

The QCD phase diagram from the method of analytic continuation



A. Papa

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References

- P. Cea, L. Cosmai, M. D'Elia, A.P., Phys. Rev. D77 (2008) 051501 [arXiv:0712.3755]
- P. Cea, L. Cosmai, M. D'Elia, C. Manneschi, A.P., Phys. Rev. D80 (2009) 034501 [arXiv:0905.1292]
- P. Cea, L. Cosmai, M. D'Elia, A.P., Phys. Rev. D81 (2010) 094502 [arXiv:1004.0184]
- P. Cea, L. Cosmai, M. D'Elia, A.P., F. Sanfilippo, Phys. Rev. D 85 (2012) 094512, [arXiv:1202.5700]

Fermions and Extended Objects on the Lattice
Benasque, June 16 - 22, 2013

Outline

1 Introduction

- QCD phase diagram
- QCD with non-zero baryon density and the sign problem
- The method of analytic continuation

2 Investigations in QCD-like theories free of the sign problem

- Two-color QCD with $n_f = 8$
- Finite isospin SU(3) with $n_f = 8$

3 Application to QCD with $n_f = 4$ and $n_f = 2$

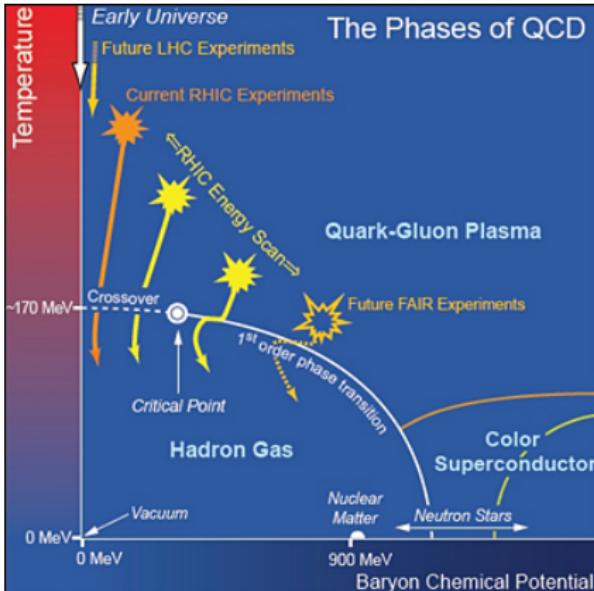
- SU(3) with $n_f = 4$
- Finite isospin SU(3) with $n_f = 2$
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4 Conclusions and Outlook

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QCD phase diagram



(from bnl.gov)

Important implications in heavy ion collisions, in cosmology and in physics of compact stars.

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QCD at non-zero temperature and density

- Lattice is the main non-perturbative tool for the investigation of the QCD phase diagram

- Non-zero temperature:  $T = \frac{1}{N_\tau a(\beta)}$, $\beta = \frac{2N}{g^2}$
- Non-zero density:  sign problem!

Importance sampling requires positive weights, but in

$$Z(T, \mu) = \int [dU] e^{-S_G[U]} \det[M(\mu)]$$

the fermionic determinant $\det[M(\mu)]$ is **complex** for $\mu \neq 0$ in $SU(3)$.

Exceptions:

- **imaginary chemical potential**: $\mu = i\mu_I$
- **$SU(2)$ or two-color QCD**
- **isospin chemical potential**: $\mu_u = -\mu_d$

Ways around I

- Perform simulations at $\mu=0$ and take advantage of physical fluctuations in the thermal ensemble for extracting information at (small) non-zero μ , after suitable reweighting

[I.M. Barbour et al., 1997]

[Z. Fodor, S.D. Katz, 2002 →]

- Taylor-expand in μ the v.e.v. of interest and calculate the coefficients of the expansion by numerical simulations at $\mu = 0$

[S.A. Gottlieb, 1988]

[QCD-TARO coll., 2001]

[C.R. Allton et al., 2002-2003-2005]

[R.V. Gavai, S. Gupta, 2003-2005]

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Ways around II

- Build canonical partition functions by Fourier transform of the grand canonical function at imaginary chemical potential
 - [A. Hasenfratz, D. Toussaint, 1992]
 - [M.G. Alford, A. Kapustin, F. Wilczek, 1999]
 - [P. de Forcrand, S. Kratochvila, 2004-2005-2006]
 - [A. Alexandru et al., 2005]
- Reorder the path integral representation of the partition function, by first calculating expectation values with constrained parameters and then weighting over the density of states
 - [G. Bhanot et al., 1987]
 - [M. Karliner et al., 1988]
 - [A. Gocksch, 1988]
 - [V. Azcoiti, G. Di Carlo, A.F. Grillo, 1990]
 - [X.-Q. Luo, 2001]
 - [J. Ambjorn et al., 2002]
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The method of analytic continuation

- Perform Monte Carlo numerical simulations at some selected **imaginary** values of the chemical potential, $\mu = i\mu_I$, thus getting data points with their statistical uncertainties
- Interpolate the results obtained by a suitable function of μ_I^2
- Analytically continue to **real** chemical potentials: $\mu_I \rightarrow -i\mu$

A bit of history:

- idea of formulating a theory at imaginary chemical potential
[M.G. Alford, A. Kapustin, F. Wilczek, 1999]
- test of effectiveness in strong-coupling QCD [M.P. Lombardo, 2000]
- thereafter, a lot of applications to QCD and tests in QCD-like theories and in spin models

- Applications in QCD:

- $n_f = 2$ staggered
- $n_f = 3$ staggered
- $n_f = 4$ staggered
- $n_f = 2 + 1$ staggered
- $n_f = 2$ Wilson
- $n_f = 4$ Wilson

[Ph. de Forcrand, O. Philipsen, 2002]
[M. D'Elia, F. Sanfilippo, 2009]
[Ph. de Forcrand, O. Philipsen, 2003]
[M. D'Elia, M.P. Lombardo, 2003-2004]
[V. Azcoiti *et al.*, 2004-2005]
[M. D'Elia, F. Di Renzo, M.P. Lombardo, 2007]
[Ph. de Forcrand, O. Philipsen, 2007]
[L.-K. Wu, X.-Q. Luo, H.-S. Chen, 2007]
[K. Nagata, A. Nakamura, 2011]
[H.-S. Chen, X.-Q. Luo, 2005]

- Tests:

- $3d$ SU(3) + adj. Higgs
- SU(2), $n_f = 8$ staggered
- SU(3), $n_f = 8$ staggered
- SU(2) via chiral RMT model
- $3d$ 3-state Potts model
- $2d$ Gross-Neveu at large N

[A. Hart, M. Laine, O. Philipsen, 2001]
[P. Giudice, A.P., 2004]
[S. Conradi, M. D'Elia, 2007]
[Y. Shinno, H. Yoneyama, 2009]
[S. Kim *et al.*, 2005]
[F. Karbstein, M. Thies, 2006]

