Estimating $\chi_{\text{top}}$ Lattice Artifacts from Flowed SU(2) Calorons

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Abstract: We consider calorons on the lattice under different types of gradient flow. We identify the amount of gradient flow required to “collapse” calorons as a function of their initial size and the type of gradient flow, and we estimate the severity of $a^2$ corrections as a function of gradient flow depth when computing the topological susceptibility at high temperatures.
1 Introduction

Ever since the discovery of instantons in non-abelian gauge theories more than 40 years ago [1, 2], a lot of work has been devoted to these mysterious objects. They are believed to play a fundamental role in QCD. In the context of chiral symmetry breaking, the Banks-Casher relation [3] establishes a connection between the order parameter of spontaneous symmetry breaking and the mean-squared fluctuations of the topological charge. Phenomenological motivations have been found in the past related to the $\eta - \eta'$ mass difference through the Witten-Veneziano formula [4, 5]. Indeed, instantons may play a rather broad role in the infrared dynamics of QCD [6].

Another place where instantons are relevant is in the strong CP problem. The QCD vacuum may contain a CP violating phase $\Theta_{\text{QCD}}$ which plays a physical role only because of instantons [7, 8]. Peccei and Quinn showed that additional degrees of freedom may eliminate this problem [9]. But again, the properties of the new particle, the axion [10, 11], are sensitive to the topological susceptibility. Of special note is the possibility that the axion plays the role of the dark matter of the Universe [12–14]. In this case, besides the now rather well-determined [15] value of the topological susceptibility in vacuum, we also
need the topological susceptibility in the temperature range $3 T_c - 7 T_c$ [16, 17], which has recently become the topic of intense investigation [18–24]. (For a recent review of the axion see Ref. [25].)

An instanton is defined as the minimum-action gauge configuration which carries unit topological charge $Q = 1$, defined as

$$Q \equiv \frac{1}{32\pi^2} \int d^4x F_{\mu\nu}^a(x) \tilde{F}^{\mu\nu}_a(x), \quad \tilde{F}^{\mu\nu}_a \equiv \frac{1}{2} \epsilon^{\mu\nu\rho\sigma} F_{a \rho\sigma}(x).$$

(1.1)

By the triangle inequality $|F \tilde{F}| \leq F^2$, so (anti)instantons are (anti)self-dual solutions, $F_{\mu\nu} = \pm \tilde{F}_{\mu\nu}$, which also ensures that they are classical in the sense that they obey the equation of motion $D_\nu F^{\mu\nu} = 0$. In SU(2), BPST instantons [1] are described by a single length parameter $\rho$ which is a measure of its size. At the classical level the action is size independent,

$$S(\rho) = 8\pi^2 |Q|/g^2,$$

(1.2)

but because the coupling runs with scale, instantons are expected to be most important in the infrared, where the theory becomes nonperturbative [26]. Therefore, a lattice approach seems ideal to investigate topological configurations and indeed a lot of studies have been performed in the past (see for instance Ref. [6] for an extensive review on the subject). Unfortunately, the lattice introduces its own limitations.

Strictly speaking, there is no perfectly clean and unambiguous definition for topology on the lattice. After all, on a compact space without boundary, topology partitions the space of smooth continuum configurations into path-disconnected subspaces with different integer $Q$ values. But the space of lattice configurations is $[SU(N)]^{N_\ell}$ (with $N_\ell$ the number of lattice links), which is path connected, precluding a continuous and integer definition of $Q$. This problem has long been appreciated; Lüscher showed that topology becomes well defined if we restrict to sufficiently “smooth” lattice configurations, in the sense that all plaquettes are suitably close to the identity [27]. That means that the failure for a perfectly clean definition of topology on the lattice lies with certain very non-smooth configurations, termed “dislocations.” These configurations have no good continuum limit and should be thought of, roughly, as representing instantons which are of order one lattice spacing across. Such configurations are necessary and relevant because lattice Markov chain procedures generally explore the configuration space in a continuous way and must pass through dislocations to explore multiple $Q$ value sectors. On the other hand, we need that dislocations become rare in the continuum limit so that almost all configurations have a well defined $Q$ and the continuum limit of the topological susceptibility is well defined. Therefore, the smaller the lattice spacing, the more difficult it is to move between topological sectors, and the more difficult it becomes to sample topological sectors with good statistical power. This makes the sampling of topology at fine lattice spacings problematic in a compact space without boundary.

