Two flavor QCD and confinement - II

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This paper is part of a program of investigation of the chiral transition in $N_f = 2$ QCD, started in Ref. [1]. Progress is reported on the understanding of some possible systematic errors. A direct test of first order scaling is presented.

I. INTRODUCTION

The order of the chiral transition of two-flavor QCD is not established yet, despite its great relevance to understand important aspects of color confinement and of the structure of the QCD phase diagram [2]. A natural order parameter in that limit is the chiral condensate, even if empirically one finds that also deconfinement happens at the same critical temperature T_c, as found by looking at the susceptibility of the Polyakov loop or by direct studies of order parameters constructed in the framework of specific models of color confinement [3, 4, 5].

A renormalization group analysis plus ϵ-expansion can be made around $m \simeq 0$, assuming that the relevant degrees of freedom for the chiral transition are scalar and pseudoscalar fields [6, 7, 8]. The result is that for $N_f = 2$, if the $U_A(1)$ anomaly term is still effective at the transition, i.e. if the η' mass does not vanish at T_c, an infrared stable fixed point may exist in the universality class of the three dimensional $O(4)$ spin model. Two possibilities are therefore left open: a first order order phase transition, or a second order phase transition with $O(4)$ critical indexes.

Two completely different scenarios correspond to those two possibilities. Since, contrary to the first order case, second order phase transitions are unstable against the explicit breaking of the underlying symmetry, in the second case one would have a crossover instead of a real phase transition for small but non-zero quark masses. That would imply the possibility of going continuously

from a confined to a deconfined state of matter, in contrast with the idea of confinement being an absolute property of strongly interacting matter at zero temperature and of deconfinement being an order-disorder transition associated to a change of symmetry [9]. A second consequence would be the presence of a crossover line, at finite mass, in the region of high temperature and small baryon chemical potential μ_B of the QCD phase diagram, thus implying a critical point [10] to connect with the first order line which is supposed to exist at low temperatures and large chemical potentials. No such point is expected to exist if the transition at $\mu_B = 0$ is first order. No critical point has been found up to now in experiments with heavy ions, but the question is still open [11, 12, 13].

The problem can in principle be solved numerically using lattice QCD simulations, by means of a finite size scaling (FSS) analysis leading eventually to a precise determination of the critical indexes of the transition. However technical difficulties are encountered in this program. First of all, huge computational resources are needed to make numerical simulations of the system which are close enough both to the chiral and to the thermodynamical limit (i.e. with small enough quark masses and large enough spatial volumes). Second, a FSS analysis is made intricate by the fact that the system has two relevant scales: the correlation length ξ of the order parameter and the inverse quark mass $1/m_q$. In particular it is possible to write the following FSS ansatz for the free energy density $\mathcal{L}/kT$ around the chiral critical point

$$\frac{\mathcal{L}}{kT} \simeq L_s^{-d} \phi \left(\tau L_s^{1/\nu}, am_q L_s^{y_h} \right) . \qquad (1)$$

$\mathcal{L}$ depends on two different scaling variables instead of one as is the case for simpler systems, like e.g. the quenched theory. L_s is the spatial size, τ is the reduced temperature $\tau = (1 - T/T_c)$, ν is the critical index of

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the correlation length ($\xi \sim \tau^{-\nu}$) and y_h is the magnetic critical index. From Eq. (1) one can then derive the FSS for the specific heat

$$C_V - C_0 \simeq L_s^{\alpha/\nu} \phi_c \left(\tau L_s^{1/\nu}, am_q L_s^{y_h} \right) , \qquad (2)$$

where C_0 stems from an additive renormalization [14], and for the susceptibility χ of the chiral order parameter

$$\chi_m - \chi_0 \simeq L_s^{\gamma/\nu} \phi_\chi \left(\tau L_s^{1/\nu}, am_q L_s^{y_h} \right) . \qquad (3)$$

A few groups have investigated the problem on the lattice with staggered [15, 16, 17, 18, 19, 20, 21] or Wilson [22] fermions. The common procedure has been to use approximate versions of the scaling laws (2) and (3), usually assuming to be already in the infinite volume limit. No clear answer has been found, but there exists a general prejudice in favor of a second order chiral transition.