Drawbacks

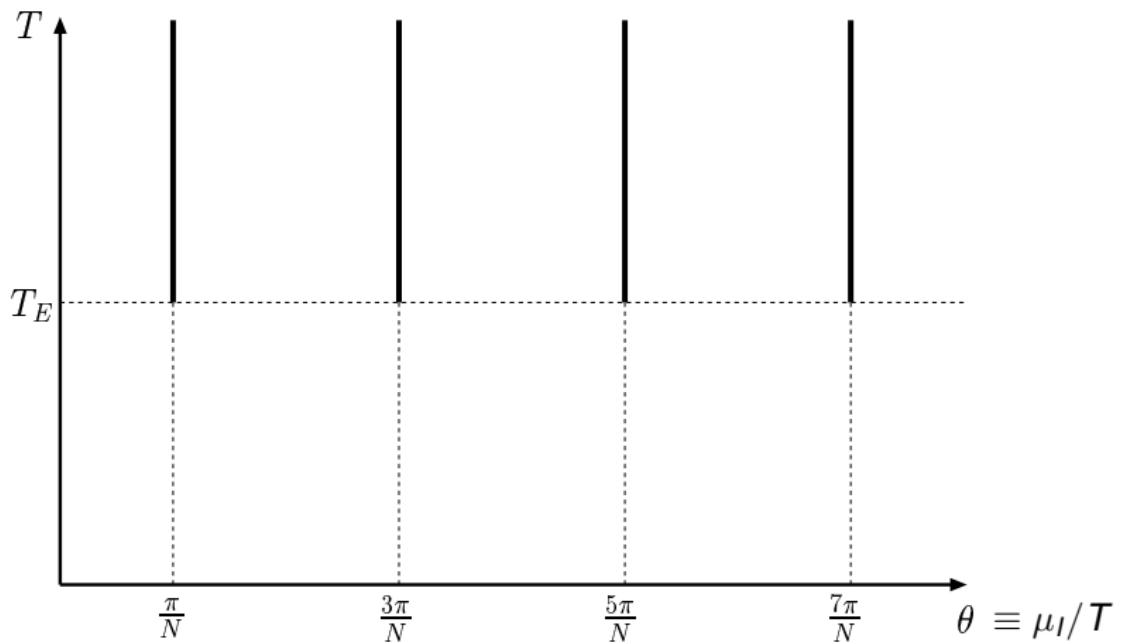
- ➊ a practical one: Monte Carlo simulations yield data points with statistical uncertainties at fixed values of the imaginary chemical potential; the **interpolation** of these points is **not unambiguous**
- ➋ a principle one: the theory at imaginary chemical potential has its own **non-analyticities** and is **periodic** in the variable $\theta = \mu_I/T$ (period $2\pi/N_c$)

[A. Roberge, N. Weiss, 1986]

⇒ the region effectively available for Monte Carlo simulations is limited by the condition $\mu_I/T \lesssim 1$

▶ Roberge-Weiss

- The combination of these two drawbacks implies that the analytic continuation is expected to work for **real chemical potentials satisfying $\mu_R/T \lesssim 1$.**



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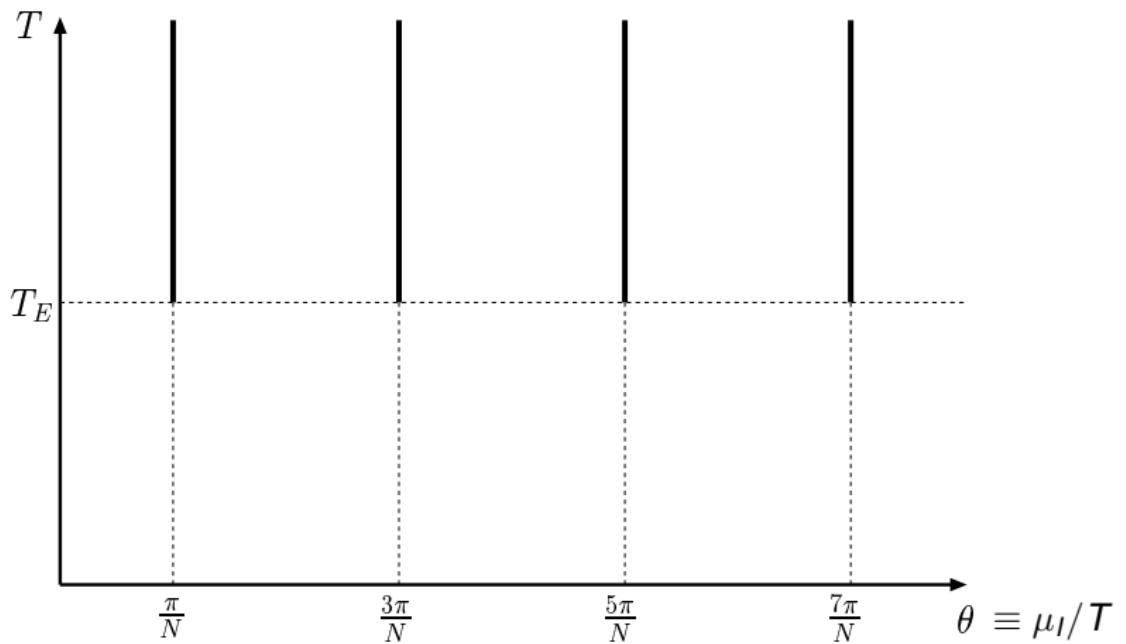
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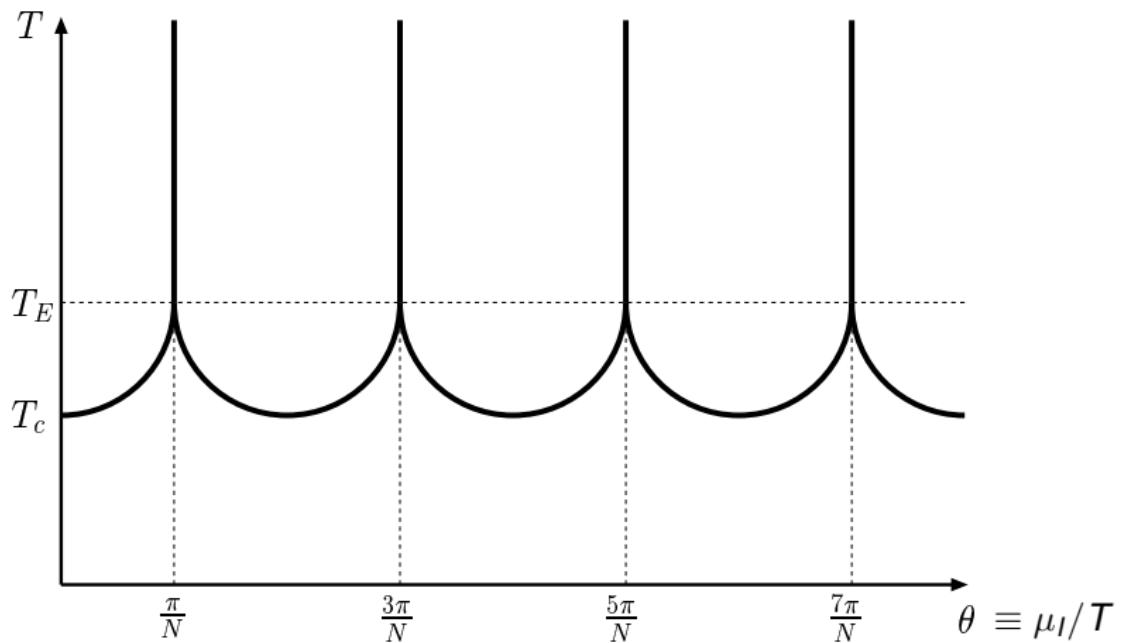
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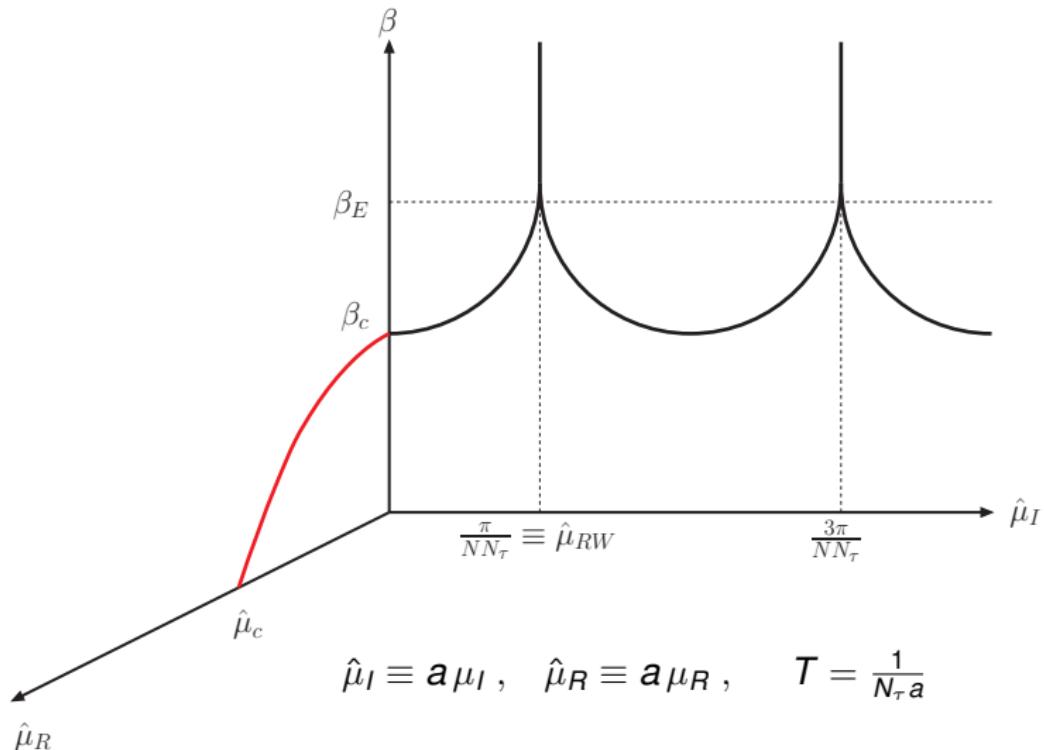
▶ Roberge-Weiss