A modern tool for studying topology on the lattice is the integration of a lattice discretized version of $Q$ after the lattice fields have been subjected to gradient flow [28, 29]. This definition has its roots in older studies employing cooling [30–33], with gradient flow representing a better-controlled and better-understood form of gauge-link cooling. With
gradient flow, a well-defined parameter $t$ controls the extent of smearing applied. The
gradient flow tends to eliminate dislocations [34], but since there is no clean distinction
between dislocations and small-but-physical instantons, it may also destroy the smallest
instantons which we want to keep. In this paper we shall explore this issue in more detail,
studying exactly how much gradient flow destroys exactly what size of BPST instantons
[1] and Harrington-Shepard calorons [35]. This requires a lattice implementation of the
colonon, which we supply. We also explore different implementations of flow; Wilson flow
[29], a recently proposed $O(a^2)$-improved flow dubbed Zeuthen flow [36], and an “overim-
proved” flow in which we force the $a^2$ errors in the flow action to have the opposite sign
as in Wilson flow. We are hardly the first to implement calorons on the lattice [37, 38] or
to consider topology after cooling [31–33]. But our emphasis is a little different; we want
to understand and control what size of dislocation/caloron survives what amount of flow,
and what impact this may have on the determination of topological susceptibility at finite
lattice spacing.

Once we know the rate at which calorons are destroyed for the different flow types
as a function of the flow time $t$, we use this information to provide an estimate of how
lattice artifacts affect the calculation of the topological susceptibility at high temperatures.
Discretization effects will in general modify the density of calorons; for the Wilson action,
small-radius calorons are enhanced (as we show explicitly). We therefore study the fraction
of calorons that is being flowed away and more importantly, we make a statement about
their contribution to the topological susceptibility, providing an example study at $T = 4 T_c$.
This helps estimate what lattice spacing will be needed to be in the scaling regime where
a continuum extrapolation can be attempted.

The paper is structured as follows: In Sec. 2 we collect our definitions and define
our topology configurations. Sec. 3 then introduces the different flows and flow actions.
In Sec. 4 we show our results and Sec. 5 addresses an application of our results to the
topological susceptibility at high temperatures. Our conclusions can then be found in
Sec. 6.

## 2 Instanton and Caloron Discretizations

Nothing in this section is really new, but we include it to make our presentation self-
contained. Readers well familiar with instantons and calorons can skip to the next section.

Instantons are defined as those Euclidean solutions of the Yang-Mills equation of mo-
motion $D^\mu F_{\mu\nu} = 0$ that satisfy the self-duality condition

$$ F_{\mu\nu} = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} F_{\rho\sigma}, $$

(2.1)

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]$ is the usual field-strength tensor, $A_\mu(x) = A_\mu^a(x) T^a$
with $T^a$ the anti-hermitian algebra generators of SU($N$) satisfying $\text{tr}[T^a T^b] = -\frac{1}{2} \delta^{ab}$, and
$D_\mu = \partial_\mu + [A_\mu, \cdot]$ is the covariant derivative. Concentrating on SU(2) instantons, the gauge
field continuum form is best derived from a scalar superpotential $\Phi(x)$ [39] as

$$ A_\mu^a(x) = \eta_{a\mu\nu} \partial_\nu \ln \Phi(x), $$

(2.2)
where \( \eta_{\alpha\mu\nu} = \epsilon_{0\alpha\mu\nu} + \delta_{\alpha\mu}\delta_{\nu0} - \delta_{\alpha\nu}\delta_{\mu0} \) is the 't Hooft symbol (equivalently for \( \bar{\eta}_{\alpha\mu\nu} \) the sign of the last two terms is reversed and one obtains an anti-instanton with \( Q = -1 \)) [2]. The self-duality condition implies that a valid solution for \( A_\mu(x) \) is obtained if \( \Phi(x) \) obeys the Poisson equation \( \Box \Phi = 0 \). The specific form of \( \Phi(x) \) is now needed to obtain instanton and caloron continuum expressions with topological charge \( Q \).

### 2.1 BPST Lattice Instanton with \( Q = 1 \)

't Hooft's solution for the BPST instanton reads

\[
\Phi_{\text{BPST}}(x) = 1 + \frac{\rho^2}{(x-z)^2}, \tag{2.3}
\]

where \( \rho \) has length-units and will be playing the role of the instanton radius. The position of the instanton is defined through a Lorentz vector \( z \). Using Eq. (2.2), one readily obtains

\[
A_\mu^a(x) = -\frac{2\rho^2}{(x-z)^2} \eta_{\alpha\mu\nu}(x-z)_\nu \tag{2.4}
\]

