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Moving topological charge over the Great Wall in the HMC algorithm

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With highly improved lattice actions and increasing lattice sizes the problem of accurate sampling of the topological sectors of the QCD vacuum has become more difficult. A possible solution is presented which enhances the appearance of a hypercube sized dislocation in a controlled manner. This dislocation can then grow into a topology changing instanton. The effect of this perturbation of the lattice action is removed in measurements by adjusting the Boltzman weight by an appropriate reweighting factor. The method and initial tests are discussed.

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1. The problem with improved actions

The 21st century has seen exciting advances in lattice gauge theory, both in terms of computing power, which has allowed simulations with very large (Vol. $\sim 100^4$) lattices, as well as the development of highly improved actions which suppress lattice artifacts and produce smooth fields. However a drawback of these developments is that they suppress configurations which tunnel between topological sectors of the QCD vacuum, so that the autocorrelation (in monte carlo time) of the topological charge becomes extremely long, or in some cases such as domain wall fermions, infinite. These simulations then effectively sit in one topological sector. While new instantons still appear and disappear they occur mostly in +/- pairs such that the net topological charge does not change.

The root of this problem is that lattice simulations use fixed boundary conditions so that, in principle, the topology of the gauge field is fixed. In practice, instantons can appear on the lattice via a singular configuration (or a smooth configuration with a singular gauge transformation)—a *dislocation*. If this singularity is located in the interior of a hypercube, the links of the lattice gauge field will be finite, but the periodic configuration will have non-zero topological charge. In a monte carlo update with say, the Wilson gauge action, these objects are easily generated, and facilitate tunneling between topological vacua. Improved actions and reduced lattice spacings suppress the occurance of local singularities in the gauge field configuration and thus reduce the occurance of these objects.

There are three main approaches to dealing with this problem:

1. Ignore the issue, as is done widely.
2. Understand the effect of fixed topology on simulations;
   for example, [1] and [2].
3. Develop new updating algorithms which overcome the problem
   as in [3] and [4].

2. A modest proposal

In [5] a method was introduced which addressed this issue in two dimensional QED, the Schwinger Model. The difference between the topological transition rate with and without this modification is shown in Figure 2. As can be seen, the algorithm was quite effective in 2-D QED.

The algorithm[1] works as follows. We wish to enhance the possibility of tunneling to a different topological sector of the vacuum by the appearance of an ultralocal gauge object. Since tunneling is achieved via configurations with non-zero topological charge, we construct an algorith which increases the likelihood of a hypercube (plaquette in the case of 2D QED) that carries topological charge 1/2. Other fluctuations of in the gauge field will move the configuration over the barrier or perhaps not, randomly.

Since topological charge in 2D QED is simply $Q = 1/2\pi \int dx^2 F_{\mu\nu}$, we want to induce a *sphaeleron* ($Q = 1/2$) configuration which has all (or most) of its charge density, $q(x) = F_{\mu\nu} \sim \pi$