- The combination of these two drawbacks implies that the analytic continuation is expected to work for **real chemical potentials satisfying** $\mu_R/T \lesssim 1$.





Analytic continuation of the critical line



The most important application of the method is the analytic continuation of the critical line itself.

Strategy

- locate the (pseudo-)critical β 's for several fixed values of the **imaginary** chemical potential, by looking for peaks in the susceptibilities of a given observable
- interpolate the critical β 's obtained at **imaginary chemical potential** with an analytic function of μ^2 , to be then extrapolated to real chemical potential
- if the theory is free of the sign problem, compare the extrapolated curve with the determinations of the critical β 's at **real** chemical potential.

Observables: chiral condensate, Polyakov loop, plaquette.

Investigations in QCD-like theories

- Early approaches in QCD: pseudocritical line $\beta_c(\mu^2)$ well interpolated by $\beta_c(\mu^2) = \beta_c(0) + A\mu^2$, for $\mu = i\mu_I$, at small μ_I
[Ph. de Forcrand, O. Philipsen, 2002-2003]
[M. D'Elia, M.P. Lombardo, 2003-2004]
- Later on, systematic investigations aimed at extending the domain of reliability of the method
 - wider range of μ_I values in numerical simulations
 - larger statistics
 - several trial interpolations[P. Cea, L. Cosmai, M. D'Elia, A.P. et al, 2006→]

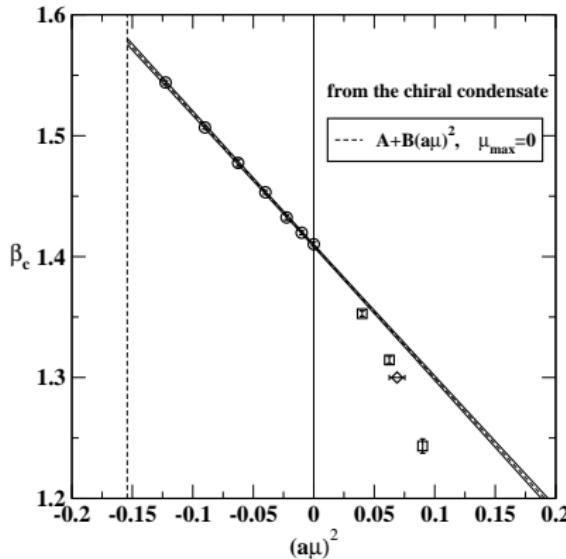
Testfield: QCD-like theories (**two-color QCD** and **finite isospin QCD**) free of the sign problem, where the analytic continuation can be compared with Monte Carlo determinations obtained directly at real chemical potentials.

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$SU(2)$, $n_f = 8$ staggered, $16^3 \times 4$ lattice, $am = 0.07$

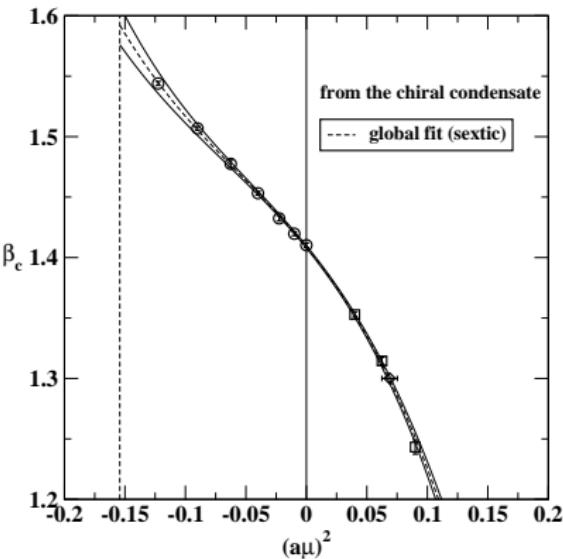
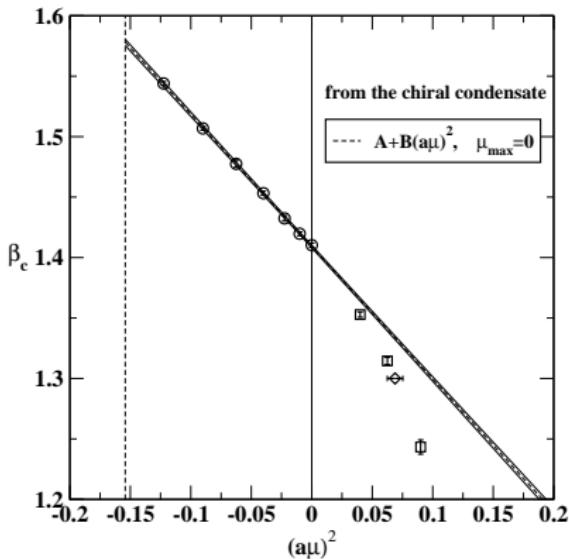
[P. Cea, L. Cosmai, M. D'Elia, A.P., Phys. Rev. D77 (2008) 051501]



No room for fitting functions different from $A + B\hat{\mu}^2$ at $\mu^2 < 0$;
extrapolation fails!

SU(2), $n_f = 8$ staggered, $16^3 \times 4$ lattice, $am = 0.07$

[P. Cea, L. Cosmai, M. D'Elia, A.P., Phys. Rev. D77 (2008) 051501]



A global fit with $A_0 + A_1(a\mu)^2 + A_2(a\mu)^4 + A_3(a\mu)^6$ works nicely;
remark: all $A_i > 0$.

