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Winding number on 3D lattice

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We propose a simple numerical method which computes an approximate value of the winding number of a mapping from 3D torus T^3 to the unitary group $U(N)$, when T^3 is approximated by discrete lattice points. Our method consists of a “tree-level improved” discretization of the winding number and the gradient flow associated with an “over-improved” lattice action. By employing a one-parameter family of mappings from T^3 to $SU(2)$ with known winding numbers, we demonstrate that the method works quite well even for coarse lattices, reproducing integer winding numbers in a good accuracy. Our method can trivially be generalized to the case of higher-dimensional tori.

Subject Index B31,B34,B38

1 Introduction

One of the topological numbers, the winding number of a differential mapping from a 3D closed manifold $\mathcal{M}$ to the unitary group $U(N)$,

$$W_3 := \frac{1}{24\pi^2} \int_{\mathcal{M}} \mathrm{tr}\big(g^{-1}\mathrm{d}g\big)^3 \in \mathbb{Z}, \qquad g \in U(N), \tag{1.1}$$

appears in various branches of physics, ranging from particle physics (see, for example, Refs. [1–3]) to condensed matter physics (see Ref. [4] and references cited therein). In some occasions, one wants to (approximately) determine the winding number only given the mapping only discrete points of $\mathcal{M}$. This problem, which is closely related to a lattice formulation of the 3D non-Abelian Chern–Simons theory, is revisited recently [5–8].[1] In this paper, we propose a numerical method which approximately computes the winding number W_3. Explicitly, we consider the situation in which a mapping from 3D torus T^3 is given approximately on discrete cubic lattice points. By employing a one-parameter family of mappings with known winding numbers, we first demonstrate that a simple discretization of Eq. (1.1) with a "tree-level improvement" (that eliminates the leading lattice discretization error) works quite well, approximately reproducing non-trivial integer winding numbers. Then, as a possible treatment of data given only on a coarse lattice, we formulate a smearing based on the gradient flow [11]. We find numerically that, as recently studied in the context of lattice gauge theory [12],[2] the gradient flow associated with an "over-improved" lattice action provides a strong stabilization of the lattice winding number along the gradient flow. A combination of the discretized winding number and an appropriate gradient flow thus provides a simple and versatile method to approximately compute the winding number; we note that this method requires neither the diagonalization of $g(x)$ nor the interpolation of $g(x)$ on the lattice.

2 Discretization of W_3

We assume that the group elements $g(x) \in U(N)$ are residing on lattice points x (i.e., sites) of the periodic cubic lattice $\Lambda_L = (\mathbb{Z}/L\mathbb{Z})^3$, $x \in \Lambda_L$. The Lorentz indices are labeled by μ, ν, … and the unit vector in the μ direction is denoted by $\hat{\mu}$. We discretize W_3

[1] The winding number is related to the second Chern number on a 4D discrete lattice. For the computation of the first Chern number on discrete lattice, there exists a very effective computational method [9, 10].

[2] This study is closely related to studies in Refs. [13, 14].

in Eq. (1.1) by substituting the derivative by[3]

$$g(x)^{-1}\partial_\mu g(x) \to \frac{1}{4}H(x,\mu), \tag{2.1}$$

where

$$\begin{aligned} H(x,\mu) := g(x)^{-1}\Big\{&g(x+\hat{\mu}) - g(x-\hat{\mu}) \\ &- \frac{\eta}{6}\left[g(x+2\hat{\mu}) - 2g(x+\hat{\mu}) + 2g(x-\hat{\mu}) - g(x-2\hat{\mu})\right]\Big\} - \text{H.c.} \end{aligned} \tag{2.2}$$

In this expression, the term proportional to the parameter η is introduced to control the leading discretization error of the order of $a^2 g^{-1}\partial_\mu^3 g$ (a being the lattice spacing) in the classical continuum limit. The choice $\eta = 1$ eliminates the leading discretization error but we will later utilize this freedom of η to realize a gradient flow that stabilizes the lattice winding number along the flow. We then define a lattice counterpart of W_3 (1.1) by

$$W_3^{\text{lat}} := \frac{1}{4^3 \cdot 24\pi^2} \sum_{x\in\Lambda_L} \sum_{\mu,\nu,\rho} \epsilon_{\mu\nu\rho} \operatorname{tr}\left[H(x,\mu)H(x,\nu)H(x,\rho)\right]. \tag{2.3}$$

We examine the validity of this very simple prescription by using a one-parameter family of mappings with known winding numbers. It is the following mapping from T^3 to $SU(2)$:[4]

$$g(\theta) := \bar{\xi}_0 \mathbf{1} + i\sum_{\mu=1}^{3} \bar{\xi}_\mu \sigma_\mu, \qquad \bar{\xi}_A := \frac{\xi_A}{\sqrt{\sum_{A=0}^{3} \xi_A^2}}, \tag{2.4}$$

where σ_μ are Pauli matrices and

$$\xi_0 := m + \sum_{\mu=1}^{3}(\cos\theta_\mu - 1), \qquad \xi_\mu := \sin\theta_\mu, \qquad -\pi \le \theta_\mu \le \pi. \tag{2.5}$$

Since $g(\theta) \to -g(\theta)$ under $\theta \to \theta + \pi$ and $m \to 6 - m$, W_3 (1.1) for this mapping is invariant under $m \to 6 - m$. This mapping appears, for instance, in the computation of the Chern–Simons term [15, 16] and the axial anomaly [17] in lattice gauge theory; there, the parameter m is related to the number of species doublers in a lattice Dirac operator. It can

[3] Here, the lattice spacing a is set to be unity.

