Some recent results on the QCD phase diagram from the lattice

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1 – OUTLINE

- **The order of the Roberge-Weiss endpoint and the QCD phase diagram** **(based on M. D’E. and F. Sanfilippo, Phys. Rev. D 80, 111501 (2009) arXiv:0909.0254)**

- **Analytic continuation of the critical line**

  (P. Cea, L. Cosmai, M. D’E., C. Manneschi and A. Papa, Phys. Rev. D 80, 034501 (2009) arXiv:0905.1292 and work in progress)

2 – Introduction: analytic continuation and the Roberge-Weiss line

Knowledge about the QCD phase diagram is important from a purely theoretical and from a phenomenological point of view, but we are still lacking a complete description of it.

The problem is of non-perturbative nature and lattice QCD simulations are the ideal tool to approach it. However, getting definite answer is non-trivial already when considering the simple finite temperature theory (i.e. without chemical potentials).

We know that the system passes through a (pseudo)critical temperature T_c at which both confinement and chiral symmetry breaking disappear.

Whether a simple rapid change (crossover) or a real phase transition takes place, and which is the order of the transition in the latter case, are non-trivial questions.

The QCD thermal partition function, e.g. given in the lattice path integral representation, has exact symmetries, which are spontaneously broken at T_c, only in the quenched or in the chiral limit.

$$Z(T) \equiv \int \mathcal{D}U e^{-S_G[U]} \det M[U]$$

$$M[\mu]_{i,j} = am\delta_{i,j} + \frac{1}{2}\sum_{\nu=1}^{4} \eta_{i,\nu} \left(U_{i,\nu}\delta_{i,j-\hat{\nu}} - U^{\dagger}_{i-\hat{\nu},\nu}\delta_{i,j+\hat{\nu}} \right)$$

U **are gauge link variables,** M **is the fermion matrix,**

S_G **is the pure gauge (e.g. plaquette) action,** $S_G = \beta \sum_{\Box}(1 - \mathrm{ReTr}\Box/N_c)$**;**

$T = 1/(N_t a(\beta))$**. Boundary conditions are periodic (antiperiodic) for bosons (fermions).**

- **infinite quark masses (quenched limit, no fermion determinant) $\longrightarrow$ center symmetry (i.e. twist of temporal boundary conditions by a center element). Weak first order transition. Order parameter: Polyakov loop.**

- **zero quark masses (chiral limit) $\longrightarrow$ chiral symmetry. Order parameter: chiral condensate. Universality class: depend on the number of light flavors.**

In the case of finite quark masses no exact symmetry is known. Chiral symmetry is broken explicitly and the presence of the fermion determinant in breaks Z_3 center symmetry explicitly. Consider the loop expansion of $\det M$

$$M[U] = m\mathrm{Id} + D[U]$$

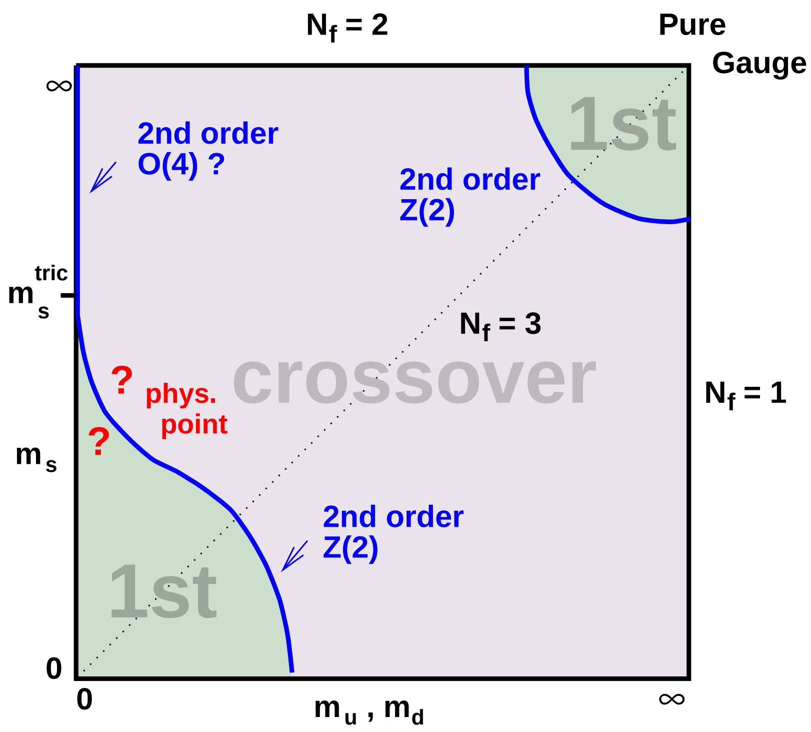
where $D[U]$ involves terms hopping from one site to the other. We can write formally:

$$\det M = e^{\mathrm{Tr}\ln M} = \exp\left(\mathrm{Tr}\ln\left(m + D[U]\right)\right) \propto \exp\left(\mathrm{Tr}\left(\frac{1}{m}D - \frac{1}{2m^2}D^2 + \ldots\right)\right)$$

only traces over closed paths are non-zero. That includes Polyakov loops, which are not invariant under Z_3.

That's like adding a magnetic field proportional to some power of $1/m$ in a three state 3D Potts model. Since the transition is first order at $m = \infty$, we expect the first order transition to persist for relatively large masses.

In general the transition and its order is flavor spectrum dependent.

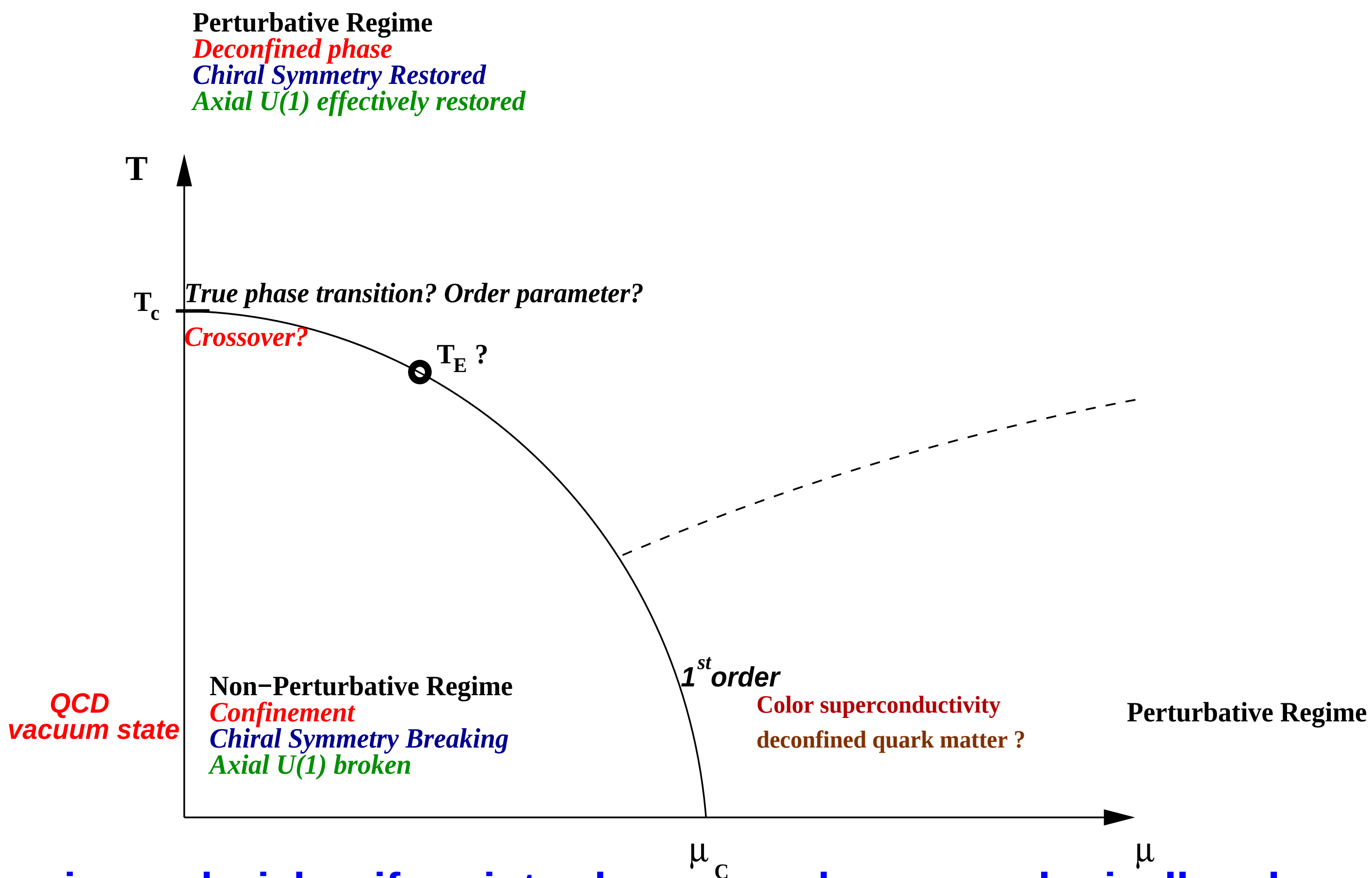


This is the commonly accepted scenario for 2+1 flavors (Columbia plot). The regions of low masses and high quark masses are first order and are separated from an intermediate crossover region by second order lines. The physical point is presently believed to be in the crossover region.

A still unsettled issue regards the chiral limit of $N_f = 2$ (upper-left corner): second order in the O(4) universality class or first order? (G. Cossu, M. D'E., A. Di Giacomo, C. Pica 2005, 2007):

Data are not consistent with O(4), they are consistent with first order, but a clear signal of phase coexistence still not visible on the largest available lattices ($48^3 \times 4$).

Very weak first order or very small scaling region around the chiral point?



The phase structure is much richer if we introduce new phenomenologically relevant parameters, like a finite baryon chemical potential μ.

If the transition at $\mu = 0$ is a crossover, a critical endpoint is possible in the phase diagram for a first order line starting in the low T, high μ region of the phase diagram.

There is a tremendous hunt, both at a theoretical and experimental level, for this possible endpoint.

Unfortunately, exploring the phase diagram of QCD at finite T and finite baryon chemical potential μ by lattice QCD simulations is highly non-trivial because of the sign problem. The fermion determinant appearing in the expression for the full QCD partition function

$$Z(T) \equiv \int \mathcal{D}U e^{-S_G[U]} \det M[U]$$

is a complex quantity if $\mu \neq 0$. That makes usual Monte-Carlo importance sampling not feasible.

There are various, possible partial solutions to this problem, one of them is using a purely imaginary chemical potential.

The sign problem disappears for imaginary values of the chemical potential

$$Z(T,\mu^2) \equiv \int \mathcal{D}U e^{-S_G} \det M[\mu] \longrightarrow \int \mathcal{D}U e^{-S_G} \det M[\mu = i\mu_I]$$

$$M[\mu]_{i,j} = am\delta_{i,j} + \frac{1}{2}\sum_{\nu=1}^{3} \eta_{i,\nu} \left(U_{i,\nu}\delta_{i,j-\hat{\nu}} - U^{\dagger}_{i-\hat{\nu},\nu}\delta_{i,j+\hat{\nu}} \right) + \eta_{i,4} \left(e^{a\mu} U_{i,4}\delta_{i,j-\hat{4}} - e^{-a\mu} U^{\dagger}_{i-\hat{4},4}\delta_{i,j+\hat{4}} \right)$$

$$M[i\mu_I]_{i,j} = am\delta_{i,j} + \frac{1}{2}\sum_{\nu=1}^{3} \eta_{i,\nu} \left(U_{i,\nu}\delta_{i,j-\hat{\nu}} - U^{\dagger}_{i-\hat{\nu},\nu}\delta_{i,j+\hat{\nu}} \right) + \eta_{i,4} \left(e^{ia\mu_I} U_{i,4}\delta_{i,j-\hat{4}} - e^{-ia\mu_I} U^{\dagger}_{i-\hat{4},4}\delta_{i,j+\hat{4}} \right)$$

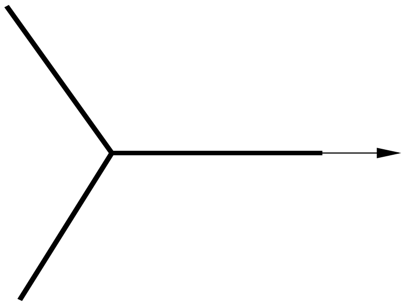
An imaginary $\mu = i\mu_I$ is like adding a background U(1) field in the Euclidean temporal direction. The fermion determinant is real, numerical simulations are feasible again.