It is a straightforward exercise to check that indeed this gauge field yields \( Q = 1 \) and \( S = 8\pi^2 \). Notice that it is given in singular gauge, meaning that there is a singularity at the center of the instanton\(^1\) when \( x = z \). Next, we use the path-ordered exponential map to obtain the expression for the lattice links as

\[
U_\mu(x) = \mathcal{P} \exp \left[ a \int_0^1 \, dt \, A_\mu(\Gamma_\mu(x,t)) \right], \tag{2.5}
\]

where \( \Gamma_\mu(x,t) = x + ta\hat{\mu} \) is an appropriate parameterization for the corresponding path connecting the two neighboring lattice sites \( x \) and \( x + a\hat{\mu} \) with \( t \in [0,1] \) (no summation over \( \mu \) is implied in Eq. (2.5)). All gauge fields along the path in a given direction commute with each other: \( [A_\mu(\Gamma_\mu(x,t)), A_\mu(\Gamma_\mu(x,t'))] = 0 \) \( \forall t, t', x, \mu \). Therefore, the path-ordered exponential can be done exactly by simply performing the integral analytically and exponentiating the result. Finally, we apply periodic boundary conditions at the boundaries of the lattice. The discontinuities caused by this are minimized by our use of singular gauge, but we will nevertheless need to smooth out the boundary behavior, cf. Subsec. 4.1.

### 2.2 Harrington-Shepard Lattice Caloron with \( Q = 1 \)

A natural extension of Eq. (2.3) for \( n \) pseudo particles with parameters \( \rho_k \) and positions \( z_k \) reads

\[
\Phi(x) = 1 + \sum_{k=1}^n \frac{\rho_k^2}{(x-z_k)^2}. \tag{2.6}
\]

The Harrington-Shepard caloron [35] can be understood as the finite temperature generalization of the BPST instanton. The most straightforward way of constructing the solution is to recognize that we have to take into account the infinite time copies that arise due to

\(^1\)On the lattice, we will avoid the singularity by placing our topology objects in between lattice points and unless stated otherwise we always consider \( z = (z_0, \vec{z}) = \frac{1}{2}(\beta - a, L - a) \).
the compactification of the Euclidean time direction whose inverse length plays the role of
temperature ($\beta \equiv T^{-1}$). We consider therefore a specific case of Eq. (2.6) for which we ask
for $\rho_k \equiv \rho$ and $z_k = (z_0 + k\beta, \vec{z})$ and obtain [35]

$$\Phi_{HS}(x) = 1 + \sum_{k \in \mathbb{Z}} \frac{\rho^2}{(x - z_k)^2} = 1 + \frac{\pi \rho^2 \sinh \frac{2\pi |\vec{x} - \vec{z}|}{\beta}}{\frac{1}{\beta} |\vec{x} - \vec{z}| \left( \cosh \frac{2\pi |\vec{x} - \vec{z}|}{\beta} - \cos \frac{2\pi (x_0 - z_0)}{\beta} \right)}.$$  (2.7)

It is straightforward to check that

$$\lim_{\beta \to \infty} \Phi_{HS}(x) = \Phi_{BPST}(x).$$  (2.8)

A simple evaluation of Eq. (2.2) with $\Phi(x) = \Phi_{HS}(x)$ yields the continuum HS caloron
gauge field in singular gauge whose analytic expression we do not reproduce here. Links
are obtained in a similar way. At finite temperature, however, the gauge fields along the
path of a link do not commute with each other and the path ordering is crucial. The reason
is that not all directions are treated democratically due to the loss of Lorentz invariance.
A systematically improvable way of solving this is to divide the path in $n$ subintervals and
evaluate the integrand at the midpoints numerically. In this way, Eq. (2.5) turns into the
limit

$$U_\mu(x) = \lim_{n \to \infty} \mathcal{P} \prod_{k=1}^n \exp \left[ \frac{\alpha_n}{n} A_\mu(\Gamma_\mu(x, 2k-1/2n)) \right].$$  (2.9)

The only approximation here comes from the truncation of the product by not considering
intervals finer than $1/n$. Since the setup of this configuration is very cheap, we can afford
big values of $n \sim 40$ with negligible round-off errors.

Finally the embedding into an SU(3) background is trivial since a particular lattice
gauge exists in which the links take the following form:

$$U_\mu^{SU(3)} = \begin{pmatrix} U_\mu^{SU(2)} \\ 0 \\ 0 \\ 1 \end{pmatrix}. \quad (2.10)$$

Therefore we are effectively considering SU(2) configurations in this paper. This makes our
study less general than Ref. [37], who also consider calorons in the background of nontrivial
holonomy. Note however that if we are primarily interested in high temperatures, nontrivial
holonomy is not likely to be relevant, since fluctuations create an effective potential for the
Polyakov loop which favors trivial holonomy.

