THE ORDER OF THE QCD PHASE TRANSITION WITH TWO LIGHT FLAVORS

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OUTLINE

- The QCD phase diagram and the chiral transition for $N_f = 2$
- Predictions from effective models.
- Present evidence from lattice QCD simulations.
- Some new preliminary results
- Conclusions and discussion



The low temperature phase of QCD is characterized by non-perturbative phenomena, such as color confinement and chiral symmetry breaking, which are expected to disappear in the high temperature perturbative regime.



Cabibbo and Parisi (1975) suggested the presence of a transition leading to quark liberation, which has been observed in lattice QCD simulations (1980, Kuti, Polonyi, Szlachanyi, SU(2) pure gauge theory) and is still the subject of theoretical and experimental investigation.



Numerical simulations show that, in QCD with fundamental fermions, deconfinement and chiral symmetry restoration take place at very close or coincident temperatures. The question whether there is a true phase transition or simply a rapid change (crossover) and, in the first case, about which is a sensible order parameter, is fundamental.



The order of the finite temperature QCD transition may have a great relevance to the early evolution of our Universe



The presence or absence of a true phase transition is essential to understand whether it is sensible or not to try interpret confinement/deconfinement in terms of some exact (and yet unknown) symmetry of QCD. Confinement is an absolute property of Nature or a fine tuned suppression of color charge?



The answer is relevant to the description of the QCD phase diagram in presence of a finite baryon density. Models predict a density driven first order transition at T = 0 crossover at $\mu = 0 \implies$ critical endpoint T_E with clear experimental signatures in heavy ion collisions.



Exact symmetries with associated order parameters are only known in the infinite or zero quark mass limits:

- At infinite mass (quenched QCD) center symmetry Z_3 (corresponding to a twist by a center element of periodic temporal parallel trasports) is exact. The Polyakov loop $\langle L \rangle$ is a good order parameter, associated to confinement/deconfinement.
- At zero quark mass chiral symmetry is exact, and the chiral condensate $\langle \psi \psi \rangle$ is a good order parameter, associated to chiral symmetry breaking/restoration.
- At intermediate masses there is no known exact symmetry. The answer is not obvious, may depend on dynamics, may give hints for further symmetries.

There is a general tendency to accept the crossover scenario in the real QCD case ($N_f = 2 + 1$ with physical quark masses): it has been shown (Y. Aoki, Z. Fodor, S. D. Katz and K. K. Szabo, Phys. Lett. B 643, 46 (2006); Nature 443, 675 (2006)) that the susceptibility of a possible order parameter for the transition (the chiral condensate) does not show any signal of growing with the spatial volume, till $L_s \sim 6$ fm.

Theoretical exploration is however still open (the critical endpoint has not yet been found by experiments) and in this context $N_f = 2$ with massless quarks (exact chiral symmetry) is a fundamental testground:

- It is quite close to the physical case:
 first order ⇒ likely first order for small quark masses
 second order ⇒ crossover for two light flavors
- Clear theoretical predictions exist, based on universality considerations (effective models) on the analysis of effective chiral models in 3 dimensions, which can be confronted with numerical QCD simulations.
- Despite several efforts by different groups, it is still an open problem.

Model predictions

Predictions about the nature of the transition in the chiral limit can be obtained by a renormalization group analysis of an effective chiral model:

R. D. Pisarski and F. Wilczek, Phys. Rev. D 29, 338 (1984)

$$\tilde{\phi}: \phi_{ij} \equiv \langle \bar{q}_i(1+\gamma_5)q_j \rangle \quad (i,j=1,\ldots,N_f)$$

Under chiral and $U_A(1)$ transformations of the group $U_A(1) \otimes SU(N_f) \otimes SU(N_f)$, $\tilde{\phi}$ transforms as

$$\tilde{\phi} \to e^{i\alpha} U_+ \tilde{\phi} U_-$$

so that by the usual symmetry arguments, and neglecting irrelevant terms

$$\mathcal{L}_{\phi} = \frac{1}{2} Tr\{\partial_{\mu}\phi^{\dagger}\partial^{\mu}\phi\} - \frac{m_{\phi}^{2}}{2} Tr\{\phi^{\dagger}\phi\} - \frac{\pi^{2}}{3}g_{1}\left(Tr\{\phi^{\dagger}\phi\}\right)^{2} - \frac{\pi^{2}}{3}g_{2}Tr\{(\phi^{\dagger}\phi)^{2}\} + c\left[\det\phi + \det\phi^{\dagger}\right]$$

The last term describes the anomaly: indeed it is $SU(N_f) \otimes SU(N_f)$ invariant, but not $U_A(1)$ invariant.

