Non-zero baryon density on the lattice with the method of analytic continuation

Based on
P. Cea, L. Cosmai, M. D'Elia, A.P., PoS(LATTICE 2007)214 [arXiv:0710.2068]
P. Cea, L. Cosmai, M. D'Elia, A.P., Phys. Rev. D77 (2008) 051501 [arXiv:0712.3755]
P. Cea, L. Cosmai, M. D'Elia, A.P., in progress

Alessandro Papa

Università della Calabria & INFN - Cosenza

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Outline

1. Introduction
   - QCD phase diagram
   - QCD with non-zero baryon density
   - The “sign” problem
   - Ways out
2. The method of analytic continuation
   - QCD with imaginary chemical potential
   - Description of the method
   - Numerical test
3. Conclusions

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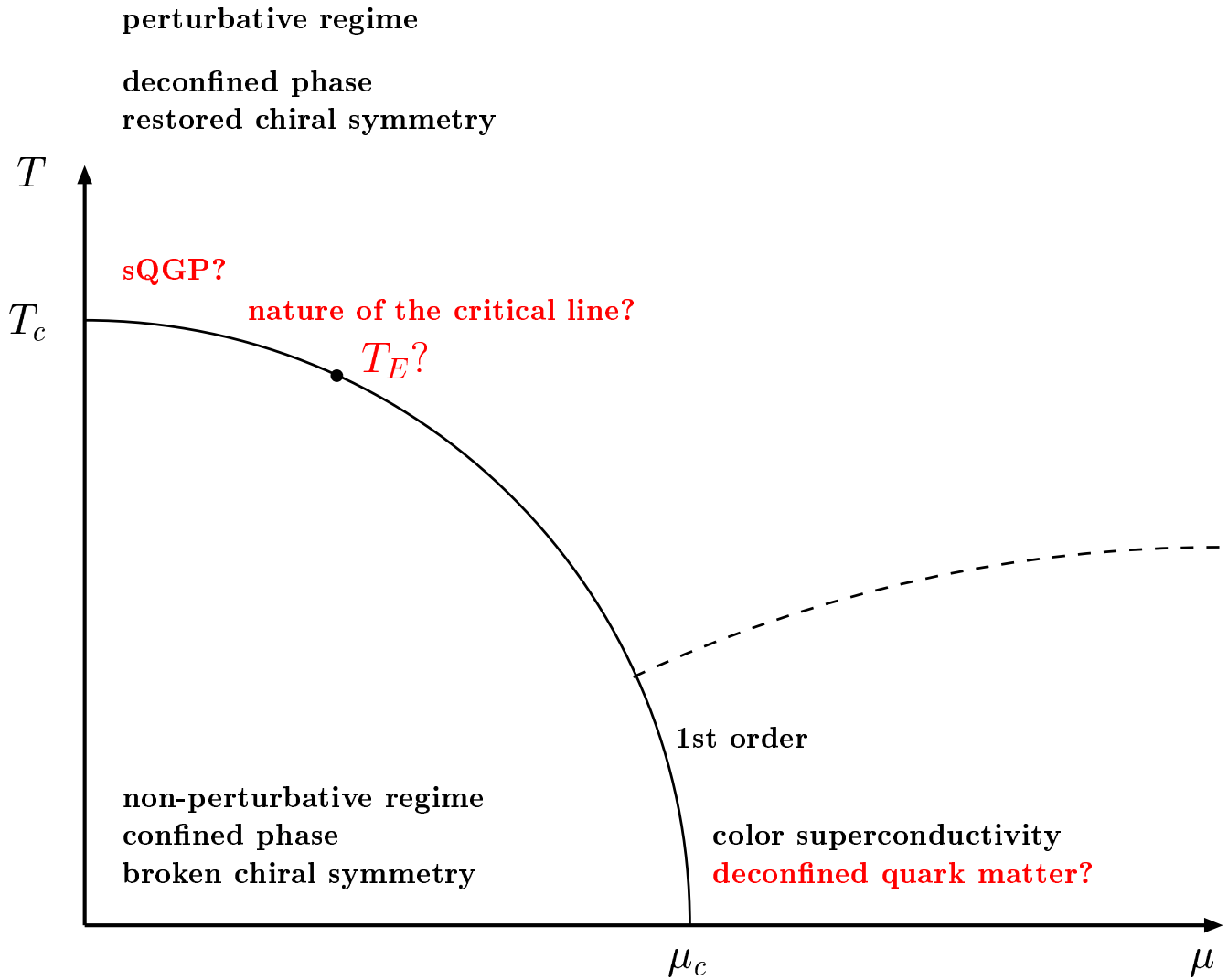
QCD phase diagram



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QCD with non-zero baryon density

- Continuum: $\mathcal{L} = \mathcal{L}_{QCD} + \mu J_0, \quad J_\mu = \overline{\psi}\gamma_\mu\psi, \quad \int d^3x J_0 = N_q - N_{\overline{q}}$

$$Z(\mu) = \mathrm{Tr}\left(e^{-(H_{\mathrm{QCD}} - \mu N)/T}\right)$$

- Lattice: μ as the temporal component of a U(1) imaginary background field

$$U_4(n) \to e^{a\mu} U_4(n)\,, \qquad U_4^\dagger(n) \to e^{-a\mu} U_4^\dagger(n)$$

[F. Karsch, P. Hasenfratz, 1983]

$$\langle O \rangle = \frac{\int DU\, D\overline{\psi} D\psi\; O[U,\psi,\overline{\psi}]\; e^{-S_F[U,\psi,\overline{\psi}] - S_G[U]}}{\int DU\, D\overline{\psi} D\psi\; e^{-S_F[U,\psi,\overline{\psi}] - S_G[U]}}$$

$$S_F = \sum_{n,m} \overline{\psi}(n) M_{nm}[U,\mu]\psi(m) \longrightarrow \int D\overline{\psi} D\psi\; e^{-S_F[U,\psi,\overline{\psi}]} = \det M[U,\mu]$$

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The "sign" problem

$$\langle O \rangle = \frac{\int DU \, \langle O \rangle_{S_F} e^{-S_{eff}[U]}}{\int DU \, e^{-S_{eff}[U]}} \, , \quad \langle O \rangle_{S_F} = \frac{\int D\overline{\psi} D\psi \, O[U,\psi,\overline{\psi}] \, e^{-S_F[U,\psi,\overline{\psi}]}}{\int D\overline{\psi} D\psi \, e^{-S_F[U,\psi,\overline{\psi}]}}$$

$$S_{eff}[U] = S_G[U] - \ln \det M[U]$$

- In order to perform Monte Carlo simulations "det M" must be real
  - OK for $\mu = 0$ in SU(3), since $M^\dagger = PMP^{-1}$, with $P = \gamma_5$ for Wilson, $P = I$ for staggered fermions
  - NO for $\mu \neq 0$ in SU(3), since $M^\dagger(\mu) = M(-\mu)$
  - OK for finite isospin density; e.g., for $N_f = 2$, $(M(\mu)M(-\mu))^\dagger = M(\mu)M(-\mu)$
  - OK for $\mu \neq 0$ in SU(2), owing to $M^* = \tau_2 M \tau_2$
  - OK for $\mu = i\mu_I$ in SU(N_c), being $M^\dagger(i\mu) = M(i\mu)$

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Ways' out I

- to perform simulations at μ=0 and to take advantage of physical fluctuations in the thermal ensemble for extracting information at (small) non-zero μ, after reweighting

$$\langle O \rangle_{\mu \neq 0} = \left\langle O \frac{\det(M(\mu))}{\det(M(0))} \right\rangle_{\mu=0} \Big/ \left\langle \frac{\det(M(\mu))}{\det(M(0))} \right\rangle_{\mu=0}$$

[I.M. Barbour et al., 1998]

Multiparameter reweighting: reweighting also in β

[Z. Fodor, S.D. Katz, 2002 →]

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

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Ways' out II

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$$U_4(n) \to e^{ia\mu_I} U_4(n)\,, \qquad U_4^\dagger(n) \to e^{-ia\mu_I} U_4^\dagger(n) = \left(e^{ia\mu_I} U_4(n)\right)^\dagger$$

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Ways' out III

1. to build the canonical partition function $Z(n)$ by Fourier transform of the grand canonical function at imaginary chemical potential:

$$
\begin{aligned}
Z(n) &= \mathrm{Tr}\left(e^{-H_{\mathrm{QCD}}/T}\delta(N-n)\right) = \mathrm{Tr}\left(e^{-H_{\mathrm{QCD}}/T}\int_0^{2\pi}\frac{d\theta}{2\pi}\,e^{i\theta(N-n)}\right) \\
&= \frac{1}{2\pi}\int_0^{2\pi} d\theta\; e^{-i\theta n} e^{-(H_{\mathrm{QCD}}-i\theta TN)/T} \\
&= \frac{1}{2\pi}\int_0^{2\pi} d\theta\; e^{-i\theta n} Z(\mu = i\theta T)
\end{aligned}
$$

[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]

Ways' out IV

2. Method of analytic continuation: to perform numerical simulations at *imaginary* chemical potential and to analytically continue the results to real μ

[M.P. Lombardo, 2000] [A. Hart, M. Laine, O. Philipsen, 2001]
[Ph. de Forcrand, O. Philipsen, 2002-2003-2004]
[M. D'Elia, M.P. Lombardo, 2002-2003-2004]
[P. Giudice, A.P., 2004] [V. Azcoiti et al., 2004-2005]
[H.-S. Chen, X.-Q. Luo, 2005] [S. Kim et al., 2005]
[M.P. Lombardo, 2005] [M. D'Elia, F. Di Renzo, M.P. Lombardo, 2005]
[P. Cea, L. Cosmai, M. D'Elia, A.P., 2006 $\rightarrow$]
[F. Karbstein, M. Thies, 2006]
[L.-K. Wu, X.-Q. Luo, H.-S. Chen, 2007]

