

Scale setting of $SU(N)$ Yang–Mills theory, topology and large- N volume independence

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We set the scale of $SU(N)$ Yang–Mills theories for $N = 3, 5, 8$ and in the large- N limit via gradient flow, as a first step towards the computation of the large- N Λ -parameter using step scaling. We adopt twisted boundary conditions to achieve large- N volume reduction and the Parallel Tempering on Boundary Conditions algorithm to tame topological freezing. This setup allows accurate determinations of the gradient-flow scales even on extremely fine lattices for all the explored values of N . Moreover, we are able to precisely estimate the finite-size systematics related to topological freezing, and to show the suppression of finite-volume effects expected by virtue of large- N twisted volume reduction.

I. INTRODUCTION

In the last decade, it has become increasingly common for lattice studies of QCD and QCD-like systems to reach percent or even sub-percent levels of accuracy. Recent paramount examples are the lattice computation of the hadronic contribution to the muon anomaly—see the review [1] and references therein—or the lattice computation of the strong coupling constant—see Ref. [2] and references therein. As a higher precision is achieved, new possible sources of systematic effects must be investigated and controlled. In this regard, *scale setting* plays a crucial role, as its uncertainties and systematics propagate to any observable which needs to be converted from lattice to physical units.

Gradient flow [3–6] scales have become a standard choice for scale setting, requiring only the numerical integration of the gradient flow equation and computation of the energy density on the lattice. These are considered to be reliable reference scales, as numerical integration can be performed with arbitrarily small systematic error, and the energy density can be determined with high statistical precision. However, it is widely acknowledged that the scale-setting procedure via gradient flow may be subject to a bias due to finite-volume effects and *topological freezing* [7, 8]. Topological freezing [9–11] constitutes a computational challenge that pervades Monte Carlo simulations of all lattice field theories possessing non-trivial topological properties when employing conventional local algorithms in the vicinity of the continuum limit. As the lattice spacing decreases, the Markov chain tends to

remain trapped in a fixed topological sector, thereby losing ergodicity. It is well-known that expectation values taken at fixed topology suffer for power-like finite-volume effects [12, 13], thus a fixed topology enhances finite-size corrections with respect to the usual exponentially suppressed ones. Moreover, after the gradient flow, the energy density used to extract gradient-flow scales becomes highly-correlated with the topological charge of the underlying gauge fields. Thus, the ergodicity problem due to the incorrect topological sampling could also introduce unwanted biases in the scales themselves [7].

The goal of this paper is to perform the scale setting of large- N Yang–Mills theories via the gradient flow on lattices with lattice spacings as fine as ~ 0.025 fm. Our main motivation is related to the fact that this is a necessary first step towards the determination of the large- N Λ -parameter via step-scaling [14] from a finite-volume renormalization scheme based on the use of twisted boundary conditions [15]. This is an ongoing project we are carrying on [16–19]. In the regime we are interested in, due to the well-known worsening of topological freezing at large N , systematic effects discussed above are particularly relevant, requiring to be addressed with particular care. Apart from our principal goal, our setup allows to illustrate the behavior of systematic effects on gradient-flow scales in the presence of a frozen topology. Such topic is of much broader interest, and goes beyond the study of scale setting in large- N gauge theories. Thus, our investigation may also be a useful reference on the subject even for communities working on other lattice field theories.

To pursue the goal of this paper, it is imperative to devise a numerical strategy to mitigate topological freezing. This is achieved by employing the *Parallel Tempering on Boundary Conditions* (PTBC) algorithm in combination with *Twisted Boundary Conditions* (TBCs). The PTBC algorithm is a well-established method of mitigating topological freezing, which has been shown to effectively reduce the auto-correlation time of the topological

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charge in a variety of systems and physical regimes (fine lattice spacings, large N , zero and finite temperature), both in $2d$ models [20–22], and in $4d$ non-abelian gauge theories with [23] and without fermion content [19, 24–28]. The choice of TBCs over standard *Periodic Boundary Conditions* (PBCs) is driven by the concept of *twisted volume reduction* [29–31] (references [32, 33] provide comprehensive reviews on this subject). It has been demonstrated that, under certain conditions that are satisfied thanks to TBCs, Yang–Mills theories enjoy a dynamical equivalence between color and space-time degrees of freedom in the large- N limit [34]. In the context of a finite N , and when considering specific choices of the twist, the finite-volume effects associated with an $L \times L$ lattice plane with TBCs should be equivalent to those with PBCs and $L \rightarrow NL$, up to $1/N^2$ corrections. This enables a reduction in the volume of the simulated lattices as N increases, whilst maintaining control over finite-volume effects.

This paper is organized as follows. In Sec. II we define the several gradient-flow scales we will compute. In Sec. III we describe our lattice discretization, Monte Carlo algorithm and numerical strategies. In Sec. IV we present our numerical results for $N = 3, 5, 8$ and in the large- N limit. Finally, in Sec. V we draw our conclusions and discuss future outlooks of this investigation.

II. SCALE SETTING WITH GRADIENT FLOW

The scale of $SU(N)$ Yang–Mills theories can be conveniently set using the gradient flow [3–6], a smoothing procedure that evolves the gauge fields $A_\mu(x)$ in a time t according to the flow equation

$$\partial_t B_\mu(x, t) = D_\nu F_{\nu\mu}(x, t), \quad B_\mu(x, t=0) = A_\mu(x), \quad (1)$$

where D_μ and $F_{\mu\nu}$ are the covariant derivative and the field strength tensor of the flowed fields $B_\mu(x, t)$. The gradient-flow scale t_0 is defined for $SU(3)$ as [5]:

$$\langle t^2 E(t) \rangle|_{t=t_0} = \frac{3}{10} = 0.3, \quad (2)$$

where $E(t)$ is the energy density of the flowed gauge fields,

$$E(t) = \frac{1}{2} \text{Tr} [F_{\mu\nu}(x, t) F_{\mu\nu}(x, t)]. \quad (3)$$

In physical units, this corresponds to $\sqrt{8t_0} \simeq 0.475$ fm [35]. To generalize this definition to $SU(N)$, consider that, in the small- t perturbative limit, the scaling with N of $t^2 E(t)$ gives [5]

$$\langle t^2 E(t) \rangle \underset{N \rightarrow \infty}{\sim} \frac{N^2 - 1}{N}. \quad (4)$$

Thus, a definition of t_0 that remains finite in the large- N limit and coincides with Eq. (2) for $N = 3$ is given by [36]

$$\varphi(t_0) = \frac{9}{80} = 0.1125, \quad (5)$$

where

$$\varphi(t) \equiv \frac{N}{N^2 - 1} \langle t^2 E(t) \rangle. \quad (6)$$

Analogously, one defines w_0^2 [37] in the large- N limit through the logarithmic derivative of $\varphi(t)$,

$$t \frac{d\varphi(t)}{dt} \Big|_{t=w_0^2} = \frac{9}{80} = 0.1125. \quad (7)$$

In addition to these two, we will also consider the scale t_1 , defined as cutting $\varphi(t)$ at half the threshold of t_0 [38]:

$$\varphi(t_1) = \frac{9}{160} = 0.05625. \quad (8)$$

The preference for one or other of these scales is dictated by the need to minimize finite-volume effects and/or lattice artifacts on the flow. Given that the gradient flow smears the gauge fields on a ball of radius $\sqrt{8t}$, a condition to minimize both effects at a given flow time t would be $a \ll \sqrt{8t} \ll l$, with a the lattice spacing and $l \equiv La$ the physical size of the lattice.

The normalization of $\varphi(t)$ chosen in Eq. (6) cancels the leading and sub-leading scaling with N predicted by perturbation theory. Alternative definitions, canceling only the leading N -dependence of the flow, can also be found in the literature [39, 40]:

$$\varphi'(t'_0) = \frac{1}{10} = 0.1, \quad (9)$$

$$\varphi'(t'_1) = \frac{1}{20} = 0.05, \quad (10)$$

and

$$t \frac{d\varphi'(t)}{dt} \Big|_{t=w_0'^2} = \frac{1}{10} = 0.1. \quad (11)$$

where

$$\varphi'(t) \equiv \frac{1}{N} \langle t^2 E(t) \rangle. \quad (12)$$

These definitions, adopted in twisted-reduced models where $N \sim \mathcal{O}(10^2 - 10^3)$ is so large that $N^2 - 1 \simeq N^2$, define scales with a finite large- N limit too, but only coincide with the previous ones for $N = 3$.

Finally, to study the effect of topology on the scale setting, we will also compute all the scales obtained when the flow is projected into the sector with topological charge $Q = 0$. This is achieved replacing $\varphi(t)$ with

$$\varphi_0(t) \equiv \frac{N}{N^2 - 1} \frac{\langle t^2 E(t) \delta_{Q,0} \rangle}{\langle \delta_{Q,0} \rangle}, \quad (13)$$

with $\delta_{Q,n} = 1$ when $Q = n$ and 0 otherwise, and the same for $\varphi'(t)$. As explained in the introduction, a fixed topological sector should not affect the gradient-flow scales defined in the thermodynamic limit. However, taking into account both the projected and non-projected definitions enables us to identify the finite-volume effects introduced by a frozen or poorly sampled topology.

III. NUMERICAL SETUP

In this section, we describe our lattice setup and the algorithm used for the simulations. We also present a general discussion on the expected lattice artifacts and finite volume effects on the flow.