The phase diagram in the T-μ_I plane can explored systematically.

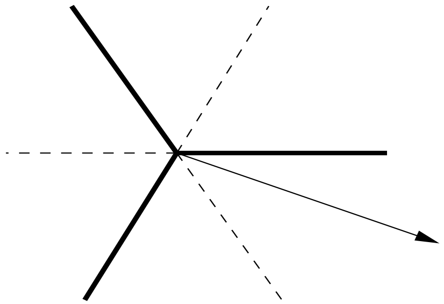
What do we learn from doing that?

Sketch of the T-μ_I phase diagram

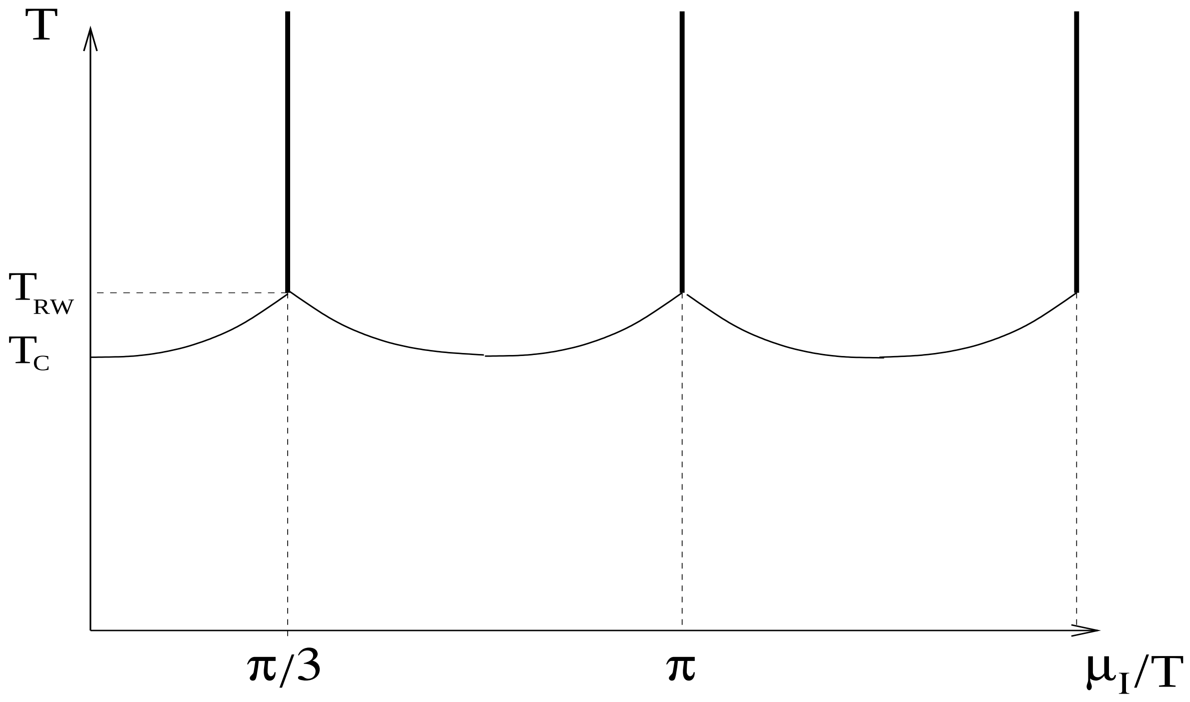
- an imaginary chemical potential is equivalent to a rotation of fermion boundary conditions in temporal direction by an angle $\theta_q = N_t a \mu_I = \mu_I / T$
- an amount $2\pi k / N_c$ of this rotation, with k integer, can be cancelled by a center transformation. Hence the partition function has periodicity $2\pi/N_c$ in θ_q (Roberge and Weiss)
- the periodicity is smoothly realized at low T. Instead in the high T regime first order phase transitions occur for $\theta_q = (2k+1)\pi/N_c$ at which the Polyakov loop $\langle L \rangle$ suddenly jumps from one center sector to the other (RW lines). One may think of θ_q as a rotation angle for the external field of the 3 state 3D Potts model.



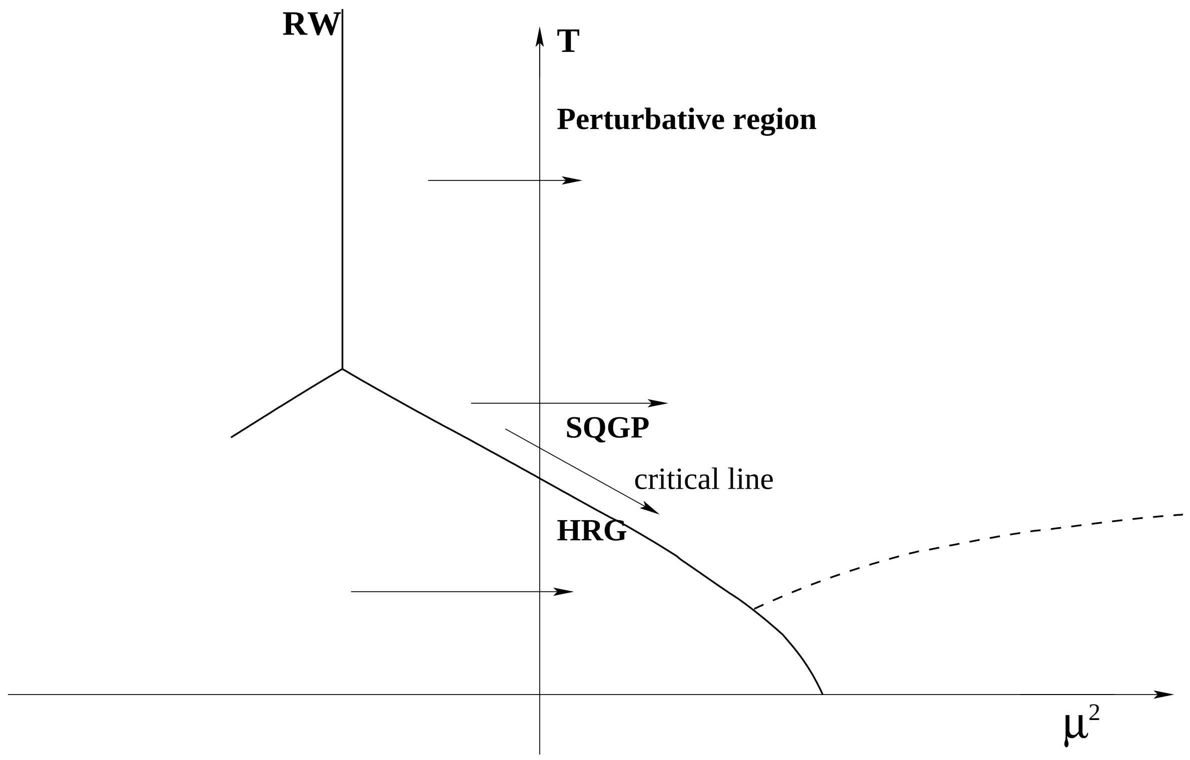
zero chemical potential



non zero imaginary chemical potential



- **The RW line must end at some endpoint T_{RW}**
- **The diagram is completed by the analytic continuation of the physical deconfinement/chiral transition line, which repeats periodically over the plane. Numerical results show that such line touches the RW line right on its endpoint.**



One way to exploit information gathered at imaginary chemical potentials is to perform ANALYTIC CONTINUATION $\equiv$ a given ansatz for the dependence of physics on μ^2 can be continued to $\mu^2 < 0$ and checked (fitted) against numerical data at imaginary chemical potentials

Predictivity restricted by domains of analyticity

Systematics affected by the choice of the ansatz.

Determining the location of the deconfinement line may be useful to get part of the physical line by analytic continuation (see later)

Ph. de Forcrand and O. Philipsen, Nucl. Phys. B 642, 290 (2002); Nucl. Phys. B 673, 170 (2003)

M. D'Elia and M.P. Lombardo, Phys. Rev. D 67, 014505 (2003); Phys. Rev. D 70, 074509 (2004)

V. Azcoiti, G. Di Carlo, A. Galante and V. Laliena, Nucl. Phys. B 723, 77 (2005).

H. S. Chen and X. Q. Luo, Phys. Rev. D 72, 034504 (2005).

P. Giudice and A. Papa, Phys. Rev. D 69, 094509 (2004)

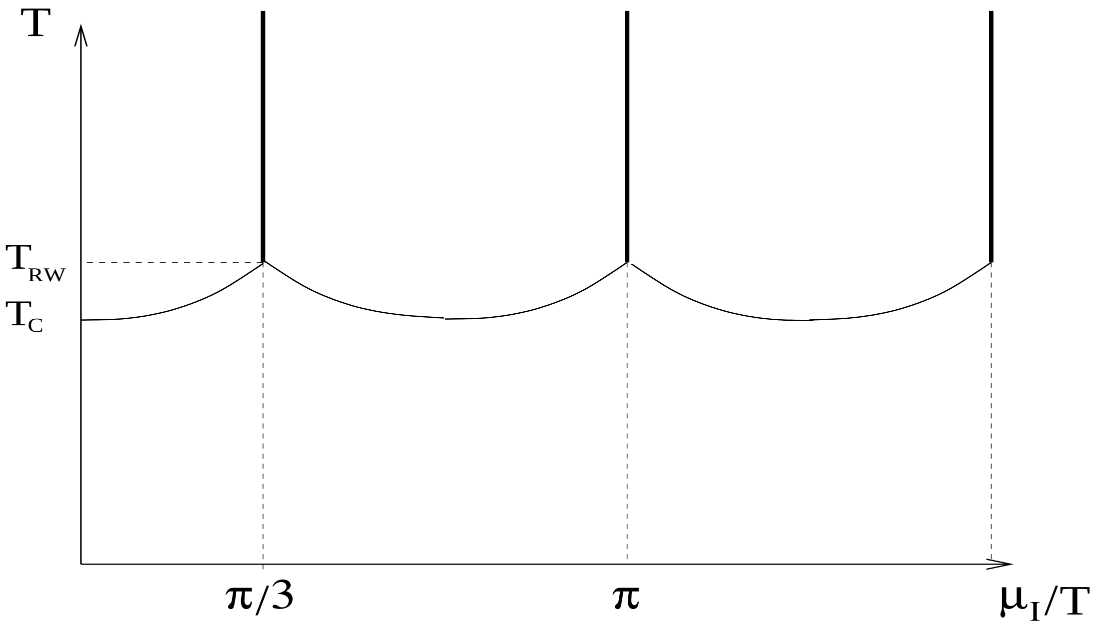
P. Cea, L. Cosmai, M. D'Elia and A. Papa, Phys. Rev. D 77, 051501 (2008); Phys. Rev. D 80, 034501 (2009).

Here we are interested in a different question:

What is the order of the RW endpoint?

The issue has been partially addressed in some previous studies

de Forcrand and Philipsen for SU(3) $N_f = 2$(2002), Kouno et al. (2009) in a PNJL model, G. Cortese for 2 color QCD (2007)



Along the RW lines the theory possesses an exact Z_2 symmetry: the system is in perfect equilibrium between two center sectors. The symmetry is spontaneously broken for $T > T_{\rm RW}$, where a phase transition in T takes place.

Such symmetry is better appreciated at $\theta_q = \pi$ (periodic b.c.), where it corresponds to charge conjugation. The RW endpoint is equivalent to the finite spatial size transition at which charge symmetry is spontaneously broken which has been studied in other contexts T. DeGrand, R. Hoffmann and J. Najjar, JHEP 0801, 032 (2008); B. Lucini, A. Patella and C. Pica, Phys. Rev. D 75, 121701 (2007); B. Lucini and A. Patella, Phys. Rev. D 79, 125030 (2009)

Two possibilities

- **The endpoint is second order.**

  In this case the universality class is Ising 3d by symmetry, the corresponding critical behaviour may in principle influence physics at $\theta_q = 0$ M. D'Elia, F. Di Renzo and M.P. Lombardo, Phys. Rev. D 76, 114509 (2007); H. Kouno, Y. Sakai, K. Kashiwa and M. Yahiro, arXiv:0904.0925 [hep-ph].

