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Chiral transition in two-flavor QCD: an update

Guido Cossu
Scuola Normale Superiore and INFN Sezione di Pisa, P.zza dei Cavalieri 7, I-56127 Pisa, Italy
E-mail: `g.cossu@sns.it`

Massimo D'Elia
Dipartimento di Fisica, Università di Genova and INFN Sezione di Genova, Via Dodecaneso 33, I-16146 Genova, Italy E-mail: `delia@ge.infn.it`

Adriano Di Giacomo
Dipartimento di Fisica, Università di Pisa and INFN Sezione di Pisa, largo Pontecorvo 3, I-56127 Pisa, Italy E-mail: `digiaco@df.unipi.it`

Claudio Pica*
Dipartimento di Fisica, Università di Pisa and INFN Sezione di Pisa, largo Pontecorvo 3, I-56127 Pisa, Italy E-mail: `pica@df.unipi.it`

On the basis of our earlier investigations, we present an extended analysis of the chiral transition in two-flavor QCD. The focus of the present work is twofold. First, the systematic uncertainties present in the data from past numerical simulations are checked against new Monte Carlo data generated using an exact RHMC algorithm. No significant deviations from old data are observed, meaning that the systematics in old data were under control. Secondly, an explicit consistency check of the hypothesis that the transition is of the first order is performed based on a new set of MC simulations.

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*Speaker.

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1. Introduction

The nature of the finite temperature transition in QCD with two light mass degenerate fermions has been the subject of a considerable number of investigations in the literature [1, 2, 3, 4, 5, 6, 7]. Nonetheless a clarifying and definitive study on this subject do not seem to be yet viable, mostly due to the subtle nature of the system and the huge computing power required to simulate dynamical fermions in the chiral limit.

In the present contribution we report on the progress made in trying to improve our analysis in [7]. This improvement is twofold: we eliminate some sources of systematic errors and we make a direct check of the hypothesis that the transition is first order.

2. Previous analysis

In this section some basic facts on the chiral transition in $N_f = 2$ QCD and our strategy of analysis presented in [7] are briefly recalled.

The first prediction on the order of the chiral transition in QCD with N_f flavors of mass degenerate quarks goes back to 1984 and it is due to Pisarski and Wilczek [8]. By using the idea of universality of critical systems undergoing a second order phase transition they studied the simplest effective model with the same symmetry and symmetry breaking pattern of QCD looking for IR stable fixed point of the RG flow corresponding to possible second order universality classes. We summarize in Table 1 their findings for the chiral transition $m_q = 0$. The presence or absence of the axial $U(1)$ anomaly at the critical temperature is important in this analysis because it changes the symmetry of the system. For the case $N_f = 2$ the transition at $m_q = 0$ can be first order or second order in the universality class of $O(4)$ but only if the anomaly is still present at T_c. When massive quarks are persent, they can be included in the effective model as an external magnetic field with strength proportional to the mass of the quarks. Thus the prediction in this case $m_q > 0$ is a crossover if the transition were second order at $m_q = 0$ or it remains a first order transition for sufficiently small quark masses.

Inspired by this seminal paper, many investigation on the lattice were made [1, 2, 3, 4, 5, 6]. A general tendency towards the claim that the transition was second order emerged, although no conclusive evidence in favor of $O(4)$ was found. In [7] we addressed the question whether the transition is second order $O(4)$ or not using a novel strategy. The idea was the following. The critical behavior of a system is described by the singular part of the free energy density $\mathscr{F}_s$, which is a function of the scaling variables

$$\mathscr{F}_s(\tau, m_L, L_s) = L_s^{-d} \mathscr{F}'_s(\tau L_s^{y_t}, m_L L_s^{y_h}) \tag{2.1}$$

where the relevant quantities are the reduced temperature τ, the quark mass m_L and the system size L_s. Eq. 2.1 gives the scaling law for the free energy density from which the singular behavior of all other thermodynamic quantities can be derived. It is important to notice that $\mathscr{F}'_s$ depends on the relevant quantities only in certain combinations fixed by the critical exponents y_t and y_h. In principle starting form Eq. 2.1 one can study the quality of the scaling and determine the universality class of the transition, but the presence of two scaling variables makes this procedure unpractical. To test a given universality class, in [7] we adopted a different strategy: we fixed one of the two scaling

	$U(1)_A$ broken	$U(1)_A$ restored at T_c
$N_f = 1$	first order / crossover	first order / $O(2)$
$N_f = 2$	first order / $O(4)$	first order
$N_f \geq 3$	first order	first order

Table 1: Possible universality classes for the chiral transition $m_q = 0$.

