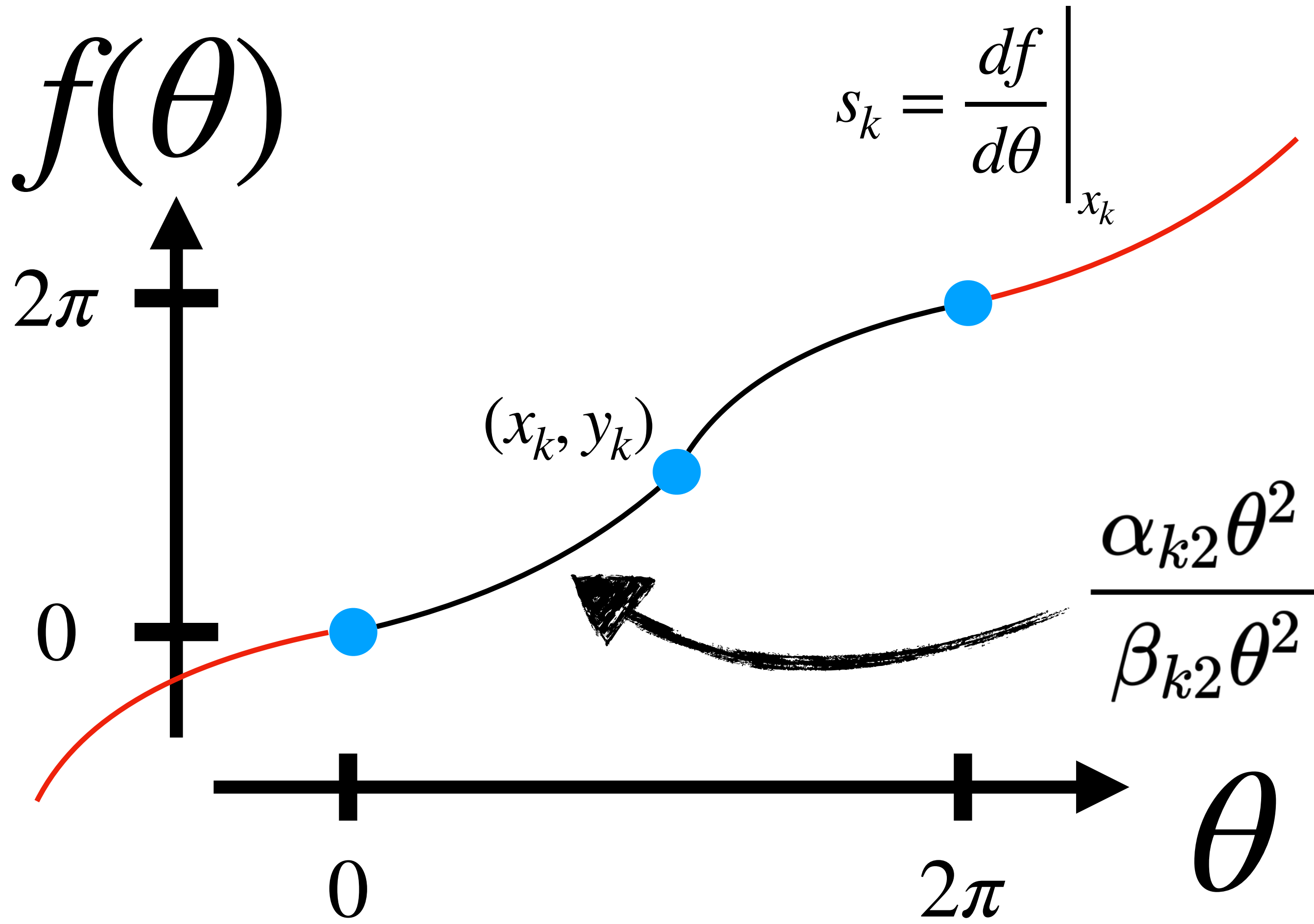
monotonic, invertible

Circular splines:

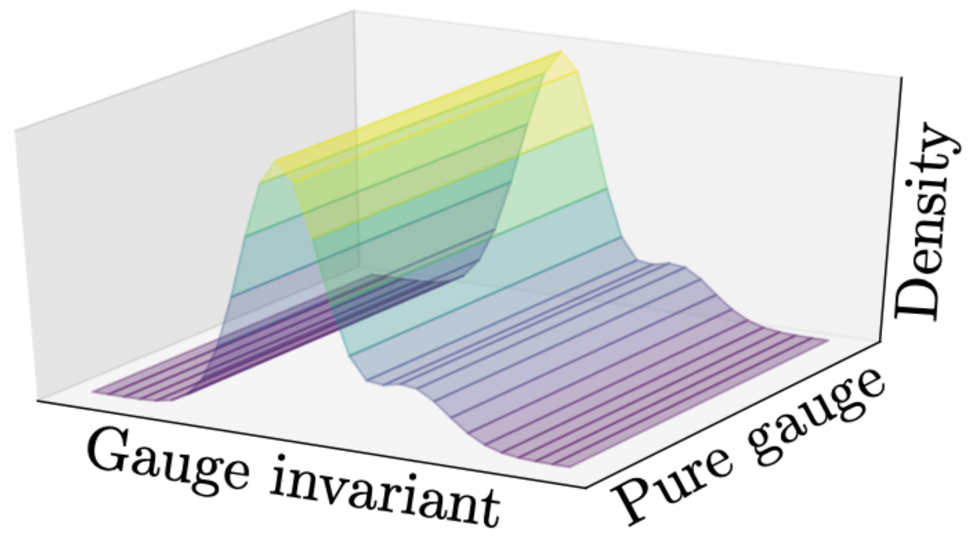
- Trainable positions and slopes
- Expressivity with more knots



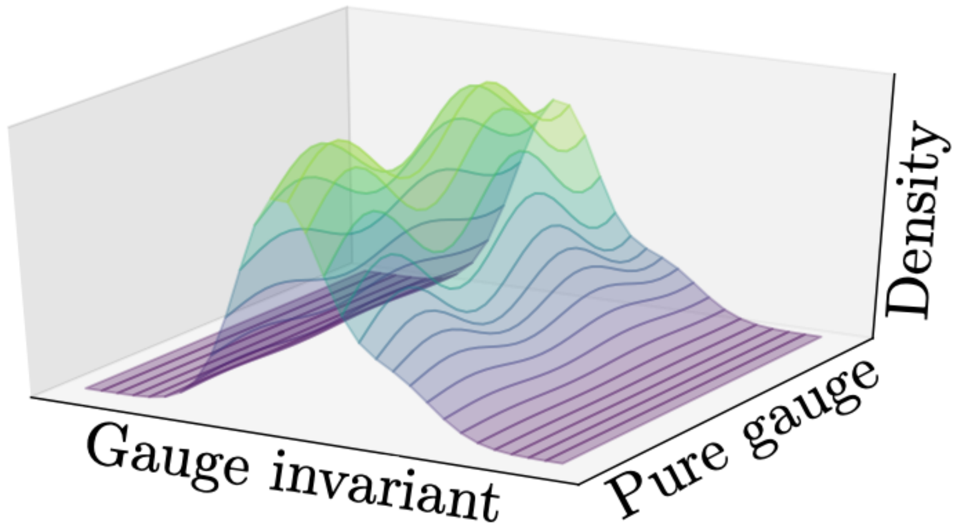
Incorporating symmetries

- Not essential, but:
  - ✓ Reduces complexity of training
  - ✓ Reduces parameter count

Gauge symmetries:



True distribution



Learned by naive ML

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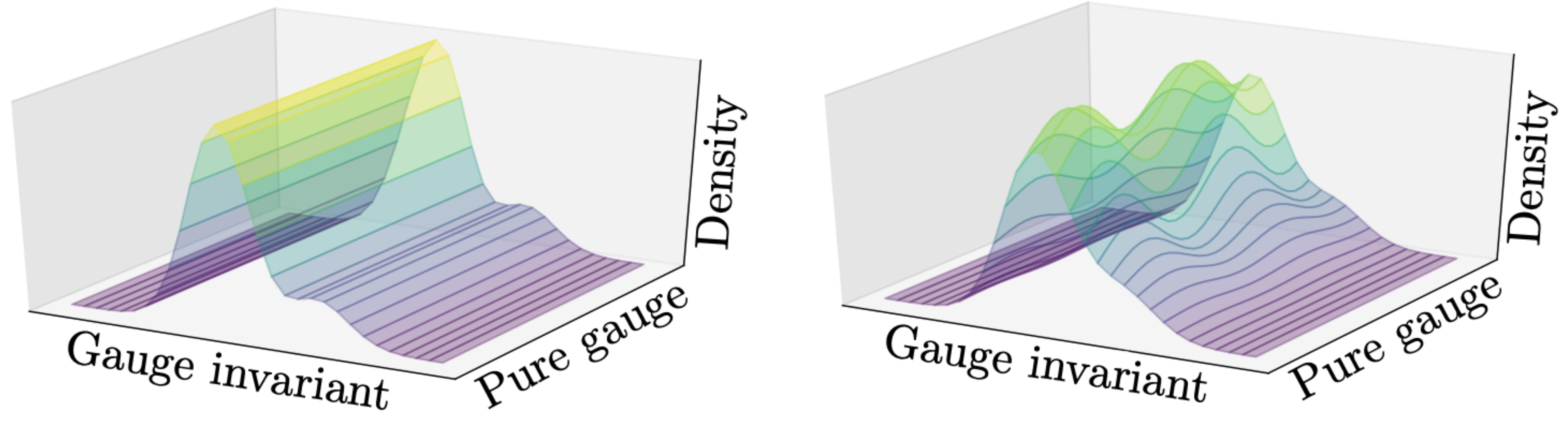
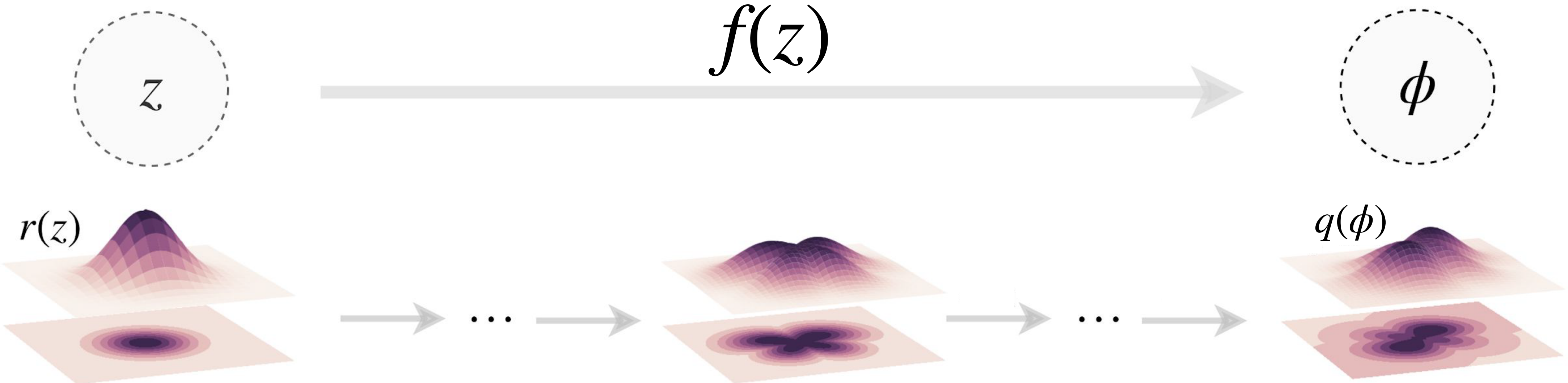


True distribution **Learned by naive ML**

General approach:

1. Invariant base distribution

$$r(z) = r(t(z))$$



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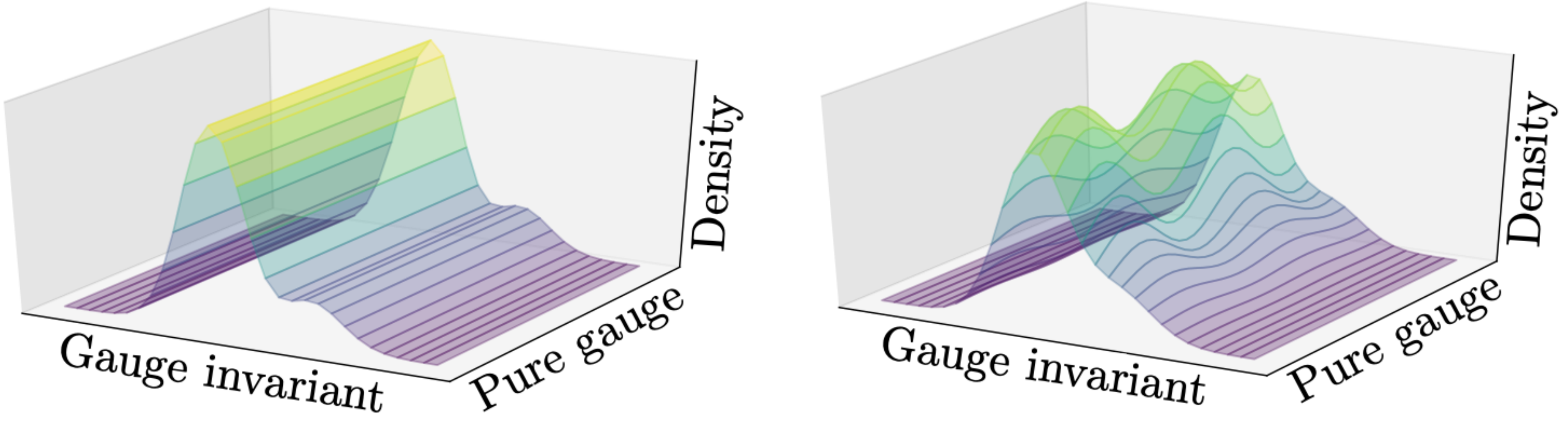


True distribution | **Learned by naive ML**

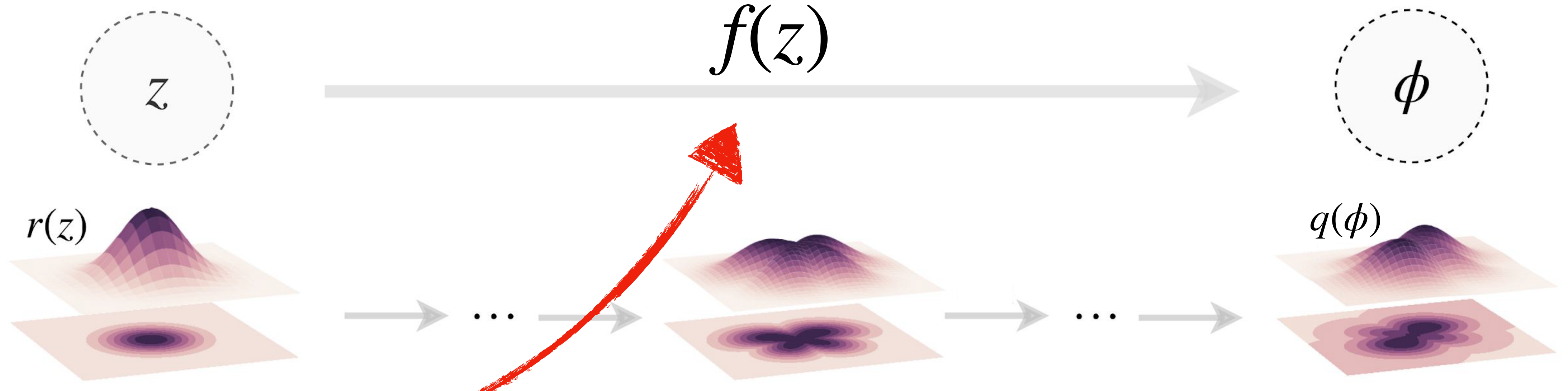
General approach:

1. Invariant base distribution

$$r(z) = r(t(z))$$

2. Equivariant flow

$$f(t(\phi)) = t(f(\phi))$$



Fernando Romero-López, MIT

Flows with gauge variables

- **Gauge invariant prior + gauge-equivariant transformations:**

$$\theta \sim \mathrm{Uniform}(0, 2\pi)$$
$$g\big(\Omega(x)U_\mu(x)\Omega^\dagger(x+\mu)\big) = \Omega(x)\, g(U_\mu(x))\, \Omega^\dagger(x+\mu)$$

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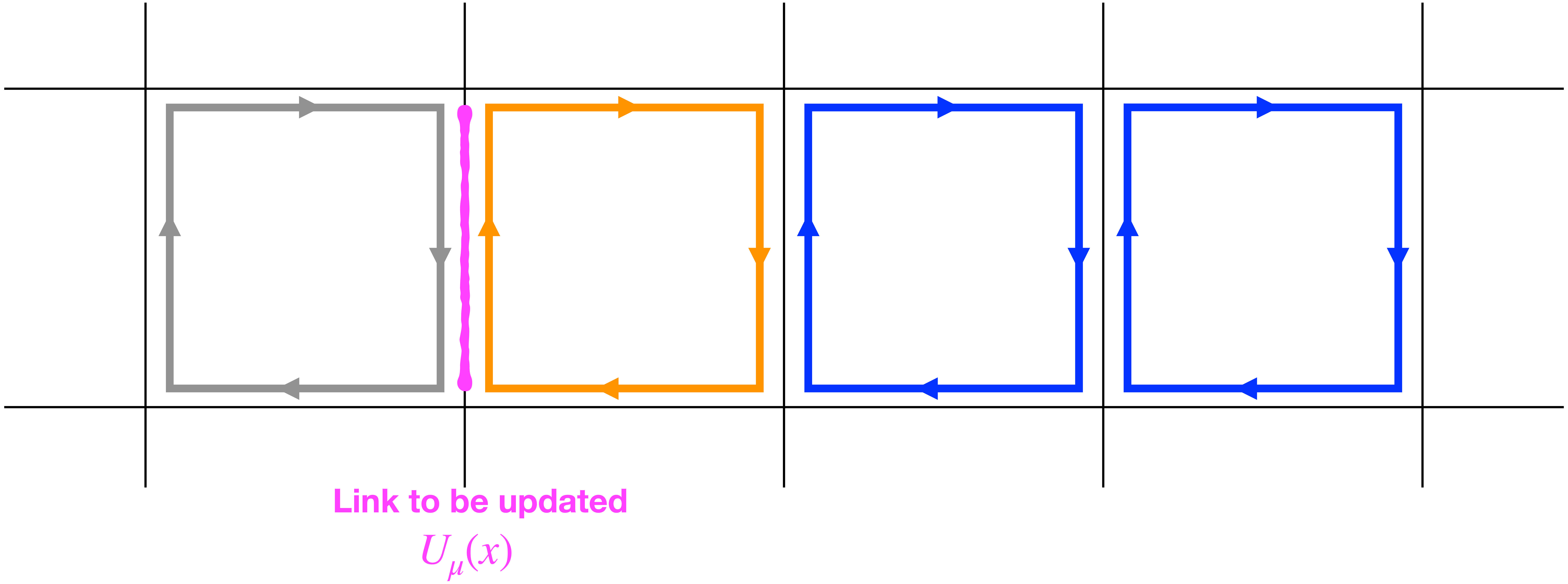

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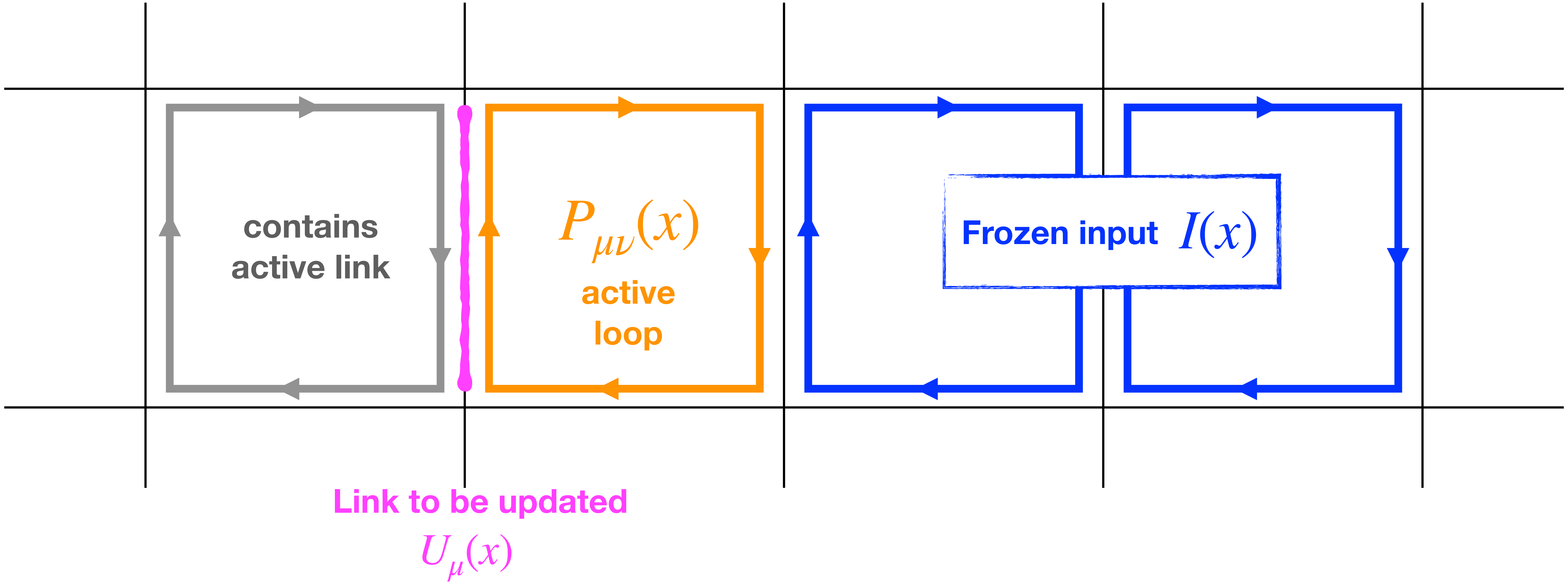

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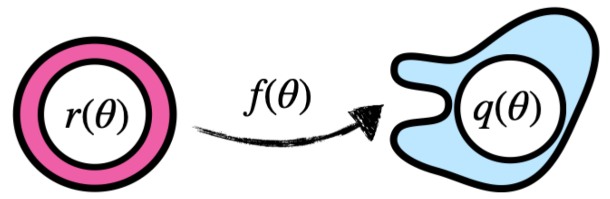
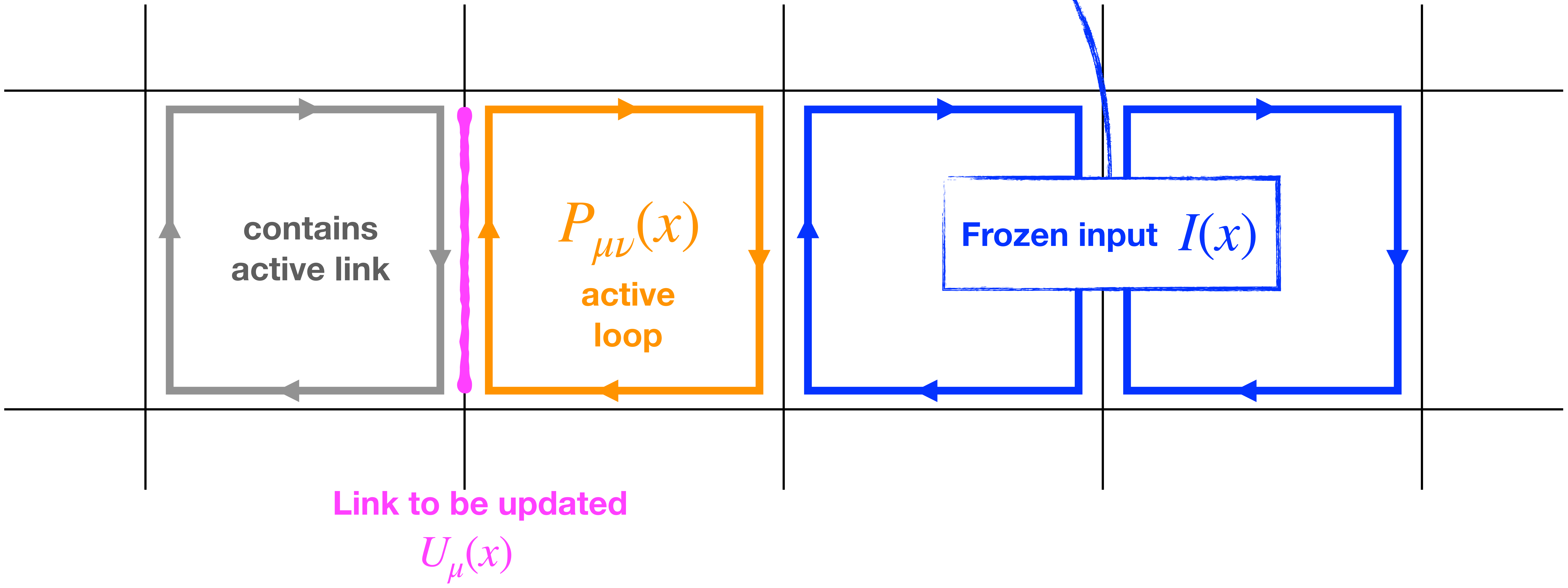
$$P'_{\mu\nu}(x) = h\left(P_{\mu\nu}(x) \,|\, I(x)\right)$$

e.g. circular splines





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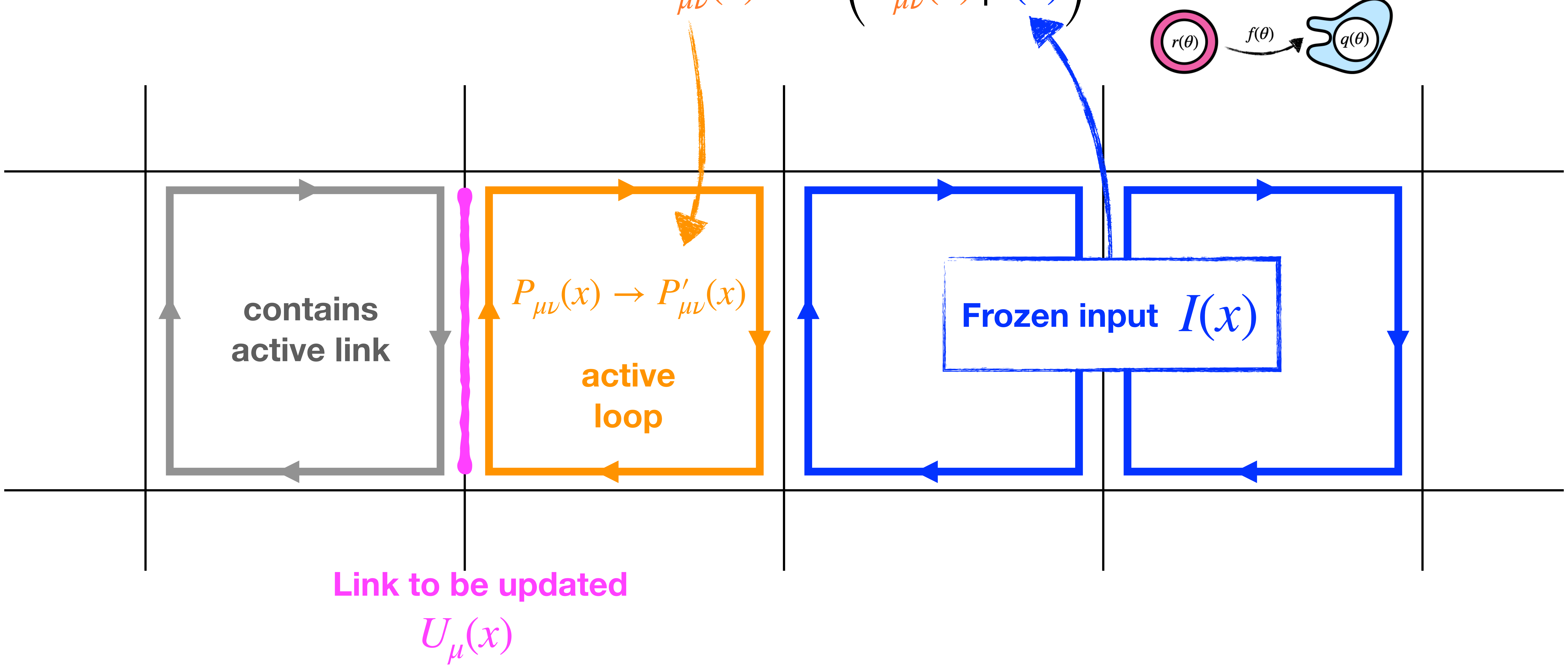

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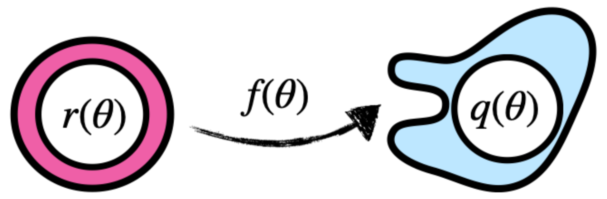

