

## Universal and non-universal finite-volume effects in the vicinity of chiral phase transition in (2+1)-flavor QCD

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Sabarnya Mitra,<sup>a,\*</sup> Jishnu Goswami<sup>a</sup> and Frithjof Karsch<sup>a</sup>

<sup>a</sup>Fakultät Für Physik, Universität Bielefeld, D-33615 Bielefeld, Germany

E-mail: [smitra@physik.uni-bielefeld.de](mailto:smitra@physik.uni-bielefeld.de), [jishnu@physik.uni-bielefeld.de](mailto:jishnu@physik.uni-bielefeld.de),  
[karsch@physik.uni-bielefeld.de](mailto:karsch@physik.uni-bielefeld.de)

In this proceeding, we discuss the finite-size scaling analysis of the order parameter related to the chiral phase transition in QCD with two massless quarks. We use data obtained in lattice QCD calculations performed with highly improved staggered quarks (HISQ) for a range of light quark masses,  $1/240 \leq m_\ell/m_s \leq 1/27$  for different spatial volumes ( $N_\sigma$ ) on Euclidean lattices with temporal extent  $N_\tau = 8$ , satisfying  $3 N_\tau \leq N_\sigma \leq 10 N_\tau$ . We observe that infinite volume extrapolated data for the order parameter agree reasonably well with the expected  $O(2)$  scaling behavior even for physical ratios of the light-to-strange quark mass ratio. We quantify deviations from asymptotic scaling and perform a detailed analysis of the influence of finite-size effects in terms of temperature and quark masses at a fixed lattice cutoff. This is crucial for improving the reliability of the infinite-volume extrapolated estimate of the chiral order parameter and for a more precise determination of chiral phase transition temperature from direct Lattice QCD simulations.

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\*Speaker

## 1. Introduction

Despite having commendable lattice Quantum Chromodynamics (QCD) evidences for the restoration of spontaneously broken chiral symmetry,  $SU(2)_L \times SU(2)_R$ , in the limit of vanishing light quark masses through a second order phase transition<sup>1</sup> along with the explicitly broken nature of the  $U(1)_A$  symmetry at the QCD transition temperature [2, 3], the role of the axial anomaly in the vicinity of the chiral phase transition, in particular the strength of its breaking and its impact on physical QCD thermodynamic observables continues to remain to be an open question. It is therefore quite crucial to provide further concrete support for the universal critical behavior of chiral phase transition, which in the limit of two vanishing light quark masses does resemble the universality class of the 3-dimensional,  $O(4)$  spin model [4], and which is also supposed to provide stringent constraints on the location of the elusive QCD critical point in the QCD phase diagram [5, 6]. Although several studies, comparing lattice QCD calculations with expected universal critical behavior close to the chiral limit, are already existent in the related state-of-the-art literature, a majority of these numerical studies base their point for observation of universal critical behavior on the very presumption that the transition belongs to the 3-d,  $O(4)$  universality class and on subsequently constructing the corresponding universal scaling ansatz to parameterize deviations away from criticality in terms of additional non-singular terms contributing to the relevant observables. Thus, a direct lattice QCD determination of the critical parameters influencing the QCD chiral phase transition obviously is desirable.

In this work, we systematically approach towards a direct lattice QCD based calculation of the critical universal parameters related to the QCD chiral phase transition. We remark that we will not yet aim at presenting continuum extrapolated results in this work. We rather focus on a detailed analysis of finite volume and non-vanishing quark mass effects on chiral observables that eventually will allow a direct determination of universal amplitudes and critical exponents in QCD, without relying on any form of presumption regarding the underlying universality class. For recent developments and progress already made, kindly refer to our previous works [7–9]. Working within the domain of zero density here, we will analyze an improved order parameter for quantifying the extent of chiral symmetry restoration in (2+1)-flavor, lattice regularized QCD for a non-zero value of the lattice cut-off or spacing.

The proceedings is organised as follows: In the next Section 2, we briefly introduce the basic quantities of relevance for this work along with the core theory concerning the finite-volume analysis of QCD chiral phase transition. In Section 3, we briefly describe the setup and present the main results of our current study. We summarise the present state of the work in Section 4.

## 2. Finite-size scaling analysis of (2+1)-flavor QCD chiral phase transition with HISQ fermions

In this section we present a brief summary of the basic equations [10–12] relevant for finite-size scaling analysis of chiral phase transitions. It is well-known that staggered fermion discretization preserves only part of the full  $SU(2)_L \times SU(2)_R$  chiral symmetry on the lattice. For (2+1)-flavor QCD at finite lattice spacing, the remnant chiral symmetry group is associated with the 3-d,  $O(2)$

<sup>1</sup>For a recent overview and further references, see [1].

universality class, which governs the universal critical behavior close to the chiral phase transition. In the limit of vanishing light quark masses, the chiral condensate  $M_\ell$  ( $\ell = u, d$ ), and the chiral susceptibility  $\chi_\ell$  are the order parameter and the corresponding susceptibility of the chiral phase transition [13], defined as :

$$M_\ell = \frac{m_s}{f_K^4} \langle \bar{\psi}\psi \rangle_\ell^{n_f=2}, \quad \chi_\ell = m_s \frac{\partial M_\ell}{\partial m_\ell} = \frac{m_s^2}{f_K^4} \chi_\ell^{n_f=2}, \quad (1)$$

with  $m_s$  denoting the strange quark mass, which is used to define a multiplicatively renormalized chiral condensate, and appropriate factors of the kaon decay constant  $f_K$  to arrive at a dimensionless order parameter and its susceptibility. To remove the ultraviolet (UV) divergence of the bare chiral condensate, we define a renormalization group invariant (RGI) improved order parameter in a temperature-independent normalisation,

$$M(T, H, L) = M_\ell - H\chi_\ell, \quad (2)$$

which is a function of temperature  $T$ , light-to-strange quark mass ratio  $H = m_\ell/m_s$  and the aspect ratio  $L = N_\sigma/N_\tau$ , where  $N_\sigma$  and  $N_\tau$  denote the spatial and temporal extent of the lattice, respectively. Chiral observables are obtained by taking derivatives with respect to  $m_\ell$  of the (2+1)-flavor QCD partition function  $Z$  given as :

$$Z(N_\tau, N_\sigma, m_\ell, m_s) = \int DU e^{-S_s[U]} [\det D_\ell(U, m_\ell)]^{1/2} \times [\det D_s(U, m_s)]^{1/4}, \quad (3)$$

where  $D_\ell$  and  $D_s$  denote the light and strange quark staggered Dirac operator, respectively. We use the 2-flavor normalisation for the light quark chiral condensate and its susceptibility,

$$\langle \bar{\psi}\psi \rangle_\ell^{n_f=2} = \frac{T}{V} \frac{\partial \ln Z}{\partial m_\ell} = \frac{1}{2} \frac{1}{N_\sigma^3 N_\tau} \langle \text{Tr} D_\ell^{-1} \rangle, \quad \text{and} \quad \chi_\ell^{n_f=2} = \frac{\partial}{\partial m_\ell} \langle \bar{\psi}\psi \rangle_\ell^{n_f=2} \quad (4)$$

In the vicinity of the critical point, the order parameter  $M_\ell$  and the susceptibility  $\chi_\ell$  are predominantly controlled by the so-called singular parts, which can be represented in terms of scaling functions  $f_G$  and  $f_\chi$ , respectively. They are functions of scaling variables  $z, z_L$ ,

$$M_\ell(T, H, L) = h^{1/\delta} f_G(z, z_L), \quad (5)$$

$$\chi_\ell(T, H, L) = h_0^{-1} h^{1/\delta-1} f_\chi(z, z_L), \quad (6)$$

where,

$$f_\chi(z, z_L) = \frac{1}{\delta} f_G(z, z_L) - \frac{z}{\beta\delta} \frac{\partial f_G(z, z_L)}{\partial z} - \frac{v z_L}{\beta\delta} \frac{\partial f_G(z, z_L)}{\partial z_L}, \quad (7)$$

and  $h = H/h_0$  with  $h_0$  being a non-universal constant that sets the scale for the symmetry breaking parameter  $H$ . Similar non-universal parameters  $t_0, \ell_0$  appear as respective scales for the reduced temperature  $\tau = (T - T_c)/T_c$  and the dimensionless volume<sup>2</sup>  $L$ . The scaling variables  $z$  and  $z_L$  are defined as

$$z = z_0 z_b, \quad z_L = z_{L,0} z_{L,b}, \quad (8)$$

<sup>2</sup>We denote by  $L$ , the spatial extent of a three dimensional lattice expressed in units of the inverse temperature,  $L = V^{1/3} T$ . In the context of lattice QCD, this is identical to the aspect ratio  $L \equiv N_\sigma/N_\tau$ .

with  $z_0 = h_0^{1/\beta\delta} / t_0$ ,  $z_{L,0} = h_0^{\nu/\beta\delta} \ell_0$ , and the bare scaling variables  $z_b$ ,  $z_{L,b}$ , obtained directly from the ‘bare’ parameters entering any numerical computation are :

$$z_b = \frac{\tau}{H^{1/\beta\delta}}, \quad z_{L,b} = \frac{1}{LH^{\nu/\beta\delta}}. \quad (9)$$

The critical exponents  $\beta$ ,  $\delta$  are well-known for the 3-d,  $O(2)$  universality class [14, 15], which we use,

$$\beta = 0.34864(7), \quad \delta = 4.7798(5). \quad (10)$$

Furthermore, the critical exponent  $\nu$  entering the definition of  $z_L$  is related to these two critical exponents through a hyper-scaling relation,

$$\frac{\nu}{\beta\delta} = \frac{1}{3} \left( 1 + \frac{1}{\delta} \right). \quad (11)$$

Universal scaling functions for the order parameter and the order parameter susceptibility have been analyzed in quite some detail for the 3-d,  $O(2)$  universality class (see e.g. [12, 16]), although an explicit parametrization for finite volume scaling functions in this universality class has been given in terms of a Taylor series in  $z$  and  $z_L$ , only recently [10] :

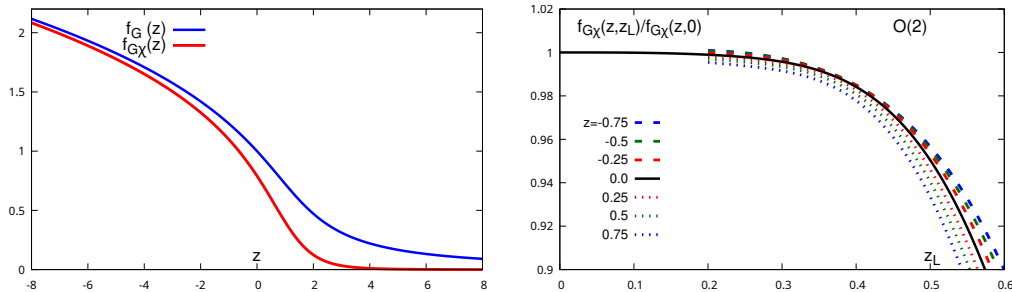
$$f_G(z, z_L) = f_G(z) + \sum_{n=0}^5 \sum_{m=3}^8 a_{nm} z^n z_L^m, \quad (12)$$

in the range  $z \in [-1 : 2]$  and  $z_L \in [0.4 : 1.0]$  with coefficients  $a_{nm}$  given in [10]. In the infinite volume limit,  $z_L = 0$ , the volume-dependent term of the scaling functions obviously vanishes and we obtain the standard one-parameter form of the infinite volume scaling function  $f_\chi(z)$ .

Using Eqs. (5) and (6) we find for the improved order parameter introduced in Eqn. (2) can be written as:

$$M = h^{1/\delta} f_{G_\chi}(z, z_L), \quad \text{with} \quad f_{G_\chi}(z, z_L) = f_G(z, z_L) - f_\chi(z, z_L). \quad (13)$$

In Fig. 1 (left) we show the infinite volume order parameter scaling function  $f_{G_\chi}(z)$  for the improved order  $M$  and compare it to the scaling function  $f_G(z)$  for the conventional order parameter. Its finite-size dependence is shown in Fig. 1 (right) for a few values of  $z$  that are relevant for the study



**Figure 1:** *Left:* The 3-d,  $O(2)$  infinite volume scaling functions  $f_G(z)$  and  $f_{G_\chi}(z)$  versus  $z$ . *Right:* The ratio of the 3-d,  $O(2)$  finite volume scaling function  $f_{G_\chi}(z, z_L)$  and the infinite volume result,  $f_{G_\chi}(z, 0) \equiv f_{G_\chi}(z)$ , versus  $z_L$ .

of universal critical behavior close to  $T_c$  and for the range of symmetry breaking parameters  $H$  used in our current study.

For  $z = z_L = 0$ , *i.e.* at the critical point, the scaling function  $f_{G\chi}(z)$  obeys the normalization  $f_{G\chi}(0) = 1 - 1/\delta$ . The scaled order parameter  $M/H^{1/\delta}$  at this critical point thus is proportional to the non-universal constant  $h_0^{-1/\delta}$ ,

$$M(T_c, H)/H^{1/\delta} = h_0^{-1/\delta}(1 - 1/\delta). \quad (14)$$

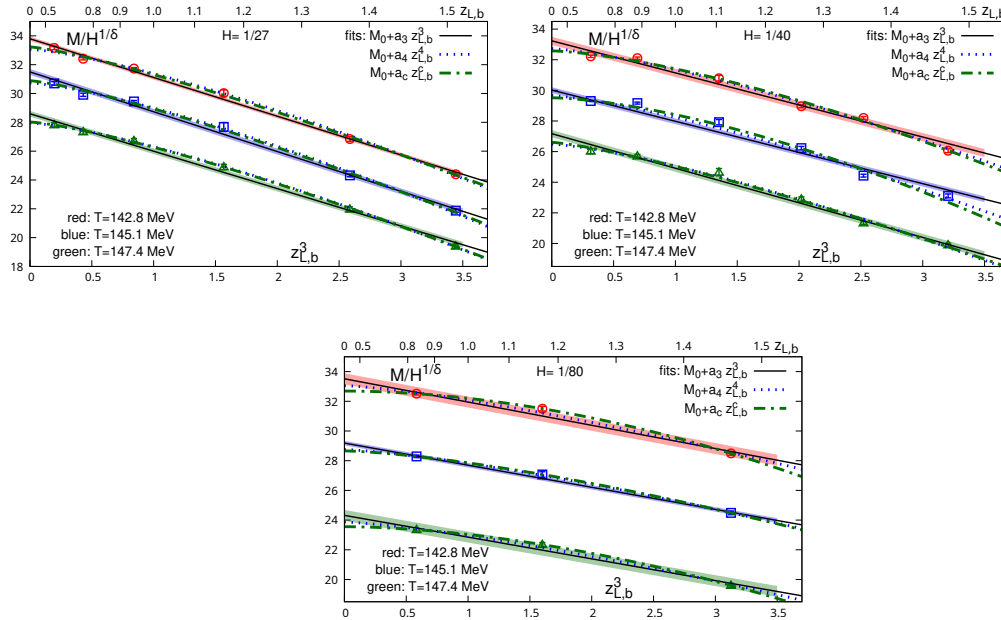
Also note that  $M(T, H)/H^{1/\delta}$  will diverge in the chiral limit for  $T < T_c$  and vanishes for  $T > T_c$ . This feature, arising from the asymptotic expansion of scaling function  $f_{G\chi}$ , actually is quite insensitive to a particular choice of the exponent  $\delta$ . For  $z = 0$  *i.e.* at  $T = T_c$ , the parametrization of finite volume corrections take on a simple form in terms of a polynomial in  $z_L$  only,

$$f_G(0, z_L) = 1 + \sum_{m=4}^8 a_{0m} z_L^m, \quad (15)$$

with coefficients  $a_{0m}$  given in Ref. [10].

### 3. Results

The main purpose of this proceedings contribution is to achieve a better understanding of basic chiral observables in the vicinity of the chiral phase transition temperature in (2+1)-flavor QCD and quantify their finite-size dependence. Although this should eventually been done in



**Figure 2:** The scaled order parameter,  $M/H^{1/\delta}$ , for three values of the light-to-strange quark mass ratio,  $H = 1/27, 1/40$  and  $1/80$ , versus the bare finite volume scaling variable  $z_{L,b}$ .

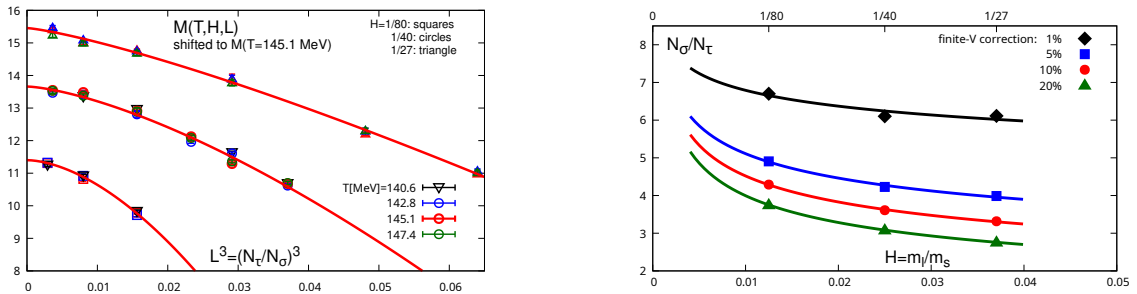
the continuum limit of QCD, we stick here to an analysis of the improved order parameter  $M$ , introduced in Eqn. (2), on lattices with fixed temporal extent  $N_\tau = 8$ . For our calculations with highly improved staggered quarks and an  $O(a^2)$  Symanzik-improved gauge action, we use the RHMC package embedded within the *SIMULATEQCD* repository [17, 18]. We present here results from our ongoing calculations obtained by using roughly  $10K$  statistics or more for each parameter set  $(T, m_\ell, V)$  or  $(t, H, L)$  in equivalent dimensionless lattice terms.

In Fig. 2, we show the scaled order parameter  $M/H^{1/\delta}$  which in the chiral limit, is proportional to the order parameter scaling function  $f_{G\chi}(z, z_L)$  as discussed in the previous section. We show results for three temperature values in the vicinity of the chiral phase transition temperature on lattices with temporal extent  $N_\tau = 8$ . This temperature has been estimated previously as  $T_c^{N_\tau=8} = 143.7(2)$  MeV [5]. We note that the finite-size dependence of  $M/H^{1/\delta}$  is close to being linear in the inverse volume  $z_L^3 \sim 1/L^3$  (see filled bands in Fig. 2). A slight curvature, however, is visible. This is reminiscent of the  $z_L$ -dependence of the 3-d,  $O(2)$  scaling function, which for small  $z_L$  has been found to be well described by  $f_G(0, z_L) \sim z_L^4$  in the vicinity of  $T_c$  [10]. We thus fitted the data for  $M/H^{1/\delta}$  obtained for fixed  $H$  as function of  $z_{L,b}$ , to an ansatz,

$$M = M_0 + a_c z_{L,b}^c, \quad (16)$$

where we (i) either fixed the exponent to  $c = 3$  or  $4$ , or (ii) kept  $c$  as an additional fit parameter. The latter ansatz indeed yields values for  $c$  close to  $4$ . We also note that the  $T$ -dependence of the finite volume slope of  $M$  is statistically not significant for the three temperatures shown in Fig. 2. In fact, fits with fixed  $c = 4$ , as well as with free exponents  $c$ , give amplitudes  $a_c$ , which agree within errors for the fits performed at three values of  $T$ , namely at  $T = 142.8, 145.1$  and  $147.4$  MeV.

We therefore performed joint fits to the data obtained for all three  $T$ -values, using the ansatz given in Eqn. (16) with  $a_c$  and  $c$  being  $T$ -independent and allowing only  $M_0$  to be  $T$ -dependent. Results of such a fit are shown in Fig. 3 (left), where we have shifted the data obtained at  $T_1 = 142.8$  MeV and  $T_2 = 147.4$  MeV, respectively, to  $T = 145.1$  MeV by using the difference  $s_i = M_0(T_i) - M_0(T)$  as shift parameters. Results obtained for the fits shown in Fig. 3 (left) are given in Table 1.



**Figure 3:** *Left:* The improved order parameter at  $T = 145.1$  MeV as well as at  $T = 142.8$  MeV and  $T = 147.4$  MeV. The latter two data sets have been shifted to the former (see discussion in the text). *Right:* Aspect ratio  $N_\sigma/N_\tau$  needed to reduce finite-volume effects in the improved order parameter  $M$  below a certain level, for different light quark masses  $m_\ell \equiv m_s H$ .

We may use these fits to estimate the aspect ratio  $N_\sigma/N_\tau$ , that is needed in lattice QCD calculations at fixed  $H$  to reduce finite-size effects in calculations of the improved order parameter below a certain percentage level. Such estimates are shown in Fig. 3 (right). This figure shows that in order to reduce finite-size effects on  $M$  below the one percent level, aspect ratios larger than 6 are needed for physical light-to-strange quark mass ratios,  $H = 1/27 \sim 0.037$  while an aspect ratio of about 7.5 is needed at  $H = 1/80 = 0.0125$ , which corresponds to a Goldstone pion mass of about 80 MeV. We also note that the fits performed here are valid for  $z_{L,b} \lesssim 1.5$ . For physical quark mass values or  $H = 1/27$ , this corresponds to an aspect ratio  $N_\sigma/N_\tau \simeq 2.5$ . For larger values of  $z_{L,b}$ , higher order corrections in  $z_{L,b}$  need to be taken into account for an accurate description of the finite-size dependence of the order parameter.

$H$	$M_0(T)$	$a_c$	$c$	$s_1$	$s_2$
1/27	15.46(7)	-0.95(8)	3.77(18)	1.21(6)	-1.32(7)
1/40	13.66(5)	-0.56(8)	4.39(37)	1.42(6)	-1.50(8)
1/80	11.40(4)	-0.23(4)	5.16(43)	1.68(3)	-1.96(3)

**Table 1:** Results for fits of  $M/H^{1/\delta}$  using the ansatz given in Eqn. (16) with  $M_0(T)$  for  $T = 145.1$  MeV and  $M_0(142.8\text{MeV}) = M_0(T) + s_1$ ,  $M_0(147.4\text{MeV}) = M_0(T) + s_2$ . The data for  $T_1 = 142.8$  MeV and  $T_2 = 147.4$  MeV have been shifted by  $s_1$  and  $s_2$ , respectively.

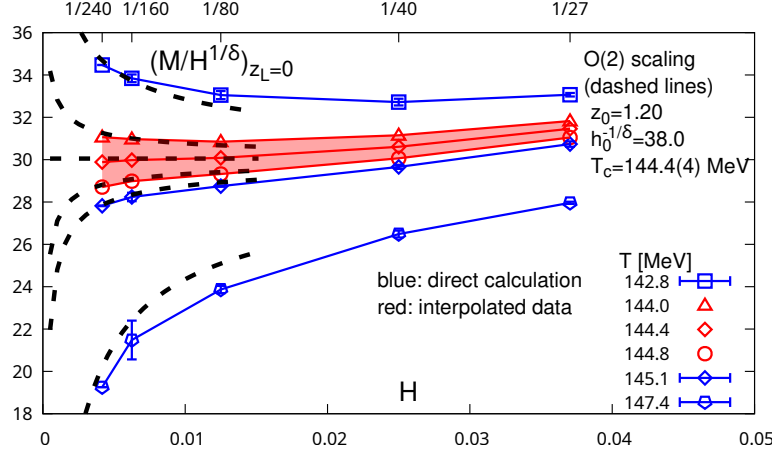
Finally, we want to use the infinite volume extrapolated results for  $M/H^{1/\delta}$  to obtain a new estimate for the chiral phase transition temperature on lattices of temporal extent  $N_\tau = 8$ . In Fig. 4, we show the scaled order parameter  $M/H^{1/\delta}$  versus  $H$  for the three temperature values examined so far. In addition to the infinite volume extrapolation of the data for  $H \geq 1/80$  shown in Fig. 2, we also added some preliminary results obtained for  $H = 1/160$  and  $H = 1/240$ . The tendency for  $M/H^{1/\delta}$  to diverge in chiral limit at  $T = 142.8$  MeV and vanish at  $T = 147.4$  MeV is clearly observed, following theoretical expectations based on the asymptotic expansion of the scaling functions. At  $T = 145.1$  MeV, the data continues to decrease for reducing value of  $H$  in chiral limit, suggesting that this temperature value also is above  $T_c^{N_\tau=8}$ .

Also shown in Fig. 4 are results for  $M/H^{1/\delta}$  obtained from a linear interpolation of data at  $T = 142.8$  MeV and  $T = 145.1$  MeV, respectively. Demanding that the interpolated data at  $H = 1/160$  and  $1/240$  agree within errors, yields an estimate for  $T_c^{N_\tau=8}$ . As our data generation and analysis is not yet complete for the two lowest values of  $H$ , the new estimate of the chiral transition temperature based on a well-controlled infinite volume extrapolation, also is still preliminary. At present, we find  $T_c^{N_\tau=8} = 144(4)$  MeV, which is in reasonable agreement with earlier estimates [5].

Using this estimate for  $T_c$  and the value  $h_0^{-1/\delta}$  obtained as,

$$h_0^{-1/\delta} = \lim_{H \rightarrow 0} \left[ \frac{M(144 \text{ MeV}, H)}{H^{1/\delta} \left(1 - \frac{1}{\delta}\right)} \right] \simeq 38, \quad (17)$$

we can determine the only remaining non-universal parameter  $z_0$  from a fit to the three values for  $M/H^{1/\delta}$  at  $H = 1/240$ . We obtain this as  $z_0 \simeq 1.2$ . The resulting asymptotic scaling curves are shown as dashed lines in Fig. 4. As can be seen, the asymptotic scaling curve  $f_{G_\chi}(z)$  gives a fairly



**Figure 4:** The infinite volume extrapolated, scaled order parameter versus  $H$  for three values of the temperature (blue) and interpolated values (red) used to estimate the chiral phase transition temperature on lattices with temporal extent  $N_\tau = 8$ . Dashed lines show the infinite volume, asymptotic scaling results using the non-universal parameters given in the figure.

good approximation to the scaled order parameter data for  $H \leq 1/160$  and in an even larger range,  $H \leq 1/80$ , at as well as close to  $T_c$ .

#### 4. Summary and Outlook

We presented first results from an ongoing study of finite-size effects in calculations of an improved order parameter for chiral symmetry breaking in (2+1)-flavor QCD, in which we attempt to quantify the finite-size effects as function of lattice volume and the light quark masses for a given temperature close to the chiral phase transition. Our calculations on lattices with fixed lattice cut-off corresponding to a temporal extent of  $N_\tau = 8$  show that precision studies of the order parameter require aspect ratios for the lattice size in units of temperature,  $N_\sigma/N_\tau \geq 6$  at physical values of the quark masses, which increases to about 8 for the currently used smallest quark mass ratio  $H = m_\ell/m_s = 1/240$ . This is currently a work in progress.

We also show that the improved order parameter  $M$  receives corrections to the leading order universal critical behavior from corrections-to-scaling and/or regular terms for  $m_\ell/m_s > 1/160$ . These corrections stay below the 10% level at the physical value of the light-to-strange quark mass ratio  $H = 1/27$ .

A more detailed, quantitative analysis of corrections to leading order universal scaling does require further calculations at small values of  $m_\ell/m_s$ , which are ongoing.

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