New simulation strategies for lattice ~~QCD~~ Gauge Theory

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Lattice 2016 • Southampton, UK
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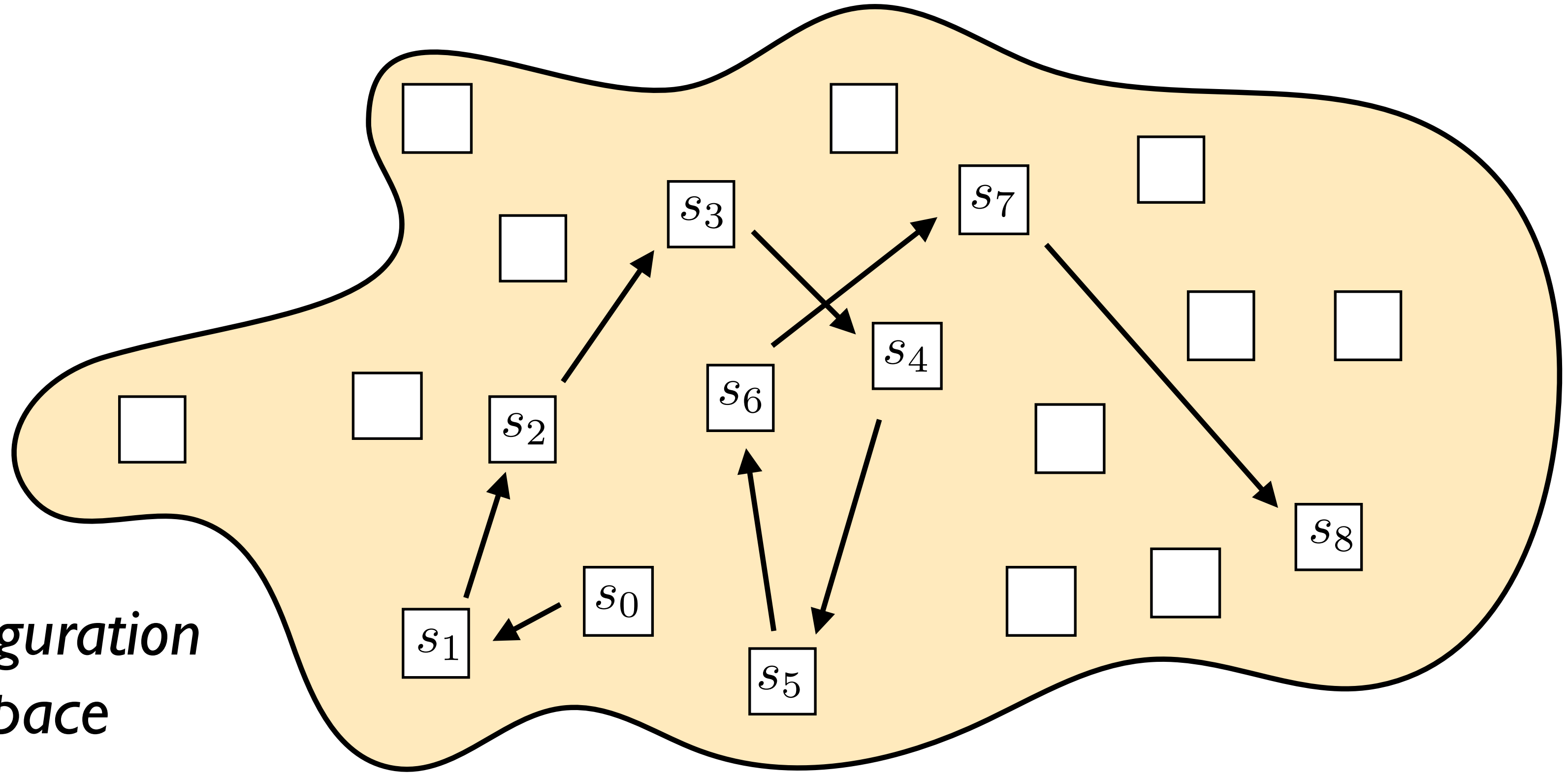
Statistical uncertainties

A reliable determination of statistical uncertainties requires an understanding of correlations in generated configurations

- Arise due to sequential nature of Markov Chain Monte Carlo (MC) algorithms
- Highly dependent on the times scales that govern the Markov process



configuration space

Critical slowing down

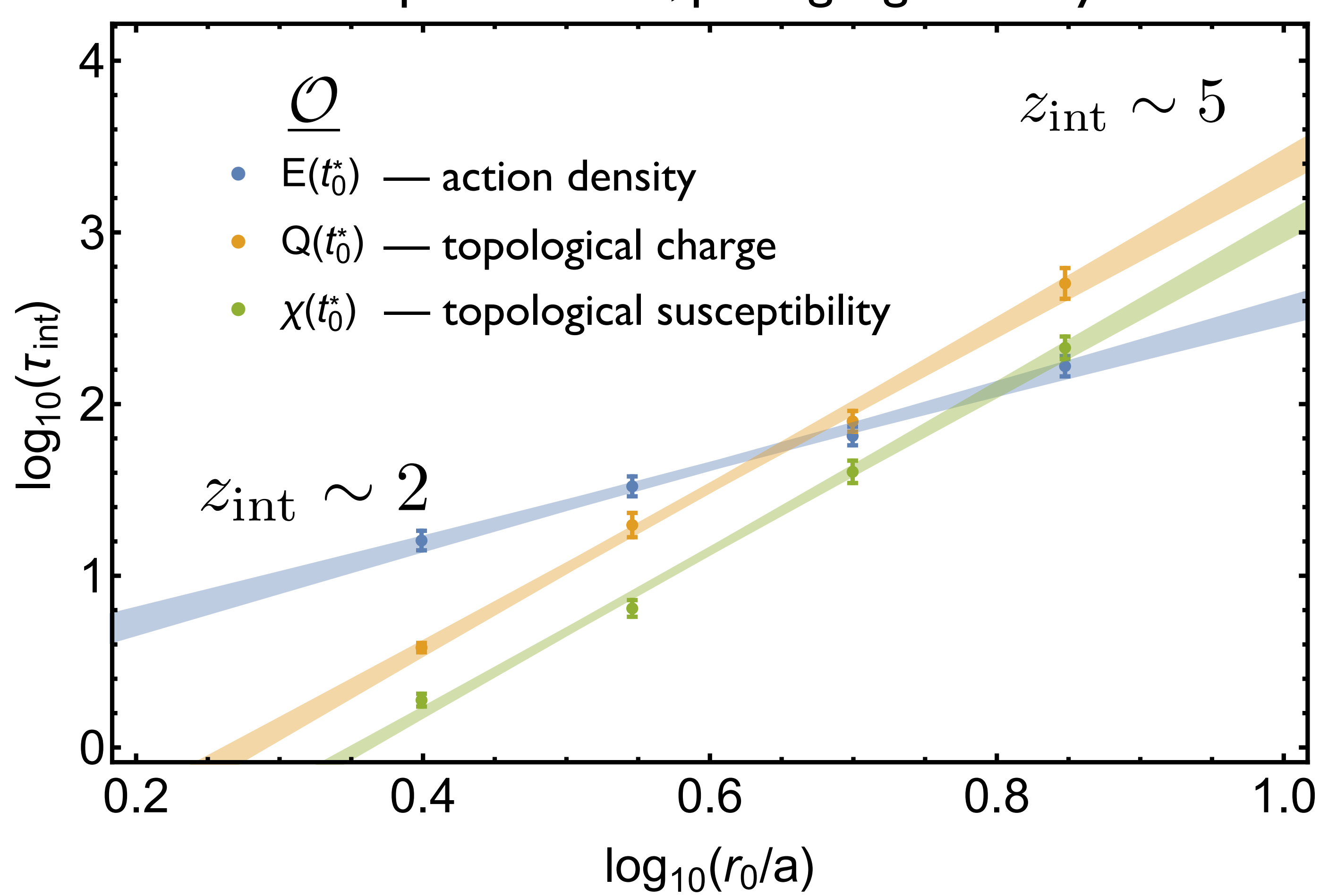
Coarse lattices decorrelate faster than fine lattices

- Observables are probes for determining decorrelation times
- Autocorrelations are influenced by how well observables couple to slow modes
  - topological charge (Q) couples strongly

$$\tau_{\text{int}}(\mathcal{O}) \sim \left(\frac{1}{a}\right)^{z_{\text{int}}(\mathcal{O})}$$

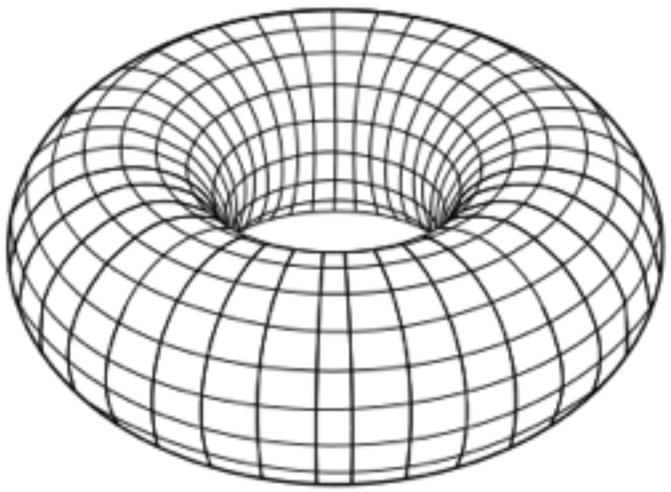
$$cost \sim \left(\frac{1}{a}\right)^{\overbrace{D+\max_{\mathcal{O}} z_{\text{int}}(\mathcal{O})}^{\sim 9}}$$

D=4 with periodic BC; pure gauge theory w/HB



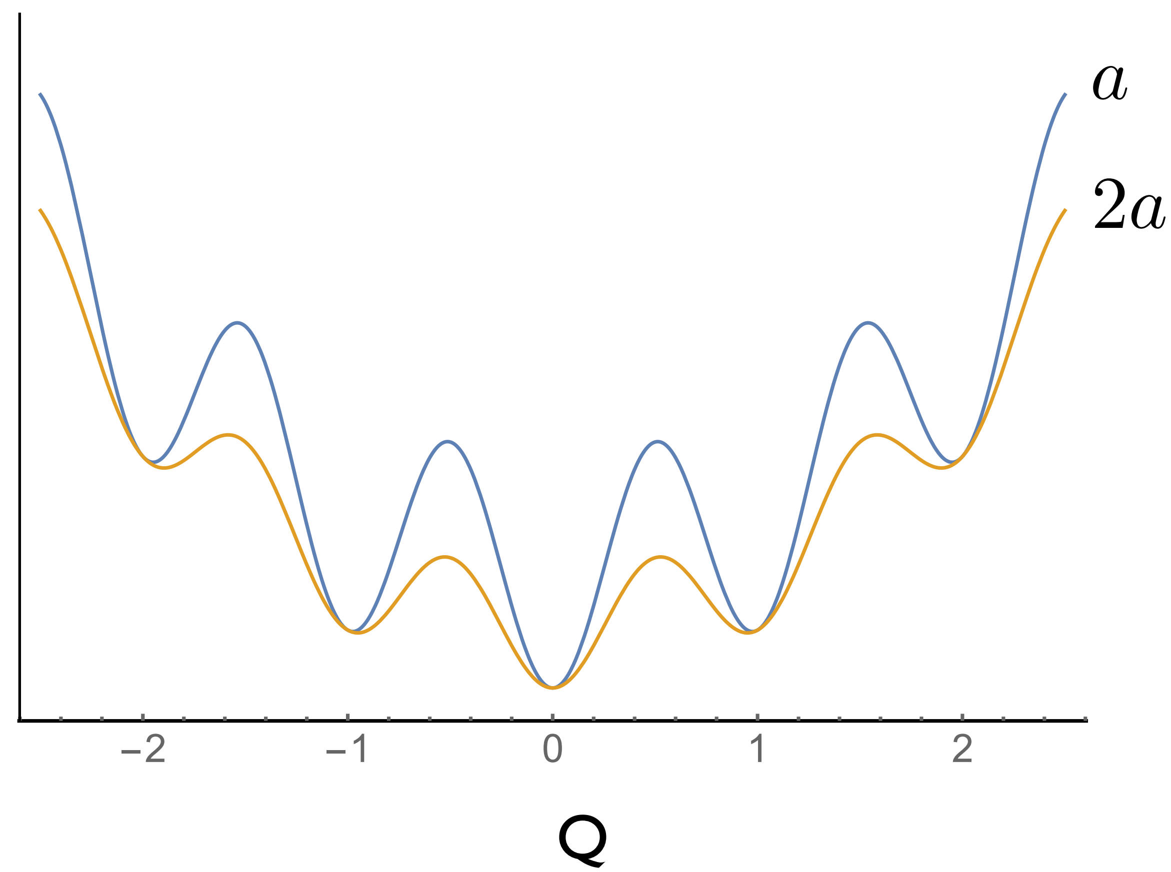
Topological charge on a space-time torus

