Finite-temperature Yang-Mills theories with the density of states method: towards the continuum limit

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A first-order, confinement/deconfinement phase transition appears in the finite temperature behavior of many non-Abelian gauge theories. These theories play an important role in proposals for completion of the Standard Model of particle physics, hence the phase transition might have occurred in the early stages of evolution of our universe, leaving behind a detectable relic stochastic background of gravitational waves. Lattice field theory studies implementing the density of states method have the potential to provide detailed information about the phase transition, and measure the parameters determining the gravitational-wave power spectrum, by overcoming some of the challenges faced by importance-sampling methods. We assess this potential for a representative choice of Yang-Mills theory with $Sp(4)$ gauge group. We characterize its finite-temperature, first-order phase transition, in the thermodynamic (infinite volume) limit, for two different choices of number of sites in the compact time direction, hence taking the first steps towards the continuum limit extrapolation. We demonstrate the persistence of non-perturbative phenomena associated to the first-order phase transition: coexistence of states, metastability, latent heat, surface tension. We find consistency between several different strategies for the extraction of the volume-dependent critical coupling, hence assessing the size of systematic effects. We also determine the minimum choice of ratio between spatial and time extent of the lattice that allows to identify the contribution of the surface tension to the free energy. We observe that this ratio scales non-trivially with the time extent of the lattice, and comment on the implications for future high-precision numerical studies.

I. INTRODUCTION

Finite-temperature, first-order phase transitions in gauge theories are critical to our understanding of particle physics and cosmology. Yet, their characterization on the lattice requires overcoming algorithmic and technological challenges. It is hence the subject of a vast literature, both for $SU(3)$ gauge theories—see for example the discussion in Ref. [1], the review [2], and references therein, in particular Refs. [3, 4], but also Refs. [5–17] and Refs. [18–24]—and for other gauge groups, relevant for new physics [25–39].

Appealing extensions of the Standard Model (SM) of particle physics postulate the existence of new dark sectors [40–46], taking a variety of forms: composite dark matter models [47–56], strongly interacting massive particle (SIMP) models [57–69], dark dilaton effective field theories [70–72]. They address puzzles in the Standard Model of cosmology, such as observational evidence that dark energy and dark matter, that have no SM explanation, dominate our present universe (see, e.g., the review in Ref. [73]). Even explaining the observed baryonic component requires a matter-antimatter asymmetry that admits no dynamical SM origin—see Refs. [74, 75] for reviews, and references therein. In particular Refs. [76–83] show the failure of the Sakharov's out-of-equilibrium

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condition [84] for electroweak baryogenesis.

If the dark sector gauge theory undergoes, in the early universe, a strong first-order phase transition, it leads to the emission of gravitational waves [85–90], potentially detectable by future experimental programmes [91–108]—see also Ref. [109]. Appraising the viability of experimental searches necessitates a precise characterization of the physics in proximity of the transition, including a measurement of the parameters that control the gravitational wave (GW) power spectrum. Of particular interest are α, which is a measure of the strength of the transition, and β/H_* [107], where β corresponds to the duration of the phase transition and H_* is the Hubble parameter at the transition. The latent heat can be related to α and the bubble nucleation rate (and bubble surface tension) can be related to β/H_*.[1]

The main challenge for the direct lattice numerical calculation of these quantities (that act as input values in numerical packages such as PTPlot [107]) is that first-order phase transitions are accompanied by phase coexistence and metastability. These phenomena compromise ergodicity and detailed balance requirements of traditional importance-sampling techniques, based on Markov chain Monte Carlo update algorithms, and lead to critical slowing down [111]. Indirect routes can be pursued to estimate the power spectrum in strongly coupled theories [112–117], using effective Polyakov-loop theory [118–126] and matrix models [127–135]. Most recently, gauge-gravity duality techniques [136–139], adapted to capture confinement and chiral symmetry breaking [140–150], have also been used for the treatment of first-order phase transitions in strongly coupled field theories—see, e.g., Refs. [151–163].

This paper adopts a new, alternative strategy to gain direct access to the proximity of first-order phase transitions, that takes inspiration from flat histogram [111] and density of states [164] methods. The Logarithmic Linear Relaxation (LLR) algorithm [165–168]—see also Ref. [169]—is precisely described in the body of the paper. The underlying idea is to scan the space of configurations with a density function inspired by the microcanonical (rather than canonical) ensemble in statistical mechanics, and treat on equal footing stable, metastable, as well as unstable configurations of the lattice system, overcoming the difficulties connected with importance sampling methods. A number of increasingly sophisticated analyses have already been performed, pertaining to Abelian gauge theories [167], and to $SU(3)$ theories at zero [168] and finite temperature [170–172]. Finite-temperature studies exist also for $Sp(4)$ [173], $SU(4)$ [174, 175] and $SU(N_c)$ [176, 177], all of which yield encouraging preliminary results.

We consider a non-Abelian gauge theory—the $Sp(4)$ Yang–Mills theory in four dimensions—characterize its finite-temperature deconfinement transition using the LLR algorithm, and perform the first scaling test to approach the continuum and infinite-volume limits. To this purpose, we discretize the theory on hypercubic lattices with varying number of sites on the temporal, $N_t = 4$ and $N_t = 5$, and spatial, N_s, directions, measure a set of observables, extrapolate them to the physical limits, and assess the magnitude of methodological systematic uncertainties. The free energy density of the theory displays its multivalued nature in a region of parameter space in proximity of the first-order phase transition. We estimate the critical couplings at finite volume, β_{CV}, (in the following referred to as critical couplings, for brevity) extracted in several complementary ways, with finite spatial volume of the lattice. We also measure the specific heat and surface tension. We study in detail how all the lattice observables converge to continuum field theory quantities in the limits of $N_s \to +\infty$ (the infinite-volume, or thermodynamic, limit) and $N_t \to +\infty$.

The TELOS collaboration has been carrying out a systematic programme of lattice studies of the $Sp(2N)$ gauge theories, both in the pure gauge case [178–182], as well as in the presence of fermion matter fields [178, 183–196], reshaping our understanding of these theories—see also the review in Ref. [197], as well as Refs. [68, 198–200]. The $Sp(4)$ Yang-Mills theory is the most accessible and best understood one in this class, and hence a natural target of the present study, though our results are expected to be relevant also for the study of other gauge groups (see Ref. [172] for $SU(3)$). The study presented in this paper uses some of the technology TELOS developed and made publicly available, such as the implementation within the HiRep code [201, 202] of the adaptations needed for the study of $Sp(N_c = 2N)$ theories [178, 203], and the implementation of the heat bath and domain decomposition initially implemented for $SU(N_c)$ gauge groups [172, 204], extended to symplectic gauge groups [173, 205].

The paper is organized as follows. In Sect. II, we outline the methodology based on the density of states. We describe pedagogically the relevant aspects of the density of states methods, and the implementation of the LLR algorithm in the (continuum) field theory context of relevance. In Sect. III, we discuss the numerical lattice field theory of interest and the formulation of the LLR algorithm on a finite lattice. We report our new results in Sec. IV. This section contains also critical discussions, which include direct comparisons to the existing, published data, obtained with smaller time and space extents of the lattice. We conclude in Sec. V, by summarizing the main results of the study, and outlining future avenues for investigation. We collect some technical aspects of the numerical study in the Appendix.