Ways' out V

– coupling β and chemical potential μ can be varied independently

– no limitation from increasing lattice sizes

– extent of the attainable domain with real μ is limited

1. by the periodicity and non-analyticities for imaginary μ
2. by the accuracy of the interpolation of data for imaginary μ

All the mentioned methods have roughly the same range of applicability ($\mu/T \lesssim 1$), although with different systematics, and agree inside this range

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QCD with imaginary chemical potential

- SU(N_c) gauge theory with imaginary μ

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

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

- [A. Roberge, N. Weiss, 1986] have shown that
  - $Z(\theta)$ is always periodic with $2\pi/N_c$
  - $F(\theta) = -\ln Z(\theta)/\beta$
    $T < T_E$: 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)

- This scenario has been confirmed in numerical simulations in SU(3) [Ph. de Forcrand, O. Philipsen, 2002; M. D'Elia, M.P. Lombardo, 2003] and in SU(2) [P. Giudice, A.P., 2004]

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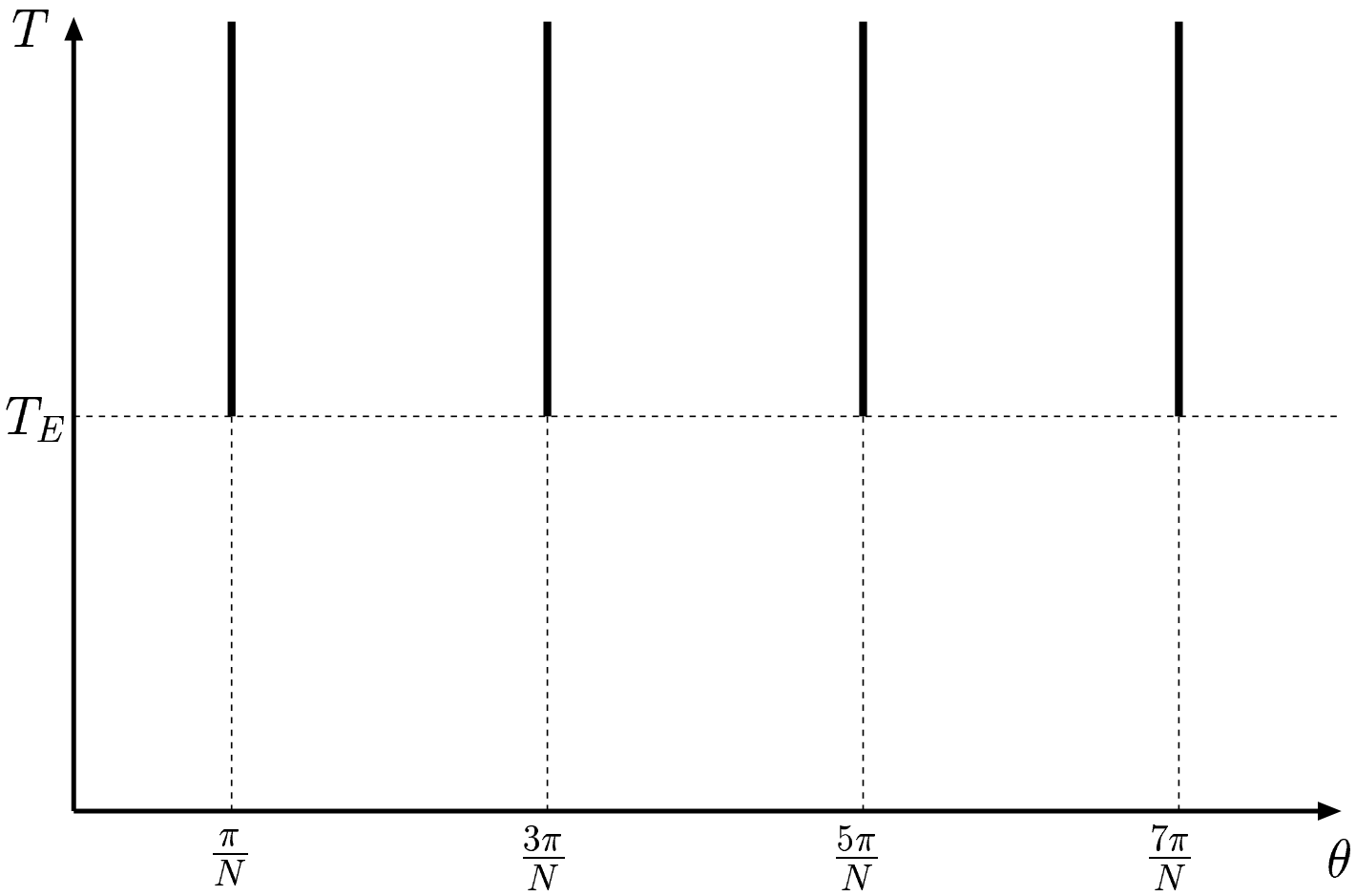
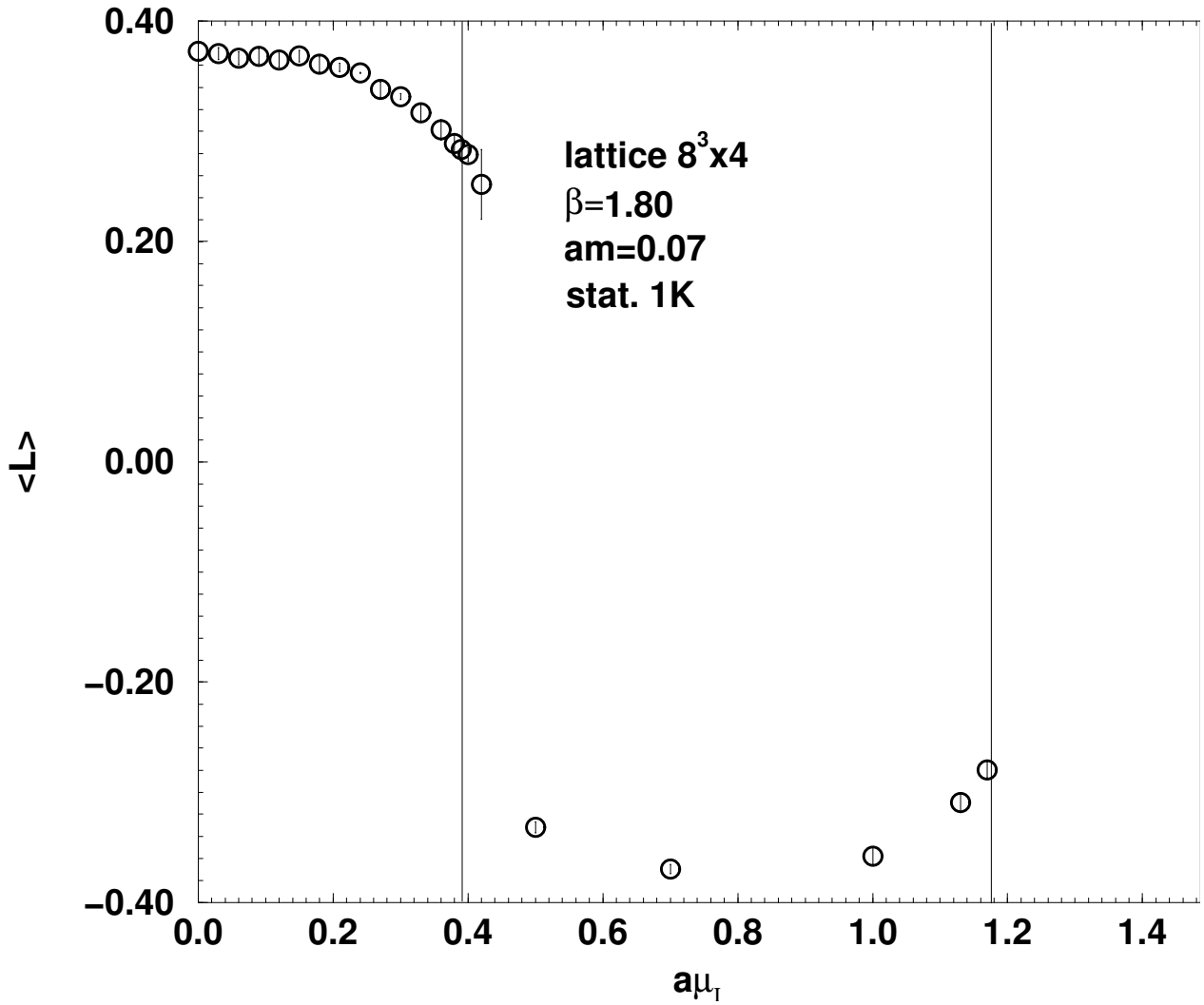
Phase diagram on the (T,θ)-plane