In Ref. [1] we have approached the problem by use of staggered fermions and a novel strategy for the FSS analysis which, together with the availability of relevant resources of computer power, has allowed us to achieve some progress. We have decided to keep one of the scaling variable fixed, so as to reduce the FSS analysis, Eqs. (2) and (3), again to one variable. In order to do that, after choosing a value for the critical index y_h appropriate to a given universality class, we have performed a series of runs at variable spatial size L_s and quark mass m_q, keeping the quantity $am_q L_s^{y_h}$ fixed. The choice for the index y_h implies an a priori assumption about the critical behavior, which can then be carefully checked without any approximation looking at the residual scaling. In particular in Ref. [1] we have chosen to test the $O(4)$ critical behavior, or better $O(2)$, which is more appropriate for the case of staggered fermions at non zero lattice spacing [20]: we have therefore fixed $y_h = 2.49$, which happens to be the same both for $O(4)$ and for $O(2)$. Our results for the chiral susceptibility, for the specific heat and for the equation of state have then shown a clear inconsistency with both the $O(4)$ and $O(2)$ scaling hypothesis, thus giving clear evidence against the possibility that those critical behaviors can describe the QCD phase transition for $N_f = 2$ in the chiral limit. In Ref. [1] we did not perform the analogous scaling test assuming a first order. We do that in the present paper (see Sect. III). In Ref. [1] we have obtained some evidence in favor of a first order transition, by keeping the first scaling variable fixed. We then do the approximation of spatial size large compared to the inverse pion mass. With this approximation the scaling laws read

$$C_V - C_0 \simeq am_q^{-\alpha/(\nu y_h)} \phi_c \left(\tau L_s^{1/\nu} \right) , \qquad (4)$$

$$\chi_m - \chi_0 \simeq am_q^{-\gamma/(\nu y_h)} \phi_\chi \left(\tau L_s^{1/\nu} \right) . \qquad (5)$$

We have checked Eqs. (4)-(5) and we found disagreement with $O(4)$, $O(2)$ and agreement with a weak first order.

A further result of our study was that a simple analysis of the dependence of the pseudocritical temperature on the quark mass, when correctly taking into account the dependence of the physical lattice scale on m_q, does not allow to discriminate between a second order and a first order critical behavior. In Ref. [1] also the magnetic equation of state was consistent with weak first order (see also Sect. III below).

The results obtained in Ref. [1] must be considered as the starting point of an accurate study of the problem. Indeed several questions have been left open, which deserve further analysis. First of all, the preliminary evidence in favor of a first order transition should be directly confirmed by a series of runs in which $am_q L_s^{y_h}$ is kept fixed according to first order critical behavior, i.e. $y_h = 3$. Second, our evidence against a second order transition in the universality class of $O(4)$ or $O(2)$ should be verified against all possible systematic effects which could have influenced our results, in particular: *i)* In Ref. [1] we have used an non-exact R algorithm [23], even if being quite conservative in the choice of the integration step for molecular dynamics; that could lead to systematic errors which, in principle, could influence the determination of the order of the phase transition. *ii)* In Ref. [1] we have used a standard gauge and fermionic action, and a temporal extent $L_t = 4$, corresponding to a lattice spacing $a \sim 0.3$ fm around the phase transition ($T = 1/(aL_t)$). Critical behavior is a typical infrared phenomenon. Nevertheless ultraviolet cut-off effects could in principle have some influence on it so that the continuum limit of our results should be checked by using a smaller lattice spacing, i.e. an improved action and/or a larger value of L_t. Finally, if the chiral transition is really first order, however weak, one should find signals of metastability in the physical observables when going to large enough volumes; no convincing signals were found in previous literature, nor in Ref. [1], and the question should be clarified, by exploring larger volumes.

Answering to all previous questions represents a difficult and computationally demanding program, which we partially carry out in the present paper. In particular we address the question related to the use of a non-exact algorithm in Section II, where some of the results obtained with the R algorithm in Ref. [1] are checked by using an exact RHMC algorithm. In Section III we directly test the first order hypothesis by using a new set of numerical simulations performed by keeping $am_q L_s^{y_h}$ fixed with $y_h = 3$. Our conclusions and perspectives for the continuation of our program will be presented in Section IV.