II. FIELD THEORY FORMULATION OF THE LLR ALGORITHM

In this section, we introduce the density of states methodology for non-Abelian gauge theories, and its im-

[1] Calculating the nucleation rate is itself a challenging task [110].

plementation in the LLR algorithm. The presentation is self-contained and pedagogical, and we refer to the literature for additional details [165–169]. We also discuss our implementation of the replica exchange, to enforce ergodicity, and comment on our estimation of errors.

A. Density of states

We write the partition function of the Yang-Mills gauge theory with group $Sp(2N)$, treated in isolation from any other fields (including SM ones) as follows:

$$Z(\beta) \equiv \int [DA]\, e^{-\beta S[A]}\,, \quad (1)$$

where $\beta \equiv 4N/g_0^2$, with g_0 the bare gauge coupling, and $[DA]$ the (Haar) measure. The Euclidean action, $S[A]$, is expressed as a function of the gauge fields, $A = \sum_B A_\mu^B T^B$, where T^B are the generators of the group, while

$$S[A] \equiv \int \mathrm{d}^4x\, \mathrm{Tr}\left[\frac{1}{2}F_{\mu\nu}(x)F_{\mu\nu}(x)\right]\,, \quad (2)$$

and the field-strength tensor is

$$F_{\mu\nu}(x) \equiv \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + i[A_\mu(x)\,,\, A_\nu(x)]\,. \quad (3)$$

Notice how we made explicit the dependence on β in the exponential weight, rather than in the action.

The expectation value of a generic operator, $O[A]$, that depends on the gauge fields, is

$$\langle O\rangle_\beta \equiv \frac{1}{Z(\beta)}\int [DA]\, O[A] e^{-\beta S[A]}\,. \quad (4)$$

This expression implicitly defines a probability density in the space of the fields, $\mathrm{d}P_\beta[A]$, taking the form

$$\mathrm{d}P_\beta(A) = \frac{1}{Z(\beta)}\,[DA]\, e^{-\beta S[A]}\,. \quad (5)$$

In the presence of a first-order transition, this probability density may show multiple, inequivalent stationary points, corresponding to coexisting phases. On the lattice, importance-sampling (Markov chain) algorithms have exponentially suppressed transition rates in Monte-Carlo time between regions near different local maxima of the probability distribution. The resulting freezing of the updates near one of the local maxima introduces the aforementioned violations of ergodicity and detailed balance (hysteresis). Ultimately, the resulting critical slowing down [111] makes it unfeasible to overcome the problem with realistic amounts of computational resources.

The approach based upon the density of states, $\rho(E)$, is designed to overcome these challenges. One constrains the action, $S[A]$, to match the energy, $S[A] = E$:

$$\rho(E) \equiv \int [DA]\, \delta(S[A] - E)\,, \quad (6)$$

and then rewrites the ensemble average of any operator that is only a function of the action $O(E = S[A])$ as[2]

$$\langle O\rangle_\beta = \frac{1}{Z(\beta)}\int \mathrm{d}E \rho(E) O(E) e^{-\beta E}\,. \quad (7)$$

The calculation of $\langle O\rangle_\beta$ for a value of β therefore requires determining the density of states, $\rho(E)$, at all values of the energy $S[A] = E$. As in the process we explore all values of E individually, there is no concern about transitions between inequivalent configurations (phases), that have different energy, E. The probability distribution density for a given energy is then written as

$$P_\beta(E) = \frac{1}{Z(\beta)}\rho(E) e^{-\beta E}\,. \quad (8)$$

This method can yield a precise determination of the critical coupling, since β is no longer a parameter entering the Monte Carlo calculations, but rather can be tuned freely once $\rho(E)$ has been determined numerically. The non-trivial algorithm leading to such determination is the subject of the next subsection.

B. Linear logarithmic relaxation (LLR)

When computing ensemble averages with Eq. (7), one finds that they are dominated by integrations over finite energy intervals. We use this empirical observation to guide our heuristic choice of the range $[E_{\mathrm{min}}, E_{\mathrm{max}}]$, which includes all such intervals, but requires deploying only limited amounts of computational resources, as we neglect exponentially suppressed contributions from other energies. A caveat to this approach is that it compromises the implementation of the third law of thermodynamics, which would require the continuous mapping of $\rho(E)$ to reach the low energy regime close to zero temperature. The drawback is the appearance of an arbitrary constant, to which we return shortly.

We cover the energy range, $[E_{\mathrm{min}}, E_{\mathrm{max}}]$, with intervals of finite width, $\Delta_E/2$,[3] centered around regularly spaced energies, $E_0^{(n)}$, for $n = 1, \ldots, N$. We characterize the density of states in terms of its logarithmic derivative, $a(E)$, defined as

$$a(E) \equiv \frac{\mathrm{d}}{\mathrm{d}E}\log\rho(E)\,, \quad (9)$$

which we determine by modelling it with the approximation $\log\tilde\rho(E) \simeq \log\rho(E)$, consisting of a piecewise-linear function defined so that

$$\log\rho(E) \;\simeq\; \log\tilde\rho(E) \equiv a^{(n)}\left(E_0^{(n)} - E\right) + c^{(n)}\,, \quad (10)$$
$$\text{for } E \in \left[E_0^{(n)} - \frac{\Delta_E}{4}, E_0^{(n)} + \frac{\Delta_E}{4}\right]\,.$$

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[2] This approach can be generalized to other observables, such as the Polyakov loop, in which case additional information may be required—see, e.g., the discussion in Ref. [167].

[3] We follow the notation from Ref. [173].

The determination of $\tilde{\rho}$ is then equivalent to the reconstruction of all $a^{(n)}$, and $c^{(0)}$. The coefficients $c^{(n)}$, with $n > 0$, are determined by requiring continuity. The first coefficient, $c^{(0)}$, is left undetermined by this approach, but as anticipated only results in an overall normalization of the partition function, $Z(\beta)$, that drops out of ensemble averages such as those in Eq. (7).

In order to illustrate how we determine the numerical values of $a^{(n)}$, we introduce the restricted expectation value, for which we use the double-bracket notation:

$$\langle\langle f \rangle\rangle_n(\hat{a}) \equiv \frac{1}{\mathcal{N}_n(\hat{a})}\int D[A] f[A] e^{-\hat{a}\left(S[A]-E_0^{(n)}\right)} W(S[A]-E_0^{(n)},\delta)\,, \tag{11}$$

$$\text{where} \quad \mathcal{N}_n(\hat{a}) \equiv \int D[A] e^{-\hat{a}\left(S[A]-E_0^{(n)}\right)} W(S[A]-E_0^{(n)},\delta)\,, \tag{12}$$

$$\text{and} \quad W(x,\delta) \equiv \begin{cases} 1\,, & \text{if} \quad -\delta/2 < x < \delta/2 \\ 0\,, & \text{otherwise} \end{cases}\,, \tag{13}$$

for any function, $f(A)$, of the fields, A.[4] Here, $\hat{a}$ is a generic parameter, while $W(x,\delta)$ restricts the energy to an interval centered around x with fixed width, δ.