If the chiral transition is second order, its universality class is determined by the fixed point of the corresponding chiral model, hence:

- If the chiral model does not have a fixed point, the chiral transition is not expected to be second order, but first order instead (this is verified for $N_f > 2$).
- However, even if the chiral model has a fixed point, the chiral transition could still be first order (interplay with degrees of freedom other than chiral could be essential)

For
$$N_f = 2$$

- $U_A(1)$ anomaly effective (no light $\eta', c \neq 0$) \implies the model has a fixed point \implies second order in the 3d O(4) universality class or first order
- $U_A(1)$ anomaly not effective (η' is light, $c \sim 0$) \implies no stable fixed point F. Basile, A. Pelissetto, E. Vicari, 2005 \implies U(2)_L \otimes U(2)_R/U(2)_V or first order

The problem can be settled by lattice QCD simulations and a Finite Size Scaling (f.s.s.) analysis.

The QCD partition function is rewritten in terms of a path integral over a discretized euclidean lattice with periodic boundary condition in the time direction (antiperiodic for fermion fields).

$$Z = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi}e^{-(\beta S_G + \bar{\psi}M[U, m_q]\psi)} = \int \mathcal{D}U e^{-\beta S_G} \det M[U, m_q]$$

 βS_G the pure gauge (e.g. plaquette) action, $\beta \equiv 2N_c/g^2$ is the inverse bare gauge coupling and M is the fermion matrix, e.g. in the staggered formulation:

$$M_{i,j} = am\delta_{i,j} + \frac{1}{2} \sum_{\nu=1}^{4} \eta_{i,\nu} \left(U_{i,\nu} \delta_{i,j-\hat{\nu}} - U_{i-\hat{\nu},\nu}^{\dagger} \delta_{i,j+\hat{\nu}} \right)$$

In this formulation thermal expectation values can be computed through Monte Carlo simulations, using $e^{-\beta S_G} \det M[U, m_q]$ as a probability distribution function for gauge configurations.

The physical temperature is given by the inverse temporal extension

$$T = \frac{1}{N_t a} \tag{1}$$

and the approach to the continuum field theory links the lattice spacing a to the bare parameters of the theory, $a \equiv a(\beta, m_q)$. Therefore at fixed N_t the temperature is a function of β and the bare quark mass m_q .

The lattice formulation of fermions in general breaks chiral symmetry explicitly, therefore, in case of second order, one does not expect to see the expected universal behaviour (e.g. O(4)) but in the continuum limit.

However in the staggered fermion formulation (in contrast to Wilson fermions) a residual symmetry of the lattice action leads to a predicition for O(2) universal behaviour also at finite lattice spacing.

The critical behaviour of QCD at the transition can be investigated by looking at various thermodynamical quantities:

- order parameter ($\langle ar{\psi}\psi
 angle$), energy density, ...
- susceptibility of the order parameter $\chi \equiv (T/V)(\partial^2/(\partial h)^2) \ln Z$
- specific heat $C_V \equiv (T^2/V)(\partial^2/(\partial T)^2) \ln Z$

which can be measured directly or reconstructed in terms of other susceptibilities.