II. RESULTS OBTAINED WITH THE RHMC ALGORITHM

Keeping under control the systematic errors introduced by a non-exact algorithm like the Hybrid-R is a very expensive task in terms of computer power. In principle one should carry out multiple MC simulations with smaller
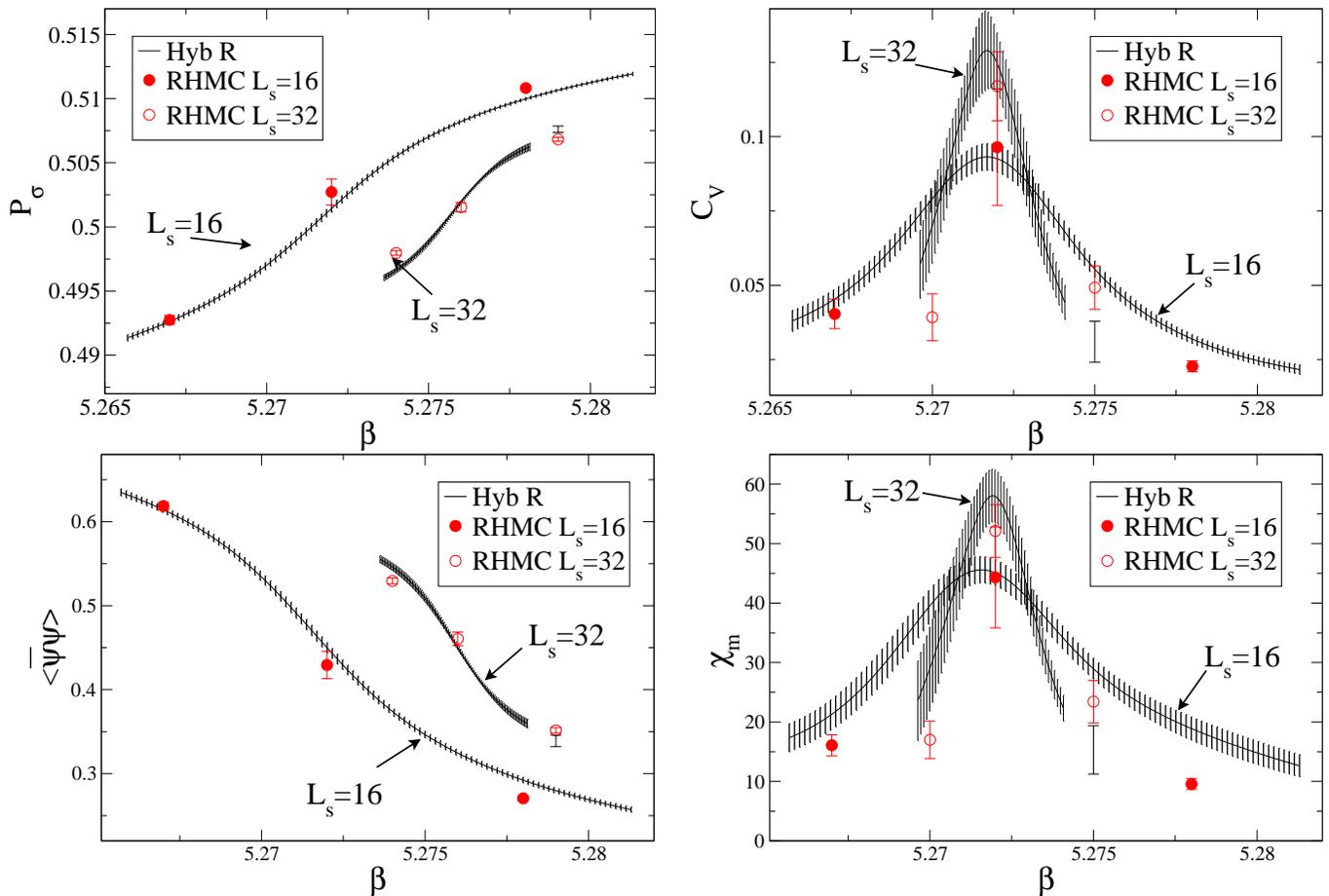
FIG. 1: Comparison between MC estimates obtained by the exact RHMC algorithm and the Hybrid-R for the average value (left column) and susceptibility (right) of the plaquette (top row) and chiral condensate (bottom) on lattices with $L_s = 16, 32$ and $m_L = 0.01335$. The average values for $L_s = 32$ in the left figures have been shifted to the right ($\Delta\beta = 0.004$) for sake of visual clarity.

and smaller molecular dynamics integration steps for every value of the simulation parameters. This extrapolation is in practice unfeasible - especially if one aims at the investigation of the chiral limit. What can be done is to choose the integration step size as a function of the simulation parameters, in our case the lattice quark mass $am_q \equiv m_L$, in such a way that discretization errors are negligible as compared to the statistical ones. The right functional form can be determined by a preliminary study on a representative subset of the parameters or using known results present in the literature (see e.g. [20]). For standard Kogut-Susskind fermions the simple choice: $\delta t = m_L/4$ is believed to lead to an accuracy of $\approx 5\%$ in the thermodynamic susceptibilities for masses as low as $m_L \approx 0.01$. That was the choice we used in Ref. [1] for all but the largest volume $L_s = 32$ at the smallest mass $m_L = 0.01335$ where, for computational limitations, we took $\delta t = m_L/2$, which is expected to introduce errors of about 10%.