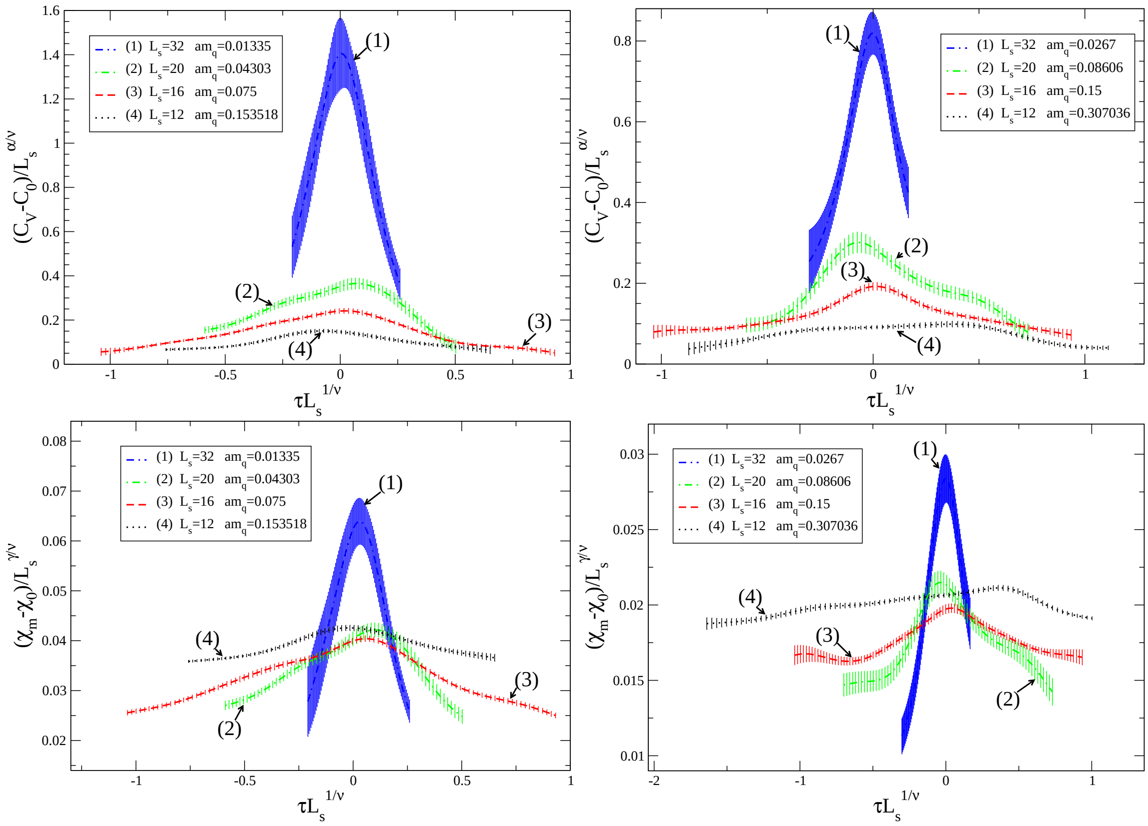

Figure 1: Test of $O(4)$ scaling of C_V (top row) and χ_m (bottom) for Run1 (left column) and Run2 (right).

variables and studied the dependence on the other. Namely we made a number of measurement at a fixed value of the quantity $m_L L_s^{y_h}$, i.e. we changed m_L as a function of L_s in our simulations. We collected two different set of data, called Run1 and Run2, on lattices with $L_s = 12, 16, 20, 32$ differing only for the value of the constant $m_L L_s^{y_h}$. Since the functional relation between the quark mass m_L and the lattice size L_s depends on the critical exponent y_h, one can only test one given universality class: in [7] we tested $O(4)$, fixing $y_h = 2.49$.