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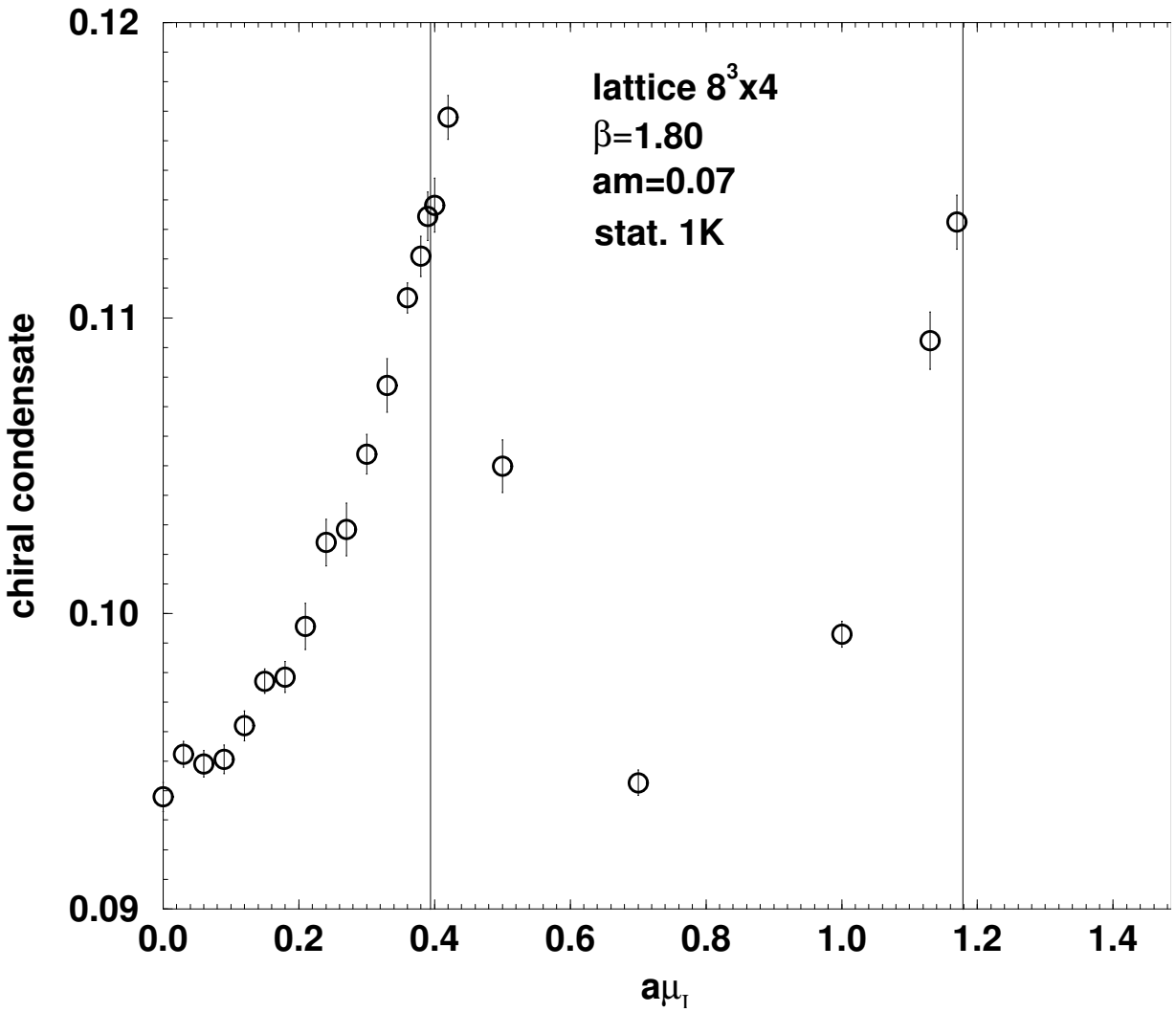
stat. 1K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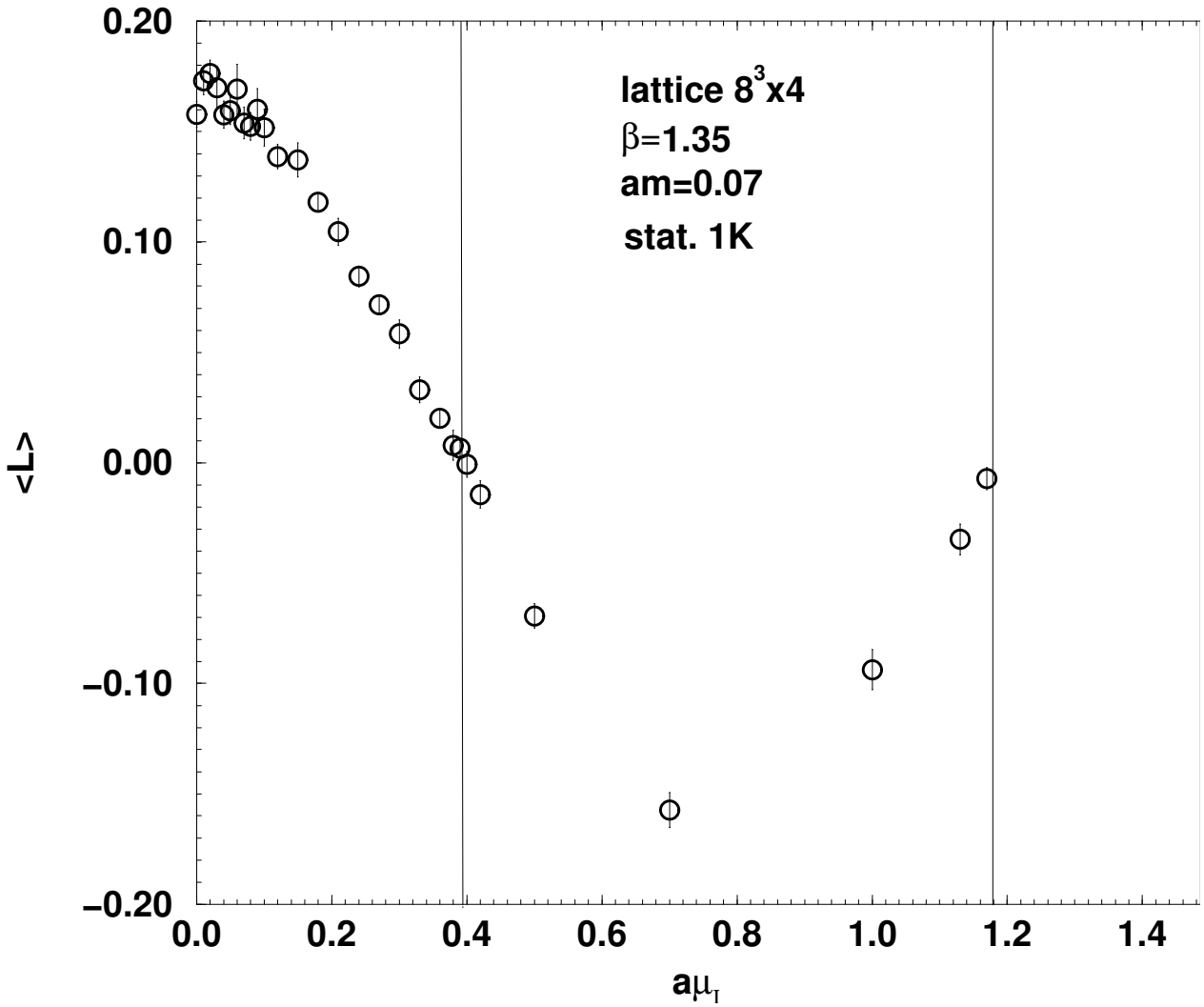
$a\mu_I$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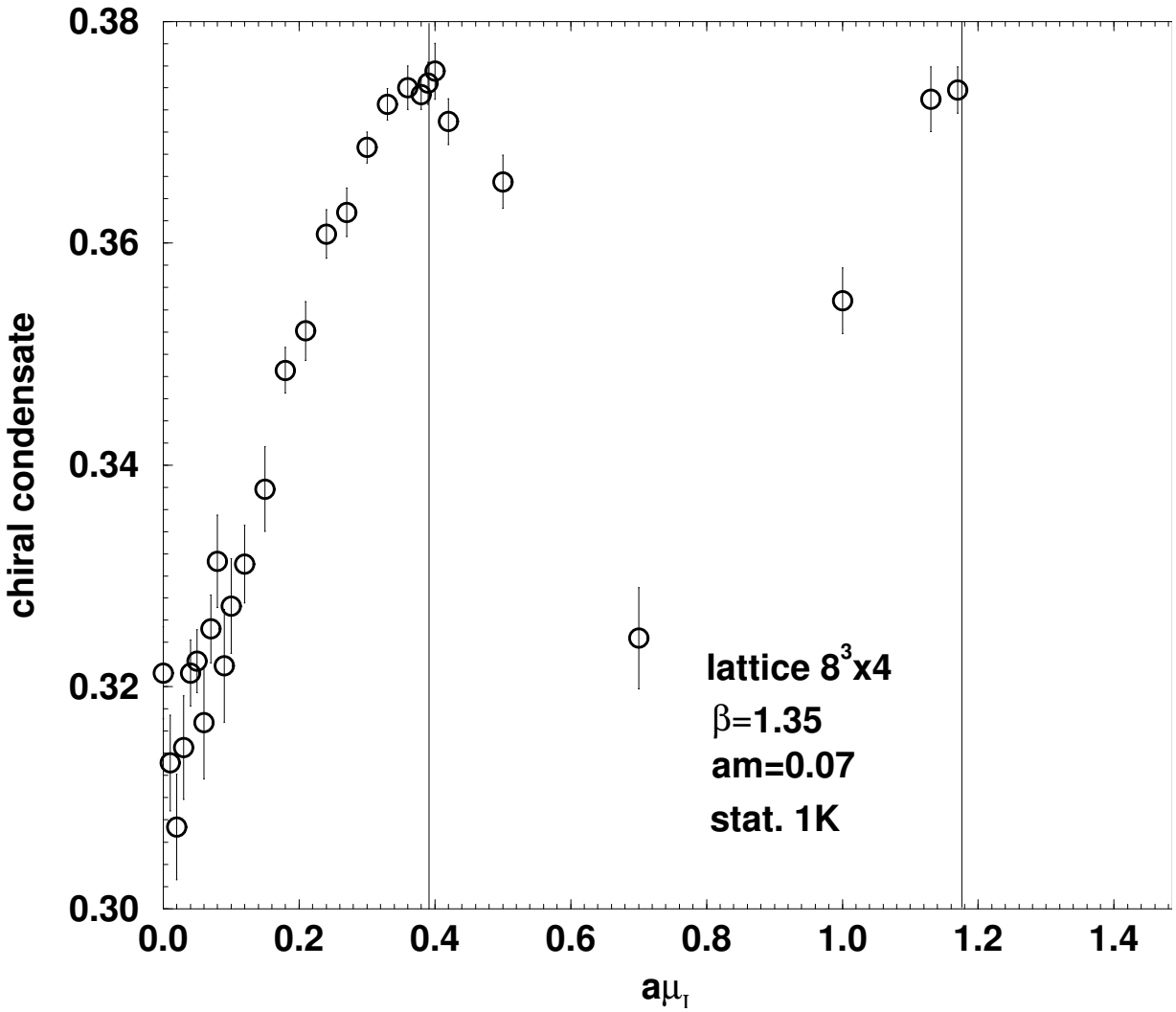
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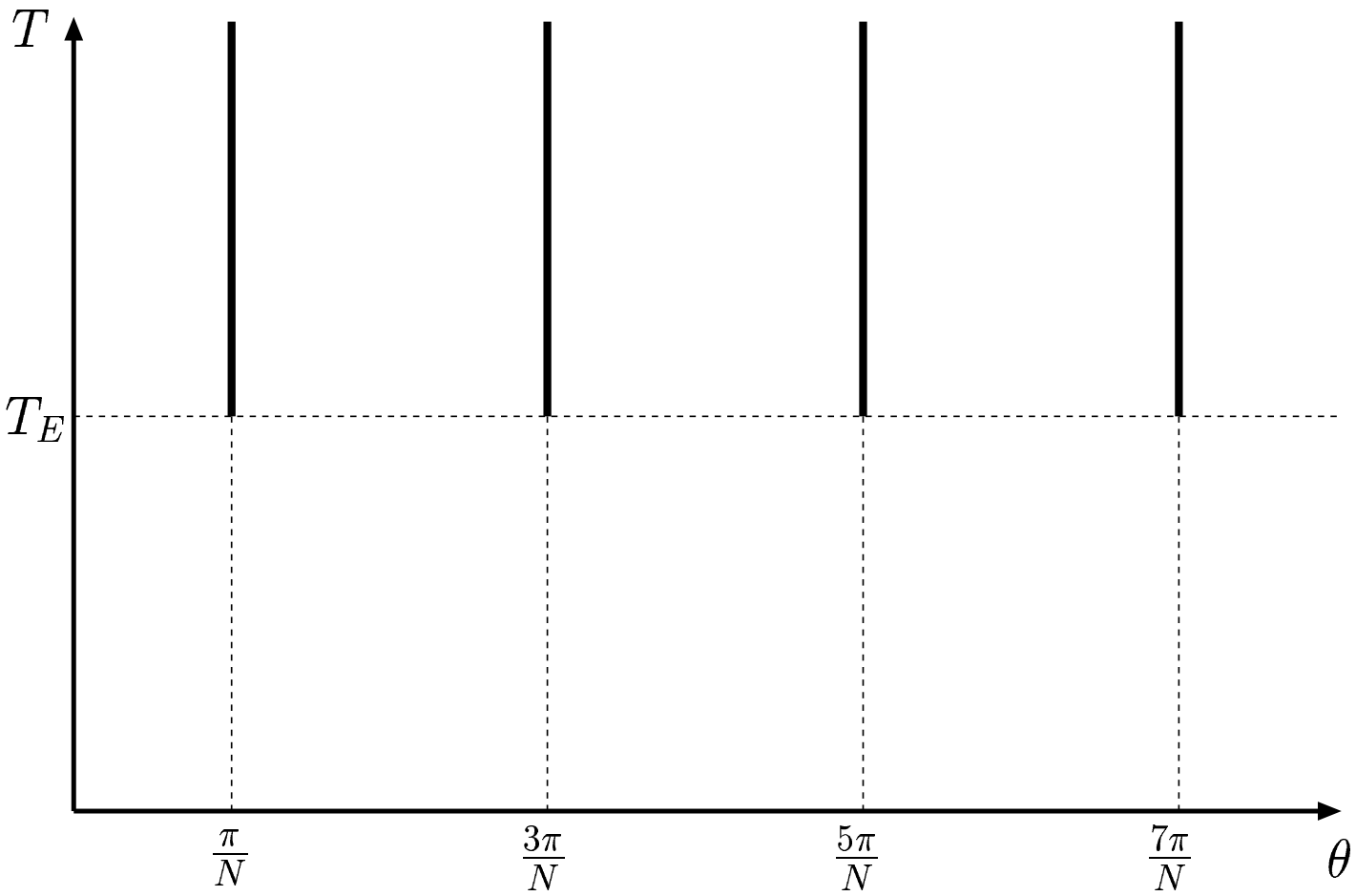