Continuum: *field space splits into disconnected topological sectors (labeled by quantized Q)*



Lattice: *topological sectors are connected, however separated by large action barriers*

$$f(Q) = -\frac{1}{V}\log\langle\delta\left(Q - Q[U]\right)\rangle$$



- Change in topology requires tunneling; probability exponentially suppressed by barrier height
- Barrier height depends on the discretization of the action

Topological freezing

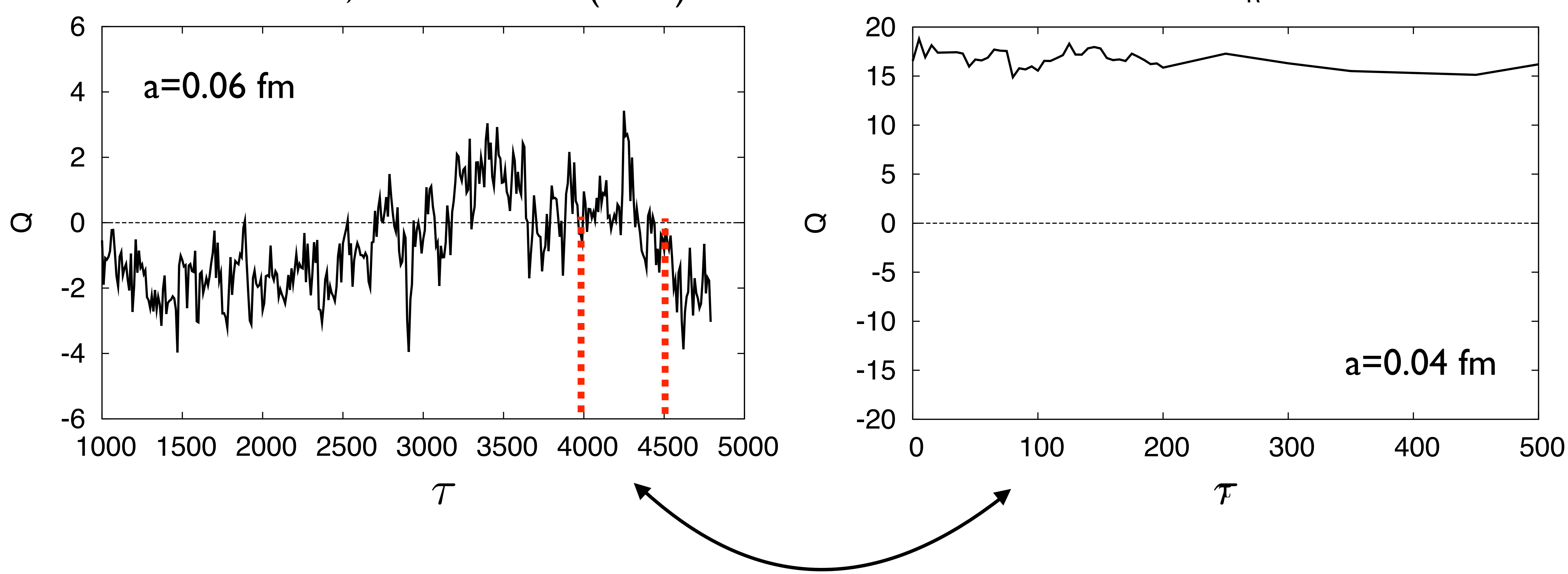
At very fine lattice spacing, the timescale for topology change can exceed the total time of the simulation

- Problem for HB and HMC
- Fixed topology → 1/V corrections to observables
- Particularly severe for a ≲ 0.05 fm

R. Brower, S. Chandrasekharan, J. Negele and U.-J. Wiese, Phys.Lett. B **560** (2003) 64-74

S. Schaefer *et al.*, PoS **LAT2009** (2009) 032

m_π ~ 360 - 480 MeV

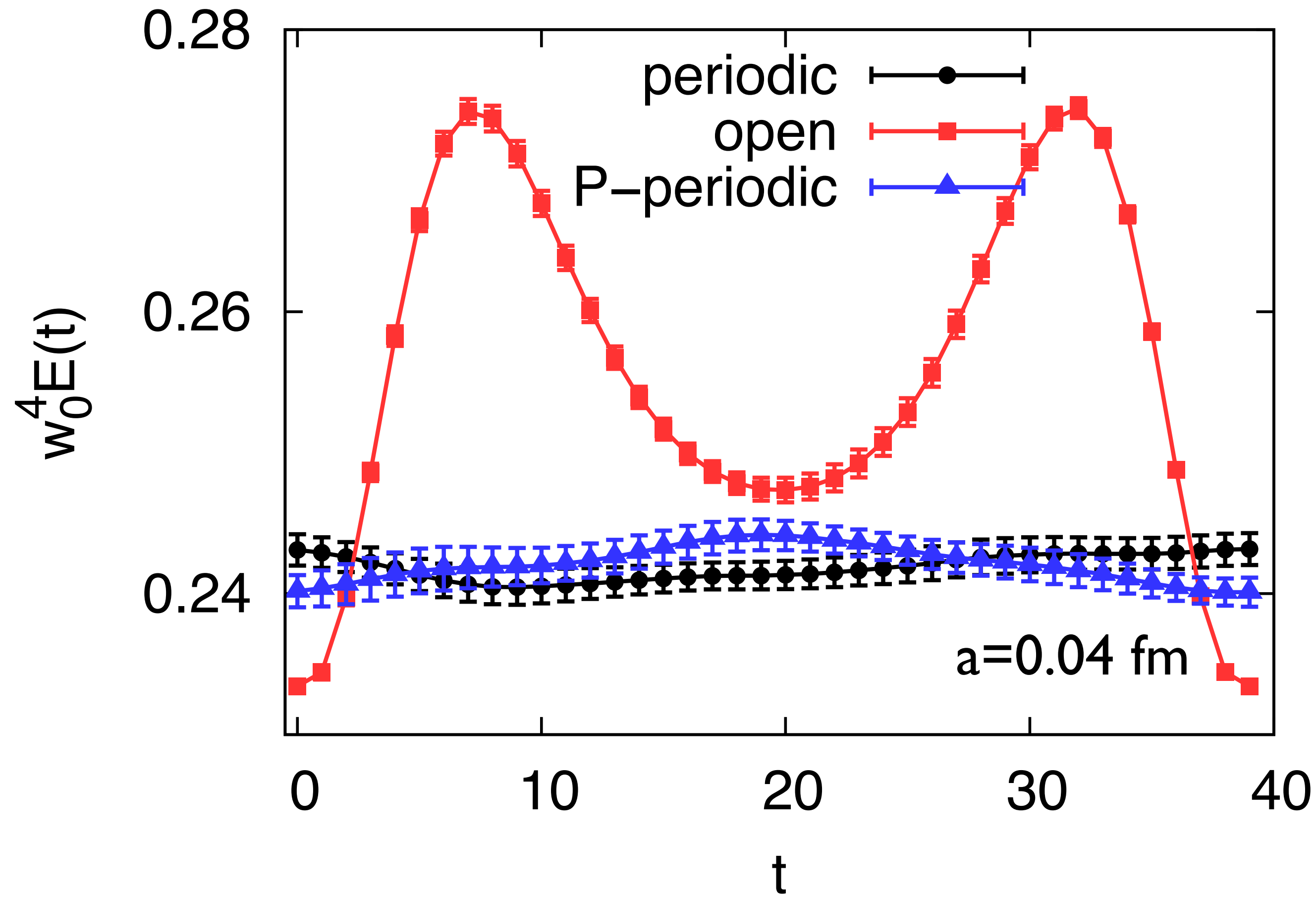


Overcoming topological freezing/critical slowing down

(Some) strategies for attacking the problem

- **Infrared** — choice of boundary conditions
  - open boundary conditions
    - M. Lüscher and S. Schaefer, JHEP **07** (2011) 036
  - non-orientable manifolds
    - S. Mages, B. C. Toth, S. Borsanyi, Z. Fodor, S. Katz, and K. K. Szabo, arXiv:1512.06804
- **Ultraviolet** — exploiting lattice artifacts, ambiguity in the definition of Q
  - metadynamics
    - A. Laio, G. Martinelli, and F. Sanfilippo, arXiv:1508.07270
  - multiscale methods
    - M. G. E., R. C. Brower, W. Detmold, K. Orginos, and A V. Pochinsky, Phys.Rev. D **92** (2015) 114516
    - W. Detmold and M. G. E., arXiv:1605.09650

Some recent proposals



Lattice QCD on Non-orientable Manifolds
Theoretical Developments

— July 25, 2016 @ 15:15 (Simon Mages)
— July 25, 2016 @ 15:35 (Balint Toth)

- Open boundary conditions
  - connected field space
  - translational symmetry broken; large boundary effects
- Non-orientable manifolds: P-periodic BCs (parity transformation at boundary)
  - topological charge not quantized; improved scaling of $\tau_{int}(Q)$ with 1/a
  - suppressed translational symmetry breaking effects
  - non-trivial to implement fermions (but possible)