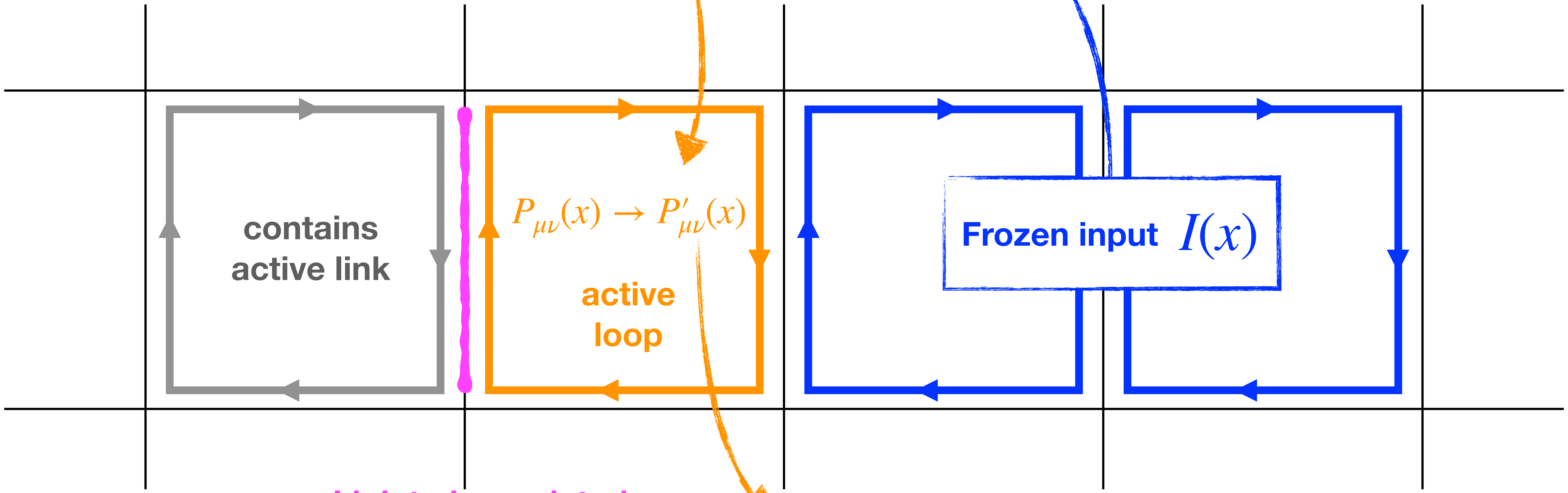

Link to be updated

$$U_\mu(x) \to U'_\mu(x) = P'_{\mu\nu}(x) P^\dagger_{\mu\nu}(x) U_\mu(x)$$

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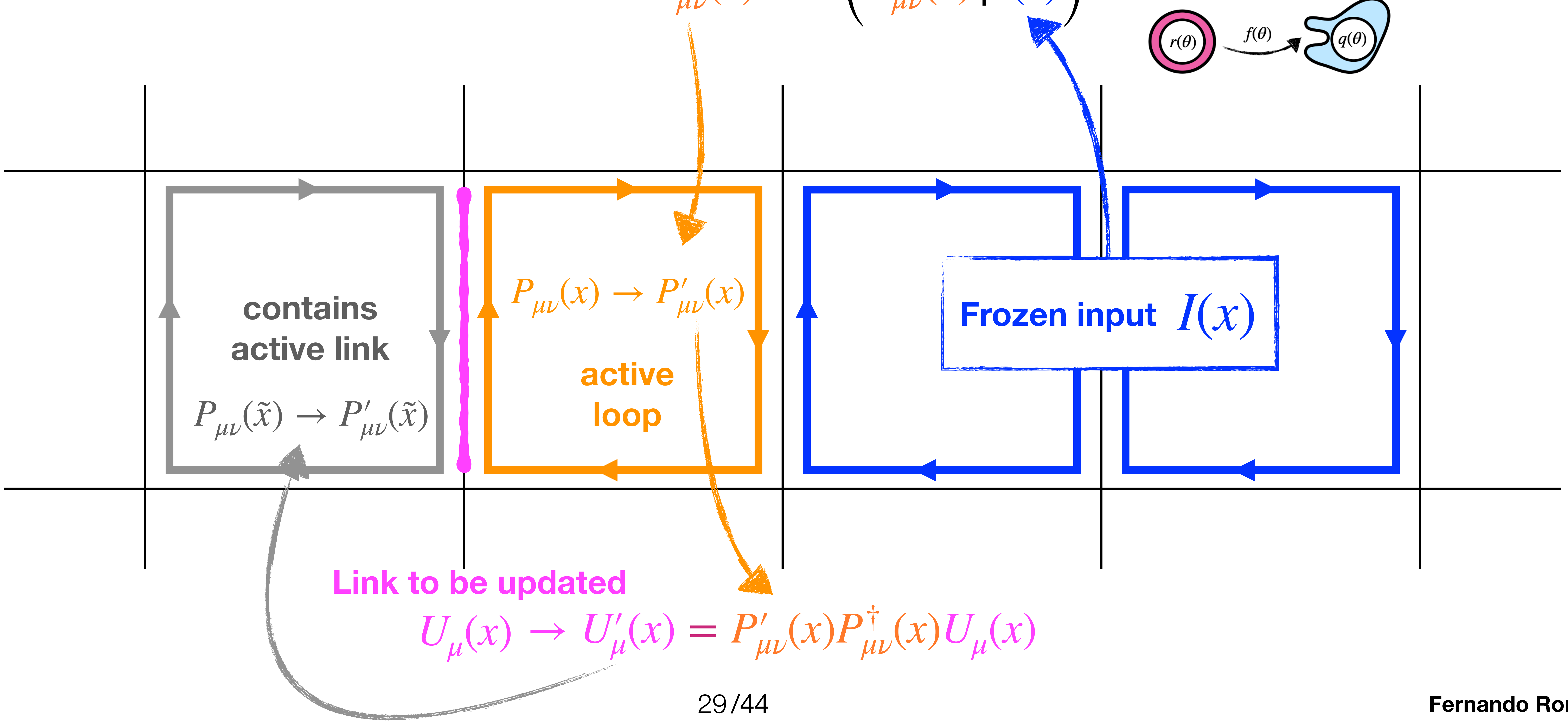

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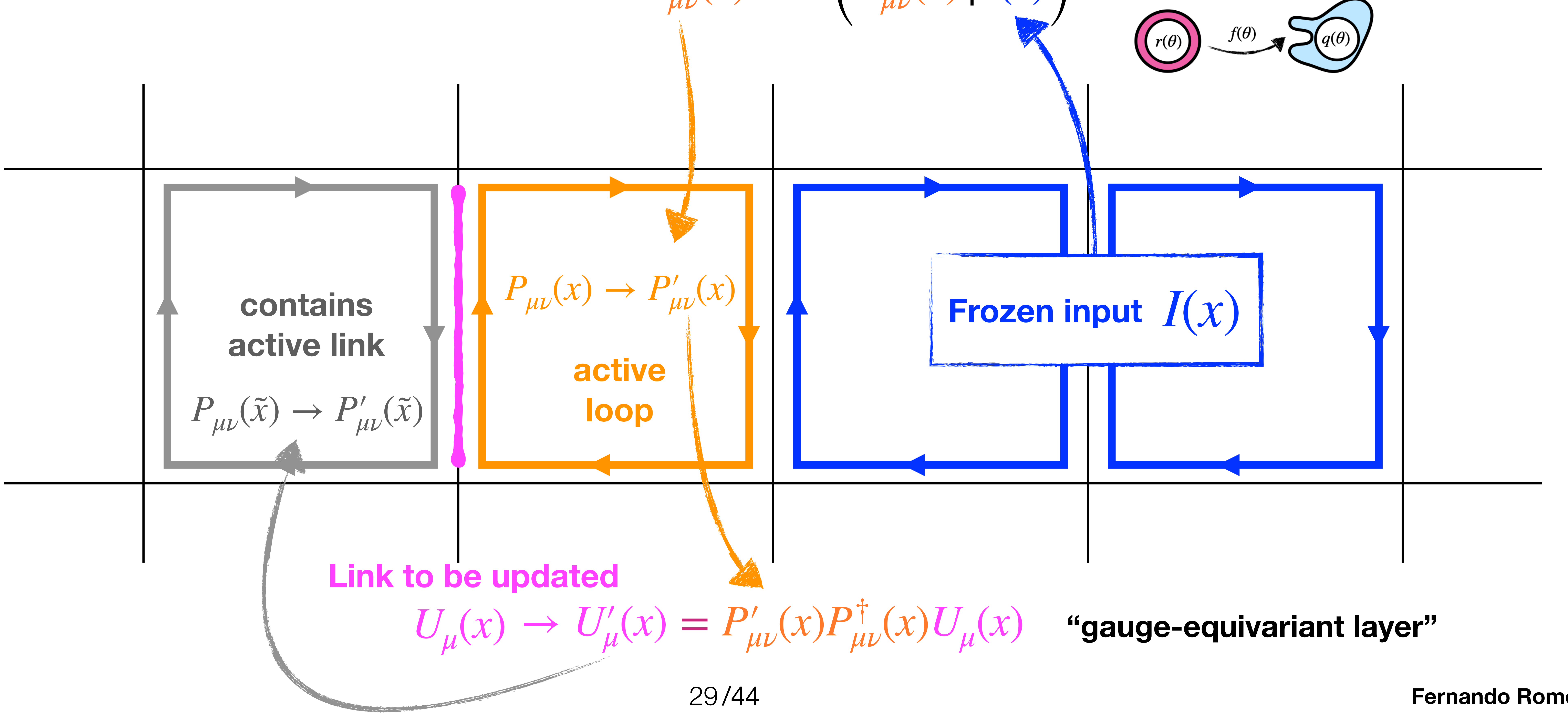

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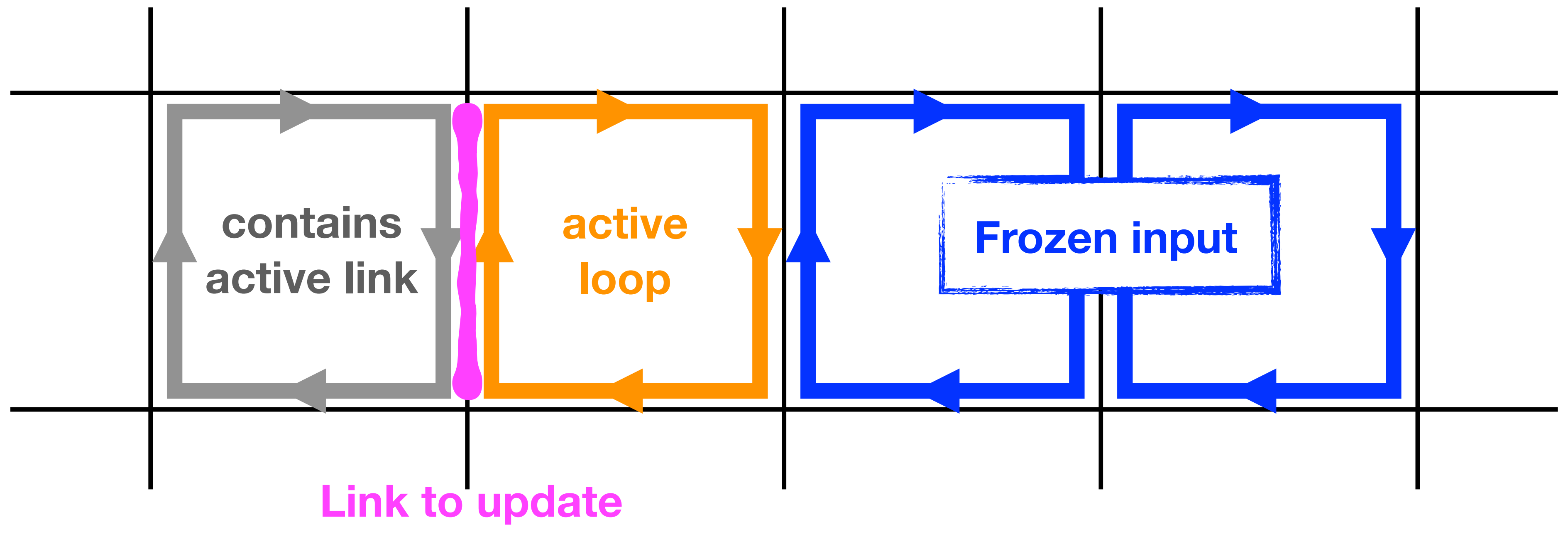
"gauge-equivariant layer"

Gauge-equivariant models



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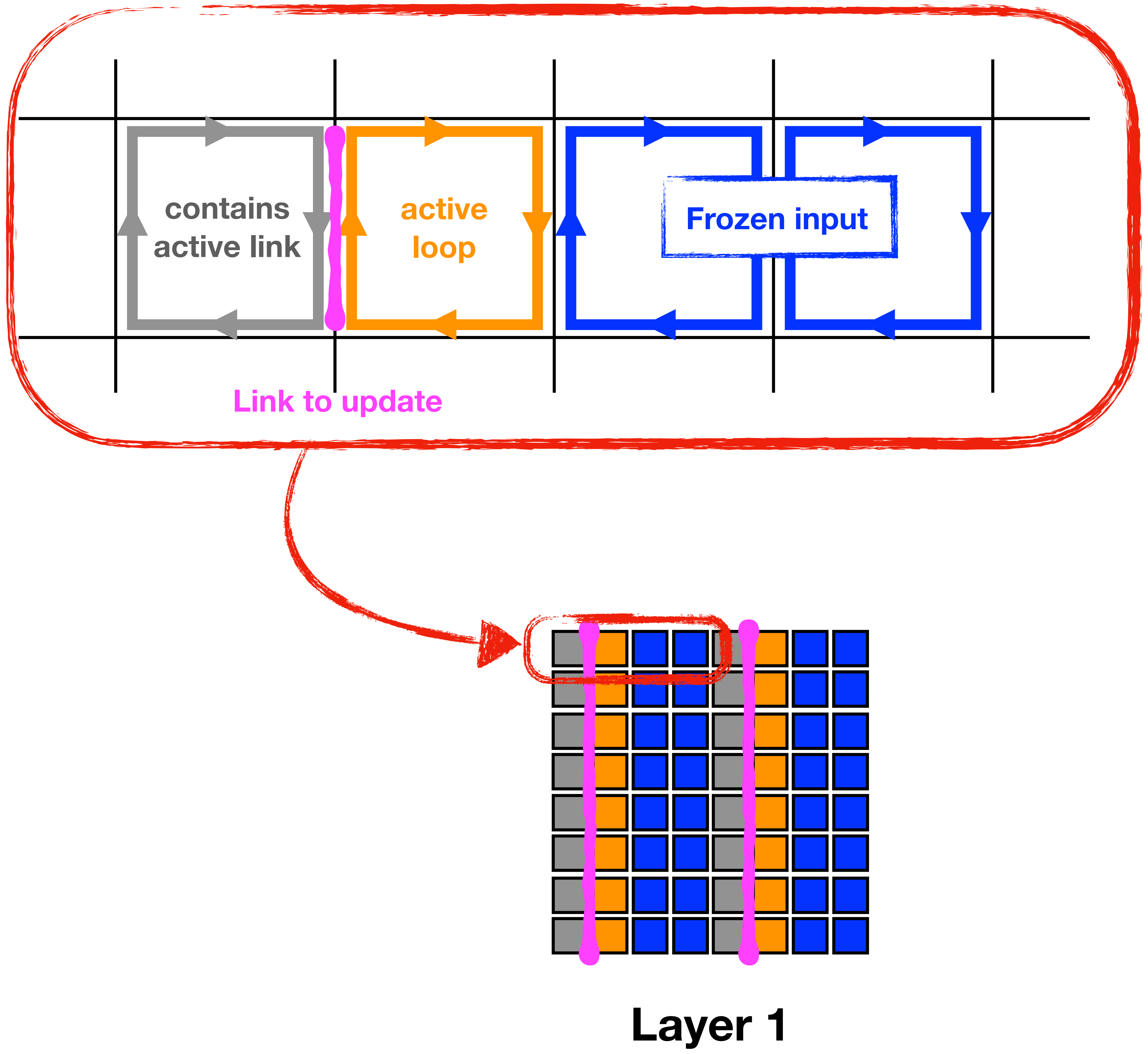
Gauge-equivariant models