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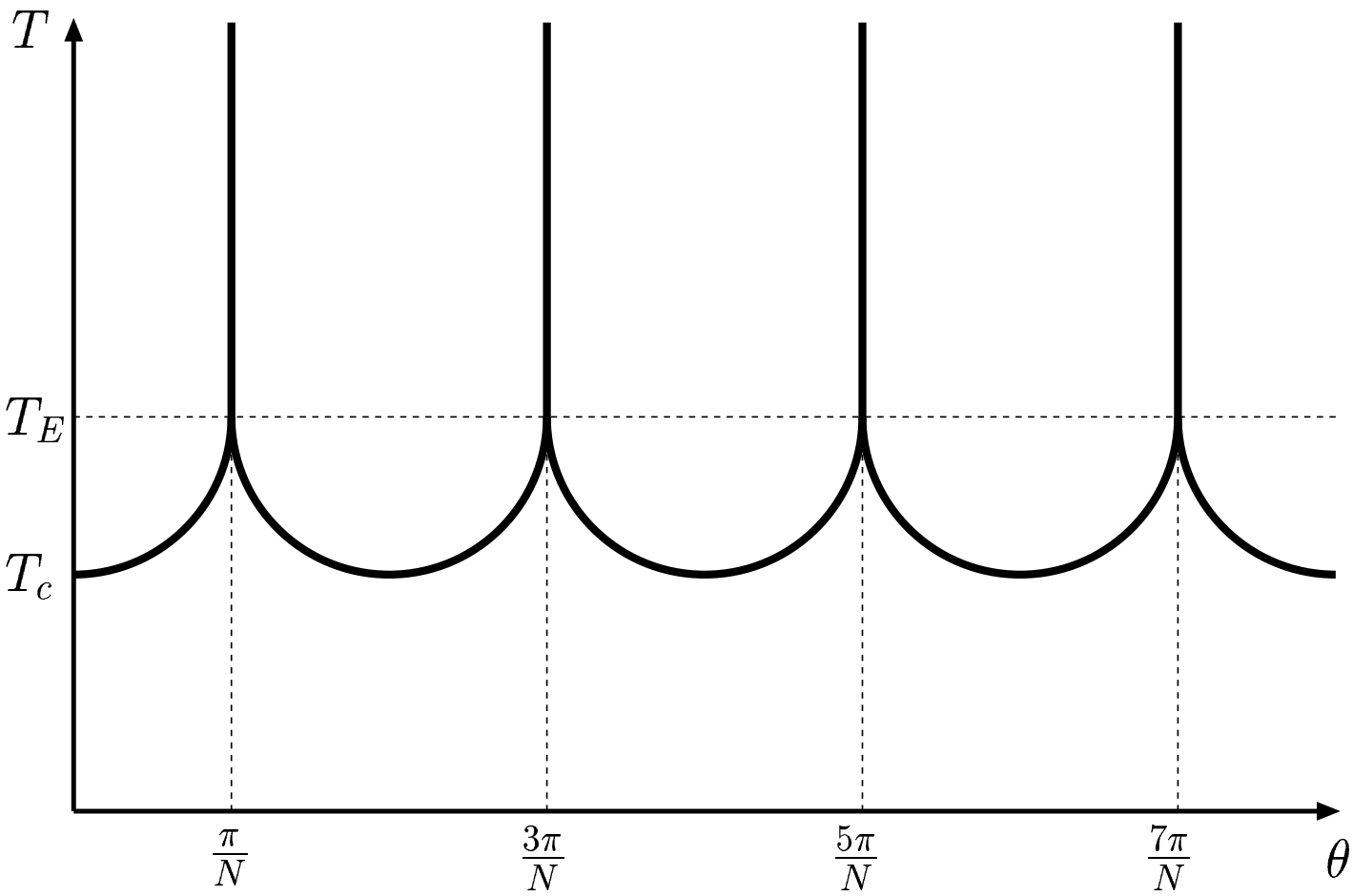

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Description of the method

- Strategy of the method of analytic continuation
  - determine $\langle \mathcal{O} \rangle$ for a set of value of imaginary chemical potential, $\mu = i\mu_I$
  - interpolate $\langle \mathcal{O} \rangle(\mu)$ with a polynomial:

$$\langle \mathcal{O} \rangle(\mu) = a_0 + a_2\mu^2 + a_4\mu^4 + a_6\mu^6 + O(\mu^8)$$

  - analytically continue to $\mu = \mu_R$ by the replacement $\mu^2 \to -\mu^2$

$$\langle \mathcal{O} \rangle(\mu) = a_0 - a_2\mu^2 + a_4\mu^4 - a_6\mu^6 + O(\mu^8)$$