As the double-bracket expectation value, $\langle\langle f \rangle\rangle_n(\hat{a})$, in Eq. (11) can be explicitly rewritten in the form of Eq. (4), it can be calculated using standard Monte-Carlo techniques. But because the energy is restricted to an interval, this calculation (for sufficiently small choices of interval, δ) is not affected by the aforementioned challenges, due to possible metastability and phase coexistence. Furthermore, it can be shown that [165]

$$\langle\langle S[A] - E_0^{(n)} \rangle\rangle_n(\hat{a} = a^{(n)}) = 0\,. \tag{14}$$

This observation allows to translate the problem of determining $a^{(n)}$ (and the density of states) into the algebraic solution of Eq. (14), for each interval labeled by n. We do so iteratively, with a combination of the Newton-Raphson (NR) and Robbins-Monro (RM) updates as defined below [206]—see also Tab. I for the exact number of the respective number of iterations. After estimating the derivative of $\langle\langle S[A] - E_0^{(n)} \rangle\rangle_n$ [165, 167], we arrive at the iterative equation

$$a_{k+1}^{(n)} = a_k^{(n)} - \alpha_{k+1}\frac{12}{\delta^2}\langle\langle S[A] - E_0^{(n)} \rangle\rangle_n(a_k^{(n)})\,, \tag{15}$$

where $\alpha_k = 1$ for the standard Newton-Raphson method, and $\alpha_k = 1/k$ for the Robbins-Monro updates. The Robbins-Monro algorithm guarantees that the iteration prescription converges for stochastic estimations, which we use when calculating the double-bracket expectation values, as $\sum_k \alpha_k \to \infty$ while $\sum_k \alpha_k^2$ remains finite [206].

[4] The double bracket in the notation reflects the fact that this object closely resembles the simultaneous application of microcanonical and canonical ensembles, as it amounts to restricting the integration to a narrow interval around a given value of the energy, $E_0^{(n)}$, but also to multiplying the integrand by a weight function depending exponentially on $S[A]$—an overall factor of $e^{\hat{a}E_0^{(n)}}$ drops from the ratio with the normalization, $\mathcal{N}_n(\hat{a})$.

C. Ergodicity and replica exchanges

A potential ergodicity flaw of the algorithm ensues from the fact that configurations with an energy in the same interval might only be connected via local updates by allowing intermediate energies outside the interval which is not possible within the framework defined by Eq. (11). Following Ref. [167], we apply the *replica exchange method* [207, 208] to overcome this impasse. The number of replicas equals that of energy intervals used in the algorithm, $N_{\rm rep} = N$. Furthermore, we choose the energy intervals to overlap with the neighboring ones and simulate all intervals in parallel, by fixing the central energies to be spaced by half the interval width [172, 173], so that

$$E_0^{(n+1)} - E_0^{(n)} = \Delta_E/2\,, \tag{16}$$

and setting $\delta = \Delta_E$.

When two Markov chains of neighbor intervals are in the overlap region, we swap them with a probability of

$$P_{\rm swap} = \min\left(1, e^{\left(S[A^{(n)}]-S[A^{(n+1)}]\right)\left(a^{(n)}-a^{(n+1)}\right)}\right)\,. \tag{17}$$

We further modify Eq. (11) for the first and last energy intervals, $n = 1$ and $n = N = N_{\rm rep}$, by allowing the Monte Carlo to probe energies outside the range $[E_{\rm min}, E_{\rm max}]$, with probability distribution proportional to the Boltzmann weight $\exp(-\beta S[A])$, as in typical importance sampling calculations. This allows the Markov chains to probe all possible energies and thus ensure ergodicity.

D. Error estimation

In our numerical calculations, we terminate the iteration in Eq. (15) after a fixed number of updating steps. We initialise the system by performing a fixed number of Newton-Raphson updates, $n_{\rm NR}$. We follow this by a fixed number of Robbins-Monro updates, $n_{\rm RM}$ We estimate the error by repeating the same iteration prescription multiple times, while starting from a different random configuration. Error estimates are then obtained using a jackknife analysis over the final result of the repeated calculations, $N_{\rm repeats}$.

III. LATTICE FORMULATION

The ensemble averages entering Eq. (14), and hence the reconstruction of the density of states, are computed by discretising the theory on a hypercubic lattice with finite spacing, a, and space-time volume, $\tilde{V} = (N_t a) \times (N_s a)^3$. We impose periodic boundary conditions in all directions, and interpret the temporal extent of the lattice, characterized by $N_t < N_s$, in terms of the temperature of the system at equilibrium.

We adopt the Wilson gauge action, expressed in terms of the plaquette, $U_{\mu\nu}(x)$, itself a function of a (gauge) link configuration as

$$S[U] \equiv \frac{1}{N_c} \sum_x \sum_{\mu<\nu} {\rm Re}\,{\rm Tr}\left[1 - U_{\mu\nu}(x)\right] . \qquad (18)$$

It is notationally convenient to express the action, $S[U]$, in terms of the average value of the plaquette

$$u_p \;\equiv\; \frac{a^4}{6\tilde{V}} \frac{1}{N_c} \sum_x \sum_{\mu<\nu} {\rm Re}\,{\rm Tr}\left[U_{\mu\nu}(x)\right] , \qquad (19)$$

where $N_c = 4$, for $Sp(4)$, and use the equivalent expression

$$S[U] = \frac{6\tilde{V}}{a^4}\left(1 - u_p[U]\right) . \qquad (20)$$

Our measurements are characterized by the extent of the lattice, the range of energies considered—equivalently, the average plaquette, u_p—the number of intervals/replica, $N = N_{\rm rep}$, and repeats. We report the lattice sizes and parameters used in this work in Tab. I, in which we indicate explicitly also the number of NR and RM iterations, for each lattice. As anticipated, the HiRep code [201, 202], supplemented with the symplectic adaptations [178, 203], has been used, in particular for the domain decomposition of the heat bath algorithm [173, 205]. We decompose each replica into four domains, along one of the spatial dimensions, as in Ref. [173]. Every double-bracket expectation value is based on a restricted Monte Carlo Markov chain. We first perform 300 updates to thermalize the energy-restricted Markov chain. We then measure the operator of interest on 700 thermalized configurations, generated using the restricted heat bath method.

A. Thermodynamics

Borrowing notation from Ref. [173], we can make use of the following identifications, that bring the system back into a form familiar from statistical mechanics. We define the entropy as

$$s \;\equiv\; \log\left(\rho\right) , \qquad (21)$$

noting that this definition is valid up to an additive constant—see the earlier discussion about the constant $c^{(0)}$. The energy, $E = S$, is identified with the internal energy, and hence the temperature, t, is given by

$$t \;\equiv\; \frac{\partial E}{\partial s} \;=\; \frac{1}{a^{(n)}} . \qquad (22)$$

A Legendre transform yields the free energy, F, as

$$F = E - ts . \qquad (23)$$

A second additive constant appears in this definition, and, following Ref. [173], we conventionally set it so that F vanishes at criticality.

Having reconstructed the density of states, and by making use of Eq. (8), we can provide a first measurement of the critical coupling, $\beta_{CV}(P)$, for a given value of N_t and N_s, by dialing β so that the probability distribution of the partition function, $P_\beta(E)$—equivalently the probability distribution of the average plaquette, $P_\beta(u_p)$, obtained by inverting Eq. (20)—displays a double Gaussian shape, with two peaks of equal height at different values of u_p.[5]

TABLE I. Characterization of the lattice studies used for this work. We report the lattice size, $N_t \times N_s^3$, the energy range, given in terms of the average plaquette, $\left[u_p^{\rm min}, u_p^{\rm max}\right]$, as well as the number of replicas/intervals, $N_{\rm rep} = N$, and the number of repeats, $N_{\rm repeats}$. We further report the total number of Newton-Raphson and Robbins-Monro iteration steps, $N_{\rm NR}$ and $N_{\rm RM}$, respectively. We also include the ensembles from Ref. [173], for $N_t = 4$, which we use to recalculate all quantities considered in this paper to facilitate comparison with the new data at $N_t = 5$.