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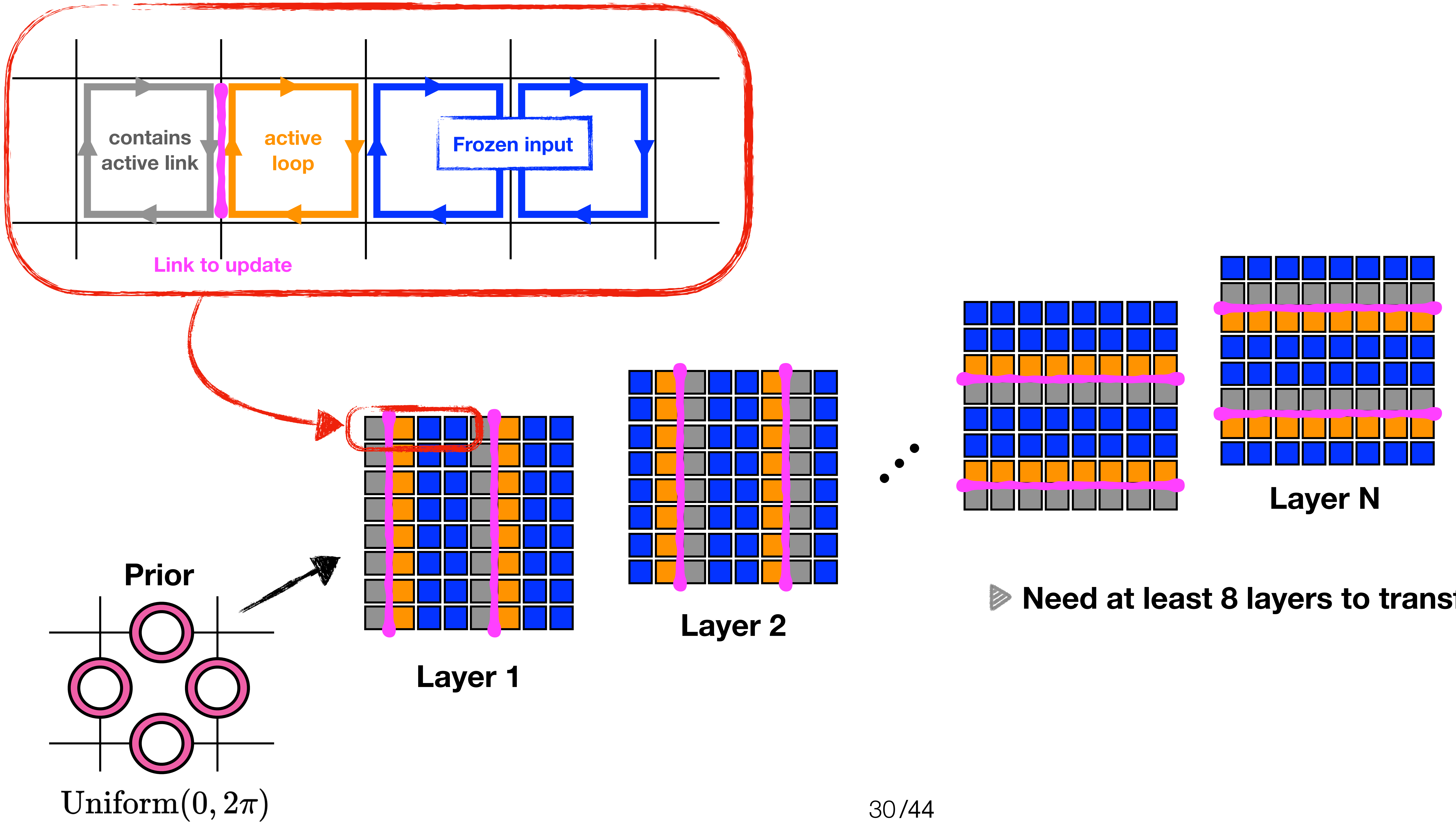
Gauge-equivariant models



- Need at least 8 layers to transform all links

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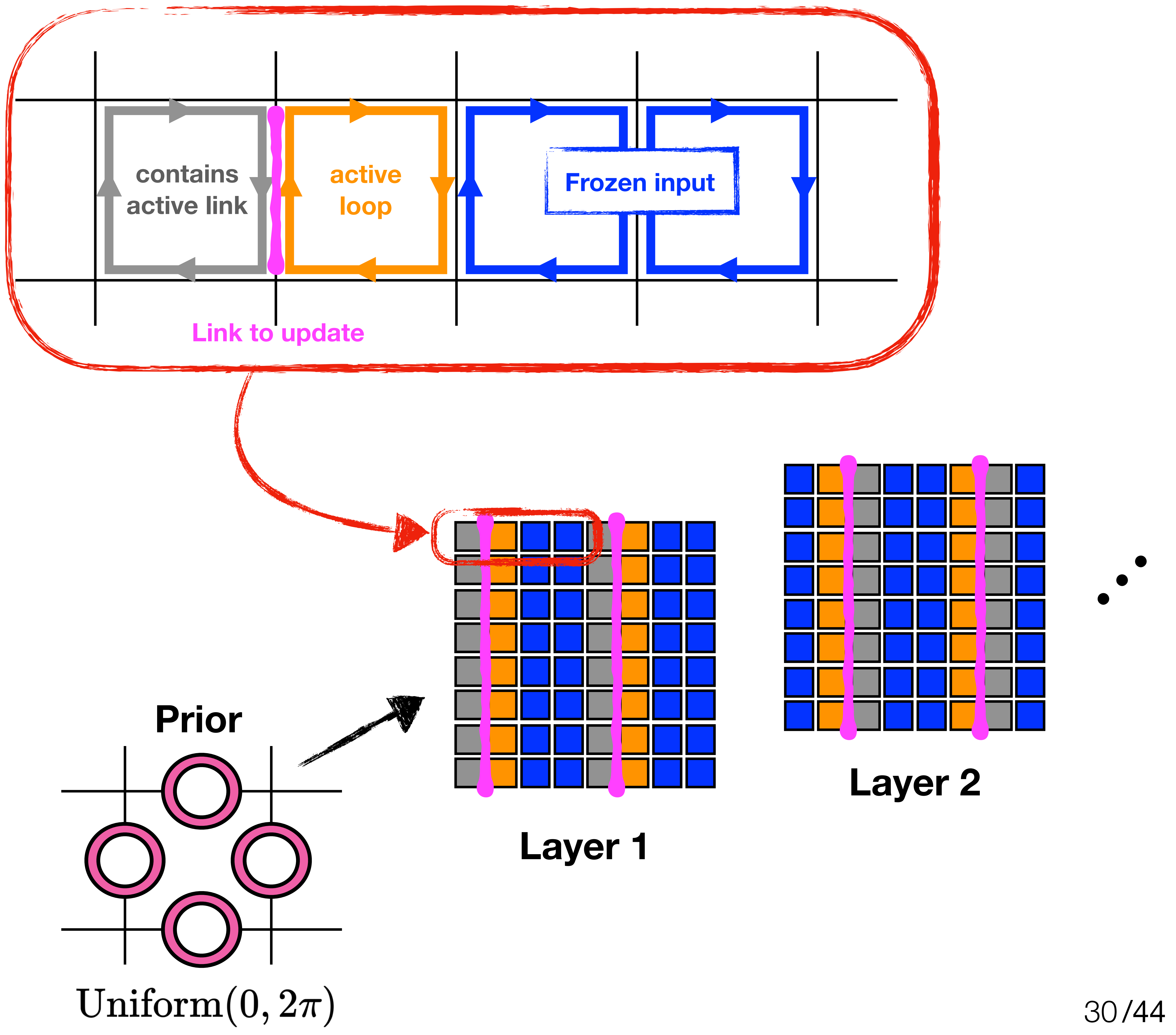
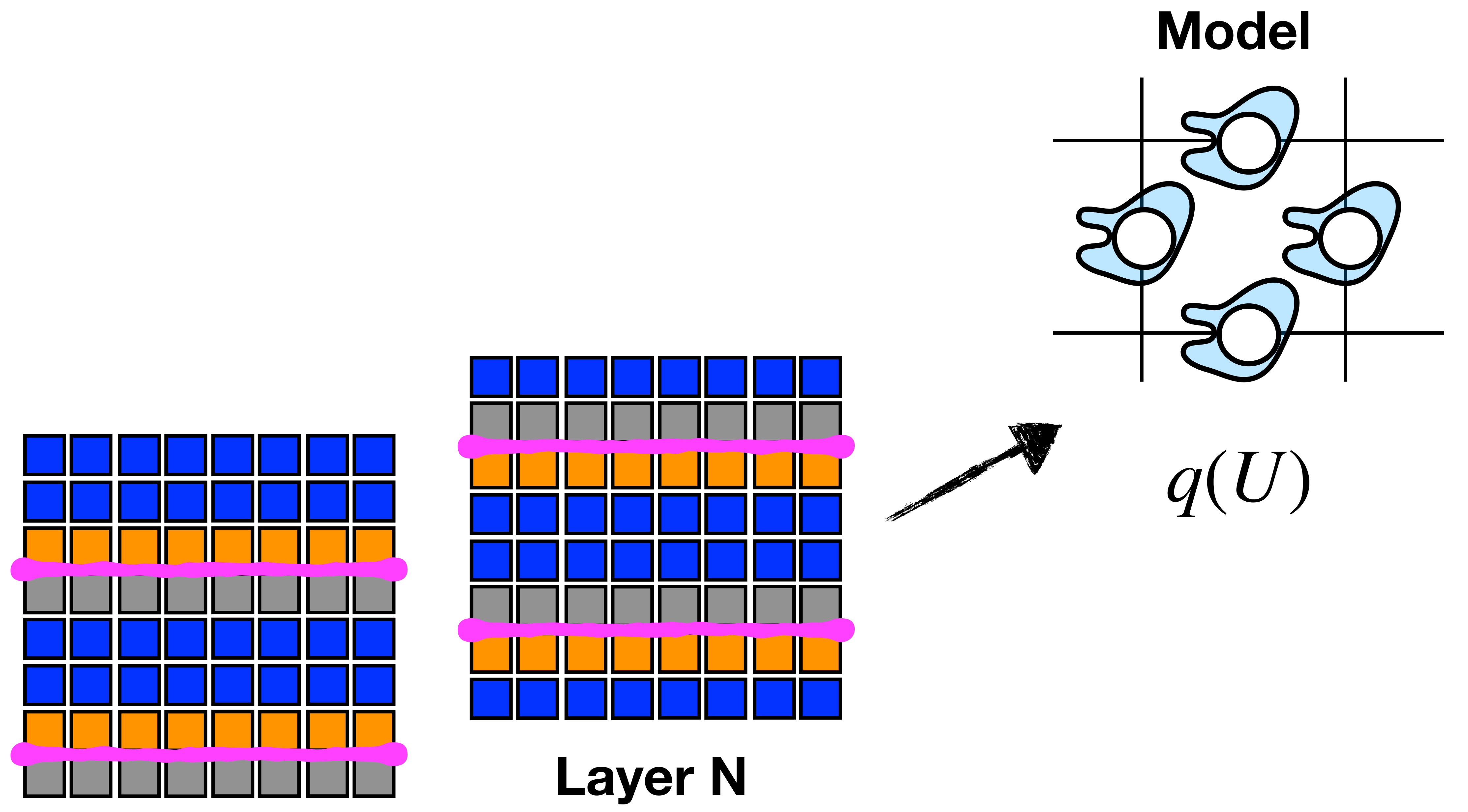
Gauge-equivariant models





- Need at least 8 layers to transform all links
- ✓ Similar approach can be applied to SU(N)
  [Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan 2003.06413]

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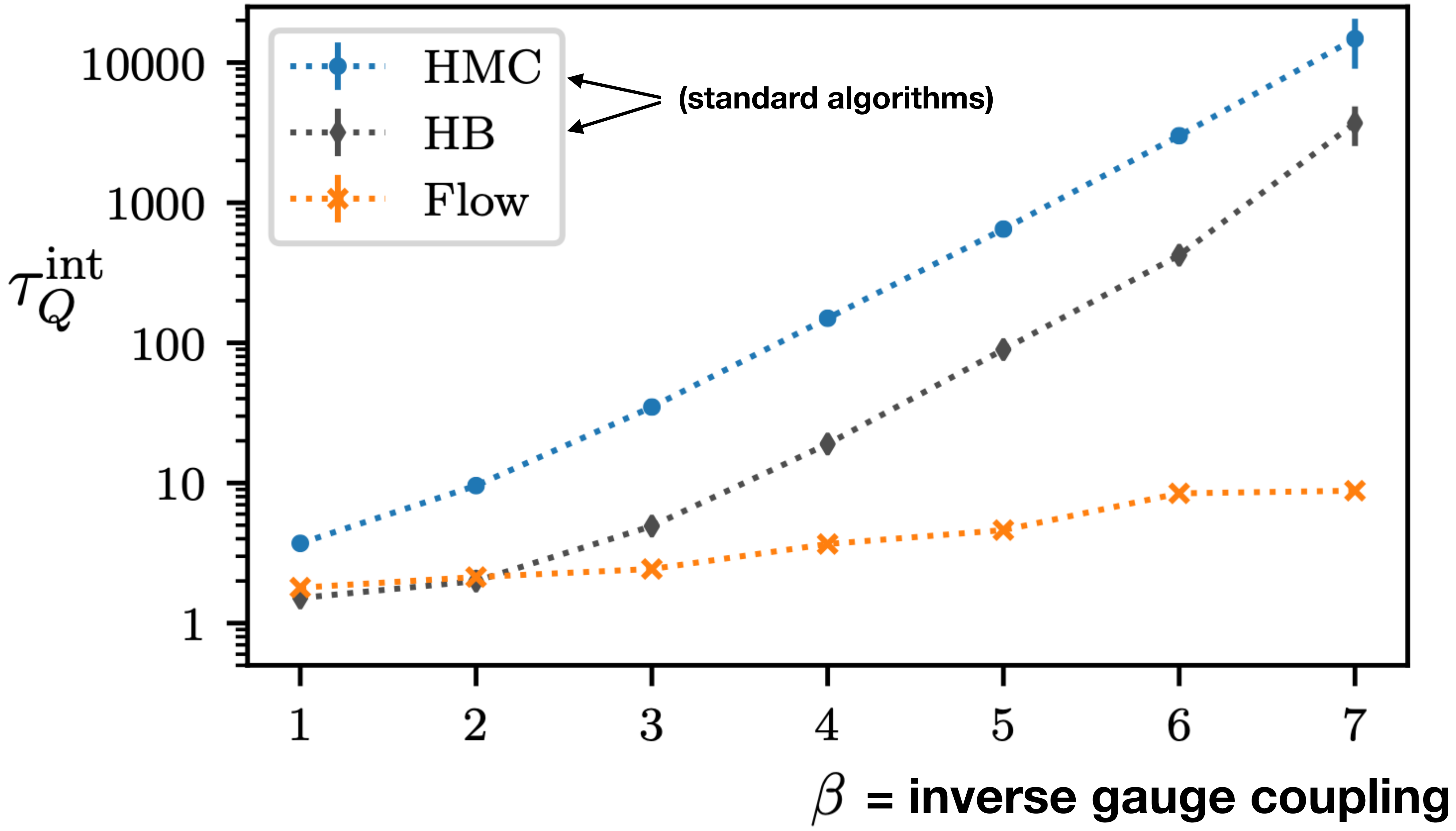
Results in 2D U(1) theory

Cost per independent sample



Autocorrelation time
of the topological charge

Continuum limit

✓ **Flow-based sampling has no topological freezing**

[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan 2003.06413]

Fernando Romero-López, MIT

Flows for fermionic gauge theories

The Schwinger Model

QED in 1+1 dimensions with Nf=2 fermions

$$\mathcal{L} = -\frac{1}{4g^2} F_{\mu\nu} F^{\mu\nu} + \sum_{f=1,2} \bar{\psi}_f (i\gamma^\mu D_\mu - m)\psi_f$$

Fernando Romero-López, MIT

The Schwinger Model

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Toy model for QCD

1. Confinement
2. Chiral symmetry breaking
3. Topology

Machine Learning challenges

1. Gauge symmetry
2. Fermion degrees of freedom
3. Long-range correlations

Fernando Romero-López, MIT

Fermionic theories

- **The fermionic part of the action**

Dirac-Wilson operator

$$S_{\text{ferm}}(U,\psi,\bar{\psi}) = \sum_{f=1}^{N_f} \sum_{x,y} \bar{\psi}_f^{\beta}(y) D[U](y,x)^{\beta\alpha} \psi_f^{\alpha}(x)$$

$$D[U](y,x)^{\beta\alpha} = \delta(y-x)\delta^{\beta\alpha} - \kappa \sum_{\mu=0,1} \left\{ [1-\sigma_\mu]^{\beta\alpha} U_\mu(y)\delta(y-x+\hat{\mu}) + [1+\sigma_\mu]^{\beta\alpha} U_\mu^\dagger(y-\hat{\mu})\delta(y-x-\hat{\mu}) \right\},$$