The results of our investigation are shown in Fig. 1 where the quality of the $O(4)$ scaling is shown for two different thermodynamical susceptibilities: the specific heat C_V and the chiral condensate susceptibility χ_m. No signal of scaling was observed for both of our datasets which led to the conclusion that the $O(4)$ universality class is incompatible with the lattice data. Excluding the second order nature of the transition, the only other possibility is that the transition is first order. Indeed in [7] some hint of a first order transition was found reusing the data at our's disposal, but this required some further assumption on the scaling functions.

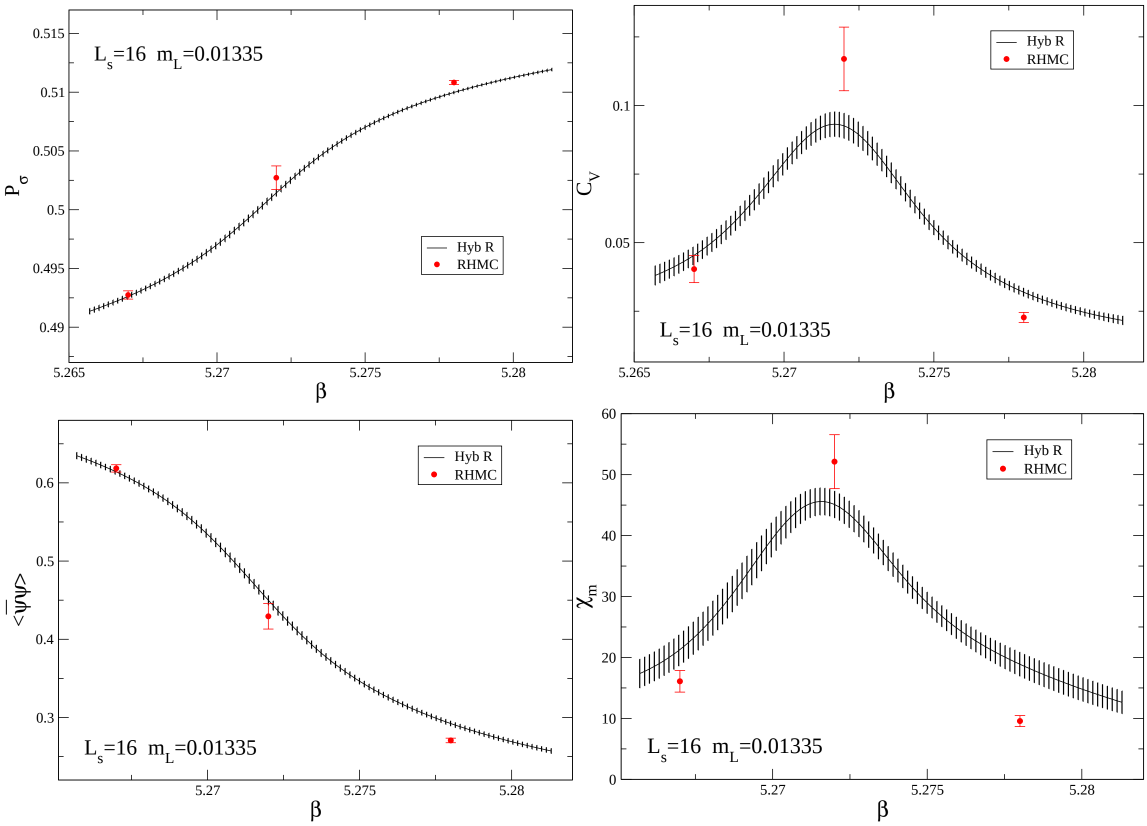

Figure 2: Comparison between MC estimates obtained by the exact RHMC algorithm and the Hybrid-R for the average value (left column) and susceptibility (right) of the plaquette (top row) and chiral condensate (bottom) on a lattice with $L_s = 16$ and $m_L = 0.01335$.