In simulations at finite quark mass and finite lattice volume, the strategy to investigate the order of the transition can be the following:

- locate pseudocritical values T_c (β_c) of the temperature (of the inverse coupling) looking at peaks of the relevant susceptibilities.
- try the easiest (?) thing: look for metastabilities and double peak structure of the order parameter and of the energy density around the transition, i.e. coexistence of phases, which is a clear signature for first order.
- perform a finite size scaling analysis around the chiral critical point to extract critical indexes

Finite Size Scaling

Approaching the transition the correlation length of the order parameter ξ goes large compared to the lattice spacing a, so that the dependence of physical quantities on a/ξ can be neglected. It is then possible to write the following scaling ansatz, e.g. for the free energy density:

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

 L_s is the spatial size

 $au \equiv 1 - T/T_c$ is the reduced temperature,

u is the critical index of the correlation length ($\xi \sim au^{u}$)

 y_h is the magnetic critical index (the quark mass playing the role of the external magnetic field, i.e. the symmetry breaking parameter)

From that a f.s.s. ansätz for other quantities can be deduced, like:

specific heat \implies $C_V - C_0 \simeq L_s^{\alpha/\nu} \phi_c \left(\tau L_s^{1/\nu}, am_q L_s^{y_h}\right)$ order parameter susceptibility \implies $\chi \simeq L_s^{\gamma/\nu} \phi_\chi \left(\tau L_s^{1/\nu}, am_q L_s^{y_h}\right)$

The problem is well defined but quite difficult:

- Simulations on large volumes and with light quark masses are necessary for a reliable f.s.s. analysis => huge computational power required
- f.s.s. behavior is given in terms of two different scales (two scaling variables).

A possible approach, adopted in some studies, is to assume L_s large enough to neglect finite size effects (this is reasonable for a continuous transition). At finite m_q the dependence on $am_q L_s^{y_h}$ must cancel that on L_s in front of scaling functions:

$$C_V - C_0 \simeq (am_q)^{-\alpha/(\nu y_h)} f_c \left(\tau(am_q)^{-1/(\nu y_h)} \right)$$
$$\chi \simeq (am_q)^{-\gamma/(\nu y_h)} f_{\chi} \left(\tau(am_q)^{-1/(\nu y_h)} \right).$$

one can also write a scaling ansätz for the pseudocritical temperatures

 $\tau(am_q)^{-1/(\nu y_h)} = \operatorname{const}(am_q)^{1/(\nu y_h)}.$

or for the so-called magnetic equation of state

 $\langle \bar{\psi}\psi \rangle \simeq m^{1/\delta} f(\tau m^{-1/(\nu y_h)})$

This is a table of the critical indexes which can be relevant to the f.s.s. analysis for $N_f=2$

	y_t	y_h	ν	α	γ
O(4)	1.336(25)	2.487(3)	0.748(14)	-0.24(6)	1.479(94)
O(2)	1.496(20)	2.485(3)	0.668(9)	-0.005(7)	1.317(38)
MF	3/2	9/4	2/3	0	1
$1^{st}Order$	3	3	1/3	1	1

Last column refer to the effective critical indexes predicted for a weak first order transition in three dimensions.

The critical indexes of the $U(2)_L \otimes U(2)_R/U(2)_V$ universality class proposed in case of effective $U(1)_A$ restoration (F. Basile, A. Pelissetto, E. Vicari, 2005) are numerically very close to those for O(4) and O(2).

A brief history of previous investigations

M. Fukugita, H. Mino, M. Okawa, A. Ukawa, PRL 65, 816 (1990); PRD 42, 2936 (1990) F. R. Brown, *et al*, PRL 65, 2491 (1990)

- A first order transition was detected for $N_f = 3, 4$ staggered quarks at small m_q .
- $N_f = 2$: no clear metastabilities or size dependence of susceptibilities was found for masses down to $am_q = 0.01$ and lattice sizes up to $16^3 \times 4$ ($aL_s = 4/T$).