N_t	N_s	$u_p^{\rm min}$	$u_p^{\rm max}$	$N_{\rm rep}$	$N_{\rm repeats}$	$n_{\rm NR}$	$n_{\rm RM}$
5	48	0.588	0.592	48	25	10	60
5	48	0.588	0.592	96	25	10	50
5	56	0.588	0.592	128	25	10	50
5	56	0.588	0.592	48	25	10	50
5	56	0.588	0.592	96	25	10	50
5	64	0.588	0.592	95	20	7	50
5	72	0.588	0.592	95	20	11	50
5	80	0.588	0.59	64	20	15	30
4	20	0.565	0.58	64	20	10	300
4	24	0.565	0.58	64	20	10	300
4	28	0.565	0.58	64	20	10	200
4	40	0.568	0.576	128	25	10	100
4	48	0.568	0.576	128	26	10	100

[5] We could as well require the appearance of two peaks with height ratio fixed to a difference conventional factor. As long as the thermodynamic limit leads to two δ-functions, the same critical coupling will be recovered—see Appendix A.

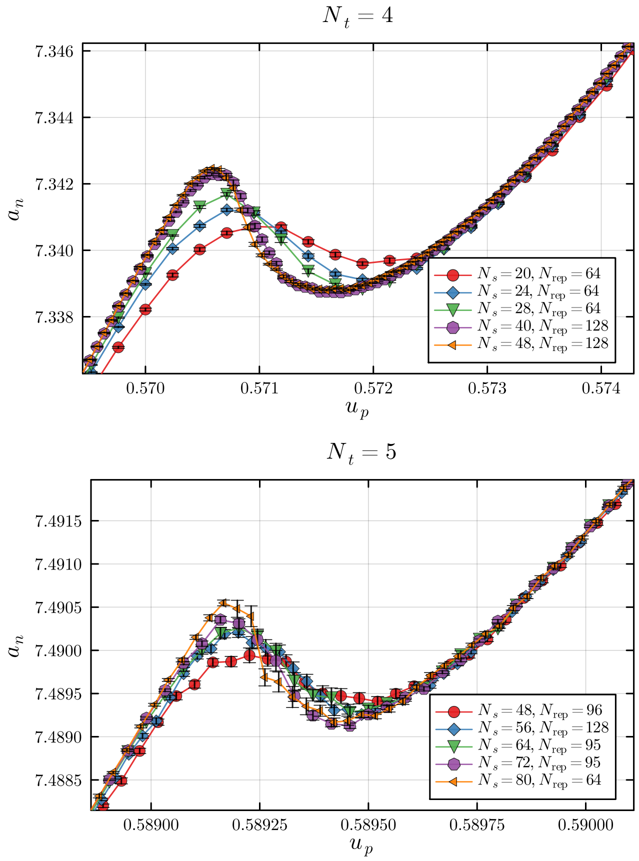

FIG. 1. Results for the coefficients, $a^{(n)}$, entering the piecewise-linear approximation of the logarithm of the density of states, as a function of the average plaquette, u_p, computed in the middle of each finite energy interval, $\Delta_E/2$. In both cases with $N_t = 4$ (top panel) and $N_t = 5$ (bottom), we show results for all available volumes. For volumes for which we performed the calculations with more than one choice of the interval size, we display only the results with the smallest Δ_E.

Alternative definitions of critical coupling rely on other observables. For example, we consider both the specific heat, C_V, and the Binder cumulant, B_V. Both can be expressed in terms of moments of the average plaquette, given, respectively, by

$$C_V(\beta) \equiv \frac{6V}{a^4}\left[\langle u_p^2\rangle_\beta - \langle u_p\rangle_\beta^2\right], \tag{24}$$

$$B_V(\beta) \equiv 1 - \frac{\langle u_p^4\rangle_\beta}{3\langle u_p^2\rangle_\beta^2}. \tag{25}$$

At the critical coupling, the specific heat displays a maximum, whereas the Binder cumulant exhibits a minimum. The resulting definition of $\beta_{CV}(C_V)$ and $\beta_{CV}(B_V)$ converge to the same physical temperature in the thermodynamic and continuum limit as $\beta_{CV}(P)$, hence the study of the discrepancy between them provides a useful indicator of the methodological systematics appearing in our calculations.

Assuming that the aspect ratio, N_s/N_t, is sufficiently large, we can extract the surface tension, σ_{cd}, of the bubble walls separating different phases at the confinement/deconfinement transition. Following Ref. [28, 209], the interface tension is related to the minimum and maximum of the probability distribution obtained by tuning β to the critical value defined by the appearance of peaks with equal heights. One expects that the probabilities computed at the peaks and at the minimum in the valley between them scale as follows:

$$\frac{P_{\rm min}}{P_{\rm max}} \propto \sqrt{N_s}\exp\left(-2\left(\frac{N_s}{N_t}\right)^2\frac{\sigma_{cd}}{T_c^3}\right), \tag{26}$$

where T_c is the critical temperature, In our numerical data, we study the quantity [28]:

$$\tilde{I} = -\frac{1}{2}\left(\frac{N_t}{N_s}\right)^2\log\left(\frac{P_{\rm min}}{P_{\rm max}}\right) + \frac{1}{4}\left(\frac{N_t}{N_s}\right)^2\log(N_s). \tag{27}$$

In the thermodynamic limit, $\lim_{N_s/N_t\to\infty}\tilde{I} = \sigma_{cd}/T_c^3$.

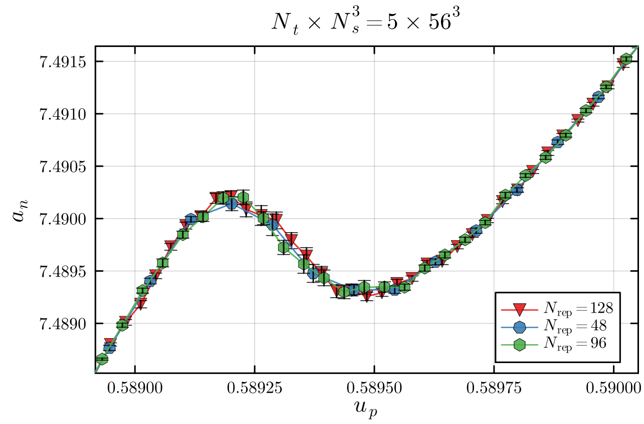

FIG. 2. Results for the coefficients, $a^{(n)}$, entering the piecewise-linear approximation of the logarithm of the density of states, as a function of the average plaquette, u_p, computed in the middle of each finite energy interval, Δ_E. Having fixed the other parameters, for the representative choice of lattice with extent $N_t \times N_s^3 = 5 \times 56^3$, we compare three different choices of number of replicas (and intervals), $N_{\rm rep}$, and hence different energy interval sizes, Δ_E. We observe no statistically significant difference between the sequences of $a^{(n)}$ obtained with these alternative choices of interval sizes.