A. Lattice action and observables

We discretize the pure-gauge $SU(N)$ theories for $N = 3, 5, 8$ using the Wilson plaquette action on lattices with a long size $l \equiv La$ along the two directions $\mu = 0, 3$ and a short size $l_s \equiv L_s a < l$ along $\mu = 1, 2$. We impose standard Periodic Boundary Conditions (PBCs) along the long directions and Twisted Boundary Conditions (TBCs) [15, 29] in the plane with two short directions. The lattice action is given by:

$$S_w[U] = -Nb \sum_{x, \mu \neq \nu} Z_{\mu\nu}^*(x) \text{Tr}[P_{\mu\nu}(x)], \quad (14)$$

where $b = 1/\lambda$ is the inverse 't Hooft bare coupling ($\lambda = Ng^2 = 2N^2/\beta$, with β the usual lattice coupling) and $P_{\mu\nu}(x)$ is the plaquette,

$$P_{\mu\nu}(x) = U_\mu(x)U_\nu(x + a\hat{\mu})U_\mu^\dagger(x + a\hat{\nu})U_\nu^\dagger(x). \quad (15)$$

The factor $Z_{\mu\nu}(x)$ implements TBCs. For $\mu < \nu$,

$$Z_{\mu\nu}(x) = Z_{\nu\mu}^*(x) = \begin{cases} e^{i\frac{2\pi k}{N}}, & (\mu, \nu) = (1, 2) \\ & x_\mu = x_\nu = 0 \\ 1, & \text{otherwise,} \end{cases} \quad (16)$$

where k is an integer co-prime with N . We take $k = 1, 2, 3$ for $N = 3, 5$ and 8 , respectively, for reasons that will become clear below.

This setup is analogous to the one of Refs. [16, 19], which was used to determine the renormalized strong coupling in the Twisted Gradient Flow scheme. In that instance, the aspect-ratio $l/l_s = N$ and k were predetermined as part of the scheme definition. However, the gradient-flow scales that are of interest in this study are defined in the thermodynamic limit. Consequently, they should not be dependent on the lattice geometry or the boundary conditions. Nevertheless, their choice can be optimized to reduce finite-volume effects. In this work, the same choice of twist as in [16, 19] is maintained, selecting k and N such that they are separated by two steps in the Fibonacci sequence. In the Twisted Gradient Flow scheme, this choice allows to circumvent the emergence of tachyonic instabilities in the large N limit that invalidates the property of reduction [41].

Furthermore, in contrast to Refs. [16, 19], the aspect ratio l/l_s is not fixed to the number of colors. Instead, a series of simulations are conducted, encompassing various combinations of l and l_s . The objective is to quantify and control finite-volume effects, but also to analyze the reduction of finite-size effects in the short and twisted

directions, expected from TBCs over PBCs. It is anticipated that finite size effects in l_s will fully disappear in the limit of large N .

As dimensionless energy density on the lattice, we use the clover definition

$$a^4 E(t) = E_{\text{clov}}(t) = -\frac{1}{2} \text{Tr}[C_{\mu\nu}(x, t)C_{\mu\nu}(x, t)], \quad (17)$$

where $C_{\mu\nu}(x, t)$ is the clover operator on the (μ, ν) plane in the site x evaluated after the gauge links have been evolved for a flow time t . It is defined as the anti-hermitian and traceless part of:

$$\begin{aligned} \frac{1}{4} \left[Z_{\mu\nu}^*(x)P_{\mu\nu}(x, t) + Z_{\mu\nu}^*(x - a\hat{\nu})P_{-\nu\mu}(x, t) \right. \\ \left. + Z_{\mu\nu}^*(x - a\hat{\mu})P_{\nu-\mu}(x, t) \right. \\ \left. + Z_{\mu\nu}^*(x - a\hat{\mu} - a\hat{\nu})P_{-\mu-\nu}(x, t) \right], \end{aligned} \quad (18)$$

where $U_{-\mu}(x, t) = U_\mu^\dagger(x - a\hat{\mu}, t)$.

The flow equation in Eq. (1) is discretized and integrated with the adaptive third-order Runge-Kutta method described in Ref. [42]. This procedure allows the determination of both $\varphi(t)$ and $\varphi'(t)$ for discrete times $T = t/a^2$. In order to ascertain a scale, a spline interpolation of $\varphi(t)$ and $\varphi'(t)$ (or its derivatives for w_0^2 and $w_0'^2$) and of its statistical uncertainty is performed, after which the time at which it intersects the threshold defining the scale is extracted.

In order to study the effect of topology on the scale setting, one further ingredient is required; namely, a definition of the topological charge on the lattice. Given the clover discretization

$$Q_{\text{clov}}(t) = \sum_{x, \mu\nu\rho\sigma} \frac{\varepsilon_{\mu\nu\rho\sigma}}{32\pi^2} \text{Tr}[C_{\mu\nu}(x, t)C_{\rho\sigma}(x, t)], \quad (19)$$

we assign to each configuration an integer topological charge

$$Q = \text{round}[Q_{\text{clov}}(t_0)]. \quad (20)$$

We verified that $Q_{\text{clov}}(t)$ reaches a plateau in t before t_0 and is close to an integer number, thus it can be safely rounded to the closest integer. This allows to define the projection into the $Q = 0$ topological sector in Eq. (13). As an example, in Fig. 1 we show a lattice determination of t_0 , with and without topological projection.

B. Monte Carlo algorithm

The determination of the gradient-flow scales without resorting to the $Q = 0$ projection requires a correct sampling of the topological charge. As outlined in the introduction, this is a complex task due to the occurrence of topological freezing at the fine lattice spacings that will be simulated. Topological freezing, moreover, further worsens when increasing N at fixed lattice spacing.

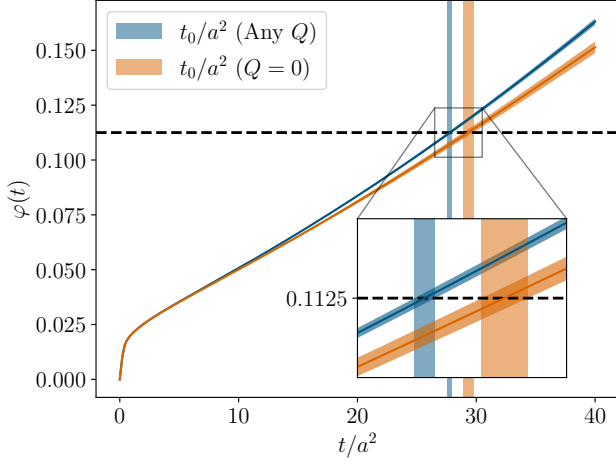


FIG. 1: Example of the determination of t_0 on an SU(3) lattice with $L = 38$, $L_s = 24$, $b = 0.37583$ and TBCs, with and without projection to $Q = 0$.

Open boundary conditions [43] or master field simulations [44] have been employed to circumvent this issue in the case of SU(N) pure gauge theories [35, 36]. In this paper, the Parallel Tempering on Boundary Conditions (PTBC) algorithm is adopted, following the implementation of Ref. [19] with TBCs in the short directions. Originally proposed for two-dimensional CP $^{N-1}$ models [20], the PTBC algorithm has been widely employed in the last few years to improve the state of the art of the lattice determination of several quantities. Various numerical studies have demonstrated that this approach leads to a substantial reduction in the auto-correlation time of the topological charge when compared with standard algorithms [19, 21–28].

The main idea of the PTBC algorithm is to consider N_r replicas $r = 0, 1, \dots, N_r - 1$ of the lattice, each one differing for the boundary conditions imposed on a small sub-region called the *defect* D . We choose D to be an L_d^3 spatial cube, placed on the time boundary $x_0 = L - 1$. Links that cross D orthogonally (i.e., temporal links) are multiplied by a real factor $c(r)$. For the physical replica (i.e., the one on which observables are computed) $c(0) = 1$, so the defect has no effect and links enjoy PBCs. The other replicas interpolate between periodic and open boundary conditions on the defect: $c(N_r - 1) = 0$ for the last replica and $0 < c(r) < 1$ for those in-between. With TBCs, the defect is implemented by taking as the action of the replica r

$$S_W^{(c(r))}[U_r] = -bN \sum_{x, \mu \neq \nu} K_{\mu\nu}^{(c(r))}(x) Z_{\mu\nu}^*(x) \text{Tr} \left[P_{\mu\nu}^{(r)}(x) \right], \quad (21)$$

where U_r denotes the gauge links of the replica r . The factor $K_{\mu\nu}^{(c(r))}(x)$ changes the boundary conditions on the defect, similarly to how the twist factor $Z_{\mu\nu}(x)$ in

Eq. (16) implements TBCs:

$$K_{\mu\nu}^{(c(r))}(x) = K_{\mu}^{(c(r))}(x) \cdot K_{\nu}^{(c(r))}(x + a\hat{\mu}) \cdot K_{\mu}^{(c(r))}(x + a\hat{\nu}) \cdot K_{\nu}^{(c(r))}(x), \quad (22)$$

$$K_{\mu}^{(c(r))}(x) = \begin{cases} c(r), & \mu = 0, x \in D, \\ 1, & \text{otherwise.} \end{cases} \quad (23)$$

For what concerns the Monte Carlo sampling, each replica is updated simultaneously and independently performing 1 lattice sweep of the standard local heat-bath algorithm [45, 46], followed by $n_{\text{ov}} = 12$ lattice sweeps of the standard local over-relaxation algorithm [47]. Then, swaps among two adjacent replicas ($r, s = r + 1$) are proposed and accepted via a Metropolis step with probability

$$p(r, s) = \min \left\{ 1, e^{-\Delta S_{\text{swap}}^{(r, s)}} \right\}, \quad (24)$$

$$\Delta S_{\text{swap}}^{(r, s)} = S_W^{(c(r))}[U_s] + S_W^{(c(s))}[U_r] - S_W^{(c(r))}[U_r] - S_W^{(c(s))}[U_s]. \quad (25)$$

The values $c(r)$ of intermediate replicas are tuned with short test simulations in order to achieve a mean acceptance p of swaps around 20% for each pair of replicas. Thus, a given field configuration performs a sort of random walk among different replicas. Moreover, to improve the performance of the algorithm, the defect is translated randomly around the lattice and local updates are more frequent around it.