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- Full action can be expressed only in terms of gauge variables: use gauge flow architectures!

$$S_E(U) = -\beta\sum_x \operatorname{Re}P(x) - \log\det D[U]^\dagger D[U]$$

"exact determinant"

(gauge part)

(assuming N_f=2)

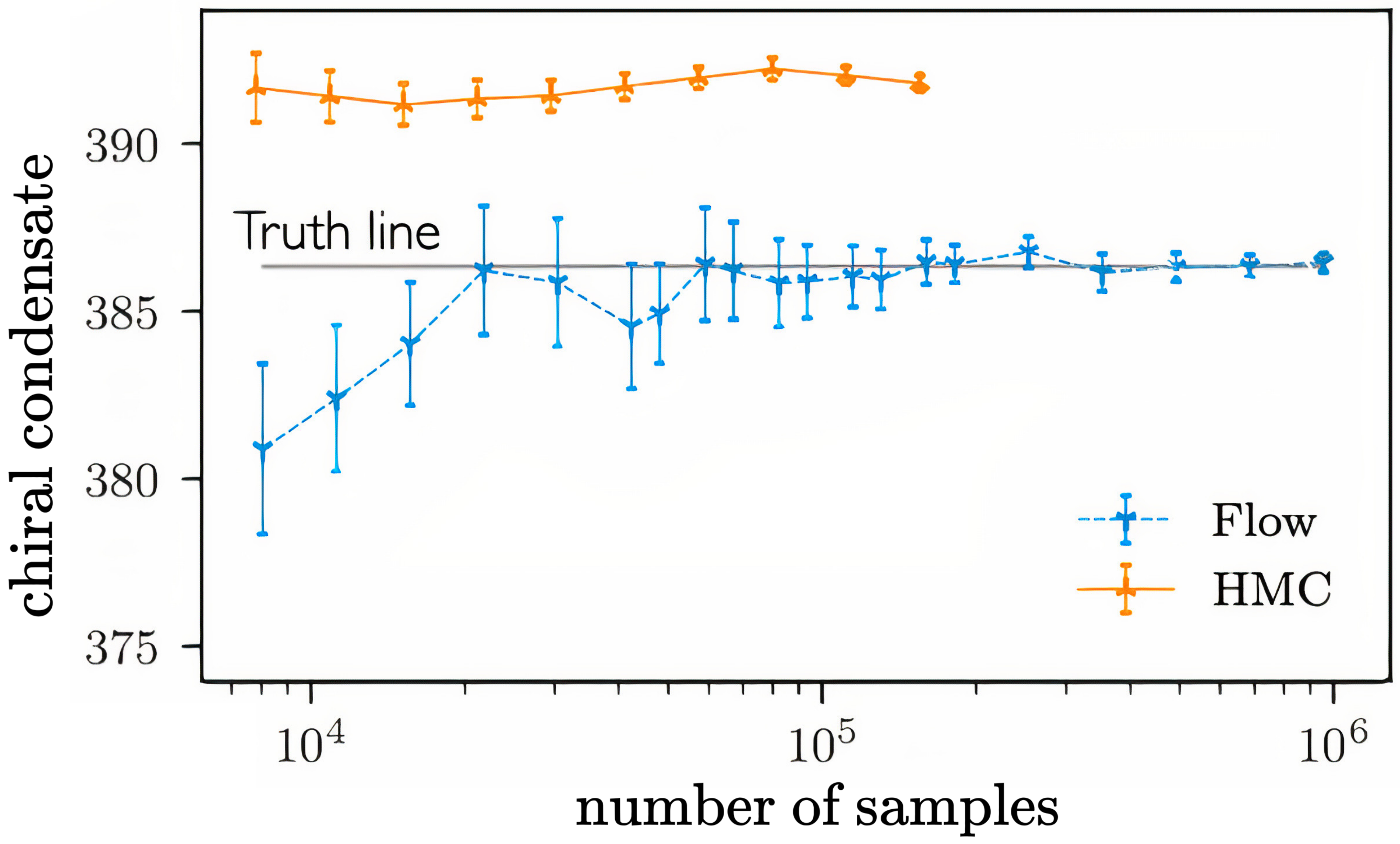
Fernando Romero-López, MIT

The Schwinger model at criticality

Critical parameters:

- **Vanishing fermion mass**
- **Diverging correlation length**

! Hardest to simulate in standard approaches



[Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Urban 2202.11712]

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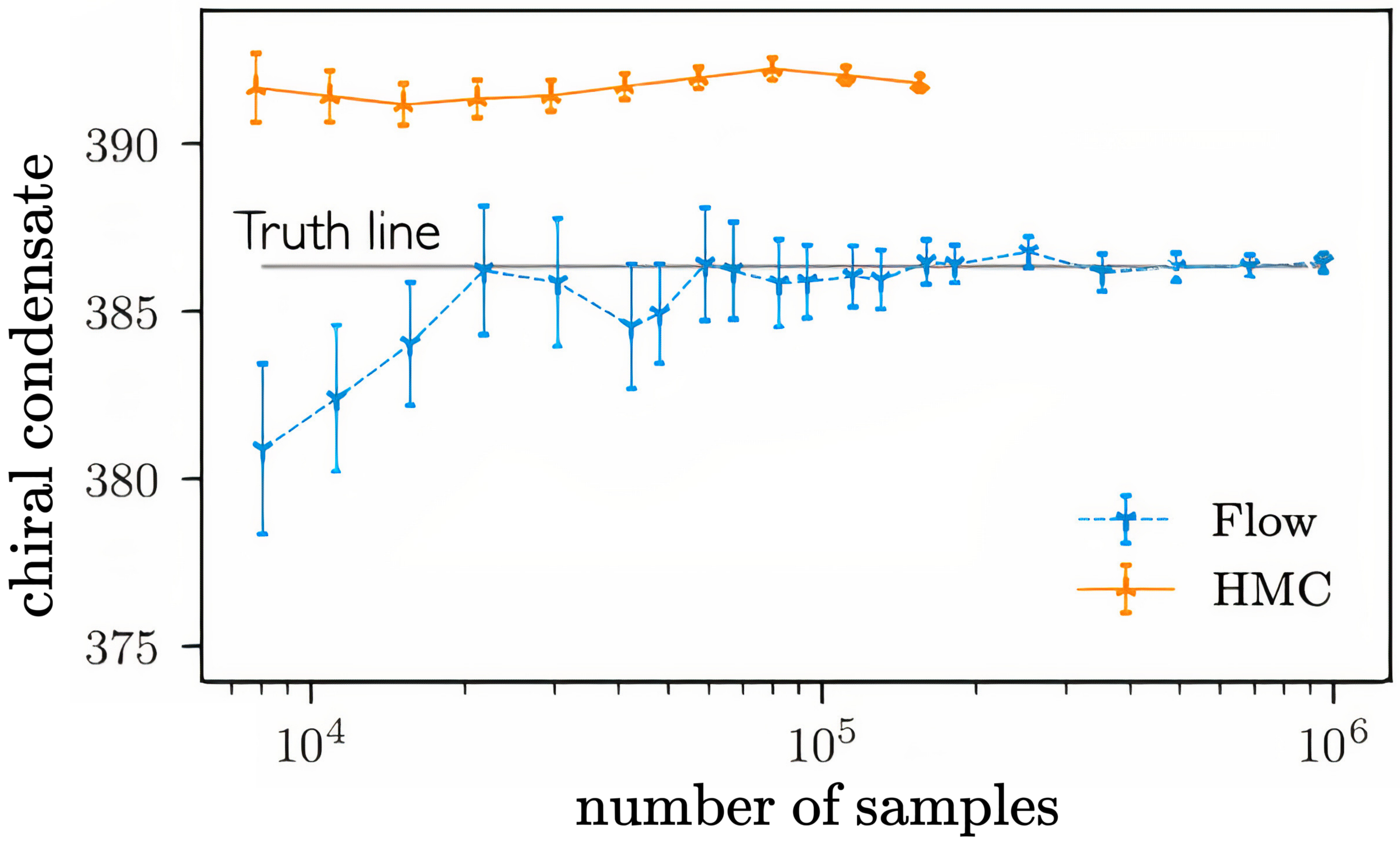

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✓ **Flow-based sampling provides correct results**

[Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Urban 2202.11712]

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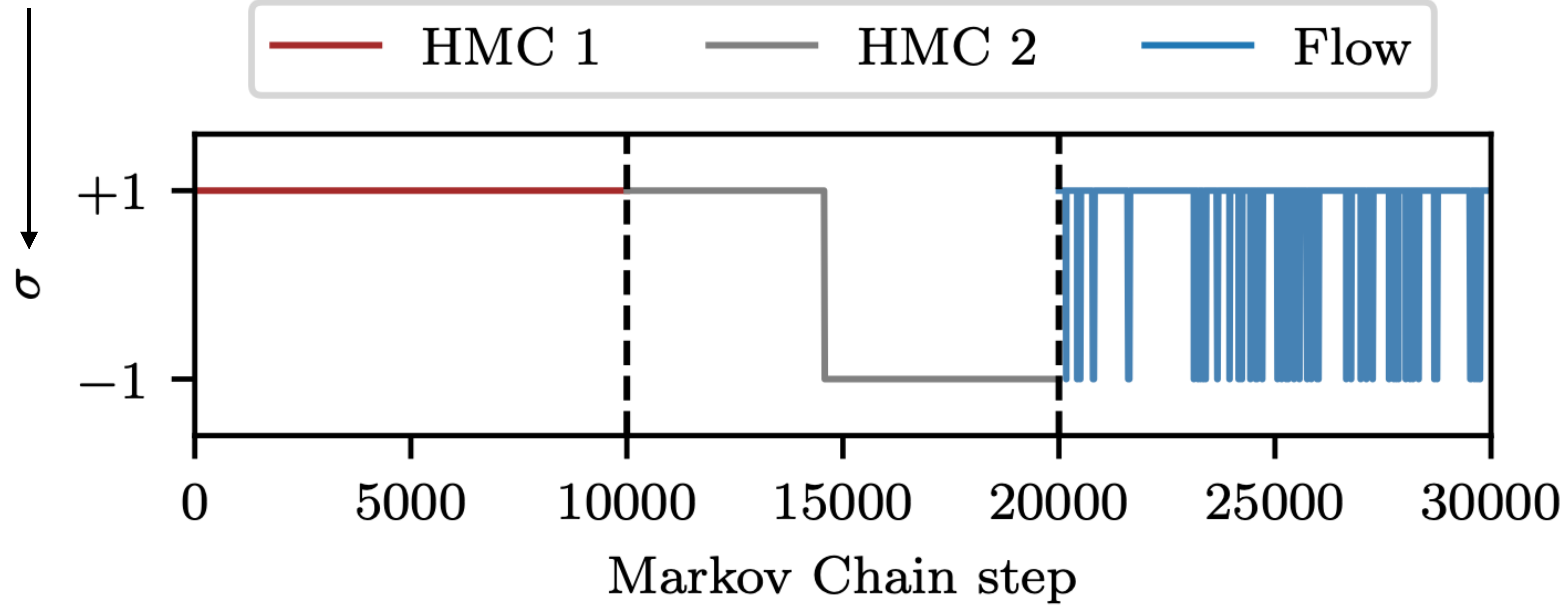
(topological observable)
sign of $\det D[U]$



✗ HMC shows biased results with underestimated errors

✓ Flow-based sampling provides correct results

✓ Flow-based sampling mitigates topology freezing even at criticality

[Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Urban 2202.11712]

The cost of the determinant

- **Evaluation of the fermion determinant is expensive.**

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- In QCD, the Dirac operator is a matrix of dimension:

$$n = 2 \times 4 \times N_c \times L^3 \times T \sim 10^9$$

Not feasible for QCD-scale calculations!

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- Scalable approach: use stochastic determinant estimators: Pseudofermions!

Fernando Romero-López, MIT

Pseudofermions

- **Stochastically estimate determinant using auxiliary degrees of freedom**

Assuming $N_f=2$ →

$$\det DD^\dagger = \frac{1}{Z_{\mathcal{N}}} \int \mathcal{D}\phi \, e^{-\phi^\dagger (DD^\dagger)^{-1} \phi}$$

Pseudofermions

Fernando Romero-López, MIT

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- Only need the Dirac operator applied to the PF field: scales linearly with the lattice volume

Fernando Romero-López, MIT

Joint flow models

$$p(U, \phi) = p(U)p(\phi \mid U)$$

$$p(U) \propto \det DD^\dagger(U) e^{-S_g(U)}$$

“marginal”

$$p(\phi|U) \propto \frac{1}{\det DD^\dagger(U)} e^{-S_{PF}(\phi|U)}$$

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$$\boxed{f_m(\chi)}$$

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Different flow models to approximate marginal and conditional distributions

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

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[Kanwar et al, 2003.06413]

[Boyda et al, 2008.05456]

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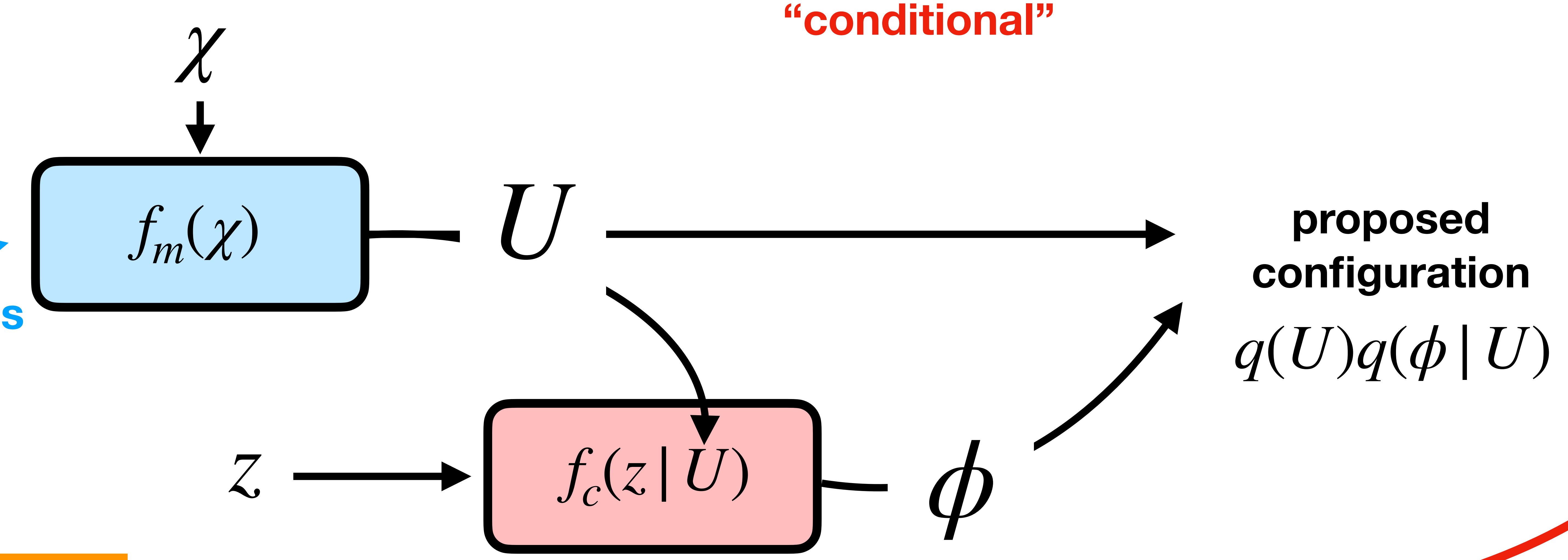

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Gauge-equivariant conditional models