3. Improving the analysis

Some sources of systematic errors are present in [7], which in principle can influence the results. The main problems are: 1) the use of a non-exact MC algorithm; 2) no explicit test of a first order phase transition was made; 3) the lattice temporal extent used was $L_t = 4$. To solve problem 3) the use of finer lattices is needed and/or the use of improved actions. In this work a preliminary attempt is made to address the first two problems.

3.1 Hyb-R vs RHMC

The dataset collected in [7] were generated using the Hybrid-R algorithm which is known to have systematic errors due to the presence of a non-zero integration step in the molecular dynamics evolution of the fields. Although care was used to reduce this systematic effect to a minimum compatibly with computational costs, one can wonder how our results are affected by this error. In the following to address this question we perform a comparison of a subset of our dataset used in [7] with new MC data obtained using the exact RHMC algorithm. The subset was chosen to be those MC simulations with the lowest quark mass value $m_L = 0.01335$ where the effects of the discretization error are expected to be more sensitive. The comparison is shown in Fig. 2 for a lattice with $L_s = 16$ and in Fig. 3 for $L_s = 32$ where we plot the average and susceptibility of both

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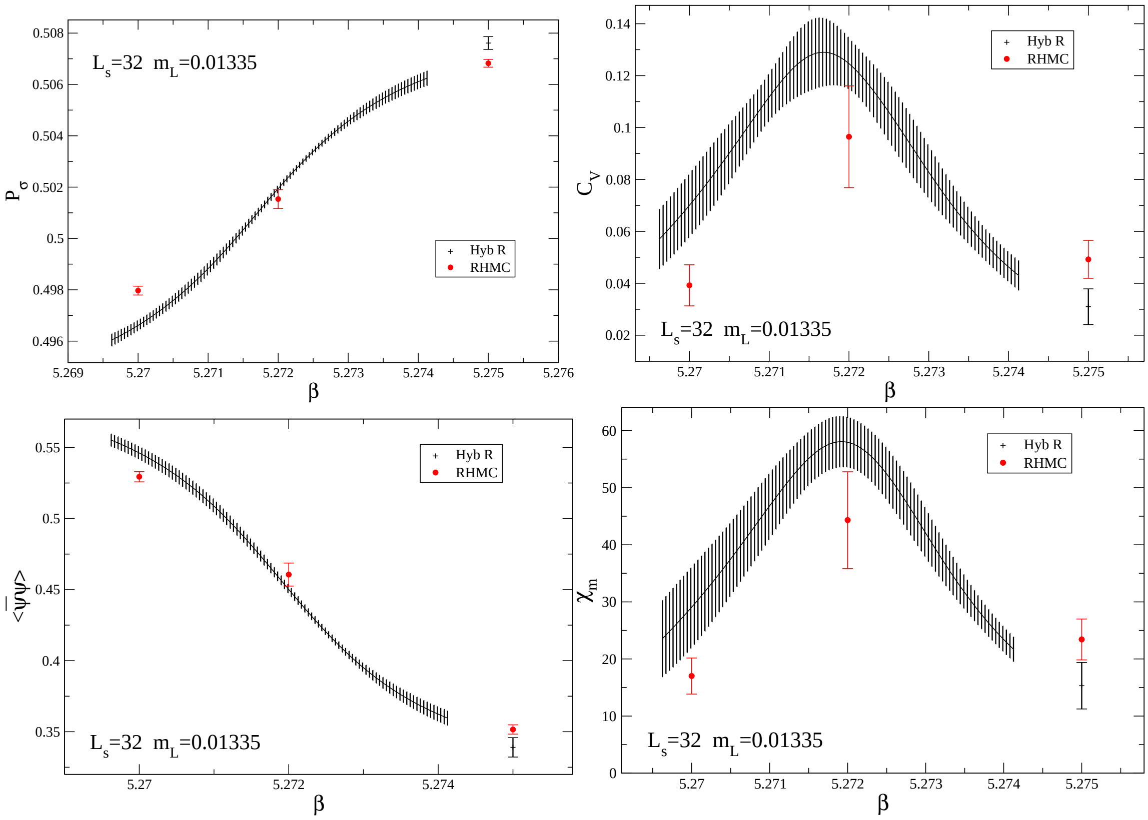