IV. NUMERICAL RESULTS

We show, in Fig. 1, our results for the values of the coefficients, $a^{(n)}$, entering the approximation of the density of states, as a function of the central value of the plaquette, u_p, for lattices with temporal extent $N_t = 4$ and $N_t = 5$. The former are exhibited for comparison purposes [173]. The sequence of values of $a^{(n)}$ approximates a multivalued (non-invertible) function of u_p, over a finite range of u_p. The difference between the peak and valley values of $a^{(n)}$

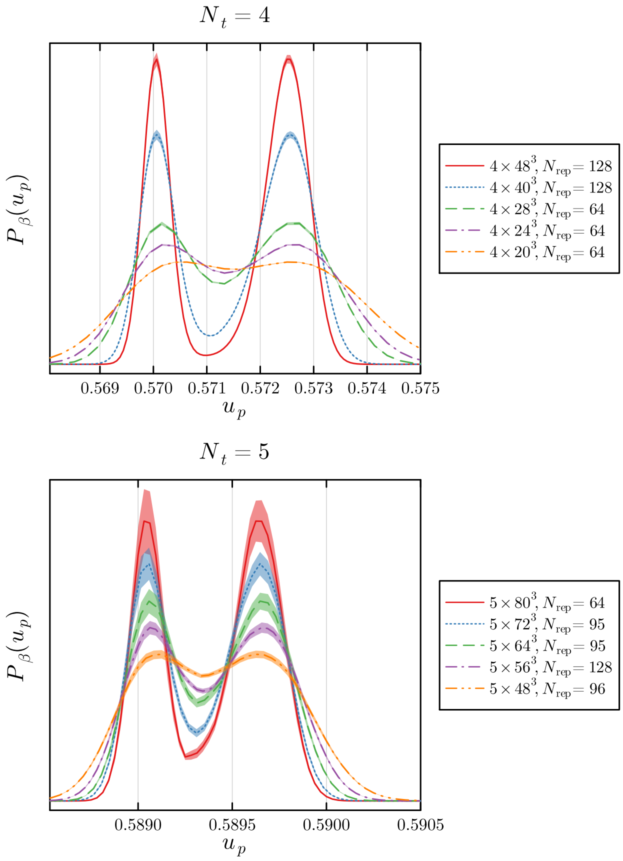

FIG. 3. Probability distribution of the plaquette, $P_\beta(u_p)$, as defined in Eq. (8), evaluated at the critical coupling, $\beta = \beta_{CV}(P)$, for $N_t = 4$ (top panel) and $N_t = 5$ (bottom panel), defined by dialing β so that the two peaks are of equal height. The probability distribution is normalised so that $\int \mathrm{d}u_p P_\beta(u_p) = 1$.

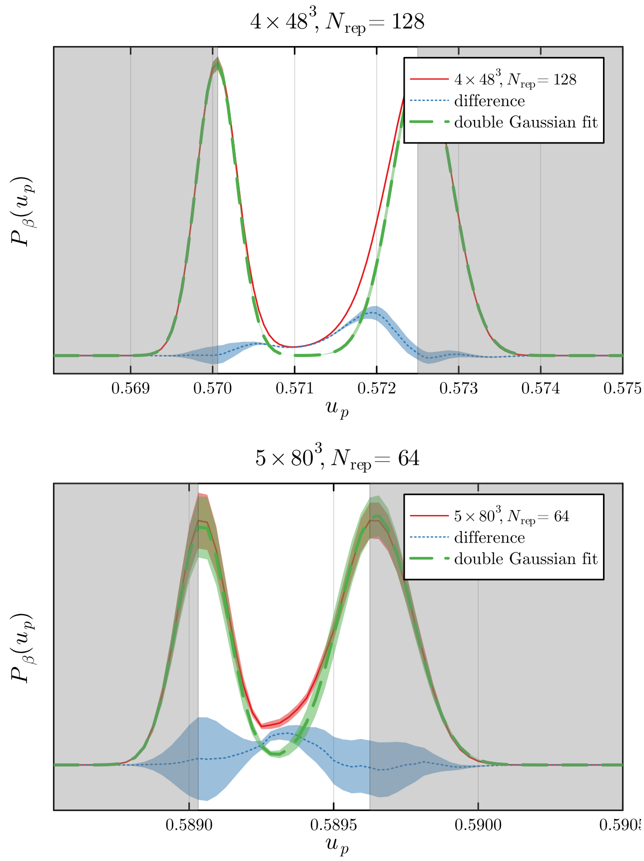

FIG. 4. Fit of the plaquette distribution, $P_\beta(u_p)$ (blue), to a bimodal Gaussian distribution (green), for the critical value of the coupling, $\beta = \beta_{CV}(P)$, and for the largest available volumes with $N_t = 4$ (top panel) and $N_t = 5$ (bottom). The gray shaded region highlights the region of the data used in the fitting procedure. We observe good agreement with the expected Gaussian behaviour for large and small values of the average plaquette, while also detecting clear evidence of the effect of interfaces in the region between the peaks, as evidenced by the non-vanishing difference between measurements and fit (orange).

inside this non-invertibility range is less pronounced in the new, $N_t = 5$, measurements—roughly by a factor of three. Furthermore, the presence of a range over which $a^{(n)}$ is not invertible as a function of u_p emerges at larger values of u_p, and is restricted to a narrower range. It further emerges only at much larger aspect ratios, up to $N_s/N_t = 16$, to become clearly discernible. In existing data on $N_t = 4$ only aspect ratios up to $N_s/N_t = 12$ are available, yet the signal of metastability is clearly visible. To the best of our knowledge, the values of aspect ratios used for this publication are the largest ones deployed in published studies of this type.

In Fig. 2, we show a representative example of the comparison between the values of $a^{(n)}$ obtained with three different choices of the size of the energy intervals, $\Delta_E/2$, holding fixed the lattice parameters $N_t = 5$ and $N_s = 56$. We find good agreement between results derived with the interval sizes studied here. We take this as indication that the interval sizes used in generating the measurements presented in this paper are sufficiently small that systematic effects connected to this choice are negligible.

A common feature of Figs. 1 and 2 is that $a^{(n)}$ is not invertible as a function of u_p, yet it is unique. To verify that this is a dynamical feature, and not the product of the algorithm we use, we monitored the evolution of the NR and RM steps, and found that, for this system, independently of the starting point of the algorithm, all solutions converge to a unique value of $a^{(n)}$, for each choice of energy interval. This can be contrasted with some of the findings in the literature on holographic studies of phase transitions (see, for example Fig. 6 in Ref. [159]) which expose the possibility that, in some regions of parameter space, multiple values of the temperature (related to $a^{(n)}$) correspond to the same energy. If that were the case in realistic theories, under special conditions the out-of-equilibrium dynamics in proximity of the transition, and the process of bubble nucleation, might appear quite different from the standard paradigm, with potentially