- Train a flow to map an uncorrelated gaussian into a correlated one:

$$r(z) \propto e^{-z^\dagger z} \xrightarrow{f_c(z\,|\,U)} \boxed{q(\phi\,|\,U)} \propto e^{-\phi^\dagger A(U)\phi} \simeq e^{-\phi^\dagger \left(D(U)D^\dagger(U)\right)^{-1}\phi}$$

approximates

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Fernando Romero-López, MIT

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(gauge-invariant inputs)

Fernando Romero-López, MIT

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(gauge equivariance)

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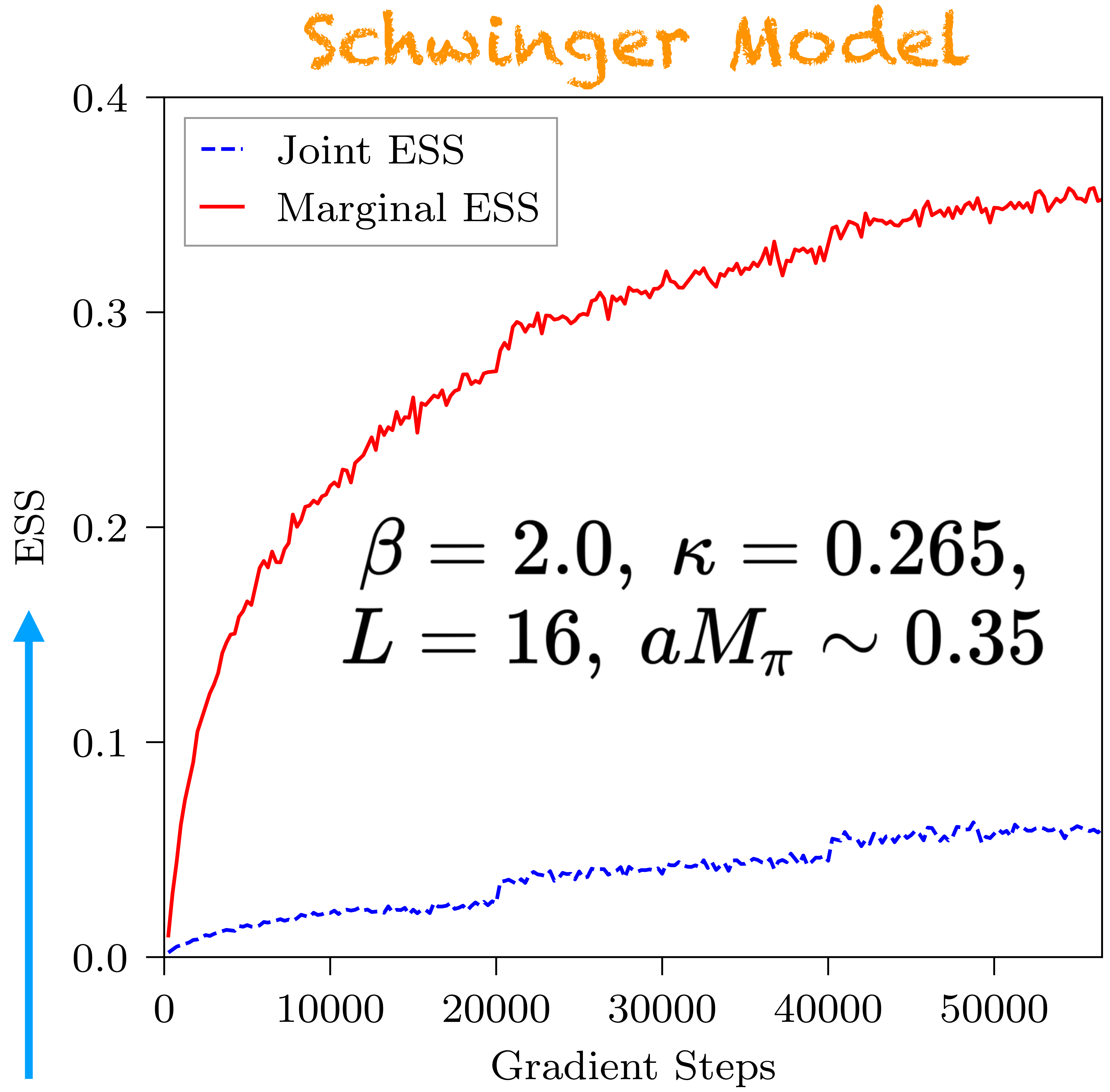
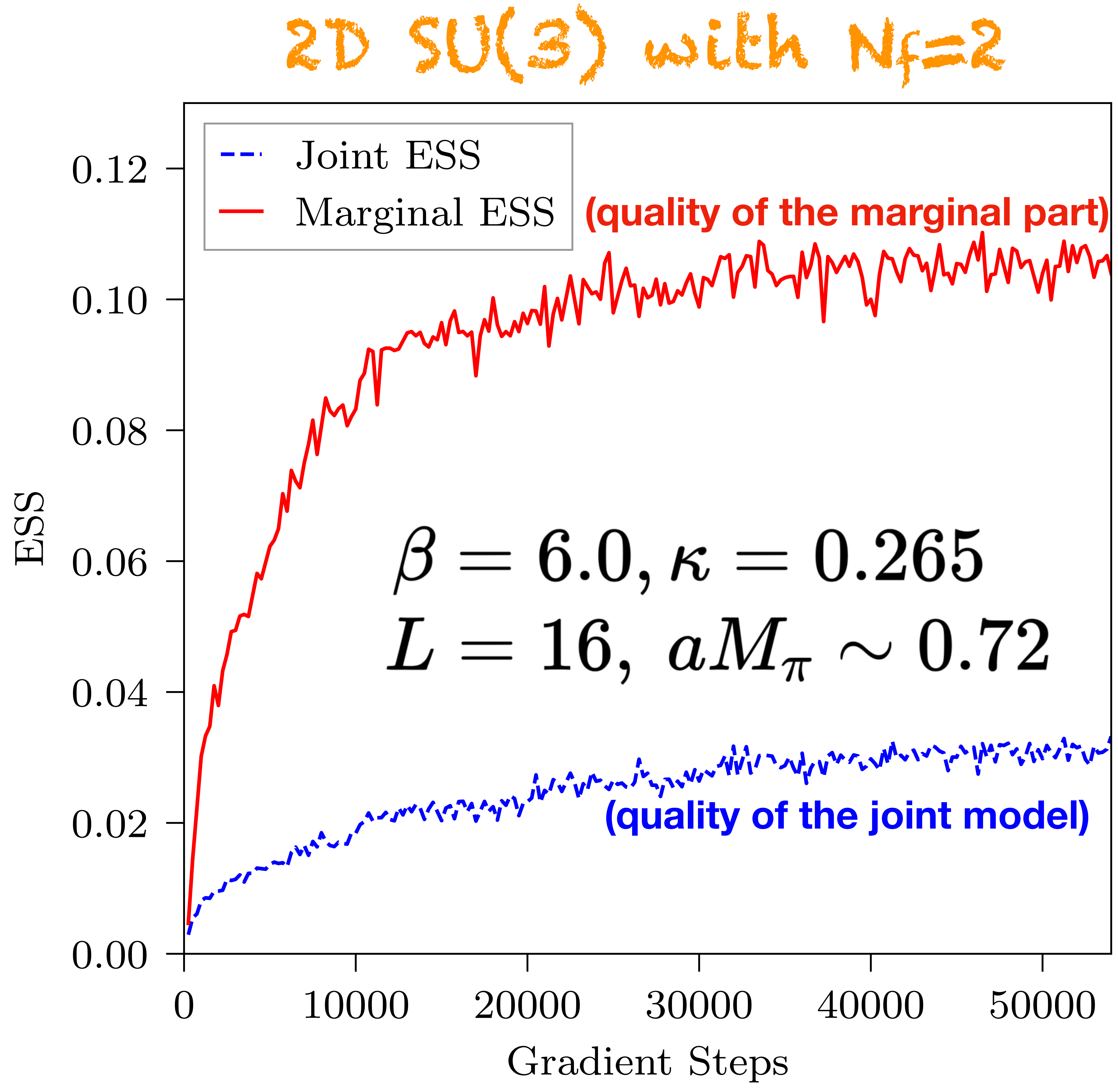
Fernando Romero-López, MIT

Examples of flow models





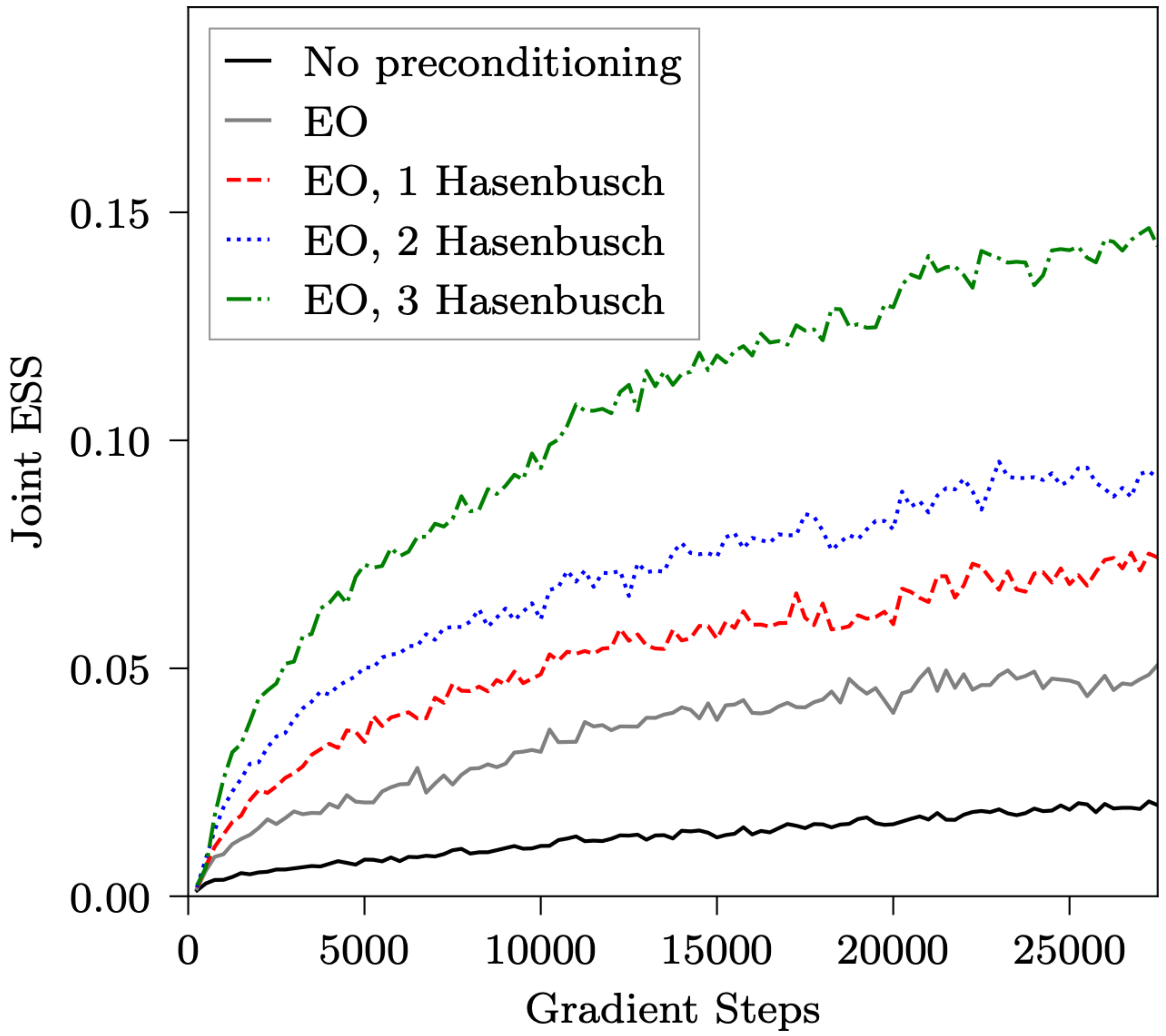
"Effective sample size" ≡ model quality
(ESS=1 for a perfect model)

[Abbott, Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Tian, Urban 2207.08945]

Fernando Romero-López, MIT

Examples of flow models

- Use of preconditioners in flow models
- ✓ Even/odd and Hasenbusch improve model quality



(Examples in Schwinger model)

Fernando Romero-López, MIT

Can we ML generate lattice QCD?

☑ **Overcoming critical slowing down in toy models: scalar theories, Schwinger model** [Abbott ...FRL... et al.] (several works)

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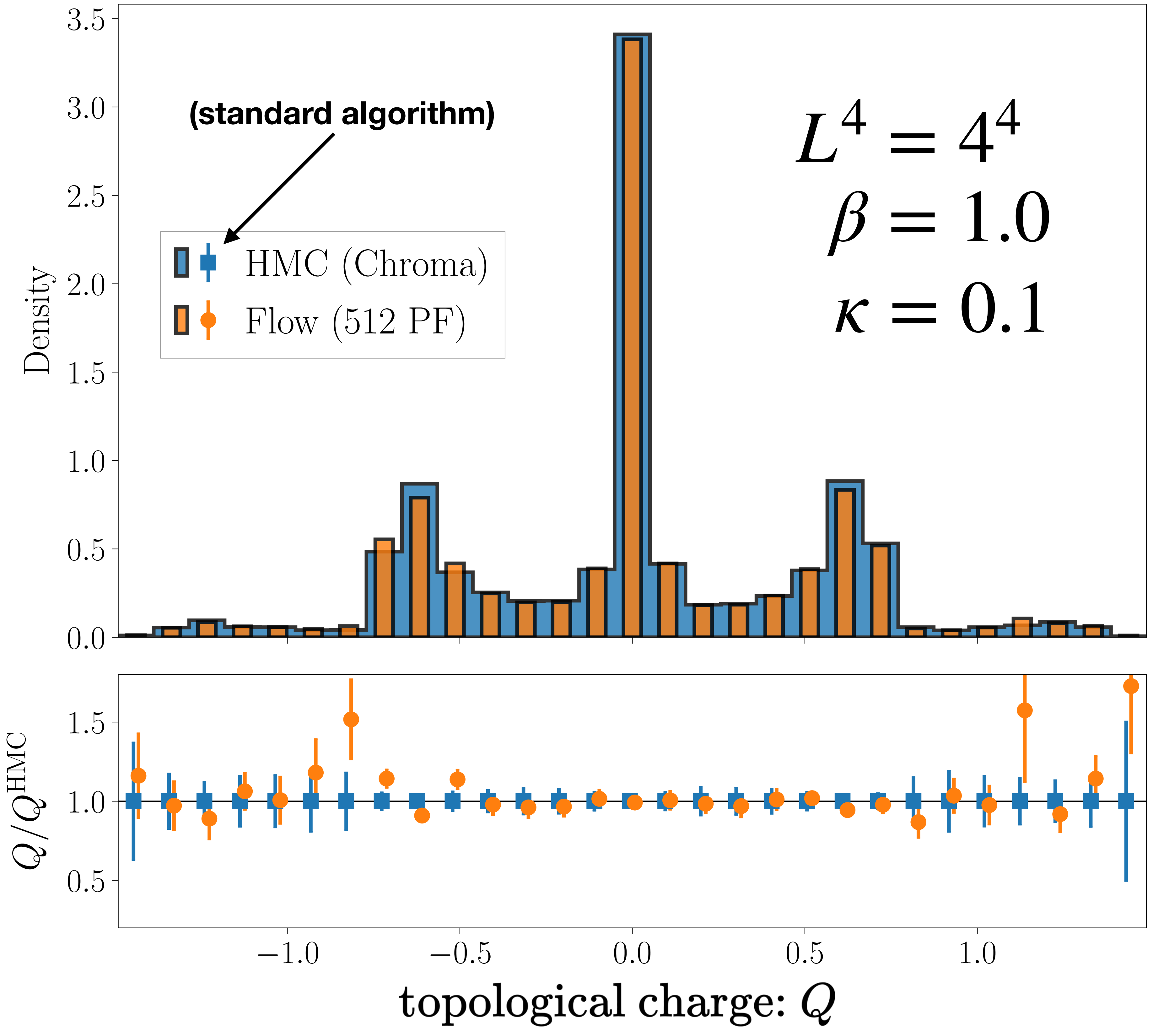