[4] This is basically identical to one of mappings considered in Refs. [5, 6].

be analytically shown that

$$W_3 = \begin{cases} 0 & \text{for } m < 0 \text{ and } 6 < m, \\ 1 & \text{for } 0 < m < 2 \text{ and } 4 < m < 6, \\ -2 & \text{for } 2 < m < 4. \end{cases} \tag{2.6}$$

Now, Tables 1 and 2 show W_3^{lat} (2.3) with $\eta = 0$ (i.e., no improvement) and $\eta = 1$ (i.e., tree-level improvement) in Eq. (2.2), respectively, for various lattice sizes (i.e., the number of 1D discretization points) L.

Table 1: The lattice winding numbers W_3^{lat} (2.3) for the mapping (2.4) with $\eta = 0$ in Eq. (2.2) (i.e., no improvement). L is the lattice size. These should be compared with the exact values in Eq. (2.6).

m	$L = 10$	$L = 20$	$L = 30$	$L = 40$	$L = 50$
-1	2.46937×10^{-3}	1.01207×10^{-3}	4.88982×10^{-4}	2.83336×10^{-4}	1.83861×10^{-4}
1	7.49024×10^{-1}	9.28484×10^{-1}	9.67423×10^{-1}	9.81515×10^{-1}	9.88121×10^{-1}
3	-1.51316	-1.86086	-1.93661	-1.96402	-1.97688

Table 2: Same as Table 1 but computed with $\eta = 1$ in Eq. (2.2); this value of η eliminates the leading discretization error in W_3^{lat} (i.e., tree-level improvement).

m	$L = 10$	$L = 20$	$L = 30$	$L = 40$	$L = 50$
-1	1.75038×10^{-3}	2.49312×10^{-4}	5.64141×10^{-5}	1.87146×10^{-5}	7.83516×10^{-6}
1	9.45947×10^{-1}	9.95024×10^{-1}	9.98940×10^{-1}	9.99655×10^{-1}	9.99857×10^{-1}
3	-1.89778	-1.99036	-1.99794	-1.99933	-1.99972

We observe that the winding numbers are basically well approximately reproduced even with a simple discretization as in Eqs. (2.2) and (2.3); this was somewhat surprising to us. Moreover, we observe that the tree-level improvement $\eta = 1$, which removes the leading lattice discretization error of $O(a^2)$ in W_3^{lat} improves the situation drastically; practically, $L \simeq 20$ would be sufficient to extract the integer winding number reliably.

In the above example, the continuous form of the mapping is a priori known and one can approximate the mapping in an accuracy as much as one wishes. In practical problems, however, the number of lattice points could be limited due to various reasons. For such a mapping in a coarse lattice or a noisy form of mappings, in the next section, we propose a smearing of the configuration by the gradient flow.

3 Gradient flow of $g(x)$

Going back to the continuum theory, we consider a one-parameter evolution of the group valued field $g(x) \in U(N)$ along a fictitious time $t \geq 0$. We postulate that the evolution is given by

$$\partial_t g(t,x) = g(t,x)\partial_\mu \left[g(t,x)^{-1}\partial_\mu g(t,x)\right], \qquad g(t=0,x) = g(x). \tag{3.1}$$

This "flow equation" is actually the gradient flow associated with the action S, i.e.,

$$\partial_t g(t,x) = -g(t,x)\frac{\delta S}{\delta\eta^a(t,x)}T^a, \tag{3.2}$$

where we have parametrized the variation of $g(t,x)$ as $\delta g(t,x) := g(t,x)\eta(t,x)$ and $\eta(t,x) = \eta^a(t,x)T^a$ with $U(N)$ generators T^a.[5] The action S is given by

$$S := -\int_{T^3} d^3x \ \mathrm{tr}\left[g^{-1}(t,x)\partial_\mu g(t,x) \cdot g^{-1}(t,x)\partial_\mu g(t,x)\right] \geq 0. \tag{3.3}$$

Then, noting the relation $\delta(g^{-1}\partial_\mu g) = \partial_\mu(g^{-1}\delta g) + [g^{-1}\partial_\mu g, g^{-1}\delta g]$, it is straightforward to see that Eq. (3.2) gives the flow equation (3.1). Also, from $\partial_t(g^{-1}\partial_\mu g) = \partial_\mu\varphi + [g^{-1}\partial_\mu g, \varphi]$, where $\varphi := \partial_\nu(g^{-1}\partial_\nu g)$, we see that $\partial_t S \leq 0$, the action monotonically decreases along the flow. The winding number W_3 (1.1), being an integer, is constant along the flow. Therefore, in the continuum theory, the flow is confined within a topological sector specified by W_3 and it comes to a stop at a local minimum of the action (i.e., a classical solution of S). In lattice theory, we want to approximately realize this property of the gradient flow in continuum.