That was interpreted as evidence for an analytic crossover at finite m_q , hence a second order transition at $m_q = 0$, leading to the following standard scenario



Future studies were mostly devoted to verify the correct universality class predicted by chiral models (i.e. O(4) or O(2) at finite lattice spacing) in case of second order. That effort was started in

- F. Karsch, PRD 49, 3791 (1994)
- F. Karsch and E. Laermann, PRD 50, 6954 (1994)

Assuming scaling laws in the $L_s \rightarrow \infty$ limit they found, for $am_q = 0.02 \rightarrow 0.075$:

- good scaling with ${\cal O}(2)$ indexes for pseudocritical couplings
- good scaling for the peak of chiral susceptibility
- no good scaling for other susceptibilities (related to specific heat)

These non-conclusive results were confirmed on larger lattices (up to $24^3 \times 8$) and smaller quark masses (down to $am_q = 0.008$) by

- S. Aoki et al. (JLQCD collaboration), PRD 57, 3910 (1998)
- C. Bernard et al, PRD 61, 054503 (2000)

In the last paper also an inconsistent scaling of the equation of state was revealed. Since failure of the predicted universality class points back to first order, a further search for metastabilities was done, with negative outcome.

A. A. Khan et al. (CP-PACS collaboration), PRD 63, 034502 (2001)

found, using Wilson fermions, consistency with O(4) for the pseudocritical temperature scaling and for the equation of state. No analysis of the specific heat.

S. Chandrasekharan and F.J. Jiang, PRD 68, 091501 (2003)

found good agreement with O(2) in the strong coupling limit of staggered fermions (i.e. pure gauge contribution to the action completely neglected).

J. B. Kogut and D. K. Sinclair, PRD 73 (2006) 074512

confirmed scaling violations with respect to O(4) (O(2)) critical indexes, but compared finite size effects in QCD and in the O(2) spin model claiming they could be similar.

Our contribution

M. D'E, A. Di Giacomo and C. Pica, PRD 72, 114510 (2005)

We have approached the problem for the case of staggered fermions, using the finite size scaling approach common to previous studies, with a few improvements and exploring a wide range of quark masses and lattice sizes (thanks to the APEmille computer resources).

- In order to deal with the two scales problem, we have performed series of runs at variable L_s and quark mass am_q, keeping am_qL^{y_h} fixed. That reduces the problem again to one scale without any approximation.
 Assume one particular behavior (fix y_h) ⇒ check it carefully.
 Our choice has been for O(4) (O(2)) ⇒ y_h = 2.49 (also consistent with U(2)_L⊗U(2)_R/U(2)_V)
- We have considered also the dependence of T on the quark mass, $T = 1/(N_t a(\beta, m_q))$, which slightly changes the definition of the reduced temperature

$$\tau \simeq \beta - \beta_{\chi} + k_m a m_q + \dots$$

We have performed two series of runs ($am_q L_s^{y_h} = 74.7$ and $am_q L_s^{y_h} = 149.4$) with fixed $N_t = 4$ and varying L_s in the range $12 \rightarrow 32$ and am_q in the range $0.01335 \rightarrow 0.15$. $aL_s m_{\pi} \sim O(10)$ in all of our runs.

Analysis of the psudocritical couplings



Our determinations are in perfect agreement with previous works

A fit of the pseudocritical reduced temperature

$$\tau_c \propto (\beta_{\chi} - \beta_c) + k_m a m_q + k_{m^2} (a m_q)^2 + k_{m\beta} a m_q (\beta_{\chi} - \beta_c) \,.$$

to the expected scaling with the quark mass $au_c = k_{ au} (am_q)^{1/
u y_h}$

gives good results, in the range $0.01335 \le am_q \le 0.075$, with O(4) critical indexes, but also with first order ones. A much lower mass would be needed to distinguish the two possibilities using pseudocritical indexes alone.

F.S.S. of susceptibilities

In our framework, i.e. at fixed $am_q L_s^{y_h}$, the f.s.s. laws for susceptibilities become

$$C_V(\tau, L_s) - C_0 = L_s^{\alpha/\nu} \Phi_C(\tau L_s^{1/\nu})$$

$$\chi_m(\tau, L_s) = L_s^{\gamma/\nu} \Phi_\chi(\tau L_s^{1/\nu})$$

As in previous works, we have not measured the whole specific heat, but various singular contributions to it, which have the same critical behaviour in the thermody-namical limit. In particular we show results for the spatial plaquette susceptibility.



The subtraction of a regular contribution C_0 must be performed, which we have done by fitting data well outside (12 peak half widths) the peak location. The subtraction is well described by a linear function of β for all of our data.