[Abbott, … , FRL, …, et al 2208.03832]

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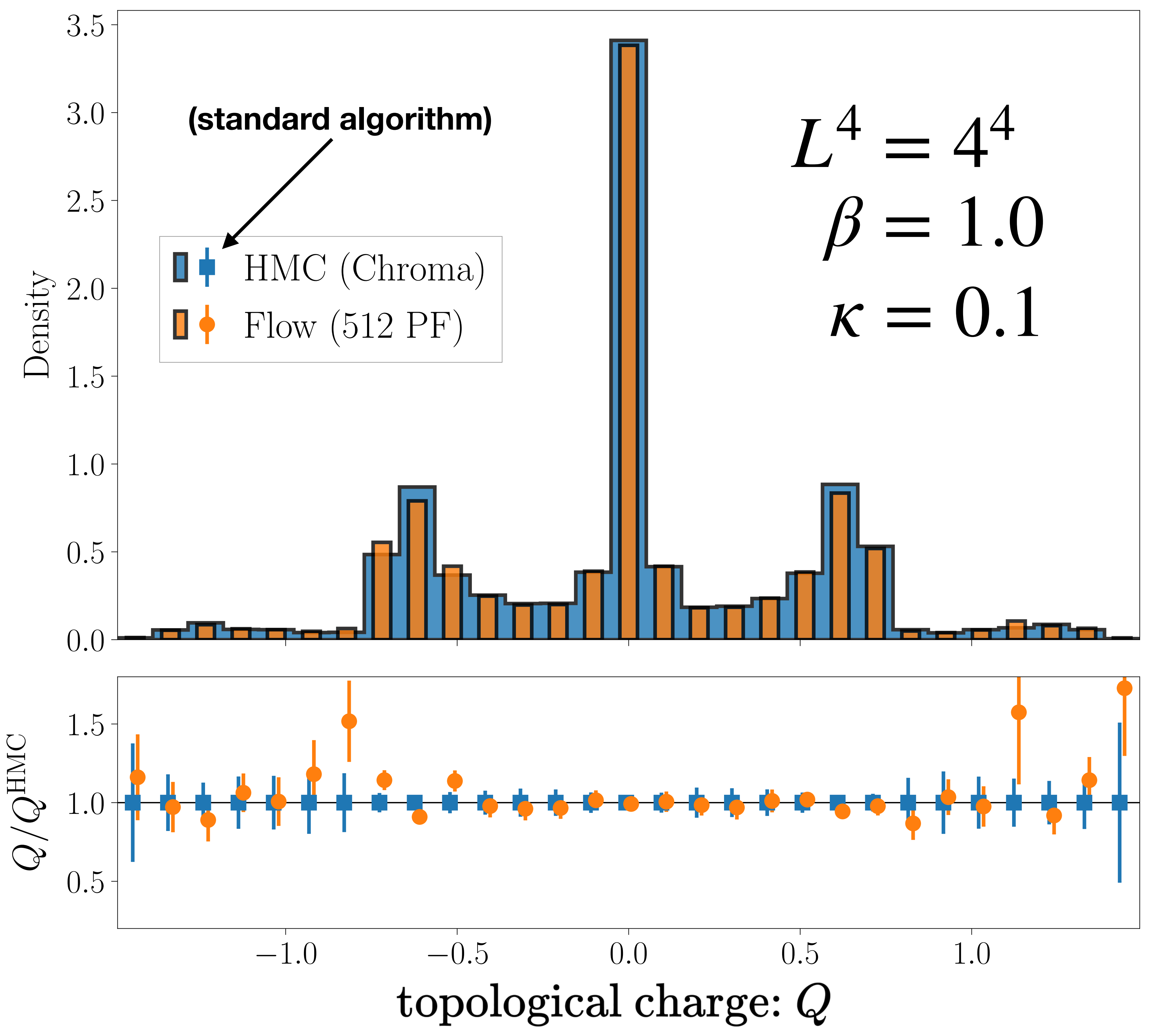

[Abbott, ... , FRL, ..., et al 2208.03832]

☐ **Will it work for state-of-the-art Lattice QCD?**

Aspects of scaling and scalability for flow-based sampling of lattice QCD

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

[arXiv:2211.07541]

"For flow-based methods, assessing scalability will require direct, experimental investigation of applications to QCD itself, which has only just begun."

Summary & Outlook

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- Lattice QCD is the first-principle treatment of the strong interaction at hadronic energies

- Continuum limit in lattice QCD is limited by the performance of algorithms (critical slowing down)

- Flow-based sampling has the potential to mitigate this problem

- Success has been demonstrated in 2D fermionic gauge theories: Schwinger model
  [Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Urban 2202.11712]

- Demonstration in QCD at small scale
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- Next steps: scale flow-based sampling to state-of-the-art QCD
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Thanks!

Back-up slides

The road to QCD

(1+1)d real scalar field theory
[Albergo, Kanwar, Shanahan 1904.12072]
[Hackett, Hsieh, Albergo, Boyda, JW Chen, KF Chen, Cranmer, Kanwar, Shananan 2107.00734]

(1+1)d Abelian gauge theory
[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan 2003.06413]

(1+1)d non-Abelian gauge theory
[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan 2003.06413]

(1+1)d Yukawa model
i.e. real scalar field theory + fermions
[Albergo, Kanwar, Racanière, Rezende, Urban, Boyda, Cranmer, Hackett, Shanahan 2106.05934]

Schwinger model
i.e. (1+1)d QED
[Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Urban 2202.11712]

2D fermionic gauge theories with pseudofermions
[Abbott, Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Tian, Urban 2207.08945]

QCD in the strong-coupling region
[Abbott et al, 2208.03832]

…

State-of-the-art lattice QCD!

Fernando Romero-López, MIT

Recap of Pseudofermions

- **Action:** $$S(\psi,\bar\psi,U) = S_{\rm g}(U) + S_F(\psi,\bar\psi,U)$$

Gauge fields

Fermions

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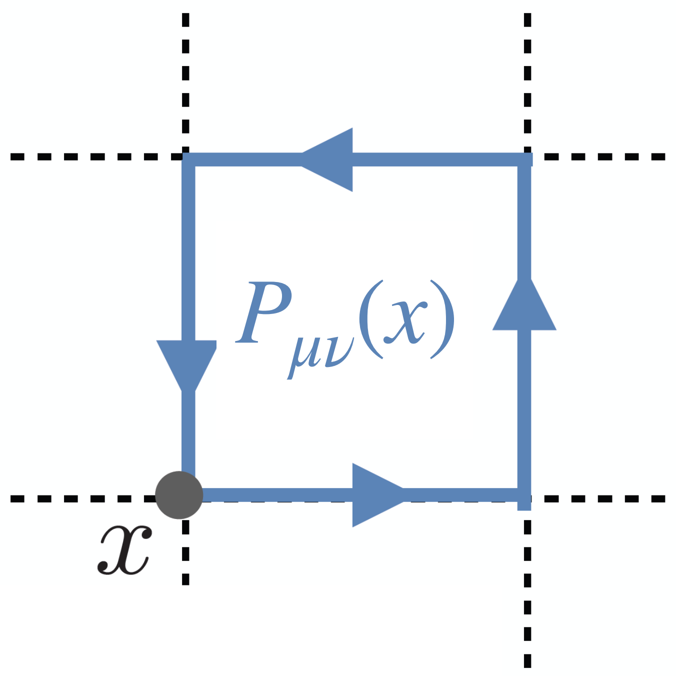
Fernando Romero-López, MIT

Flows on SU(3)

- **Gauge transformations maintain the eigenvalues of SU(3) matrices:**



$$P_{\mu\nu} = X \begin{pmatrix} e^{i\theta_1} & 0 & 0 \\ 0 & e^{i\theta_2} & 0 \\ 0 & 0 & e^{i\theta_3} \end{pmatrix} X^\dagger$$

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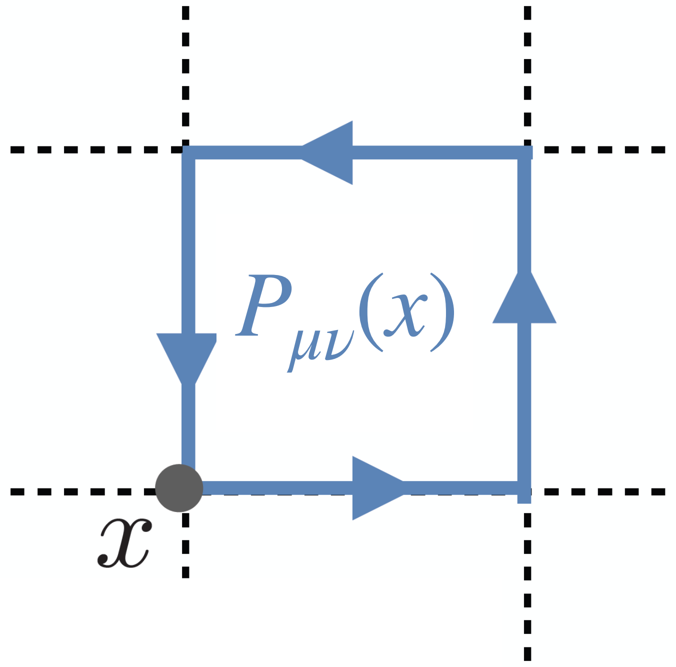

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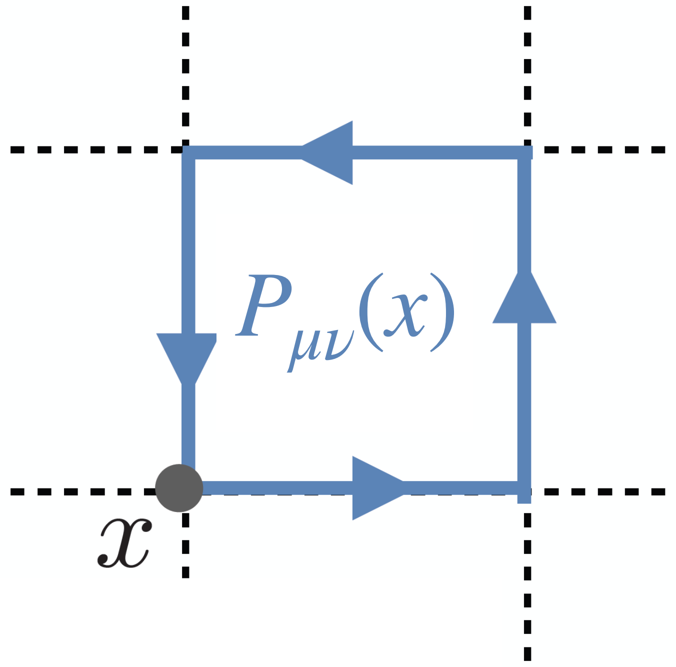

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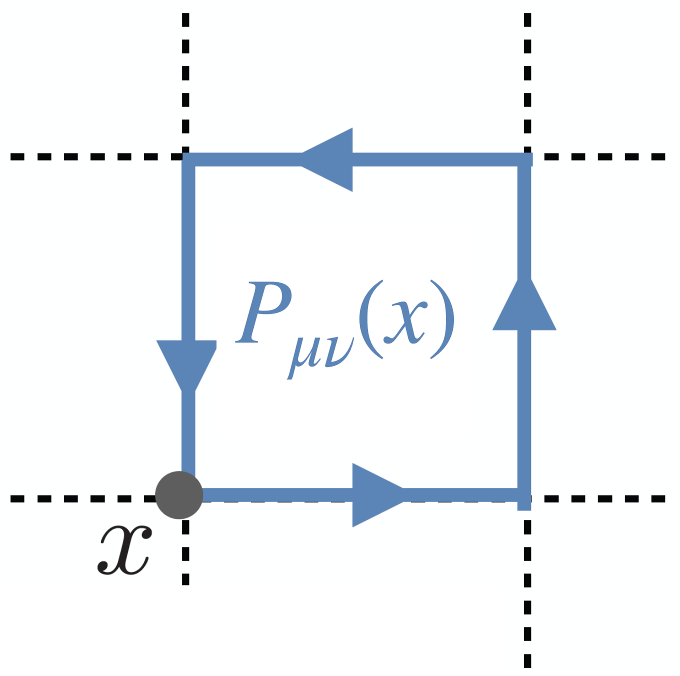

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Use transformation on eigenvalues

- **However, ordering of the eigenvalues is not unique: <u>need permutation equivariance</u>**
  - **Place eigenvalues in canonical ordering**
  - **Transform eigenvalues**
  - **Undo canonical ordering**

$$\mathrm{iscanon}(\theta_1, \theta_2, \theta_3) = \begin{cases} \theta_3 \geq \theta_2 \geq \theta_1 & \sum_i \theta_i = 0 \\ \theta_1 \geq \theta_3 \geq \theta_2 & \sum_i \theta_i = 2\pi \\ \theta_2 \geq \theta_1 \geq \theta_3 & \sum_i \theta_i = -2\pi \end{cases}$$

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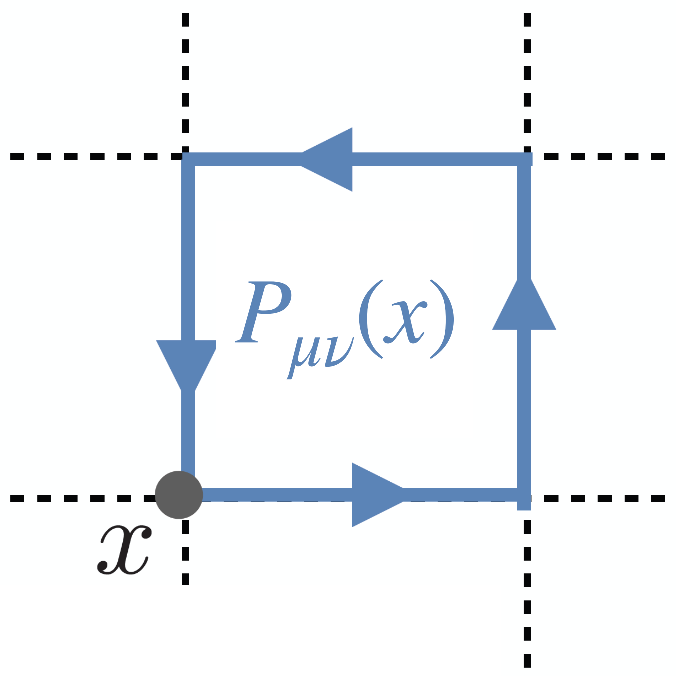
Flows on SU(3)

- Gauge transformations maintain the eigenvalues of SU(3) matrices:



$$P_{\mu\nu} = X \begin{pmatrix} e^{i\theta_1} & 0 & 0 \\ 0 & e^{i\theta_2} & 0 \\ 0 & 0 & e^{i\theta_3} \end{pmatrix} X^\dagger$$

Use transformation on eigenvalues

- However, ordering of the eigenvalues is not unique: <u>need permutation equivariance</u>

  - Place eigenvalues in canonical ordering
  - Transform eigenvalues
  - Undo canonical ordering

$$\mathrm{iscanon}(\theta_1, \theta_2, \theta_3) = \begin{cases} \theta_3 \geq \theta_2 \geq \theta_1 & \sum_i \theta_i = 0 \\ \theta_1 \geq \theta_3 \geq \theta_2 & \sum_i \theta_i = 2\pi \\ \theta_2 \geq \theta_1 \geq \theta_3 & \sum_i \theta_i = -2\pi \end{cases}$$

✓ Successfully applied to SU(3) in 2D

[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan 2003.06413]

Fernando Romero-López, MIT

Exactness via Markov Chain

❗ **Trained models are not perfect but exactness is essential.**

Exactness via Markov Chain

❗ Trained models are not perfect but exactness is essential.