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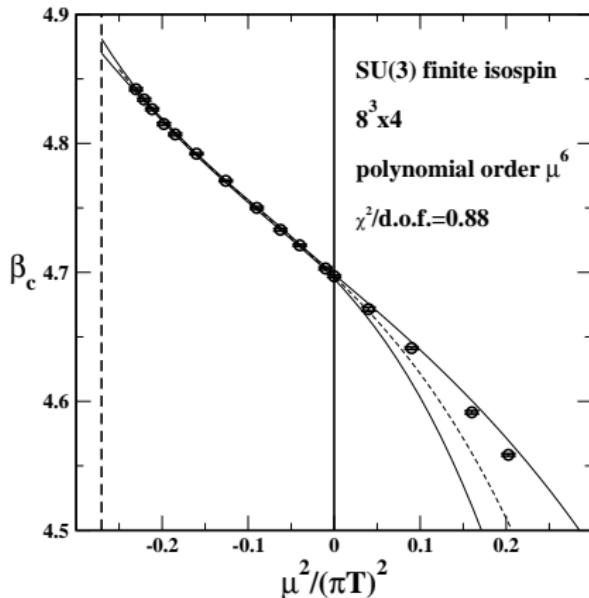
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Finite isospin SU(3), $n_f = 8$ staggered, $8^3 \times 4$ lattice, $am=0.1$

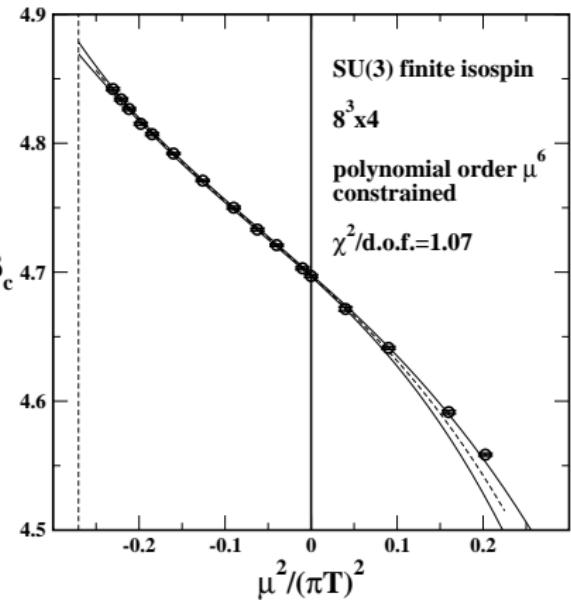
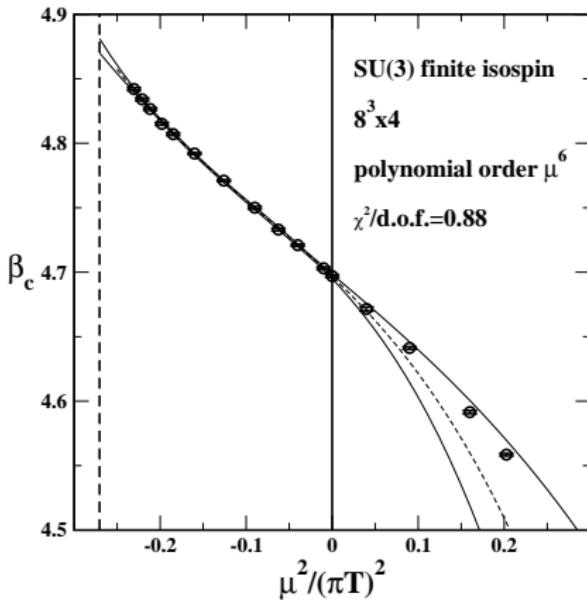
[P. Cea, L. Cosmai, M. D'Elia, C. Manneschi, A.P., Phys. Rev. D80 (2009) 034501]



Deviations from the linear behavior in μ^2 are evident at $\mu^2 < 0$. At least a 3rd order polynomial in μ^2 is needed; extrapolation OK.

Finite isospin SU(3), $n_f = 8$ staggered, $8^3 \times 4$ lattice, $am=0.1$

[P. Cea, L. Cosmai, M. D'Elia, C. Manneschi, A.P., Phys. Rev. D80 (2009) 034501]



Predictivity is increased if the coefficient of μ^2 in the 3rd order polynomial in μ^2 is constrained by a linear fit in the region near $\mu = 0$.

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- SU(3) with $n_f = 2$

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SU(3) with $n_f = 4$

SU(3), $n_f = 4$ staggered, $12^3 \times 4$ lattice, $am = 0.05$

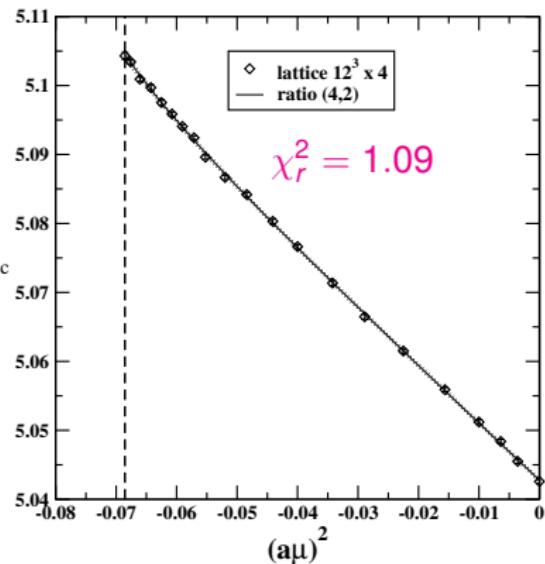
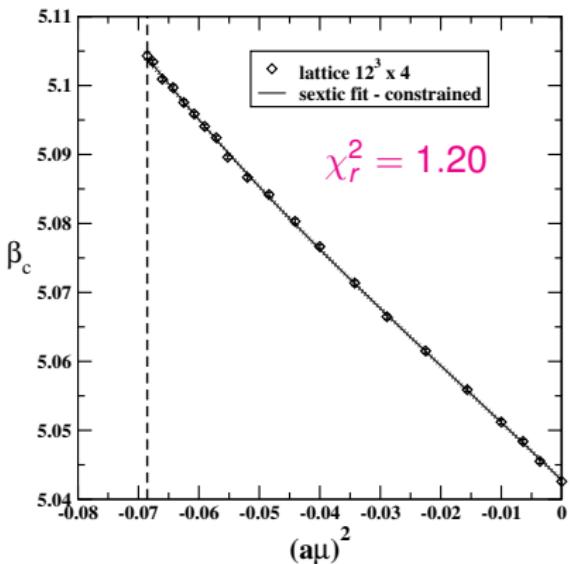
[P. Cea, L. Cosmai, M. D'Elia, A.P., Phys. Rev. D81 (2010) 094502]

Setup:

- Φ -hybrid Monte Carlo algorithm, with $dt=0.01$
[S.A. Gottlieb *et al.*, 1987]
- statistics: 10k trajectories of 1 Molecular Dynamics unit
(up to 100k for a few β 's near $\beta_c(\mu^2)$)
- $\beta_c(\mu^2)$ determined as the position of the peak in the susceptibility
of the (real part of) the Polyakov loop
- simulations on apeNEXT and on the PC cluster of the INFN Bari
Computer Center for Science

$SU(3)$, $n_f = 4$ staggered, $12^3 \times 4$ lattice, $am = 0.05$

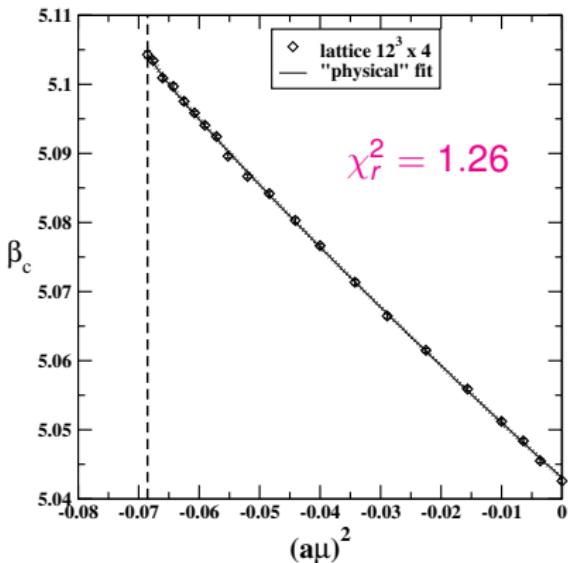
[P. Cea, L. Cosmai, M. D'Elia, A.P., Phys. Rev. D81 (2010) 094502]