- **The endpoint is first order.**

  In this case it is actually a triple point with two further first order lines departing from it. Those are naturally identified with (part of) the analytic continuation of the physical critical line. More interesting consequences follows ...

For $N_c = 3$, the first order hypothesis is surely realized close enough to the quenched limit, $am_q \to \infty$, where θ_q becomes completely irrelevant and the RW endpoint coincides with the usual quenched deconfining transition, $T_{\rm RW} = T_c$

3 – NUMERICAL RESULTS

We have investigated QCD with two degenerate flavors, standard plaquette action, standard staggered fermion formulation (square root), RHMC algorithm.

Two values of the bare quark mass: $am_q = 0.075$ **and** $am_q = 0.025$

Lattices $L_s^3 \times L_t$ **with** $L_t = 4$ **and** $L_s = 8,\ 12,\ 16,\ 20,\ 32$**.**

We have worked at fixed $\theta_q = \pi$ **and the temperature** $T = 1/(L_t a(\beta, m_q))$ **has been changed by tuning the inverse gauge coupling** β**.**

Collected statistics are of the order of $50 - 100$**K trajectories for the** β **values closest to the critical point.**

At $\theta_q = \pi$, the broken symmetry is charge conjugation and the imaginary part of the Polyakov loop is a possible order parameter.

$\mathrm{Im}(L) \to \mathrm{magnetization}$ $\qquad (\theta_q - \pi) \to \mathrm{magnetic\ field}$

We study its susceptibility

$$\chi \equiv L_s^3 \left(\langle \mathrm{Im}(L)^2 \rangle - \langle |\mathrm{Im}(L)| \rangle^2 \right) \tag{1}$$

its expected finite size scaling behaviour is the following

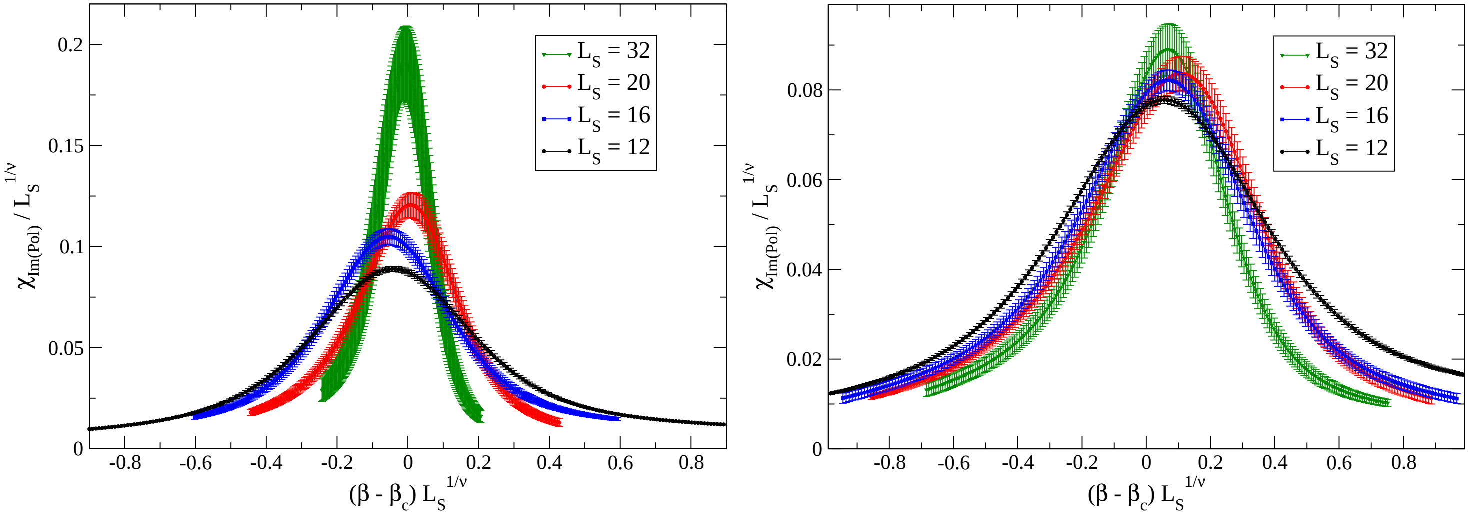
$$\chi = L_s^{\gamma/\nu}\, \phi(\tau L_s^{1/\nu}) \quad \Longrightarrow \qquad \chi / L_s^{\gamma/\nu} = \phi(\tau L_s^{1/\nu}) \tag{2}$$

where $\tau \equiv (T - T_{\mathrm{RW}})/T_{\mathrm{RW}} \sim (\beta - \beta_{\mathrm{RW}})$**,**