O(4) or O(2) are clearly excluded by our data.

The discrepancy is particularly strong for the specific heat: a non-divergent behaviour is predicted by O(4) ($\alpha < 0$) but a divergence with $\sim L_s^3$ is observed.

On the other hand, approximate scaling laws are marginally compatible with first order critical indexes, especially for the specific heat



Approximate scaling, assuming $L_s
ightarrow \infty$ (top) or at $au L_s^{1/
u}$ fixed (bottom)

Similar results are obtained for the equation of state of the order parameter

The non-exact R-algorithm may be source of systematic error: we have excluded that comparing with an exact RHMC at our lowest mass, $am_q = 0.01335$, and on two different lattice sizes, $L_s = 16$ and $L_s = 32$. no significant discrepancy has been

found (G. Cossu, M. D'E, A. Di Giacomo and C. Pica, arXiv:0706.4470)



We also made a direct test of the first order hypothesis (scaling with $am_qL_s^3$ fixed)



• The chiral susceptibility shows deviations.

• The specific heat shows a good scaling: not only the peak heights, but also the peak widths are well described by the first order hypothesis

The non-scaling of χ_m could be due to the large mass range explored (up to 0.1), which could be well outside the region where $\langle \bar{\psi} \psi \rangle$ is a good order parameter. The specific heat, instead, which is a good probe of critical properties indipendently of the order parameter choice, could have a wider scaling region. Our partial conclusion, at the lattice cut-off $a = 1/(N_t T_c) \sim 0.3$ fm explored:

- O(4) (O(2)) seems to be ruled out
- some evidence for weak first order

First order and scaling analysis

Consider again the scaling law $C_V - C_0 \simeq L_s^{\alpha/\nu} \phi_c \left(\tau L_s^{1/\nu}, a m_q L_s^{y_h} \right)$

- continuous transition $\implies L_s$ dependence must cancel as $L_s \rightarrow \infty$ at finite m_q . The scaling function can be expanded in terms of $1/(am_q L_s^{y_h})$: the leading term must be $1/(am_q L_s^{y_h})^{\alpha/(\nu y_h)} \implies$ no discontinuity (no latent heat) at finite m_q .
- First order chiral transition \implies a first order singularity is expected also at some $m_q \neq 0$, leading to a non-zero latent heat: we can allow for a constant term in the expansion in powers of $1/(am_q L_s^{y_h})$

$$C_V - C_0 \sim a m_q^{-1} \phi_c \left(\tau V\right) + V \tilde{\phi}_c \left(\tau V\right)$$

In the second case the relative weight of the singular to the regular contribution is not known apriori, may be very small for small volumes and weak first order transitions.

Our partial conclusion leaves many open questions:

- If first order, where are metastabilities and double peaked distributions around the transition? Never clearly observed
- where is the linear growth of susceptibilities with the volume at fixed m_q expected for first order? Never clearly observed

On the other hand, if it is not first order, why we do not observe the predicted second order critical indexes?

Of course one could question about the finite lattice spacing effects, but the puzzle still remains, at least for this values of N_t (of a).

There are essentially two ways out of this puzzle:

- 1. There is really a first order transition which however is so weak that metastabilities will not show up but on very large, still unexplored volumes.
- 2. We observe "wrong" critical indexes because the scaling region around the chiral point is so small that the "correct" O(4) indexes will not show up but at very small, still unexplored quark masses.

In principle both ways could be followed for a long while, with a great numerical effort. We have decided to give a "last chance" to the first (order) hypothesis.

In a weak first order transition, a tiny discontinuity in physical observables (e.g. latent heat) may stay hidden in thermal fluctuations until large values of the volume. It is easy to built simple double gaussian distributions mimicking that:



The linear behaviour of the "susceptibility" $V(\langle x^2 \rangle - \langle x \rangle^2)$ with the volume, will not be visible but on large V. In the real case mixed states due to a possibly small interface tension may worsen the situation.