Recently the RHMC algorithm [24] has emerged as a convenient and exact algorithm for staggered fermion

simulations. Not only it has no systematic errors to control (i.e. no estrapolation is needed), but it also outperforms the R algorithm for 2 flavors in terms of computer time. This makes the RHMC algorithm the ideal candidate to put the data of Ref. [1] to the test (and to produce the new data).

The subset of simulations used for this comparison was the one with the smallest lattice quark mass, namely $m_L = 0.01335$ with $L_s = 16, 32$, where discretization errors are expected to be more significant and where a larger δt was used for the biggest lattice. We made three different simulations for each value of L_s at couplings just below, just above and at the transition point. For each value of β we accumulated a statistics of order 3k trajectories for $L_s = 32$ and of order 15k trajectories for $L_s = 16$.

The results are shown in Fig. 1. The two most significant quantities, the average plaquette and the chiral condensate, used in Ref. [1] are displayed together with their respective susceptibilities for both the lattices.

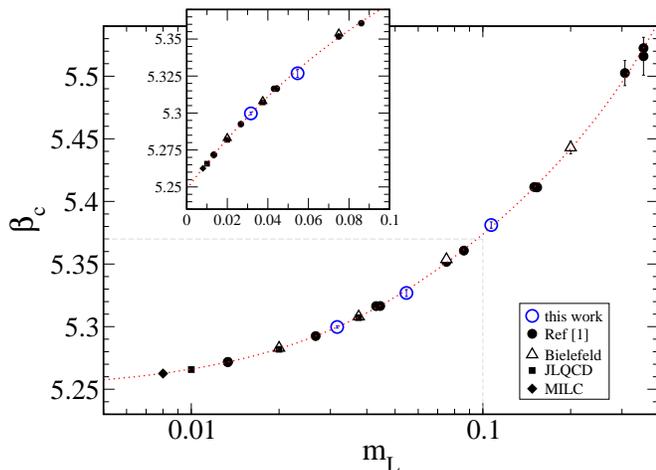A clear agreement at a 1σ level for all of these quan-

FIG. 2: Pseudocritical coupling curve in the (β, m_L) plane. The newly added points are drawn using open circles. To be compared with Fig. 3 of Ref. [1].

tities is observed at the transition point. The other points agree within 2σ except for the one corresponding to $L_s = 16$ above the transition. The reason for this discrepancy can be traced back to the limited statistics used for the end tail in this simulation of Ref. [1], in a coupling region of small importance. In the scaling region of interest the results obtained in Ref. [1] are proved to be well within the expected errors.

We confidently conclude that the use of the R algorithm in Ref. [1] did not introduce artefacts invalidating the finite-size scaling analysis.

III. DIRECT TEST OF THE FIRST ORDER HYPOTHESIS

Some hints of a first order transition were observed in Ref. [1], by use of Eqs. (4)-(5) using the dataset generated to directly check the $O(4)$, $O(2)$ universality classes. We now repeat the scaling analysis of Ref. [1] assuming weak first order. We generate a dataset with a fixed value of $am_q L_s^{y_h}$, with $y_h = 3$ as expected for a first order transition. The most convenient way to proceed is to use the already available and checked MC simulations at $L_s = 32$ and $m_L = 0.01335$. This enables a major saving in computer time. This also automatically fixes the value of $m_L L_s^3 \simeq 437.45$. Three other sets of simulations were made to construct the dataset for the first order scaling test: one with $L_s = 16$ and $m_L = 0.1068$, one with $L_s = 20$ and $m_L = 0.054682$ and one with $L_s = 24$ and $m_L = 0.03164444$. For each of them ten different values of β spanning the entire critical region were simulated with a total statistics of about 90k trajectories collected for each of the lattices.

The pseudocritical couplings β_c of the three new lattices are in excellent agreement with the pseudocritical curve determined in Ref.[1] (see Fig. 2). Given such an

agreement, no modification is necessary to Sect. IVA of Ref.[1].