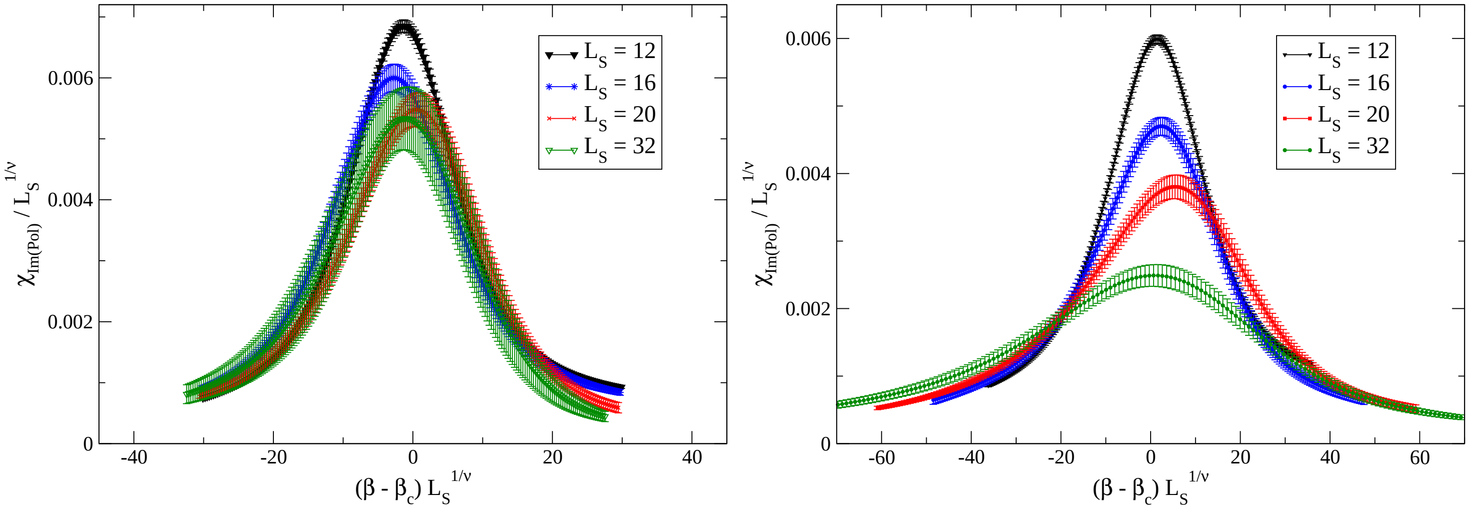
Table of relevant critical indexes

	ν	γ
Ising 3d	**0.63**	**1.24**
$1^{st} Order$	$1/3$	**1**

2nd order



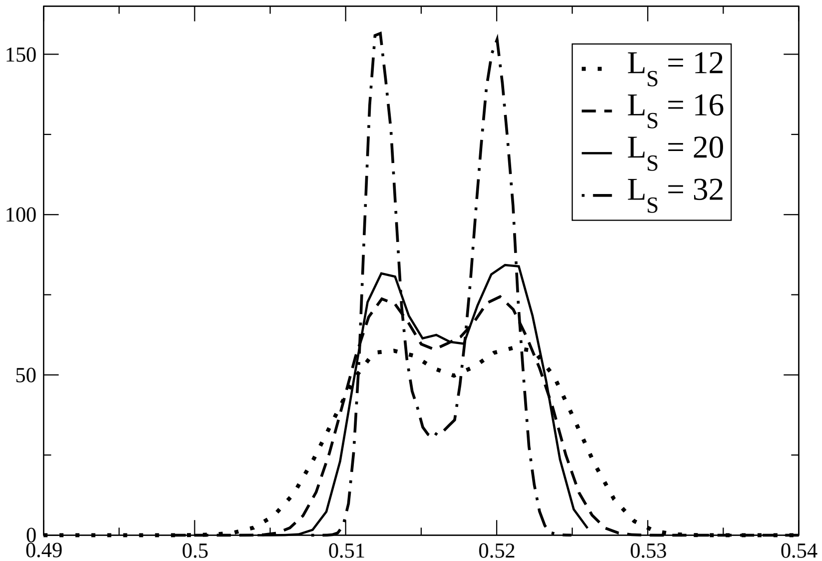
1st order



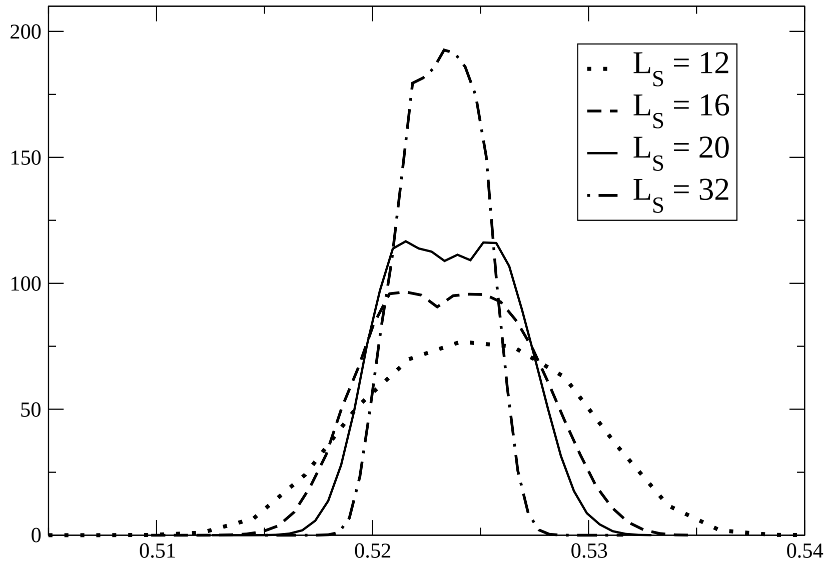
$am_q = 0.025$ $\qquad$ $am_q = 0.075$

$\beta_{\text{RW}} = 5.33885$ $\qquad$ $\beta_{\text{RW}} = 5.3965$

reweighted plaquette distribution at the critical coupling



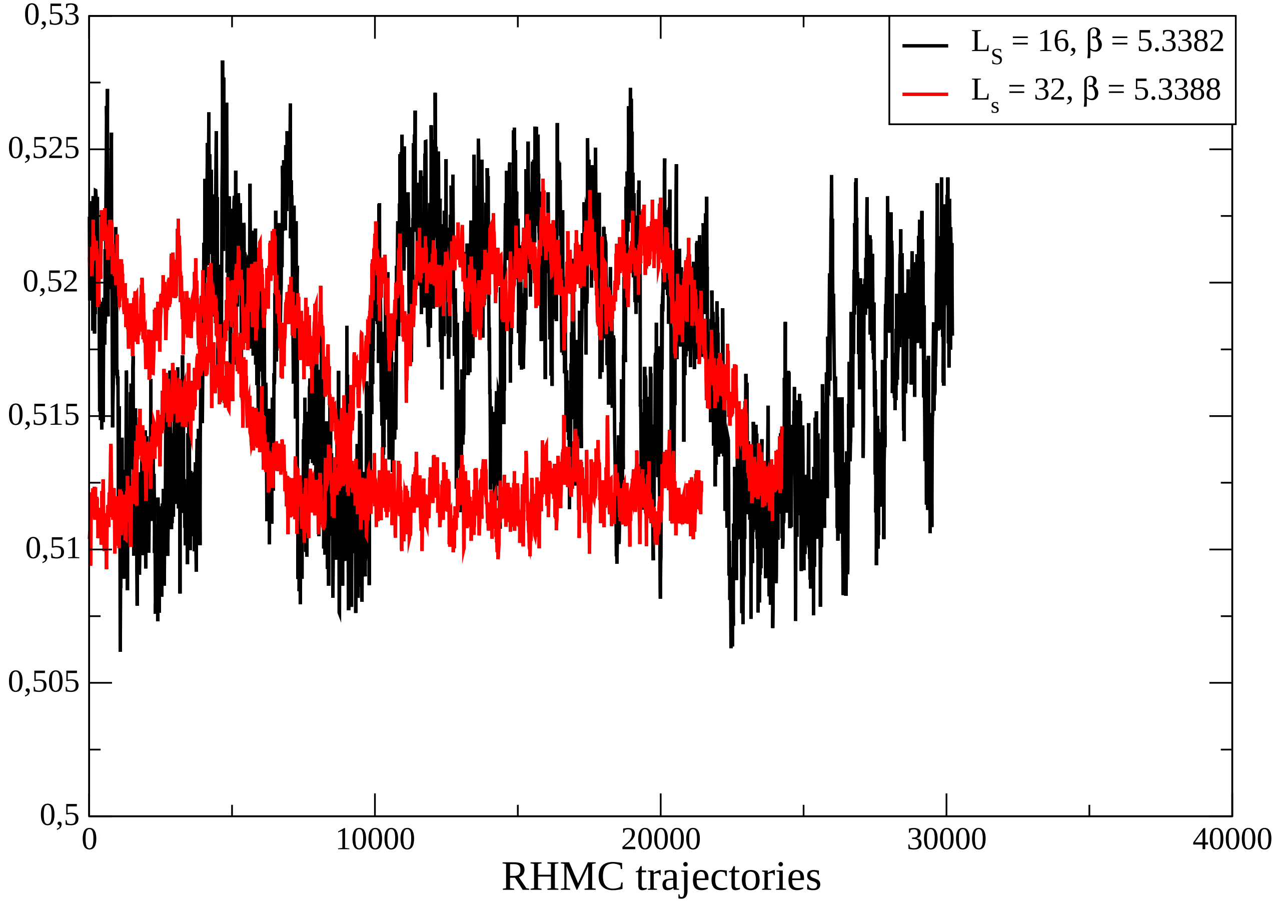
$am_q = 0.025$



$am_q = 0.075$

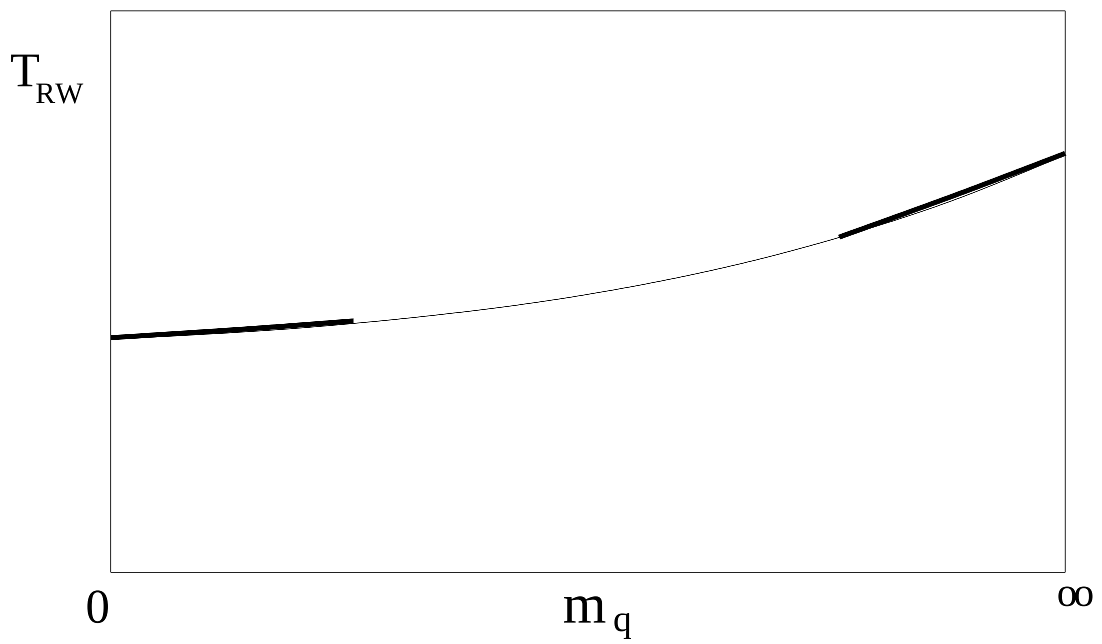
Double peak distributions are visible at the lower quark mass, but not at the higher quark mass

The development of metastabilities as $L_s \to \infty$ for the lower quark mass is also visible from Monte-Carlo histories of the plaquette:

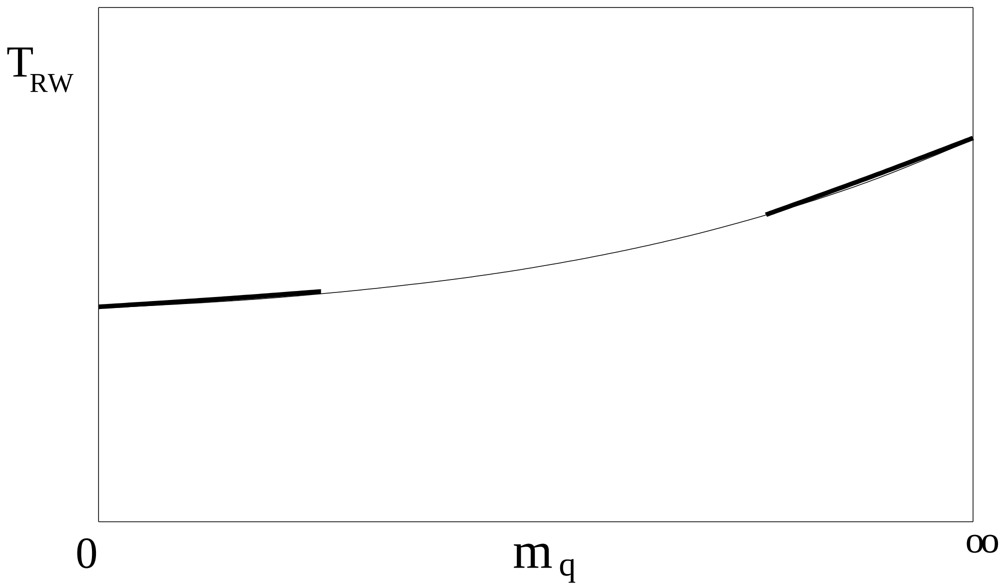


Both the scaling of the order parameter susceptibility and the search for double peak distribution lead to the following conclusion:

The transition is first order at the lower quark mass $am = 0.025$. It is weaker and likely second order at the higher quark mass $am_q = 0.075$. Since at $am_q = \infty$ the transition must be first order again, the following scenario is likely:



Since for $am_q = 0.025$ the pion is already quite heavy, the first order chiral region includes physical quark masses.



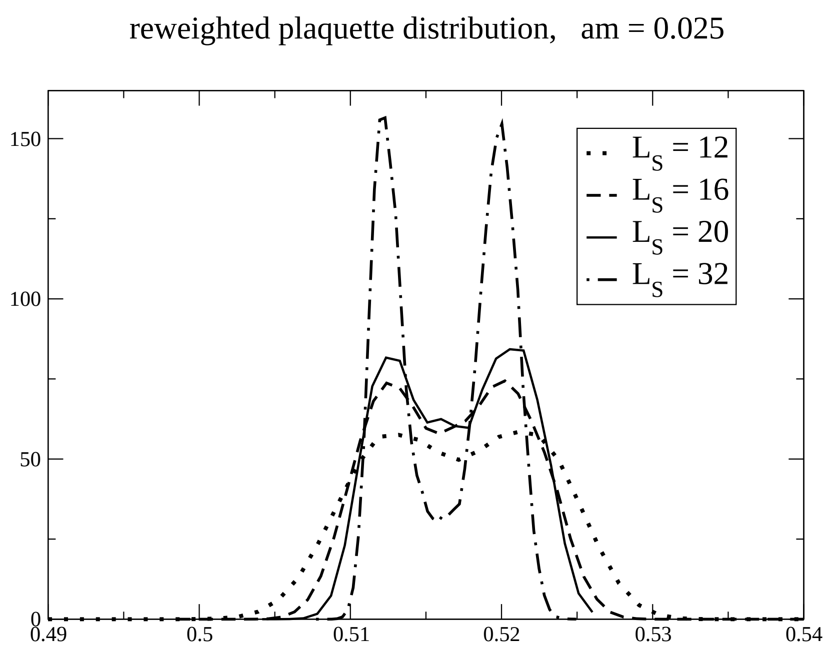
The right, high mass region of this phase diagram is the exact mapping of what happens for a 3-state 3D Potts model in a negative external field, where the residual Z_2 symmetry breaks spontaneously (C. Bonati, M. D'E., in progress).

The left, low mass region comes unexpected: the strengthening of the transition for low masses is likely due to an interplay with chiral degrees of freedom which should be better understood.

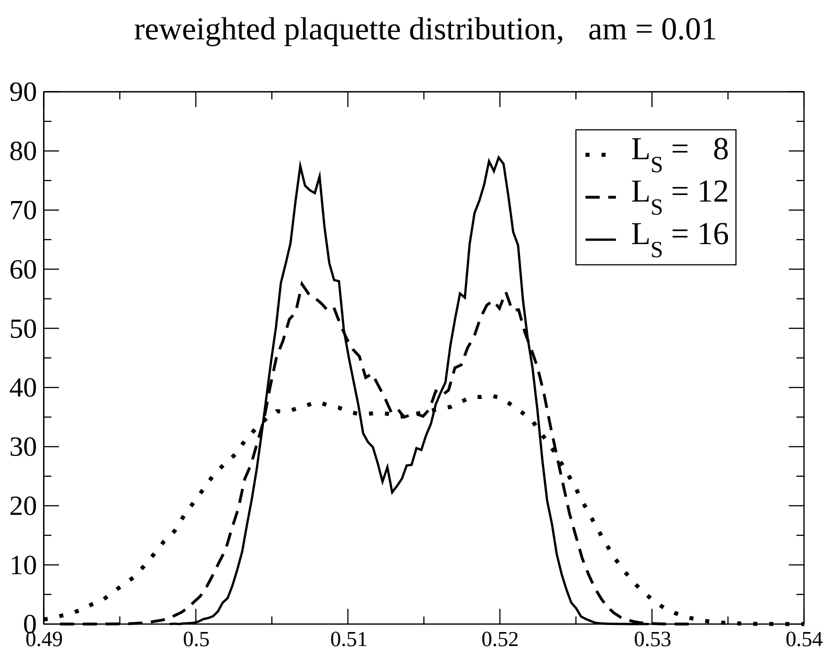
We are currently trying to put this scenario on a firmer basis by investigating more quark masses, preliminary results are positive

Further preliminary evidence collected in favour of the above scenario

(M. D'E., F. Sanfilippo, in progress)