Of course we cannot think that the first order will show up at scales order of magnitudes distant from the typical QCD scale. At some stage the "hunt" has to finish. Our present data show that some clear signal could be within reach. Let us look again at the spatial plaquette susceptibility, $\chi_{\sigma\sigma}$, at fixed quark mass $am_q = 0.01335$ on $L_s = 16$ and $L_s = 32$.



The presence of a slight increase from $L_s = 16$ to $L_s = 32$ could be consistent with the presence of a term proportional to the volume:

 $\chi_{\sigma\sigma} = A + BL_s^3$. The decrease in the width of the peaks is also consistent with that.

We estimate $A \sim 0.35$ and $B \sim 0.163/32^3$. The "divergent" contribution is still 30% on $L_s = 32$, should be dominant on $L_s = 80$ but already 60% on $L_s = 48$. According to this rough estimates the discontinuity in the spatial plaquette should be ~ 0.002 . In order to clarify the issue, we have judged worth dedicating a large numerical effort to a run at $am_q = 0.01335$ on a $48^3 \times 4$ lattice (thanks to apeNEXT!)

That corresponds to $m_\pi \sim$ twice the physical value and to a spatial size \sim 13-14 fm.



We are exploring 4 β values around the transition point. We have collected a total of about 30K trajectories till now: that has required \sim 1 teraflopyear (apeNEXT) with an RHMC algorithm using two pseudofermion fields.

Spatial plaquette and chiral condensate histories are shown for $\beta = 5.272$. Some signals of metastability are visible.



The plaquette probability distribution function around the transition shows double peak structures: their significance must be clarified by further statistics



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Similar double peak structures are present in the chiral condensate distribution function.



Spatial plaquette probability distribution function at the transition

Looking back at the same distributions on smaller lattice sizes: the plaquette distribution is clearly single peaked on $L_s = 16$



Spatial plaquette probability distribution function at the transition

Looking back at the same distributions on smaller lattice sizes: the plaquette distribution is clearly single peaked on $L_s = 16$ as well as on $L_s = 32$



Spatial plaquette probability distribution function at the transition

Looking back at the same distributions on smaller lattice sizes: the plaquette distribution is clearly single peaked on $L_s = 16$ as well as on $L_s = 32$ only in the new run at $L_s = 48$ a double peak structure seems to be present the distance between the peaks is ~ 0.0015 , well compatible with our previous estimate from the B coefficient (~ 0.0020)



Evidence from the (reweighted) susceptibility is less clear:

going from $L_s = 32$ to $L_s = 48$ the peak width shrinks but no clear peak height growth is still visible. More statistics is probably required.

In conclusion, present evidence is surely still not conclusive but indicates that our efforts are worth being continued. We hope to completely clarify this issue within a few months.

CONCLUSIONS AND DISCUSSION

Conclusion 1: With present UV cutoff effects ($N_t = 4$, non-improved action) and within the present quark mass range a second order chiral transition in the O(4) (and O(2) and $U(2)_L \otimes U(2)_R/U(2)_V$) seems to be excluded

Conclusion 2: First order critical indexes seems to be preferred

Preliminary: we have some signals for a first-order bistability at $am_q = 0.01335$, however the bistability does not show up until $L_s = 12/T \sim 13 - 14$ fm

If confirmed, should we change the standard scenario for a second order chiral transition (crossover at any finite mass) in $N_f = 2$ QCD? Not yet.

Our results have been obtained with a quite large lattice spacing $N_t = 4 \implies a \sim 0.3$ fm and with a non-improved action. If our results will be confirmed on $N_t = 6$ and/or using an improved lattice action, then the scenario must be changed.

- Going to $N_t = 6$ with an improved action will be much more time consuming. We cannot expect, with present computer resources, to say a definite word within a short time, but we will go on.

- Another issue will be the complete reconstruction of the specific heat or of some other quantity directly coupled to it (e.g. quartic baryon susceptibility).

- A final consideration: Could such a weak first order be phenomenologically relevant, e.g. to the early Universe evolution or to heavy ion collisions? Probably not directly: not easily distinguishable from a crossover. However it would have important consequences:

- Critical endpoint
- Theoretical interpretation of confinement/deconfinement