# Equation of state for SU(3) gauge theory via the energy-momentum tensor under gradient flow

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The energy density and the pressure of SU(3) gauge theory at finite temperature are studied by direct lattice measurements of the renormalized energy-momentum tensor obtained by the gradient flow. Numerical analyses are carried out with  $\beta = 6.287 - 7.500$  corresponding to the lattice spacing  $a = 0.013$ –0.061 fm. The spatial (temporal) sizes are chosen to be  $N_s = 64$ , 96, 128 ( $N<sub>\tau</sub> = 12$ , 16, 20, 22, 24) with the aspect ratio,  $5.33 \le N_s/N_\tau \le 8$ . Double extrapolation,  $a \to 0$  (the continuum limit) followed by  $t \to 0$  (the zero flow-time limit), is taken using the numerical data. Above the critical temperature, the thermodynamic quantities are obtained with a few percent precision including statistical and systematic errors. The results are in good agreement with previous high-precision data obtained by using the integral method.

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# I. INTRODUCTION

Thermodynamic observables in QCD such as the energy density  $\varepsilon$  and the pressure p as functions of temperature T and baryon chemical potential  $\mu_B$  provide fundamental information for studying the physics of relativistic heavyion collisions and compact stars. Because of their importance, high precision lattice simulations of  $\varepsilon$  and p in SU(3) gauge theory  $[1-5]$  $[1-5]$  and in full QCD  $[6,7]$  on the lattice at finite  $T$  have been carried out extensively for the past few decades. In most of these studies the integral method [\[1\]](#page-12-0) is adopted, where  $\varepsilon$  and  $p$  are obtained by integrating so-called the interaction measure  $\Delta \equiv \varepsilon - 3p$  calculated on the lattice.

Recently, a new method to calculate thermodynamic quantities has been proposed [\[8,9\]](#page-12-2) on the basis of the gradient flow [\[10](#page-12-3)–14]. In this method, one makes use of the renormalized energy-momentum tensor (EMT) operator  $T_{\mu\nu}$  constructed from the "flowed field" at nonzero flow time  $t$  [\[8\]](#page-12-2). Once EMT is defined,  $\varepsilon$  and  $p$  can be calculated by simply taking thermal averages at any given temperature,

<span id="page-0-6"></span>
$$
\varepsilon = -\langle T_{44} \rangle, \qquad p = \frac{1}{3} \sum_{i=1}^{3} \langle T_{ii} \rangle. \tag{1}
$$

This method has been tested for the thermodynamics of SU(3) gauge theory in Ref. [\[9\]](#page-12-4) for the first time with  $\beta = 6/g_0^2 = 5.89$ –6.56 corresponding to the lattice spacing  $a = 0.041-0.11$  fm and the spatial (temporal) size  $N_s = 32$  $(N<sub>\tau</sub> = 6, 8, 10)$ . It was found that the  $\varepsilon$  and p obtained by the gradient flow with small statistics can be comparable to those obtained by the integral method with high statistics. An extension of this method to full QCD has been also formulated [\[15\]](#page-12-5) and numerical results were reported recently [\[16,17\]](#page-12-6).

In the present paper, we report an improved analysis of the thermodynamics of SU(3) gauge theory with the gradient flow. Numerical analyses are carried out with  $\beta = 6.287 - 7.500$  corresponding to the lattice spacing  $a = 0.013-0.061$  fm. The spatial (temporal) sizes are chosen to be  $N_s = 64$ , 96, 128 ( $N_\tau = 12$ , 16, 20, 22, 24) with the aspect ratio  $5.33 \le N_s/N_\tau \le 8$ . The double extrapolation,  $a \rightarrow 0$  (the continuum limit) followed by  $t \to 0$  (the zero flow-time limit), is taken using the data on these fine lattices. We note that such a double limit could not be taken in Ref. [\[9\]](#page-12-4) due to the coarse lattice. The lattice spacing *a* required for these analyses has been determined on the basis of the gradient flow (see Ref. [\[18\]](#page-12-7) and Appendix A 1).

After taking the double limit, the final results of  $\varepsilon$  and  $p$ above the critical temperature  $T_c$  reach a few percent precision with both statistical error and systematic errors. The latter errors are associated with the  $a \to 0$  and  $t \to 0$ extrapolations as well as the scale setting and lambda parameter. Our high precision results based on the gradient flow are found to be in good agreement with the previous high precision results with the integral method.

This paper is organized as follows. In the next section we introduce the gradient flow and the EMT operator used in our study. After describing the setup of numerical

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simulations in Sec. [III](#page-2-0), the numerical results are presented in Sec. [IV.](#page-4-0) The last section is devoted to a short summary. In the Appendix, the analyses of the lattice spacing and the lambda parameter are described in detail.

# II. BASIC FORMULATION

#### A. Yang-Mills gradient flow

Let us first recapitulate the essential features of the Yang-Mills gradient flow [\[10\]](#page-12-3) and its application to define the renormalized EMT [\[8\].](#page-12-2)

<span id="page-1-0"></span>The gradient flow of the Yang-Mills field is generated by the differential equation with a flow time  $t$ , which has a dimension of inverse mass squared,

$$
\frac{dA_{\mu}(t,x)}{dt} = -g_0^2 \frac{\delta S_{\text{YM}}(t)}{\delta A_{\mu}(t,x)} = D_{\nu} G_{\nu\mu}(t,x). \tag{2}
$$

Here the Yang-Mills action  $S_{YM}(t)$  and the field strength  $G_{\mu\nu}(t, x)$  are composed of the flowed field  $A_{\mu}(t, x)$ , which is a function of  $t$  and the four-dimensional Euclidean coordinate x. Color indices are suppressed for simplicity. The initial condition at  $t = 0$  is taken to be  $A_\mu(0, x) = A_\mu(x)$ with  $A_u(x)$  being the ordinary gauge field in fourdimensional Euclidean spacetime.

With Eq. [\(2\),](#page-1-0) the gauge field flows along the steepest descent direction of  $S_{YM}(t)$  as t increases. At the tree level, Eq. [\(2\)](#page-1-0) is rewritten as

$$
\frac{dA_{\mu}}{dt} = \partial_{\nu}\partial_{\nu}A_{\mu} + \text{(gauge dependent terms)},\qquad(3)
$$

which is a diffusion-type equation. Therefore, the gradient flow for  $t > 0$  acts as a cooling of the gauge field with the smearing radius  $\sqrt{8t}$  in the four-dimensional Euclidean spacetime. In Ref. [\[19\]](#page-12-8), it is proved in pure gauge theory that all composite operators composed of  $A<sub>u</sub>(t, x)$  take finite values for  $t > 0$ . Also, the idea of the gradient flow can be generalized to gauge theory with fermions [\[20\]](#page-12-9).