3 Gradient Flows

Gradient flow and its discretized version on the lattice [28, 29, 40–43] have become an
essential tool to reduce UV fluctuations. In the continuum it defines a mapping of the
gauge fields $A_\mu(x)$ to smeared gauge fields $B_\mu(x, t)$, where $t$ is the so-called flow time, via
the flow equation

$$\partial_t B_\mu = D_\nu F_{\nu\mu}, \quad B_\mu(x, 0) = A_\mu(x).$$  (3.1)
The right-hand side of this differential equation is nothing but the classical equations of motion. Consequently, it will drive the gauge field along the trajectory of steepest descent minimizing the action along the way. On the lattice the simplest form reads

\[ a^2 \partial_t V_\mu(x, t) = -g_0^2 \partial_{x, \mu} S_W[V] V_\mu(x, t), \]  

where \( V_\mu(x, t) \) is the flowed gauge field with initial condition \( V_\mu(x, 0) = U_\mu(x) \) and \( S_W \) denotes the Wilson plaquette action. The Lie-algebra valued derivative of a general function of the link variables \( f(U_\mu) \) is given by

\[ \partial^a_{x, \mu} f(U_\mu(x)) = T^a d \frac{d}{ds} f(e^{sT^a U_\mu(x)}) \bigg|_{s=0}. \]  

Recently, an \( O(a^2) \) improved version of the flow equation was developed in Ref. [36]. The so-called Zeuthen flow equation reads

\[ a^2 \partial_t V_\mu(x, t) = -g_0^2 \left( 1 + \frac{a^2}{12} \nabla^* \nabla \right) \partial_{x, \mu} S_{\text{Sym}}[V] V_\mu(x, t), \]  

where \( S_{\text{Sym}} \) is the tree-level improved Symanzik action [44] and the discretized adjoint covariant derivative is given by

\[
\begin{align*}
    a \nabla_\mu f(x) &= U_\mu(x) f(x + a \hat{\mu}) U^\dagger_\mu(x) - f(x), \\
    a \nabla^*_\mu f(x) &= f(x) - U^\dagger_\mu(x - a \hat{\mu}) f(x - a \hat{\mu}) U_\mu(x - a \hat{\mu}).
\end{align*}
\]  

The unexpected additional factor \( (1 + a^2 \nabla^*_\mu \nabla^{\mu} / 12) \) can be understood as follows. We know that improvement requires replacing square plaquettes with a linear combination of squares and rectangles. The Symanzik action does this in the four spacetime directions. The added term does it in the flow-time direction. Ref. [36] have proven that this gives a (tree-level) \( O(a^2) \) improvement of the flow equation. In addition to these two we investigate a flow equation with an overimproved action (precise definitions of these actions are given in Subsec. 4.2)

\[ a^2 \partial_t V_\mu(x, t) = -g_0^2 (\partial_{x, \mu} S_{\text{OI}}[V]) V_\mu(x, t), \]  

We expect this flow equation to allow for stable topological solutions under flow.

The goal is to study the effect of Eqs. (3.2), (3.4), and (3.6) on our constructed clean topological configurations to learn about how their topological properties are changed. This can represent interesting information to better control systematic errors when performing lattice calculations of topological observables with the help of flow.

4 Lattice Caloron and Instanton Properties

Mainly we will focus on the measurement of the topological charge \( Q \) and the action \( S \) which in the continuum take the values \( Q = 1 \) and \( S = 8\pi^2 \), respectively. Deviations from these numbers occur on a finite lattice due to cutoff and boundary effects. We will try to disentangle those and reduce them as much as possible to more deeply understand the effect of flow.
4.1 Caloron vs. Instanton

First of all, it is interesting to check whether the caloron and instanton implementations work as expected. Notice that boundary effects coming from the spatial directions are unavoidable and need special treatment; otherwise our results will suffer tremendously. In order to reduce them as much as possible, we “flow the boundaries away.” What this means is that we perform a space-time dependent flow where the core of the configuration (where most of the topological charge is localized) is unaffected while boundary effects are smoothed out. A similar idea was used in Ref. [32] where a discretized version of $D_\mu F_{\mu\nu}(x)$ was measured on every space-time point and an improved form of cooling was performed on those lattice points that satisfied the bound $D_\mu F_{\mu\nu}(x) > \epsilon$. In App. B we explain our own procedure for reducing boundary effects which we utilize throughout this work. Note that we do not smooth the time periodic surface for instantons, meaning that we will see the damage from the lack of time periodicity in the instanton solution. From now on, when setting up a topological configuration, we always implicitly apply this procedure. Note that the gradient flow used to reduce the boundary effects should not be confused with the usual gradient flow that we apply for some calculations in the remainder of this work.