The gradient flow equation (3.2) is naturally transcribed to the lattice theory as

$$\partial_t g(t,x) = -g(t,x)\partial_x^a S^{\mathrm{lat}} T^a, \tag{3.4}$$

where the Lie-algebra derivative is defined by

$$\partial_x^a f(g) = \frac{d}{ds} f(ge^{sX})\bigg|_{s=0}, \qquad X(y) = \begin{cases} T^a & \text{if } y = x, \\ 0 & \text{otherwise.} \end{cases} \tag{3.5}$$

[5] We adopt a convention that T^a are anti-Hermitian and normalized as $\mathrm{tr}(T^aT^b) = -(1/2)\delta^{ab}$.

From these relations, we have

$$\partial_t g(t,x) = -\sum_{x\in\Lambda_L} \partial_x^a S^{\mathrm{lat}} \partial_x^a S^{\mathrm{lat}} \tag{3.6}$$

and, assuming that the lattice action S^{lat} is real, S^{lat} monotonically decreases along the flow. We set the form of the lattice action as

$$S^{\mathrm{lat}} := -\frac{1}{16}\sum_{x\in\Lambda_L}\sum_{\mu} \operatorname{tr} H(x,\mu)^2 \geq 0, \tag{3.7}$$

where $H(x,\mu)$ is given by Eq. (2.2) and here it is understood that the substitution $g(x) \to g(t,x)$ is made.

The gradient flow equation (3.4) can be numerically solved by the Runge–Kutta method described in Appendix C of Ref. [11].[6] In the notation of Ref. [11], the Lie-algebra valued function $Z(t,x)$ in

$$\partial_t g(t,x) = Z(t,x) g(t,x) \tag{3.8}$$

is given by (omitting the argument t)

$$\begin{aligned}
&Z(x)\\
&= -g(x)\partial_x^a S T^a g(x)^{-1}\\
&= -\frac{1}{16}\sum_{\mu}\Bigl(-\Bigl\{g(x+\hat\mu) - g(x-\hat\mu)\\
&\qquad\qquad - \frac{\eta}{6}\left[g(x+2\hat\mu) - 2g(x+\hat\mu) + 2g(x-\hat\mu) - g(x-2\hat\mu)\right]\Bigr\} H(x,\mu) g(x)^{-1}\\
&\qquad + g(x)\Bigl\{H(x-\hat\mu,\mu)g(x-\hat\mu)^{-1} - H(x+\hat\mu,\mu)g(x+\hat\mu)^{-1}\\
&\qquad\qquad - \frac{\eta}{6}\bigl[H(x-2\hat\mu,\mu)g(x-2\hat\mu)^{-1} - 2H(x-\hat\mu,\mu)g(x-\hat\mu)^{-1}\\
&\qquad\qquad\qquad + 2H(x+\hat\mu,\mu)g(x+\hat\mu)^{-1} - H(x+2\hat\mu,\mu)g(x+2\hat\mu)^{-1}\bigr]\Bigr\}\Bigr)\\
&\quad - \text{H.c.}
\end{aligned} \tag{3.9}$$

When $g \in SU(N)$, we may replace $Z(x)$ by its traceless part:

$$Z(x) \to Z(x) - \frac{1}{N}\operatorname{tr}\left[Z(x)\right]\mathbf{1}. \tag{3.10}$$

The gradient flow acts as a smearing on the lattice field. After the flow with a certain appropriate flow time t, we may employ the discretized formula for the winding number,

[6] Our numerical calculation employs `Gaugefields.jl` in the JuliaQCD package [18]. The actual code set can be found in `https://github.com/o-morikawa/Gaugefields.jl`; the numerical data for this paper is stored in `https://github.com/o-morikawa/Wind3D`