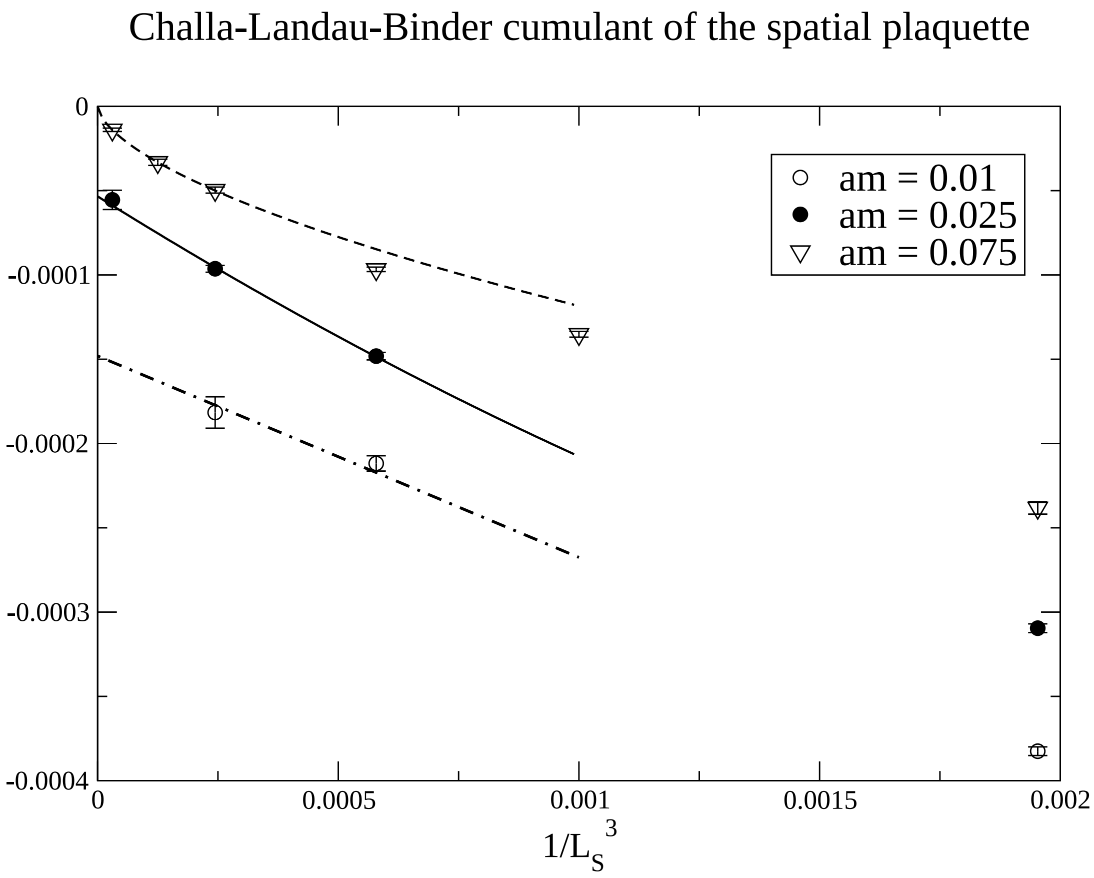


$am_q = 0.025$



$am_q = 0.010$

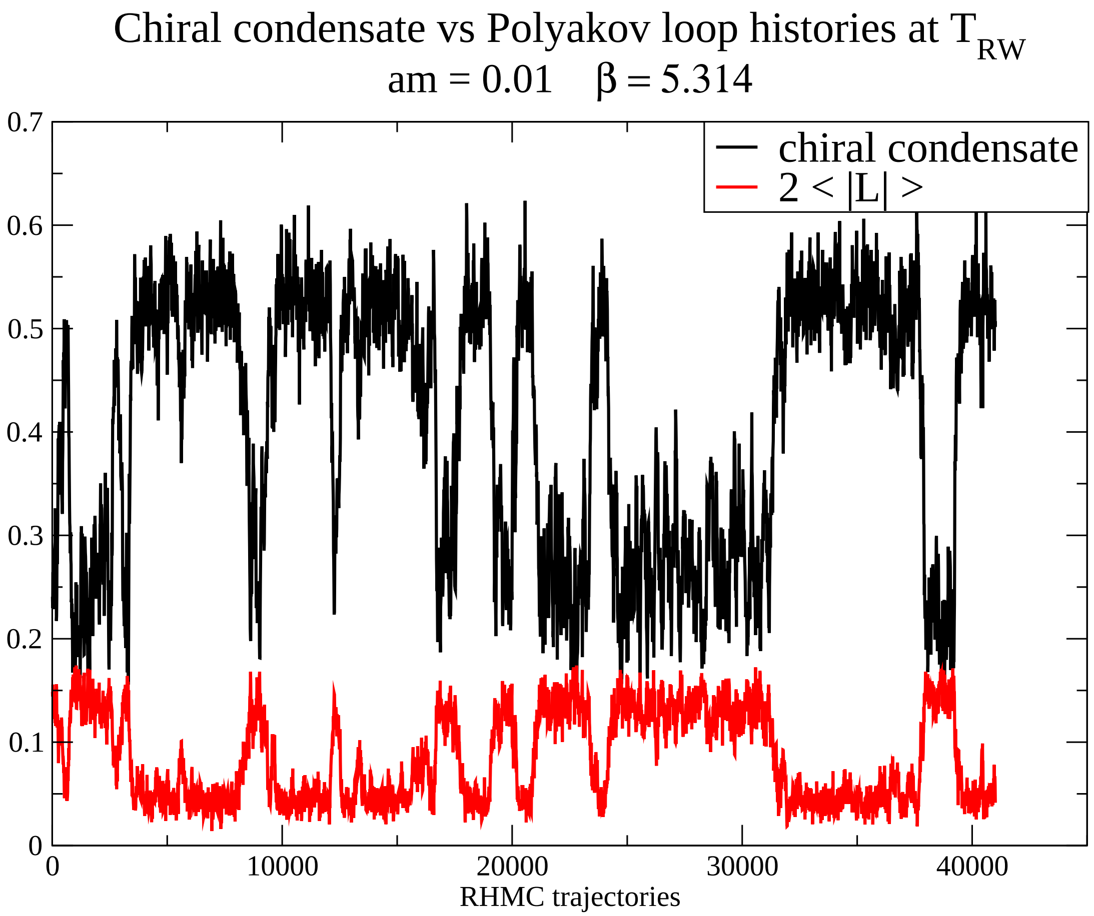
The first order transition at $am = 0.010$ is sensibly stronger than at $am = 0.025$.



this is also visible from the infinite volume limit of the Binder-Challa-Landau cumulant (at the transition temperature) of the plaquette

$$\frac{1}{3}\left(1-\frac{\langle P^4\rangle}{\langle P^2\rangle^2}\right)$$

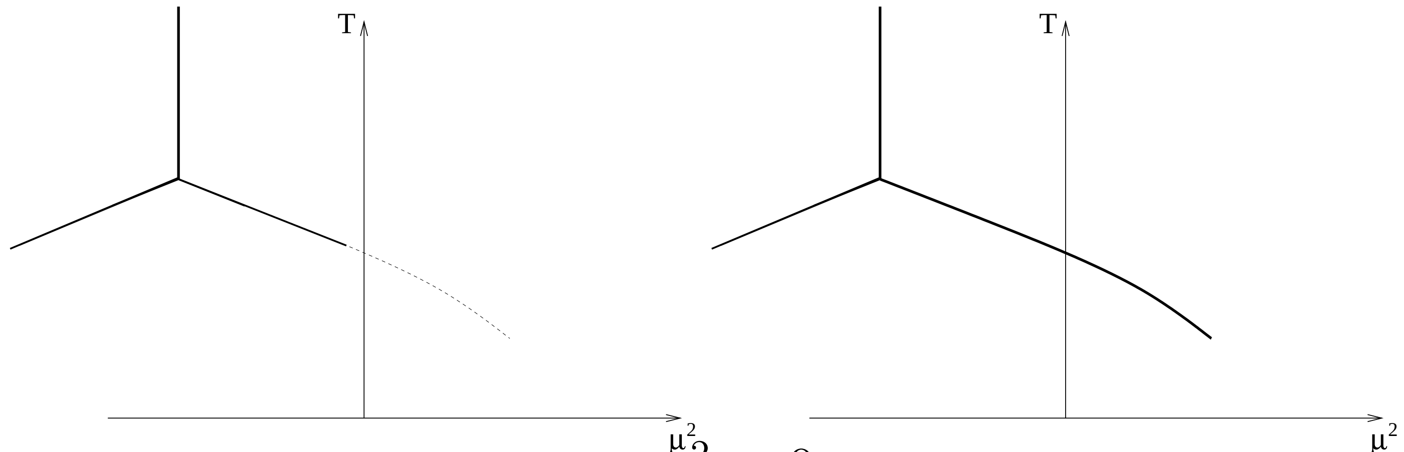
whose non-zero value signals a first order (it is proportional to the gap squared)



Monte-Carlo histories show that chiral dynamics are strictly entangled with Polyakov loop dynamics: at the RW endpoint also chiral symmetry restoration takes place.

4 – Discussion and speculations

When the RW endpoint is first order, what is the fate of the departing first order line?



1) It could have a 2nd order endpoint at $\mu^2 < 0$: its critical behaviour could strongly influence $\mu^2 = 0$ physics above T_c, which is known to be highly non-trivial.

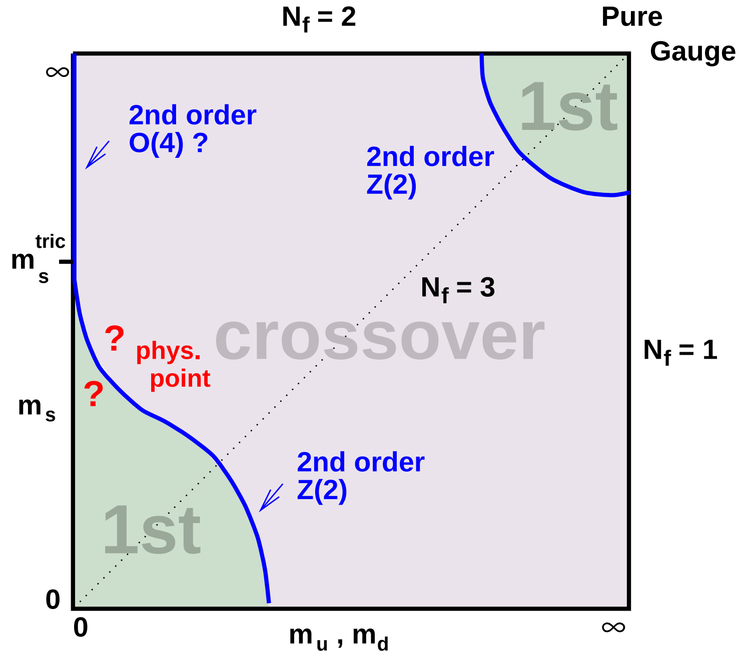
2) It could cross the $\mu^2 = 0$ axis, leading to first order at $\mu^2 = 0$.

One expects that the extension of the departing first order line depends on the strength of the starting RW endpoint. The second possibility is surely verified in the quenched limit, it could be likely again in the chiral limit where the RW endpoint gets stronger.

The answer is of course strictly interrelated to the solution of the puzzle about the $N_f = 2$ critical behaviour at $m_q = 0$ mentioned before.

A pure speculation ...

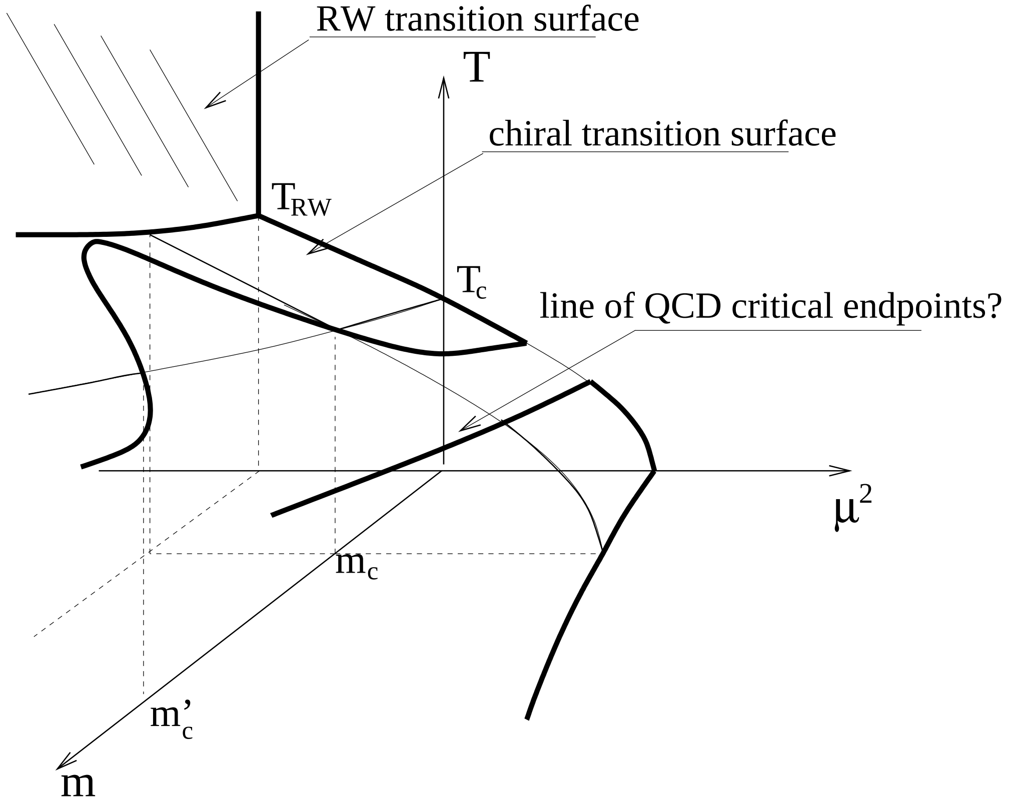
Suppose a similar scenario happens for different number of flavors (i.e. RW endpoint weakens and gets stronger again when decreasing the quark masses)



What if the first order regions in the Columbia plot are interesections with the first order line (hyper-surface) departing from the RW endpoint?