Some recent proposals

Lattice QCD on Non-orientable Manifolds
Theoretical Developments

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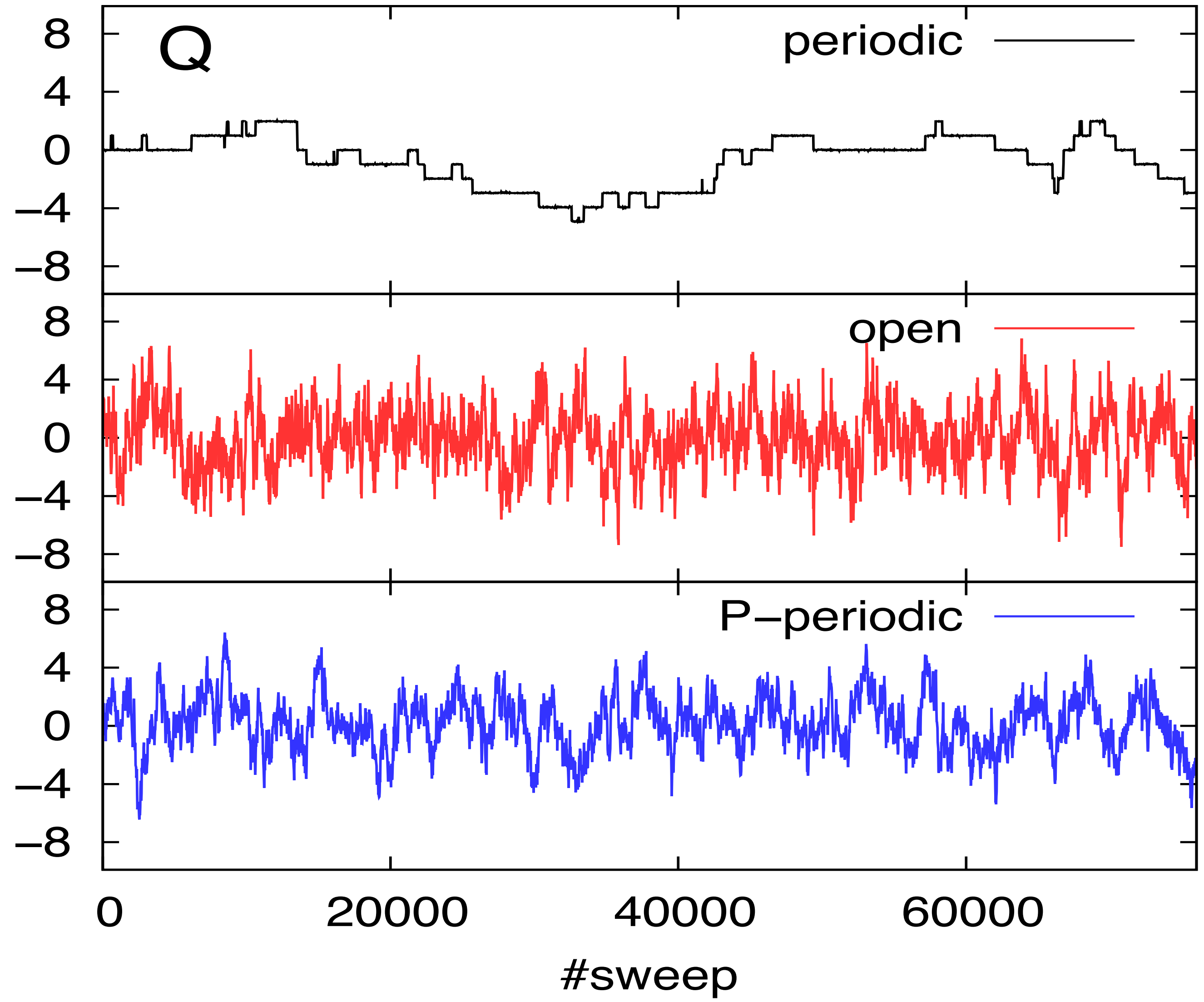
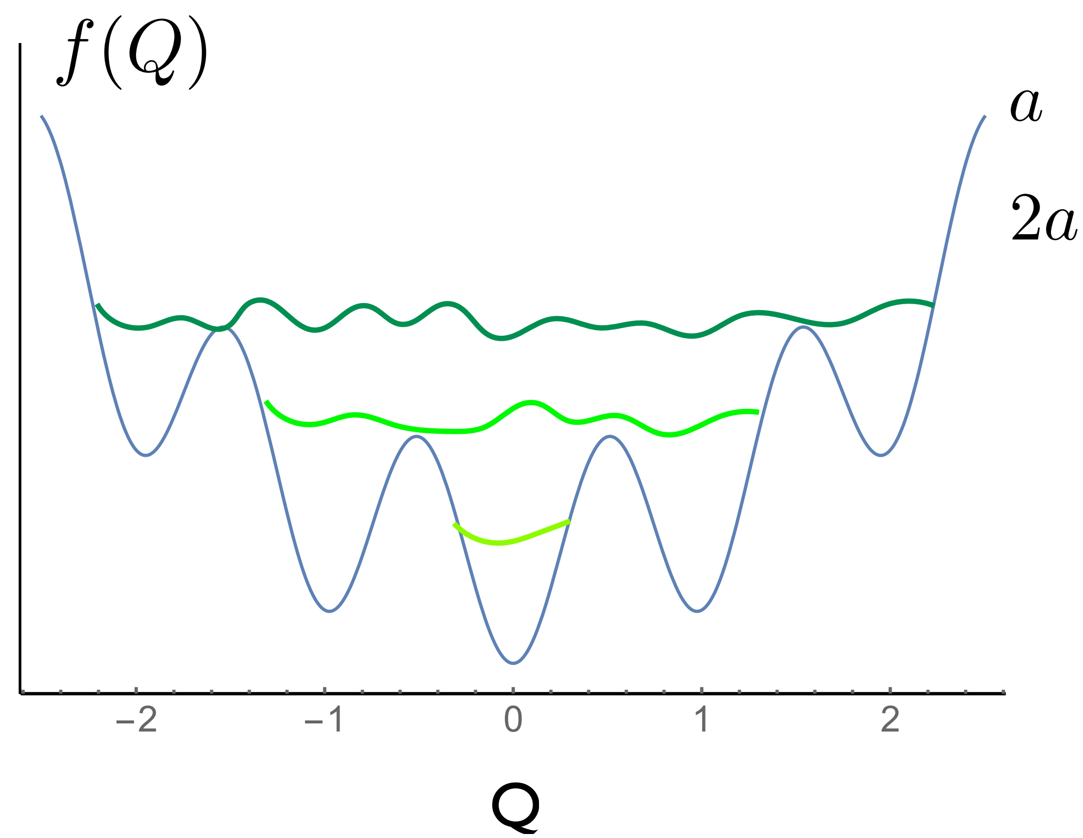
Pure gauge theory
(a=0.04 fm)



Some recent proposals



Metadynamics Remedies for Topological Freezing
Algorithms and Machines
— July 26, 2016 @ 18:10 (Francesco Sanfilippo)

$$f(Q) = -\frac{1}{V}\log\langle\delta\left(Q - Q[U]\right)\rangle \quad \approx -v(Q)$$

- Introduces a MC time-dependent potential bias which <u>disfavors</u> revisiting configurations; effectively fills the potential wells with MC time
- Takes advantage of the fact that MC time-averaged potential bias is an estimator for -f(Q)
- Recover expectation values via reweighting: $\langle\mathcal{O}\rangle \approx \frac{\sum_i \mathcal{O}(U_i)e^{-Vv(Q(U_i))}}{\sum_i e^{-Vv(Q(U_i))}}$

Some recent proposals

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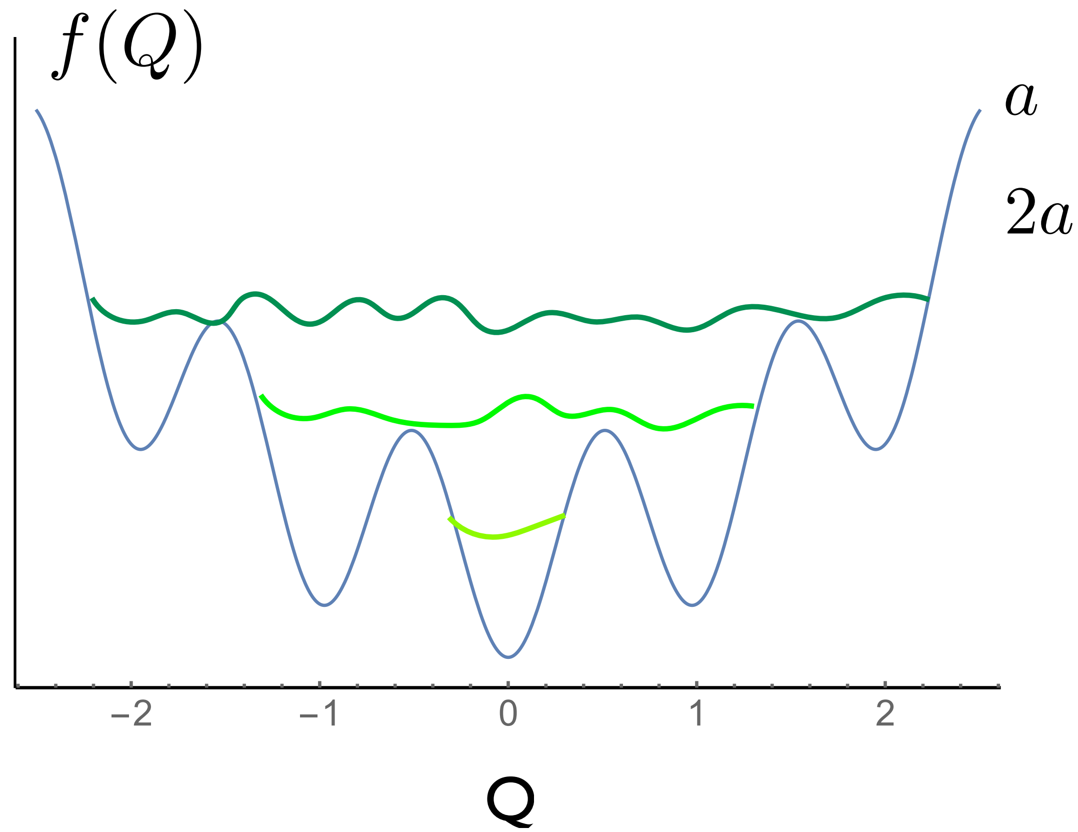
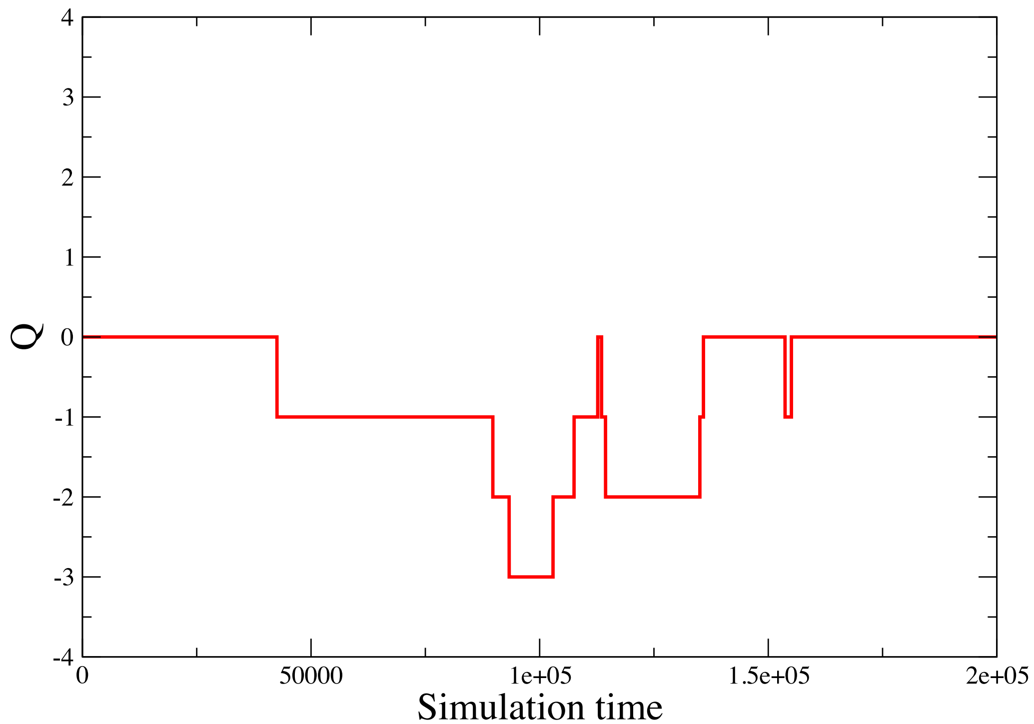
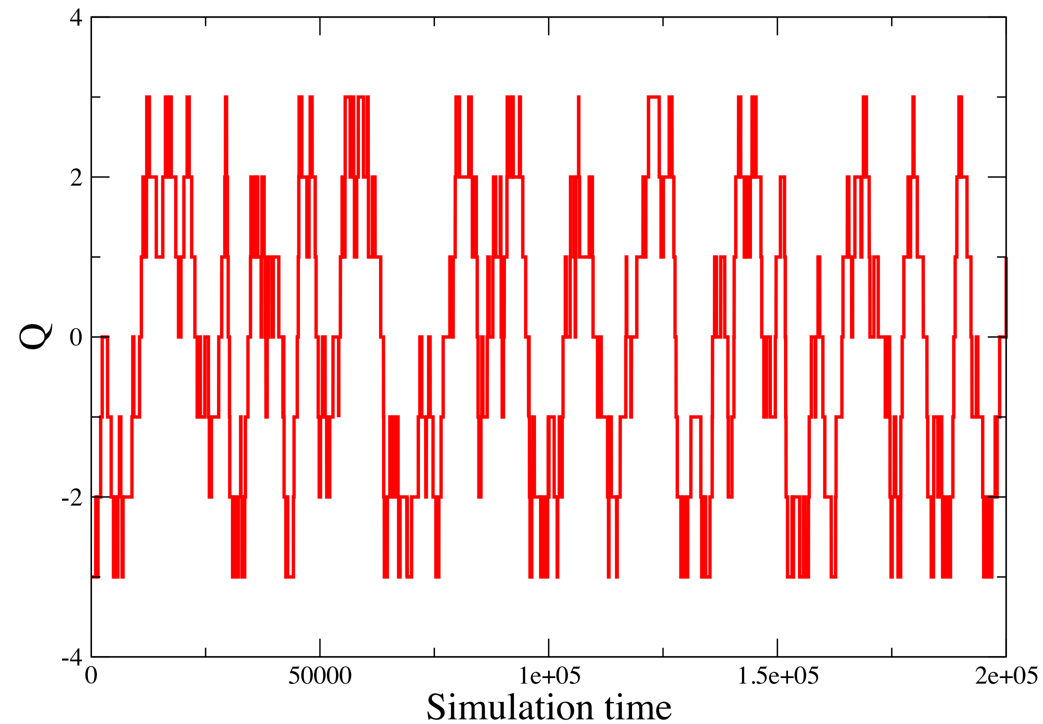