Figure 3: The same comparison as in Fig. 2 on a lattice with $L_s = 32$ and $m_L = 0.01335$.

the plaquette and the chiral condensate. In all the cases the systematic effects are comparable with our statistical errors, except for a point far from the transition temperature on the larger lattice. We can safely conclude that this systematic error were under control in the critical region of interest and thus the claim that $O(4)$ scaling is incompatible with lattice data remains unchanged.

3.2 Explicit test of first order scaling

The dataset used in [7] was generated to test the $O(4)$ universality class using a value of the magnetic critical exponent of $y_h = 2.49$ and it was suitable to test first order according to the strategy explained in Sect. 2. Here we repeat the whole analysis assuming first order from the start, i.e. using the value $y_h = 3$ for the effective critical exponent. This means that a new set of MC simulations, called Run3 in the following, must be performed at different values of matching m_L, L_s. In the following a preliminary analysis is presented using two different lattice sizes of $L_s = 16, 32$. The value of m_L for the lattice with $L_s = 32$ was chosen to be $m_L = 0.01335$, i.e. the same as for Run1, so that old data can be reused. A new set of MC simulations was made for $L_s = 16$ at $m_L = 0.1068$, which is shown in Fig. 4 where raw data point and the reweighting confidence region is shown for the average and susceptibility of both the plaquette and the chiral condensate.

Comparing the two matching lattice data we can esteem the quality of the first order scaling, shown in Fig. 5. The scaling is good for the specific heat C_V as the two curves collapse on each