![Figure 1](image1.png)

**Figure 1**: Left: Topological charge for caloron and instanton as a function of the radius $\rho$. Right: Caloron and instanton Wilson actions. Both instanton and caloron are placed at the center of an $8 \times 32^3$ lattice.

In Fig. 1 we show how temperature effects are fully taken into account in the case of the caloron while instantons suffer from temperature corrections as soon as $\rho/\beta \gtrsim 1/4$. The right panel shows that the Wilson action starts small for small values of the radius, and is suppressed until about $\rho = 1.5a$. Therefore this is about the scale where we should switch from considering the configurations as dislocations to thinking of them as small instantons. Above this size, the topological charge for the caloron plateaus to 1 while the instanton rapidly drops due to boundary effects in the temperature direction.
4.2 Actions

Throughout this work we consider Lüscher-Weisz actions of the form [44, 45]

\[ S(c_0, c_1) = \frac{2}{g_0} \left( c_0 \sum_x \text{Re} \, \text{tr}(1 - U_P(x)(1,1)) + c_1 \sum_x \text{Re} \, \text{tr}(1 - U_R(x)(2,1)) \right), \]  

(4.1)

where \( U_P(x)(1,1) \) denotes the simple closed plaquette and \( U_R(x)(2,1) \) are \( 2 \times 1 \) (and \( 1 \times 2 \)) rectangles where both loop orientations are taken into account by the \( \text{Re} \, \text{tr} \) operation. A correct normalization requires \( c_0 + 8c_1 = 1 \). The three actions going into the three different flow equations can be summarized as follows:

\[
\begin{align*}
S(1, 0) &= S_W \quad \text{(Wilson),} \\
S(5/3, -1/12) &= S_{\text{Sym}} \quad \text{(Symanzik),} \\
S(7/3, -1/6) &= S_{\text{OI}} \quad \text{(Overimproved).}
\end{align*}
\]

(4.2)

From Fig. 2 one sees that all actions start small and rapidly rise towards a value of \( 8\pi^2 \). We also show an estimate, based on expanding Eq. (4.2) in operator dimension and evaluating the first non-vanishing high-dimension correction in the caloron background, see App. A. This estimate works well in a range \( 1.0 \lesssim \rho/a \lesssim 3.0 \). Beyond this value, finite-volume boundary effects become larger than \( a^2 \) effects, despite our attempts to reduce them as explained in App. B. The overimproved action possesses positive \( a^2 \) corrections and therefore develops a maximum. This will be of importance when flowing with this action as it will stabilize calorons larger than the size where \( S \) is maximum, preventing them from shrinking, “falling through the lattice,” and being lost.

4.3 Topological Charges

The field-strength tensor \( F_{\mu\nu}(x) \) is the main building block for constructing gauge operators like the topological charge (cf. Eq. (1.1)). Apart from the popular geometrical clover definition (4-plaquette average), we considered an improved version thereof. To this end, we implement an improved field-strength tensor \( \hat{F}^{\text{imp}}_{\mu\nu} \) free of \( O(a^2) \) errors by considering weighted averages of \( 1 \times 1 \) plaquettes and \( 2 \times 1 \) rectangles [47, 48].

We then study the two definitions

\[ Q_{\text{clov/imp}} = -\frac{1}{16\pi^2} \epsilon_{\mu\nu\rho\sigma} \sum_x \text{tr} \left( \hat{F}^\text{clov}_{\mu\nu}(x) \hat{F}^\text{clov}_{\rho\sigma}(x) \right), \]  

(4.3)

where in each case

\[ \begin{align*}
\hat{F}^\text{clov}_{\mu\nu}(x) &= F_{\mu\nu}(x) + O(a^2), \\
\hat{F}^\text{imp}_{\mu\nu}(x) &= F_{\mu\nu}(x) + O(a^4).
\end{align*} \]

(4.4)

As can be seen from Fig. 3, the improved topological charge operator shows a much better behavior at all investigated values of the radius. Notice that boundary effects are milder for the topological charge than for the action. We see only advantages to using the improved definition.
4.4 Critical Radius