- Deviations from the linear behavior in μ^2 are seen
- Also a plain 3rd order polynomial in μ^2 works well
- It is hard to see differences among the successful interpolations

SU(3), $n_f = 4$ staggered, $12^3 \times 4$ lattice, $am = 0.05$

[P. Cea, L. Cosmai, M. D'Elia, A.P., Phys. Rev. D81 (2010) 094502]



"Physical fit":

$$\left[\frac{T_c(\mu)}{T_c(0)} \right]^2 = \frac{1 + C\mu^2/T_c^2(\mu)}{1 + A\mu^2/T_c^2(\mu) + B\mu^4/T_c^4(\mu)}$$

$$a(\beta_c(\mu^2))^2|_{2-\text{loop}} = a(\beta_c(0))^2|_{2-\text{loop}}$$

$$\times \frac{1 + A\mu^2/T_c^2 + B\mu^4/T_c^4}{1 + C\mu^2/T_c^2}$$

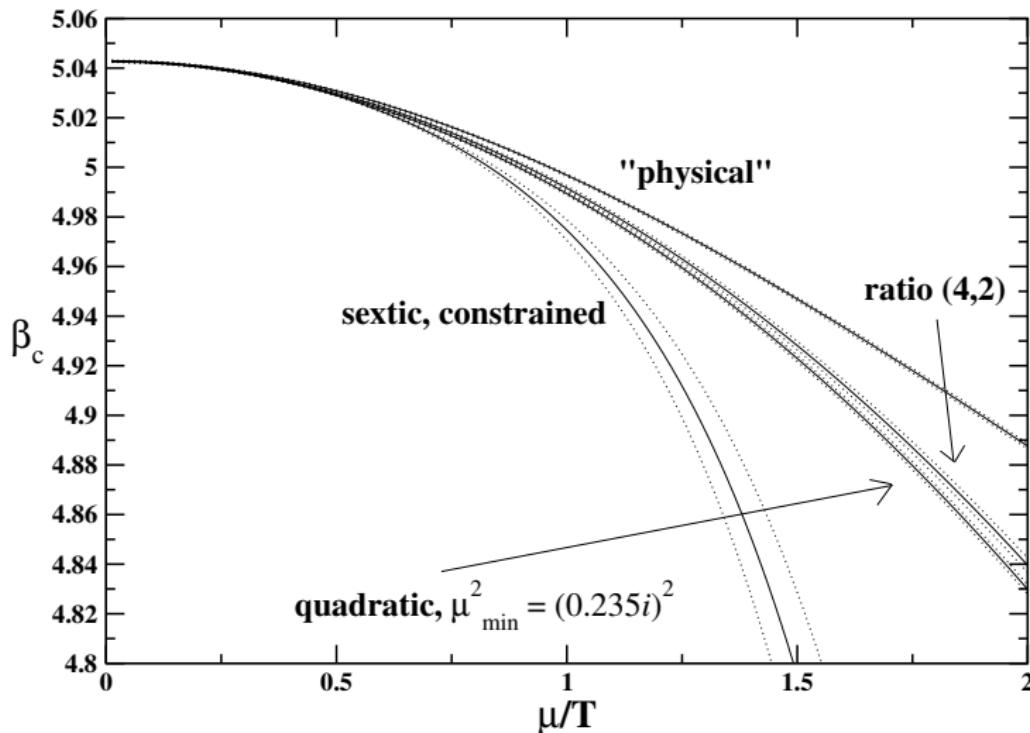
The formal limit $T_c \rightarrow 0$ leads to

$$\mu_c(T=0) = \sqrt{\frac{C}{B}} T_c(0) = 2.5904(93) T_c(0)$$

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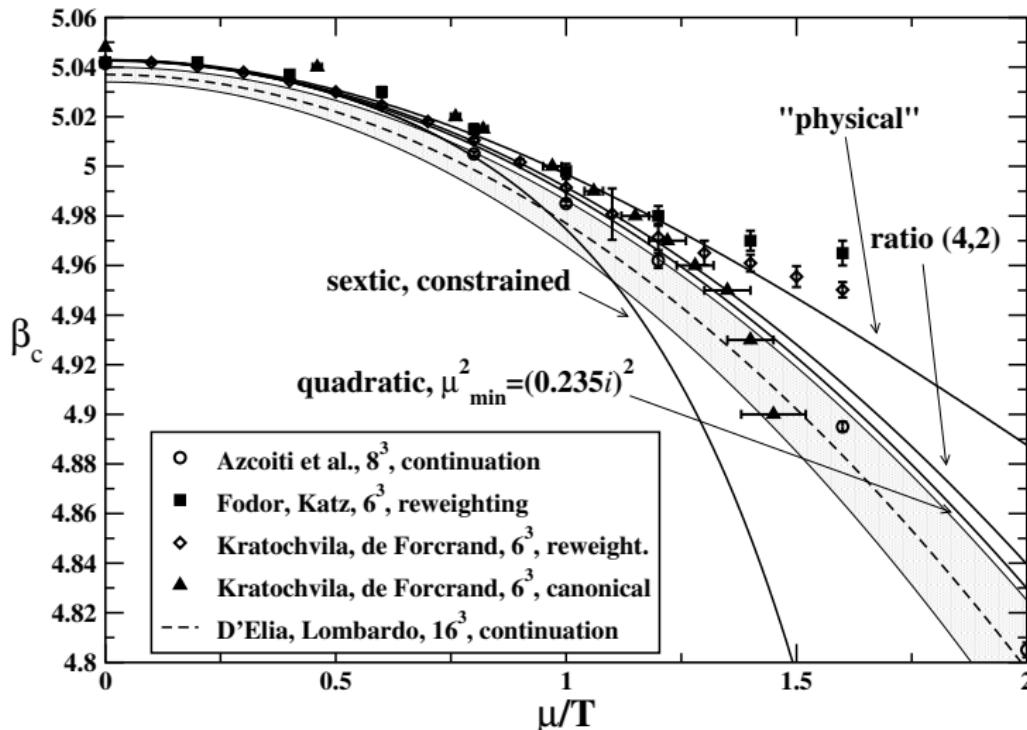
Extrapolations to positive μ^2



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- **Finite isospin SU(3) with $n_f = 2$**
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SU(3) with $n_f = 2$

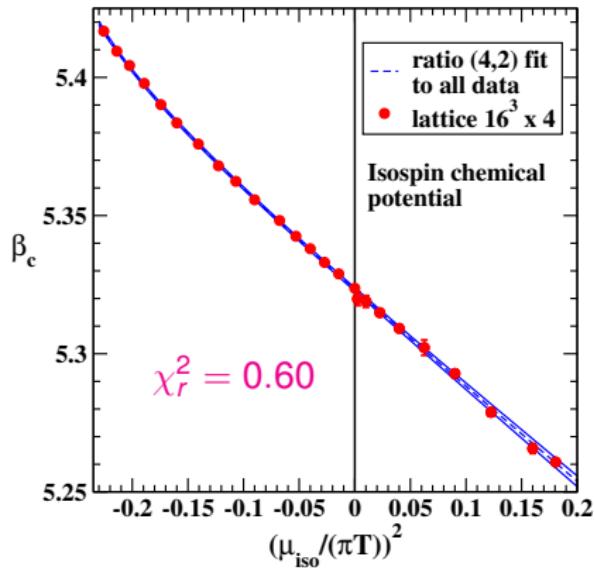
SU(3), $n_f = 2$ staggered, $16^3 \times 4$ lattice, $am = 0.05$ ($m_\pi \sim 400$ MeV)