CP^{N-1} model with conventional HMC



CP^{N-1} model with metadynamics



Some recent proposals

Multiscale Thermalization

based on

M. G. E., R. C. Brower, W. Detmold, K. Orginos and A. V. Pochinksy
Phys.Rev. D **92** (2015) 114516

W. Detmold and M. G. E., (2016) [arXiv:1605.09650]

Multiscale thermalization

Can an initial distribution of configurations be constructed such that thermalization is governed only by higher modes of evolution? (Yes!)

MCMC evolution of distributions:

evolution time scales

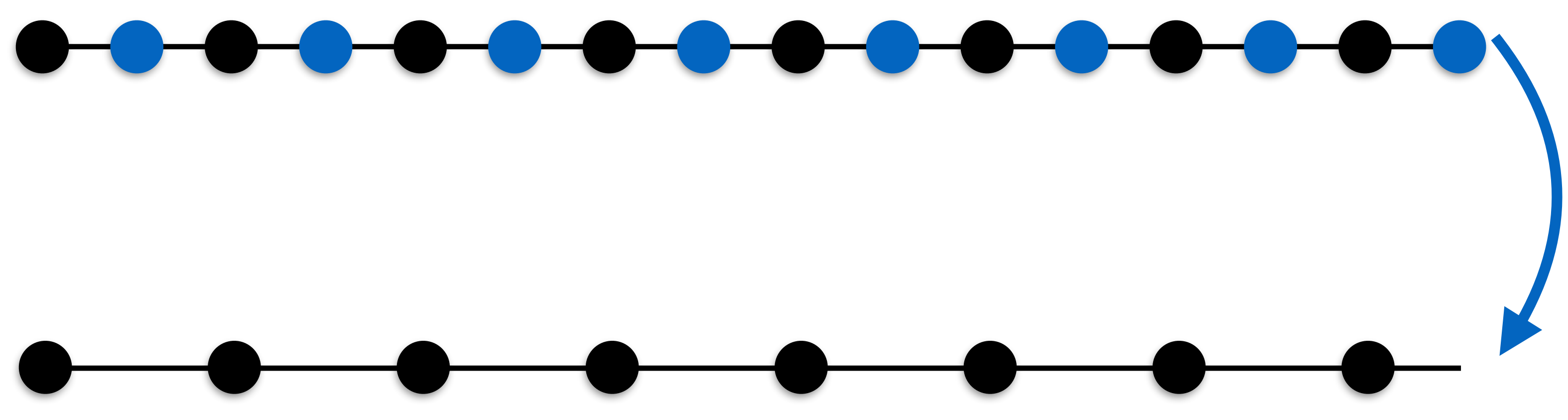
$$\mathcal{P}_\tau(s) = \mathcal{P}(s) + \sum_{n>0} \langle s|\chi_n\rangle \langle\tilde{\chi}_n|\mathcal{P}_0\rangle e^{-\tau/\tau_n}$$

stationary distribution

coupling of initial distribution to modes of evolution

Wanted: $\mathcal{P}_0$ such that $\langle\tilde{\chi}_n|\mathcal{P}_0\rangle = 0$ for small n

Lessons from a toy model

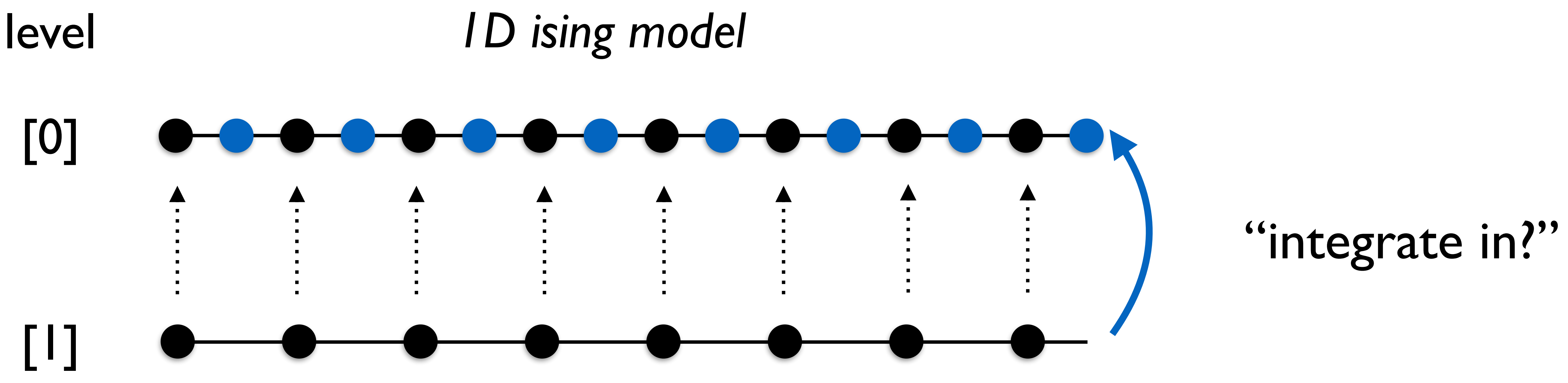


$$H^{[0]} = {\color{blue}J} \sum_i {\color{blue}S_{2i}} (S_{2i+1} + S_{2i-1})$$

$$H^{[1]} = R(J) \sum_i S_{2i+1} S_{2i-1}$$

$$R(J) = \frac{1}{2} \cosh^{-1}\left(e^{2J}\right)$$

Lessons from a toy model

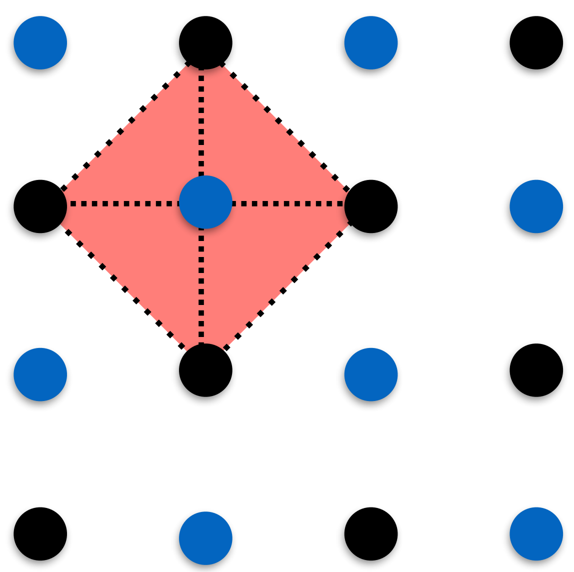


Even site probability measure: $$\mathcal{P}(S_{2i}) = \frac{e^{-J S_{2i}(S_{2i+1}+S_{2i-1})}}{\cosh\left(J(S_{2i+1}+S_{2i-1})\right)}$$

"Integrating in" remaining fine degrees of freedom requires only a single update per site

Generalization to more complicated systems

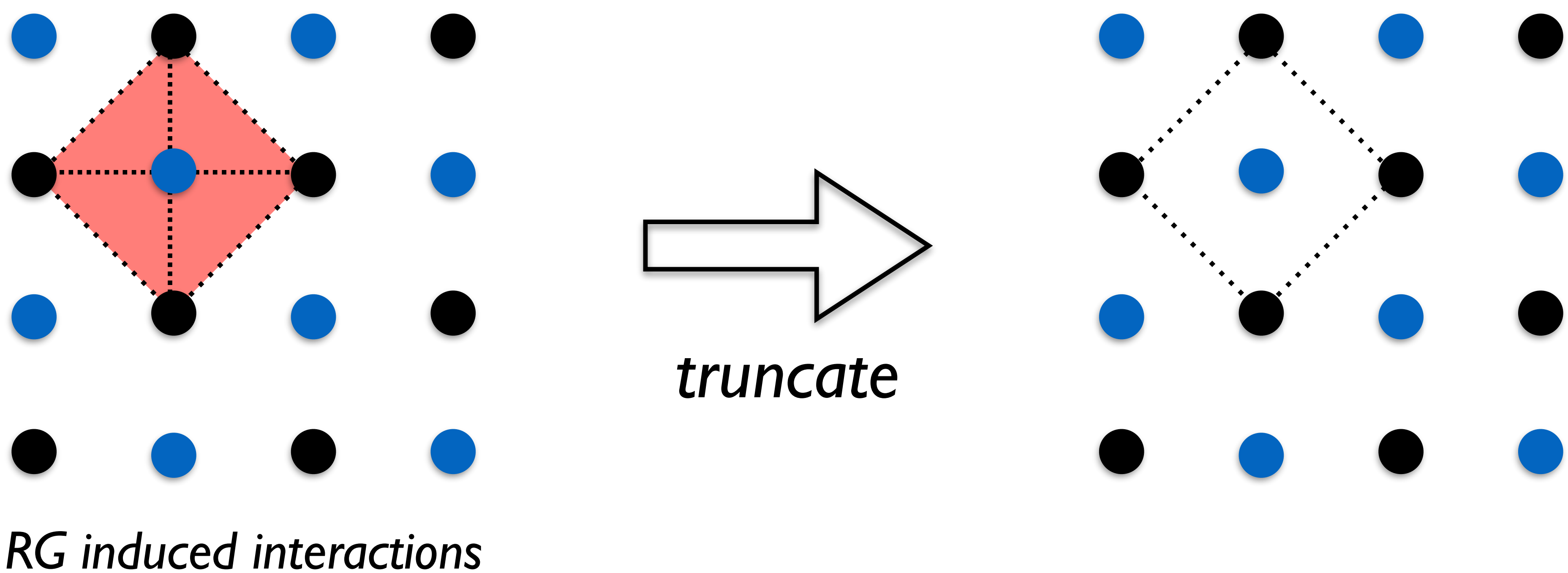
- Higher dimensions/complicated actions:
  - coarse graining induces increasingly complicated interactions
- Gauge theories with fermions:
  - nonlocal actions due to fermion determinants