As in Ref.[1] the background must be determined in order to check the scaling. For the case of the specific heat such background was observed not to depend on m_L and to be almost linear in β in the mass region of relevance for our purposes. The three new datasets at $m_L = 0.03164444$, $m_L = 0.054682$ and $m_L = 0.1068$ nicely fit together with all other data. The background estimate of Ref.[1] is only slightly modified by the new data (shifts of order 0.3σ): $C_0(\beta) = 0.417(51) - 0.0695(93)\beta$. For the chiral condensate susceptibility χ_m the background is determined by a best fit of the peaks of the curves to the function: $\chi_{peak}(L_s) = \chi_0 + kL_s^{\gamma/\nu}$ with $\gamma/\nu = 3$, appropriate to a first order transition (see Eq. (3)).

The consistency check of the first order finite size scaling is shown in Fig. 3 (the analogous figures for $O(4)$ are Fig. 6 and 17 of Ref. [1]). A reasonable scaling is observed for the specific heat C_V. As already stated in Ref.[1], C_V is independent of any prejudice on the symmetry and on the order parameter. Violations of the scaling Eq. (3) are observed for χ_m at larger values of the masses. In fact Eq. (3) is expected to be valid for the susceptibility of the order parameter. At large masses chiral symmetry is badly broken and $\langle\bar{\psi}\psi\rangle$ is possibly not a good order parameter. In our data, both of the present paper and of Ref. [1], Eq. (3) seems to be violated for $m_L > 0.05$.

An updated version of the scaling laws Eqs. (4)-(5) (Fig. 8, 9 and 18 of Ref. [1]) with the new data is shown for completeness in Fig. 4. The scaling laws Eqs. (4)-(5) correspond to taking the limit $m_L L_s^{y_h} \gg 1$ with $\tau L_s^{1/\nu}$ fixed in Eq.(1). In the mass region considered a reasonable scaling is observed for first order for the specific heat (similar considerations as above apply). For the chiral susceptibility good scaling is observed only for $m_L < 0.05$.

Both in Fig.3 and in Fig. 4, the background for the chiral susceptibility has been obtained by the fit to the curves with $m_L < 0.05$. The fact that only in a neighboorhood of $m_L = 0$ the scaling is expected is well known – but the actual mass range is not. The fitting procedure described allows us to identify a scaling window where the whole curve scaling can be verified.

The scaling of the chiral condensate (magnetic equation of state) can also be checked. The expectation for first order is:

$$\langle\bar{\psi}\psi\rangle = f(\tau m_L^{-1}) \qquad (6)$$

In Ref. [1] we found that if a subtraction is allowed on the left-hand side of Eq. (6) then a good scaling is found with the first order exponent. The subtraction was found to be numerically equal to the value of the condensate on the zero gauge field background (perturbative value). This, in the region explored, is equivalent to impose that all the curves coincide at the pseudocritical coupling.

The updated figure for the first order scaling is shown in Fig. 5 (see Fig. 14 of Ref.[1]). The scaling is very good
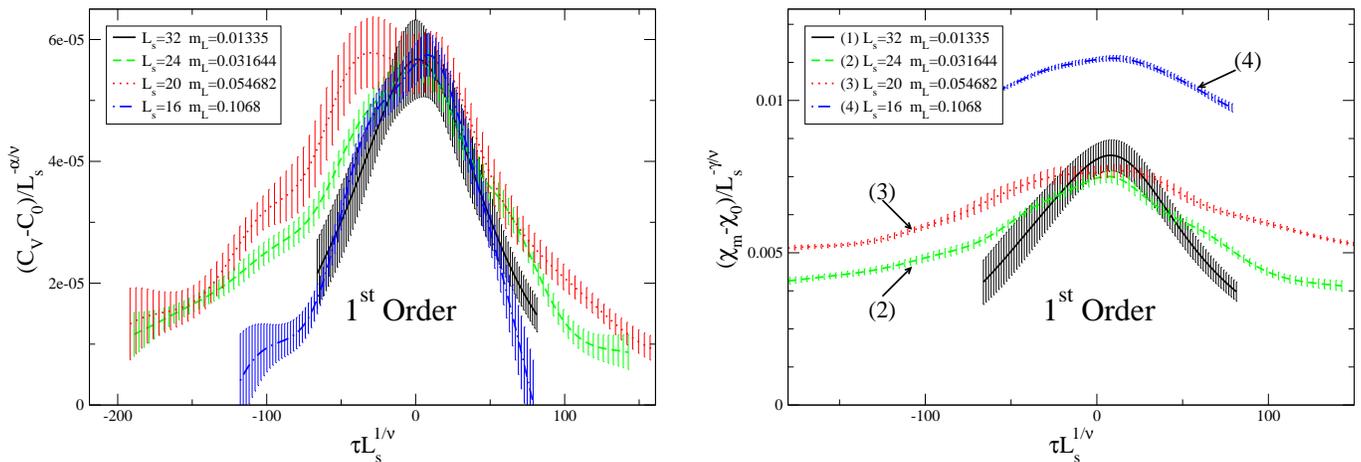
FIG. 3: Finite size scaling at $m_L L_s^3$ fixed of the subtracted specific heat $C_v - C_0$ and of the chiral condensate susceptibility $\chi_m - \chi_0$.