- Applied in
  - SU(3), $n_f = 2$ [Ph. de Forcrand, O. Philipsen, 2002]
  - SU(3), $n_f = 2$ (Wilson) [L.-K. Wu, X.-Q. Luo, H.-S. Chen, 2007]
  - SU(3), $n_f = 3$ [Ph. de Forcrand, O. Philipsen, 2003]
  - SU(3), $n_f = 4$
    [M. D'Elia, M.P. Lombardo, 2003; V. Azcoiti et al., 2004-2005]
  - SU(3), $n_f = 4$ (Wilson) [H.-S. Chen, X.-Q. Luo, 2005]

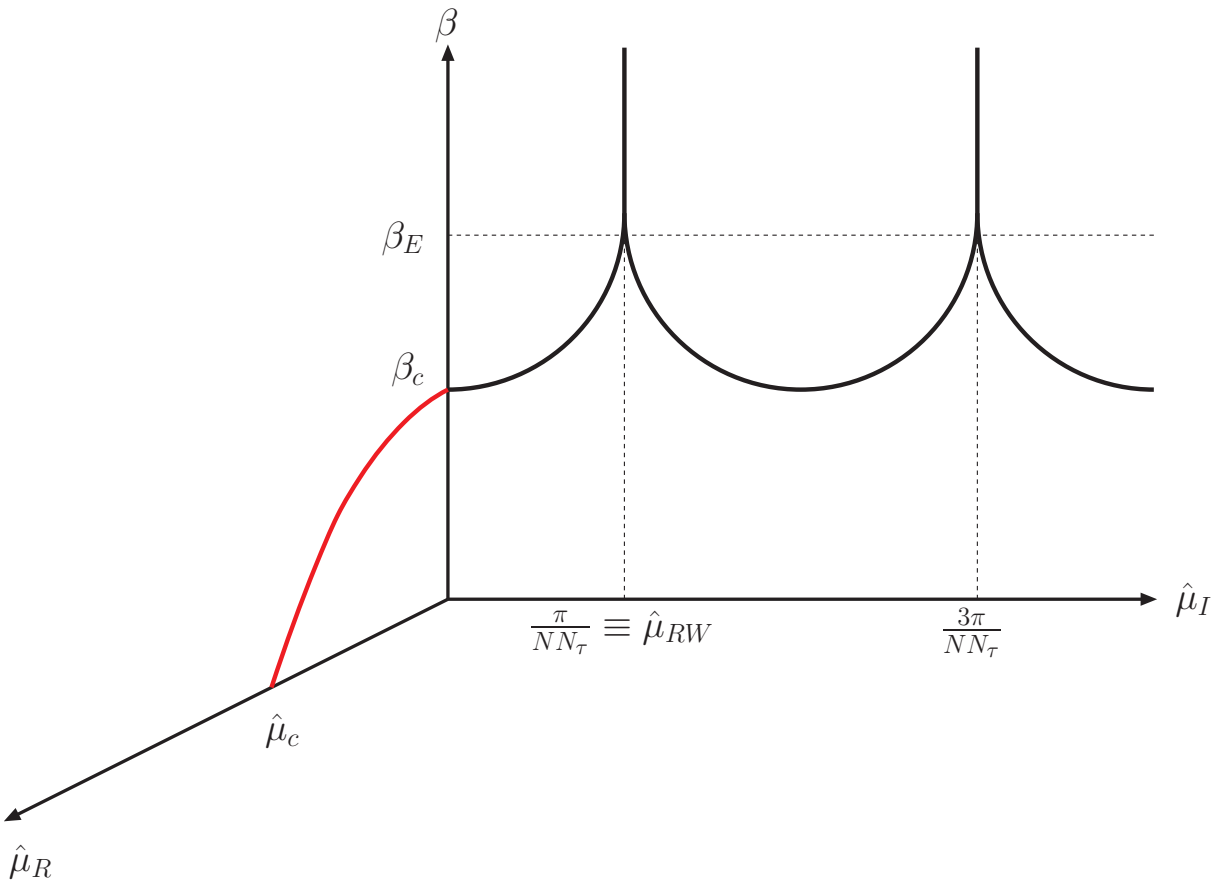
Description of the method

- Tested in
  - strong-coupling QCD [M.P. Lombardo, 2000]
  - $3d$ SU(3) + adjoint Higgs model
    [A. Hart, M. Laine, O. Philipsen, 2001]
  - SU(2), $n_f = 8$
    [P. Giudice, A.P., 2004; P. Cea, L. Cosmai, M. D'Elia, A.P., 2006]
  - $3d$ 3-state Potts model [S. Kim et al., 2005]
  - $2d$ Gross-Neveu at large N [F. Karbstein, M. Thies, 2006]

- In most cases a polynomial has been used as interpolating function, sometimes a Fourier sum for the low-temperature regime [M. D'Elia, M.P. Lombardo, 2002];

- A careful numerical analysis in SU(2) has shown that a considerable improvement can be achieved at high temperatures if ratio of polynomials [M.P. Lombardo, Lattice 2005] are used instead [P. Cea, L. Cosmai, M. D'Elia, A.P., 2006; A.P., SM&FT 2006]

Analytic continuation of the critical line



- The method of analytic continuation is extensively applied to the critical line itself.

Analytic continuation of the critical line: strategy

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, to be then extrapolated to real chemical potential
- if the theory is free from 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.

Outline

1. Introduction
   - QCD phase diagram
   - QCD with non-zero baryon density
   - The “sign” problem
   - Ways out
2. The method of analytic continuation
   - QCD with imaginary chemical potential
   - Description of the method
   - Numerical test
3. Conclusions

Numerical test

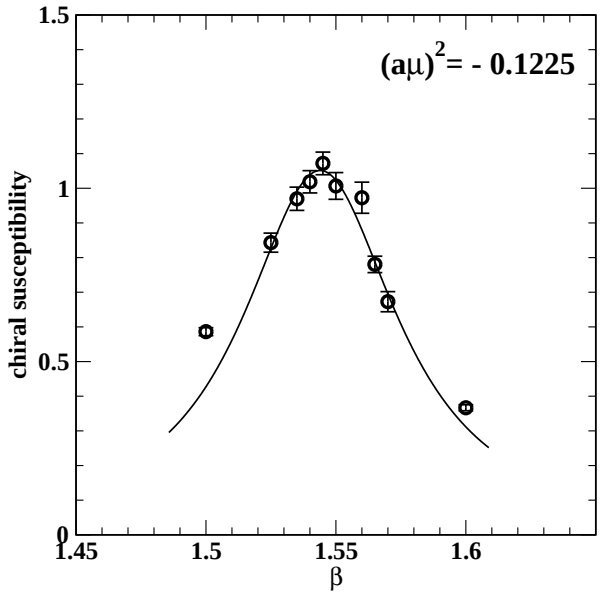
The test is performed in two theories free from the sign problem:

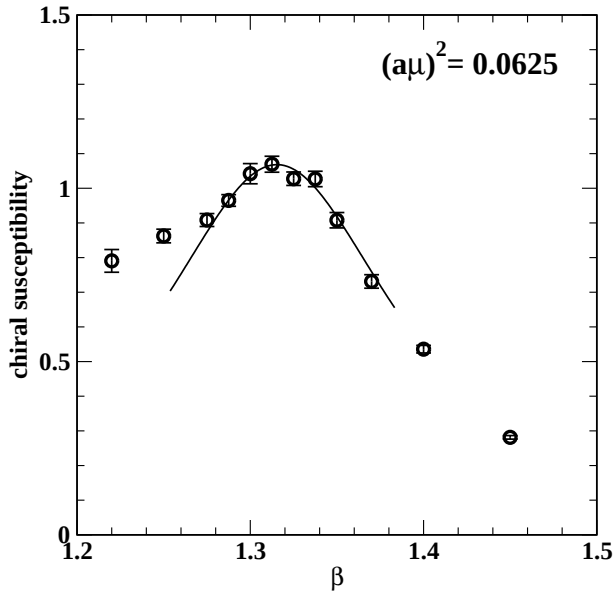
- SU(2) with n_f=8 staggered fermions
  - $16^3 \times 4$ lattice, fermion mass am=0.07 and am=0.2
  - $16^3 \times 6$ lattice, fermion mass am=0.07
- SU(3) with finite isospin density, n_f=8 staggered fermions, $8^3 \times 4$ lattice, fermion mass am=0.1

Technical details:

- hybrid Monte Carlo algorithm, with dt=0.01 (*exact* ϕ algorithm [S.A. Gottlieb et al., 1987]).
- statistics 10k $\div$ 20k
- simulations performed mostly on the computer facilities at the INFN APEnext Computing Center