RG induced interactions

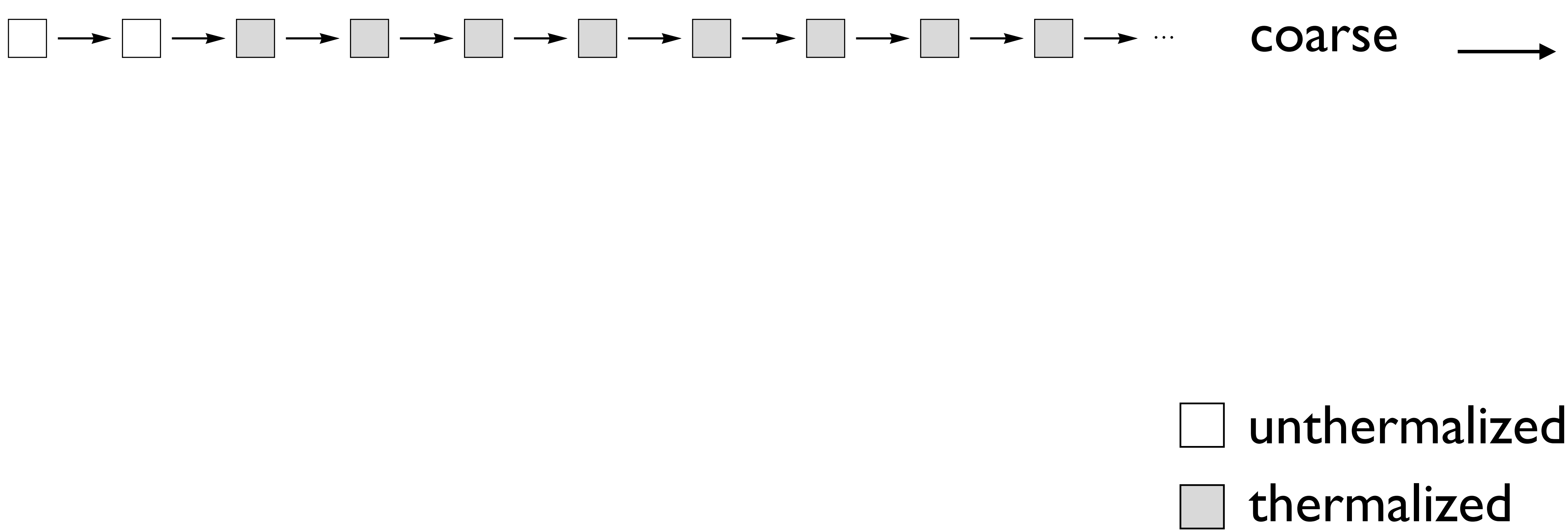
Generalization to more complicated systems

- Generalization is achieved with approximations:
  - truncated coarse action; implies inexact RG matching
  - inexact (one-to-one) refinement prescription
- *Rethermalize* using conventional algorithms to correct errors induced by approximations



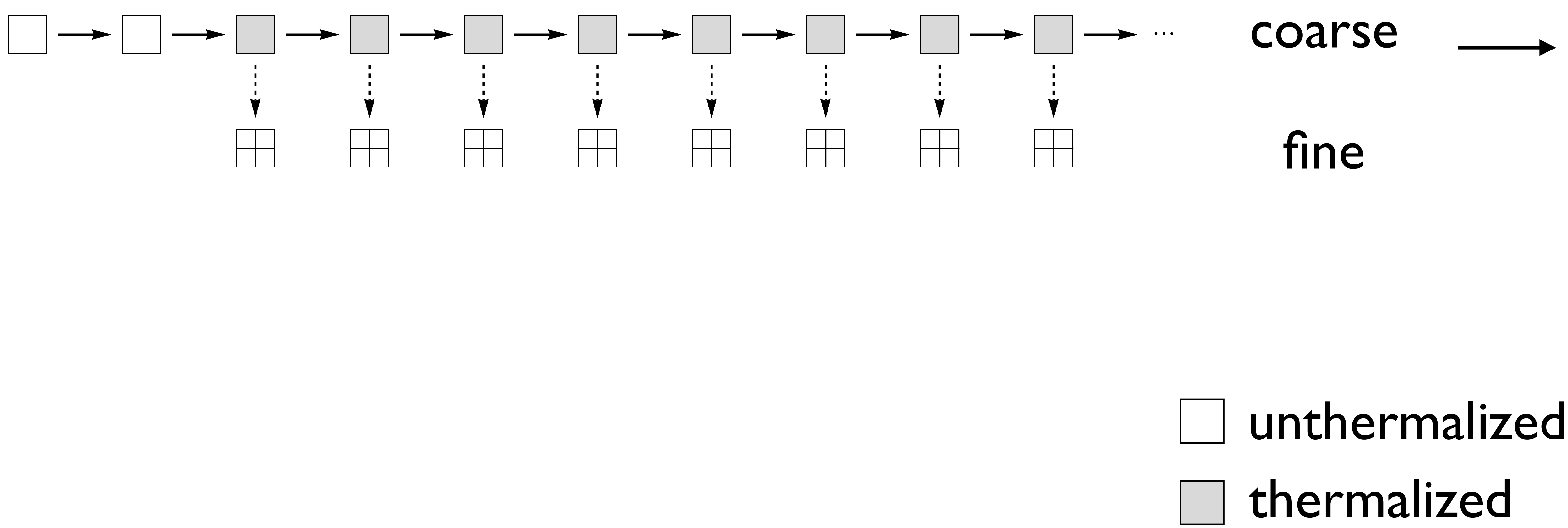
A new proposal for ensemble generation

- Generate *decorrelated* coarse ensemble using an RG matched coarse action



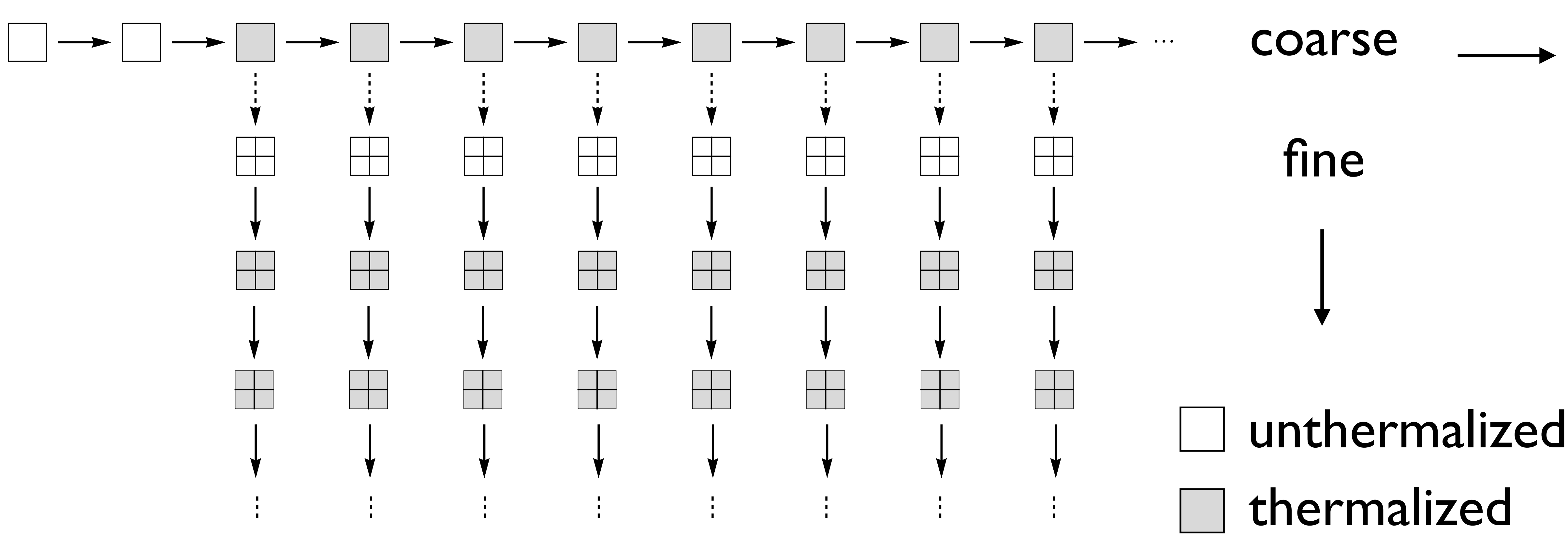
A new proposal for ensemble generation

- Generate *decorrelated* coarse ensemble using an RG matched coarse action
- Map coarse ensemble onto a fine lattice, *while preserving long distance properties*