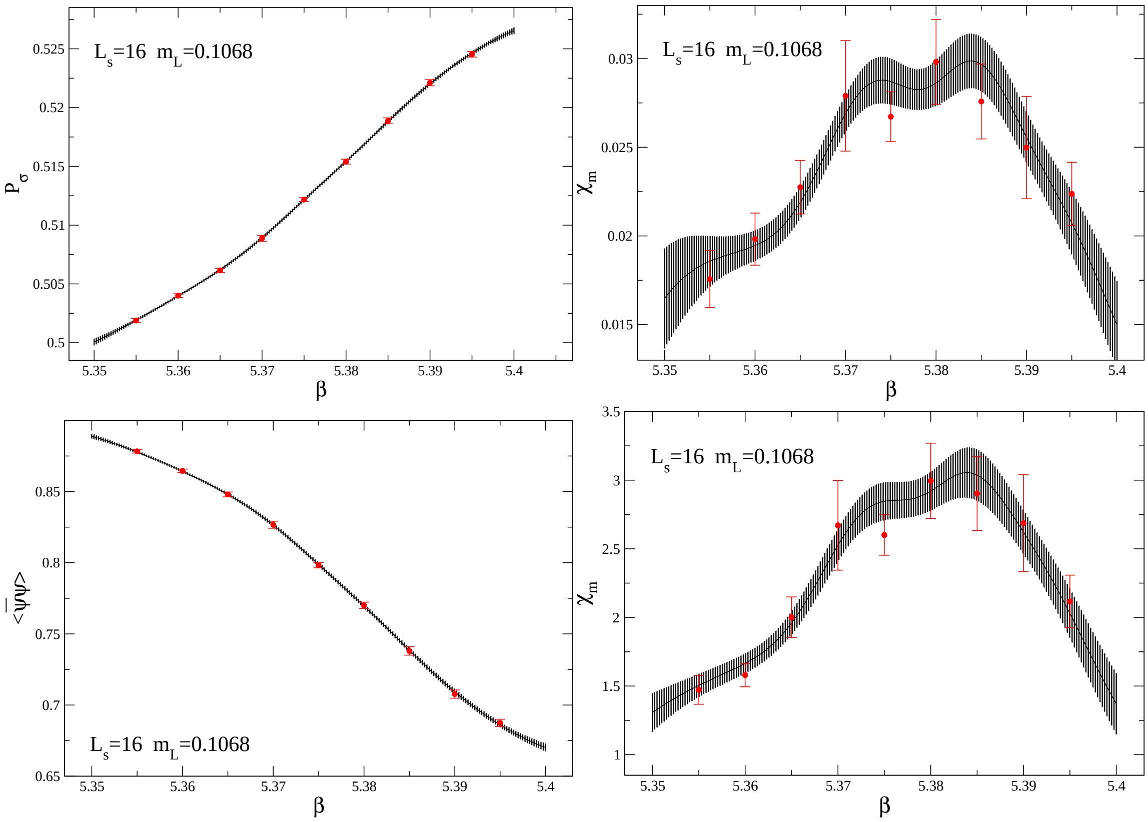

Figure 4: MC data obtained using the RHMC algorithm on a lattice with $L_s = 16$ and $m_L = 0.1068$ (Run3). Plaquette related quantities are shown in the first row; the ones related to the chiral condensate in the second.

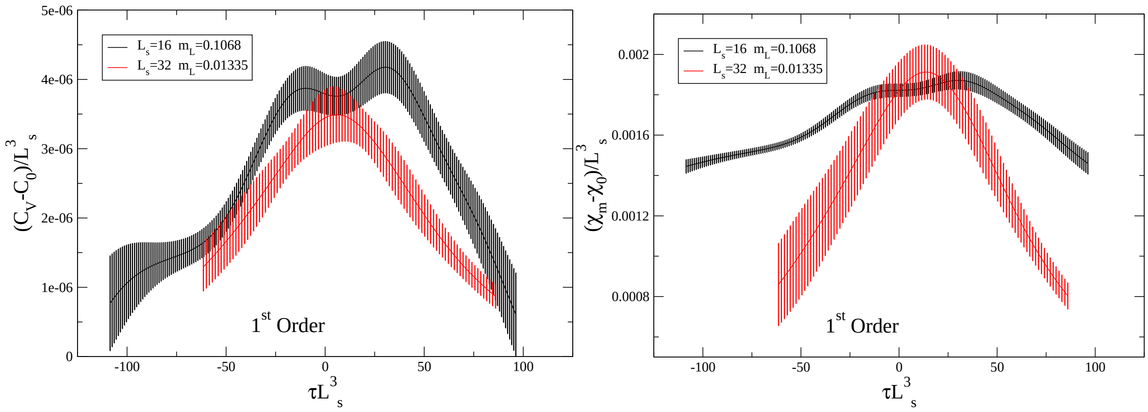

Figure 5: Test of first order scaling (Run3). Specific heat scaling is shown on the left; χ_m scaling on the right.

other within errors around the critical temperature. However for the susceptibility of the chiral condensate χ_m this is not the case. This may be due to the high value of the quark mass for the smaller lattice but further investigation is needed to understand the issue.

4. Conclusions

We have addressed two main sources of systematic errors which were present in our analysis [7] on the nature of the chiral transition in $N_f = 2$ QCD.

The first one is related to the use of the non-exact Hybrid-R algorithm. We have made a direct comparison between the old MC data with new simulations made using the exact RHMC algorithm and we have found that the systematic errors were comparable with the statistical ones and thus under control. The results found in [7] remain valid.

The second one is a direct check of the first order nature of the transition. Following the same strategy developed in [7], a preliminary analysis have been made using two matching lattices of size $L_s = 16, 32$ with the same value of the scaling variable $m_L L_s^{y_h}$ with $y_h = 3$. While the specific heat shows a good scaling, the susceptibility χ_m does not, probably due to the large value of the quark mass $m_L = 0.1068$ corresponding to $L_s = 16$.

This work was done using the INFN APEmille machines in Pisa and the apeNEXT facility in Rome.

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