#### B. EMT from gradient flow

<span id="page-1-1"></span>In the present study, we use the EMT defined by the short flow-time expansion [\[8\]](#page-12-2). Let us consider a composite local operator  $O(t, x)$  defined from the field  $A<sub>\mu</sub>(t, x)$  at positive flow time  $t > 0$ . The short flow-time expansion [\[19\]](#page-12-8) asserts that in the small  $t$  limit this operator can be written as a superposition of local operators of the original gauge theory at  $t = 0$  as

$$
O(t,x) \to \sum_{t \to 0} C_i(t) O_i^{\mathbb{R}}(x),\tag{4}
$$

where  $O_i^R(x)$  in the right-hand side are renormalized operators of the original gauge theory at  $t = 0$  with the subscript *i* denoting a set of operators, while  $c_i(t)$  are associated c-number coefficients calculable in perturbation theory for small  $t$ .

In order to define the EMT using Eq. [\(4\),](#page-1-1) we consider the short flow-time expansion of dimension-four gaugeinvariant operators [\[8\].](#page-12-2) In pure gauge theory, there are two such operators;

<span id="page-1-2"></span>
$$
U_{\mu\nu}(t,x) = G_{\mu\rho}^a(t,x)G_{\nu\rho}^a(t,x) - \frac{1}{4}\delta_{\mu\nu}G_{\rho\sigma}^a(t,x)G_{\rho\sigma}^a(t,x),
$$
\n(5)

$$
E(t,x) = \frac{1}{4} G_{\mu\nu}^a(t,x) G_{\mu\nu}^a(t,x).
$$
 (6)

<span id="page-1-3"></span>Since they are gauge invariant, only gauge invariant operators appear in the right-hand side of Eq. [\(4\):](#page-1-1) Such an operator with dimension-zero is an identity operator, while operators with dimension-four are EMTs  $T_{\mu\nu}(x)$ . Up to this order, the short flow-time expansion of Eqs. [\(5\)](#page-1-2) and  $(6)$  thus gives<sup>1</sup>

<span id="page-1-5"></span><span id="page-1-4"></span>
$$
U_{\mu\nu}(t,x) = \alpha_U(t) \left[ T_{\mu\nu}(x) - \frac{1}{4} \delta_{\mu\nu} T_{\rho\rho}(x) \right] + O(t), \quad (7)
$$

$$
E(t,x) = \langle E(t,x) \rangle_0 + \alpha_E(t) T_{\rho \rho}(x) + O(t). \tag{8}
$$

We normalize EMT so that the vacuum expectation values vanish,  $\langle T_{\mu\nu}(x)\rangle_0 = 0$ . This determines the coefficient of the unit operator in the right-hand side of Eq. [\(8\)](#page-1-4) to be  $\langle E(t, x) \rangle$ <sub>0</sub>. The unit operator does not appear in Eq. [\(7\)](#page-1-5) since  $U_{\mu\nu}(t, x)$  is traceless. Contributions from the operators of dimension-six or higher are proportional to  $t$  or higher from the dimensional reason, and thus they are suppressed for small  $t$ .

<span id="page-1-6"></span>Combining relations Eqs. [\(7\)](#page-1-5) and [\(8\),](#page-1-4) we have

$$
T_{\mu\nu}(x) = \lim_{t \to 0} T_{\mu\nu}(t, x),
$$
\n(9)

<span id="page-1-7"></span>with

$$
T_{\mu\nu}(t,x) = \frac{1}{\alpha_U(t)} U_{\mu\nu}(t,x)
$$

$$
+ \frac{\delta_{\mu\nu}}{4\alpha_E(t)} [E(t,x) - \langle E(t,x) \rangle_0]. \tag{10}
$$

<span id="page-1-8"></span>The coefficients  $\alpha_U(t)$  and  $\alpha_E(t)$  are calculated perturbatively in the  $\overline{\text{MS}}$  scheme in Ref. [\[8\],](#page-12-2)

<span id="page-1-9"></span>
$$
\alpha_U(t) = \bar{g}(1/\sqrt{8t})^2 [1 + 2b_0 \bar{s}_1 \bar{g}(1/\sqrt{8t})^2 + O(\bar{g}^4)], \quad (11)
$$

$$
\alpha_E(t) = \frac{1}{2b_0} [1 + 2b_0 \bar{s}_2 \bar{g} (1/\sqrt{8t})^2 + O(\bar{g}^4)], \quad (12)
$$

<sup>&</sup>lt;sup>1</sup>This useful combination was first given in Ref. [\[21\]](#page-13-0).

where  $\bar{g}(q)$  denotes the running gauge coupling in the  $\overline{\text{MS}}$ scheme with  $q = 1/\sqrt{8t}$  and

$$
\bar{s}_1 = \frac{7}{22} + \frac{1}{2}\gamma_E - \ln 2 \simeq -0.08635752993, \quad (13)
$$

$$
\bar{s}_2 = \frac{21}{44} - \frac{b_1}{2b_0^2} = \frac{27}{484} \approx 0.05578512397, \qquad (14)
$$

with  $b_0 = \frac{1}{(4\pi)^2} \frac{11}{3} N_c$ ,  $b_1 = \frac{1}{(4\pi)^4} \frac{34}{3} N_c^2$  with  $N_c = 3$ .

<span id="page-2-1"></span>We note here that (i) the right-hand side of Eq. [\(9\)](#page-1-6) is independent of the regularization because of its UV finiteness, so that one can take, e.g., the lattice regularization scheme, and (ii) the small t expansion of  $U_{\mu\nu}(t, x)$  and  $E(t, x)$  implies

$$
T_{\mu\nu}(t,x) = T_{\mu\nu}(x) + \mathcal{O}(t).
$$
 (15)

#### <span id="page-2-4"></span>C. Energy density and pressure on the lattice

The thermodynamic quantities are obtained from the expectation values of diagonal elements of the EMT as in Eq. [\(1\)](#page-0-6). A combination of  $\varepsilon$  and  $p$  called the interaction measure  $\Delta$  is related to the trace of the EMT (the trace anomaly):

$$
\Delta = \varepsilon - 3p = -\langle T_{\mu\mu}(x) \rangle. \tag{16}
$$

Also, the entropy density s at zero chemical potential is given by  $\varepsilon$  and  $p$  as

$$
sT = \varepsilon + p = -\langle T_{44}(x) \rangle + \frac{1}{3} \sum_{i=1}^{3} \langle T_{ii}(x) \rangle.
$$
 (17)

In the practical numerical analysis, we calculate Eq. [\(10\)](#page-1-7) on a flowed gauge field with  $t > 0$ . With finite a, the lattice gauge field has to be smeared by the gradient flow sufficiently to suppress the lattice discretization effect. Since the smearing length of the gradient flow is given by  $\sqrt{8t}$ , this condition requires  $\sqrt{8t} \gtrsim a$ . On the other hand, the value of  $\sqrt{8t}$  has to be small enough compared with half the temporal extent of the lattice,  $1/(2T)$ , so that the smearing by the gradient flow does not feel the periodic boundary condition. From these requirements, the measurement has to be performed in the range

$$
a \lesssim \sqrt{8t} \lesssim \frac{1}{2T}.\tag{18}
$$

<span id="page-2-2"></span>When Eq. [\(10\)](#page-1-7) shows approximate linear dependence as shown in Eq.  $(15)$  in a range of t given by Eq.  $(18)$ , one can take the small  $t$  limit and obtain Eq.  $(9)$ . The linear dependence Eq.  $(15)$  can also be violated for large t when the perturbative results of the coefficients in Eqs. [\(11\)](#page-1-8) and

[\(12\)](#page-1-9) are no longer applicable. This happens when  $\sqrt{8t}$ approaches the lambda parameter  $\Lambda_{\overline{\text{MS}}}.$ 

For the measurement of  $\Delta$ , we have to calculate  $\langle E(t, x) \rangle$  to carry out vacuum subtraction. This means that the numerical analysis for vacuum configuration is needed in addition to  $T > 0$  simulation. On the other hand, the analysis of  $sT$ , which depends only on the traceless part, does not require the vacuum subtraction and hence can be performed solely with a nonzero  $T$  simulation. This is an advantage of our method compared with the integral method.<sup>2</sup>

# III. SIMULATION SETUP

<span id="page-2-0"></span>We have performed numerical simulations of  $SU(3)$ gauge theory on four-dimensional Euclidean lattices. We considered the Wilson plaquette gauge action under the periodic boundary condition with several different values of  $\beta = 6/g_0^2$  with  $g_0$  being the bare coupling constant. Gauge configurations are generated by the pseudo-heat-bath algorithm with the over-relaxation, mixed in the ratio of 1∶5. We call one pseudo-heat-bath update plus five over-relaxation sweeps as a "Sweep." Each measurement is separated by 200 Sweeps. Statistical errors are then estimated by the jackknife method. The binsize  $N_{\text{bin}}$  of the jackknife analysis is determined so that the total number of jackknife bins is 50 unless otherwise stated. We have checked that the  $N_{\text{bin}}$  dependence of the statistical error is not observed with this binsize.

We use the Wilson gauge action for  $S_{YM}(t)$  in the flow equation, Eq.  $(2)$ . The gradient flow in the *t*-direction is numerically solved by the third order Runge-Kutta (RK) method [\[10\].](#page-12-3) The RK time step is taken to be 0.01 for small  $t$  and is increased gradually as  $t$  increases. Accumulation errors due to the RK method are found to be more than 2 orders of magnitude smaller than the statistical errors in all the analyses discussed below.

<span id="page-2-3"></span>For the operator  $U_{\mu\nu}(t, x)$  in Eq. [\(5\)](#page-1-2) necessary to analyze  $s/T<sup>3</sup>$ , we use  $G_{\mu\nu}^a(t, x)$  written in terms of the clover leaf representation. For  $E(t, x)$  in Eq. [\(6\)](#page-1-3) necessary to analyze  $\Delta/T^4$ , we use the mixed representation [\[23,24\],](#page-13-1)

$$
E(t, x)_{\text{imp}} = \frac{3}{4}E(t, x)_{\text{clover}} + \frac{1}{4}E(t, x)_{\text{plaq}},
$$
 (19)

where  $E(t, x)_{\text{clover}}$  is constructed from the clover leaf representation of  $G_{\mu\nu}^a(t, x)$  in Eq. [\(6\),](#page-1-3) while  $E(t, x)_{\text{plaq}}$  is defined as [\[10\]](#page-12-3)

$$
E(t, x)_{\text{plaq}} = \frac{1}{18} P(t, x),
$$
 (20)

<sup>&</sup>lt;sup>2</sup>An alternative method to analyze  $sT$  without vacuum subtraction is recently proposed in Refs. [\[5,22\].](#page-12-10)

with the plaquette  $P(t, x) = 1/(6N_c) \sum_{\mu,\nu} \text{ReTr} [U_\mu(t, x) \times$  $U_{\nu}(t, x + \hat{\mu}) U_{\mu}^{\dagger}(t, x + \hat{\nu}) U_{\nu}^{\dagger}(t, x)$ . If the Wilson gauge action is employed for both the gauge action and  $S_{YM}(t)$ in Eq. [\(2\),](#page-1-0) the  $O(a^2)$  discretization errors in  $E(t, x)_{\text{imp}}$  are canceled out in the tree level [\[23\].](#page-13-1)

To specify temperature of a lattice as well as to perform the continuum extrapolation, we need to relate  $\beta$  to the lattice spacing a. For this purpose, we have previously performed measurements of a in the range  $6.3 \le \beta \le 7.5$ using the gradient flow [\[18\]](#page-12-7). As summarized in the Appendix, we derived a relation between the dimensionless reference scale  $w_0/a$  and  $\beta$  as

<span id="page-3-0"></span>
$$
\frac{w_0}{a} = \exp\left(\frac{4\pi^2}{33}\beta - 9.1268 + \frac{41.806}{\beta} - \frac{158.26}{\beta^2}\right), \quad (21)
$$

which is applicable in the range  $6.3 \le \beta \le 7.4$ . The statistical error of Eq. [\(21\)](#page-3-0) associated with the fitting parameters is less than 0.4%. Topological freezing of the data may also introduce an extra 1% error to this result (see Appendix  $A_1$  for more details). To determine  $T_1$  of a lattice in the unit of  $T_c$ , we use the critical coupling after the infinite volume extrapolation  $\beta_c = 6.33552(47)$  at  $N_{\tau} = 12$  [\[25\]](#page-13-2) and Eq. [\(21\)](#page-3-0), which gives

$$
w_0 T_c = 0.25244(17). \tag{22}
$$

In the definition of the EMT operator, Eq. [\(10\)](#page-1-7), we need the running coupling  $\overline{q}(q)$  in the  $\overline{MS}$  scheme which appears in the coefficients  $\alpha_U(t)$  and  $\alpha_E(t)$  given by Eqs. [\(11\)](#page-1-8) and [\(12\)](#page-1-9). To obtain  $\bar{g}(q)$  at  $q = 1/\sqrt{8t}$ , we need a functional form of  $\bar{g}(q)$  and the relation between the lattice spacing and  $\Lambda_{\overline{\text{MS}}}$ . We use the iterative formula for four-loop running coupling [\[26\]](#page-13-3) and

$$
w_0 \Lambda_{\overline{\text{MS}}} = 0.2154(5)(11). \tag{23}
$$

See Appendix [A 2](#page-10-0) as well as Ref. [\[18\]](#page-12-7) for more details. Note that topological freezing would introduce an extra 1% error to this result, too.

The simulation parameters are summarized in Tables [I](#page-3-1) and [II.](#page-3-2) We perform the numerical simulations for eight different temperatures in the range  $0.93 \leq T/T_c \leq 2.69$ on the lattice of volume  $N_s^3 \times N_\tau$  as summarized in Table [I](#page-3-1). For each  $T/T_c$ , we perform numerical simulations for three different values of  $N_{\tau}$ . The value of  $\beta$ , lattice volume  $N_s^3 \times N_\tau$  and the number of configurations are shown in the table. The aspect ratios  $N_s/N_\tau$  of all lattices are within the range  $5.33 \le N_s/N_\tau \le 8$ . The values of  $N_\tau$  for two coarse lattices are fixed to  $N<sub>\tau</sub> = 12$  and 16. The finest lattice has the value of  $N_{\tau}$  in the range  $N_{\tau} = 20-24$ ; because the corresponding vacuum simulation on 128<sup>4</sup> lattice requires a large numerical cost, we make use of a single vacuum simulation for several values of T by changing  $N_{\tau}$ .

Since the lattice spacing determined by Eq.  $(21)$  has  $1\%$ error, the value of  $T/T_c$  on each lattice is expected to have

<span id="page-3-1"></span>TABLE I. Simulation parameters  $\beta = 6/g_0^2$ ,  $N_s^3 \times N_\tau$  and the number of configurations for nonzero temperature simulations at  $T/T_c$ . The \* symbol in the far right column shows the set of configurations that the corresponding vacuum simulation  $(N_s = N_\tau)$  is available.

$T/T_c$	β	$N_{\scriptscriptstyle S}$	$N_{\tau}$	Configurations	Vacuum
0.93	6.287	64	12	2125	*
	6.495	96	16	1645	∗
	6.800	128	24	2040	*
1.02	6.349	64	12	2000	*
	6.559	96	16	1600	*
	6.800	128	22	2290	∗
1.12	6.418	64	12	1875	$\ast$
	6.631	96	16	1580	∗
	6.800	128	20	2000	$\ast$
1.40	6.582	64	12	2080	*
	6.800	128	16	900	*
	7.117	128	24	2000	*
1.68	6.719	64	12	2000	*
	6.941	96	16	1680	*
	7.117	128	20	2000	*
2.10	6.891	64	12	2250	
	7.117	128	16	840	*
	7.296	128	20	2040	
2.31	7.200	96	16	1490	
	7.376	128	20	2020	
	7.519	128	24	1970	
2.69	7.086	64	12	2000	
	7.317	96	16	1560	
	7.500	128	20	2040	

a similar-size uncertainty. Also, there is a possible finite volume effect, although it is expected to be small due to our large aspect ratio,  $5.33 \leq N_s/N_t$ . These small uncertainties are not considered in the final results of  $\Delta/T^4$  and  $s/T^3$  to be shown at the end of this paper.

For the measurement of  $\Delta/T^4$ , we need the vacuum simulation for vacuum subtraction. We carry out the simulations on  $N_{\tau} = N_{s}$  lattices corresponding to the temperatures in the range  $0.93 \leq T/T_c \leq 1.68$ . The simulation parameters are shown in Table [II.](#page-3-2) The configuration

<span id="page-3-2"></span>TABLE II. Parameters for vacuum simulations  $(N_s = N_\tau)$ .

$\beta$	$N_{s,\tau}$	Configurations
6.287	64	2125
6.349	64	950
6.418	64	1000
6.582	64	800
6.719	64	1000
6.495	96	840
6.559	96	840
6.631	96	900
6.941	96	837
6.800	128	992
7.117	128	1028

sets whose vacuum subtraction is available are shown by the  $*$  symbol in the far right column in Table [I](#page-3-1).

To obtain the expectation values of the EMT with Eqs. [\(9\)](#page-1-6) and [\(10\)](#page-1-7), the double extrapolation  $(t, a) \rightarrow (0, 0)$ has to be taken. To proceed this analysis, we first take the continuum limit,  $a \to 0$ , with fixed t in physical unit. Since the leading lattice discretization effect on the thermodynamic quantities with the Wilson plaquette gauge action is of order  $a^2$  [\[1\],](#page-12-0) we take the following parametrization to take the continuum limit:

<span id="page-4-3"></span>
$$
\langle T_{\mu\nu}(t,x) \rangle_{\text{lat}} = \langle T_{\mu\nu}(t,x) \rangle_{\text{cont}} + \frac{b_{\mu\nu}(t)}{N_{\tau}^2}.
$$
 (24)

<span id="page-4-4"></span>Here,  $\langle T_{\mu\nu}(t, x) \rangle_{\text{lat}}$  is the expectation value obtained on the lattice with  $N_{\tau}$ . One has to determine  $b_{\mu\nu}(t)$  for each t independently. Then, we take  $t \to 0$  extrapolation by fitting the continuum extrapolated result,

$$
\langle T_{\mu\nu}(t,x) \rangle_{\text{cont}} = \langle T_{\mu\nu}(x) \rangle + C_{\mu\nu}t,\tag{25}
$$

according to Eq. [\(15\).](#page-2-1)  $C_{\mu\nu}$  has in principle logarithmic t dependence, but we treat it as a constant in our extrapolation.

#### IV. NUMERICAL RESULTS

#### <span id="page-4-0"></span>A.  $\langle T_{\mu\nu}(t,x)\rangle_{\text{lat}}$  and its t and a dependences

We first focus on the result for  $T = 1.68T_c$  to see the t and a dependences of the numerical results. Shown in Fig. [1](#page-4-1) are the t dependence of  $\Delta/T^4 = (\epsilon - 3p)/T^4$  (left) and entropy density  $s/T^3 = (\varepsilon + p)/T^4$  (right) as functions of  $tT^2$  at fixed temperature,  $T/T_c = 1.68$ , for three different values of the lattice spacing,  $\beta = 6.719, 6.941$  and 7.117 ( $a = 0.033$ , 0.025 and 0.020 fm). For  $\Delta/T^4$ , the improved operator in Eq. [\(19\)](#page-2-3) is adopted. Let us discuss the three regions of t separately: (i) For  $0 < \sqrt{8t} \lesssim a$ , the lattice discretization effect becomes prominent as discussed in Sec. [II C.](#page-2-4) One finds, particularly in the right panel, that

<span id="page-4-1"></span>

FIG. 1. Flow-time t dependences of trace anomaly  $\Delta/T^4 = (\varepsilon - 3p)/T^4$  (left) and entropy density  $s/T^3 = (\varepsilon + p)/T^4$  (right) for  $T/T_c = 1.68$  with  $N_\tau = 12$ , 16 and 20.

<span id="page-4-2"></span>

FIG. 2. t dependence of  $\Delta/T^4$  for  $T/T_c = 1.68$  with  $N_\tau = 12$  (left) and  $N_\tau = 20$  (right) calculated by different discretizations,  $E(t, x)_{\text{imp}}$ ,  $E(t, x)_{\text{clover}}$  and  $E(t, x)_{\text{plaq}}$ .

<span id="page-5-0"></span>

FIG. 3. N<sub>r</sub> dependence of  $\Delta/T^4$  at  $T^2 = 0.005$ , 0.01, 0.015 and 0.02 together with the result of continuum extrapolation using Eq. [\(24\).](#page-4-3) The results with three discretizations for  $E(t, x)$  are plotted.

this region becomes narrower as  $a$  decreases. (ii) For the smallest a in this figure (red points),  $\Delta/T^4$  has a plateau and  $s/T^3$  has a linear behavior in the range  $0.005 \leq tT^2 \leq$ 0.015 in accordance with Eq. [\(15\).](#page-2-1) (iii) The deviation from the linear behavior is seen for  $tT^2 \geq 0.015$ , which is attributed to the over-smearing as discussed in Sec. [II C](#page-2-4). These considerations indicate that there exists a window of t from which the values of  $\Delta/T^4$  and  $s/T^3$  at  $t = 0$  can be extracted.

To check the effect of different choices for the operator  $E(t, x)$  in  $\Delta/T^4$ , we compare three cases in Fig. [2](#page-4-2),  $E(t, x)_{\text{imp}}$ ,  $E(t, x)_{\text{clover}}$  and  $E(t, x)_{\text{plaq}}$ , for  $T/T_c = 1.68$ and  $N_{\tau} = 12, 20$ . In both figures, the improved operator, Eq. [\(19\)](#page-2-3), shows the least discretization error for  $\Delta/T^4$ .

#### B. Double extrapolation

Let us now describe the procedure for the double extrapolation  $(t, a) \rightarrow (0, 0)$ . As discussed in Sec. [III](#page-2-0), we first take the continuum limit with  $t$  fixed. This extrapolation is taken by fitting the results with three different values of  $N<sub>\tau</sub>$  with Eq. [\(24\).](#page-4-3) To obtain the values of  $\langle T_{\mu\nu}(t, x) \rangle_{\text{lat}}$  at the same t for different  $N_{\tau}$ , we apply the cubic spline interpolation to the data for each  $N_{\tau}$ .

In Figs. [3](#page-5-0) and [4,](#page-6-0) we show the  $N<sub>\tau</sub>$  dependences of  $\Delta/T^4$  and  $s/T^3$  at  $tT^2 = 0.005$ , 0.01, 0.015 and 0.02 together with the result of continuum extrapolation with Eq. [\(24\).](#page-4-3) In Fig. [3,](#page-5-0) three results obtained by the different choices for the operator  $E(t, x)$  are shown. The value of  $\chi^2$ /dof is within the range  $\chi^2$ /dof  $\lesssim$  2.0 for  $0.005 \le tT^2 \le 0.02$ . The error of the continuum extrapolation is estimated by the jackknife analysis. For values of  $tT<sup>2</sup>$  smaller than 0.005, the fitting becomes worse particularly for  $s/T<sup>3</sup>$ . Therefore, in the following, we will use the results only for  $0.005 \le tT^2 \le 0.02$ . Figure [3](#page-5-0) also shows that the continuum extrapolated results with different discretizations for  $E(t, x)$  agree with each other.

In Fig. [5](#page-6-1), we show the t dependences of  $\Delta/T^4$  and  $s/T<sup>3</sup>$  after the continuum extrapolation by the black line with the error band together with the data for finite lattice spacings,  $N_{\tau} = 12$ , 16 and 20. We make linear t extrapolation by using the continuum extrapolated data for  $0.005 \leq tT^2 \leq 0.02$  according to Eq. [\(25\).](#page-4-4) We employ three fitting ranges,

*Range-1* 0.01 ≤  $tT^2$  ≤ 0.015, Range-2  $0.005 \leq tT^2 \leq 0.015$ ,  $Range-3$  0.01 ≤  $tT^2$  ≤ 0.02.

<span id="page-6-0"></span>

FIG. 4.  $N<sub>\tau</sub>$  dependence of  $s/T<sup>3</sup>$  at  $tT<sup>2</sup> = 0.005, 0.01, 0.015$  and 0.02 together with the result of continuum extrapolation using Eq. [\(24\).](#page-4-3)

<span id="page-6-1"></span>

FIG. 5. Results of continuum extrapolation (black band) for  $\Delta/T^4$  (left) and s/T<sup>3</sup> (right) as functions of  $tT^2$ . The extrapolation to  $t = 0$  using the data in Range-1 is shown by the dashed line, and the extrapolated value with the error is given by the filled square at  $t = 0$ . The extrapolated values with Range-2 and Range-3 are also shown around the origin.

In Fig. [5,](#page-6-1) the black solid bar at  $t = 0$  with a squared symbol denotes the result of the extrapolation with Range-1, while the open circle and triangle symbols denote the results with Range-2 and Range-3, respectively.  $\chi^2$ /dof in these fittings is smaller than unity. Then, we use the result of Range-1 as a central value, while those of Range-2 and Range-3 are used to estimate the systematic error associated with the fit range. $3$ 

<sup>&</sup>lt;sup>3</sup>In our previous exploratory study of  $\Delta/T^4$  and  $s/T^3$  in Ref. [\[9\]](#page-12-4), the continuum limit has been taken, while the flow time was fixed to be  $tT^2 = 0.02$ . There was no resolution to detect the slope  $C_{\mu\nu}$  owing to limited statistics and coarse lattice.

<span id="page-7-0"></span>

FIG. 6. Systematic errors originated from  $\pm 1\%$  of change of  $\Lambda_{\overline{MS}}$ .

<span id="page-7-1"></span>

FIG. 7. Similar plots with the left panel of Fig. [5](#page-6-1) for different values of  $T/T_c$ .

In order to estimate the systematic error from the uncertainly of  $a\Lambda_{\overline{\text{MS}}}$  discussed in Sec. [III](#page-2-0), we show the continuum extrapolated results under  $\pm 1\%$  change of  $a\Lambda_{\overline{\text{MS}}}$ in Fig. [6](#page-7-0). As the figure shows, the systematic error for  $\Delta/T^4$  $(s/T<sup>3</sup>)$  is negligible (comparable) to the other statistical and systematic errors.

#### C. Temperature dependence

The analysis in the previous subsection for  $T/T_c = 1.68$ is repeated for all  $T/T_c$  listed in Table [I](#page-3-1). We show the results of these analyses with different values of  $T/T_c$  in Fig. [7](#page-7-1) for  $\Delta/T^4$  and in Fig. [8](#page-8-0) for  $s/T^3$ . The values of  $\chi^2/d$ of are within a reasonable range  $\chi^2$ /dof  $\lesssim$  2 for all fits with an exception for  $s/T^3$  at  $T/T_c = 1.40$ . As these figures show, the double extrapolation works rather stably for all  $T/T_c$ .

The numerical results after double extrapolation are summarized in Table [III](#page-9-1). The table shows that  $\Delta/T^4$  and  $s/T<sup>3</sup>$  are determined within 3% precision including all systematic errors except for those at  $T/T_c = 0.93$ . Note that we do not have  $\Delta/T^4$  for the highest three temperatures owing to the lack of vacuum simulations needed to make vacuum subtraction (see Table [I](#page-3-1)).

Finally, we depict the  $T/T_c$  dependences of our  $\Delta/T^4$ and  $s/T^3$  in Fig. [9](#page-9-2) together with the previous data obtained by the integral method in Refs. [\[1,4\]](#page-12-0). By taking into the estimated errors of the previous results, three results are consistent with each other.<sup>4</sup>

<sup>&</sup>lt;sup>4</sup>We note that  $s/T^3$  recently studied in the shifted boundary method [\[5,22\]](#page-12-10) also seems to agree.

<span id="page-8-0"></span>

FIG. 8. Similar plots with the right panel of Fig. [5](#page-6-1) for different values of  $T/T_c$ .

# V. SUMMARY

We performed measurements of thermodynamic quantities of the SU(3) Yang-Mills theory from the direct analysis of the expectation value of energy-momentum tensor (EMT), Eq. [\(9\),](#page-1-6) constructed by the Yang-Mills gradient flow with a flow time  $t$ . The numerical simulations with the Wilson plaquette gauge action have been performed at finite temperature with the lattice spacing  $a = 0.013{\text -}0.061$  fm and the aspect ratio,  $5.33 \leq N_s/N_\tau \leq 8$ .

Using the lattice data, the double extrapolation ( $t \to 0$ ) after  $a \rightarrow 0$ ) has been performed to obtain the interaction measure  $\Delta(T)$  and the entropy density  $s(T)$  with a few percent precision including statistical and systematic errors. The results agree quite well with the previous highprecision data using the integral method.

The present approach with EMT provides a new tool not only to calculate QCD equation of state accurately but also to study correlation functions and transport coefficients of the quark-gluon plasma with firm theoretical

<span id="page-9-2"></span>

FIG. 9. Temperature dependences of  $\Delta/T^4$  and  $s/T^3$  (red circles) together with the previous studies based on the integral method (solid and dashed lines) [\[1,4\].](#page-12-0) The error bars of the red circles are smaller than the size of symbols.

basis. The first step along these directions will be reported in the forthcoming paper [\[27\]](#page-13-4).

given in Ref. [\[18\].](#page-12-7) A possible error originating from the topological freezing is also mentioned.

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# APPENDIX: LATTICE SPACING AND Λ PARAMETER

In this Appendix, we summarize our analysis of the lattice spacing and  $\Lambda_{\overline{MS}}$ . The numerical data used are those

<span id="page-9-1"></span>TABLE III. Summary of the equation of state with statistical and systematic errors. The first error is the statistical one, while the second error shows the systematic error associated with the choice of the fit range. The last error comes from 1% uncertainties of  $\Lambda_{\overline{\text{MS}}}$  from possible topological freezing.  $\Delta/T^4$  at  $T/T_c = 2.10$ , 2.31 and 2.69 are not available due to the lack of corresponding vacuum configurations.

$T/T_c$	$\Delta/T^4$	$s/T^3$
0.93	$0.066(32)(\frac{+3}{2})(0)$	$0.082(33)(\frac{+3}{-6})(0)$
1.02	$1.945(57)(^{+8}_{-7})(0)$	$2.104(63)(^{+16}_{-2})(8)$
1.12	$2.560(33)(\frac{+12}{-8})(0)$	$3.603(46)(^{+39}_{-0})(13)$
1.40	$1.777(24)(\frac{+14}{-3})(0)$	$4.706(35)(^{+49}_{-0})(17)$
1.68	$1.201(19)(^{+10}_{-0})(0)$	$5.285(35)(^{+44}_{-0})(18)$
2.10		$5.617(34)(^{+66}_{-0})(18)$
2.31		$5.657(55)(^{+82}_{-15})(18)$
2.69		$5.914(32)(^{+70}_{-0})(18)$

#### 1. Reference scale and lattice spacing

<span id="page-9-0"></span>Numerical simulations of the SU(3) Yang-Mills theory with the Wilson plaquette action were performed on  $N_s^4 = 64^4 - 128^4$  lattices under the periodic boundary condition. The values of  $\beta = 6/g_0^2$ , N<sub>s</sub> and the number of configurations  $N_{\text{conf}}$  are summarized in the three left columns in Table [IV.](#page-9-3)

We adopt the reference scale  $w_0$  defined by [\[29\]](#page-13-5)

$$
t\frac{d}{dt}t^2\langle E(t)\rangle\Big|_{t=w_0^2} = 0.3,\tag{A1}
$$

with the operator  $E(t)$  constructed by the clover-type representation of the flowed field  $G_{\mu\nu}^a$  at time t. We use the Wilson gauge action  $S_{YM}$  for the flow equation in Eq. [\(2\)](#page-1-0), and each measurement is separated by 1000 Sweeps. The values of  $w_0/a$  with statistical errors are summarized in the fourth column of Table [IV.](#page-9-3) The lattice spacings in physical unit estimated by  $w_0 = 0.1670(10)$  fm [\[28\]](#page-13-6) are also given in

<span id="page-9-3"></span>TABLE IV. Simulation parameters for scale setting,  $\beta = 6/g_0^2$ , the lattice size  $N_s$ , and the number of configurations  $N_{\text{conf}}$ , as well as the numerical results of  $w_0/a$ . The lattice spacing a and the physical length  $N_s a$  in the physical unit determined from  $w_0 = 0.1670(10)$  fm [\[28\]](#page-13-6) are also shown.

$N_{\rm s}$	$N_{\text{conf}}$	$w_0/a$	$a$ [fm]	$N_s a$ [fm]
64	30	2.877(5)	0.058(4)	3.72(22)
64	100	3.317(4)	0.050(3)	3.22(19)
64	49	3.797(8)	0.044(3)	2.81(17)
64	100	4.356(9)	0.038(2)	2.45(15)
64	30	4.980(23)	0.034(2)	2.15(13)
64	100	5.652(17)	0.030(2)	1.89(11)
96	60	7.297(18)	0.023(1)	2.20(13)
96	53	9.348(66)	0.018(1)	1.71(10)
128	40	12.084(61)	0.014(1)	1.77(11)

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<span id="page-10-1"></span>

FIG. 10. Result of the three parameter fit of  $w_0/a$  in Eq. [\(A2\).](#page-10-2) The shaded band shows the uncertainties from the fit parameters.

the table together with the physical lattice volume  $L = N_s a$ . Extra error due to topological freezing is estimated to be about the 1% level as discussed later.<sup>5</sup>

For the parametrization of  $w_0/a$  as a function of  $\beta$ , we introduce the fitting function motivated by the one-loop perturbation theory. It provides a reasonable result  $(\chi^2/\text{dof} = 1.104)$  for nine data points in 6.3  $\leq \beta \leq 7.4$ without overfitting as shown in Fig. [10:](#page-10-1)

<span id="page-10-2"></span>
$$
\frac{w_0}{a} = \exp\left(\frac{4\pi^2}{33}\beta - 9.1268 + \frac{41.806}{\beta} - \frac{158.26}{\beta^2}\right)
$$
  
× [1 ± 0.004(stat)]. (A2)

The difference from other fitting Ansätze (such as polynomial functions as shown in Appendix A in Ref. [\[18\]\)](#page-12-7) is found to be less than  $1\%$ . The 0.4% error in Eq.  $(A2)$ originates from the statistical errors of  $w_0/a$  except for the topological freezing.

For the analysis of  $w_0/a$  in Table [IV,](#page-9-3) we have used 30–100 configurations separated by 1000 Sweeps. In order to estimate the effect of the topological freezing on these simulations, we have performed an independent measurement at  $\beta = 6.88$  on  $N_s^4 = 64^4$  lattice by accumulating  $N_{\text{conf}} = 1290$  configurations with each measurement separated by 2000 Sweeps. This lattice setup corresponds to the physical size,  $64 \times 0.027$  fm  $\simeq 1.7$  fm, which is comparable to the smallest lattice volume in Table [IV.](#page-9-3) Since observables depend more on the topological sector for smaller spatial volume [\[33\]](#page-13-7), this analysis would serve as the most severe test for the topological freezing of the data sets in Table [IV.](#page-9-3)

The topological charge is defined by  $Q \equiv$  $-\frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \int_V d^4x \text{tr}[G_{\mu\nu}(x)G_{\rho\sigma}(x)]$ . We take the value of Q at  $t = t_0$  defined by  $t^2 \langle E(t) \rangle |_{t=t_0} = 0.3$  [\[10\]](#page-12-3). From this measurement of  $Q$ , we find that the autocorrelation

<span id="page-10-3"></span>

FIG. 11. (a) Histogram of  $Q^2$  for  $\beta = 6.88$  and  $N_s^4 = 64^4$ . (b) The values of  $w_0/a$  with fixed  $Q^2$  normalized by the expectation values using all configurations.

length is about  $100 \times 2000$  Sweeps which is 2–6 times larger than the maximum number of Sweeps used to obtain  $w_0/a$  in Table [IV.](#page-9-3) Therefore, there is indeed a danger of the topological freezing. Shown in Fig. [11\(a\)](#page-10-3) is a histogram of  $Q^2$  obtained in the simulation. The resultant fluctuation of Q reads  $\langle Q^2 \rangle = 12.2 \pm 3.2$ . Corresponding topological susceptibility is estimated as  $\chi a^4 \equiv \langle Q^2 \rangle / V =$  $(7.3 \pm 1.9) \times 10^{-7}$ , with the error by the jackknife analysis with binsize 100. By using Eq. [\(A2\)](#page-10-2) and the reference values  $w_0 = 0.1670(10)$  fm and  $r_0 = 0.49$  fm [\[28\]](#page-13-6), we find  $\chi r_0^4 = 0.084(22)$  which is in the 1.5 $\sigma$  level of agreement with the accurate determination,  $\chi r_0^4$  =  $0.0544(18)$  [\[34\]](#page-13-8).

In Fig. [11\(b\)](#page-10-3), we plot  $w_0/a$  at fixed topology,  $\langle w_0/a \rangle_0$ , normalized by the expectation value  $\langle w_0/a \rangle$  without fixing Q. The red band corresponds to the error of  $\langle w_0/a \rangle$  with total configurations. By combining the typical value expected from the topological susceptibility ( $|Q|$  <  $\sqrt{\langle Q^2 \rangle} \lesssim 4$ ) and the results of Fig. [11,](#page-10-3) we estimate the effect of the topological freezing is about 1% level.

# 2. Determination of  $\Lambda_{\overline{\text{MS}}}$

<span id="page-10-0"></span>For the value of  $w_0 \Lambda_{\overline{\text{MS}}}$ , we adopt a procedure similar to the one in Ref. [\[35\]](#page-13-9) for the determination of  $r_0 \Lambda_{\overline{MS}}$ .

<sup>&</sup>lt;sup>5</sup>See Refs. [30–[32\]](#page-13-10) for simulation strategies which are supposed to avoid the topological freezing.

<span id="page-11-0"></span>TABLE V. Simulation parameters  $\beta$  and  $N_s$ . The plaquette value,  $w_0/a$  and  $w_0\Lambda_{\overline{MS}}$  using Method I, II and II with Padé approximation. The last row corresponds to the values at the continuum limit obtained from linear extrapolation without using two coarse lattice data at  $\beta = 6.3$  and 6.4 (the italic numbers).

		Plaquette	$w_0/a$	$w_0 \Lambda_{\overline{\rm MS}}$		
$\beta$	$N_{\rm s}$			Method I	Method II	Method II Padé
6.3	64	$0.622$ 420 85(30)	2.877(5)	0.2017(3)	0.2021(3)	0.2004(3)
6.4	64	$0.630\ 632\ 88(13)$	3.317(4)	0.2046(2)	0.2050(2)	0.2033(2)
6.5	64	0.63836133(35)	3.797(8)	0.2063(5)	0.2067(5)	0.2051(4)
6.6	64	0.64566958(12)	4.356(9)	0.2087(4)	0.2091(4)	0.2075(4)
6.7	64	0.65260839(39)	4.980(23)	0.2106(10)	0.2109(10)	0.2095(10)
6.8	64	$0.659$ 215 11(11)	5.652(17)	0.2112(6)	0.2115(6)	0.2101(6)
7.0	96	$0.671$ 556 729(89)	7.297(18)	0.2133(5)	0.2136(5)	0.2123(5)
7.2	96	$0.682$ 891 86(22)	9.348(66)	0.2142(15)	0.2144(15)	0.2132(15)
7.4	128	$0.693$ 365 795(68)	12.084(61)	0.2173(11)	0.2176(11)	0.2164(11)
$\infty$			$\infty$	0.2163(5)	0.2165(5)	0.2154(5)
			$(\chi/dof)$	(0.927)	(0.902)	(0.991)

The dimensionless parameter  $a\Lambda_{\overline{\text{MS}}}$  can be obtained by matching the tadpole improved lattice perturbation theory. The boosted coupling constant  $g_{\Box}$  is defined by

$$
g_{\Box}^2 \equiv g_0^2(a)/u_0^4,
$$
 (A3)

where  $u_0^4 \equiv P = \langle \text{Tr} U_{\square} \rangle / 3$ .

As for the choice of the renormalization scale and the running coupling constant, we take the following two methods:

(i) Method I

$$
a\Lambda_{\overline{\rm MS}} = a\mu_* F^{\overline{\rm MS}}(g_{\overline{\rm MS}}(\mu_*)) \tag{A4}
$$

at the scale

$$
a\mu_* = \exp\left(\frac{t_1^{\Box}}{2b_0}\right), \tag{A5}
$$

and

$$
\frac{1}{g_{\overline{\rm MS}}^2(\mu_*)} = \frac{1}{g_{\square}^2(a)} + \left(\frac{b_1}{b_0}t_1^{\square} - t_2^{\square}\right)g_{\square}^2(a) + O(g_{\square}^4).
$$
\n(A6)

(ii) Method II

$$
a\Lambda_{\overline{\rm MS}} = a\Lambda_{\square} \exp\left(\frac{t_1^{\square}}{2b_0}\right), \tag{A7}
$$

with

$$
a\Lambda_{\square} = F^{\square}(g_{\square}(a)). \tag{A8}
$$

This scheme corresponds to choosing a scale at

$$
a\mu_{=} = \exp\left(\frac{t_1^{\Box}}{2b_0}\right) \frac{F^{\Box}(g_{\Box}(a))}{F^{\overline{\rm MS}}(g_{\Box}(a)} \tag{A9}
$$

in Method I.

At the three-loop order,  $F^S$  ( $S = \Box$ ,  $\overline{MS}$ ) is expressed as

$$
\frac{\Lambda^S}{M} = F^S(g_S(M)) = \exp\left(-\frac{1}{2b_0g_S^2}\right)(b_0g_S^2)^{-\frac{b_1}{2b_0}}
$$

$$
\times \left(1 + \frac{b_1 + \sqrt{b_1^2 - 4b_0b_S^S}}{2b_0}g_S^2\right)^{-p_A^S}
$$

$$
\times \left(1 + \frac{b_1 + \sqrt{b_1^2 + 4b_0b_S^S}}{2b_0}g_S^2\right)^{-p_B^S}, \tag{A10}
$$

where

$$
p_A^S = -\frac{b_1}{4b_0^2} - \frac{b_1^2 - 2b_0b_2^S}{4b_0^2\sqrt{b_1^2 - 4b_0b_2^S}},
$$
 (A11)

<span id="page-11-1"></span>

improvement as a function of lattice spacing  $a^2$ . The continuum limit is shown at  $a^2/w_0^2 = 0$ . The finest lattice data at  $\beta = 7.4$ deviates from the fitting line. We note that the continuum extrapolation is consistent within the statistical error without using the result at  $\beta = 7.5$ .

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$$
p_B^S = -\frac{b_1}{4b_0^2} + \frac{b_1^2 - 2b_0b_2^S}{4b_0^2\sqrt{b_1^2 - 4b_0b_2^S}}.\tag{A12}
$$

In the [1,1] Padé approximation, it leads to

$$
F_{[1,1]}^S(g_S(M)) = \exp\left(-\frac{1}{2b_0g_S^2}\right) \left[\frac{b_0g_S^2}{1 + \left(\frac{b_1}{b_0} - \frac{b_2^S}{b_1}\right)g_S^2}\right]^{-\frac{b_1}{2b_0}}.
$$
\n(A13)

In SU(3) Yang-Mills theory, the coefficients are given by

$$
b_0 = \frac{11}{(4\pi)^2}, \qquad b_1 = \frac{102}{(4\pi)^4}, \qquad b_2^{\overline{\text{MS}}} = \frac{1}{(4\pi)^6} \frac{2857}{2},
$$
  

$$
b_2^{\Box} = b_2^{\overline{\text{MS}}} + b_1 t_1^{\Box} - b_0 t_2^{\Box}, \qquad (A14)
$$

with

$$
t_1^{\Box} = 0.1348680,
$$
  $t_2^{\Box} = 0.0217565.$  (A15)

The expectation values of the plaquette,  $w_0$  and  $w_0 \Lambda_{\overline{MS}}$ with three schemes are summarized in Table [V.](#page-11-0) Following Ref. [\[35\],](#page-13-9) we adopt Method II with Padé improvement to estimate the central value of  $w_0 \Lambda_{\overline{MS}}$ . The values in the continuum limit are obtained by a linear fit as a function of  $a^2/w_0^2$  without using the coarse results at  $\beta = 6.3$  and 6.4 (see Fig. [12](#page-11-1)). We used the results of the other methods to estimate the systematic error. From this analysis we find

$$
w_0 \Lambda_{\overline{\text{MS}}} = 0.2154(5)(11). \tag{A16}
$$

Note that the topological freezing discussed in Appendix [A 1](#page-9-0) would introduce another 1% error to this number.

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