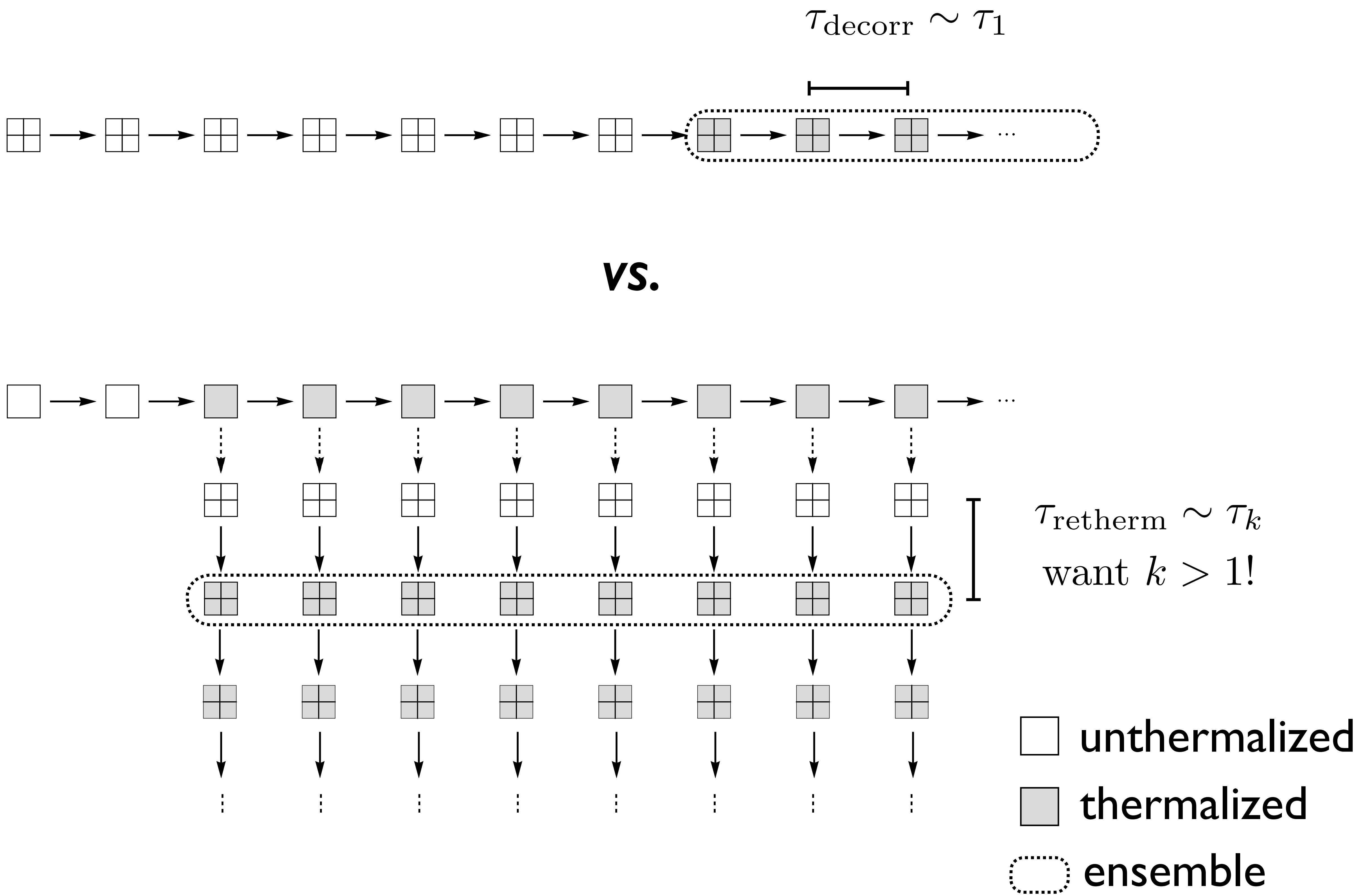


A new proposal for ensemble generation

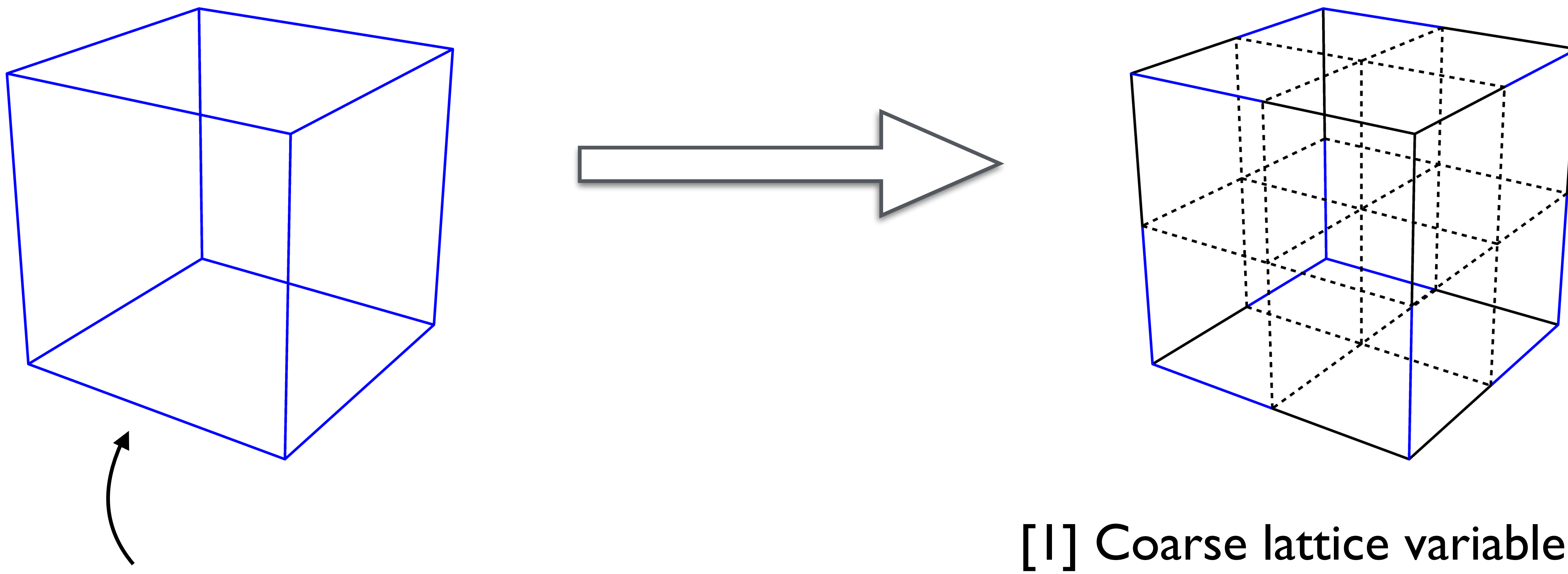
- Generate *decorrelated* coarse ensemble using an RG matched coarse action
- Map coarse ensemble onto a fine lattice, *while preserving long distance properties*
- Rethermalize and evolve multiple refined streams using fine action



A new proposal for ensemble generation



Refinement via interpolation of gauge fields (à la ’t Hooft)



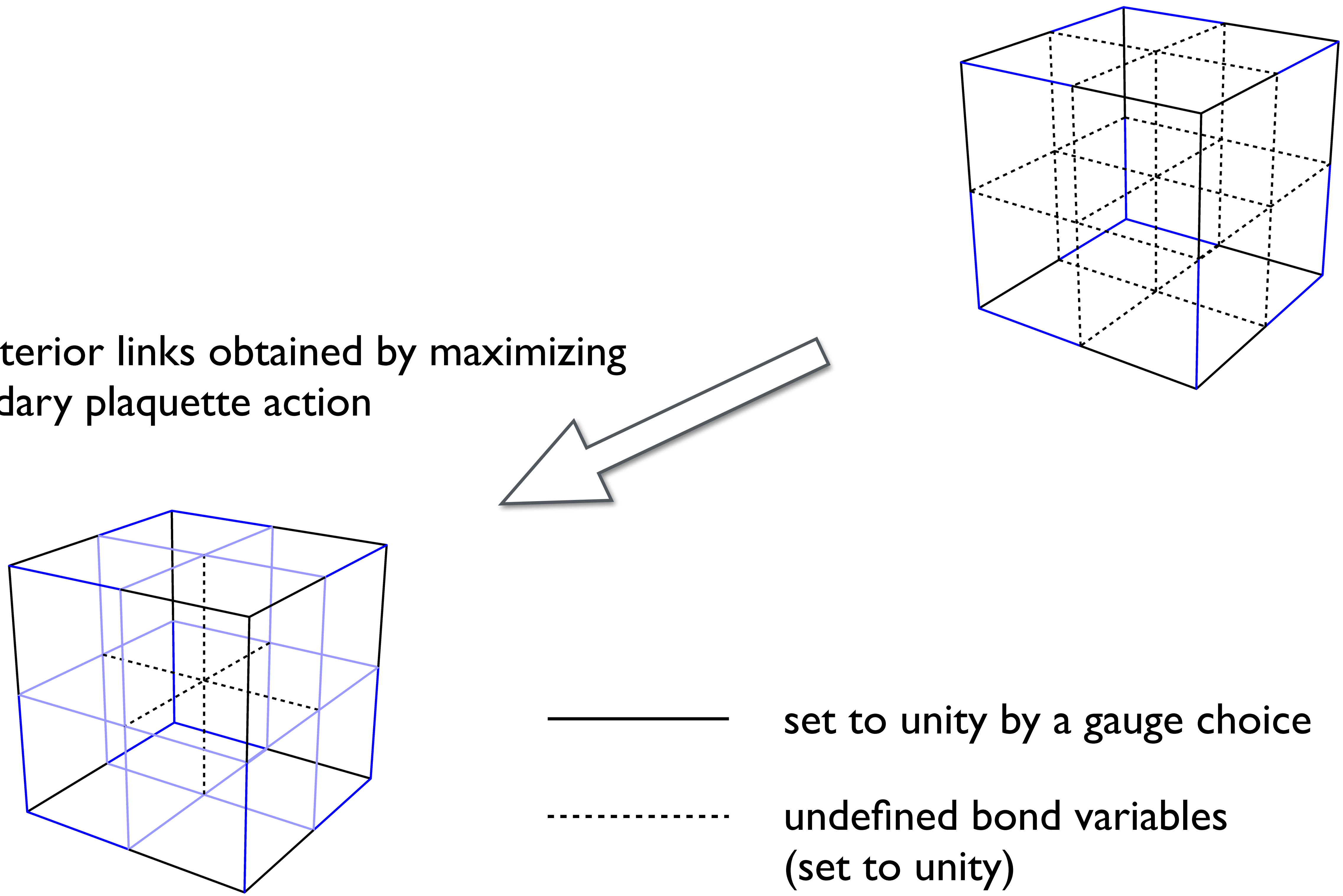
$$U_\mu(x) = e^{iaA_\mu(x)}$$

[1] Coarse lattice variables are transferred to the fine lattice

———— set to unity by a gauge choice

- - - - - - - - undefined bond variables (set to unity)

Refinement via interpolation of gauge fields (à la ’t Hooft)



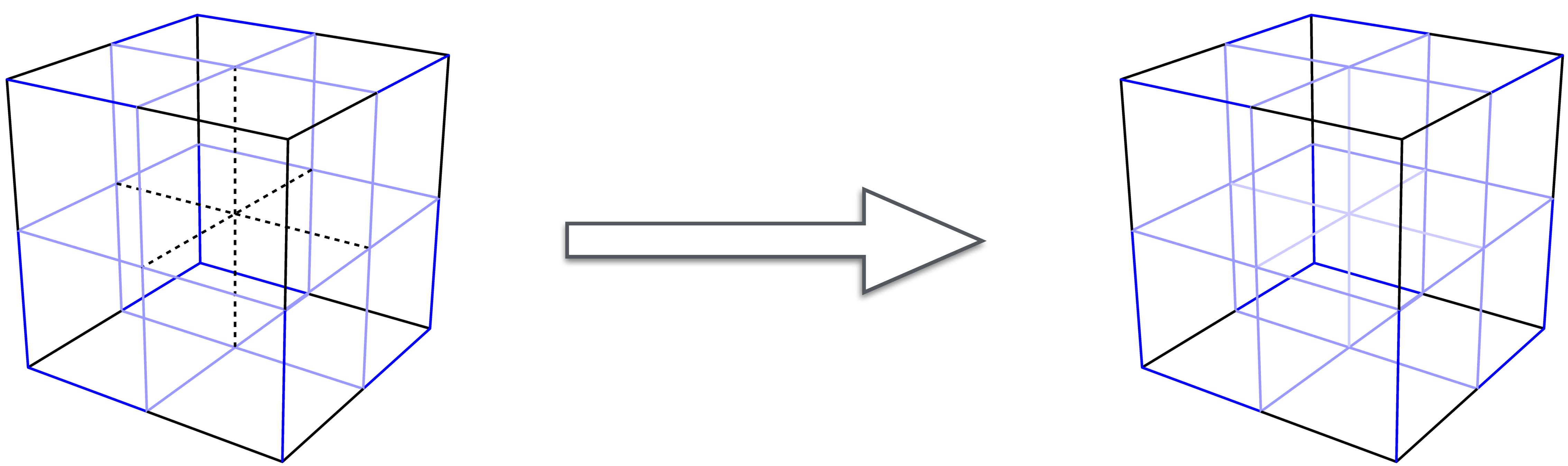
[2] Interior links obtained by maximizing boundary plaquette action

set to unity by a gauge choice

undefined bond variables (set to unity)

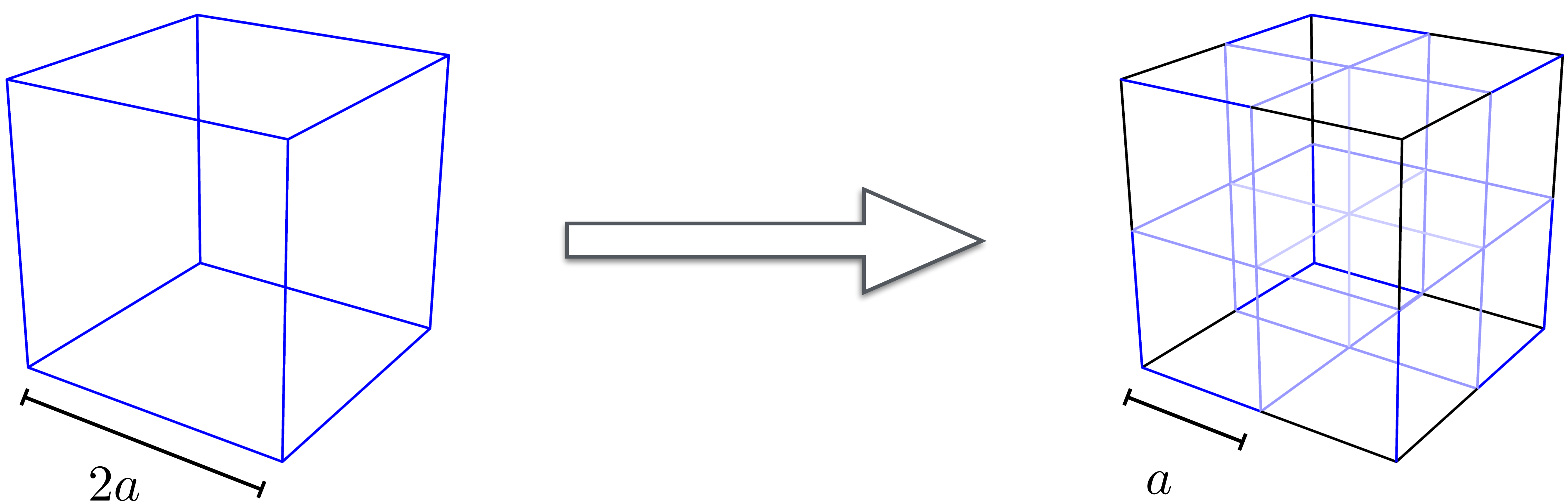
Refinement via interpolation of gauge fields (à la ’t Hooft)