[1] the idea was that of Ph. de Forcrand

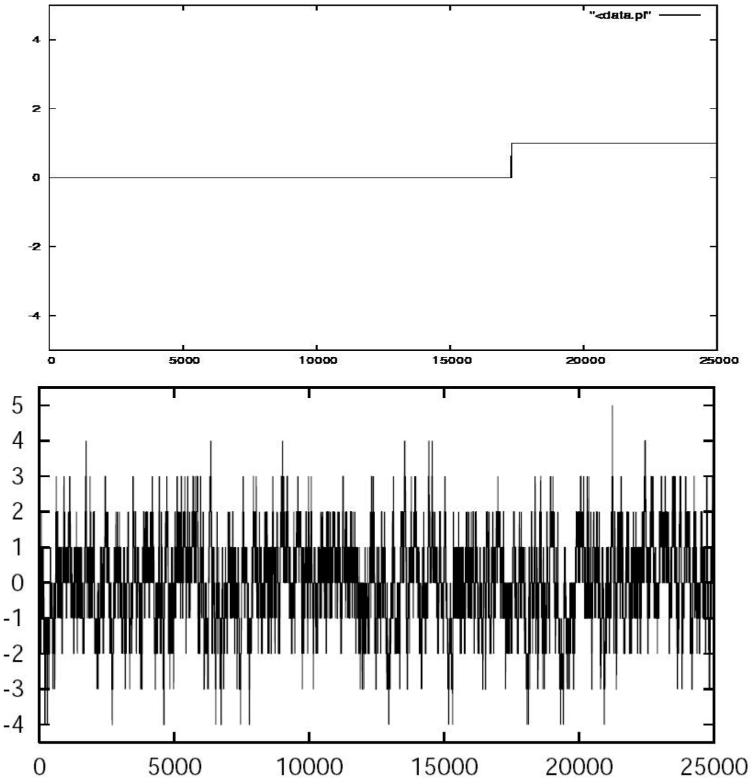

Figure 1: Top: Normal updates with R-algorithm updates, Bottom: Updating with modified action

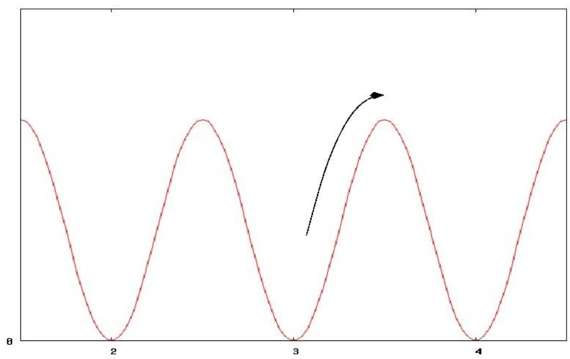

Figure 2: Move the configuration halfway to the next topological sector

at one site. Such a plaquette has links which "wrap" halfway around the group manifold of U(1) as shown below.

This is accomplished by modifying the gauge action $S = S_g + \Delta S$

$$\Delta S = -\sum_x \alpha \exp\left[-\frac{(\ |F_{\mu\nu}(x)| - \pi\ )^2}{2\theta_0^2}\right] \delta_{x,x_0} \tag{2.1}$$

where α and θ_0 are constants. x_0 is the site where the plaquette angle is *already* closest to π. This

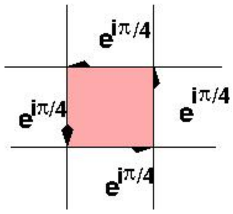

Figure 3: A half-winding plaquette configuration in 2D QED.

then, enhances–in a controlled way–the probability that the already-largest plaquette increases to become a $|Q| = 1/2$ site.

This modification to the action is compensated by reweighting observables to remove the modification to the Yang-Mills action.

$$\langle \mathscr{O} \rangle_{\text{corrected}} = \left\langle \mathscr{O} e^{\beta \Delta S} \right\rangle$$

Detailed Balance

While x_0 may vary from one configuration to the next, the prescription assigns a unique action to each configuration. Suppose we start from configuration A with maximum plaquette is at x_a. The update evolves to configuration B whose maximum plaquette is at x_b, The intermediate momenta at the midpoint, $p(A)$, are functions of the coordinates A. The update in Monte Carlo time, t, looks like this:

$$\begin{array}{ccccc} A, x_a & \rightarrow & p(A) & \rightarrow & B, x_b \\ t = 0 & & t = 1/2 & & t = 1 \end{array}$$

Starting from B and reversing Monte Carlo time looks like this:

$$\begin{array}{ccccc} A, x_a & \leftarrow & p(B) & \leftarrow & B, x_b \\ t = 0 & & t = 1/2 & & t = 1 \end{array}$$

Again, reversing the momenta at $t = 1/2$ returns the configuration to its starting place, B. Thus the molecular dynamics is reversible. As long as the integration method of the Hybrid Monte Carlo update uses a midpoint velocity method (as does the Leap Frog and most other intergrators), this procedure leads to reversible molecular dynamics ensuring detailed balance.