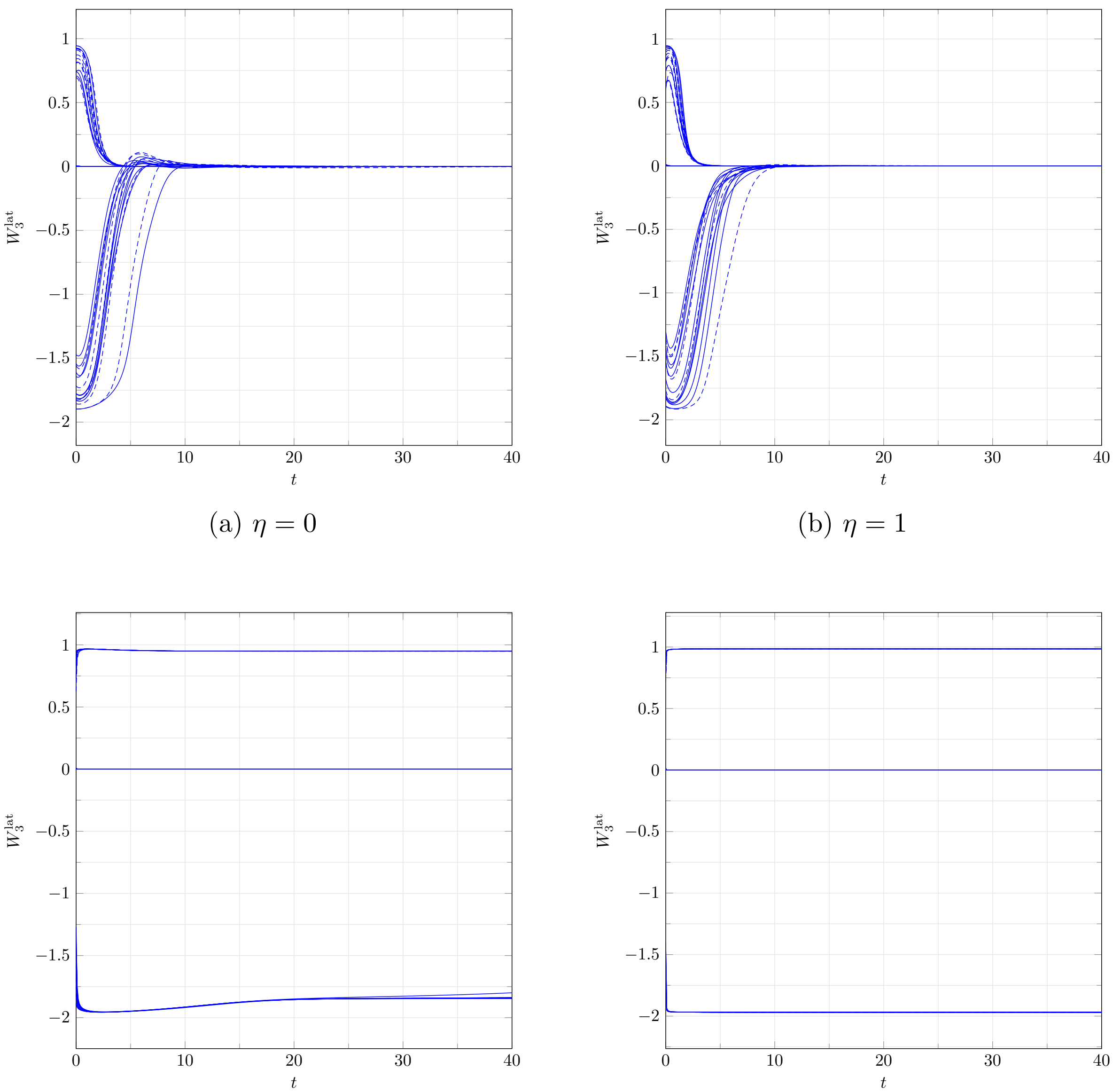
Eq. (2.3). In Figs. 1 and 2, we plot W_3^{lat} (2.3) with $\eta = 1$ (i.e., tree-level improved) as the function of the flow time t.[7] The flow is on the other hand defined by Eqs. (3.8) and (3.9) with various values of η, $\eta = 0$ (no improvement), $\eta = 1$ (tree-level improvement), $\eta = -10$, and $\eta = -20$ ("over-improved" ones), respectively. We set the initial configuration $g(t = 0, x)$ for the flow as Eq. (2.4) with $\xi_A(\theta) \to \xi_A(\theta) + \varepsilon r_A(\theta)$, where ε and $r_A(\theta)$ are uniform random numbers, $\varepsilon \in [0, 1]$ and $r_A(\theta) \in [-1/2, 1/2]$. We take 15 random initial configurations for each of $m = -1$, $m = 1$, and $m = 3$; these parameters correspond to the winding numbers $W_3 = 0$, $W_3 = 1$, and $W_3 = -2$, respectively. The lattice sizes are $L = 10$ in Fig. 1, and $L = 20$ in Fig. 2. We observe that the behaviors drastically change depending on the value of η in the flow; for $\eta = 0$ and $\eta = 1$, the flow acts to eliminate non-trivial winding numbers, while the over-improved cases ($\eta = -10$ and $\eta = -20$), the flow stabilizes the winding number around the desired integer values. For a usage of the gradient flow associated with an over-improved lattice action for the winding number stabilization, we got a hint from a recent study [12] in lattice gauge theory.

We may observe these (de)stabilization effects of the gradient flow as the evolution of the action density distribution along the flow. In Figs. 3 and 4, we see that a non-trivial structure of the configuration dies out along the flow for $\eta = 1$ (Fig. 3) but it survives for $\eta = -20$ (Fig. 4).

These (de)stabilization of the topological sector under the gradient flow could be understood by considering the lattice action S^{lat} (3.7) of the mapping (2.4) as the function of the parameter m (this argument is analogous to the study of the one instanton action as the function of the size moduli in Refs. [12, 13, 19]). In Fig. 5, we plot the value of the lattice action S^{lat} as the function of m. First, for $\eta = 0$ and $\eta = 1$, we see that the lattice action as the function of m does not have any local minimum. Since the lattice action monotonically decreases along the flow (recall Eq. (3.6)), this fact indicates that, for $\eta = 0$ and $\eta = 1$, the flow would effectively make the parameter $|m| \to \infty$ that results in $g(x) \to \mathbf{1}$ and the trivial winding number $W_3^{\mathrm{lat}} = 0$. This well explains the observation which can be made in Figs. 1a, 1b, 2a, 2b, and 3. On the other hand, for $\eta = -20$ (i.e., the over-improved one), the lattice action as the function of m acquires local minima in regions of m which correspond to distinct topological sectors. This fact indicates that the lattice winging number is stable under the gradient flow for $\eta = -20$ at least until the lattice size $L = 30$.[8] This also well explains the

[7] Since the diffusion length of the flow equation (3.4) is $\sim \sqrt{8t}$, the flow time larger than $t \sim L^2/32$ would be regarded as an over-smearing.

