Scaling, Topological Tunneling, And Actions For Weak Coupling DWF Calculations

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Outline

1 Motivation: challenge of topological tunneling at weak coupling

2 Fixing slow topological tunneling at weak coupling
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Why we need weak coupling simulations

We need fine lattice spacings for things like correct charm physics, GIM cancellations, and better matching to perturbation theory. We want $a^{-1} > 4$ GeV.

| Table: Exploratory weak coupling simulation |
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| Gauge action | Iwasaki |
| Fermion action | 2+1 flavors DWF |
| $a$ | 0.065(2) fm |
| $a^{-1}$ | 3.03(7) GeV |
| Lattice volume | $32^3 \times 64 \times 12$ |
| Physical volume | $(2.1\text{fm})^3$ |
| $m_{\pi}$ | 360 MeV |
| $m_{\pi}L$ | 3.8 |
| $m_K$ | 540 MeV |
| MD time units | 6950 |

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Slow topological tunneling in the $2+1f$ 3 GeV simulation

Autocorrelation time $\sim 250$ configurations. Will be much worse at $a^{-1} = 4$ GeV. This needs to be fixed.
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Quenched experiments in improving topological tunneling

Quenched simulations provide cheap testing ground for attempts to improvement topological tunneling.

- Adding dynamical fermions back in will improve tunneling somewhat, but not enough.
- Quenched experiments use **HMC algorithm**, since that is what full simulations will use.

Results for two ideas:

- **Open boundary conditions** (Lüscher and Schaefer, arXiv:1105.4749)
- **Dislocation-enhancing determinant**

We look at the MD time evolution of the 5Li definition of the topological charge (de Forcrand et al., arXiv:hep-lat/9701012).
Open boundary conditions

Lüscher and Schaefer proposed to open the boundary conditions in the time direction.

- Global topology can now change smoothly. There is no quantization of topological charge and no disconnected topological sectors.
- Regions near the time boundary now have wrong physics: need to do measurements away from the boundaries.
- So global topology isn't the right thing to compare. We look at interior regions, and hope to see smaller autocorrelations with open BC’s.

Parameters of this experiment:

- Iwasaki gauge action
- $a^{-1} \approx 3$ GeV.
- $24^3 \times 64$ lattice volume ($L = 1.6$ fm).
Open BC’s: periodic reference ensemble

Global topological charge $Q$, periodic boundary conditions

Autocorrelation time seems to be $>10000$ configurations.
Open BC’s: comparing open and periodic BC’s

Topological charge on central half of lattice (excludes boundary regions)

No quantization, but long autocorrelations still present and seemingly not reduced by open BC’s.
Open BC’s: autocorrelations by time slice

We can look at the autocorrelation time of the charge on each time slice to see the effects of the boundary.

As expected, autocorrelation time of $Q(t)^2$ is time-translation invariant on the periodic lattice, within statistics.
Open BC’s: autocorrelations by time slice

We can look at the autocorrelation time of the charge on each time slice to see the effects of the boundary.

The open lattice has smaller autocorrelation times near the time boundaries, but the same autocorrelation time in the bulk, within statistics.
Open boundary conditions: conclusions

- Open boundary conditions only seem to improve autocorrelation times near the open boundaries.
- But that is the part of the lattice that we have to throw away, since it has the wrong physics.
- So open boundary conditions are probably not useful for reducing autocorrelation times.
Dislocation-enhancing determinant: idea

- Idea: encourage tunneling by **seeding small instantons** ("dislocations").
- Dislocations show up in the spectrum of the Wilson Dirac operator: they produce zeromodes of $D_w(-M)$ for negative mass $-M$ of order $-1$.
Dislocation-enhancing determinant: idea

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**Graph:**

Smallest eigenvalue of $\gamma_5 D_w(M = -1)$ for a lattice-scale instanton

Free field + classical instanton

- Instanton size in lattice units
- Smallest eigenvalue of $\gamma_5 D_w(M = -1)$
Dislocation-enhancing determinant: idea

- We can encourage dislocations by introducing the determinant

\[
\det \left[ f(D_w^\dagger D_w) \right] = \prod_i f(\lambda_i^2)
\]

This generalizes the “dislocation-suppressing determinant ratio” of RBC/UKQCD (arXiv:1208.4412).

- Choose \( f(\lambda^2 = 0) \) large to encourage dislocations (which are zeromodes):

\[
f(\lambda_2)
\]

\( \lambda \) (eigenvalue of \( \gamma_5 D_w \))

\[
\begin{align*}
0 & \quad 1 \\
& \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad
\end{align*}
\]
Dislocation-enhancing determinant: experiment

We compare a reference evolution to one that includes a dislocation-enhancing determinant.