Finally, concerning the defect size, we chose it to be approximately constant in physical units, $l_d = aL_d \sim 0.18 - 0.20$ fm, which was proven to be the optimal choice in previous PTBC studies [19, 24, 28]. Once l_d is fixed, the number of replicas is scaled with b and N as $N_r \sim NL_d^{3/2}$ to keep $p \simeq 20\%$ constant, see [19, 24, 28] for more details.

C. Improvement of lattice artifacts

In order to obtain a tree-level improvement of the lattice observables used to compute $\varphi(t)$ and $\varphi'(t)$, one can resort to perturbation theory. In the continuum and at leading order in the 't Hooft coupling constant [39, 48, 49]:

$$\varphi'(t) = \mathcal{N}_{\text{cont}}(N, l, l_s, t)(\lambda + \dots) \quad (26)$$

where:

$$\mathcal{N}_{\text{cont}}(N, l, l_s, t) = \frac{3}{128\pi^2} \mathcal{A}(x, x_s, N), \quad (27)$$

with

$$\mathcal{A}(x, x_s, N) = \tilde{\theta}^2(x) \left[\tilde{\theta}^2(x_s) - \frac{1}{N^2} \tilde{\theta}^2(N^2 x_s) \right] \quad (28)$$

and

$$x = \frac{8\pi t}{l^2}, \quad x_s = \frac{8\pi t}{(Nl_s)^2}, \quad \tilde{\theta}(x) = \theta_3\left(0, \frac{i}{x}\right), \quad (29)$$

with θ_3 the Jacobi theta function.

On the lattice, with the clover definition of the energy density given in Eq. (17), one should replace the normalization $\mathcal{N}_{\text{cont}}$ by the expression obtained when expanding the clover energy density in lattice perturbation theory [39, 48]:

$$\mathcal{N}_{\text{latt}}(N, L, L_s, T) = \frac{T^2}{2V_{\text{eff}}} \sum_{\mu \neq \nu, q} \frac{e^{2T\hat{q}^2} \sin^2(q_\nu) \cos^2(q_\mu/2)}{\hat{q}^2} \quad (30)$$

where $t = Ta^2$, $l = La$, $l_s = L_s a$, $V_{\text{eff}} = (NL_s L)^2$, and $\hat{q}_\mu = 2 \sin(q_\mu/2)$ is the lattice momentum, with $q_\mu = 2\pi n_\mu / L_{\text{eff}}$ for $n_\mu = 0, \dots, L_{\text{eff}} - 1$. The effective size L_{eff} is L along the directions $\mu = 0, 3$ with PBCs and NL_s along $\mu = 1, 2$ with TBCs. The prime in the sum denotes the exclusion of momenta with both components on the twisted plane multiple of $2\pi/L_s$, that is $n_1 \bmod N = 0$ and $n_2 \bmod N = 0$. Thus, a tree-level improvement of lattice artifacts in the flow can be attained by multiplying $\varphi(t)$ and $\varphi'(t)$ by

$$\tilde{\mathcal{N}}(N, L, L_s, T) = \frac{\mathcal{N}_{\text{cont}}(N, l, l_s, t)}{\mathcal{N}_{\text{latt}}(N, L, L_s, T)}. \quad (31)$$

It should be noted that this choice only removes classical lattice artifacts in the observable used to define flow, while those associated to the discretization of the lattice action and of the flow equation are left untouched [50].

D. Twisted volume reduction in the large- N limit

One of the objectives of the present paper is to examine how the effects of finite volume are mitigated when using twisted boundary conditions at finite N . One of the consequences of reduction is an enlargement of the effective size in the directions subject to TBCs. For our particular choice of twist, this amounts to replacing $l_s \rightarrow l_s^{(\text{eff})} \equiv Nl_s$. While this holds exactly in the large- N limit, there is an explicit dependence on the actual torus size at finite N , which becomes suppressed in inverse powers of N . In order to illustrate this point, consider the leading order in perturbation theory, where the leading volume- and N -dependence of the flow can be straightforwardly derived from Eq. (26). Taking into account that

$$\tilde{\theta}(x) = \sum_{n \in \mathbb{Z}} \exp\left[-\frac{\pi n^2}{x}\right], \quad (32)$$

one gets, at leading order in the coupling:

$$\varphi'(t) = \frac{3(N^2 - 1)}{128\pi^2 N^2} \left[1 - \frac{4}{N^2 - 1} e^{-l_s^2/(8t)}\right] \lambda, \quad (33)$$

up to exponential corrections in $l^2/(8t)$ and $[l_s^{(\text{eff})}]^2/(8t)$. This expression reflects the underlying principle of reduction—in the large- N limit, irrespective of the size of the torus in the twisted directions, the thermodynamic limit is recovered with corrections that depend only on the effective volume. The perturbative expansion of Wilson loops has been shown to exhibit a similar behavior, with the dependence on the small size being suppressed as $1/N^2$ in the large- N limit [51, 52]. In accordance with these observations, we conjecture that, by virtue of large- N twisted volume reduction, the finite-size effects on the gradient-flow scales can be adequately characterized as follows:

$$\frac{t_0(N, l_s^{(\text{eff})}, l)}{t_0(N)} = 1 + G(l_s^{(\text{eff})}, l) + \frac{A(N)}{N^2} F\left(\frac{l_s^{(\text{eff})}}{N}, l\right), \quad (34)$$

with $A(N) \sim \mathcal{O}(N^0)$, and $t_0(N) \equiv t_0(N, \infty, \infty)$ the thermodynamic limit of t_0 for a given N . Analogous expressions hold for all the other scales. It is important to emphasize that this expression reflects the power of the large- N volume reduction: the term proportional to F tends to zero as N increases and the large- N result coincides with the one for $l_s^{(\text{eff})} = \infty$, irrespective of the value of l_s .

From the field-theoretical point of view, the actual functional form of the functions F and G depends on whether expectation values are taken in a fixed topological sector, or averaging over all topological sectors. This is crucial to determine the expected finite-size effects in the presence/absence of topological freezing. If topology is correctly sampled and expectation values are taken averaging over all relevant values of Q , finite-size effects on the energy density are expected to be exponentially suppressed in l , l_s and $l_s^{(\text{eff})}$, at least if these sizes are large enough in units of $\sqrt{8t_0}$ to be sufficiently deep in the non-perturbative domain in which t_0 is defined. Given that $l_s^{(\text{eff})}, l > l_s$, finite-size corrections at finite N will be dominantly due to the F -term and to its dependence on the short size:

$$\frac{t_0(N, l_s^{(\text{eff})}, l)}{t_0(N)} \simeq 1 + \frac{A_0}{N^2} e^{-m l_s^{(\text{eff})}/N} + \dots, \quad (35)$$

with m some physical mass scale of the theory. Instead, if the gradient-flow scales are computed in a fixed topological sector, finite-size effects in l , l_s and $l_s^{(\text{eff})}$ are expected to be power-like, and $\mathcal{O}(1/\mathcal{V})$ (for F) and $\mathcal{O}(1/\mathcal{V}_{\text{eff}})$ (for G) at leading order [12, 13], with $\mathcal{V}_{\text{eff}} \equiv N^2 \mathcal{V} = N^2 l^2 / l_s^2$. However, due to the $1/N^2$ suppression of the F -term with respect to G , eventually also that term becomes $\mathcal{O}(1/\mathcal{V}_{\text{eff}})$. Thus, in a fixed topological sector $Q = n$, the dominant finite-size correction will be:

$$\frac{t_0(N, l_s^{(\text{eff})}, l)}{t_0(N)} \Big|_{Q=n} \simeq 1 + \frac{C^{(n)}(N)}{N^2 \mathcal{V}} + \dots \quad (36)$$

with $C^{(n)}(N) \sim \mathcal{O}(N^0)$.

IV. RESULTS

In this section, we present our main results for the gradient-flow scales. After a brief introduction of the simulation parameters, we present the determination of the scales on an N -by- N basis and analyze the systematic effects associated to finite volume and topological freezing. Next, we study the dependence on the number of colors and perform a global analysis of finite-volume and finite- N effects to illustrate the effect of reduction. We finally present results on the continuum extrapolation of various ratios of scales to analyze the effect of the improvement of lattice artifacts.

A. Simulation parameters

Table I provides a comprehensive overview of all the simulation parameters employed in this study. As we will see *a posteriori*, the explored parameter space covers a range of very fine lattice spacings down to ~ 0.025 fm across all values of N . Reliable simulations with controlled autocorrelations in this regime are known to be extremely hard with standard algorithms due to the exponential growth in both $1/a$ and N of the autocorrelation time τ of Q^2 observed when sampling lattice Yang-Mills theories with periodic boundary conditions [9–11]. Probing our target parameter space was made feasible by the adoption of the PTBC algorithm. As a matter of fact, as discussed in Ref. [28], PTBC simulations show a much slower polynomial growth of $\tau(Q^2) \sim \sqrt{N}/a^2$ in the periodic replica.

The required number of replicas grows polynomially too as $N_r \sim N(1/a)^{3/2}$. Due to resource limitations related to the memory requirement to store all the necessary replicas, we could adopt PTBC for all simulation points but the finest lattice spacings of both SU(5) and SU(8). These points were instead simulated using only one periodic replica, frozen in the $Q = 0$ sector. In these cases, we will assess the size of finite-volume effects via results at coarser lattice spacings, where instead topological freezing is avoided. This, as we will discuss, will allow reliable thermodynamic extrapolations of the scale even in these extreme cases thanks to the observed independence of finite-size corrections of the lattice spacing. Finally, in a few cases we performed additional PBCs simulations to illustrate the reduction of finite-volume corrections on gradient-flow scales attained with TBCs.