[8] This does not necessarily imply that the flow preserves the winding number, because here we are assuming a simple form of the configuration, Eq. (2.4). In principle, the configuration could slip away from the form (2.4) under the flow, although Figs. 1d and 2d indicate that this is not the case.



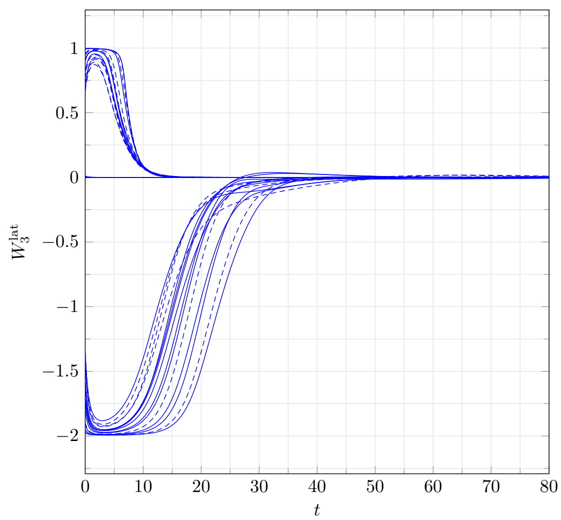
(a) $\eta = 0$

(b) $\eta = 1$

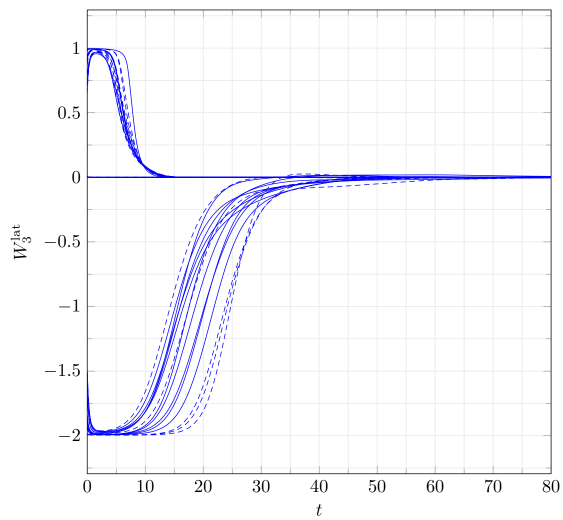
(c) $\eta = -10$

(d) $\eta = -20$

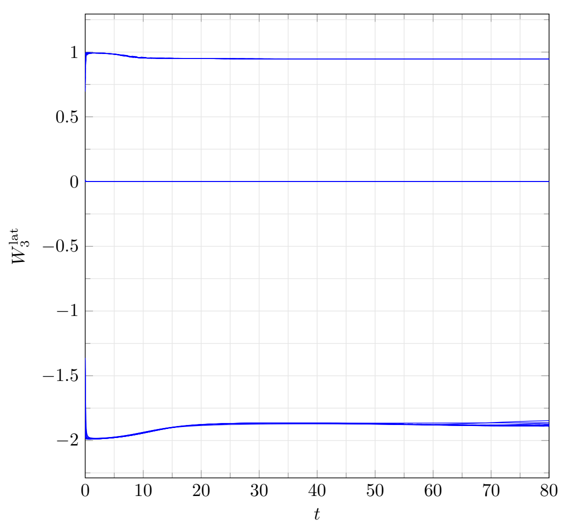
Fig. 1: W_3^{lat} (2.3) as the function of the flow time t. The flow is defined by Eq. (3.8) with various values of η, $\eta = 0$ (no improvement), $\eta = 1$ (tree-level improvement), $\eta = -10$, and $\eta = -20$ ("over-improved"), respectively. We set the initial configuration $g(t = 0, x)$ for the flow by Eq. (2.4) with $\xi_A(\theta) \to \xi_A(\theta) + \varepsilon r_A(\theta)$, where ε and $r_A(\theta)$ are uniform random numbers, $\varepsilon \in [0, 1]$ and $r_A(\theta) \in [-1/2, 1/2]$. We take 15 random initial configurations for each of $m = -1$, $m = 1$, and $m = 3$; these parameters corresponds to the winding numbers $W_3 = 0$, $W_3 = 1$, and $W_3 = -2$, respectively. The lattice size is $L = 10$.