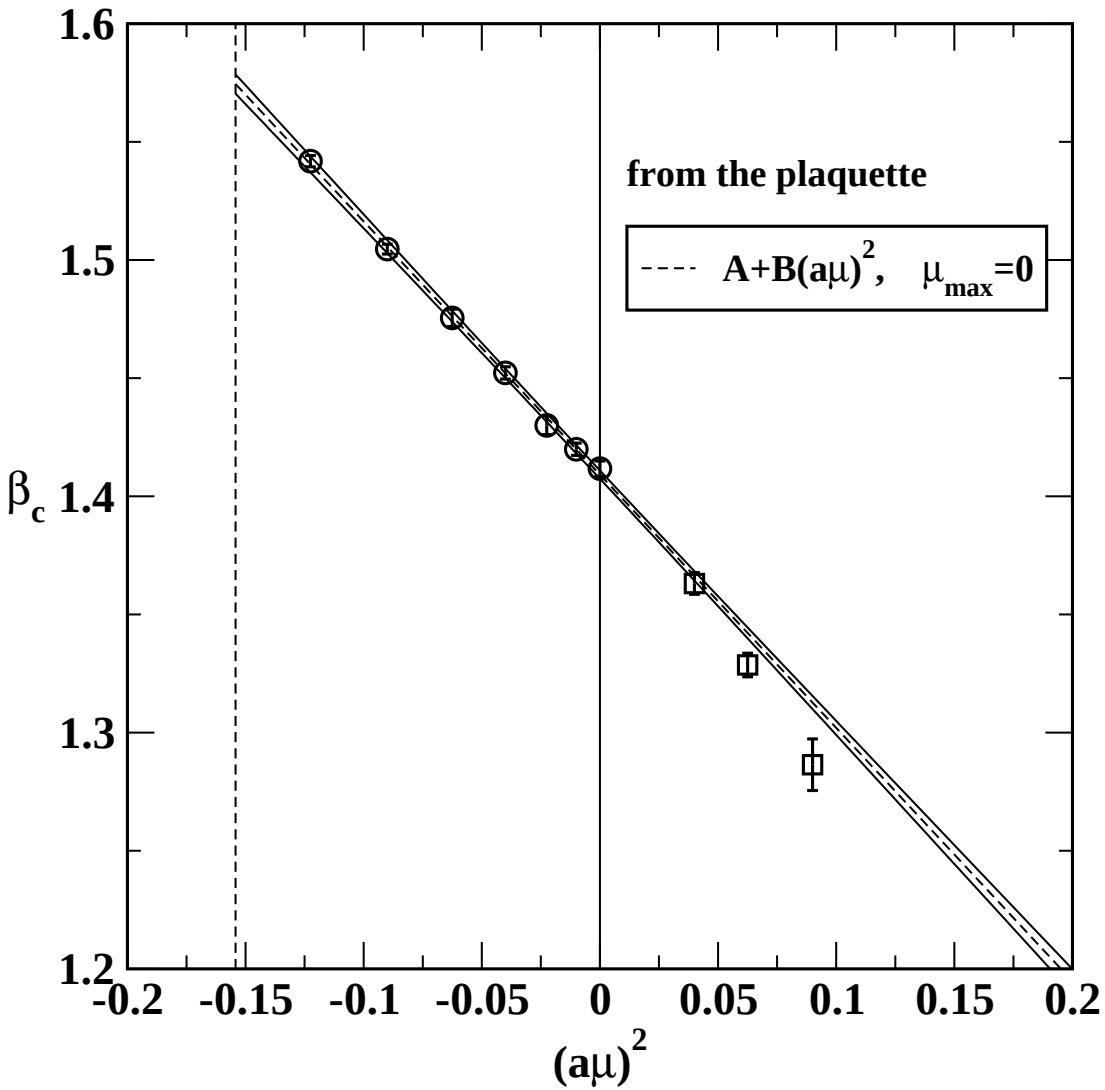
SU(2), $16^3 \times 4$, am=0.07: susceptibilities



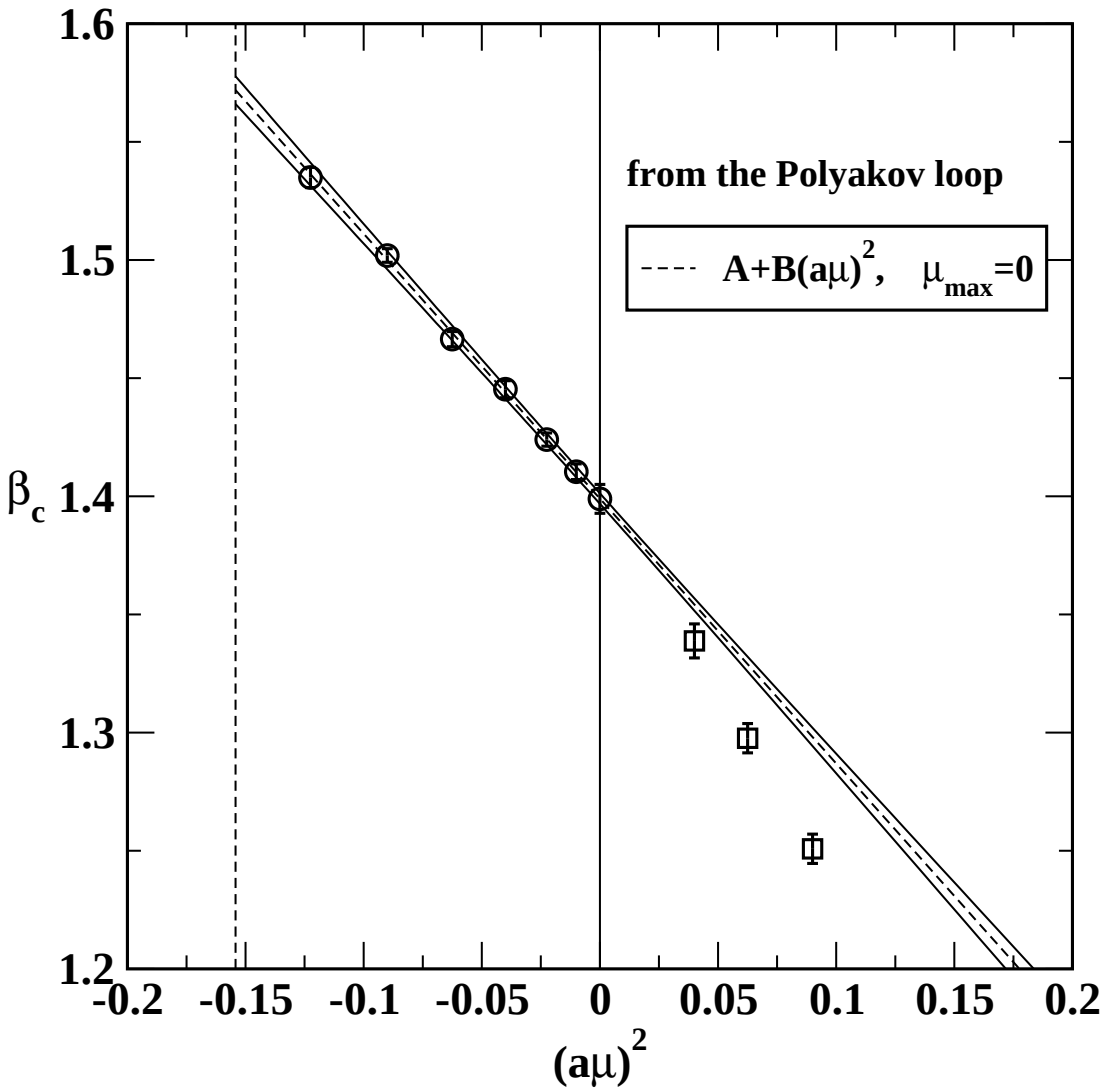


$\hat{\mu}$	chiral cond.	Polyakov loop	plaquette
0.35 *i*	1.5440(16)	1.5349(43)	1.5418(24)
0.30 *i*	1.5068(15)	1.5019(29)	1.5046(21)
0.25 *i*	1.4775(29)	1.4665(32)	1.4755(37)
0.20 *i*	1.4532(16)	1.4453(36)	1.4522(26)
0.15 *i*	1.4324(22)	1.4240(28)	1.4300(39)
0.10 *i*	1.4197(16)	1.4104(33)	1.4199(26)
0.	1.4102(18)	1.3989(61)	1.4117(32)
0.20	1.3528(22)	1.3388(72)	1.3631(46)
0.25	1.3145(30)	1.2976(62)	1.3286(50)
0.30	1.2433(59)	1.2508(62)	1.2864(109)

