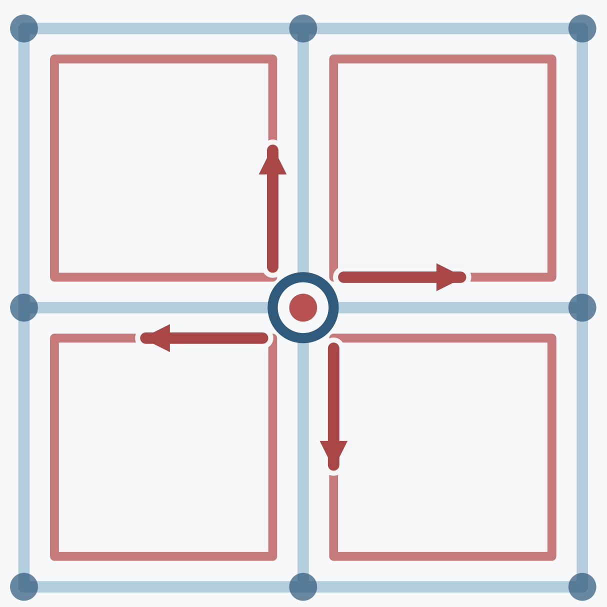

Exploration of Parallel Tempering on Boundary Conditions

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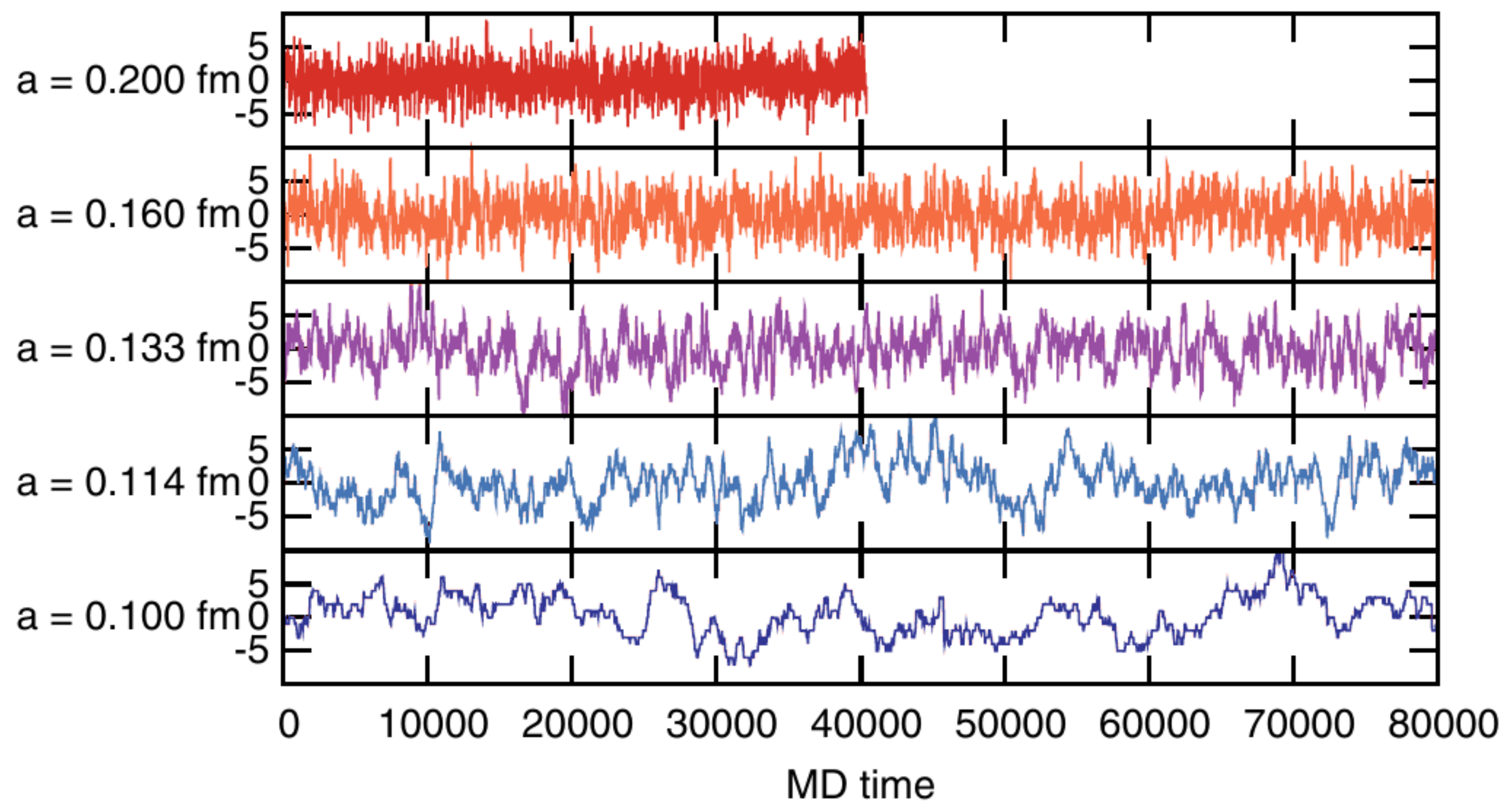
Topological Freezing

- Toward the continuum limit, local MCMC can become trapped in a single topological sector
  → Practical loss of ergodicity
- **Consequences**:
  - Biased estimates and unreliable uncertainties for observables coupled to topology
  - Specialized sampling strategies become necessary
- **Important for:**
  - QCD axion mass and cosmology.
  - QCD vacuum structure and the strong CP problem.