One of the relevant aspects we want to address in this paper is the behavior of a discretized caloron configuration under different flow equations. We consider an object to be topological if $Q_{\text{imp}} > 0.5$, and therefore define the critical radius of a caloron where it becomes topological as

$$Q_{\text{imp}}(\rho_{\text{crit}}) \equiv 0.5. \quad (4.5)$$

We can then study how flow causes calorons to shrink and disappear by investigating $\rho_{\text{crit}}$ as a function of flow time, that is, what initial caloron radii $\rho$ still have $Q_{\text{imp}} > 0.5$ after some flow depth $t$. This is shown in Fig. 4, which can be used to look up how much flow is needed to collapse calorons of a given size. Fig. 2 shows the energy contour along which the configuration should flow. An ordinary perturbative fluctuation decays as $\exp(-\rho^2 t)$, and so doubling the size requires four times the flow time, or $t \propto \rho^2$. However, the calorons are nearly extrema of the action, up to $a^2/\rho^2$ corrections in the Wilson action, so we expect $t \propto \rho_{\text{crit}}^2$. Therefore Fig. 4 plots $\rho_{\text{crit}}$ against $t^{1/4}$, which would be a straight line for $a \ll \rho \ll \beta$. The figure shows that calorons also collapse under Zeuthen flow, though more slowly (as the energy depends on scale only at $O(a^4)$, we would expect $t \propto \rho_{\text{crit}}^6$).
Figure 3: Two different discretizations of the topological charge operator as a function of the caloron size \( \rho \), on an \( 8 \times 32^3 \) lattice.

Figure 4: Critical caloron radius (separating calorons which survive from those which collapse) as a function of flow depth for three types of flow, and three different temporal lattice extents. In this plot we keep \( L/a = 32 \) fixed. Left: Wilson and overimproved flow. Right: Zeuthen flow.

and that they are preserved above some critical size \( \rho \approx 1.8a \) under overimproved flow, which was the original motivation for considering overimproved smearing [46]. The figure
also shows that finite box size effects accelerate the collapse of calorons, but the flow times where this becomes a factor are quite large for the box sizes we consider.

Another way of viewing this collapse process is to plot $Q_{\text{imp}}$ as a function of flow time for a fixed initial caloron size, see Fig. 5. For Wilson flow, the $a^2$ corrections are the main reason the caloron collapses. For Zeuthen flow the much smaller $a^4$ effects are subdominant to volume effects for the case considered here. For overimproved flow, the action maximum of Fig. 2 protects the caloron from ever collapsing.

5 Application: Estimated $a^2$ Errors in the Topological Susceptibility

As an application, we estimate the effects of $a^2$ errors in the action and of different flow depths for evaluating the instanton density at a relatively high temperature $T = 4 T_c$. To do so, we incorporate the known one-loop renormalization contributions to the caloron [26], and estimate the topological susceptibility by integrating over all instanton sizes. In the continuum this quantity is given by

$$\chi^{(T/T_c)} \simeq 2 \int_{0}^{1/\Lambda_{\text{MS}}^{N_f=0}} d\rho D(\rho)G(\pi \rho T)$$ (5.1)

with

$$D(\rho) = \frac{d_{\text{MS}}}{\rho^3} \left( \frac{8\pi^2}{g^2(\mu = \rho^{-1})} \right)^6 \exp \left( -\frac{8\pi^2}{g^2(\mu = \rho^{-1})} \right)$$ (5.2)
the vacuum density of instantons with size $\rho$, and

$$G(\lambda) = \exp(-2\lambda^2 - 18A(\lambda)), \quad (5.3)$$

$$A(\lambda) = -\frac{1}{12} \ln\left(1 + \frac{\lambda^2}{3}\right) + \alpha \left(1 + \gamma \lambda^{\frac{3}{2}}\right)^{-8} \quad (5.4)$$

the thermal corrections, first computed by Gross, Pisarski, and Yaffe [26]. The parameter values in these expressions are $\alpha = 0.0128974$, $\gamma = 0.15858$, and $d_{\text{MS}} = \frac{\alpha}{4\pi} = -4.534122$. The running of the coupling $g^2(\mu)$ can be found in Ref. [49] and $T_c/\Lambda_{\text{MS}}^{N_f=0} = 1.26$ is taken from Ref. [50]. The product of $D(\rho)$ and of $G(\pi \rho T)$ in Eq. (5.1) leads to an integrand with a broad peak near $\rho T = 0.4$ (see Fig. 6), which is then the typical size for the calorons which dominate the topological susceptibility.