The values of the inverse bare 't Hooft coupling selected for each value of N were determined based on the requirements for determining the corresponding SU(N) Λ parameter. In the context of the step-scaling procedure, the Λ parameter is initially obtained in terms of an arbitrary hadronic scale μ_{had} . This must subsequently be converted to one of the conventional scales that are employed in the literature. This reference hadronic scale is defined by the requirement that the renormalized twisted gradient flow (TGF) coupling, at each value of N , must be set to the same value across all the lattices specified in Table II. The method used to tune the lattice sizes in the

N	b	β	Algorithm	N_r	L_d	V_{max}	Δ_s	N_s
3	0.35883	6.459	PTBC	18	4	$24^2 36^2$	4	$1.4 \cdot 10^4$
	0.37583	6.765	PTBC	34	6	$30^2 54^2$	12	$1.6 \cdot 10^3$
	0.38844	6.992	PTBC	54	8	$32^2 60^2$	16	$5.7 \cdot 10^2$
5	0.35971	17.985	PTBC	21	3	$16^2 26^2$	6	$1.6 \cdot 10^4$
	0.37504	18.752	PTBC	32	4	$22^2 40^2$	8	$3.9 \cdot 10^3$
	0.38683	19.342	Std.	1	–	$28^2 46^2$	120	$3.2 \cdot 10^3$
8	0.35867	45.910	PTBC	18	2	$12^2 18^2$	4	$2.5 \cdot 10^4$
	0.38352	49.091	PTBC	46	4	$24^2 36^2$	8	$1.4 \cdot 10^3$
	0.40008	51.210	Std.	1	–	$36^2 60^2$	80	$6.1 \cdot 10^2$

TABLE I: Summary of simulation parameters using TBCs. We report both the inverse bare 't Hooft coupling $b = (N^2 g)^{-1}$ and the standard inverse bare gauge coupling $\beta = 2N^2 b$. With the Standard algorithm, only the physical replica is simulated and there is no defect. In every case, the number of over-relaxation sweeps per heat-bath sweeps is $n_{\text{ov}} = 12$. V_{max} is the largest volume simulated for each (N, b) . For the PTBC algorithm, the number Δ_s of Monte Carlo steps between measures was chosen such that the integrated auto-correlation time of $E(t \simeq t_0)$ is about one. The reported statistics N_s is the number of measures after thermalization, averaged over all the volumes simulated for each (N, b) .

N	b	L	L_s	N	b	L	L_s	N	b	L	L_s
	0.35883	24	8		0.35971	20	4		0.35867	16	2
3	0.37583	36	12	5	0.37504	30	6	8	0.38352	32	4
	0.38844	48	16		0.38683	40	8		0.40008	48	6

TABLE II: Simulation parameters of the lattices tuned to have a TGF coupling $\lambda_{\text{TGF}}^{(0)}(\mu_{\text{had}}) \simeq 44.81$ ($N = 5, 8$) and $\lambda_{\text{TGF}}^{(0)}(\mu_{\text{had}}) \simeq 34.43$ ($N = 3$), corresponding respectively to $l \simeq 1.3$ fm and 1.1 fm, where $l = 1/(0.3\mu_{\text{had}})$.

SU(3) case is described in detail in Refs. [16, 19]. A similar procedure was applied to $N = 5, 8$, for which preliminary results were presented in Ref. [18]. The TGF coupling is defined within the framework of a finite-volume renormalization scheme, wherein the coupling scale is associated with the box size. For TGF, in particular, the setup is analogous to the one presented in this paper, with the exception that the aspect ratio l/l_s is maintained fixed and equal to the number of colors. The coupling is then defined as:

$$\lambda_{\text{TGF}}^{(0)}(\mu) = \mathcal{N}_{\text{cont}}^{-1}(N, l, l/N, t) \varphi'_0(t) \Big|_{\sqrt{8t} = cl = \mu^{-1}}, \quad (37)$$

with $c = 0.3$. The particular choice of the TGF coupling taken to tune the lattices, $\lambda_{\text{TGF}}^{(0)}(\mu_{\text{had}}) \simeq 34.43$ ($N = 3$) and 44.81 ($N = 5, 8$), correspond respectively to constant lattice sizes $l \simeq 1.1$ fm and 1.3 fm (up to lattice artifacts). As we will show, these volumes are not large enough for the determination of the gradient-flow scales, exhibiting finite size effects both in l_s and $l = Nl_s$. An important final cross-check that we will provide with our results for t_0 is that lattices tuned to have the same $\lambda_{\text{TGF}}^{(0)}(\mu_{\text{had}})$ correspond indeed to the same $l/\sqrt{8t_0}$.

B. Scales on an N -by- N basis

We determined the gradient-flow scales with TBCs for three lattice spacings for each value of $N = 3, 5, 8$, with several combinations of lattice sizes. We used both Eq. (6) and Eq. (12) as definitions of the flow, with and without the improvement in Eq. (31). We report the full raw results in the Supplemental Material.

The following analysis of finite-volume effects was carried over in the same way for each N separately and for all the definitions of the scales, only distinguishing whether using the topological projection to $Q = 0$ or not. Thus, we call a generic scale in lattice units S if not projected and $S^{(0)}$ if projected. For the sake of maintaining the discussion compact, we will only show results for t_0 with the normalization of Eq. (6).

Let us start from the scales obtained considering all topological sectors. We will assume that finite-volume corrections are independent of the lattice spacing, once the lattice sizes are expressed in physical units. This allows to fit data obtained at different values of b at once. Also, since at this stage we are analyzing each N separately, we are not enforcing any particular N -dependence in the fit parameters. This will allow to check the expected $1/N^2$ suppression of finite-size corrections in the short size l_s .

Concerning possible finite-volume corrections in the long size l and the effective size $l_s^{(\text{eff})} = Nl_s$, we expect them to be exponentially suppressed as those in l_s , as discussed in Sec. III D. Given that $l_s^{(\text{eff})} > l > l_s$, we will assume them to be sub-leading and negligible. Thus, for each combination of N , b and l_s , we just took the largest $l = l_{\text{max}}$ among those simulated and fitted only the following dependence on l_s :

$$\frac{S(N, b, L_s, L_{\text{max}})}{S(N, b)} = 1 - \hat{A}(N) e^{-M(N) \hat{L}_s(N, b)}. \quad (38)$$

with $\hat{L}_s(N, b) = L_s / \sqrt{8S(N, b)}$. The underlying assumption, which we will check *a posteriori* later, is that the values of l_{max} entering the fitted dataset are large enough in physical units to neglect their associated volume corrections at our statistical precision. In particular, we anticipate that our data will satisfy $\hat{L}_{\text{max}}(N, b) \equiv L_{\text{max}} / \sqrt{8S(N, b)} \gtrsim 3$ in every case, a value which has been shown in previous studies to be sufficient to contain finite-size effects (see, e.g., Refs. [36, 53]).

In Fig. 2 we show the fitted $\hat{l}_s$ -dependence for the improved t_0 . To show all the values of N and b in the same figure, we plot the ratio $T_0(N, b, L_s, L_{\text{max}}) / T_0(N, b)$, where the numerator is our lattice determination, while the denominator is the infinite- l_s limit determined from the fits. Results for different lattice spacings fall on the same curve, confirming our hypothesis that IR finite-size effects are practically insensitive to UV discretization effects.

As it can be seen in Fig. 2, finite-size effects in the short size are well-described by an exponential suppres-

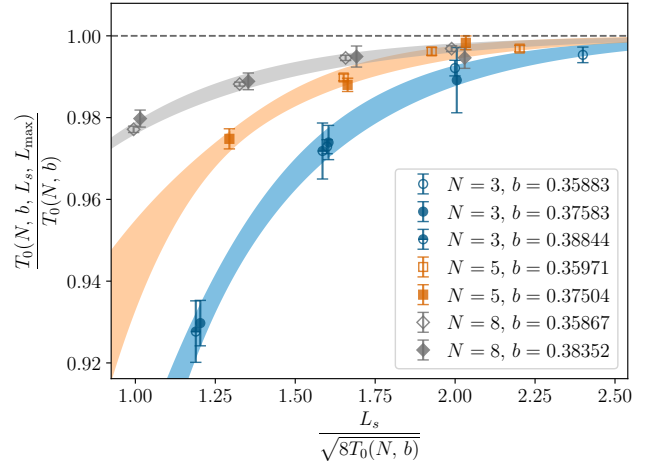


FIG. 2: Dependence on the short size $\hat{l}_s$ of the non-projected scale t_0 with improvement of lattice artifacts, see Eq. (31). The scales $T_0(N, b, L_s, L_{\text{max}})$ are determined at the largest long size $l = l_{\text{max}}$ available, and satisfy $l_{\text{max}} \gtrsim 3\sqrt{8t_0}$. All finite-volume scales are normalized with their corresponding infinite-volume result $T_0(N, b)$ obtained from the N -by- N fits.