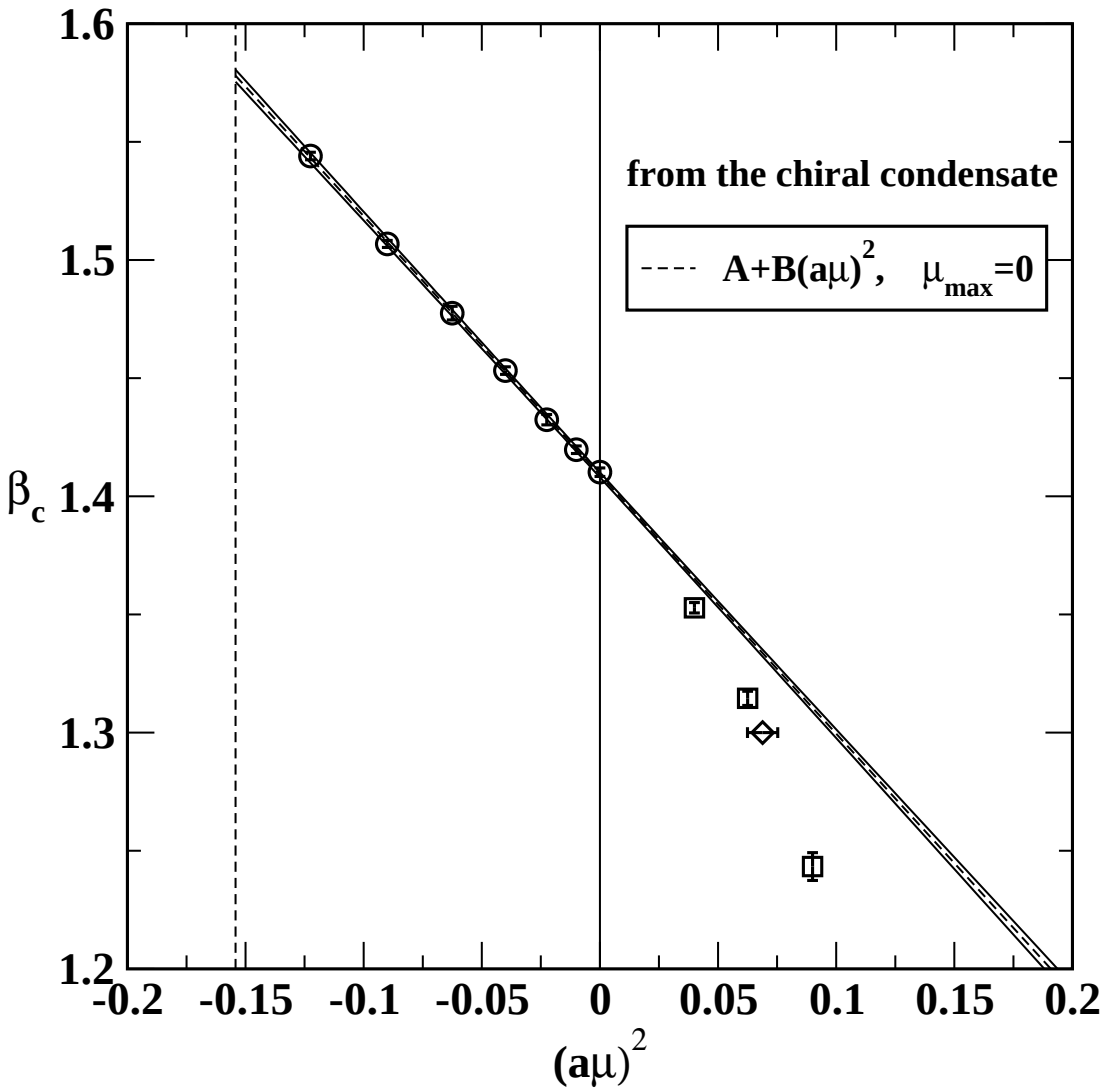
SU(2), $16^3 \times 4$, am=0.07: plaquette



SU(2), $16^3 \times 4$, am=0.07: Poyakov loop



SU(2), $16^3 \times 4$, am=0.07: chiral condensate



SU(2), $16^3 \times 4$, am=0.07: summary

- no room for fitting functions different from $A + B\hat{\mu}^2$
- $\beta_{\text{crit}}(\hat{\mu}_{RW})$ in agreement with direct determinations
- deviation between extrapolation and direct determinations at real chemical potential

$\longrightarrow$ global fit

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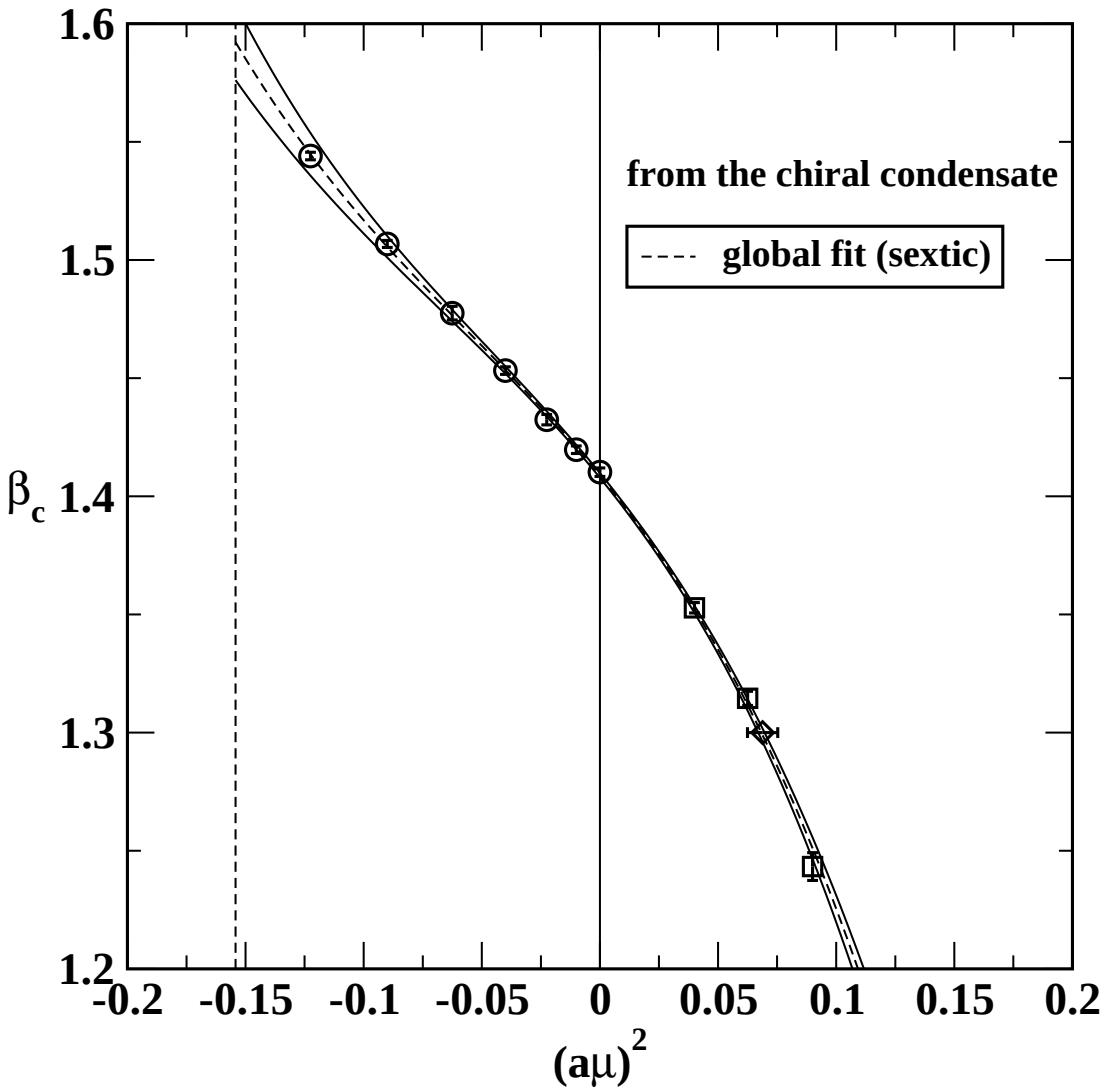
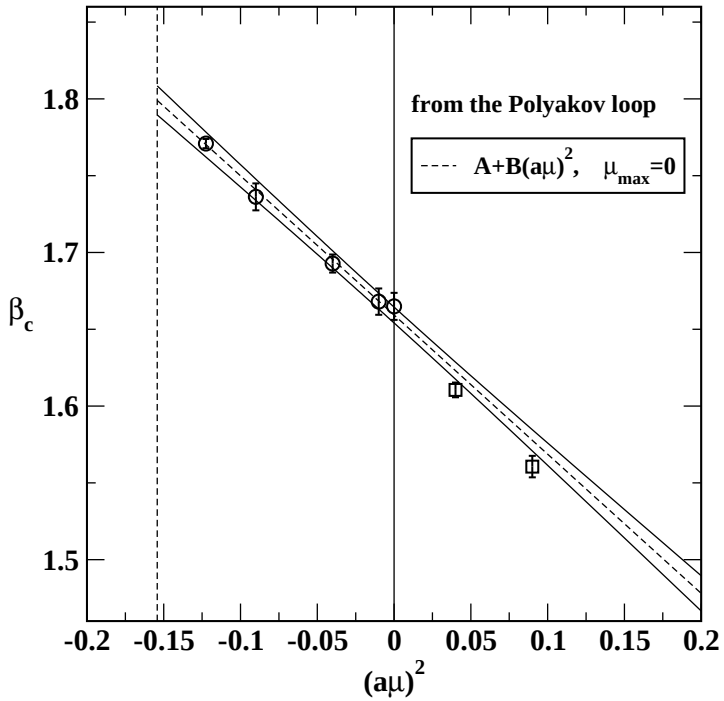
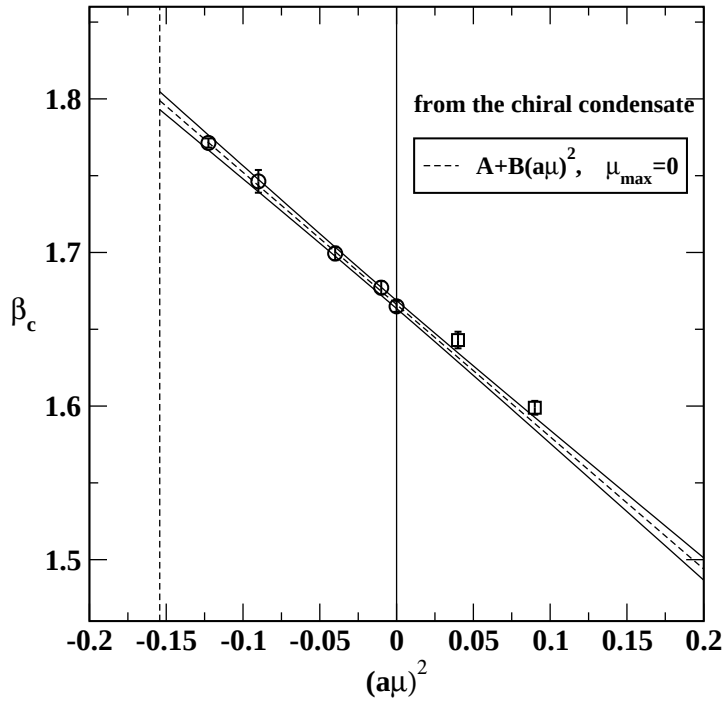
SU(2), $16^3 \times 4$, am=0.07: chiral condensate