We introduce $a^2$ corrections by replacing the continuum caloron action with the $a^2$-corrected value we found in Eq. (A.3):

$$D_{\text{lat}}(\rho, T/T_c, N_\tau) = D(\rho) \exp\left[-\frac{8\pi^2}{g^2(\mu = \rho^{-1})} \left(1 + \frac{1}{\rho T N_\tau}\right)^2 F\left(\frac{1}{\rho T}\right)\right]. \quad (5.5)$$

That is, we estimate the $a^2$ errors to be dominated by the $a^2$ corrections to the caloron action ($F$ is computed in the appendix.) This makes an assumption – that the SU(2) caloron we have found here has the same $a^2$ corrections as the more general calorons which can exist in SU(3) gauge theories [51]. Furthermore, we are assuming that the dimension-6 $a^2$-suppressed operator takes its tree level Wilson-action form; really it probably renormalizes substantially.

The other lattice correction is a cutoff on the minimum size of calorons which contribute. This cutoff is precisely what Fig. 4 displays. We therefore write

$$\chi_{\text{lat}}(T/T_c, N_\tau, t/a^2) = 2 \int_{\rho_{\text{crit}}}^{1/\Lambda_{\text{MS}}^{N_f=0}} d\rho D_{\text{lat}}(\mu = \rho^{-1}, T/T_c) G(\pi \rho T). \quad (5.6)$$

Fig. 7 shows the resulting estimate of the topological susceptibility which we would obtain by working at a given $N_\tau$ and applying a given amount of gradient flow. The lattice corrections raise the contributions in the peak of Eq. (5.1) near $\rho = 0.4/T$. But lattice artifacts also dramatically increase the number of dislocations with $\rho \sim a$, as we see from the action in Fig. 2. If these two scales, $a$ and $0.4/T$, are well separated, then gradient flow can erase the dislocations with little impact on the typical calorons; this leads to a plateau in Fig. 7 which we observe for $N_\tau = 10$. For coarser lattices such as $N_\tau = 6$, the two phenomena are not well separated. The figure suggests that $N_\tau = 6$ will not be sufficient to give results which are stable against the amount of flow, but larger $N_\tau$ will, especially if we use Zeuthen flow. Overimproved flow is good for completely “cleaning” a configuration of perturbative fluctuations, but in terms of eliminating small instantons, it is effectively equivalent to using $t = 2a^2$ of Wilson flow. Therefore it is not preferred if we want flexibility in choosing the size of caloron/dislocation which we eliminate.

Finally, we consider the extrapolation to zero lattice spacing in Fig. 8. The lattice spacing corrections are very large even for $N_\tau = 10$, and a simple extrapolation in $\chi$ can
Figure 6: Integrand of Eq. (5.6) at $T/T_c = 4$ and for $N_\tau = 6, 8, 10$. Note that there is an additional factor of $(\pi T)^4$ coming from the change of variables in Eqs. (5.1) and (5.6).

easily lead to a negative result. But that is because the $a^2$ errors are best viewed as a correction to the logarithm of $\chi$, as we see in Eq. (5.5). If we extrapolate in terms of $\ln(\chi)$, the procedure works much better – but $N_\tau = 6$ appears to be too coarse a lattice to lie in the scaling regime.

6 Conclusions

We have constructed calorons on the lattice. We find that they suffer from somewhat larger $a^2$ errors than instantons with the same $\rho/a$ value, and possess most of the action and topological charge of a continuum instanton if $\rho/a > 1$, and nearly all of the charge and action if $\rho/a > 2$. Wilson flow destroys small calorons, with progressively more flow destroying larger calorons; Fig. 4 presents our main conclusions in this regard, and shows that improved (Zeuthen) flow destroys calorons out to a smaller size, while overimproved flow preserves all calorons with $\rho/a \gtrsim 1.8$.

Using our results to estimate the $a^2$ errors which arise when computing the topological susceptibility $\chi(T)$ on the lattice, we find that $N_\tau = 6$ is probably insufficient to be in the scaling regime, and lattice spacing errors are expected to lead to a severe overestimate of $\chi(T)$ at finite $a$, which may lead to negative values if we extrapolate $\chi(T)$ against $a^2$. It is more natural to extrapolate $\ln(\chi(T))$ against $a^2$, because this corresponds better to the way which $a^2$ errors enter in the susceptibility.
Figure 7: Estimated effect of lattice artifacts on the topological susceptibility, at $T/T_c = 4$ and for $N_\tau = 6, 8, 10$, as a function of the flow depth $t/a^2$. Left: Wilson flow. Middle: Zeuthen flow. Right: Overimproved flow. The red dotted curve denotes the continuum limit.

Figure 8: Left: Result of Eq. (5.6) at $T/T_c = 4$ for $t/a^2 = 1.0, 2.0, 3.0, 5.0$ units of Wilson flow. Right: Logarithm of left plot. The black point represents the continuum value.

