Diffusion of topological charge in lattice QCD simulations

Greg McGlynn

Columbia University

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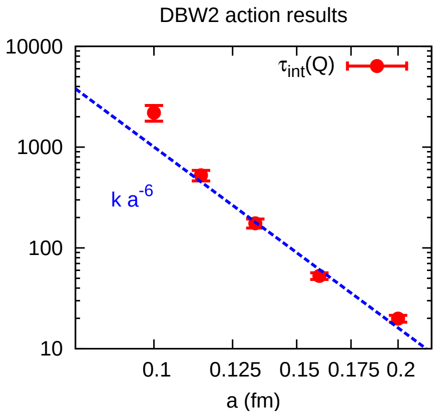
(with Bob Mawhinney)

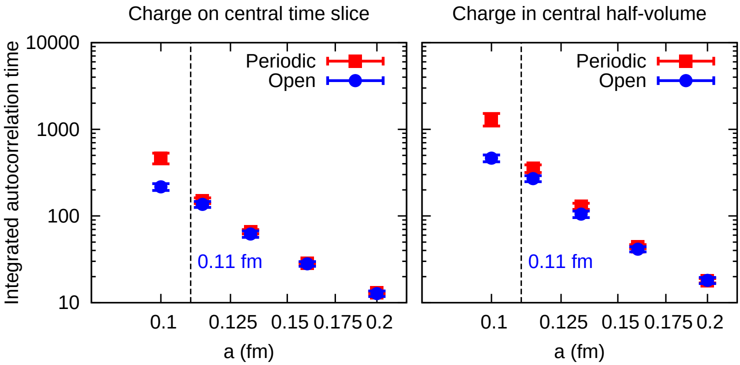
Motivation: long topological autocorrelations

- Autocorrelation time of the topological charge Q increases very rapidly as $a \to 0$.
- Open boundary conditions were proposed to help this. (Lüscher, Schaefer, 1105.4749)
  - **When** do they help?
  - **How much** do they help?
  - **How** do they work exactly—how does topological charge move in from the boundaries?



Open vs periodic boundary conditions

High-statistics simulations of pure gauge theory with DBW2 action:



For $a \lesssim 0.11$ fm, open boundary conditions are better.

- Where does 0.11 fm come from?
- What happens at even finer a?

The diffusion model

Let $Q_{\text{slice}}(t, \tau)$ be the charge on time slice t at MD time τ.

Form the correlation function:

$$C(t, t_0, \tau) = \langle Q_{\text{slice}}(t, \tau) Q_{\text{slice}}(t_0, 0) \rangle$$

This measures how much topological charge will move from time slice t_0 to time slice t in an MD time interval τ.

C turns out to obey a simple diffusion equation to very high accuracy:

$$\frac{\partial}{\partial \tau} C(t, t_0, \tau) = D \frac{\partial^2}{\partial t^2} C(t, t_0, \tau) - \frac{1}{\tau_{\text{tunn}}} C(t, t_0, \tau)$$

The diffusion model

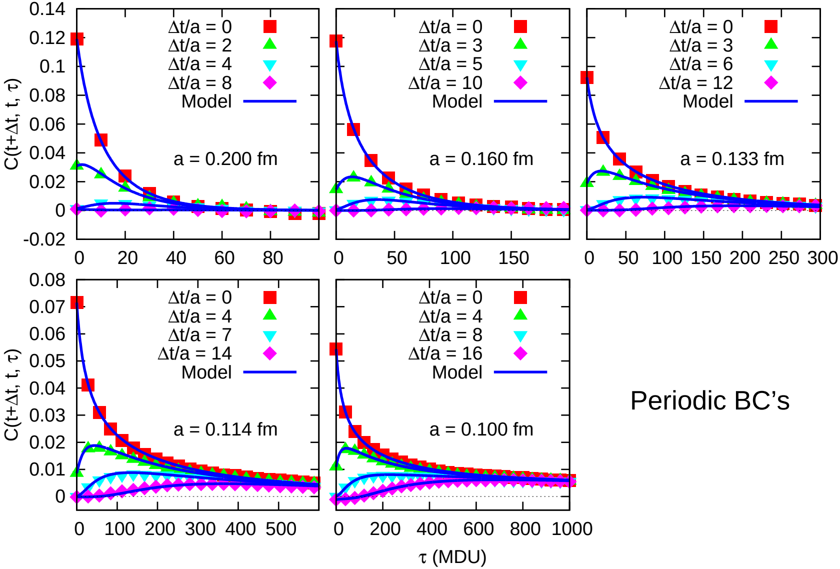
$$\frac{\partial}{\partial \tau} C(t, t_0, \tau) = \underbrace{D \frac{\partial^2}{\partial t^2} C(t, t_0, \tau)}_{\text{Diffusion}} - \underbrace{\frac{1}{\tau_{\text{tunn}}} C(t, t_0, \tau)}_{\text{Tunneling}}$$