This is true for the quenched corner, could be true also for the chiral region.

Consider the $N_f = 3$ case: at $\mu = 0$, the transition is first order for small or large m, with two critical masses m_c and m_c' delimiting an intermediate crossover region



We conjecture that, in the T-μ^2-m diagram, a first order surface departs from the line of RW endpoints and extends enough to reach $\mu^2 = 0$ only for $m < m_c$ or $m > m_c'$.

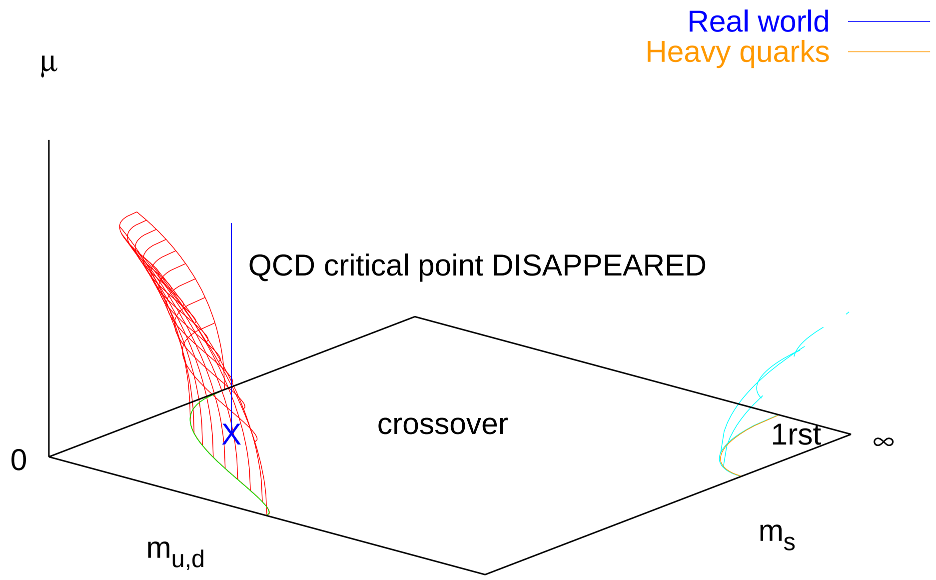
In this scenario the QCD critical endpoint, if it exists, is not related to the physics of the chiral critical region, but instead to high μ, low T physics.

Is this a reasonable conjecture?

At least for the $\mu^2 < 0$ side, future numerical studies can completely clarify that.

Moreover, it is already supported by the recent results from Ph. de Forcrand and O. Philipsen:

the chiral critical mass is a decreasing function of μ^2



From P. de Forcrand and O. Philipsen, JHEP 0811, 012 (2008)

5 – CONCLUSIONS about the RW endpoint

- For $N_f = 2$ QCD, standard staggered and plaquette action, $L_t = 4$, the RW endpoint is first order for low quark masses (including physical ones), as in the quenched limit.

  That should be checked by further studies going closer to the continuum limit.

- The first order line departing from the RW endpoint closest to the $\mu = 0$ axis could reach the axis or get very close to it. Therefore we could have a critical endpoint influencing Quark-Gluon Plasma physics, which would not be related to the traditional critical endpoint of the phase diagram.

  Future studies should investigate the position and the properties of this possible critical endpoint.

- One can make more speculative conjectures starting from that, which can be checked by systematic studies of the phase diagram in the T-μ_I plane and for different number of flavors.

6 – Analytic continuation of the critical line

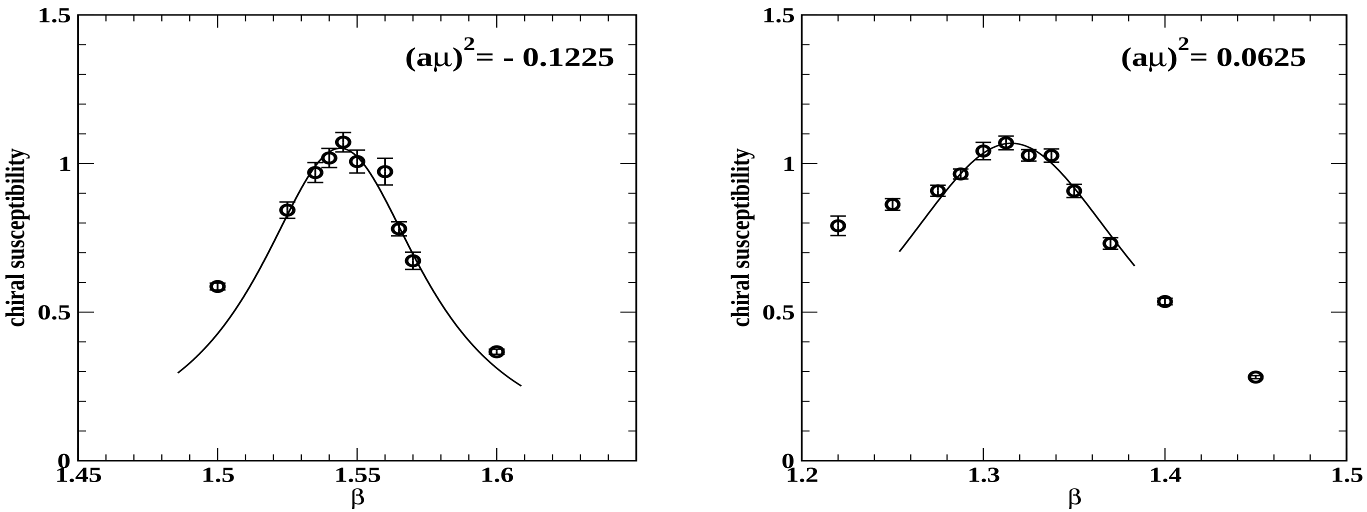
Are we able to correctly predict $T_c(\mu_B)$ by analytic continuation?

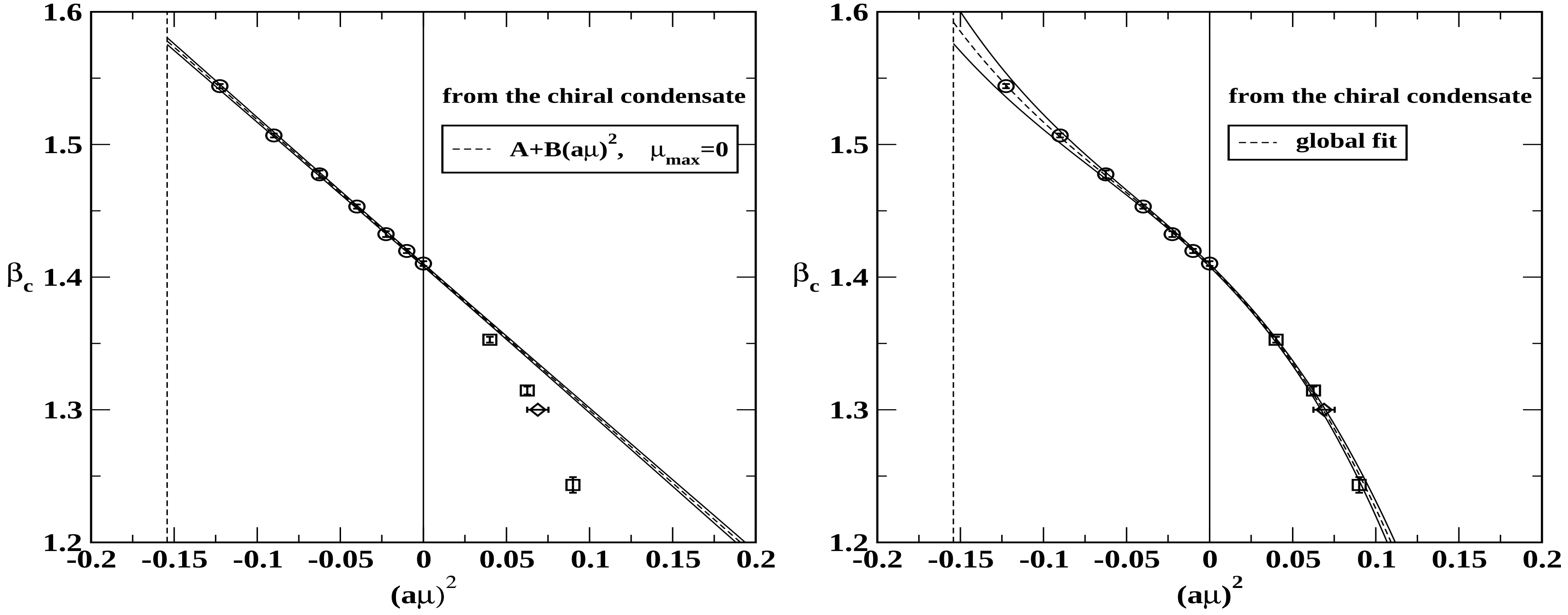
Careful checks of possible systematics in analytic continuation can be performed in theories which are free of the sign problem. An example is QCD with two colors: the fermion determinant is always real since the $SU(2)$ gauge group is real.

We have considered the continuation of the critical line in $SU(2)$ with 8 flavors, standard staggered fermions, $am = 0.07$, $L_s = 16$ and $L_t = 4$, standard HMC algorithm.

P. Cea, L. Cosmai, M. D'E., A. Papa, PRD 77, 051501(R) (2008)

Location of pseudocritical couplings performed by looking at susceptibility peaks





Data at $\mu^2 < 0$ cannot predict terms beyond the linear one in μ^2, $\beta_c(\mu) = A + B\mu^2$

$A = 1.4091(17), B = -1.095(15), \tilde{\chi}^2 = 0.27$ **but that fails to reproduce data at real μ.**

But a sixth order polynomial, $\beta_c(\mu) = A + B\mu^2 + C\mu^4 + D\mu^6$**, nicely fits all data!**

$A = 1.4088(99), B = -1.230(25), C = -3.77(25) D = -22.7(3.6), \tilde{\chi}^2 = 1.0$

Analyticity at $\mu^2 = 0$ not contradicted, but analytic continuation not predictive enough!

Suppressed, hardly visible contributions ($C\mu^4 + D\mu^6$ in our case) becoming important in different regions are a typical problem of analytic continuation.

Similar problems could apply to real QCD as well: non-linear terms in μ^2 in the critical line could be missed by analytic continuation.