- Guarantee exactness by forming a Markov chain with accept/reject Metropolis-Hastings steps

Acceptance probability ⟶

$$A\left(\phi^{(i-1)}, \phi'\right) = \min\left(1, \frac{q\left(\phi^{(i-1)}\right)}{p\left(\phi^{(i-1)}\right)} \frac{p(\phi')}{q(\phi')}\right)$$

True distribution

Model distribution

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Exactness via Markov Chain

! Trained models are not perfect but exactness is essential.

Guarantee exactness by forming a Markov chain with accept/reject Metropolis-Hastings steps

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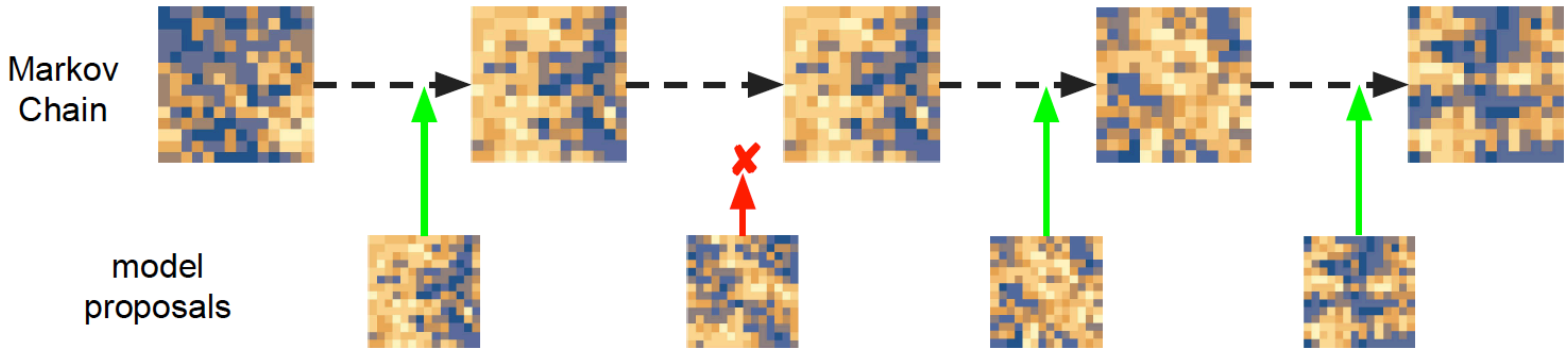

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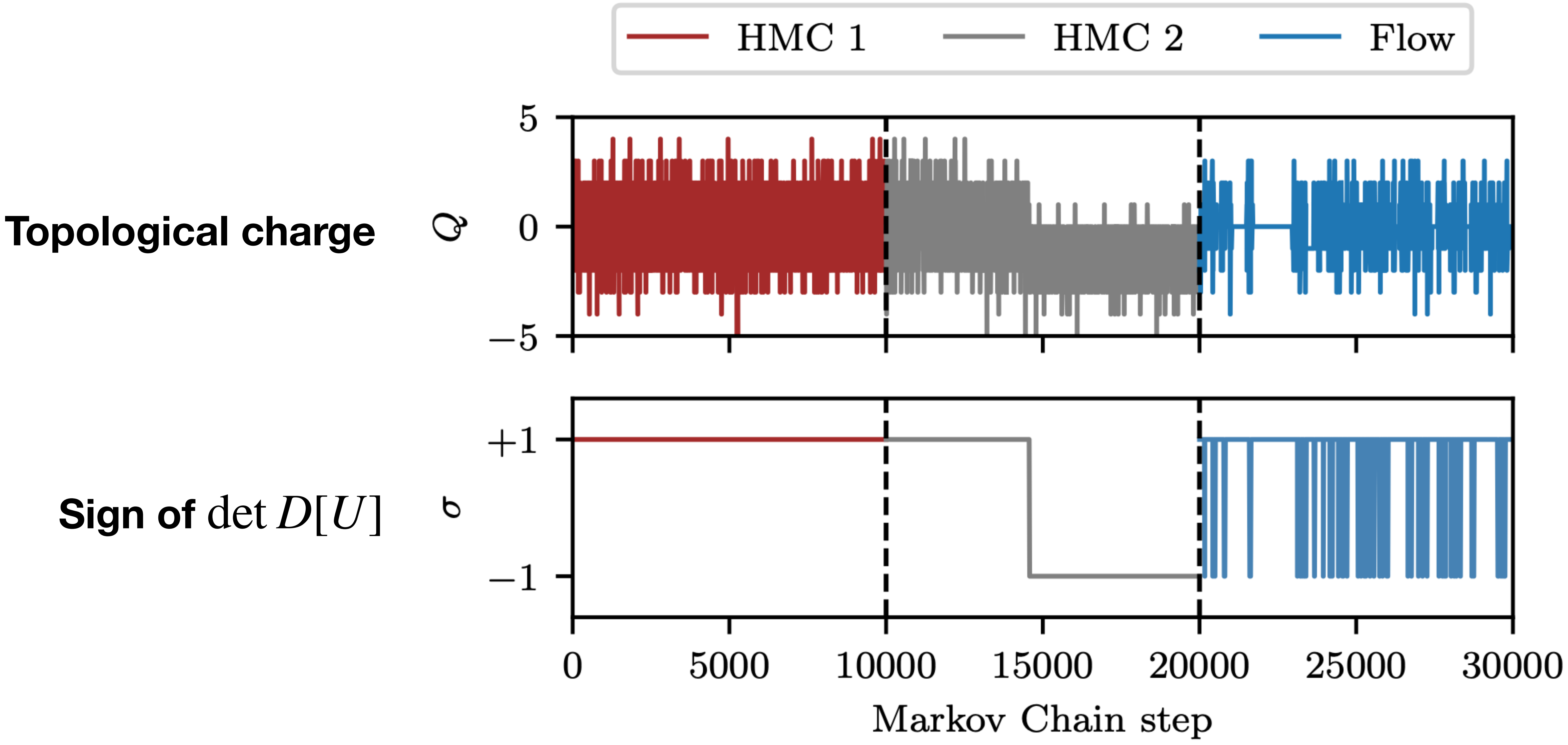
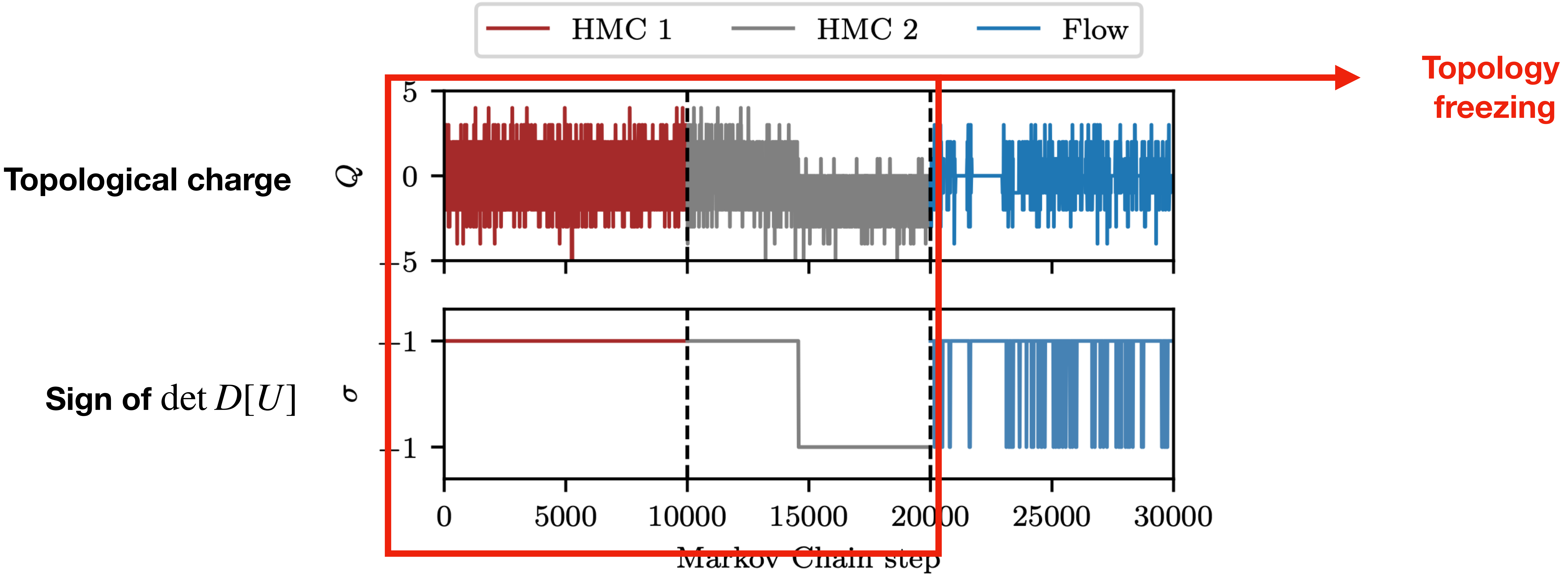
The Schwinger model at criticality



[Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Urban 2202.11712]

The Schwinger model at criticality



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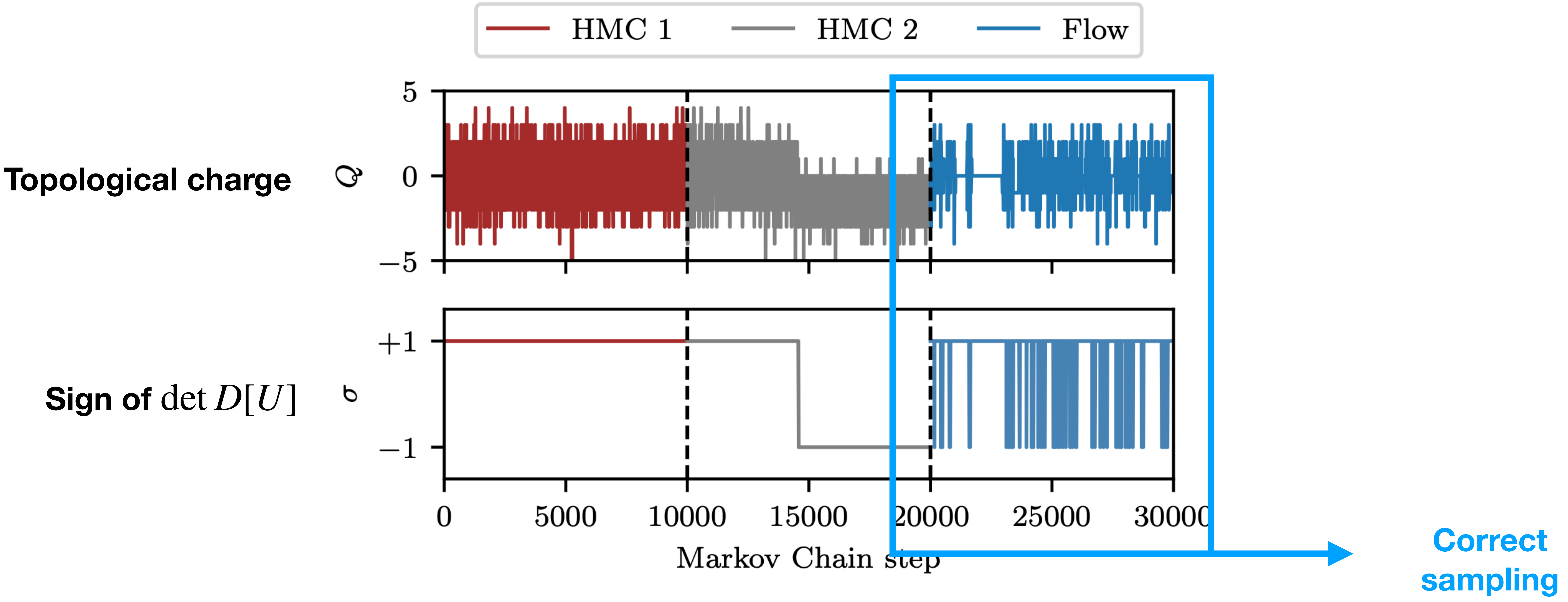

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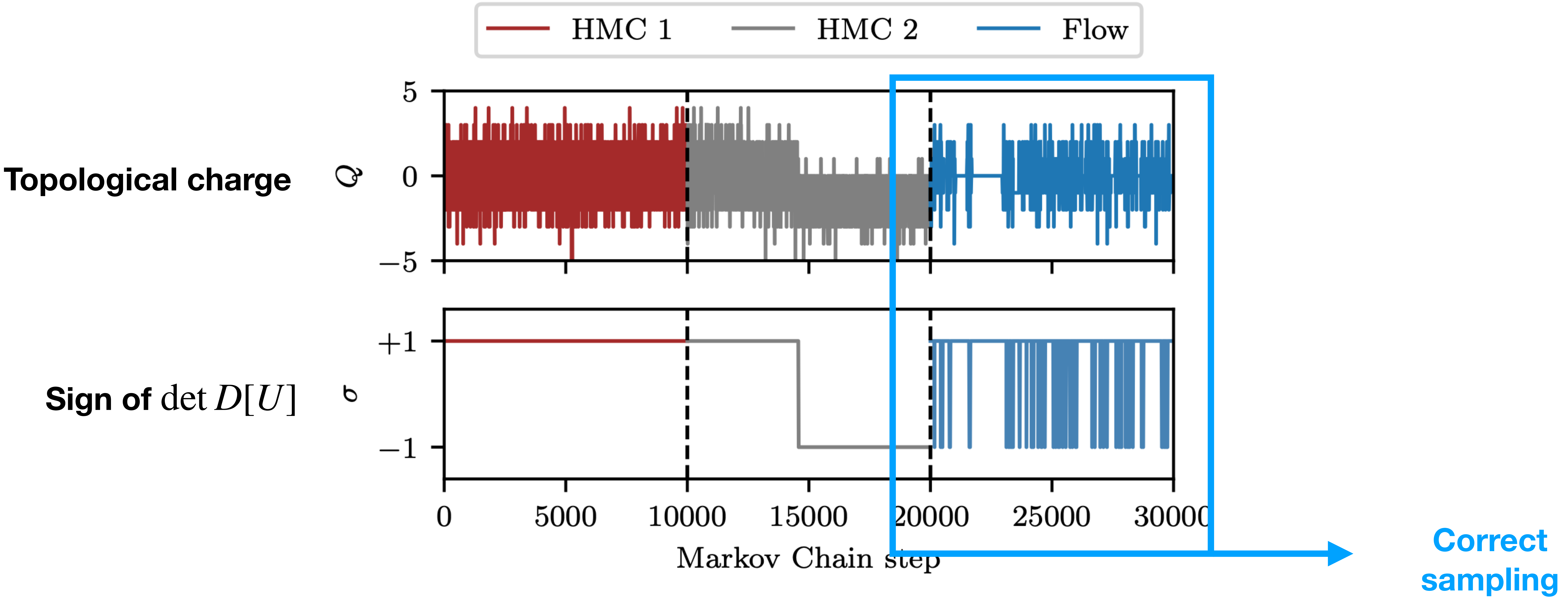
The Schwinger model at criticality



✓ **Flow-based sampling mitigates topology freezing even at criticality**

[Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Urban 2202.11712]