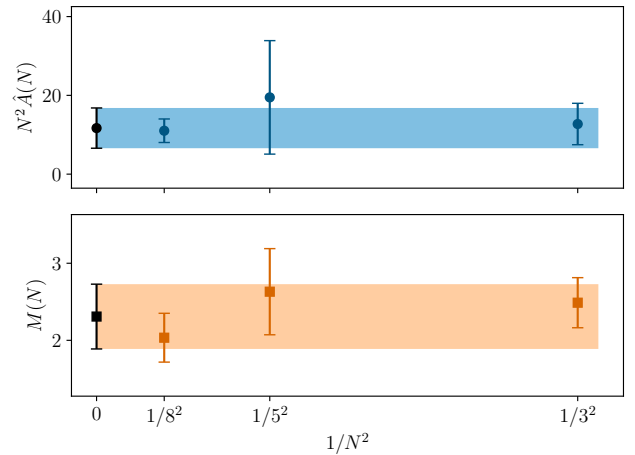


FIG. 3: Dependence on N of the best-fit parameters $\hat{A}(N)$ and $M(N)$ in Eq. (38), obtained from the N -by- N fits of the improved t_0 shown in Fig. 2. As expected, $\hat{A}(N) = \mathcal{O}(N^{-2})$ and $M(N) = \mathcal{O}(N^0)$.

sion, and become smaller at larger N , signaling a suppression of the pre-factor $\hat{A}(N)$ in the large- N limit. Such suppression is expected to be $\sim 1/N^2$, see Eq. (34). In Fig. 3 we indeed see that $N^2 \hat{A}(N)$ has a finite large- N limit, in agreement with our expectations. In the same figure we also show the exponential decay constant M , which turns out to not depend significantly on N , and to be of the same order of magnitude of the Yang-Mills mass gap. Indeed, for the large- N limit of $M = \sqrt{8t_0}m$ we find:

$$M_\infty = \sqrt{8t_0}m_\infty = 2.31(42). \quad (39)$$

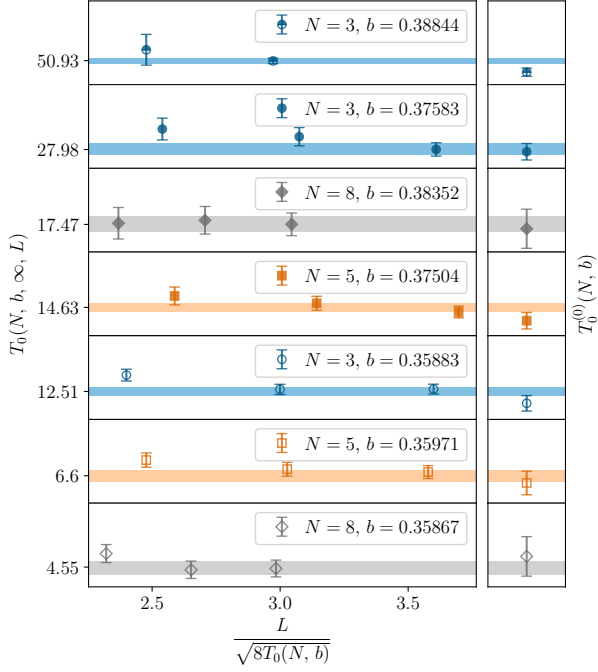


FIG. 4: Left panels: dependence of the non-projected scale t_0 on the long size l after subtraction of the exponentially-suppressed corrections in l_s . Right panels: infinite-volume results for the projected scale $t_0^{(0)}$. Colored bands represent the infinite-volume result for the non-projected scale.

Using $\sqrt{8t_0\sigma}|_{N=\infty} = 1.207(5)$ [28], we find $m_\infty/\sqrt{\sigma} = 1.91(34)$, to be compared with the large- N Yang-Mills mass gap $M_G^{(\infty)}/\sqrt{\sigma} = 3.072(14)$ [54].

To check whether the exponential corrections in the long size are negligible as we assumed, we subtracted the fitted exponential corrections in the short size from the determination of the non-projected scales obtained at different values of l and at one intermediate value of l_s . Results for the improved t_0 , showed in the left panels of Fig. 4, show no residual dependence on $\hat{l}$ for $l \gtrsim 2.7\sqrt{8t_0}$. In this case, all results are compatible among them and with the infinite-volume determination, represented by shaded bands in the figure.

Let us now discuss the scales obtained after projection to $Q = 0$. Again, we will neglect exponentially-suppressed corrections in the long sizes $l, l_s^{(\text{eff})}$, and we will assume finite-size effects to be the same for all b at fixed N . Concerning the dependence on l_s , the leading term appears through the topological correction, which scales as $1/(ll_s^{(\text{eff})})^2 = 1/(Nll_s)^2$, but in our fit we will also consider the sub-leading exponentially-suppressed term in l_s . It will turn out to be much smaller compared to the power-like one, but nonetheless present. Finally, we again fit each data set at different values of N independently and without enforcing any N -dependence in the

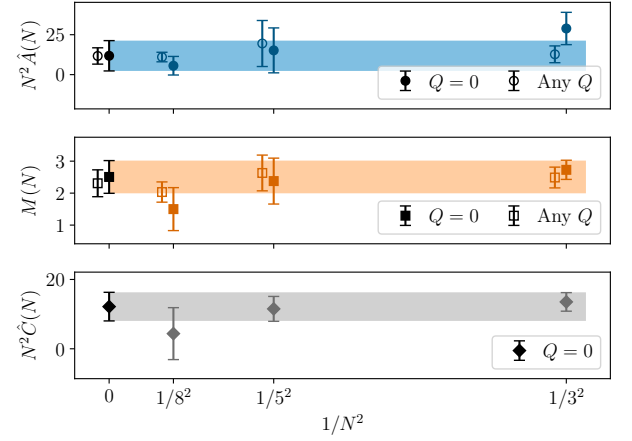


FIG. 5: Dependence on N of the best-fit parameters $\hat{A}(N)$, $M(N)$ and $\hat{C}(N)$ in Eq. (40), obtained from the N -by- N fits of the improved $t_0^{(0)}$. The values resulting from the non-projected fits are also shown. Also in this case, $\hat{A}(N) = \mathcal{O}(N^{-2})$ and $M(N) = \mathcal{O}(N^0)$, and values obtained with and without projection are compatible at each N . Moreover, also $\hat{C}(N) = \mathcal{O}(N^{-2})$ holds as expected.

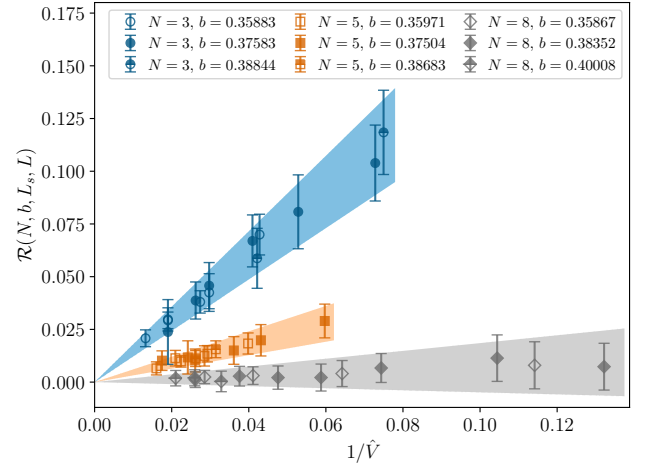


FIG. 6: Residual dependence of the projected scale $t_0^{(0)}$ on the volume $\hat{V} = \hat{L}^2 \hat{L}_s^2$ in physical units, after subtraction of the fitted sub-leading exponential corrections in the short size. The quantity $\mathcal{R}$ is defined in Eq. (41).

pre-factor. In the end, we use the following fit function:

$$\frac{S^{(0)}(N, b, L_s, L)}{S^{(0)}(N, b)} = 1 + \frac{\hat{C}(N)}{\hat{V}} - \hat{A}(N) e^{-M(N)\hat{L}_s(N, b)}, \quad (40)$$

with $\hat{V} = \hat{L}^2 \hat{L}_s^2$ and $\hat{L}_s(N, b) = L_s/\sqrt{8S^{(0)}(N, b)}$. As for the fit without projection, we are neglecting exponentially-suppressed corrections in the long sizes l and $l_s^{(\text{eff})}$. We only include in the fit those points with $\hat{L} \gtrsim 2.7$, for which we do not appreciate finite- $\hat{L}$ effects in the non-projected scales.

For $t_0^{(0)}$, we show in Fig. 5 that the pre-factor $\hat{C}(N)$ is suppressed as $1/N^2$, and that the exponential decay constant $M(N)$ and its pre-factor $\hat{A}(N)$ turn out to be in agreement with the ones found for the non-projected data. These results also hold for the other scale definitions. In Fig. 6, in order to show the finite-size effects associated with the $Q = 0$ projection, we plot the quantity

$$\mathcal{R}(N, b, L_s, L) = \frac{T_0^{(0)}(N, b, L_s, L)}{T_0^{(0)}(N, b)} - 1 + \hat{A}(N) e^{-M(N)\hat{L}_s(N, b)}, \quad (41)$$

that is, the residual finite-size corrections after the subtraction of the fitted exponential term, which is compatible with the one of the non-projected scale t_0 . It can be seen that finite-size corrections after $Q = 0$ projection are indeed dominated by power-like terms, which are suppressed as N is increased.

As a further consistency check, we compared projected scales in the thermodynamic limit, displayed in the right panels of Fig. 4, with the infinite-volume results obtained from the non-projected ones. As it can be seen, we find good agreement among the two determinations. The largest difference that we observe is about 2 standard deviations for the finest lattice spacing at $N = 3$, which is likely due to an under-sampling of topological fluctuations due to insufficient statistics.