[P. Cea, L. Cosmai, M. D'Elia, A.P., F. Sanfilippo, Phys. Rev. D 85 (2012) 094512]

Setup:

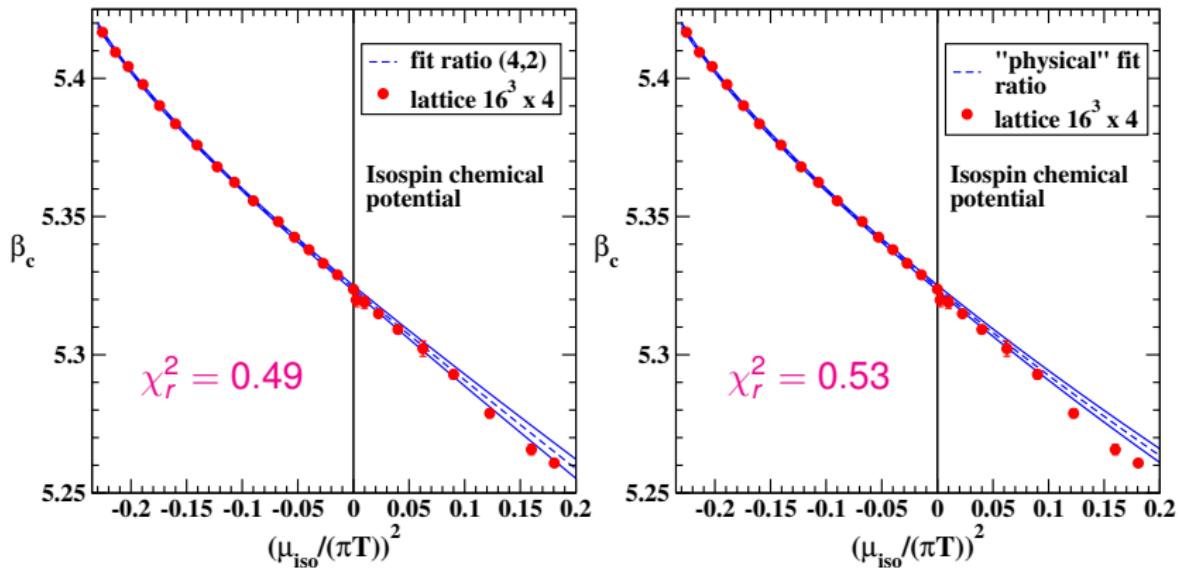
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[P. Cea, L. Cosmai, M. D'Elia, A.P., F. Sanfilippo, Phys. Rev. D 85 (2012) 094512]



- Deviations from the linear behavior in μ_{iso}^2 are seen
- Global fit: no even polynomial up to the fourth order works!

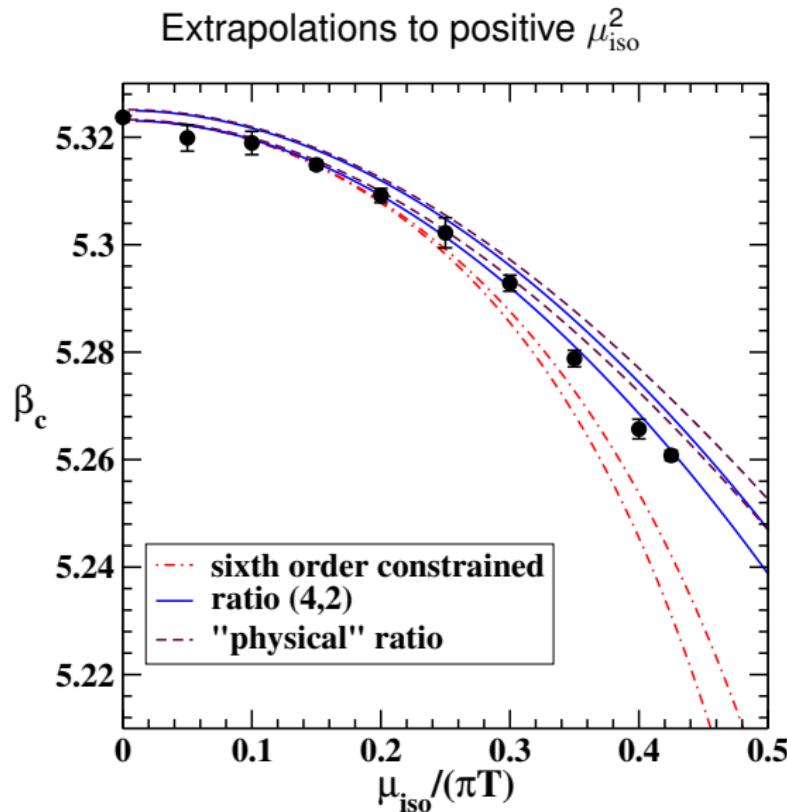
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 [P. Cea, L. Cosmai, M. D'Elia, A.P., F. Sanfilippo, Phys. Rev. D 85 (2012) 094512]



Fit to data at $\mu_{\text{iso}}^2 \leq 0$:
 ratio (4,2) of polynomials (left) and “physical fit” (right)

Finite isospin SU(3), $n_f = 2$ staggered, $16^3 \times 4$ lattice, $am = 0.05$

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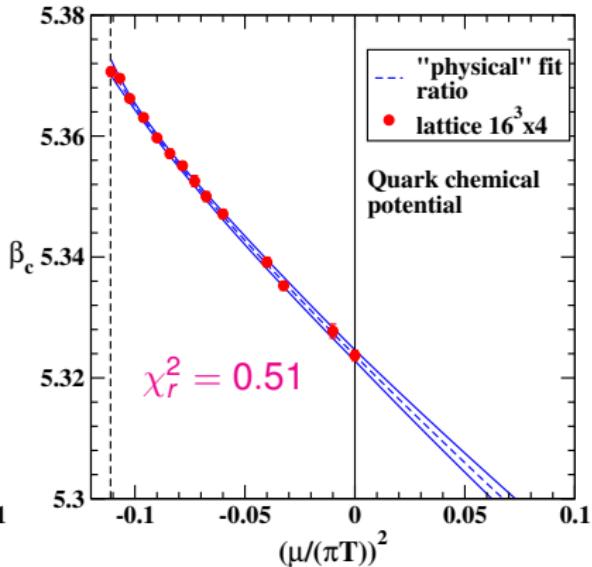
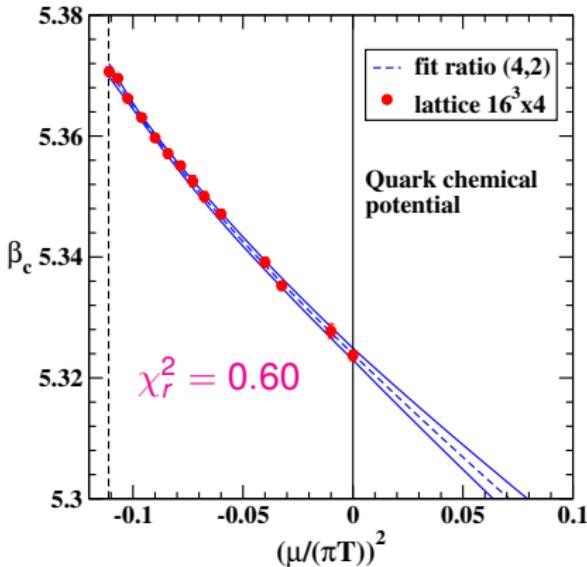
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[P. Cea, L. Cosmai, M. D'Elia, A.P., F. Sanfilippo, Phys. Rev. D 85 (2012) 094512]