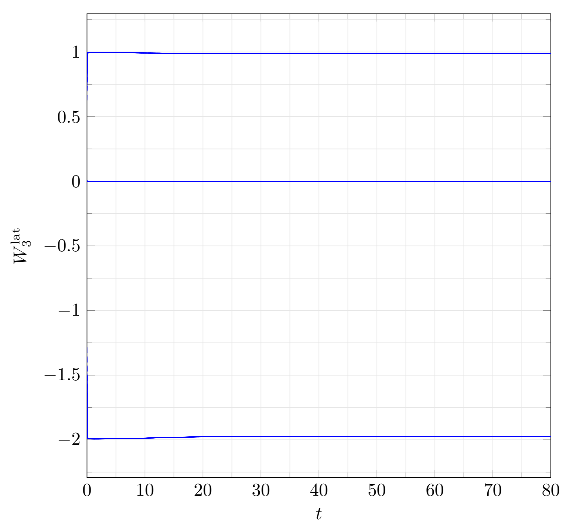
(a) $\eta = 0$



(b) $\eta = 1$



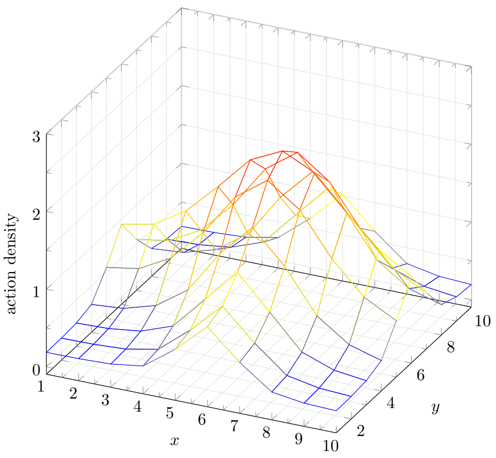
(c) $\eta = -10$



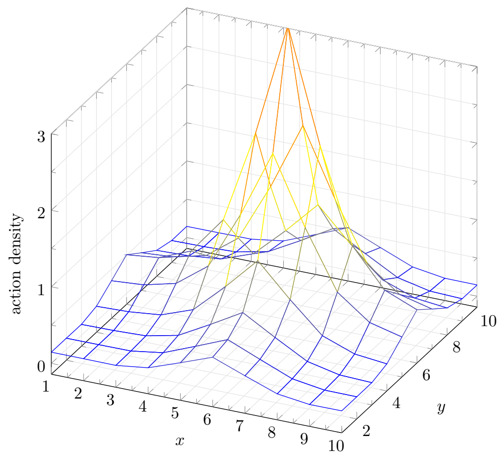
(d) $\eta = -20$

Fig. 2: Same as Fig. 1 but the lattice size is $L = 20$.

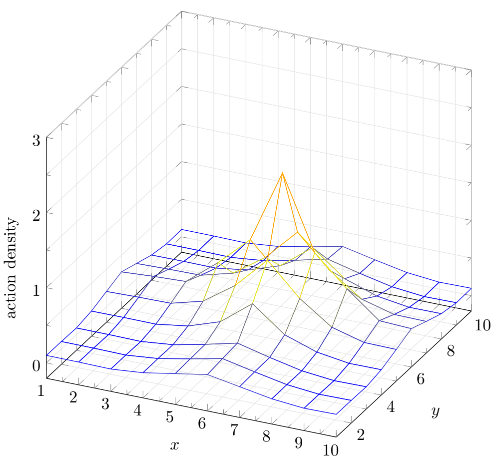
behaviors in Figs. 1d, 2d, and 4. We can understand the stabilization effect of the gradient flow associated with an over-improved lattice action in this way. Note that the stabilization comes from the discretization error in the flow equation and we thus expect that the effect becomes weaker for L larger (i.e., when the lattice becomes finer). However, when the lattice is fine enough, we may simply use the discretized winding number without relying on the gradient flow; when the lattice is coarse, we may employ the gradient flow which could