In order to give a final result for the scales, we combined the projected and non-projected extrapolated results into one determination, and assigned to each scale a statistical and a systematic error based on the differences between the two determination:

- For the central value, we took the average between the projected and the non-projected infinite-volume scales, weighted with their statistical errors.
- For the statistical error, we just took the smallest of the two.
- For the systematic error, we took the semi-difference between the projected and the non-projected scales, weighted with an estimate of the probability that this difference is not due to a statistical fluctuation:

$$\Delta_{\text{syst}} = \frac{|S - S^{(0)}|}{2} \text{erf} \left(\frac{|S - S^{(0)}|}{2\sqrt{2}\Delta_{\text{stat}}^{(\text{comb})}} \right), \quad (42)$$

with

$$\Delta_{\text{stat}}^{(\text{comb})} = \sqrt{\Delta_{\text{stat}}^2 S + \Delta_{\text{stat}}^2 S^{(0)}}. \quad (43)$$

For the finest lattice spacings of SU(5) and SU(8), we only have the scales projected into $Q = 0$ at our disposal. In these cases, we assigned as a systematic error a fraction of the finite-volume power-like correction due to

Improved — N -by- N fit strategy				
N	b	t_0/a^2	t_1/a^2	w_0^2/a^2
3	0.35883	12.483(36)[22]	5.2414(75)[41]	12.993(75)[44]
	0.37583	27.96(14)[1]	11.734(34)[1]	29.11(25)[2]
	0.38844	50.47(36)[63]	21.11(10)[10]	52.7(6)[1.1]
5	0.35971	6.597(12)[2]	2.6794(22)[19]	7.125(38)[1]
	0.37504	14.611(30)[24]	5.939(6)[11]	15.813(87)[7]
	0.38683	26.07(11)[8]	10.586(22)[17]	28.27(37)[16]
8	0.35867	4.5507(73)[13]	1.8193(10)[4]	4.987(22)[1]
	0.38352	17.470(34)[1]	7.0045(62)[4]	19.182(92)[11]
	0.40008	39.16(16)[1]	15.728(25)[1]	42.86(35)[7]

TABLE III: Infinite-volume scale-setting results of the N -by- N analysis with TBCs, flow normalized as in Eq. (6) and improvement of lattice artifacts in Eq. (31). Results with and without projection onto the $Q = 0$ topological sector are combined into a single value with a systematic error (in square brackets), as explained in the text.

Unimproved — N -by- N fit strategy				
N	b	t_0/a^2	t_1/a^2	w_0^2/a^2
3	0.35883	12.528(35)[23]	5.3052(76)[43]	13.000(75)[44]
	0.37583	28.00(14)[1]	11.797(34)[1]	29.12(25)[2]
	0.38844	50.49(36)[63]	21.17(10)[10]	52.7(6)[1.1]
5	0.35971	6.645(11)[2]	2.7463(23)[20]	7.129(39)[1]
	0.37504	14.656(29)[25]	6.005(6)[11]	15.819(88)[7]
	0.38683	26.10(11)[8]	10.652(22)[17]	28.29(37)[16]
8	0.35867	4.6020(73)[13]	1.8883(10)[4]	4.986(23)[1]
	0.38352	17.518(33)[1]	7.0691(62)[2]	19.184(95)[13]
	0.40008	39.21(16)[1]	15.795(25)[1]	42.86(35)[7]

TABLE IV: Infinite-volume scale-setting results of the N -by- N analysis with TBCs, flow normalized as in Eq. (6) and no improvement of lattice artifacts. Results with and without projection onto the $Q = 0$ topological sector are combined into a single value with a systematic error (in square brackets), as explained in the text.

the topological projection evaluated on the largest volume available: $\Delta_{\text{syst}} = \hat{C}(N)/(4\hat{V})$. We checked that this gives a good upper bound on the systematic error we took for the other cases via Eq. (42). Final results for the improved scales, cf. Eq. (6), are reported in Table III.

Let us now compare our determinations with previous results. In Fig. 7, we show that our results for the SU(3) scale t_0 without improvement, reported in Table IV, are indeed compatible within less than one standard deviations with an interpolation of the results of Ref. [35] in all cases. For SU(5), we can only compare one lattice spacing with Ref. [36], as we explore much finer lattice spacings compared to that study (our coarser lattice spacing is approximately the same as their finest one). Also in this case, our result $t_0/a^2 = 6.645(11)[2]$ is compatible with the interpolation of Ref. [36]’s data $t_0/a^2 = 6.6420(16)$ at $\beta = 17.985$.

Finally, we conclude our discussion by showing, in

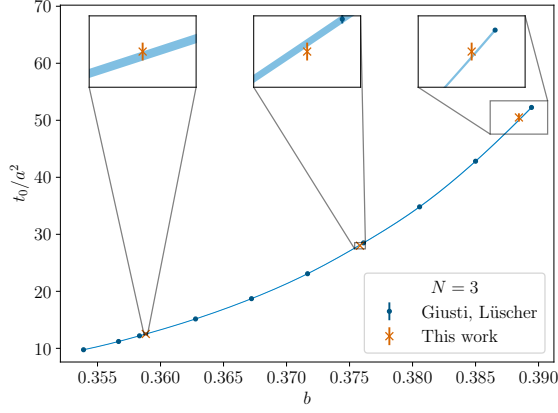


FIG. 7: Comparison of our results for the SU(3) unimproved scale t_0 with a spline interpolation of results of Ref. [35] (shaded band). Displayed errorbars on our points are the quadrature sum of statistical and systematic uncertainties.

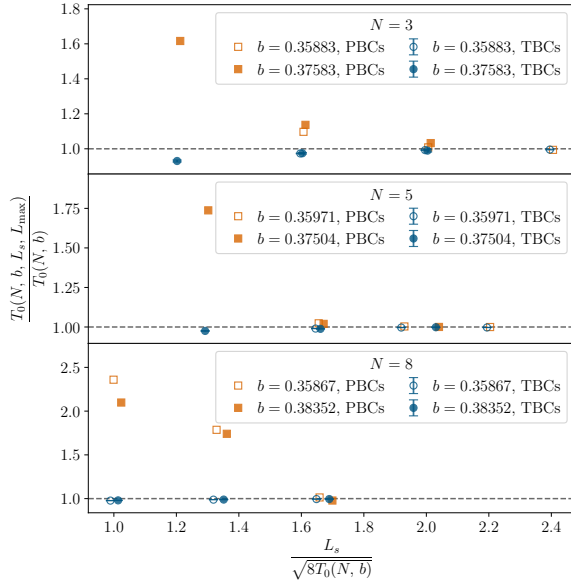


FIG. 8: Comparison of the dependence of the non-projected scale t_0 on the size l_s of the short plane with twisted (TBCs) and periodic (PBCs) boundary conditions. Finite-volume results are normalized with the thermodynamic-limit extrapolation of $t_0(N, b)$ obtained for TBCs. Results for PBCs are reported without errors because those at small l_s are obtained from a linear extrapolation of $\varphi(t)$ beyond the largest time up to which we integrated the flow equation.

Fig. 8, the reduction of finite-volume effects achieved thanks to TBCs over PBCs for the scale t_0 . With TBCs and for a short size $l_s \simeq \sqrt{8t_0} \sim 0.475$ fm, t_0 exhibits a $\sim 10\%$ deviation from the asymptotic value for SU(3), which is reduced to $\sim 2\%$ for SU(8). In the case of PBCs instead, deviations by 50 – 100% are obtained for all N at $l_s \simeq \sqrt{8t_0}$. Asymptotically, boundary conditions do not matter anymore, and the two determinations agree.

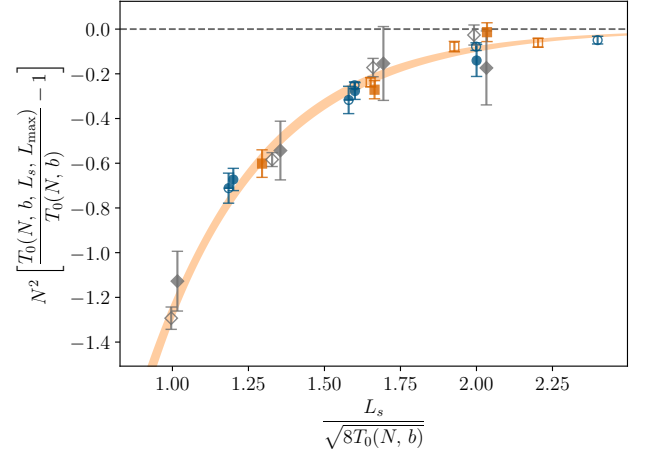


FIG. 9: Dependence of the non-projected scale t_0 on the size l_s of the short, twisted plane, as in Fig. 2, rescaling the finite-volume correction with N^2 . Results are obtained from the global fit imposing $\hat{A}(N) = A_0/N^2$ in Eq. (38).

C. Scales from a global analysis of the N -dependence

The results presented in the preceding section lend support to the hypothesis that finite-size effects in the short twisted directions are suppressed by powers of $1/N^2$. This section will undertake a more thorough examination of finite- N and finite-size effects via a global fit, encompassing all the values of N . We will proceed as before, by analyzing separately the scales obtained by taking into consideration all topological sectors and the ones derived after projection onto the trivial topology sector.