- The **diffusion coefficient** D quantifies how fast topological charge moves around.
- The **"tunneling timescale"** τ_{tunn} quantifies the rate of tunneling (spontaneous creation or destruction of instantons in the bulk).
  Equal to $\tau_{\text{int}}(Q)$ on periodic lattices.

Given these parameters, we can numerically *calculate* autocorrelation functions.

Model fits to data

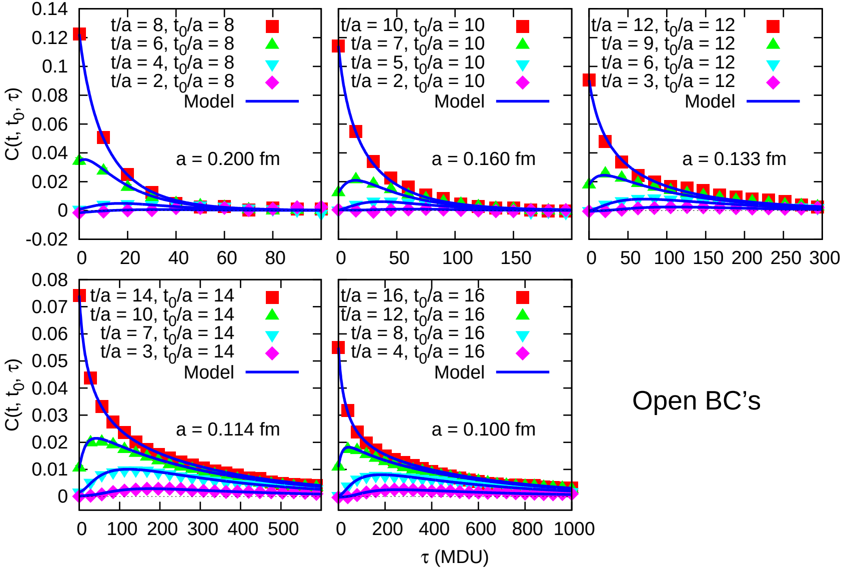
Remarkable agreement between model and data:



Periodic BC's

Model fits to data

Remarkable agreement between model and data:



Implications of the model

The diffusion model picks out a **diffusion timescale**

$$\tau_{\text{diff}} \equiv \frac{T^2}{8D}$$

This is the MD time to diffuse across a distance $T/2$.

Open boundaries help only if diffusion is *faster* than tunneling:

$$\tau_{\text{diff}} \ll \tau_{\text{tunn}} \qquad \text{i.e.} \qquad \frac{T^2}{8D} \ll \tau_{\text{int}}(Q)$$

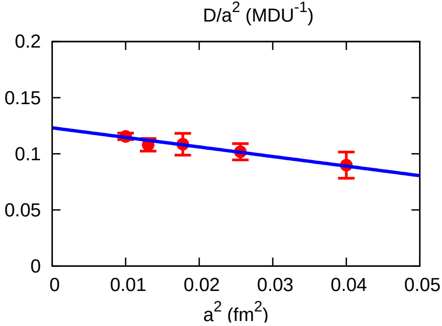
Otherwise, autocorrelations are destroyed by tunneling faster than the boundary can affect the bulk.