The formal limit $T_c \rightarrow 0$ of the “physical fit” leads to

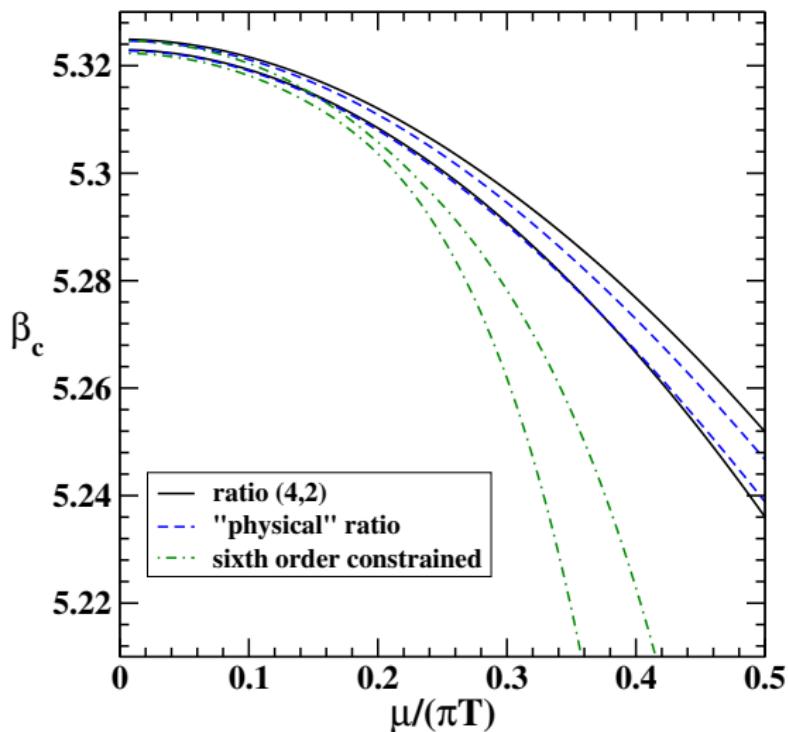
$$\mu_c(T=0) = \sqrt{\frac{C}{B}} T_c(0) = 3.284(65) T_c(0)$$

[K. Nagata, A. Nakamura, 2011]: $2.73(58) T_c(0)$ for $n_f = 2$ Wilson.

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[P. Cea, L. Cosmai, M. D'Elia, A.P., F. Sanfilippo, Phys. Rev. D 85 (2012) 094512]

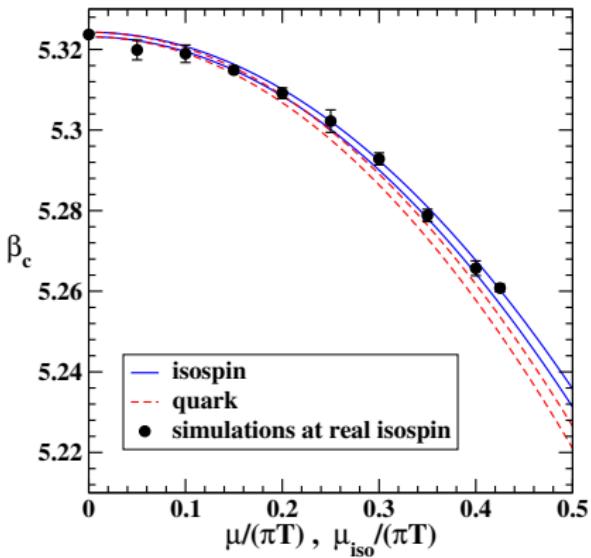
Extrapolations to positive μ^2



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Curvatures:



$$\beta_c(\mu_{q/\text{iso}}) = \beta_c(0) + a_q \left(\frac{\mu_q}{\pi T} \right)^2 + a_{\text{iso}} \left(\frac{\mu_{\text{iso}}}{\pi T} \right)^2$$

$$a_q = -0.3997(87), \quad a_{\text{iso}} = -0.3606(67)$$

about 4σ difference!

$$\frac{T_c(\mu_q, \mu_{\text{iso}})}{T_c(0)} = 1 + R_q \left(\frac{\mu_q}{\pi T} \right)^2 + R_{\text{iso}} \left(\frac{\mu_{\text{iso}}}{\pi T} \right)^2$$

$$R_{q/\text{iso}} = -\frac{1}{a} \frac{\partial a}{\partial \beta} \Big|_{\beta_c(0)} a_{q/\text{iso}}$$

$$R_q = -0.515(11), \quad R_{\text{iso}} = -0.465(9)$$

Curvatures (cont'd): $R_q = -0.515(11)$, $R_{\text{iso}} = -0.465(9)$

- $R_{\text{iso}} = -0.426(19)$ [J.B. Kogut, D.K. Sinclair (2004)]
(inexact R-algorithm and smaller spatial volume)
- $R_q = -0.500(34)$ [P. De Forcrand, O. Philipsen (2002)]
($am = 0.025$; good agreement \rightarrow mild mass dependence)
- $R_q = -0.38(12)$ [K. Nagata, A. Nakamura, 2011]
(Wilson fermions)
- $R_q = -0.792(10)$ [M. D'Elia, M.P. Lombardo (2003)]
($n_f = 4$; significant flavor dependence)

$$R_{q-\text{iso}} = \frac{R_q - R_{\text{iso}}}{R_q} = \frac{a_q - a_{\text{iso}}}{a_q} = 0.098(26)$$

Large N_c limit

[D. Toublan (2005)] [M. Hanada *et al.* (2011, 2012)] [A. Armoni, A. Patella (2012)]

$$R_{q/\text{iso}} = \mathcal{O}\left(\frac{1}{N_c}\right) , \quad \frac{R_q - R_{\text{iso}}}{R_q} = \frac{\mathcal{O}\left(\frac{1}{N_c^2}\right)}{\mathcal{O}\left(\frac{1}{N_c}\right)} = \mathcal{O}\left(\frac{1}{N_c}\right)$$