within the statistical errors. The three new curves have been inserted and have been found to scale nicely.

As a last check we looked for metastabilities in the MC histories of the new lattices. We found no metastable states. The history corresponding to the pseudo-critical coupling of the $L_s = 24$ lattice is shown in Fig. 6. No clear double-peak structure is found. If the transition is first order, increasing the lattice size, one should eventually see the metastabilities. At present, no clear sign of these states are found in the numerical data.

IV. CONCLUSIONS

The determination of the order of the chiral transition for $N_f = 2$ QCD has turned out to be a very challenging problem because of the huge computational resources required.

In Ref. [1] we proposed a novel method to deal with the double scaling Eq. (2),(3). We applied such method to test the $O(4)$, $O(2)$ critical behavior – expected for a second order transition on the basis of theoretical speculations. The conclusion was that our numerical data was not compatible with $O(4)$, $O(2)$ and we found hints of a first order transition.

In the present work we have completed our previous analysis in two different respects.

In Sect. III, we have performed a direct test of first order scaling, using new MC data with parameters, with $m_L L_s^3 = 437.45$, $L_s = 16, 20, 24, 32$. These lattices show a good scaling for the specific heat and for the chiral susceptibility at masses $m_L < 0.05$ (see Fig. 3). At larger masses scaling of the chiral susceptibility is broken, presumably because of strong breaking of the chiral symmetry.

For the sake of completeness we have also updated the scaling pictures of Ref. [1] corresponding to Eqs. (4),(5) (see Fig. 4).

The good scaling of the chiral condensate with first order pseudo-critical exponents, observed in Ref. [1], is also in complete agreement with the new MC data produced for this work (see Fig. 5).

In Sect. II, we have checked some of the systematic errors present in the previous analysis of Ref. [1], by comparing a representative subset of the old MC data generated using the non-exact R-algorithm with a new one obtained with the exact RHMC algorithm. The direct comparison has shown no significant deviations between the two datasets at the critical coupling – thus validating the result presented in Ref. [1].

Taking all the evidence together, the first order scaling is clearly preferred over the second order $O(4)$ behavior. We can say that $O(4)$, $O(2)$ are excluded and first order is consistent with data, modulo possible effects due to the discretization. Again we think that ultraviolet effects should be irrelevant with respect to the large volume behavior. However the use of finer lattices and new simulation algorithms to approach the chiral limit will possibly clarify this issue.

V. ACKNOWLEDGMENTS

[1] M. D'Elia, A. Di Giacomo and C. Pica, Phys.Rev. D **72**, 114510 (2005).