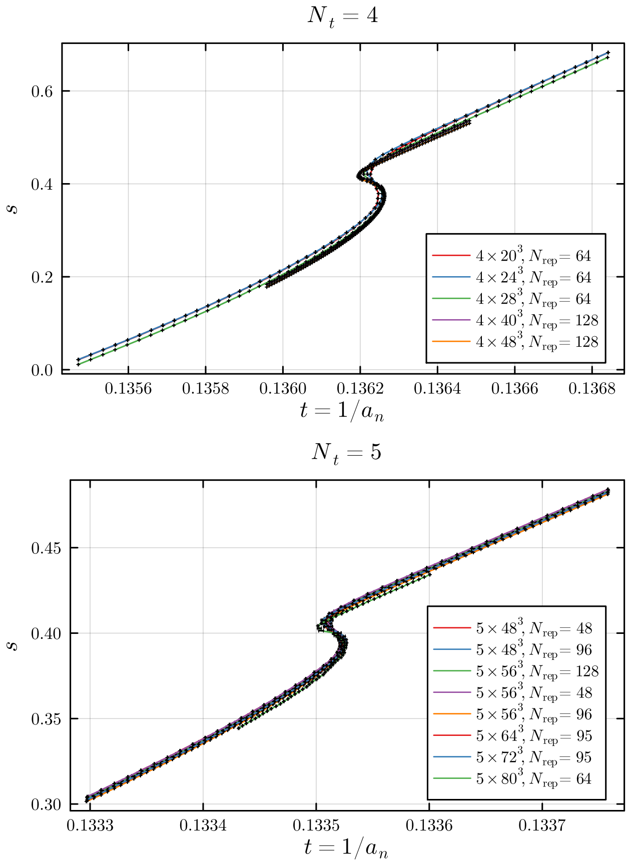

FIG. 5. The entropy, $s = \log(\rho)$, measured for $N_t = 4$ (top panel) and $N_t = 5$ (bottom), for all available calculations. We fix the unknown constant, $c^{(0)}$, in Eq. (10), and hence an additive constant in s, by requiring that the entropy is positive for all temperatures considered, and furthermore that the value of the entropy evaluated at criticality, on the unstable branch, be the same for all calculations.

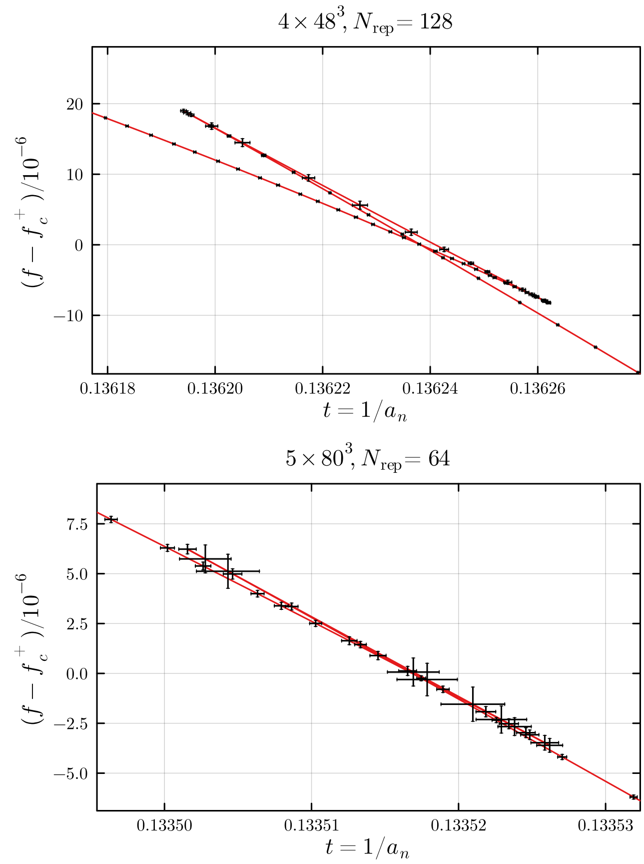

FIG. 6. Subtracted free energy density, $f - f_c^+$, determined as the Legendre transform of the internal energy, E. We fix the unknown constant in the entropy, s, by requiring that the entropy remains positive for all temperatures, and agrees across all different volumes when computed at criticality, on the unstable branch. We find the expected swallow-tail behaviour.

interesting implications for the generation of gravitational waves. We uncovered no evidence of such phenomena in our current measurements.

In Fig. 3, we show the (β-dependent) probability distribution of the average plaquette, $P_\beta(u_p)$, tuned to the critical coupling, $\beta = \beta_{CV}(P)$, obtained by requiring that the two peaks of the probability distribution are of equal height. The expected double-peaked structure is clearly visible, for both $N_t = 4$ and $N_t = 5$, for all available lattice volumes. In the $N_t = 5$ case, we were compelled to use substantially larger lattices and aspect ratios than in the case of $N_t = 4$, in order to resolve this feature, and yet the separation of the peaks is less pronounced at the spatial volumes available.

In the two panels of Fig. 4, we show our measurements of $P_\beta(u_p)$ in the largest available spatial volumes, for $N_t = 4$ and $N_t = 5$, respectively. We fit the probability, $P_\beta(u_p)$, computed with $\beta = \beta_{CV}(P)$, to a bimodal Gaussian distribution. If there were no interfaces between the two phases, the plaquette distribution would be given by two Gaussians of equal height, and hence be well reproduced by the bimodal fit. This behavior assumes that there are two independent subsystems corresponding to the two phases—see the discussion in Refs. [28] and [173]. We exclude the energy range between the two peaks from the fit and find that our data fit nicely a Gaussian behaviour, as expected in the absence of interfaces. In the central region, we clearly see the effects of an emerging interface. To help visualize this qualitative effect, the figure shows also the difference between our data and the fit. This figure provides clear evidence of a non-vanishing deviation from the Gaussian behaviour in the region between the two peaks, which encodes the physics of the mixed phases. In particular, for suitably large volumes this study would allow us to measure the surface tension, as anticipated.

A. Thermodynamic properties

Within the LLR approach, we can determine the entropy only up to an additive constant, given by $c^{(0)}$ in

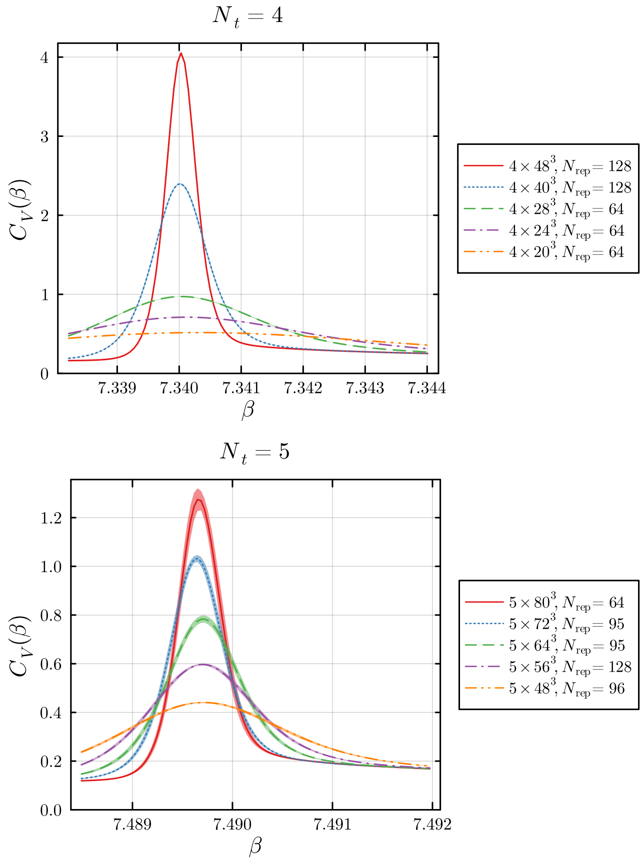

FIG. 7. Specific heat, $C_V(\beta)$, for $N_t = 4$ (top panel) and $N_t = 5$ (bottom). The peaks at $\beta = \beta_{CV}(C_V)$ scale as we approach the thermodynamic limit. We observe that the maximum at $N_t = 5$ is lower for the same aspect ratio N_s/N_t.