Curvatures (cont'd): $R_q = -0.515(11)$, $R_{\text{iso}} = -0.465(9)$

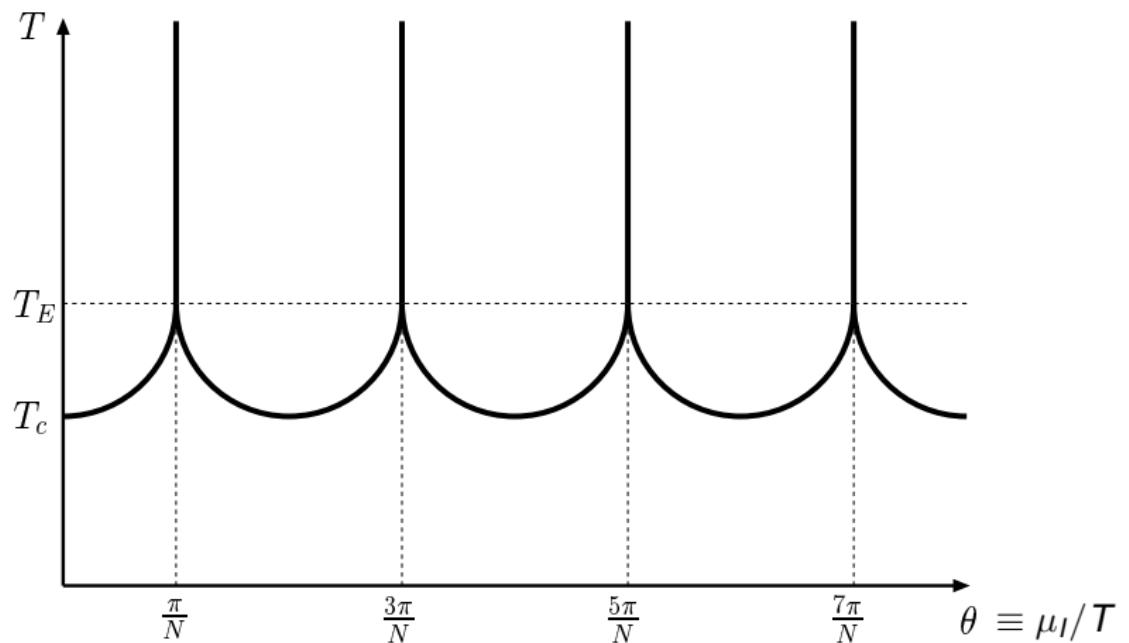
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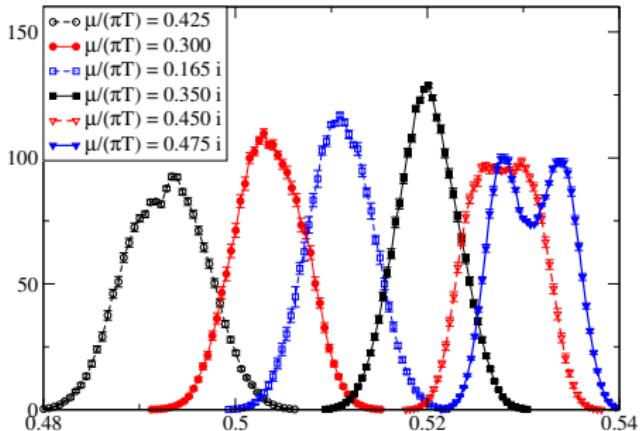
Order of the phase transition

- The order of the RW endpoint may strongly influence the nature of the pseudocritical line at imaginary μ .
- For **non-zero quark density** the RW endpoint is first order for low masses, $am < 0.043(5)$.

[C. Bonati, M. D'Elia, G. Cossu, F. Sanfilippo (2011)]

Our mass is larger, therefore we expect (and, actually, verified) that the pseudocritical line does not become first order when we approach the RW endpoint along the pseudocritical line at imaginary μ .

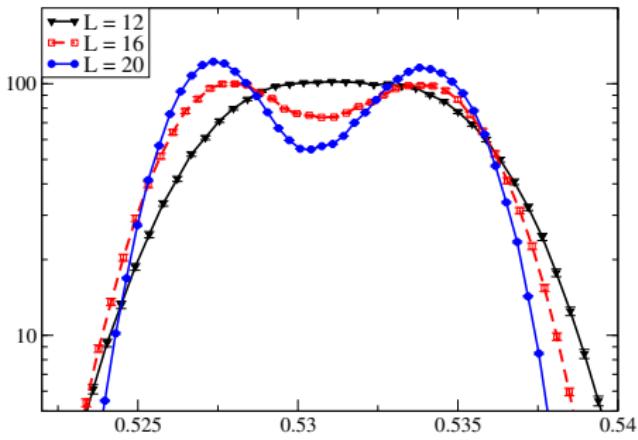
- For **non-zero isospin density** the region of $\text{Im}(\mu_{\text{iso}})$ is larger and we could expect that the pseudocritical line at imaginary μ_{iso} becomes first-order before reaching the RW endpoint.



Normalized plaquette distribution at the pseudocritical couplings for μ_{iso} approaching $\mu_{\text{iso}, \text{RW}}$
(lattice $16^3 \times 4$)

Normalized plaquette distribution at the pseudocritical coupling at $\mu_{\text{iso}} = 0.475i$ for various spatial lattices

Peaks of the plaquette susceptibility scale with the spatial volume



Conclusions

- The study of QCD at imaginary chemical potentials can bring a lot of information relevant for the region of *real* chemical potentials, not only through analytic continuation.
- Wrt the critical line
 - Deviations from the quadratic behavior in μ of the pseudocritical couplings at negative μ^2 are clearly visible in QCD with $n_f = 2$ and 4.
 - There are, however, several kinds of functions able to interpolate them, leading to extrapolations which diverge from each other at large real μ .
 - The situation is quite similar in $n_f = 2$ QCD with non-zero isospin density. The curvature of the critical line at $\mu = 0$ is less pronounced here, than in $n_f = 2$ QCD with finite baryon density.

Outlook

- Get closer to the continuum ...
 - MILC code + chemical potential
 - HISQ/tree action on $32^3 \times 8, 40^3 \times 8, 48^3 \times 8$
- ... and to physics:
 - 2+1 flavors, $m_{u,d}/m_s=0.05$ on the LCP

QCD with imaginary chemical potential

- $SU(N_c)$ gauge theory with imaginary μ

$$\mu \rightarrow i\nu, \quad Z(\theta) = \text{Tr} \left[e^{-\beta H + i\theta \hat{N}} \right] \quad \theta = \beta\nu, \quad \beta = \frac{1}{T}$$

- Free quarks ($N = 0, 1, 2, \dots$) $\longrightarrow Z(\theta)$ periodic with 2π
- Color singlets (N multiple of N_c) $\rightarrow Z(\theta)$ periodic with $2\pi/N_c$

- [A. Roberge, N. Weiss, 1986] have shown that
 - $Z(\theta)$ is **always** periodic with $2\pi/N_c$

Roberge-Weiss' proof I

$$Z(\theta) = \int D\psi D\bar{\psi} DA_\mu \exp \left\{ - \int d^4x \left[\bar{\psi}(\gamma D - m)\psi - \frac{1}{4}F^2 - i\frac{\theta}{\beta}\psi^\dagger\psi \right] \right\}$$

time interval running from $\tau = 0$ to $\tau = \beta$
periodic b.c. for A , anti-periodic b.c. for ψ

- change of variables I

$$\psi(x, \tau) \longrightarrow \exp(i\tau\theta/\beta) \psi(x, \tau)$$

$$Z(\theta) = \int D\psi D\bar{\psi} DA_\mu \exp \left\{ - \int d^4x \left[\bar{\psi}(\gamma D - m)\psi - \frac{1}{4}F^2 \right] \right\}$$

with $\psi(x, \beta) = -\exp(i\theta)\psi(x, 0)$

Roberge-Weiss' proof II

- change of variables II

$$\psi \rightarrow U\psi, \quad A \rightarrow UAU^{-1} - \frac{i}{g}(\partial U)U^{-1}$$

$U(x, \tau) \in \text{SU}(N_c), \quad U(x, \beta) = \exp(2\pi ik/N_c) U(x, 0), \quad k \text{ integer}$
i.e. U periodic up to an element of $\text{Z}(N_c)$

$$Z(\theta) = \int D\psi D\bar{\psi} DA_\mu \exp \left\{ - \int d^4x \left[\bar{\psi}(\gamma D - m)\psi - \frac{1}{4}F^2 \right] \right\}$$

with $\psi(x, \beta) = -\exp(2\pi ik/N_c) \exp(i\theta)\psi(x, 0)$

i.e. $Z(\theta) = Z(\theta + 2\pi k/N_c)$

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- $Z(\theta)$ is **always** periodic with $2\pi/N_c$
- $F(\theta) = -\ln Z(\theta)/\beta$

$T < T_E$: regular function of θ (tool: hopping parameter expansion)

$T > T_E$: discontinuous function in $\theta = 2\pi(k + 1/2)/N_c$ (tool:
perturbative evaluation of the effective potential for the Wilson line)

◀ Back