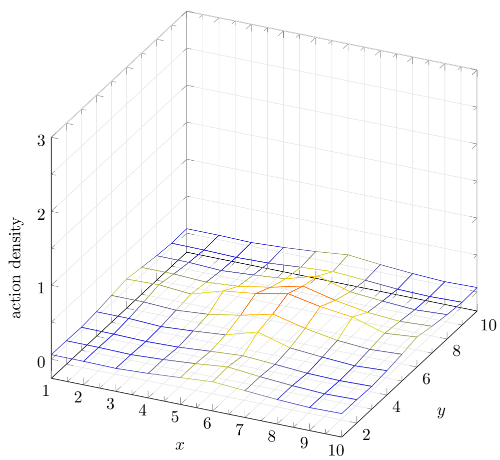
(a) $t = 0$



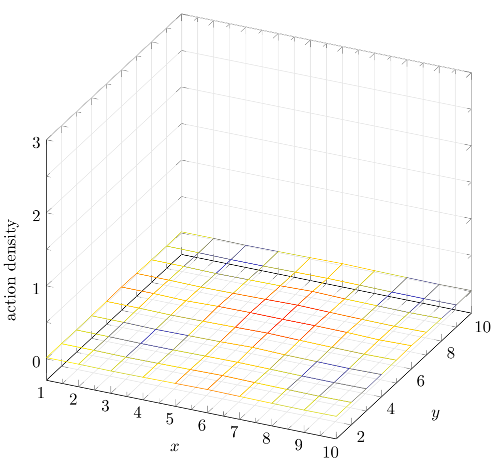
(b) $t = 1$



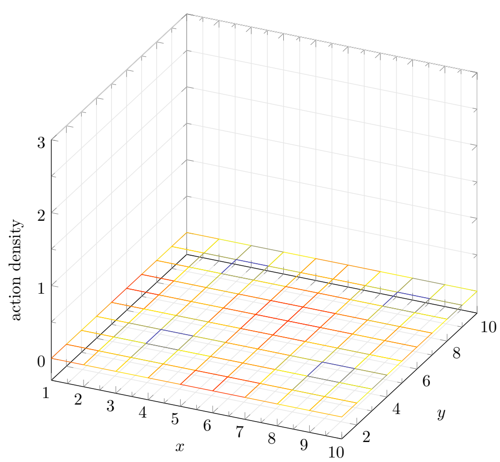
(c) $t = 2$



(d) $t = 3$

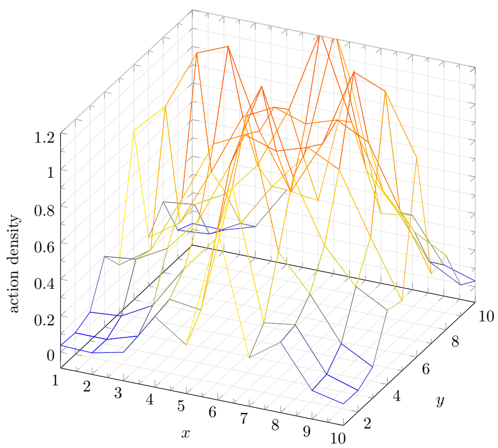


(e) $t = 5$

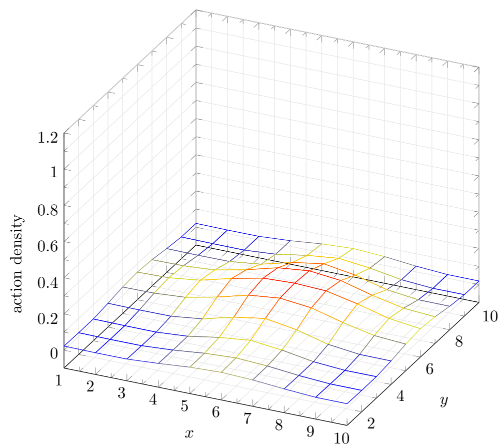


(f) $t = 8$

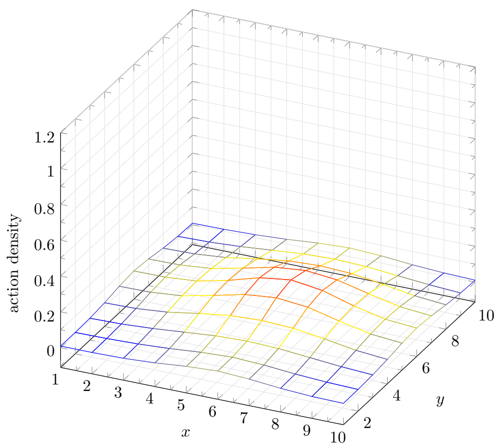
Fig. 3: 2D distribution of the action density $-(1/16)\sum_\mu \operatorname{tr} H(x, y, L/2, \mu)^2$ as the function of the flow time t. $L = 10$ and the initial configuration $g(t = 0, x)$ is Eq. (2.4) with $m = 1$. The case of the gradient flow with the parameter $\eta = 1$ in Eq. (2.2) is shown.