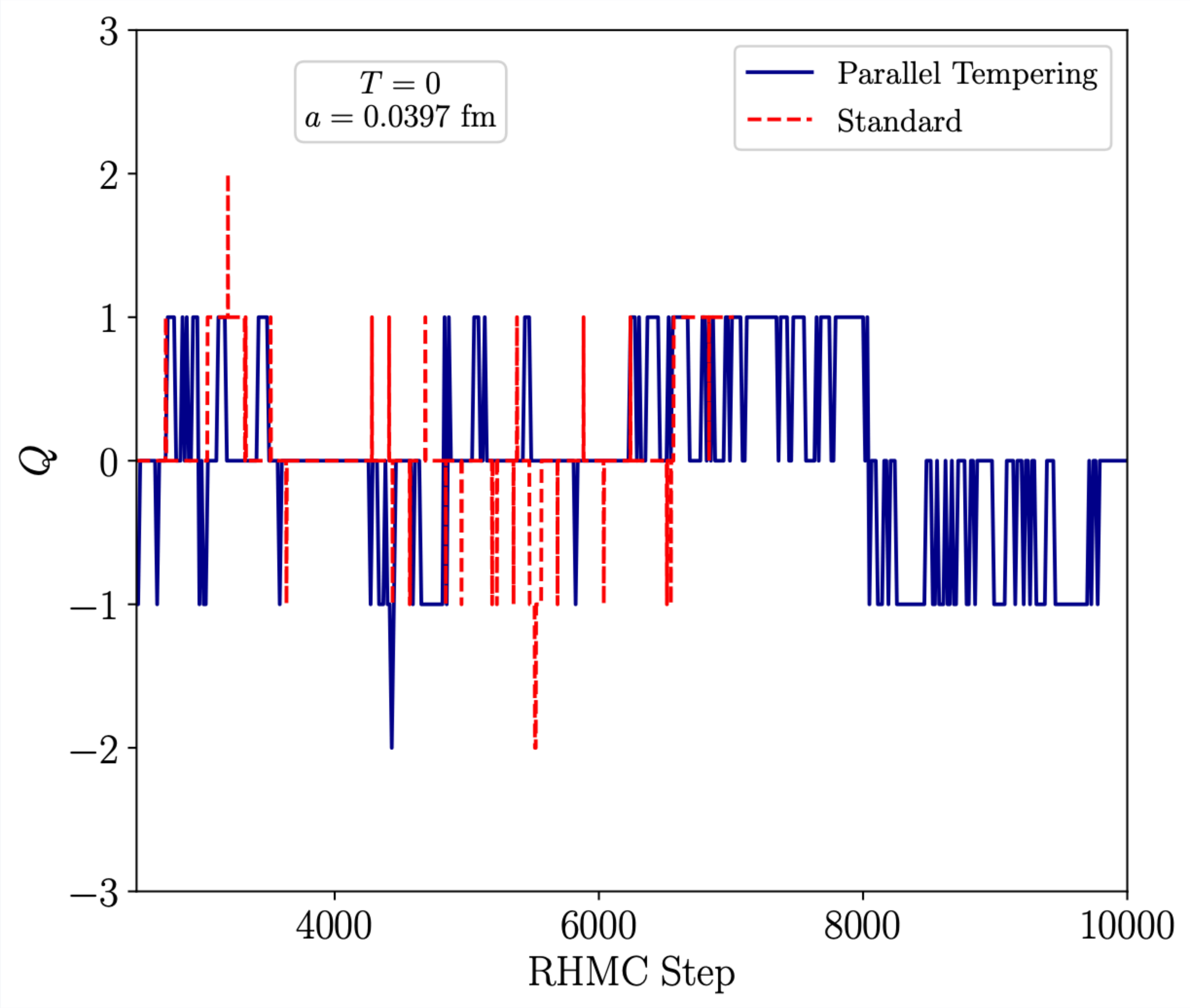
Adapted from McGlynn & Mawhinney, *Phys. Rev. D* **90**, 074502 (2014), Fig. 2.

From Open Boundaries to Parallel Tempering

- **Open boundaries** reduce topological critical slowing down: $\tau_{\text{int}}(Q^2) \sim a^{-2}$ instead of a^{-5}.
  (Lüscher and Schaefer, 2011)
- **Parallel tempering** in a line defect improves topological sampling compared to open boundary conditions in the CP^{N-1} model.
  (Hasenbusch, 2017)
- **PTBC has since been applied** to, e.g., large-N Yang-Mills, SU(3) twisted boundary conditions, and $N_f = 2 + 1$ QCD.
  (Bonanno et al., 2021; 2024a, b)

→ **PTBC substantially reduces topological freezing**

Can we find the optimal way to use PTBC?



Taken from Bonanno et al., *JHEP* **08** (2024) 236, Fig. 2.

Tempering the Boundary Conditions

Following Bonanno et al., *JHEP* **08** (2024) 236.