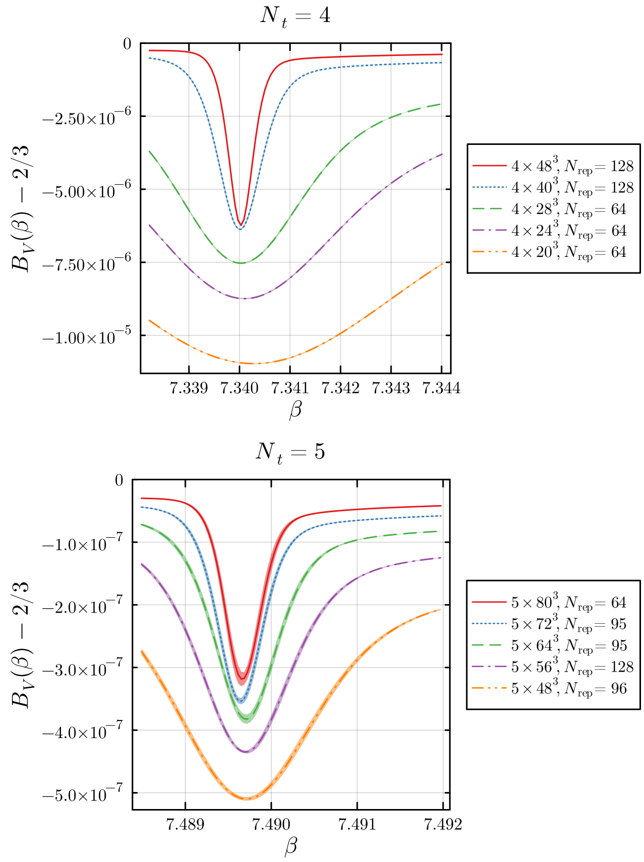

FIG. 8. Deviation of the Binder cumulant from two thirds, $B_V(\beta) - 2/3$, for $N_t = 4$ (top panel) and $N_t = 5$ (bottom). We observe a minimum at the critical coupling $\beta_{CV}(B_V)$.

Eq. (10). In principle, this constant should be fixed by imposing the third law of thermodynamics, but as anticipated we can only consider temperatures around the phase transition, for this work, and not the low temperatures entering the third law. We fix the unknown constant in the entropy by requiring that s be positive for all temperatures considered. Furthermore, we require that when evaluating the entropy at criticality, on the unstable branch in the regime of phase co-existence, we obtain the same result for all volumes studied here.

We show the entropy used in the determination of the free energy in Fig. 5. We determine the free energy as the Legendre transform of the internal energy, E, and subtract its value at the point where the two metastable branches cross. In Fig. 6, we depict the free energy density, $f = \frac{a^4}{V} F$, as a function of the micro-canonical temperature, $t = 1/a_n$. We observe the appearance of the characteristic swallow-tail shape that accompanies the phenomena of phase coexistence and metastability. If we were able to probe the system at lower temperatures and fix the unknown constant, in Eq. (23), through the third law of thermodynamics, $\lim_{t\to 0} s = 0$, the slope of the free energy would be expected to be steeper.

As a further consistency check, and to assess the size of methodological systematics, we also determine the critical coupling in two more conventional ways, by examining the specific heat (which has a maximum at $\beta = \beta_{CV}(C_V)$), and the Binder cumulant (which has a minimum at $\beta = \beta_{CV}(B_V)$), using Eqs. (24) and (25). We show the specific heat around the critical coupling in Fig. 7, and the Binder cumulant in Fig. 8.

We determine the critical coupling, $\beta_{CV}(C_V)$ ($\beta_{CV}(B_V)$), by identifying the maximum (minimum) of the respective cumulant. We show the numerical values of β_{CV} obtained at different lattice volumes and using different observables in Tab. II and Fig. 9. For the measurements with $N_t = 4$, these results have already been published in Ref. [173], and we observe the presence of statistically significant deviations between the determinations arising from the probability distribution and the specific heat as well as the Binder cumulant. We do not observe such an effect for our new measurements at $N_t = 5$ within current uncertainties.

In Fig. 10, we plot $\tilde{I}$, computed according to Eq. (27), for all available ensembles, including both the cases of $N_t = 4$ and $N_t = 5$. We find that the term $\tilde{I}$ is strongly suppressed for $N_t = 5$, in comparison to $N_t = 4$, for

TABLE II. Three complementary determinations of the critical coupling of the $Sp(4)$ Yang-Mills theory, obtained from different observables: the plaquette distribution, $P_\beta(u_p)$, the specific heat, $C_V(\beta)$, and the Binder cumulant, $B_V(\beta)$. We report our best measurements for all available lattices. For comparison, we report both results for $N_t = 4$, which were first presented in Ref. [173], and $N_t = 5$, original to this work.

N_t	N_s	$N_{\rm rep}$	$\beta_{CV}(P)$	$\beta_{CV}(C_V)$	$\beta_{CV}(B_V)$
5	48	48	7.489685(36)	7.489735(34)	7.489733(34)
5	48	96	7.489663(33)	7.489707(29)	7.489705(28)
5	56	128	7.489696(22)	7.489695(20)	7.489694(20)
5	56	48	7.489678(32)	7.489679(29)	7.489680(30)
5	56	96	7.489678(25)	7.489680(24)	7.489681(24)
5	64	95	7.489710(24)	7.489701(21)	7.489700(21)
5	72	95	7.489656(18)	7.489637(18)	7.489637(18)
5	80	64	7.489690(23)	7.489666(21)	7.489666(21)
4	20	64	7.340131(20)	7.340317(18)	7.340282(18)
4	24	64	7.340047(15)	7.340110(14)	7.340096(15)
4	28	64	7.340056(17)	7.340035(17)	7.340024(17)
4	40	128	7.3400783(97)	7.3400115(97)	7.340009(10)
4	48	128	7.3400844(57)	7.3400287(54)	7.3400275(54)

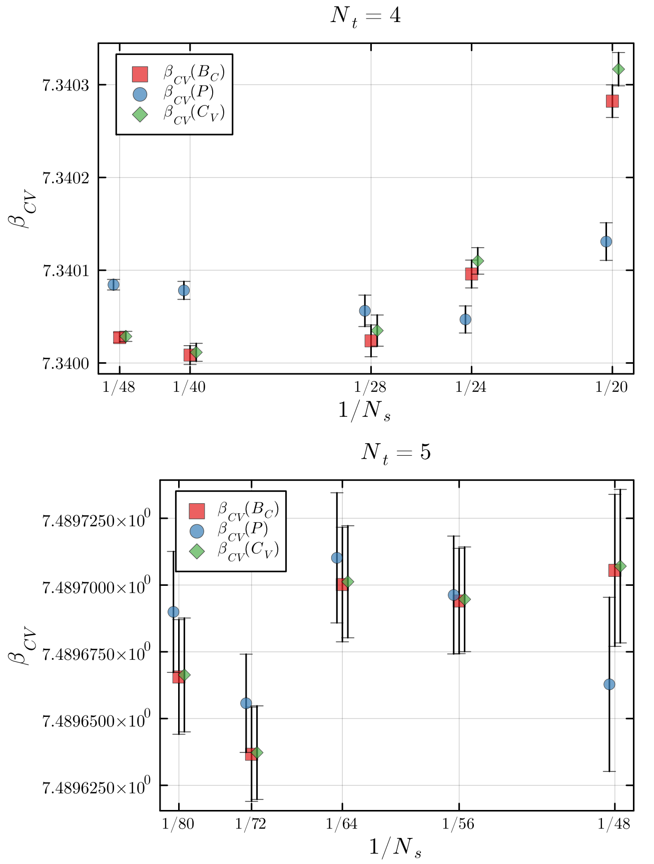

FIG. 9. Plot of the data presented in Tab. II. For comparison, we show the critical couplings for both $N_t = 4$, which were first presented in Ref. [173], and $N_t = 5$, original to this work.