The procedure enhances a local lattice artefact, which acts like a “saddle point” between topological sectors

3. Generalization to SU(N)

In 2D-QED, defining a single plaquette whose links wind halfway around gauge group, $U(1)$, is straightforward; an example is shown in Fig. 3). The comparison of the topological charge densities between 2D-U(1) and 4D-SU(N) gauge theories,

2D-U(1)	4D-SU(N)
$q(x) = F_{\mu\nu}(x)$	$q(x) = F_{\mu\nu}\tilde{F}_{\mu\nu}(x)$
$Q = \frac{1}{2\pi}\int dx^2 F_{\mu\nu}$	$Q = \frac{1}{32\pi^2}\int dx^4 F_{\mu\nu}\tilde{F}_{\mu\nu}(x)$

Leads to the following non-Abelian generalization of ΔS from eq. 2.1 valid for SU(N).

$$\Delta S = -\sum_x \alpha \exp\left[-\frac{(\ |q(x)| - 16\pi^2\ )^2}{2\theta_0^2}\right] \delta_{x,x_0} \tag{3.1}$$

The next issue is what operator to choose for $q(x)$. Since we want a very local object to be induced, we should not use a sophisticated definition which extends beyond a hypercube. The original "twisted plaquette" definition of $q(x)$, a straightforward transcription of $F_{\mu\nu}\tilde{F}_{\mu\nu}(x)$ with plaquettes, Ref. [6], is based at a lattice site as shown in Fig. 4. While this operator might work

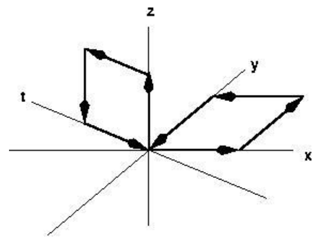

Figure 4: Site-centered topological charge density represented by the "twisted plaquette" of Ref. [6].

(it was not tested in this study), we seek an operator centered on the dual lattice whose boundary is a hypercube, analogous to the method used in 2D-QED. Such a hypercubic topological charge density operator was used by Vecchia, Fabricius, Rossi, and Veneziano in [7] and is defined by

$$q(x) = \sum_{p=1}^{48} (-1)^p W_p, \qquad p = \text{perm}(\hat{x}, \hat{y}, \hat{z}, \hat{t}). \tag{3.2}$$

W_p is an eight link Wilson loop that winds around the hypercube, changing direction at each site according to a permutation of the directions $\hat{x}, \hat{y}, \hat{z}, \hat{t}$ for the first four links, with the same directions for the last four links. One of the 48 W_p is shown schematically in Fig. 5.

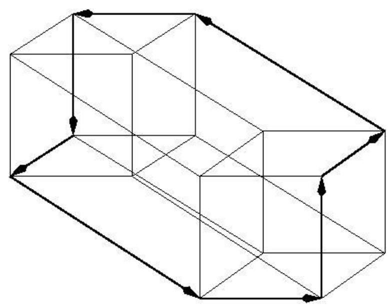

Figure 5: An example path contribution from the hypercube-centered topological charge density of Ref. [6].

With the addition of ΔS in eq. 3.1 to the action, the Hybrid Monte Carlo update of links is as usual, except for links which are part of the hypercube H_0 at x_0 which has the maximum absolute value of topological charge density, $|q(x)|$. Links that are part of this hypercube have an additional "force" coming from ΔS

$$\frac{\partial \Delta S}{\partial U_\mu(x)} = 2\alpha[|q(x)| - 16\pi^2]\exp\left\{-\frac{[\,|q(x)| - 16\pi^2\,]^2}{2\theta_0^2}\right\} \times \left.\frac{\partial |q(x)|}{\partial U_\mu}\right|_{\mathbf{x}\in\mathbf{H_0}}. \tag{3.3}$$

In addition to the usual staples, the gauge force at these sites has 7-linkstaples from the boundary of the maximal $q(x)$ hypercube. An example of one of these contributions to the update of the red link is shown below in green in Fig. 6.

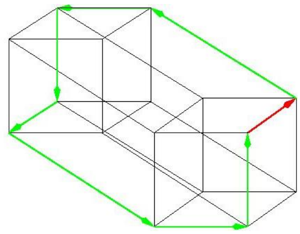

Figure 6: One of the "extra staples" contributing to the gauge force in the HMC update of the link shown in red. These staples are only added to the update for links in the hypercube with maximal topological charge density at x_0.

A summary of the update algorithm is as follows.

- Compute the topological charge density, $q(x)$, as defined in eq. 3.2.
- Find the hypercube with has maximal $|q(x)|$. This defines x_0, the base site of the maximal hypercube H_0.
- Update links as usual via HMC algoritm. For links which are part of H_0, the gauge force has an additional contributuions as shown in eq. 3.3 and Fig. 3.