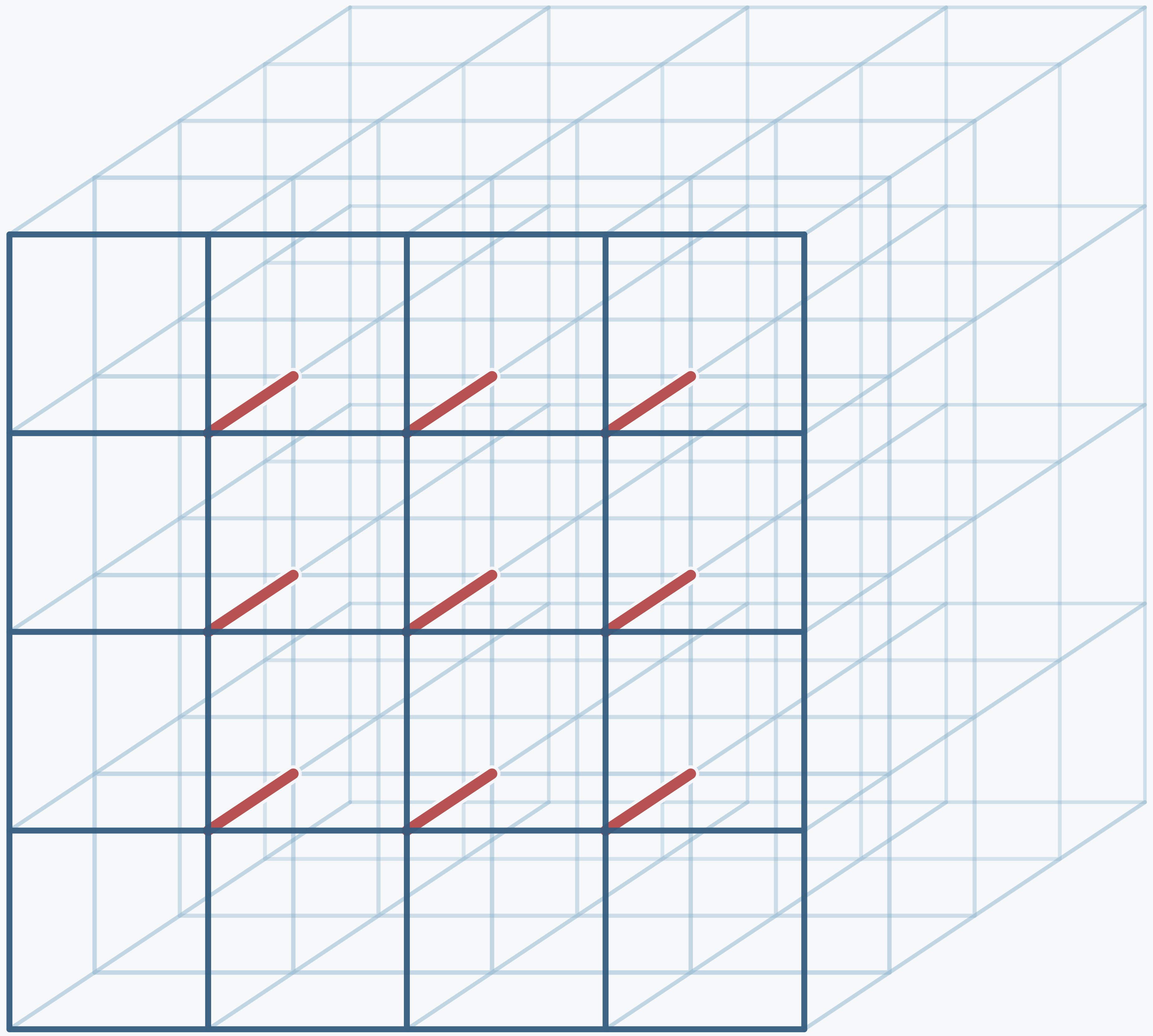
- **Interpolate** between periodic and open boundary conditions using N_r replicas.
- **Introduce a defect** of size L_d^3 on one boundary of every replica.
- **Modify the gauge interaction** for links crossing the defect:

$$K_\mu^{(r)}(x) = \begin{cases} c_r & \text{link } (x,\mu) \text{ crosses the defect} \\ 1, & \text{otherwise}\,. \end{cases}$$

$$\underbrace{c_1 = 1}_{\text{PBC}} > c_2 > \cdots > \underbrace{c_{N_r} = 0}_{\text{OBC}}$$

- **Tune** N_r and $\{c_r\}$ to obtain approximately uniform swap acceptance between neighboring replicas:

$$P_r \equiv \langle p(r, r+1) \rangle \simeq P_{\text{target}}$$



Defect with $L_d = 3$; modified links in red.

One PTBC Update

1 Local update

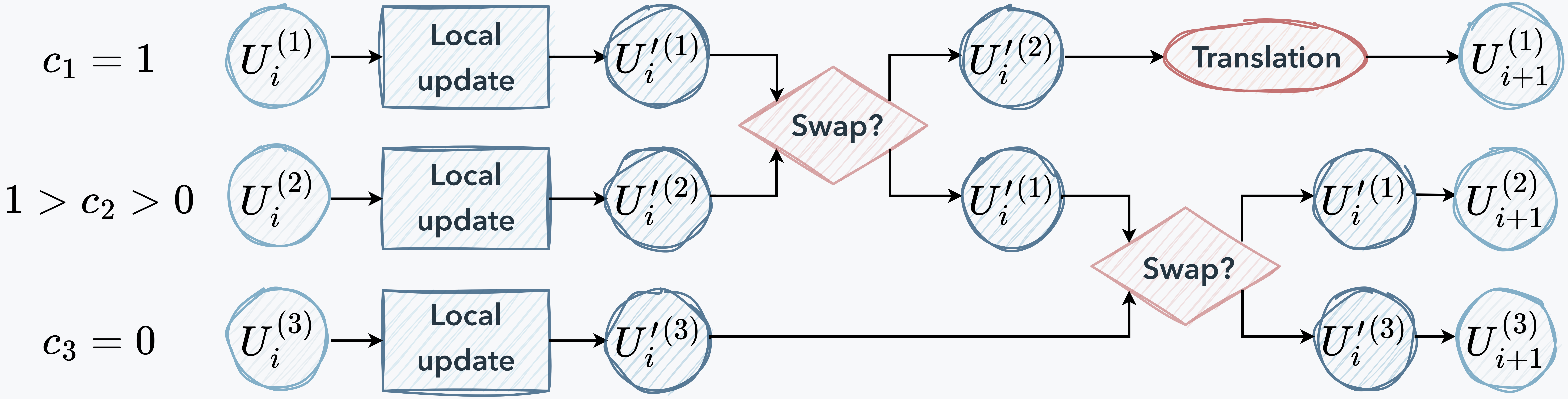
Update every replica independently according to its action $S^{(r)}$.