It is worth checking that in sign problem free theories which are closer to QCD: we have investigated QCD in presence of a finite isospin chemical potential:

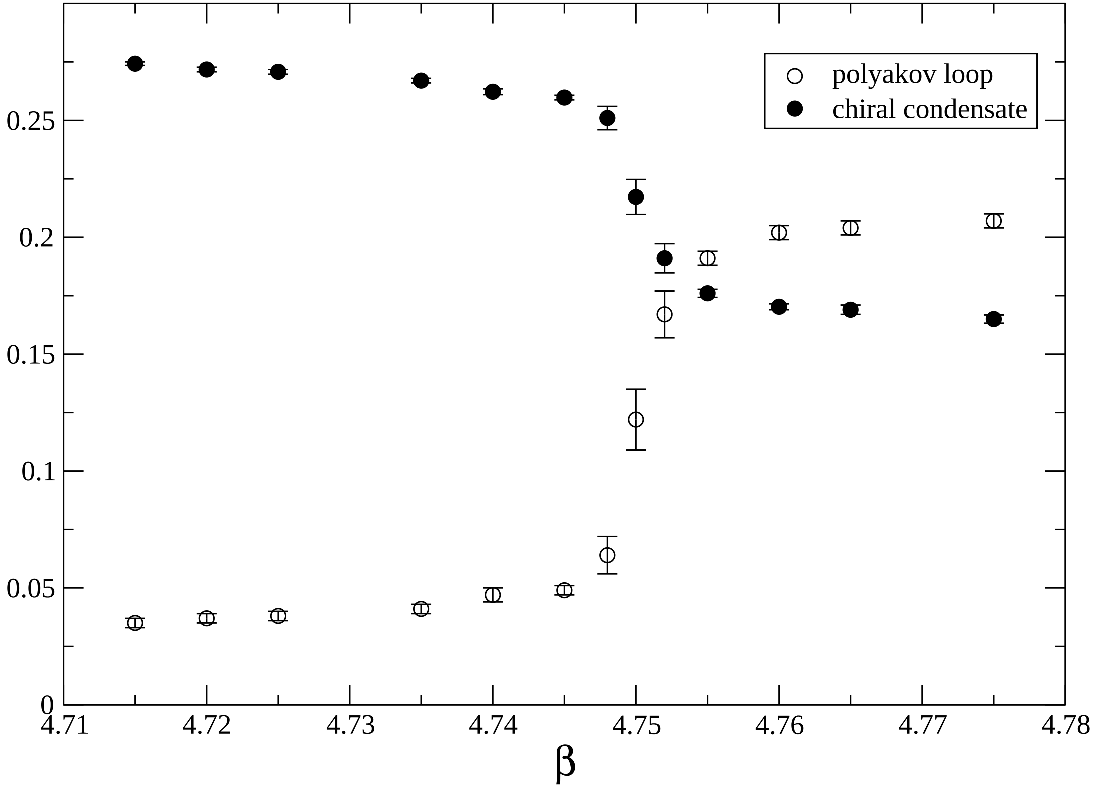
P. Cea, L. Cosmai, M. D'E., C. Manneschi, A. Papa, Phys. Rev. D 80:034501 (2009)

$$Z(T,\mu,-\mu) \equiv \int \mathcal{D}U e^{-S_G} \det M[\mu] \det M[-\mu] = \int \mathcal{D}U e^{-S_G} |\det M[\mu]|^2$$

because of $\det M[-\mu] = \det M[\mu]^*$

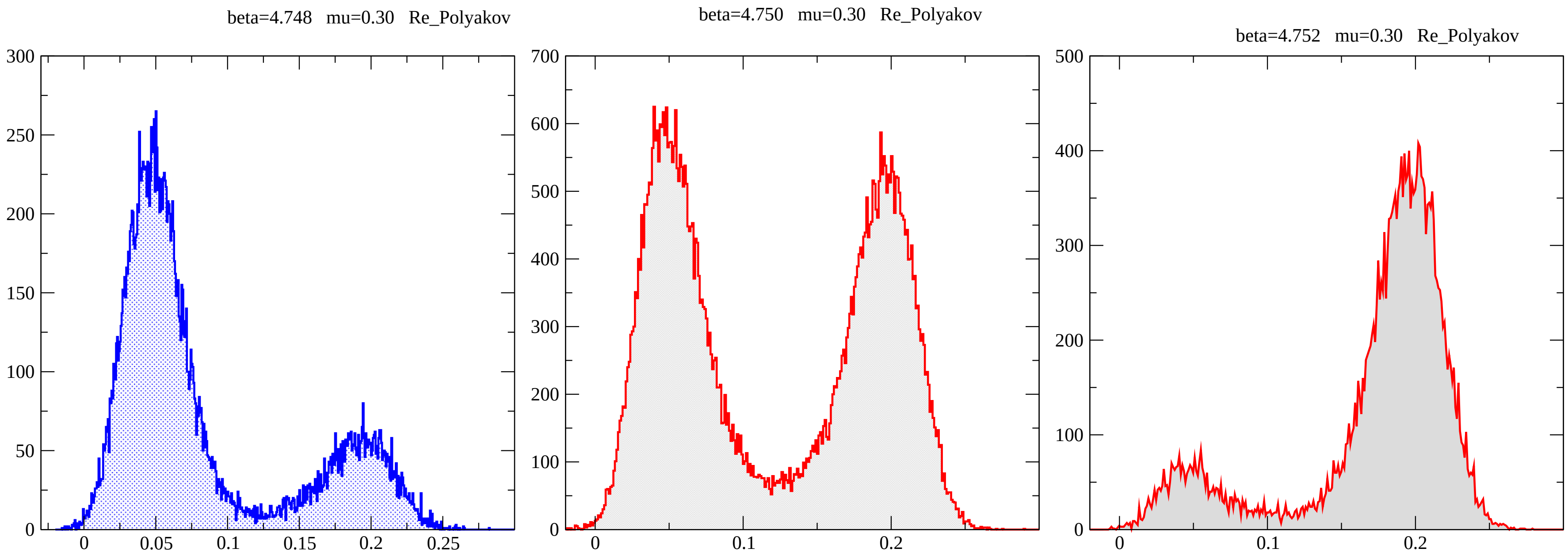
We have considered QCD with 8 flavors (4+4), standard staggered fermions, $am = 0.1$**. The transition at** $\mu^2 = 0$ **is strong first order in this case, and remains so also at** $\mu^2 \neq 0$**.**

Simulations have been done on a relatively small lattice ($8^3 \times 4$**) to avoid too long tunneling times. Critical couplings** $\beta_c(\mu^2)$ **have been determined by looking at double peak distributions around the transition.**



We show as an example how we determine the transition location for $\mu/(\pi T) = i\,0.30$.

A rough idea about β_c is obtained by looking at the behaviour of the observables

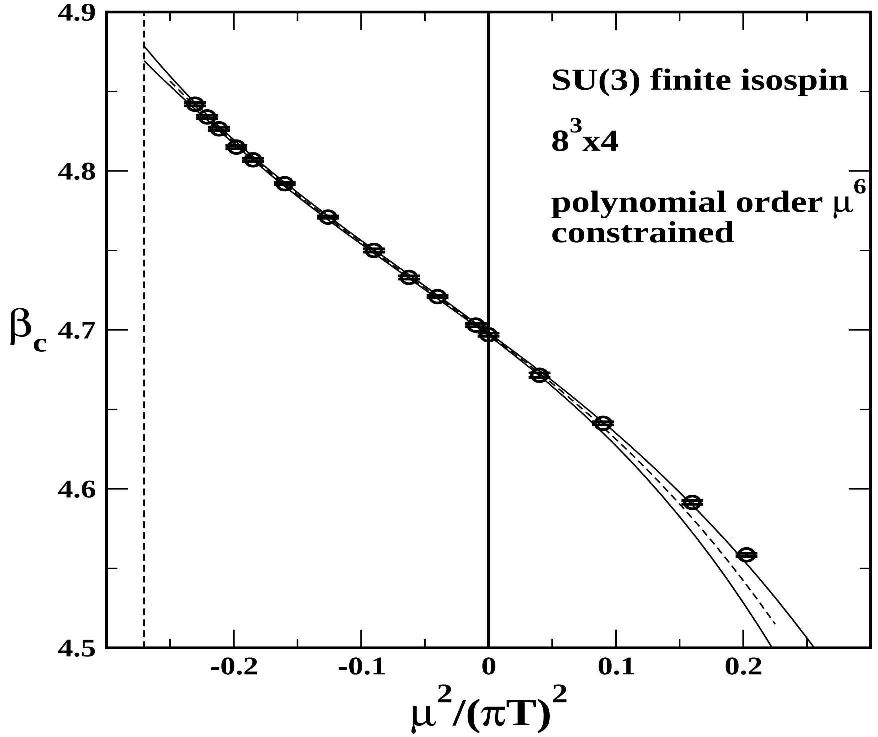


$\beta = 4.748$ $\beta = 4.750$ $\beta = 4.752$

β_c is then obtained by looking at double peak distributions (Re(Polyakov) is shown), which taken over $5 - 10 \cdot 10^4$ trajectories (about 10-20 tunneling events at β_c)

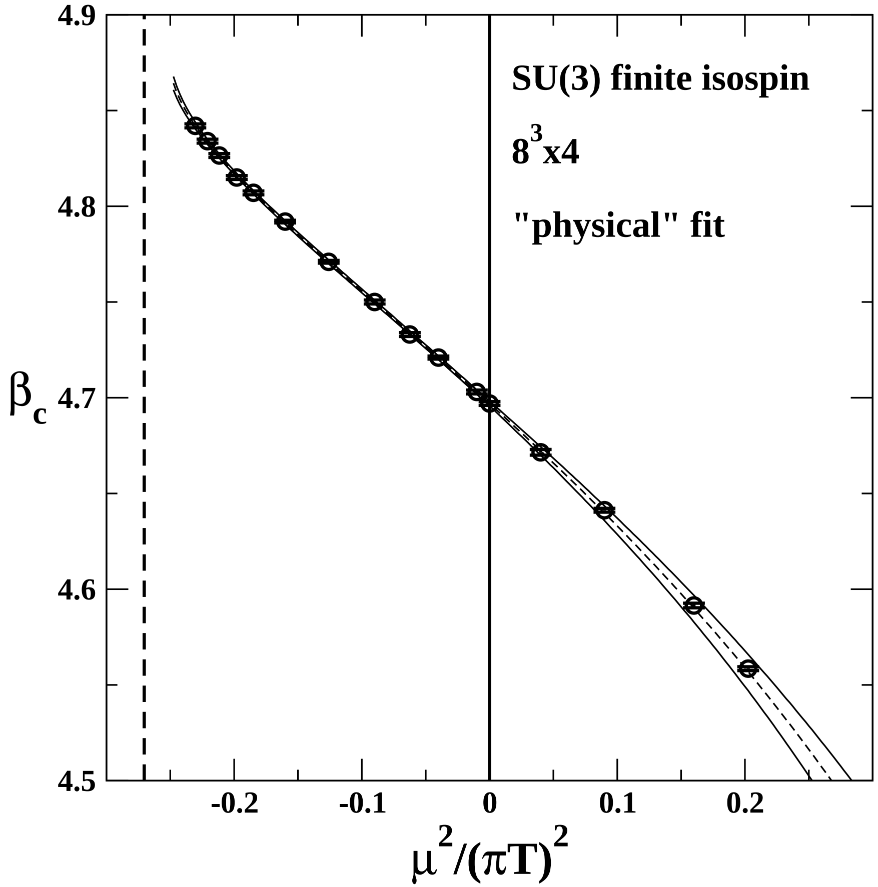
we estimate $\beta_c = 4.750(1)$ in this case

The computational problem in this case is to collect huge statistics in order to correctly sample both phase around the transition and get an high accuracy determination of $T_c = \frac{1}{N_t a(\beta_c, m_q)}$.



A polynomial fit $\beta_c(\mu) = \beta_c(0) + B\mu^2 + C\mu^4 + D\mu^6$ leads to good predictivity, if the linear term is fixed apriori by looking at a restricted region of small chemical potentials.

LESSON: fix linear term by simulations at small chemical potentials, or by other methods (reweighting or Taylor expansion), then analytic continuation is predictive enough to correctly reproduce non-linear terms.



Good predictivity is also obtained by fitting directly the dependence of $T(\mu)/T_c$ by suitable functions

$$\frac{T_c(\mu)}{T_c(0)} = \begin{cases} A + (1-A)\left[\cos\left(\frac{\mu}{T}\right)\right]^B , & \mu^2 \leq 0 \\ A + (1-A)\left[\cosh\left(\frac{\mu}{T}\right)\right]^B , & \mu^2 > 0 , \end{cases}$$

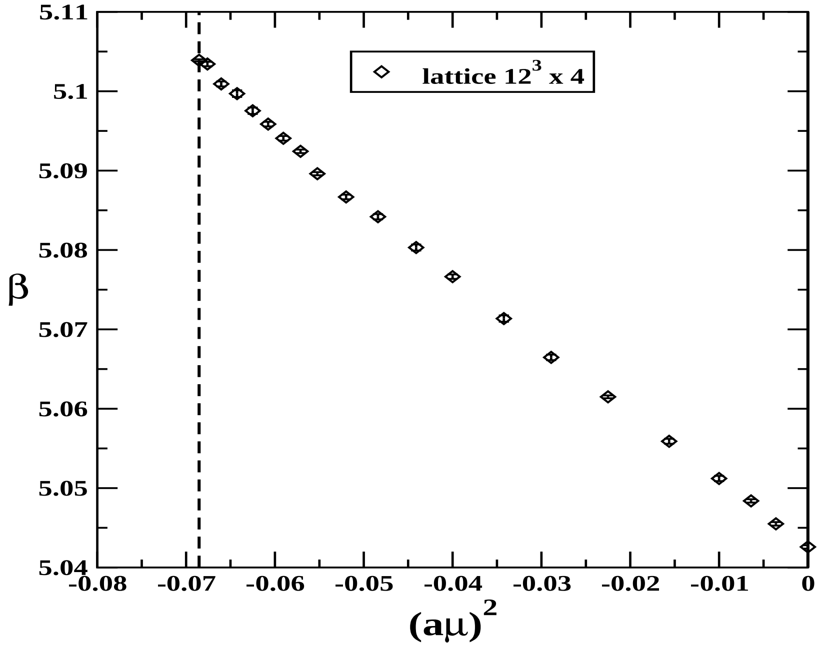
We are now revisiting existing determinations of the critical line for QCD at finite baryon density, which are mostly based on a simple linear extrapolation in μ^2.