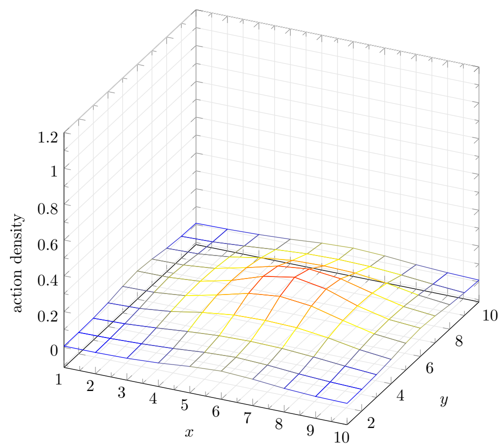
(a) $t = 0$



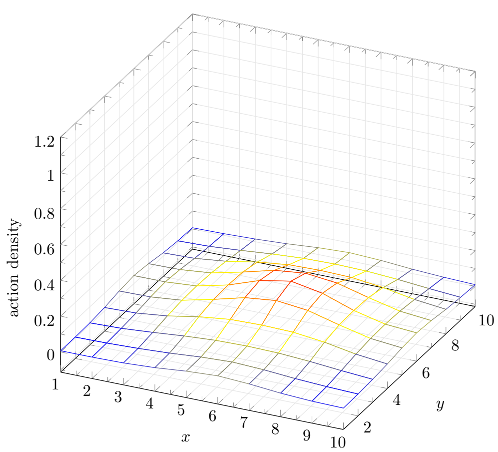
(b) $t = 1$



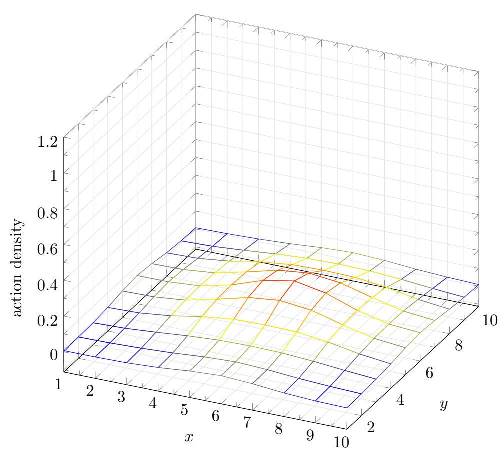
(c) $t = 8$



(d) $t = 15$



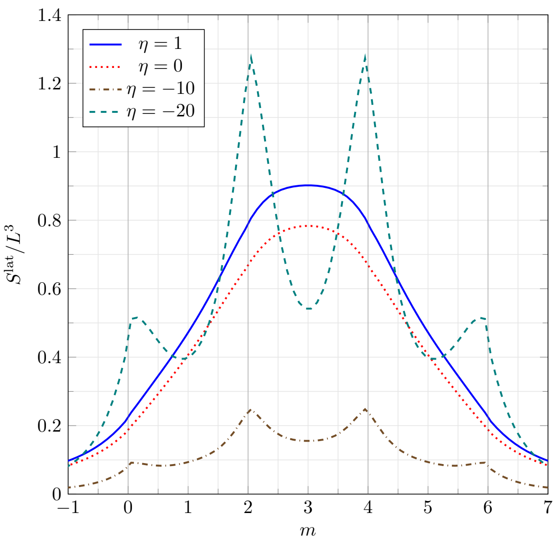
(e) $t = 25$



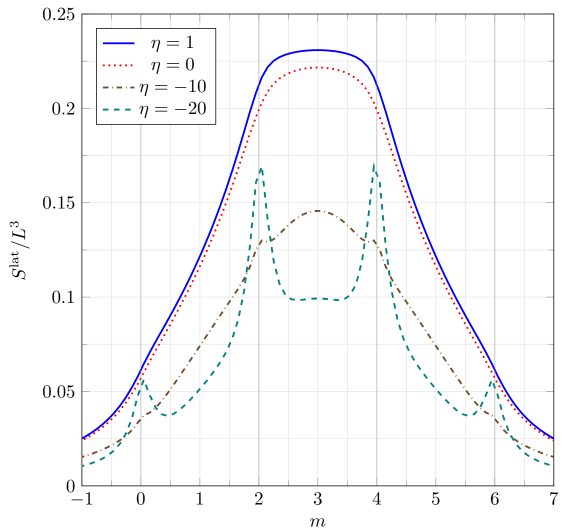
(f) $t = 40$

Fig. 4: Same as Fig. 3 but the case of the gradient flow with the parameter $\eta = -20$ in Eq. (2.2).

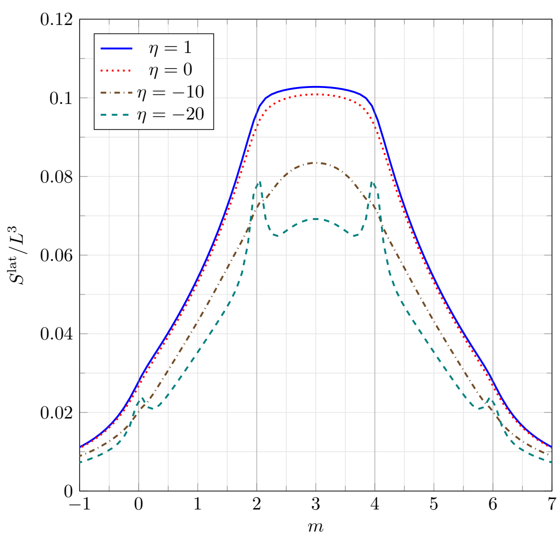
provide an enough stabilization of the winding number. In this way, both elements in our method can be complementary.



(a) $L = 10$



(b) $L = 20$



(c) $L = 30$

Fig. 5: The value of the lattice action (3.7) of the mapping (2.4) as a function of the parameter m for various values of η. The cases of lattice sizes, $L = 10$, $L = 20$, and $L = 30$, are depicted.

4 Conclusion

In this paper, we proposed a simple and versatile numerical method which computes an approximate winding number of a mapping from 3D torus T^3 to $U(N)$, when T^3 is approximated by a discrete cubic lattice. Our method consists of a tree-level improved discretization of the winding number and the gradient flow associated with an over-improved lattice action. By employing a one-parameter family of mappings from T^3 to $SU(2)$ with known winding numbers, we demonstrated that the method works quite well even for coarse lattices, reproducing integer winding numbers in a good accuracy. Since we examined the validity of our method only for a simple one-parameter mappings with known winding numbers, the implementation of our method for real problems would require some exploratory analyses especially on the optimal value of η in the gradient flow which stabilizes the lattice winding number. Nevertheless, we believe that our method will be practically useful in many problems because the computationally burden in our method is rather light. We also note that our method can trivially be generalized to the case of higher-dimensional tori. Finally, it would also be interesting to generalize the present method to a 3D lattice with boundary since the resulting system (approximately) realizes the Wess–Zumino–Witten term [20].

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