2 Replica swaps

Propose Metropolis swaps between neighboring replicas.

3 Random translation

Translate the configuration in the PBC replica in a random direction.



$$P_{\text{swap}}(r,s) = \min\left\{1, \exp\left[-\Delta S(r,s)\right]\right\}, \qquad \Delta S(r,s) = S^{(r)}[U^{(s)}] + S^{(s)}[U^{(r)}] - S^{(r)}[U^{(r)}] - S^{(s)}[U^{(s)}]\,.$$

Global and Detailed Balance

Does the complete update satisfy detailed balance?

No. The fixed ordering of reversible kernels is generally not reversible.

Is the algorithm still valid?

Yes. Both the local update and the swap kernel preserve the (joint) target distribution.

$$K_i \in \{L, S_{r,r+1}, T\}, \qquad \pi K_i = \pi \implies \pi K_1 K_2 \cdots K_m = \pi$$

L : local update, $\qquad S_{r,r+1}$: neighboring swap,

T : random PBC translation.

Detailed balance ensures stationarity for L and $S_{r,r+1}$; translation invariance ensures it for T.

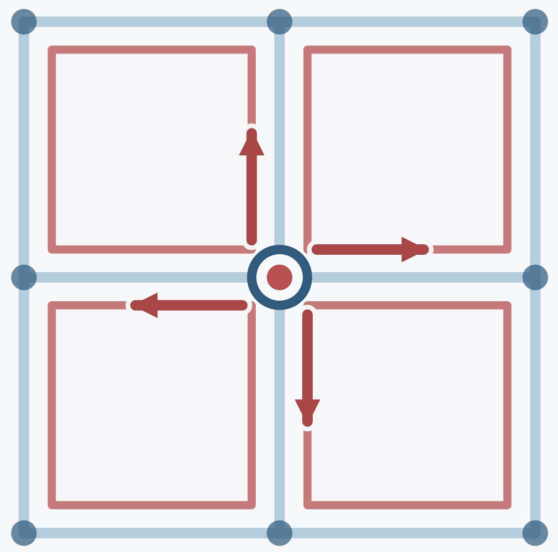
Other swap kernels that also satisfy global balance:

$$S_{EO} = \frac{1}{2}(EO + OE), \qquad E/O : \text{even/odd swaps}$$

Complete updates that satisfy detailed balance:

$$L\left(\frac{F + F^\dagger}{2}\right)L, \qquad F = S_{12}S_{23}\cdots S_{N_r-1,N_r}$$