all available choices of aspect ratio, N_t/N_s, and hence that this quantity is, with current lattices, affected by large lattice artifacts. It is likely that finer lattices at $N_t \geq 6$ are required to perform the full continuum limit. Nevertheless, the very fact that we could extract this quantity brings our current understanding of the surface tensions in the $Sp(4)$ Yang-Mills theory close to the state of the art for other theories, in particular those with $SU(N_c)$ gauge group—see, e.g., Refs. [28, 210, 211] and references therein, in particular Refs. [212–214]. Our results for $\hat{I}$ are roughly of the same size as for $SU(3)$ [28, 212–214] suggesting that the transition in $Sp(4)$ is a weak first-order transition.

V. CONCLUSION AND OUTLOOK

We presented our results for a new set of lattice studies of the finite-temperature, confinement-deconfinement phase transition in the $Sp(4)$ Yang-Mills theory. Using the LLR algorithm to implement the density of states framework, we made the first steps towards the continuum limit extrapolation, by providing an extensive set of results for lattices with temporal extent $N_t = 5$, that complement earlier measurements for $N_t = 4$. Our calculations have been performed for several choices of (large) spatial volumes, so that the thermodynamic (infinite-volume) limit can be approached. We have further shown that for our choices of finite discretization of the energy, systematic effects arising from the LLR implementation are negligible.

We demonstrated that we can resolve a first-order phase transition effectively with the LLR method on fine lattices. We have used significantly larger lattice volumes than has been done in past investigations within Yang-Mills theories. We found that larger aspect ratios were required to resolve the phase transition. We estimated the critical coupling for finite volumes, β_{CV}, through several independent prescriptions and found that the measurements are robust, being compatible with one another.

In contrast to existing results for $N_t = 4$, in the case of $N_t = 5$ this analysis suggests that the error budget is dominated by the statistical uncertainties in a_n, rather than by methodological systematics.

We provided a first quantitative assessment of the size of discretization artifacts present in the determination of the surface tension. The current measurement of the surface tension sets an upper limit on its true value, that is important as input into realistic estimates of the GW power spectrum of the continuum theory. This study provides numerical evidence for the need to deploy even larger lattices, in order to approach the continuum limit and provide a high precision measurement of this quantity.

Further progress is achievable in future studies, by considering finer lattices, and hence larger values of N_t. Doing so will require considering larger aspect ratios, N_s/N_t, which will increase the cost of the calculations, and de-

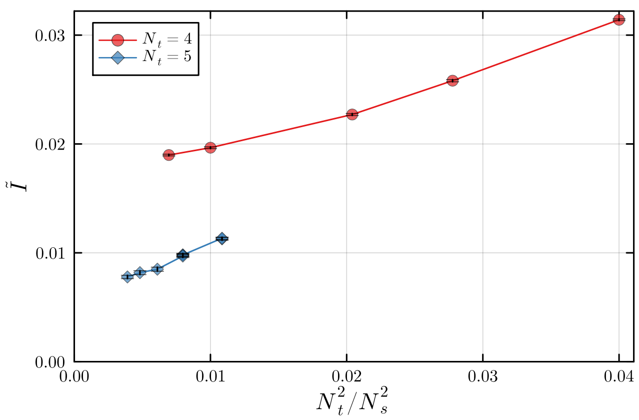

FIG. 10. Our numerical results for the term, $\tilde{I}$, giving rise to the dimensionless surface tension, σ_{cd}/T_c^3, in the limit of vanishing inverse aspect ratio, $N_t/N_s \to 0$, for all available lattices.

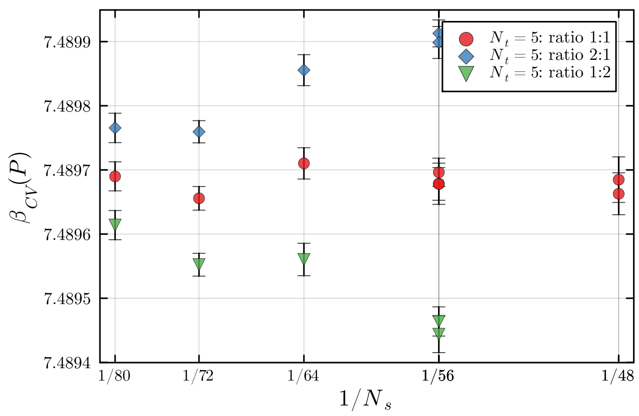

FIG. 11. Critical $\beta_{CV}(P)$ as determined (at finite volume) by analysis $P_\beta(u_p)$, and dialing β to different ratios of peak heights in the plaquette distribution: equal heights (yellow circles) and peak-height-ratio of two to one (blue hexagons) and one to two (green rectangles).

mand further algorithm and software development for the implementation of the global constraint on the internal energy underpinning the LLR algorithm, in order to optimize the parallelization of the underlying calculation.

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High performance computing—This work used the DiRAC Data Intensive service (CSD3) at the University of Cambridge, the DiRAC Data Intensive service (DIaL3) at the University of Leicester and the DiRAC Extreme Scaling service (Tursa) at the University of Edinburgh, managed respectively by the University of Cambridge University Information Services, the University of Leicester Research Computing Service and by EPCC on behalf of the STFC DiRAC HPC Facility (www.dirac.ac.uk). The DiRAC service at Cambridge, Leicester, and Edinburgh are funded by BEIS, UKRI and STFC capital funding and STFC operations grants. DiRAC is part of the UKRI Digital Research Infrastructure.

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Numerical simulations have been performed on the Swansea SUNBIRD cluster (part of the Supercomputing Wales project). The Swansea SUNBIRD system is part funded by the European Regional Development Fund (ERDF) via Welsh Government.

Research Software Availability statement—The workflow used to analyse these data is available at Ref. [215]. The modified HiRep code with support for the LLR is available at [205]. It is based upon [202, 203].

Research Data Availability Statement—The raw data generated in support of this work, and processed data derived from it, are available in machine-readable format at Ref. [216]. See also Ref. [209], for a description of our approach to reproducibility and open science.

Appendix A: More on determining $\beta_{CV}(P)$

In Sec. IV, we provided a determination of the critical coupling, $\beta_{CV}(P)$, obtained by requiring that the probability distribution of the plaquette, $P_\beta(u_p)$, displays two peaks of equal heights. In this Appendix we consider a modified prescription, in which we require that one of the peaks is twice the height of the other. In part, this is motivated by the suggestion that, in the presence of multiple choices of vacuum in the one of the phases, one might require that such mutiplicity be taken into account [217]. We hence examine how the resulting measurements of $\beta_{CV}(P)$, emerging from these three alternative prescriptions, approach the infinite volume limit.

We show the results of this analysis in Fig. 11. Finite volume corrections are much more pronounced in the case of prescriptions based on tuning $P_\beta(u_p)$ to display peaks with unequal heights. Thus, in the main body of the paper, we restrict ourselves to the definition of $\beta_{CV}(P)$ adopted in from Sec. IV.

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