4. Tests

Tests of this algorithm are underway, with two observations so far. First, the non-Abelian HMC algorithm *does* enhance the probability that some hypercube has increased topological charge density. This is shown in (the admittedly, busy) Fig. 7. What is shown is the maximal topological charge at hypercube H_0 versus update sequence number for 100 updates. Increasing the value of α in eq. 3.1, the weight of ΔS, from 10^3 to 10^5 increases $|q(x)|_{\max}$. The average value of $|q(x)|_{\max}$ for 100 updates is shown as a horizontal line. Red: $\alpha = 10^3$, Green: $\alpha = 10^4$, and Blue: $\alpha = 10^5$.

The second observation is that the algorithm seems to be rather sensitive the both the parameters α, and θ_0 in ΔS. In many cases, updates do not thermalize the configurations. In 2D-QED this sensitivity was mild; in that case, a configuration with small $q(x)$ has a $\Delta S \sim \exp(\pi) = 20$, for generic $\alpha = 1$ and $\theta_0 = 1/2$. In the non-Abelian case however, a smooth configuration ($q(x) \sim 0$) gives a $\Delta S \sim \exp(16\pi^2) = e^{158} \sim 10^{68}$. Thus, other functional forms of ΔS which enhance a hypercubic dislocation but are not so strongly peaked need to be explored.

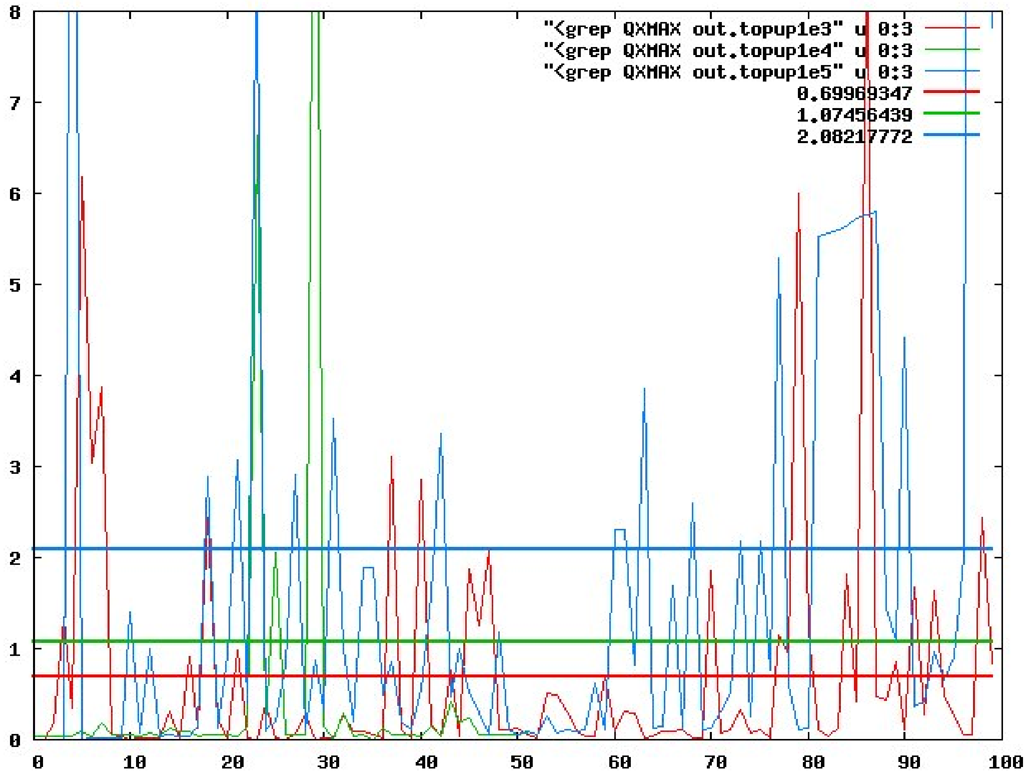

Figure 7: The maximal topological charge versus update. Increasing the value of α in ΔS from 10^3 to 10^5 increases $|q(x)|_{\max}$. The average value of $|q(x)|_{\max}$ for 100 updates is shown as a horizontal line. Red: $\alpha = 10^3$, Green: $\alpha = 10^4$, and Blue: $\alpha = 10^5$.

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