$$LEOEL$$

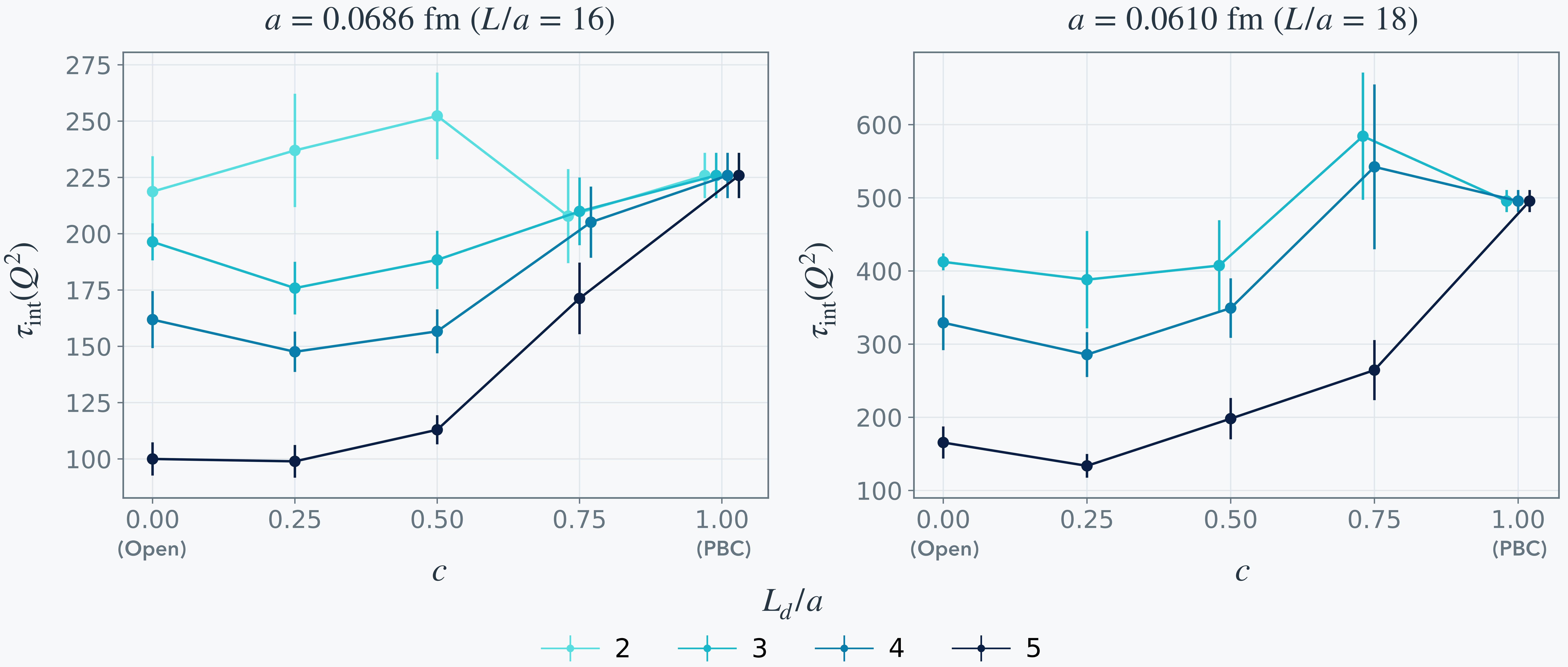


Results

Can we find the optimal way to use PTBC in SU(3) pure gauge theory?

Defect Becomes Effective for $L_d/a \geq 3$

SU(3) pure gauge · Wilson action · $V = (1.1\,\mathrm{fm})^4$ · Replicas evolved independently (no swaps)