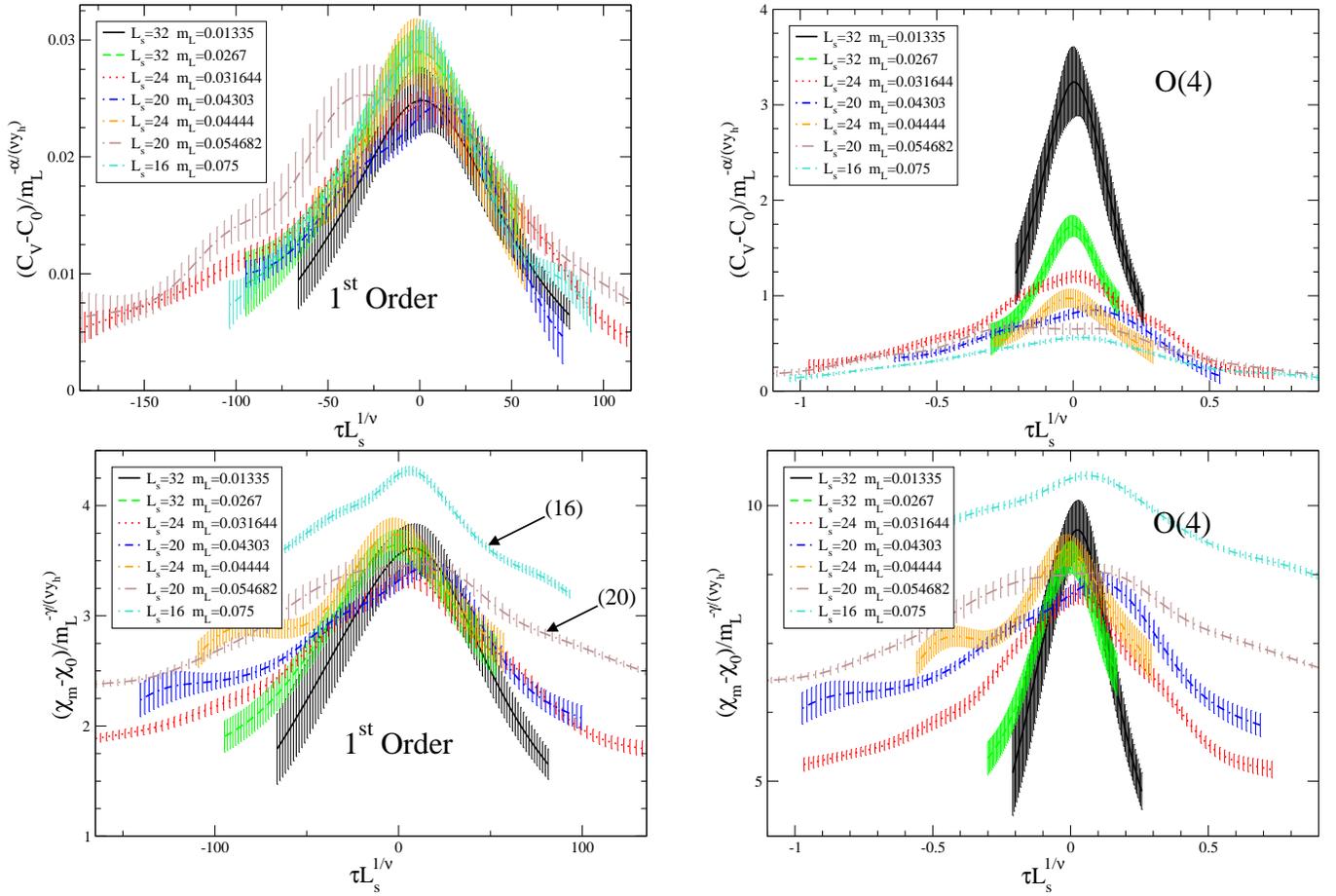[2] A recent review on QCD thermodynamics is contained

FIG. 4: Approximate scaling laws corresponding to Eqs. (4)-(5). In the fit to the background the curves (16) and (20) with $m_L > 0.05$ have been discarded.
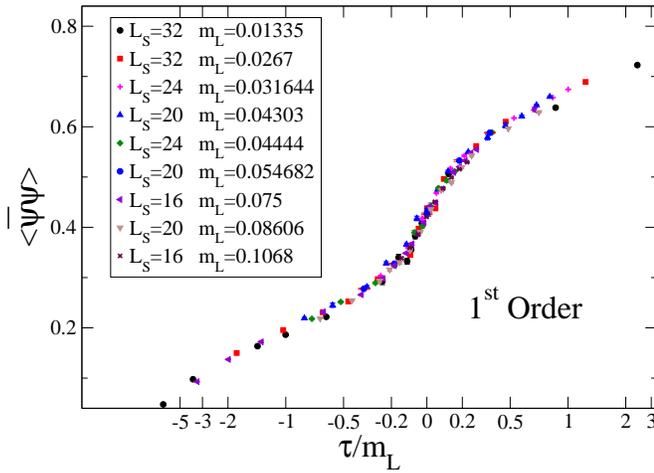

FIG. 5: Scaling of the subtracted chiral condensate with first order exponents. (x axis has been rescaled with the function atan(x) to emphasize the scaling region)

in: E. Laermann and O. Philipsen, Ann. Rev. Nucl. Part. Sci. **53** (2003) 163 [arXiv:hep-ph/0303042].