- Wilson gauge action
- $a^{-1} \approx 4$ GeV
- Lattice volume $32^4$ ($L \approx 1.6$ fm)
- We choose the enhancement function $f$ to have the form

$$f(\lambda^2) = \left(1 - \frac{a}{\lambda^2 + b_1} + \frac{a}{\lambda^2 + b_2}\right)^{-2}$$

This is easy to implement using standard RHMC codes, and for appropriate values of $a, b_1, b_2$ it has the desired form.

For convenience and speed we use the even-odd preconditioned $D_w$ in the determinant.

- Introducing the determinant can shift the lattice spacing. We therefore adjust $\beta$ to match the lattice spacing of the reference ensemble as determined by the Wilson flow (Lüscher arXiv:1006.4518, BMW arXiv:1203.4469).
Dislocation-enhancing determinant: results

Tunneling events are about 5 times more frequent with the dislocation-enhancing determinant.

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Dislocation-enhancing determinant: results

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Dislocation-enhancing determinant: outlook

- There is a lot of freedom in choosing the function $f$ and the negative mass $-M$, which could allow for a much larger improvement.
- Will enhancing dislocations increase $m_{\text{res}}$? Yes, but so far not by too much:

| Reference | DED  |
|-----------|------|
| $0.9(2) \times 10^{-4}$ | $1.5(3) \times 10^{-4}$ |

$m_{\text{res}}$ is still very small.

- Once we seed small instantons, how can we encourage them to grow?
- Can a DED exacerbate cutoff effects?
Summary

- Weak coupling simulations are needed for accurate charm and good matching to perturbation theory: we want to reach $a^{-1} > 4$ GeV. In this regime the topological charge has very long autocorrelations.
- Open boundary conditions do not seem to be useful for reducing autocorrelations.
- A dislocation-enhancing determinant can speed up topological tunneling.
Backup slides
With open BC’s, global Q sums over unphysical boundary regions.
The time history contains large rapid fluctuations from the boundary regions, superimposed on the slow fluctuations of the bulk charge.
These unphysical fluctuations artifically decrease the autocorrelation time.
No quantization, but long autocorrelations still present and seemingly **not reduced** by open BC’s.
Open BC’s: Wilson 4 GeV results

A similar open boundary conditions experiment with the Wilson gauge action at $1/a \approx 4$ GeV, $32^4$. 

![Graph showing the central 5Li topological charge over MD time for periodic and open boundary conditions.](image-url)
Open BC’s: Wilson 4 GeV results

A similar open boundary conditions experiment with the Wilson gauge action at $1/a \approx 4$ GeV, $32^4$. 

![Graph showing integrated autocorrelation time of Q(t)^2 versus time slice for Periodic BC's and Open BC's.](image)
Naik-improved DWF

HISQ-style Naik improvement is applicable to the 4D part of the DWF action. Using a two-link derivative instead of a three-link derivative is possible, but the three-link form preserves the possibility of even-odd preconditioning.

\[ \Phi_{\text{improved}} = \Phi_{w} + \Phi_{\text{Naik}} \]

\[ (\Phi_{w} \psi)_{x} = \alpha \sum_{\mu} \gamma_{\mu} \left[ U_{x,\mu} \psi_{x+\hat{\mu}} - U_{x-\hat{\mu},\mu} \psi_{x-\hat{\mu}} \right] \]

\[ (\Phi_{\text{Naik}} \psi)_{x} = \beta \sum_{\mu} \gamma_{\mu} \left[ U_{x,\mu} U_{x+\hat{\mu},\mu} U_{x+2\hat{\mu},\mu} \psi_{x+3\hat{\mu}} \right. \]

\[ \left. - U_{x-\hat{\mu},\mu} U_{x-2\hat{\mu},\mu} U_{x-3\hat{\mu},\mu} \psi_{x-3\hat{\mu}} \right] \]

|          | \( \alpha \) | \( \beta \) |
|----------|--------------|--------------|
| Unimproved | 1            | 0            |
| Improved  | \( 9/8 + O(g) \) | \( -1/24 + O(g) \) |
Definition of topological charge

We look at the topological observables

\[ Q = \sum_t \sum_{\vec{x}} \rho(\vec{x}, t) \]

\[ Q(t) = \sum_{\vec{x}} \rho(\vec{x}, t) \]

\[ Q(t_1, t_2) = \sum_{t_1 \leq t < t_2} Q(t) \]

where the topological charge density \( \rho(\vec{x}, t) \) is

\[ \rho(\vec{x}, t) = \frac{1}{16\pi^2} \epsilon_{\mu\nu\rho\lambda} \text{tr}(F_{\mu\nu}F_{\rho\lambda}) \]

and we use the 5Li definition of \( F_{\mu\nu} \) (de Forcrand et al., arXiv:hep-lat/9701012). The topological charge is always measured after cooling the gauge field with 60 rounds of APE smearing with coefficient 0.45.