Note that the inclusion of light quarks in Eq. (5.3) would change the factor $-2\lambda^2$ to $-(2 + N_f/3)\lambda^2$, which makes the dominant size of calorons smaller. Therefore, since $\rho/a$ becomes smaller, the corrections in Eq. (5.5) become larger, and the value of $N_\tau$ needed to reach scaling will be still larger. Extrapolating first in $T$ and then in $N_\tau$ may lead to an
incorrect slope for the temperature dependence of the topological susceptibility.

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A $a^2$ Corrections for Calorons

Here we compute the $a^2$ lattice spacing correction to the caloron action. The Wilson gauge action, expanded in operator dimension, takes the form

$$S_W = -\frac{1}{2} \text{tr}\{F_{\mu\nu}F_{\mu\nu}\} + \frac{a^2}{12} \text{tr}\{D_\mu F_{\mu\nu}D_\mu F_{\mu\nu}\} + \cdots,$$

(A.1)

where each index is summed once. This leads to $a^2$ corrections to the instanton or caloron action. For the instanton, using Eq. (2.4) and integrating $\int d^4x$ one readily obtains

$$S_W(\rho) = 8\pi^2 \left[ 1 - \frac{1}{5} \left( \frac{a}{\rho} \right)^2 + \mathcal{O} \left( \frac{a}{\rho} \right)^4 \right].$$

(A.2)

If now instead the caloron field is used via Eqs. (2.2) and (2.7), a corresponding finite temperature integration $\int_0^\beta d\tau \int d^3x$ yields

$$S_W(\beta/\rho) = 8\pi^2 \left[ 1 + \mathcal{F}(\beta/\rho) \left( \frac{a}{\rho} \right)^2 + \mathcal{O} \left( \frac{a}{\rho} \right)^4 \right].$$

(A.3)

A numerical evaluation of the integral yields the function $\mathcal{F}(\beta/\rho)$ depicted in Fig. 9 which nicely converges to the zero-temperature value of $-1/5$ as $\beta \to \infty$. A suitable parameterization of this curve is given in inverse powers of $\beta/\rho$ by

$$\mathcal{F}(\beta/\rho) = -\frac{1}{5} + \frac{b}{(\beta/\rho)^2} + \mathcal{O} \left( \frac{1}{(\beta/\rho)^4} \right)$$

(A.4)

with $b = -0.75766$. At $\beta/\rho = 4$ the deviation from the zero-temperature results is $\sim 17\%$.

The leading dimension-6 operator for the overimproved action has the just opposite sign and we have

$$S_{OI}(\beta/\rho) = 8\pi^2 \left[ 1 - \mathcal{F}(\beta/\rho) \left( \frac{a}{\rho} \right)^2 + \mathcal{O} \left( \frac{a}{\rho} \right)^4 \right].$$

(A.5)

Dimension-8 operators are required if one wants to see a maximum in the perturbative curve.
B Reducing Boundary Effects

In writing down the instanton and caloron field configurations, we have made no attempt to make them respect the space-periodicity of our box. We could consider extending Eq. (2.7) to include infinite sums over space-periodic copies, but the sums do not converge so this is not an option. Instead, we will try to minimize the damage from the lack of periodicity by smearing out the boundary discontinuities with gradient flow, but applied only near the boundaries so as not to affect the core regions of the instantons/calorons which we want to study. Consider the caloron placed at the center of the lattice and denote the lattice spatial extent as $L$. We then flow the links using a flow time that depends on the relative distance

$$d = \sqrt{(x - z)^2}$$

(B.1)

of the base point of the link $U_\mu(x)$ and the center of the instanton. The flow time depth gets modified as

$$t(d) = \begin{cases} 0, & d < \frac{L}{4} \\ \frac{t_0}{2} \left(1 + \sin \left[ \frac{4\pi}{L} \left( d - \frac{3}{8} L \right) \right] \right) \frac{L}{4} \leq d \leq \frac{L}{2} \\ t_0, & d > \frac{L}{2} \end{cases}$$

(B.2)
where \( t_0 \) is the “normal” flow time. This is nothing but a smooth interpolation between zero flow (close to the center of the caloron) and full flow (close to the boundary). With this procedure we reduce boundary effects while the core of the caloron remains unaffected. In Fig. 10 we show both the topological charge and the Wilson action of the caloron for different flow depths. We observe that the Wilson action suffers significantly more from boundary effects than the topological charge. Applying this modified version of Wilson flow indeed reduces boundary effects. We find that a flow time of \( t_0 = 5a^2 \) is sufficient to satisfactorily reduce most of the boundary effects.

**Figure 10:** Caloron topological charge (left) and Wilson action (right) for different values of \( t_0/a^2 \) as defined in Eq. (B.2).

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