[3] Process sequentially repeated for interior cells

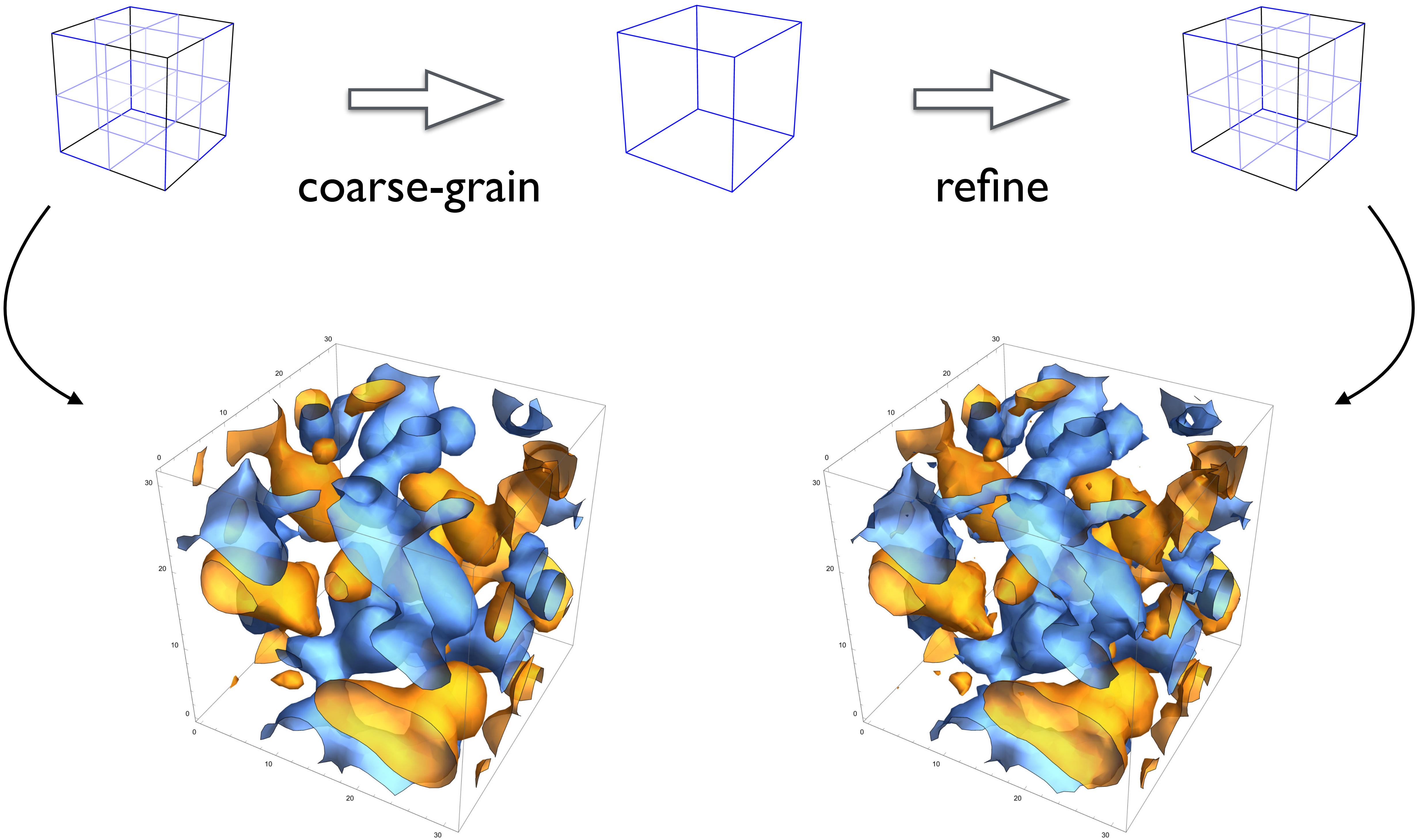


Properties of the interpolation

- Implementation is **simple**, **local** and **efficient**; preserves hypercubic **symmetries**
- Preserves long distance properties of coarse configurations
  - subset of even-shaped Wilson loops on even sites
  - topological charge/density at sufficiently fine lattice spacing
- Breaks discrete translational symmetry
  - rapidly restored upon rethermalization

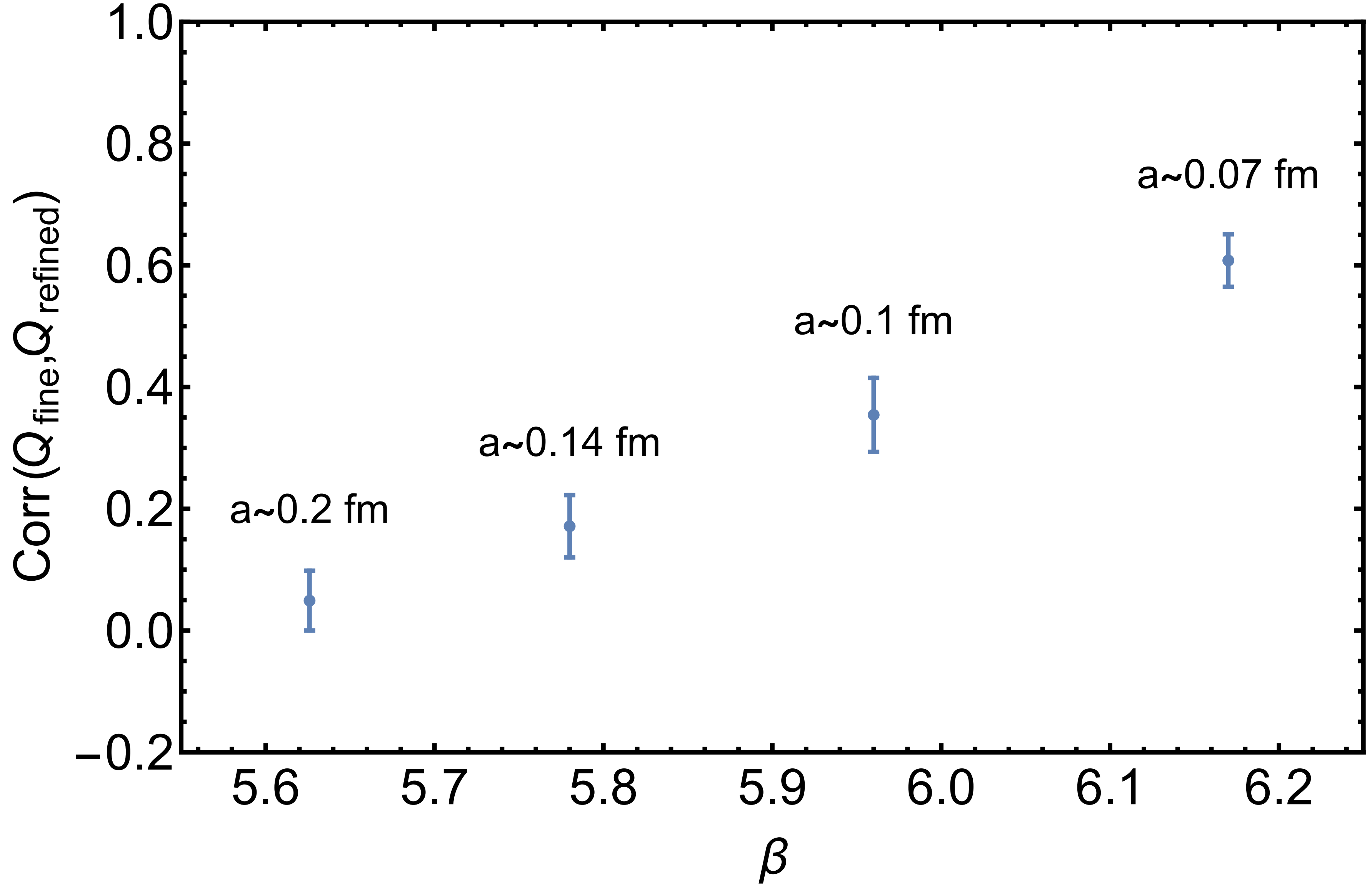


Interpolation — topological charge density



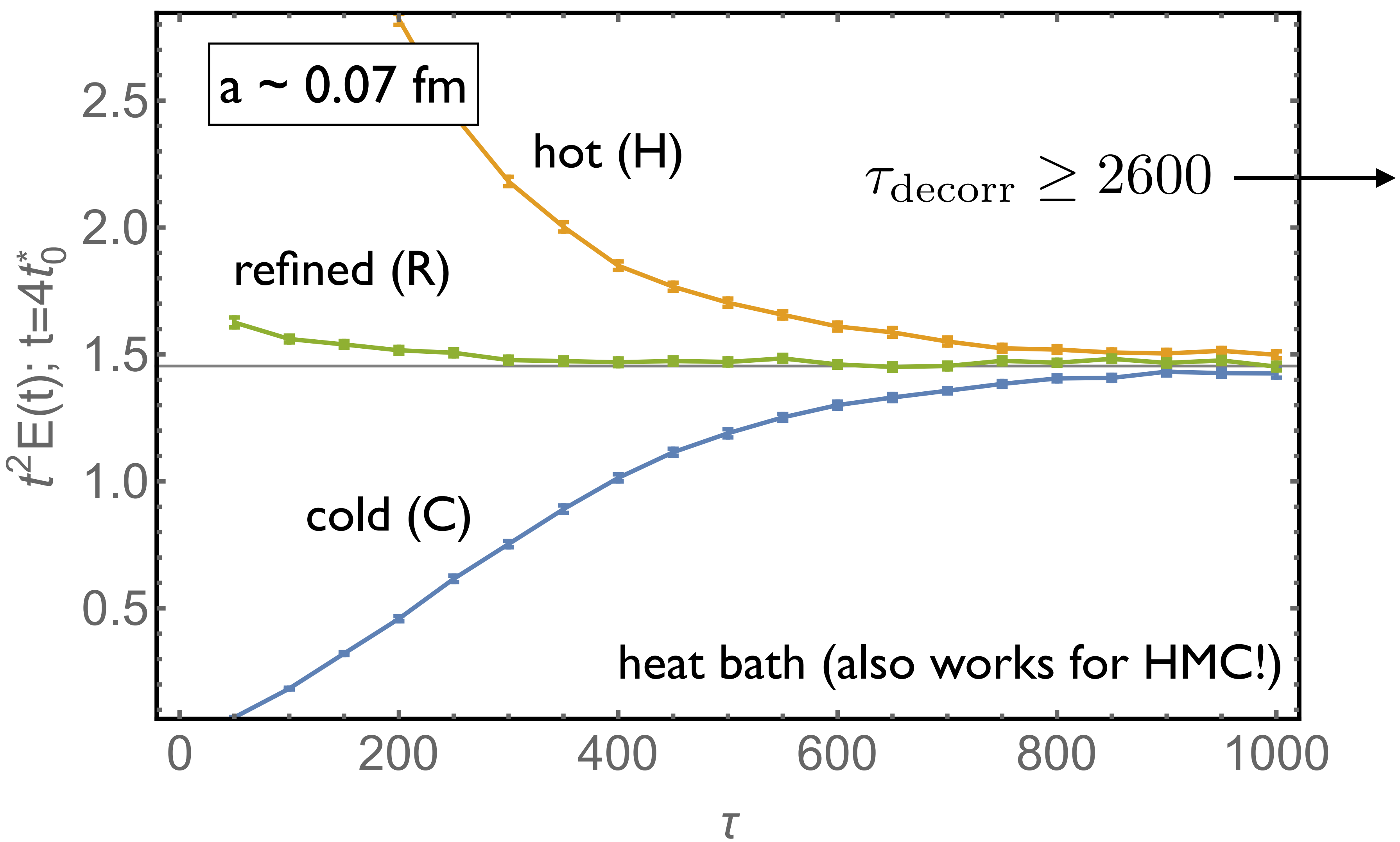
(single time slice)