$\tau_{\text{int}}(Q^2)$ Grows More Slowly with PTBC

SU(3) pure gauge

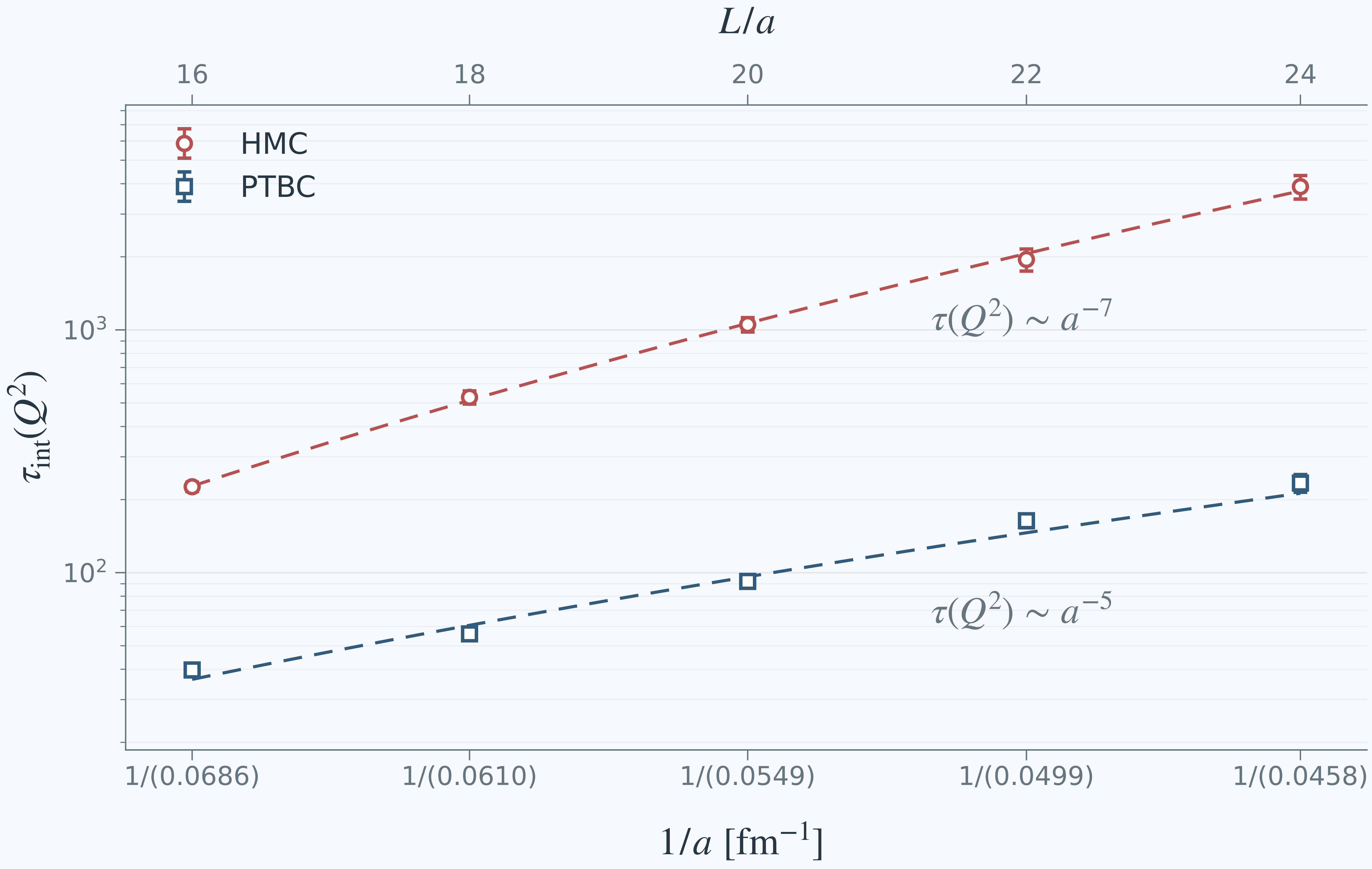
Wilson action

$V = (1.1\ \text{fm})^4$

$L_d/a = 3$

$P_{\text{swap}} \approx 20 - 25\,\%$

14 PTBC replicas



PTBC Becomes Cost-Competitive on Finer Lattices

SU(3) pure gauge

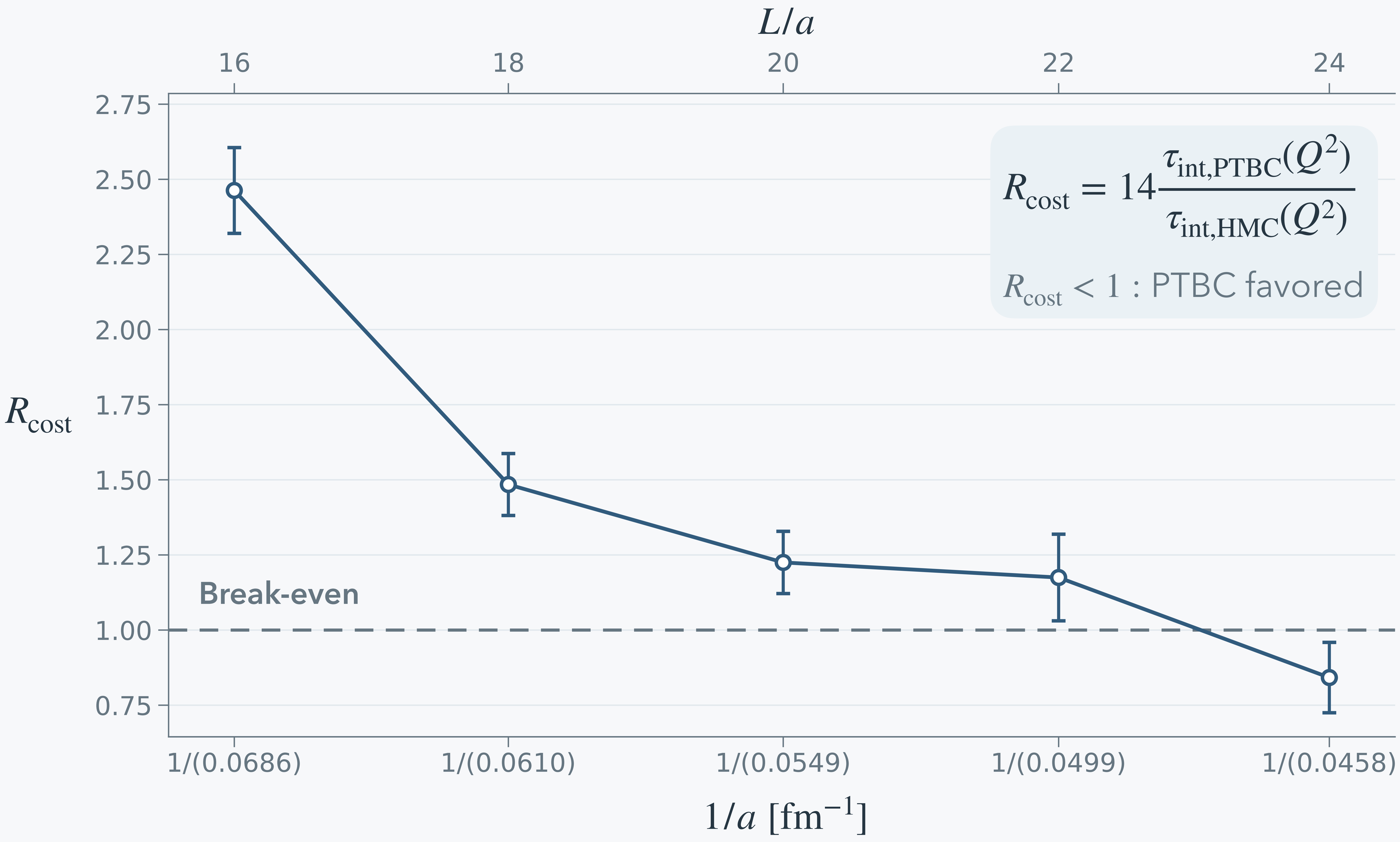
Wilson action

$V = (1.1\ \mathrm{fm})^4$

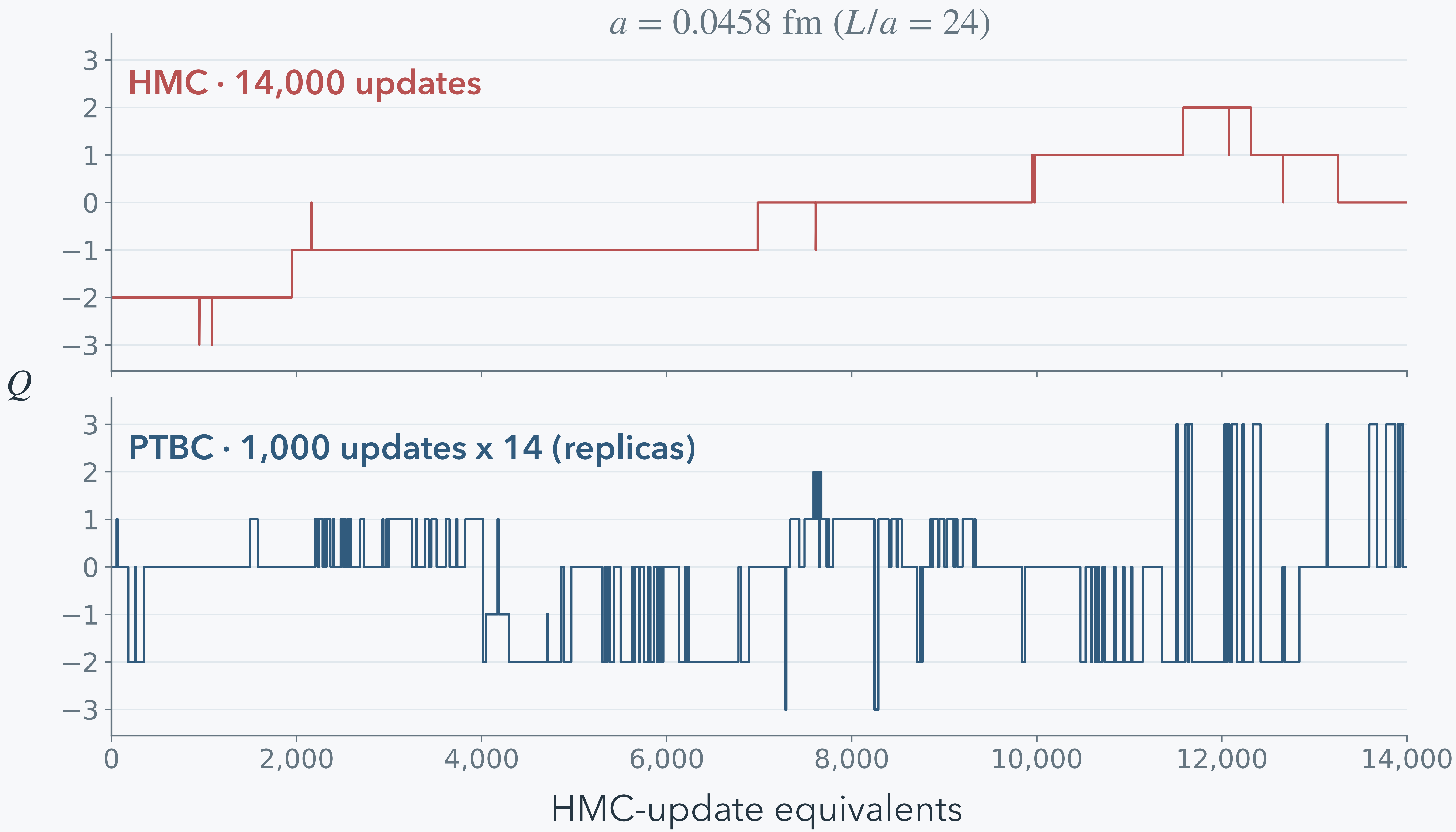
$L_d/a = 3$

$P_{\mathrm{swap}} \approx 20 - 25\,\%$