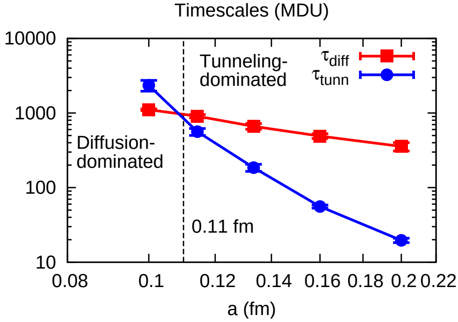
Scaling of the diffusion coefficient

The scaling of the diffusion coefficient D helps determine the scaling of autocorrelation times. We find

$$D = ka^2 + \text{ small } O(a^4) \text{ corrections}$$

$$\text{so} \quad \tau_{\text{diff}} = \frac{T^2}{8D} \propto \frac{1}{a^2}$$





Scaling of autocorrelation times

Can use diffusion model to calculate autocorrelation times.

Example: the charge on the central time slice.

Tunneling-dominated limit (coarse a)

$$\tau_{\text{int}} = \sqrt{\frac{\pi\sigma^2\tau_{\text{tunn}}}{2D}} \propto \frac{1}{a^4}$$

Diffusion-dominated limit (fine a)

$$\text{Open BC's: } \tau_{\text{int}} = \sqrt{\frac{\pi}{8}}\frac{\sigma T}{D} \propto \frac{1}{a^2}$$

$$\text{Periodic BC's: } \tau_{\text{int}} = \sqrt{2\pi}\frac{\sigma}{T}\tau_{\text{tunn}} \propto \frac{1}{a^6}$$

$1/a^2$ scaling of open boundaries confirms empirical results of Lüscher and Schaefer.

Summary

We can calculate topological autocorrelation functions with a simple differential equation.

With it we can answer several questions about open boundaries:

- **When** do open boundary conditions help?
  A: When a is fine enough that

$$\frac{T^2}{8D} \ll \tau_{\text{int}}(Q)$$

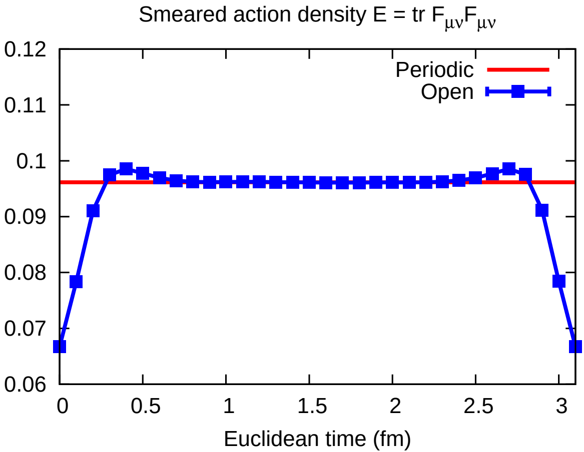
- **How much** do open boundary conditions help?
  A: Scaling of autocorrelation times is improved from $\sim 1/a^6$ to $1/a^2$ (but the coefficient is still large).
- **How** do open boundary conditions work?
  A: Topological charge moves in from the boundary via diffusion.

Q: Is the diffusion coefficient universal across lattice gauge actions?
Q: Are there algorithms with better diffusion coefficients?

Backup slides

Boundary vs bulk

Physics is not the same between periodic and open BC's in the boundary regions. Comparisons should only be done in the bulk.



Diffusion with open boundaries

$$C(t, t_0, \tau) = \langle Q_{\text{slice}}(t, \tau) Q_{\text{slice}}(t_0, 0) \rangle$$

$C(t, t_0, \tau) = 0$ if t or t_0 at a boundary.

Diffusion coefficient D is a actually a function of t near the boundaries: