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Chiral phase transition temperature in 3-flavor QCD

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Establishing whether or not the famous first order corner at small quark masses exists in the Columbia plot is one of the major open issues in studies of the phase diagram of QCD. We delve into this problem and present results from our study of the chiral limit in 3-flavor QCD using the Highly Improved Staggered Quark (HISQ/tree) action. We investigate four quark masses, which in the continuum correspond to pion masses in the range 80 MeV to 140 MeV. In our simulations, the temporal lattice size, N_τ, is fixed to be equal to 8, and we explore three different aspect ratios $N_\sigma/N_\tau = 3,\ 4$ and 5. In the pion mass range explored by us, we do not find any direct evidence of the existence of a first order phase transition. We find the quark mass and volume dependence of the chiral observables to be well-described by the finite size scaling functions belonging to 3-d, $O(2)$ universality class. We determine the chiral phase transition temperature at this value of finite lattice spacing to be $T_c = 98^{+3}_{-6}$ MeV.

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1. Introduction

In QCD, for the case of n_f massless quark flavors, left- and right- handed quarks transform under independent global $SU(n_f)$ symmetries. This symmetry group given by, $SU(n_F)_L \times SU(n_f)_R$, at low temperature gets spontaneously broken down to the diagonal subgroup $SU(n_f)_V$. This work is an investigation of the restoration of this spontaneously broken symmetry as a function of the temperature when $n_f = 3$. The nature of the QCD chiral phase transition as a function of the number of light flavors and the value of the quark masses has been the subject of intense and ongoing study ever since the first work of Pisarski and Wilczek [1]. The transition is expected to become first order when number of massless flavors is greater than or equal to 3. Our interest lies in the lower-left corner as well as the diagonal sketched in the well-known Columbia plot [2].

Lattice QCD calculations in the past performed using staggered fermions, find first order transitions with unimproved gauge and fermion actions [3], however, the bounds on the critical mass show a strong cut-off and discretization scheme dependence [4]. In calculations using HISQ action, no direct evidence for a first order transition on lattices with temporal extent $N_\tau = 6$ has been found, and a bound on the pseudoscalar Goldstone mass, above which no first order transition exists, has been estimated to be $m_\pi^c \simeq 50$ MeV [5]. In calculations with $O(a)$ improved Wilson fermions [6], first order transitions have been found at non-zero values of the quark masses and the bound on the critical mass is weaker, $m_\pi^c \lesssim 110$ MeV. This bound, however, also is consistent with a continuous transition in the continuum limit [6, 7].

A recent analysis of the order of the chiral transition as function of the number of flavors, performed with staggered fermions and extrapolated to the continuum limit [7], suggests that the chiral phase transition in 3-flavor QCD is second order, which is in contrast to RG analyses. However, as has been pointed out, such analyses are based on a Landau-Ginsburg effective action for the order parameter, which is arrived at by integrating out all gauge degrees of freedom. The role of gauge fluctuations, however, is subtle and may also influence the order of the chiral phase transition [8, 9]. It also has been argued that a ϕ^6 contribution to the effective Lagrangian for the order parameter may be of relevance and may allow for a second order chiral phase transition to occur in QCD with number of massless flavors being larger than two [7]. A continuous transition in the chiral limit of 3-flavor QCD thus may not be ruled out entirely. Ref [10] is a study of $n_f = 4$ flavors, which avoids the complication associated with rooting in staggered fermions. The results found in this unrooted study are qualitatively similar to the 3-flavor case. This provides further support to the studies based on staggered fermions, and to the possibility that the 3-flavor chiral phase transition is not first order.

The paper is organized as follows. In the next section we present simulation details. Section 3 introduces the chiral observables for 3-flavor QCD. Section 4 summarizes basic relations needed for our discussion of finite size scaling (FSS) analysis of chiral observables. In section 5 we present our results for the chiral order parameter and its susceptibility. In section 6 we finally present our results for the extraction of 3-flavor chiral phase transition temperature, T_c, from the FSS analysis of the observables constructed using chiral order parameter and its susceptibility as well as from the pseudocritical temperatures for various combinations of quark masses and volumes. We give our conclusions in section 7.

Full Details of our project can be found in our paper [11].

2. Simulation Details

In our lattice QCD simulations with three degenerate flavors, we used HISQ action and a tree-level improved Symanzik gauge action. The temporal extent of all our lattices was fixed at $N_\tau = 8$, while the spatial extent was chosen to be one of $N_\sigma = 24$, 32 or 40. In order to take into account the finite-size effects, we performed calculations at a given quark mass for at most two different values of N_σ. The larger one is chosen such that $m_\pi L \geq 3$ in the region of the pseudocritical temperatures.

We used the Bielefeld GPU code [12] to generate around 10,000-50,000 hybrid Monte Carlo trajectories separated by 0.5 Time Units (TU) for $N_\sigma = 40$, and 1 TU for the smaller volumes. These data sets have been generated in 10 independent streams that have been decorrelated initially using about 200 trajectories. The RHMC (Rational Hybrid Monte Carlo) algorithm [13, 14] was used to generate the configurations and the molecular dynamics step sizes were tuned to achieve acceptance rates of about 60-80%. We saved gauge field configurations after every 5th TU and performed calculations of various chiral observables on these configurations.

We generated data sets for different values of the quark masses at up to 17 values of the temperature in the range 110 MeV $\lesssim T \lesssim$ 170 MeV. To choose masses for three light degenerate quark flavors, we used the line of constant physics (LCP) determined in Ref. [15] for the case of (2+1)-flavor QCD. This LCP defines the value of the strange quark mass, $m_s^{\rm phys}(\beta)$, as a function of the gauge coupling β. It is tuned to its physical value by demanding the mass of the fictitious $\eta_{s\bar{s}}$ meson to stay constant on this LCP. We choose four different sets of three degenerate light quark masses, m_q, as a fraction of $m_s^{\rm phys}(\beta)$, corresponding to $m_q = H\, m_s^{\rm phys}(\beta)$, with $H = 1/27,\ 1/40,\ 1/60$ and $1/80$. We used f_K scale setting given in Ref. [16] to set the temperature scale, with $f_K = 156.1/\sqrt{2}$ MeV being the kaon decay constant.

3. Chiral observables

On each saved gauge field configuration, we calculated the chiral condensate, $\langle\bar{\psi}\psi\rangle$, and its susceptibility, $\chi_{\rm tot}$, which are obtained from the free energy density of 3-flavor QCD, $f(T, m_q) = -(T/V)\ln Z(T, V, m_q)$, as first and second derivative with respect to the quark mass m_q. $Z(T, V, m_q)$ is the QCD partition function for n_f degenerate quark flavors. The chiral susceptibility is represented in terms of disconnected, $\chi_{\rm disc}$, and connected, $\chi_{\rm con}$ contributions, $\chi_{\rm tot} = \chi_{\rm disc} + \chi_{\rm con}$. These chiral observables are given in terms of the inverse of the staggered fermion matrix, $D_q(m_q)$, and its higher powers.

$$
\begin{aligned}
\langle\bar{\psi}\psi\rangle &= -\frac{1}{N_\sigma^3 N_\tau}\frac{\partial \ln Z}{\partial m_q} = \frac{n_f}{4N_\tau N_\sigma^3}\left\langle {\rm tr} D_q^{-1}\right\rangle , \\
\chi_{\rm tot} &= \frac{\partial\langle\bar{\psi}\psi\rangle}{\partial m_q} , \\
\chi_{\rm disc} &= \frac{1}{N_\tau N_\sigma^3}\left(\frac{n_f}{4}\right)^2 \left(\left\langle {\rm tr}^2 D_q^{-1}\right\rangle - \left\langle {\rm tr} D_q^{-1}\right\rangle^2\right), \\
\chi_{\rm con} &= -\frac{n_f}{4N_\tau N_\sigma^3}\left\langle {\rm tr} D_q^{-2}\right\rangle . \qquad (1)
\end{aligned}
$$

We evaluate traces in the above equations using 100 Gaussian random vectors. After calculating the traces on each saved configuration, the observables were calculated by dividing the total number of configurations into 10 bins and using the jackknife procedure.

4. Scaling and finite-size scaling of chiral observables

Spontaneously broken symmetry restoration is generally associated with the phase transitions. Therefore, one should investigate the 3-flavor chiral transition in QCD from the lens of scaling analysis. As we are currently analyzing the chiral limit at fixed values of the cut-off, the universality class of 3-dimensional-$O(2)$ symmetric models would be appropriate, while the $Z(2)$ universality class is of relevance, if a second order phase transition occurs at a small value of the quark mass, m_q^c. In the vicinity of a critical point, (T_c, m_q^c), the thermodynamic free energy, $f(T, m_q)$, can be resolved into singular and regular contributions, $f(T, m_q) = f_s(T, m_q) + f_r(T, m_q)$. The temperature and quark mass dependence of $f_s(T, m_q)$ is expressed in terms of a universal scaling function, $f_f(z)$, which is characteristic for a particular universality class. Thus we have

$$f_s(T, m_q) = h_0 h^{1+1/\delta} f_f(z) \ \ , \ \ z = t/h^{1/\beta\delta} \ , \tag{2}$$

with t and H being dimensionless variables constructed from the temperature T and quark mass m_q,

$$t = \frac{1}{t_0}\frac{T - T_c}{T_c} \ , \ h = \frac{1}{h_0}\frac{m_q - m_q^c}{m_s^{\text{phys}}} \equiv \frac{H - H_c}{h_0}. \tag{3}$$

The constants β and δ are critical exponents of the 3-d, $O(2)$ universality class for which we use [17], $\beta = 0.3490$, $\delta = 4.7798$, while t_0 and h_0 are non-universal constants that are introduced to fix the overall normalization of the order parameter M [18].

For small quark masses, in the vicinity of the chiral transition temperature, T_c, the dominant contributions to the order parameter M and its susceptibility χ_M arise from the singular part of the free energy. Scaling relations for these observables are then obtained by taking derivatives of $f_s(z)$ with respect to H. We have

$$M(T, m_q) = -\frac{\partial f_s}{\partial H} = h^{1/\delta} f_G(z) \ , \tag{4}$$

and

$$\chi_M(T, m_q) = \frac{\partial M}{\partial H} = \frac{h^{1/\delta - 1}}{h_0} f_\chi(z) \ , \tag{5}$$

respectively. Here $f_G(z)$ and $f_\chi(z)$ are also universal functions of the scaling variable z, that can be obtained from $f_f(z)$. Both these functions have been determined numerically using high-statistics Monte Carlo simulations for the 3-d, $O(2)$ and $O(4)$ universality classes [17, 19–21]. We will make use of the implicit parameterization provided for these functions for the $O(2)$ case in Ref. [22]. We use chiral observables defined in Eq. 1, and the strange quark mass $m_s^{\text{phys}}(\beta)$ for multiplicative renormalization of the chiral observables to define the order parameter, M, and its susceptibility, χ_M as,

$$\begin{aligned} M &= m_s^{\text{phys}} \langle \bar{\psi}\psi \rangle / f_K^4 \ , \\ \chi_M &= \frac{\partial M}{\partial H} = \left(m_s^{\text{phys}}\right)^2 \chi_{\text{tot}} / f_K^4 \quad . \end{aligned} \tag{6}$$

Note that both order parameter, and its susceptibility contain the additive divergence due to UV contribution. It is possible to define a quantity, $M_\chi = M - H\chi_M$, which in the scaling regime is devoid of any regular contribution linear in H as well as of the divergent UV contributions. In terms of scaling functions it becomes,

$$M_\chi = h^{1/\delta}\left(f_G(z) - f_\chi(z)\right) \ . \tag{7}$$

M_χ is just the difference between transverse and longitudinal susceptibilities multiplied by the symmetry breaking field. At high temperatures, it vanishes as $M_\chi \sim H^3$; at low temperatures, it equals the order parameter M at $H = 0$ but receives different corrections at $O(\sqrt{H})$.

From Eqs. (4) and (5), it can be readily seen that sufficiently close to m_q^c, $f_r(T, m_q)$ can be ignored, therefore,

$$\frac{(H - H_c)\chi_M(0,h)}{M(0,h)} = \frac{f_\chi(0)}{f_G(0)} = \frac{1}{\delta} \ , \tag{8}$$

irrespective of the quark mass m_q. Curves for different quark masses will have a unique crossing point at $T = T_c$.

In addition to regular contributions, Eq. (8) also receives corrections when the system size L is finite. Then the scaling functions $f_G(z)$ and $f_\chi(z)$ in Eqs. (4) and (5) must be replaced by the corresponding Finite-Size Scaling (FSS) functions $f_{G,L}(z, z_L)$ and $f_{\chi,L}(z, z_L)$. Here $z_L = L_0/Lh^{\nu/\beta\delta}$ is a second scaling variable and $\nu = \beta(\delta + 1)/d$ with $d = 3$ is the critical exponent controlling the divergence of the correlation length at the critical point. L_0 is another non-universal constant that can be fixed through a normalization condition [23]. In the thermodynamic limit ($L \to \infty$) the finite size scaling functions, $f_{G,L}(z, z_L)$ and $f_{\chi,L}(z, z_L)$, go over to their infinite-volume equivalents $f_G(z) \equiv f_{G,L}(z, 0)$ and $f_\chi(z) \equiv f_{\chi,L}(z, 0)$.

The infinite and finite volume scaling functions have been determined for the 3-d, $O(2)$ and $O(4)$ cases [22, 23]. In our FSS analysis we use a rational polynomial parameterization of the FSS functions [24] similar to what has been used also for the analysis of FSS in $O(4)$ spin models [23]

As we will see, the observed transition is a crossover for all the quark masses that we studied. According to the standard picture of the phase diagram [2], this transition should turn into a first order phase transition if the quark mass is less than a certain value $m_q < m_q^c$. For $m_q = m_q^c$ then, the transition will be second order belonging to the 3-d, $Z(2)$ universality class. If on the other hand, the expected first order region is absent, then the transition will be second order belonging to the 3-d, $O(2)$ universality class in the three-flavor chiral limit for fixed N_τ. Since we did not find any evidence of a non-zero critical quark mass m_q^c in our study, we will assume $m_q^c = 0$ in the following and use the $O(2)$ scaling functions for the rest of this work.

5. Chiral order parameter and its susceptibility

We present our results for the chiral order parameter, M, and its susceptibility, χ_M, calculated on lattices with temporal extent $N_\tau = 8$, in Fig. 1. The order parameter M varies rapidly but smoothly, starting from a high value and decreasing to a low value over the temperature range considered here. For a given 3-flavor quark mass, we observe that the temperature range corresponding to the most rapid change in M, contains the peak of the chiral susceptibility, χ_M . Except for the case $H = 1/60$, we show in Fig. 1 results for two different volumes. While the volume dependence is

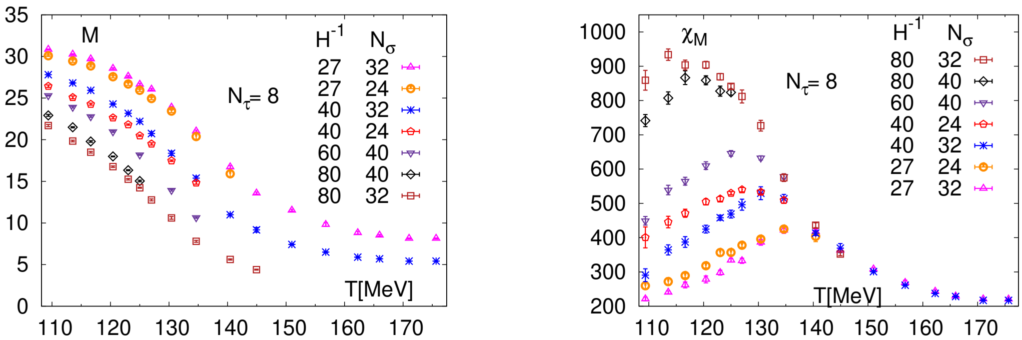

Figure 1: Results for the order parameter M (left) and its susceptibility χ_M (right) as a function of temperature for all quark masses and volumes.

negligible in M and χ_M slightly above the corresponding pseudo-critical temperatures, evidence for a characteristic volume dependence is seen at smaller temperatures. In fact, contrary to what would be expected at or close to a second or first order phase transition, we see no increase in the peak height of χ_M with increasing volume. Instead we observe a slight decrease of the peak height of χ_M and a shift of the peak position towards larger temperatures as the volume is increased. At the same time the peak becomes more pronounced with increasing volume. This behavior is reminiscent of the finite volume effects known from an analysis of finite size scaling functions in 3-d, $O(N)$ symmetric spin models [22, 23].

In Fig. 2 we show the chiral order parameter as function of H for several values of the temperature. As can be seen, for $T \geq 140$ MeV, the order parameter depends linearly on the quark mass and extrapolates smoothly to zero for $H \to 0$. At lower temperatures the quark mass dependence of the location of the maximum in χ_M suggests that in the chiral limit all our calculations correspond to a range of temperatures in the chirally symmetric phase.

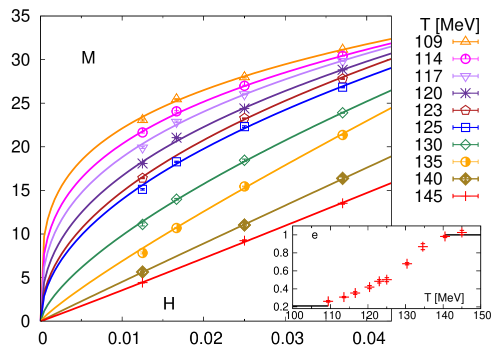

Figure 2: The chiral order parameter M as function of H at fixed temperature. Lines show fits to the ansatz $M = AH^e$. The inset shows results for the fit parameter e.

For a first analysis of the quark mass dependence of M, we thus fitted the data on the largest lattices available to an ansatz, $M = AH^e$. Results for the exponent e are shown in the inset of this figure. Within errors it is consistent with unity for $T \geq 140$ MeV and decreases continuously with decreasing temperature. At the lowest temperature, $T \simeq 110$ MeV, we find $e \simeq 0.27$, which is larger but compatible with the exponent one expects to find at a critical point belonging to the 3-dimensional $O(2)$ or $Z(2)$ universality classes, i.e. $e \equiv 1/\delta \simeq 0.21$. If we will go further down in the temperature range, we will hit the expected value for the exponent e.

6. Results

We define the pseudo-critical temperature, $T_{pc}(m_q, N_\sigma)$, on lattices with spatial extent N_σ as the location of the maximum of χ_M for a given quark mass and volume. We also define $T_{pc}(m_q)$ as the infinite volume pseudo-critical temperature for a given quark mass. As can be seen in Fig. 1, $M(T, m_q, N_\sigma)$ and $\chi_M(T, m_q, N_\sigma)$ show a sizeable volume dependence for all the quark masses and for temperatures $T < T_{pc}(m_q)$, and thus need to be treated carefully to arrive at results in the thermodynamic limit.. Above the pseudo-critical temperature this volume dependence is significantly weaker.

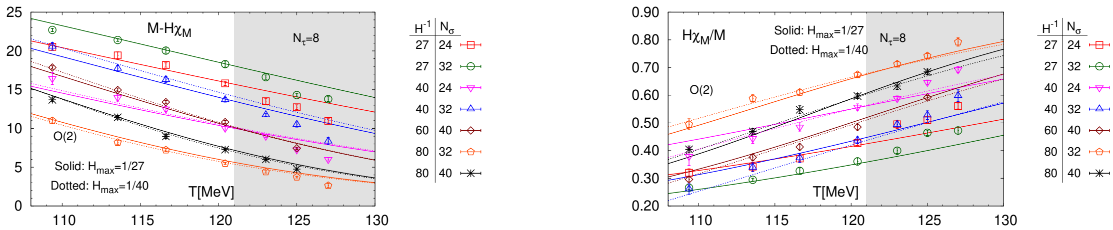

Figure 3: Finite Size Scaling fits to M_χ (left) and the ratio $H\chi_M/M$ (right) with (solid lines) and without (dotted lines) the largest quark mass ratio $H = 1/27$. The gray region has been left out of the fits. For ratio, shown is a fit as given in Eq. 9 with a regular contribution linear in temperature ($a_2 = 0$). The fit parameters are summarized in Tables III and IV of Ref [11].

Fig 3 (left) shows our fit results for $M_\chi(T, m_q, N_\sigma)$ fitted to the ansatz constructed from the difference of FSS functions as $h^{1/\delta}\left(f_{G,L}(z, z_L) - f_{\chi,L}(z, z_L)\right)$. Aside from the critical temperature in the chiral limit, T_c, a fit to this ansatz involves the three non-universal parameters, $h_0, z_0 = h_0^{1/\beta\delta}/t_0,\ z_{L,0} = L_0 h_0^{\nu/\beta\delta}$, which determine the overall amplitude of M_χ and set the scale for the scaling variables z and z_L, respectively. We perform fits only for temperatures close to the expected chiral transition temperature, *i.e.* for temperatures below 121 MeV. The results of such fits in different fit ranges for the quark masses, $H \in [0, H_{\max}]$ are given in Tab III of [11]. For $H_{\max} = 1/27$ and $1/40$, T_c values obtained from the FSS fits are 100(1) MeV and 97(1) MeV respectively.

Fig 3 (right) shows our fit results for the ratio of the chiral susceptibility multiplied by H and the chiral order parameter which has been used in [25] to determine the chiral phase transition temperature in (2+1)-flavor QCD,

$$\frac{H\chi_M(T, m_q, N_\sigma)}{M(T, m_q, N_\sigma)} = \frac{f_{\chi,L}(z, z_L) + H^{1-1/\delta} f_{\mathrm{reg}}(T)}{f_{G,L}(z, z_L) + H^{1-1/\delta} f_{\mathrm{reg}}(T)}\ . \tag{9}$$

Unlike M_χ, this ratio is sensitive to regular contributions. However, the explicit dependence on the non-universal scale parameter h_0 gets eliminated in this case. For the contributions of the regular term, we use a leading order Taylor expansion in the vicinity of the chiral transition temperature, T_c,

$$f_{\mathrm{reg}}(T) = a_0 + a_1 \frac{T - T_c}{T_c} + a_2 \left(\frac{T - T_c}{T_c}\right)^2\ . \tag{10}$$

We perform a FSS analysis of the ratio given in Eq. 9. We again performed fits in different fit intervals $H \in [0, H_{\max}]$ and a small temperature interval, $T \in [0, 121]$MeV. In this temperature interval it suffices to use a regular term, given by Eq. 10, with $a_2 = 0$. Results of these fits are summarized in the upper part of Tab. IV of Ref [11] and are shown in Fig. 3 (right) for the two cases $H_{\max} = 1/27$ and $1/40$, with T_c values obtained from fitting being 101(2) MeV and 93(4) MeV respectively.

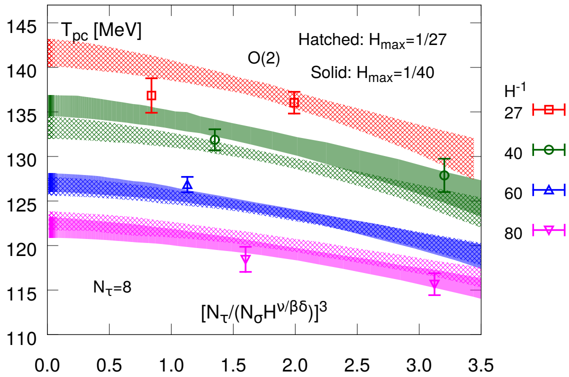

Figure 4: Results for the peak location $T_{pc}(m_q, N_\sigma)$ plotted versus the finite volume scaling variable $(z_L/z_{L,0})^3 = (N_\tau/(N_\sigma H^{\nu/\beta\delta}))^3$. The data are plotted as points whereas the bands are the fit results for two different choices of the fit interval in H.

The chiral phase transition temperature, T_c can be determined from a finite size scaling analysis of the pseudo-critical temperature $T_{pc}(m_q, N_\sigma)$, which can be obtained straightforwardly from our data for $\chi_M(T, m_q, N_\sigma)$. For the details of $T_{pc}(m_q, N_\sigma)$ extraction procedure - comprising of bootstrap sampling and quadratic fits in the peak region - see Ref [11]. The resulting estimates for the finite-volume pseudo-critical temperatures for all available lattice sizes are given in Tab. VI of [11]. We present our results for $T_{pc}(m_q, N_\sigma)$ for all the quark masses and volumes in Fig. 4.

We fitted these data using the FSS scaling ansatz for T_{pc} deduced from the fact that the finite size scaling function $f_{\chi,L}(z, z_L)$ peaks at a characteristic value z_p of the scaling variable, z. As pointed out earlier, it can be seen from Fig 1 (right), that the peak position for a given quark mass exhibits volume dependence. Hence the ansatz,

$$T_{pc}(m_q, N_\sigma) = T_c \left(1 + \frac{z_p(z_L)}{z_0} H^{1/\beta\delta}\right) , \tag{11}$$

where $z_p(0) = z_p$ gives the location of the maximum of the infinite volume $O(2)$ scaling function $f_\chi(z)$, and $z_p(z_L)$ is a parameterization of the finite volume dependence of this peak location [24],

$$z_p(z_L) = z_p \left(1 - 1.361(8)/z_L^{4.48(3)}\right) . \tag{12}$$

This parameterization holds for $z_L \leq 0.9$. The resulting fits for the pseudo-critical temperatures are also shown in Fig. 4, again for the cases with and without including the largest quark mass, $H = 1/27$, with T_c values obtained from fitting being 102(2) MeV and 95(3) MeV respectively. Details of the fit parameters z_0, z_{L0} obtained from these fits are given in Tab. VII of the Ref [11].

The chiral phase transition temperature as well as the non-universal parameters obtained from the analysis of the pseudo-critical temperatures, M_χ and the ratio $H\chi_M/M$ are in agreement within errors. We took into account the systematic differences in our fits resulting from changes of the fit range for H as well as the fit ansätze that include or leave out contributions from regular terms in the different observables we fitted. Averaging over all these fit results (see Fig 10 of Ref [11]) for T_c, we obtain the following value for the chiral phase transition temperature in 3-flavor QCD on lattices with temporal extent $N_\tau = 8$,

$$T_c = 98^{+3}_{-6} \text{ MeV} . \tag{13}$$

7. Conclusions

In our analysis of the chiral phase transition in 3-flavor QCD, performed for finite values of the lattice spacing, corresponding to $N_\tau = 8$, for the range of quark masses corresponding in the continuum limit to light pseudoscalar Goldstone masses in the range 80 MeV $\leq m_\pi \leq$ 140 MeV, we find no direct evidence for a conjectured first order phase transition. In the transition region we observe pseudo-critical behavior with a finite volume dependence, which is consistent with the expected FSS behavior in the 3-d, $O(2)$ universality class. For the chiral phase transition temperature at these non-vanishing values of the lattice spacing, we find $T_c = 98^{+3}_{-6}$ MeV.

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