In the case of the non-projected scales, we consider again the fit function in Eq. (38), but we now enforce the following N -dependent form of the pre-factor:

$$\hat{A}(N) = \frac{A_0}{N^2 + A_1} = \frac{A_0}{N^2} \left[1 - \frac{A_1}{N^2} + \mathcal{O}\left(\frac{1}{N^4}\right) \right]. \quad (44)$$

The quality of the global fits is very good, with reduced χ^2 between 0.6 and 1 over 12 degrees of freedom for all the scale definitions. To further check the assumption concerning the N -dependence of the finite-size effects, we also performed the global fits for t_0 setting $A_1 = 0$, that is, neglecting sub-leading corrections to $\hat{A}(N)$, and found a negligible effect on the infinite-volume scales and a still acceptable quality of the fits. To illustrate the goodness of the $1/N^2$ scaling of finite-size effects even with this further constraint, in Fig. 9 we show the quantity

$$N^2 \left[\frac{T_0(N, b, L_s, L)}{T_0(N, b)} - 1 \right]$$

as a function of $\hat{L}_s$ for the improved t_0 . The points, already presented in Fig. 2 with N -by- N fits, are now all

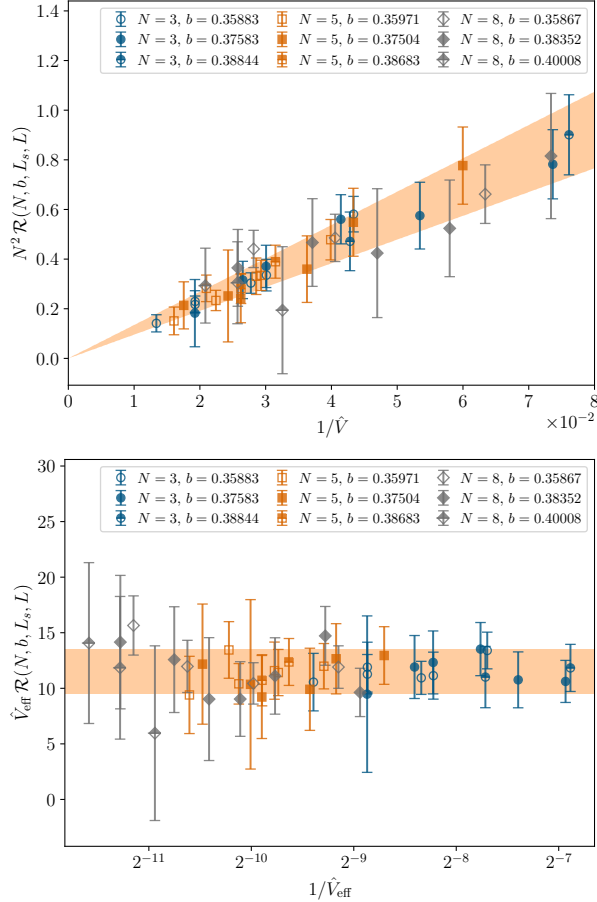


FIG. 10: Leading finite-volume correction $\mathcal{R}$, defined in Eq. (41), affecting the projected scale $t_0^{(0)}$ after the subtraction of the sub-leading exponential term, obtained from the global fit enforcing Eq. (44) and Eq. (45). In the top panel, $\mathcal{R}$ is rescaled by N^2 and showed as a function of the volume in physical units. In the bottom panel, $\mathcal{R}$ is rescaled by the effective volume to better show the quality of the global fit across all the range of volumes and values of N , with the horizontal band representing the fitted value of C in Eq. (45).

fitted together imposing $\hat{A}(N) = A_0/N^2$. As expected, when appropriately scaled with N , all the points collapse on the same curve.

An analogous analysis can be performed for the scales obtained after topological projection. The global fit function is Eq. (40), imposing the form in Eq. (44) for $\hat{A}(N)$ and similarly:

$$\hat{C}(N) = \frac{C}{N^2}, \quad (45)$$

without sub-leading terms. Again, we obtain very good fit qualities. For the improved $t_0^{(0)}$, we show in Fig. 10 the collapse of all the N -dependent curves presented in Fig. 6 when the residual volume correction Eq. (41) is multiplied by N^2 .

These results are a confirmation that the expected volume reduction tied to the use of TBCs is attained, and

Improved — Global fit strategy				
N	b	t_0/a^2	t_1/a^2	w_0^2/a^2
3	0.35883	12.517(27)[3]	5.2443(55)[21]	13.061(56)[10]
	0.37583	28.04(13)[1]	11.743(32)[1]	29.23(23)[1]
	0.38844	50.58(35)[44]	21.12(10)[8]	52.85(62)[90]
5	0.35971	6.6021(75)[35]	2.6801(13)[12]	7.119(19)[5]
	0.37504	14.622(24)[21]	5.9406(48)[65]	15.802(54)[30]
	0.38683	26.086(62)[79]	10.598(14)[15]	28.15(13)[16]
8	0.35867	4.5401(36)[41]	1.81826(73)[96]	4.9610(91)[65]
	0.38352	17.401(24)[52]	6.993(6)[12]	19.046(52)[88]
	0.40008	38.975(66)[36]	15.698(16)[7]	42.58(14)[8]

TABLE V: Infinite-volume scale-setting results of the global analysis of all values of N with TBCs, flow normalized as in Eq. (6) and improvement of lattice artifacts in Eq. (31). Results with and without projection onto the $Q = 0$ topological sector are combined into a single value with a systematic error (in square brackets), as explained in the text.

Unimproved — Global fit strategy				
N	b	t_0/a^2	t_1/a^2	w_0^2/a^2
3	0.35883	12.561(26)[4]	5.3085(56)[22]	13.074(57)[8]
	0.37583	28.07(13)[1]	11.806(32)[1]	29.25(23)[1]
	0.38844	50.60(35)[46]	21.18(10)[8]	52.90(62)[86]
5	0.35971	6.6501(74)[34]	2.7470(14)[13]	7.123(19)[5]
	0.37504	14.667(24)[21]	6.0060(49)[65]	15.809(54)[29]
	0.38683	26.129(61)[81]	10.664(14)[15]	28.16(13)[16]
8	0.35867	4.5912(36)[45]	1.8873(7)[11]	4.9593(92)[64]
	0.38352	17.450(24)[52]	7.059(6)[12]	19.047(52)[88]
	0.40008	39.021(66)[37]	15.764(16)[7]	42.59(14)[8]

TABLE VI: Infinite-volume scale-setting results of the global analysis of all values of N with TBCs, flow normalized as in Eq. (6) and without improvement of lattice artifacts in Eq. (31). Results with and without projection onto the $Q = 0$ topological sector are combined into a single value with a systematic error (in square brackets), as explained in the text.

that no residual dependence of finite-size effects in the short twisted directions remains in the large- N limit. The infinite-volume extrapolated scales extracted from these global fits are presented in Table VI, and compared with the results obtained in the previous section in Fig. 11. The two determinations agree within errors in every case.

D. Discussion of the obtained results

In this section, we calculate specific ratios of gradient-flow scales and extrapolate them to the continuum and large- N limits. These ratios are of particular utility as conversion factors between scales. To demonstrate the effectiveness of the improvement in Eq. (31) in reduc-

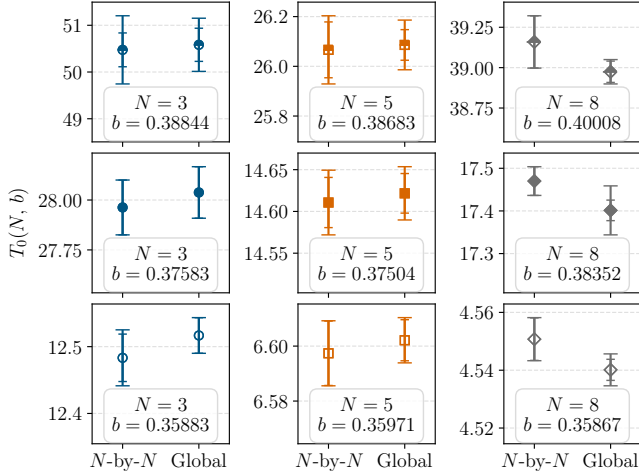


FIG. 11: Final comparison among results obtained from the N -by- N and the global fit strategies to extrapolate towards the thermodynamic limit. Plot refers to improved scales.

ing lattice artifacts, we will employ both the improved and unimproved scales. It is important to note that ratios of improved scales are not expected to be free of $\mathcal{O}(a^2)$ lattice artifacts. Besides the cut-off effects associated with the discretization of the energy and canceled at tree-level with Eq. (31), other corrections arise from the discretization of the simulated action and of the flow equation [8, 50]. Thus, we will assume leading $\mathcal{O}(a^2)$ lattice artifacts for both unimproved and improved ratios.

Ratios of scales are computed with the infinite-volume results of the N -by- N analysis discussed in Sec. IV B and presented in Tables III and IV. The statistical error assigned to each ratio is estimated by adding in quadrature the statistical errors on the numerator and denominator as if they were uncorrelated. This is a conservative option, which over-estimates the uncertainty in the ratios. Concerning systematic errors, we took them into account separately via a bootstrap analysis: each scale is resampled adding a zero-mean bias with variance equal to the systematic error. Then, the systematic error on the extrapolation is computed via the bootstrap mean of Eq. (42), considering the difference between the extrapolation obtained without systematic errors and the ones obtained in each bootstrap sample. We found that the resulting systematics are completely negligible with respect to statistical errors, which dominate the total errors on our final results.