14 PTBC replicas

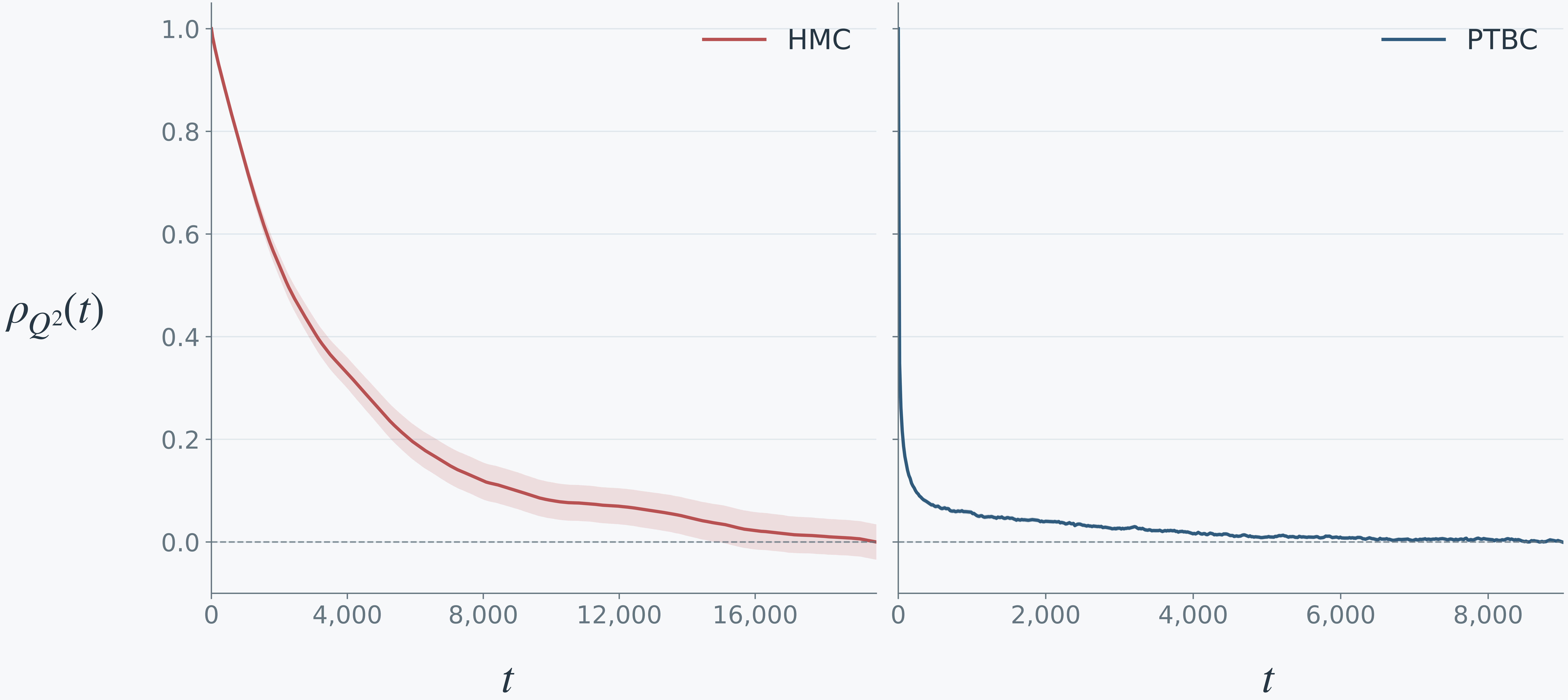


PTBC Explores Topological Sectors More Frequently



PTBC Suppresses the Slow Mode

$a = 0.0458$ fm $(L/a = 24)$



Conclusions & Outlook

Conclusions

- **Cost:** For $L_d/a = 3$, the cost of PTBC approaches break-even towards the continuum, with $a = 0.0458$ fm tentative.

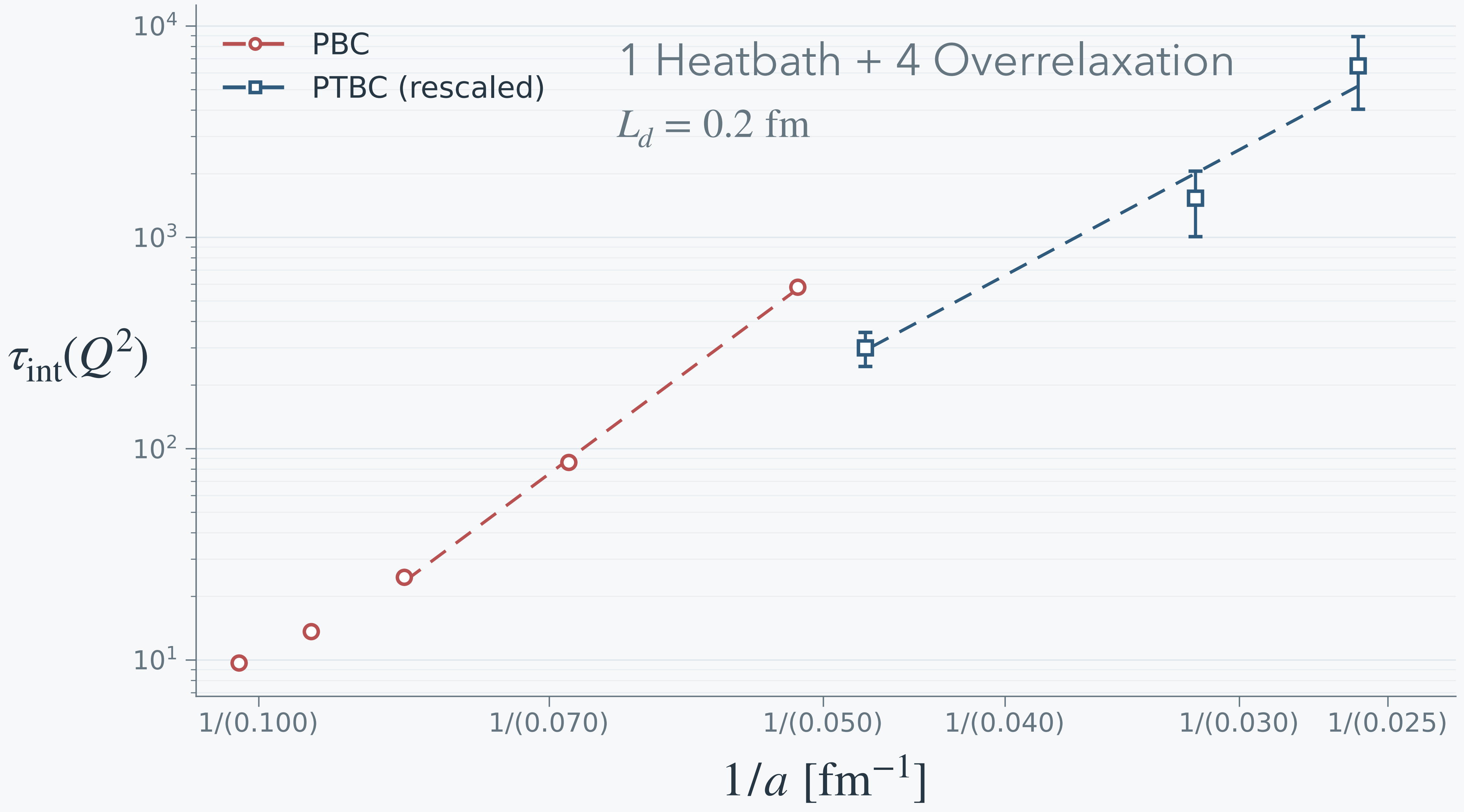
Outlook

- **Defect:** Study finer spacings at constant physical defect size L_d.
- **Swap:** Compare different swapping schemes in a cost-effective region.

This work was supported by the PASC program, *Alpenglue* project.

The authors gratefully acknowledge the resources provided by the Swiss National Supercomputing Centre (CSCS) under project ID c36.

Cost-rescaled PTBC outperforms PBC at finer lattice spacings



PBC data: C. Bonanno, *JHEP* **01** (2026) 039.
PTBC data: C. Bonanno *et al.*, *Eur. Phys. J. C* **84** (2024) 916.

Thank you