Interpolation — topological charge



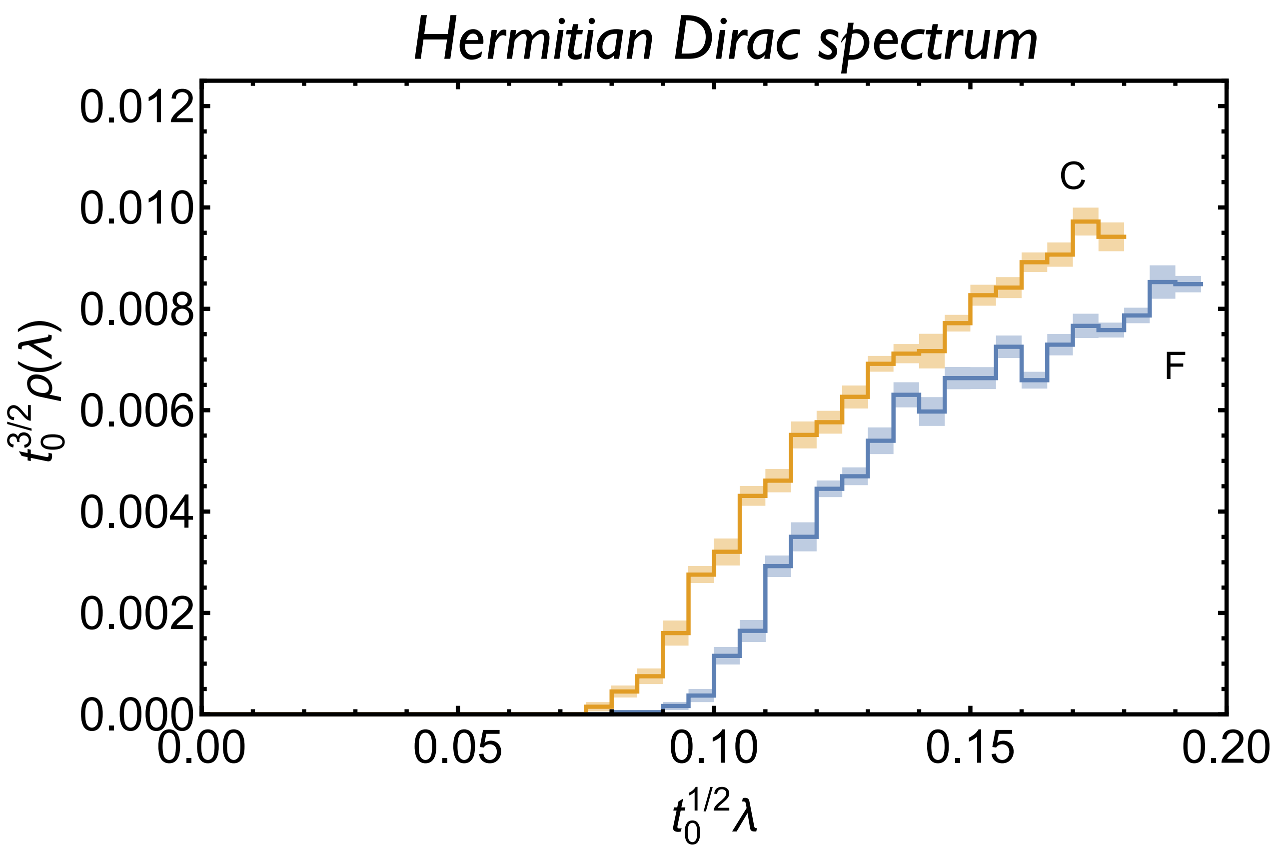
At sufficiently fine lattice spacing, refinement preserves topological charge on a per configuration basis

Demonstration of the approach — pure SU(3) YM



- Refined ensemble obtained from decorrelated RG matched (using r_0) ensemble
- Long distance observables rethermalize on time scales *shorter* than:
  - thermalization time for hot/cold starts (standard approach)
  - decorrelation time for fine evolution: $\tau_{\rm decorr} \gtrsim 2\ \tau_{\rm int}(Q)$

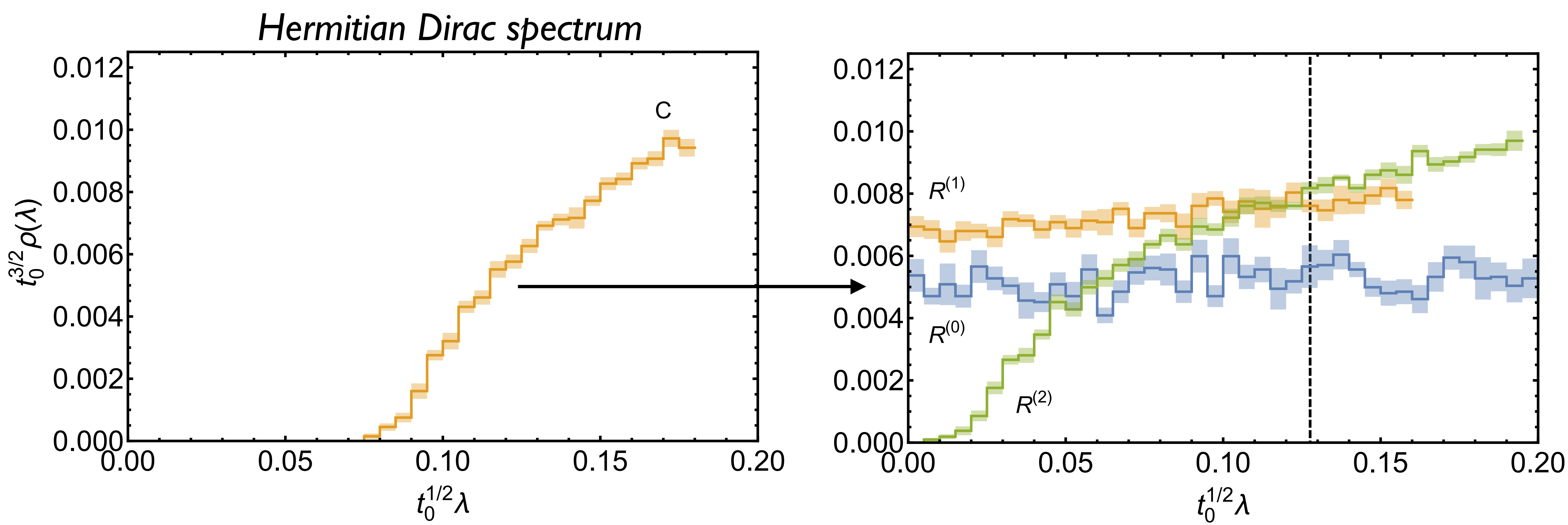
Inclusion of fermions — QCD with N_f=N_c=2



C : coarse ensemble (12^3x36)
F : fine ensemble (24^3x72)

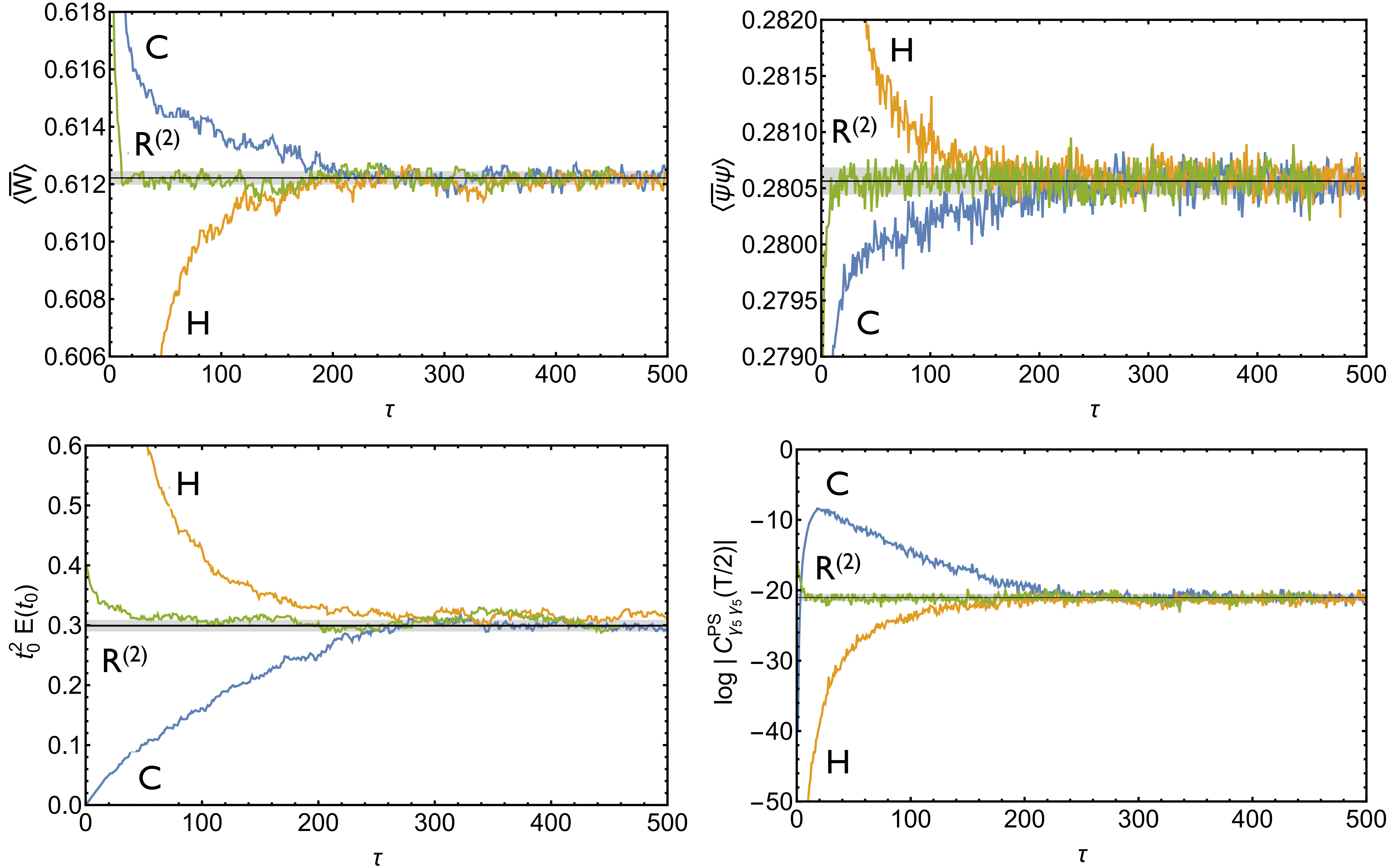
- Coarse/fine actions matched using t_0 and m_π
  - m_π/m_ρ ~ 0.85 (isospin limit)
  - differences in Dirac spectrum presumably due to lattice artifacts
- Refinement of coarse action applies **only** to gauge fields…
  - what does Dirac spectrum of refined ensemble look like?

Inclusion of fermions — QCD with $N_f=N_c=2$



- Refinement via interpolation: C → $R^{(0)}$
  - spurious zero modes; large initial fermion forces in HMC rethermalization
- Short *quenched* evolution of interpolated fields: $R^{(0)} \rightarrow R^{(1)} \rightarrow R^{(2)} \rightarrow \ldots$
  - produce a gap in the Dirac spectrum, eliminate large initial forces
  - only impacts short distance properties of ensemble (if evolution is short)

Demonstration of the approach — QCD with $N_f = N_c = 2$



Conclusion & Outlook

- Several recent promising simulation strategies for addressing critical slowing down and topological freezing:
  - **non-orientable manifolds**
  - **metadynamics**
  - **multiscale thermalization**
- Many remaining open issues for multiscale thermalization:
  - coarse/fine action matching
  - metrics for thermalization
  - removal of inherited lattice artifacts in fine topological charge distribution
  - better understanding of spurious zero-modes of refined Dirac operator and their removal