P. Cea, L. Cosmai, M. D'E., A. Papa, in progress

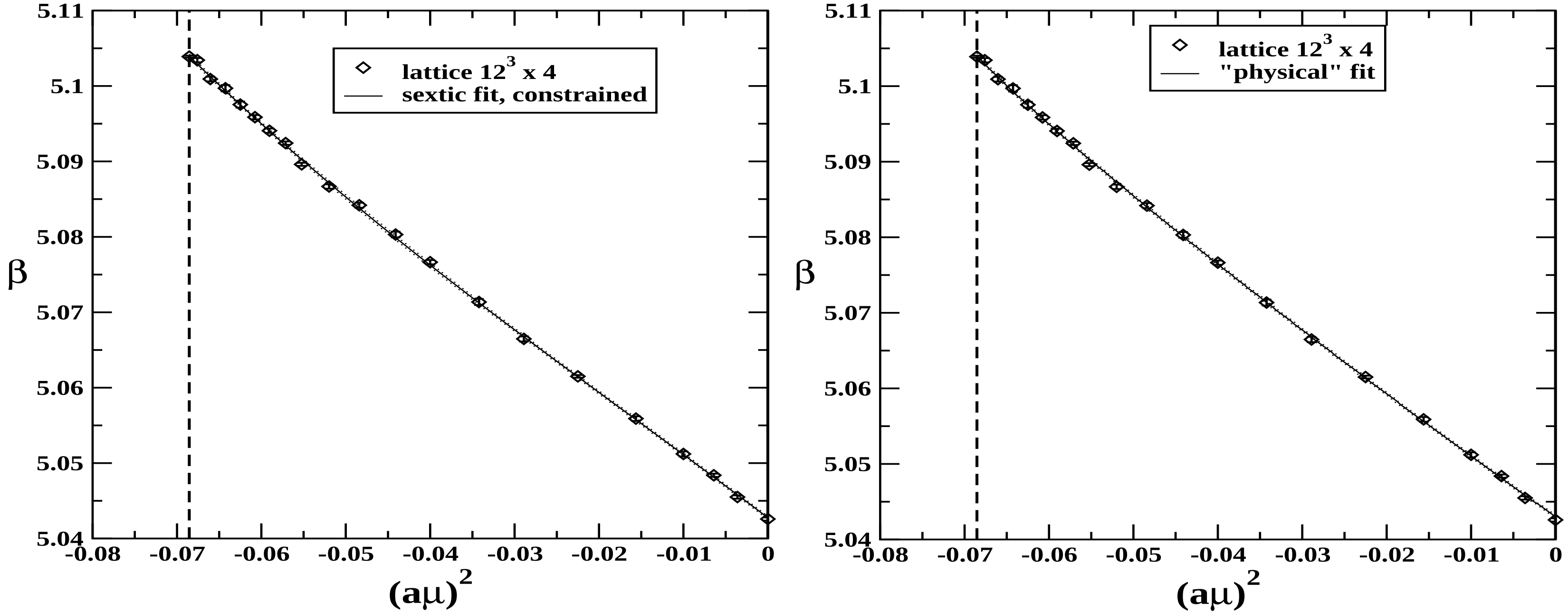
We are studying QCD with 4 degenerate flavors at a bare quark mass $am = 0.05$

(M. D'Elia and M.P. Lombardo, Phys. Rev. D 67, 014505 (2003); Phys. Rev. D 70, 074509 (2004))

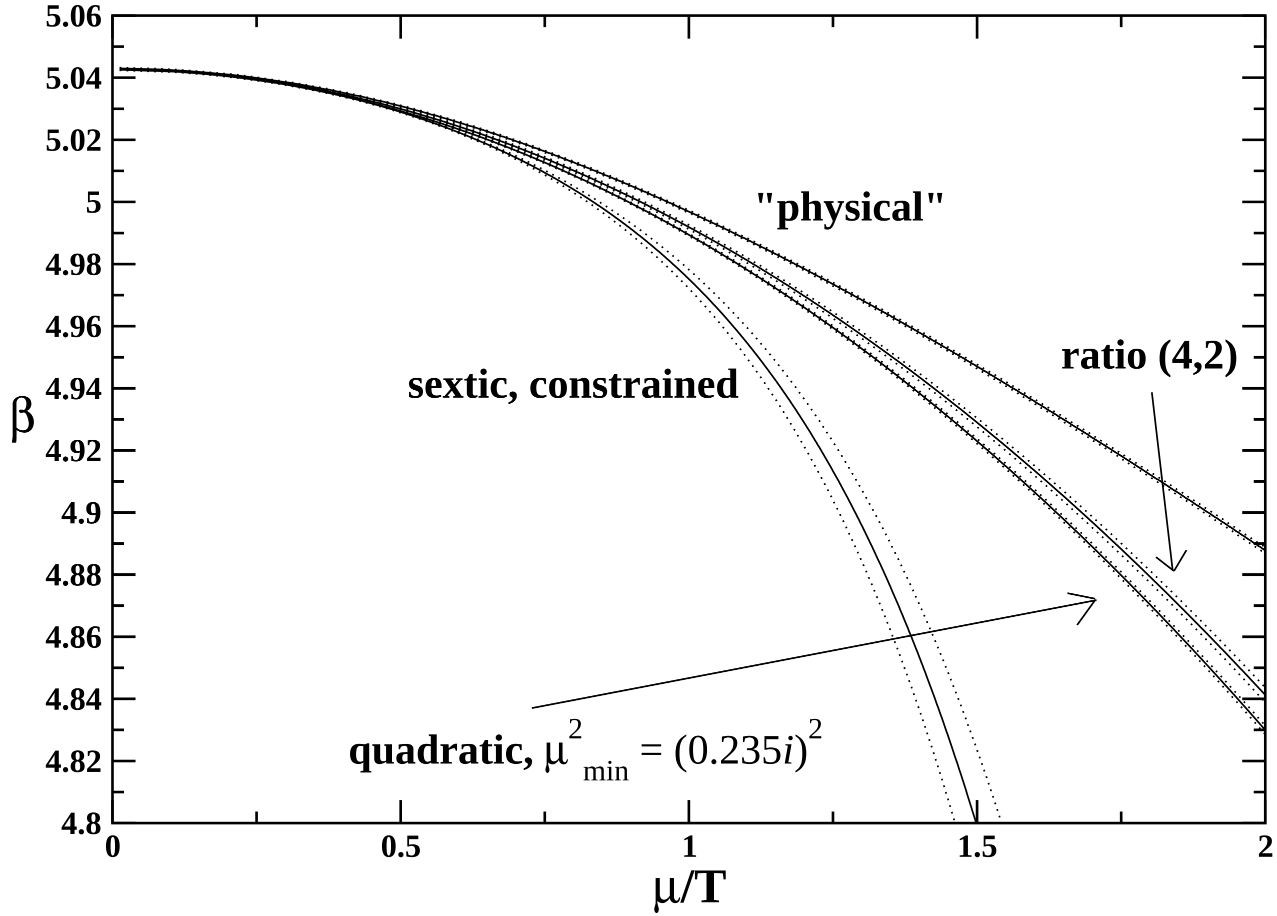
The transition is first order also in this case.



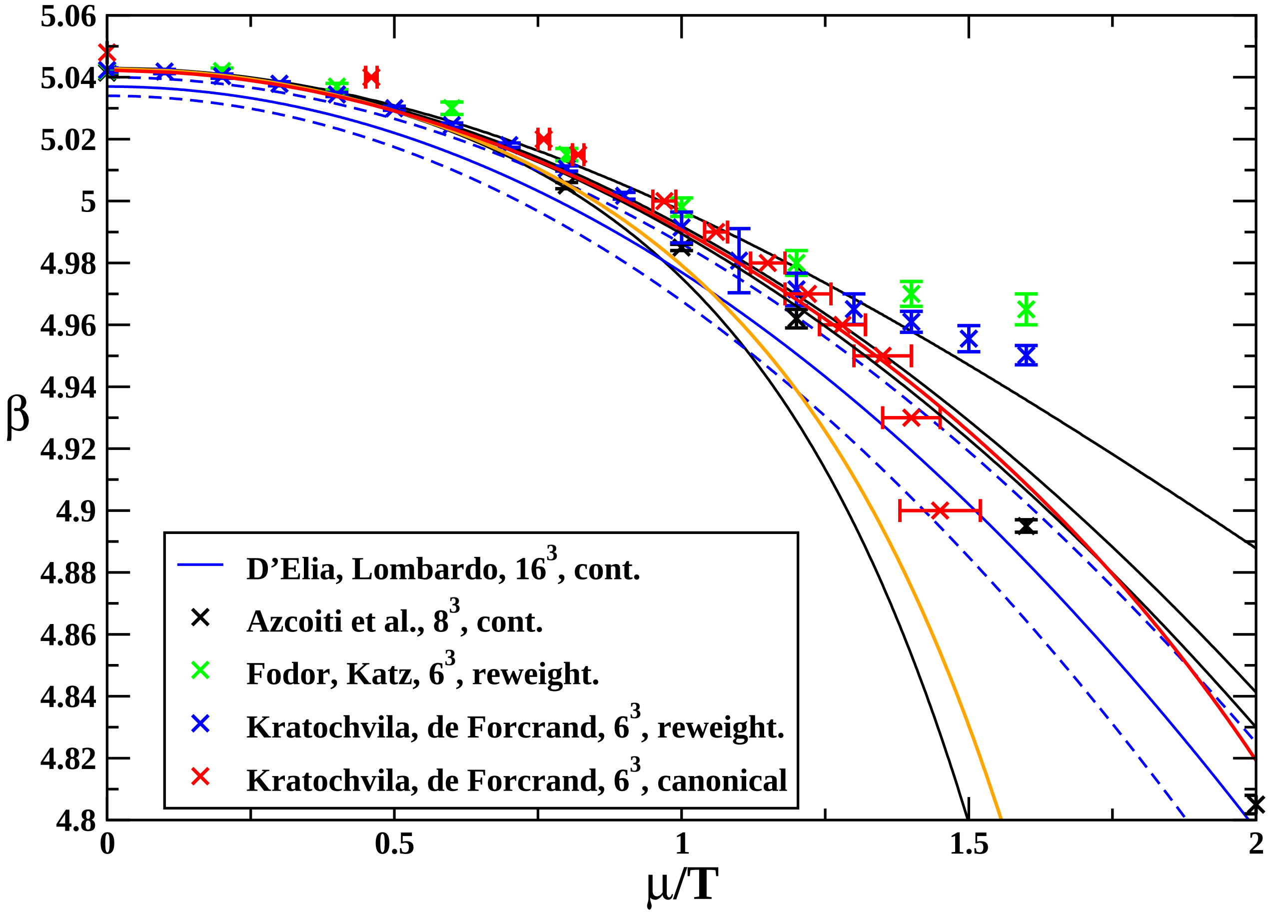
Critical couplings determined in the available region, which is smaller than in the finite isospin case: $\mu^2/T^2 > -(\pi/3)^2$ instead of $\mu^2/T^2 > -(\pi/2)^2$ as for SU(2) or SU(3) at finite isospin.



Non linear corrections are clearly visible with the small errors available and must be included to get reasonable fits. They can be included in different ways (polynomial, rational functions (fitting in β_c or T_c directly ...). Do they give consistent extrapolations to $\mu^2 > 0$?



The answer is not positive at the present stage but we are still fighting with possible extrapolation methods. The reason of the problems is likely related to the shorter range of available imaginary chemical potentials



Comparison with other determinations at real μ (canonical partition function, reweighting, previous analytic continuations .... thanks to Ph. de Forcrand for the collection) shows that our extrapolations start to diverge more or less when other determinations disagree

THANK YOU!