Similarly to the analysis of finite-volume effects, we adopt two fitting strategies to determine the continuum and large- N limits. In one case, we first perform the continuum extrapolation of each ratio for each value of N separately, then we extrapolate the continuum results to $N = \infty$. The fit function for the continuum extrapolations is

$$\frac{S_1(N, b)}{S_2(N, b)} = R(N) \left[1 + \frac{D(N)}{8S_2(N, b)} \right], \quad (46)$$

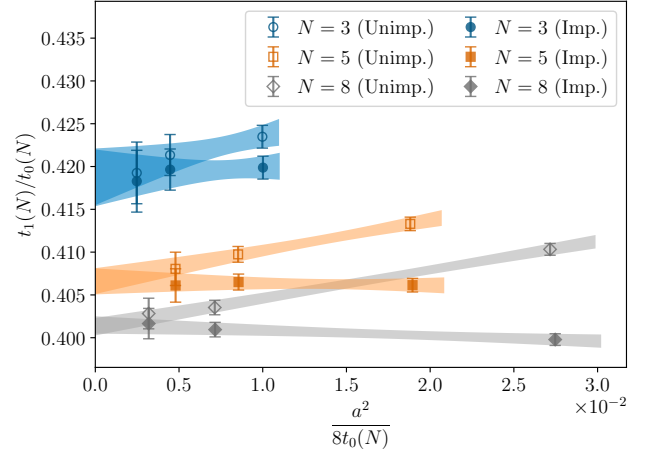


FIG. 12: Continuum extrapolations of the ratio t_1/t_0 for several values of N , with and without the improvement in Eq. (31). Each dataset at different value of N , as well as improved/unimproved datasets, have been fitted separately.

where $1/S_2(N, b)$ measures a^2 in units of the denominator scale. The fit parameters are $D(N)$ and $R(N)$, the ratio between the scales S_1 and S_2 in the continuum limit. The large- N limit R of the ratios is then obtained by fitting

$$R(N) = R \left(1 + \frac{C}{N^2} \right), \quad (47)$$

that is, assuming leading $1/N^2$ corrections. In Fig. 12 we show the continuum extrapolations of the ratio t_1/t_0 for all values of N , with and without improvement of lattice artifacts. As it is evident, the improved scale determinations demonstrate a reduced lattice-spacing dependence compared to the unimproved ones. In particular, the pre-factor $D(N)$ turns out to be very small and practically compatible with zero, possibly due to an accidental cancellation of the $\mathcal{O}(a^2)$ corrections on the scales in the ratio, at least up to our precision. The difference between the two continuum extrapolations is negligible with respect to the statistical error. These observations hold for all values of N and also for the other ratios of scales we computed. The continuum and large- N limits for the ratios of t_1 and w_0^2 over t_0 are presented in Table VII. Other ratios, best-fit parameters and the quality of the fits are reported in the Supplemental Material.

The results of the N -by- N fits show a negligible dependence on N of the pre-factor controlling the size of lattice artefacts, $D(N)$. This observation motivates our second strategy, in which we perform a global fit of finite- a and finite- N effects according to the following function:

$$\frac{S_1(N, b)}{S_2(N, b)} = R \left(1 + \frac{C}{N^2} \right) \left[1 + \frac{D}{8S_2(N, b)} \right]. \quad (48)$$

As an example of the very good quality of the global fits,

N-by-N fit strategy				
N	Unimproved		Improved	
	t_1/t_0	w_0^2/t_0	t_1/t_0	w_0^2/t_0
3	0.4188(33)	1.044(14)	0.4187(33)	1.043(14)
5	0.4066(15)	1.085(11)	0.4066(15)	1.085(11)
8	0.4013(10)	1.0976(66)	0.4015(10)	1.0973(65)
∞	0.3985(13)	1.1067(77)	0.3988(13)	1.1064(76)

TABLE VII: Continuum scale ratios from the *N*-by-*N* analysis of unimproved and improved scales.

Global fit strategy				
N	Unimproved		Improved	
	t_1/t_0	w_0^2/t_0	t_1/t_0	w_0^2/t_0
3	0.4203(11)	1.0430(55)	0.4207(11)	1.0416(55)
5	0.40637(75)	1.0839(49)	0.40655(74)	1.0832(48)
8	0.40159(88)	1.0980(58)	0.40171(88)	1.0975(57)
∞	0.3985(10)	1.1070(66)	0.3986(10)	1.1066(65)

TABLE VIII: Continuum scale ratios from the global analysis of unimproved and improved scales.

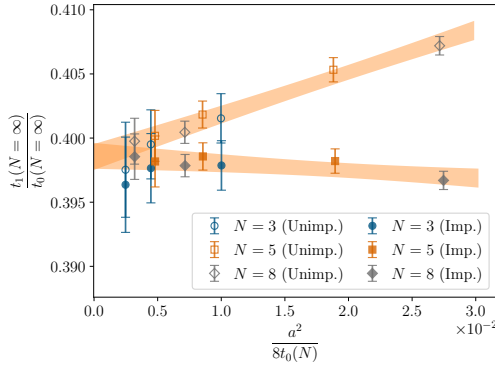


FIG. 13: Continuum extrapolation of the large-*N* ratio t_1/t_0 , with and without the improvement in Eq. (31). All values of *N* are fitted together in a global fit of both finite-*N* effects and lattice artifacts according to the fit function in Eq. (48).

we show in Fig. 13 the quantity

$$\frac{S_1(N, b)}{S_2(N, b)} \left(1 + \frac{C}{N^2}\right)^{-1},$$

representing the lattice-spacing-dependence in the large-*N* limit, for the ratio of t_1 and t_0 . The points at different values of *N*, already presented in Fig. 12, collapse into two single curves, corresponding to the ratios of scales with and without improvement. The two strategies give perfectly compatible results at each finite *N* and in the large-*N* limit, as illustrated in Fig. 14, where we show the *N*-dependence of the improved and continuum-extrapolated ratio. Results from the global fit are reported in Table VIII.

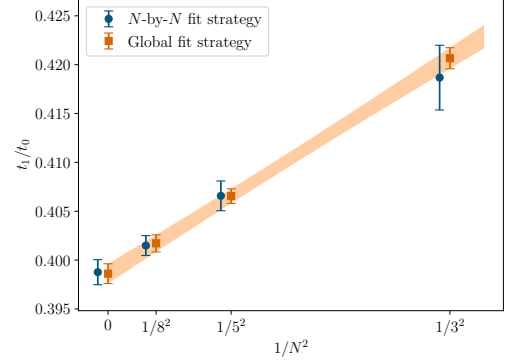


FIG. 14: Large-*N* extrapolation of the continuum-extrapolated ratio t_1/t_0 with the improvement in Eq. (31). All values of *N* are fitted together in a global fit of both finite-*N* effects and lattice artifacts. The points resulting from the *N*-by-*N* fits presented in Fig. 12 and their large-*N* extrapolation are also shown.

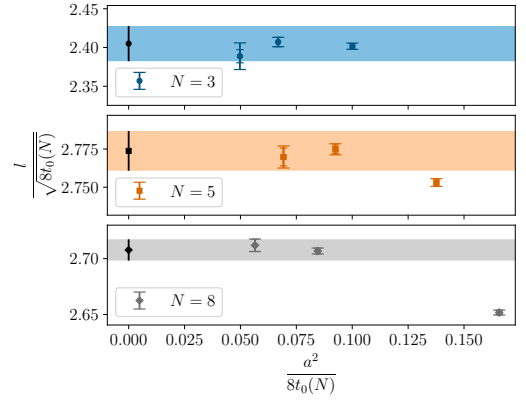


FIG. 15: Lattice sizes in units of the improved t_0 for the simulations in Table II, with parameters calibrated via the TGF coupling. Colored bands represent a fit to a constant excluding the coarsest lattice spacing with errors multiplied by 4.

As a further consistency check of our calculations, we also computed the $N = \infty$ ratios t_0/t'_0 and t'_1/t'_0 . These can be compared with the same quantities recently obtained within the Twisted Eguchi-Kawai (TEK) model [55–57] in the large-*N* limit. We find $t_0/t'_0 = 1.1433(42)$ and $t'_1/t'_0 = 0.3744(11)$, in good agreement with TEK results $t_0/t'_0 = 1.140(3)$ and $t'_1/t'_0 = 0.3953(125)$.

Finally, let us conclude our discussion by using our scale-setting results to compute the values of the lattice size in physical units for the simulation parameters calibrated via the TGF coupling reported in Table II. For each *N*, those simulation points should all correspond to the same value of $l = aL/\sqrt{8t_0}$, modulo small lattice artifacts. We show results for l in Fig. 15. As it can be observed, our results for the scale setting support our theoretical expectations. In particular, using $\sqrt{8t_0} \simeq 0.475$ fm [35], we find $l \simeq 1.14$ fm for $N = 3$ and $l \simeq 1.30$ fm

for $N = 5, 8$, as expected.

V. CONCLUSIONS

In this paper we have presented scale-setting results for large- N Yang–Mills theory obtained via the gradient flow. This is the first step within a larger project whose ultimate goal is to achieve the first lattice determination of the large- N Yang–Mills Λ -parameter using the step scaling method.

Scale setting at large- N for step scaling applications requires to explore a regime of lattice Yang–Mills theories (large values of N , fine lattice spacings), where topological freezing is extremely severe. In this study we tackled this problem by adopting the Parallel Tempering on Boundary Conditions (PTBC) to effectively reduce autocorrelation times of topological quantities, and Twisted Boundary Conditions (TBCs) to exploit large- N volume reduction and keep finite-size effects under control.

Our setup allow us to achieve control over systematic finite-size effects, both of standard nature and due to the fixed topological background that would be obtained in the presence of topological freezing. In particular, we are able to clearly probe the exponentially-suppressed finite volume effects dominating scale setting quantities in the presence of a properly-sampled topology, and the power-like ones dominating topology-projected scale determinations. Moreover, we are also able to numerically show the expected $1/N^2$ suppression of finite-volume effects in the short, twisted lattice size l_s expected on general theoretical grounds by virtue of large- N volume independence.

We concluded our study providing a series of cross checks of our results. For $N = 3$, our results for t_0 agree with those obtained from Master Field simulations. In the large- N limit, ratio of scales are found in agreement with those determined using the Twisted Eguchi–Kawai (TEK) model with N as large as 841. Finally, we verified that lattice parameters calibrated to have the same renormalized strong coupling in the so-called Twisted Gradi-

ent Flow scheme indeed corresponded to the same physical value of the lattice size $\hat{l} = aL/\sqrt{8t_0}$ (up to small lattice artifacts).

In the next future, we will employ the results presented in this study to set the scale in our forthcoming step scaling study of the large- N Yang–Mills Λ -parameter. Indeed, step scaling determines Λ in units of an arbitrary energy scale μ_{had} . Our scale-setting results will thus allow the conversion of μ_{had} , and thus of Λ , into units of $\sqrt{8t_0}$. This investigation will be presented in a forthcoming publication.

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