[3] J. M. Carmona, L. Del Debbio, M. D'Elia, A. Di Giacomo, B. Lucini, G. Paffuti, Phys. Rev. D **66**, 011503 (2002).
[4] M. D'Elia, A. Di Giacomo, B. Lucini, G. Paffuti, C. Pica, Phys. Rev. D **71**, 114502 (2005).
[5] P. Cea, L. Cosmai and M. D'Elia, JHEP **0402** (2004) 018 [arXiv:hep-lat/0401020].
[6] R. D. Pisarski and F. Wilczek, Phys. Rev. D **29**, 338 (1984);
[7] F. Wilczek, Int. J. Mod. Phys. A **7**, 3911 (1992);
[8] K. Rajagopal and F. Wilczek, Nucl. Phys. B **399**, 395 (1993)
[9] G. 't Hooft, Nucl. Phys. B **138**, 1 (1978).
[10] M. A. Stephanov, K. Rajagopal and E. V. Shuryak, Phys. Rev. Lett. **81** (1998) 4816 [arXiv:hep-ph/9806219].
[11] B. Mohanty *et al.*, Nucl. Phys. A **715**, 339 (2003) [arXiv:nucl-ex/0208019].
[12] S. Pratt, Nucl. Phys. A **715**, 389 (2003) [arXiv:nucl-th/0308022].
[13] R. Stock, AIP Conf. Proc. **756**, 1 (2005).
[14] E. Brézin, J. Physique **43** 15 (1982)
[15] M. Fukugita, H. Mino, M. Okawa and A. Ukawa, Phys. Rev. Lett. **65**, 816 (1990).
[16] M. Fukugita, H. Mino, M. Okawa and A. Ukawa, Phys. Rev. D **42**, 2936 (1990).
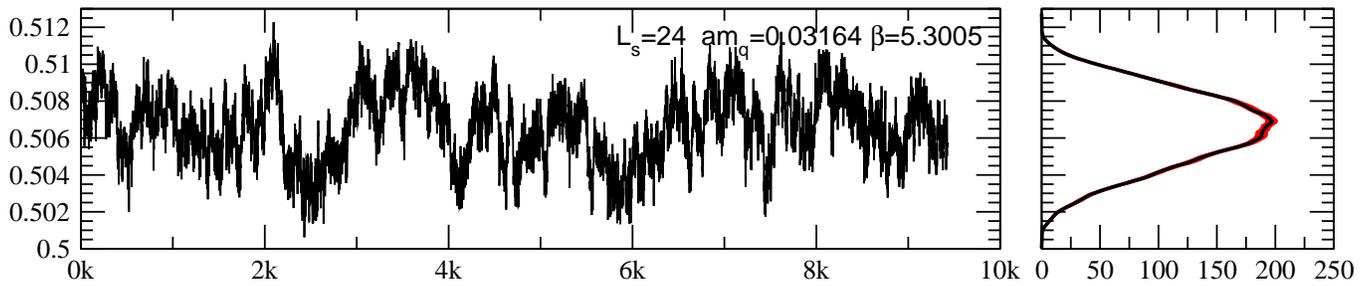[17] F. R. Brown, F. P. Butler, H. Chen, N. H. Christ, Z.

FIG. 6: MC time history at the pseudo-critical coupling for $L_s = 24, m_L = 0.03164444$. No clear metastabilities are observed.

Dong, W. Schaffer, L. I. Unger and A. Vaccarino, Phys. Rev. Lett. **65**, 2491 (1990)

[18] F. Karsch, Phys. Rev. D **49**, 3791 (1994).

[19] F. Karsch and E. Laermann, Phys. Rev. D **50**, 6954 (1994).

[20] S. Aoki et al. (JLQCD collaboration), Phys. Rev. D **57**, 3910 (1998) [arXiv:hep-lat/9710048].

[21] C. Bernard, C. DeTar, S. Gottlieb, U. M. Heller, J. Hetrick, K. Rummukainen, R.L. Sugar and D. Toussaint, Phys.Rev. D **61**, 054503 (2000)

[22] A. A. Khan et al. (CP-PACS collaboration), Phys. Rev. D **63**, 034502 (2001) [arXiv:hep-lat/0008011].

[23] S. A. Gottlieb, W. Liu, D. Toussaint, R. L. Renken and R. L. Sugar, Phys. Rev. D **35**, 2531 (1987).

[24] A. D. Kennedy, I. Horvath and S. Sint, Nucl. Phys. Proc. Suppl. **73**, 834 (1999) [arXiv:hep-lat/9809092].