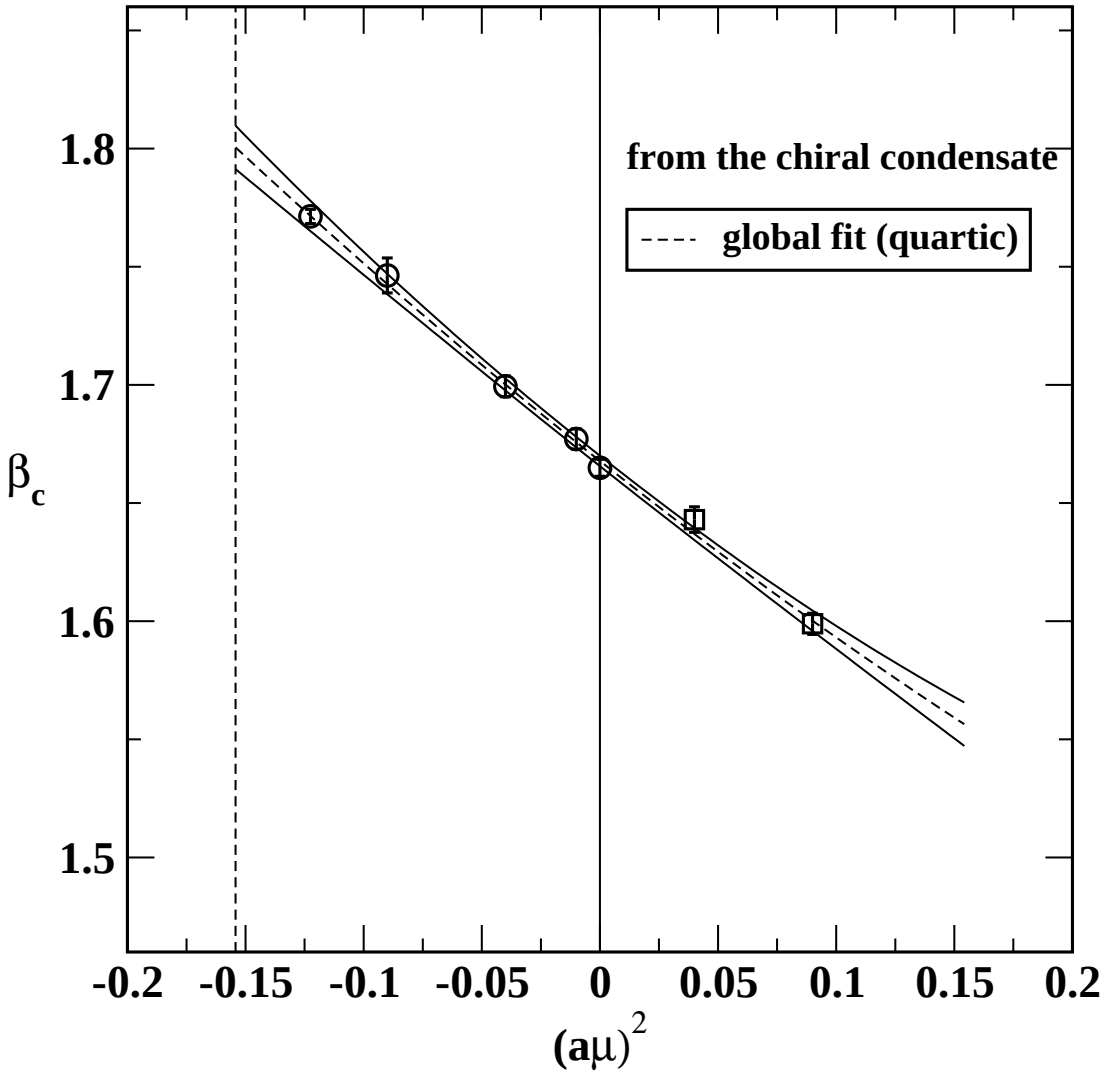
SU(2), $16^3 \times 4$, am=0.2 (preliminary)

$\hat{\mu}$	chiral cond.	Polyakov loop
0.35 i	1.7713(30)	1.7709(30)
0.30 i	1.7463(74)	1.7362(88)
0.20 i	1.6994(44)	1.6928(59)
0.10 i	1.6771(43)	1.6680(86)
0.	1.6649(36)	1.6649(88)
0.20	1.6430(54)	1.6105(48)
0.30	1.5989(45)	1.5606(70)





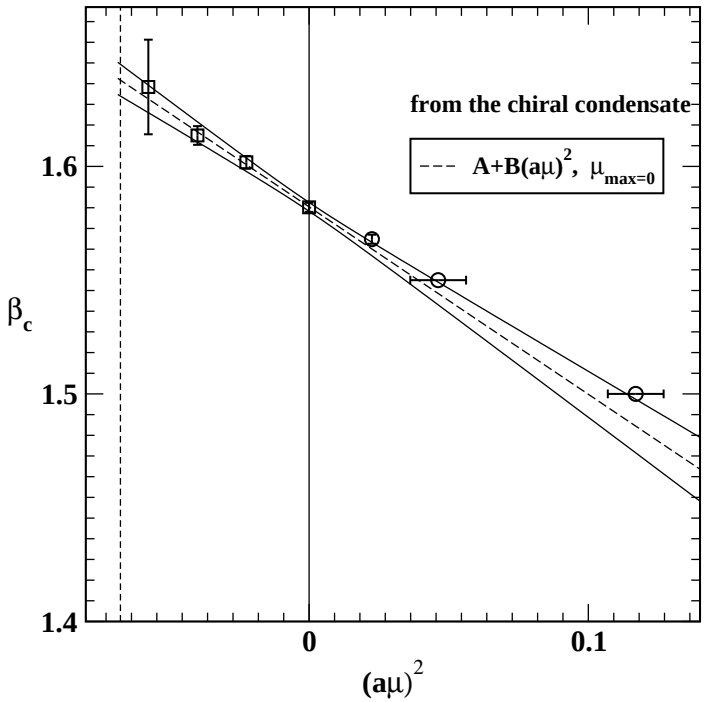
SU(2), $16^3 \times 4$, am=0.2 (preliminary)

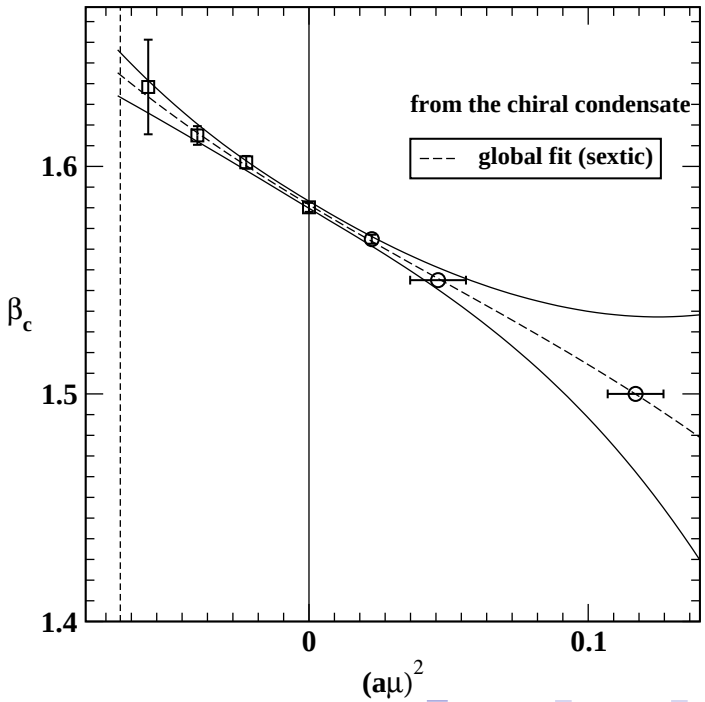


SU(2), $16^3 \times 6$, am=0.07 (preliminary)

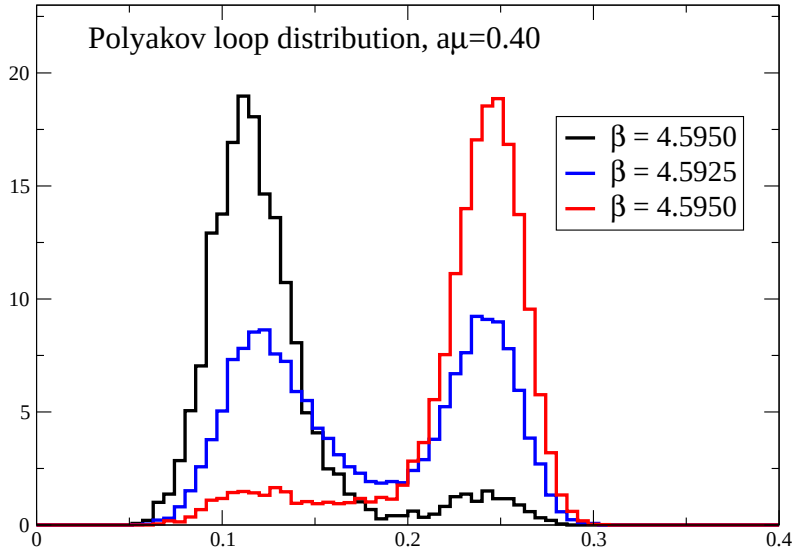
$\hat{\mu}$	chiral cond.
0.24 i	1.6349(208)
0.20 i	1.6136(41)
0.15 i	1.6018(28)
0.	1.582(2)
0.15	1.568(2)
0.215(10)	1.55
0.342(10)	1.5

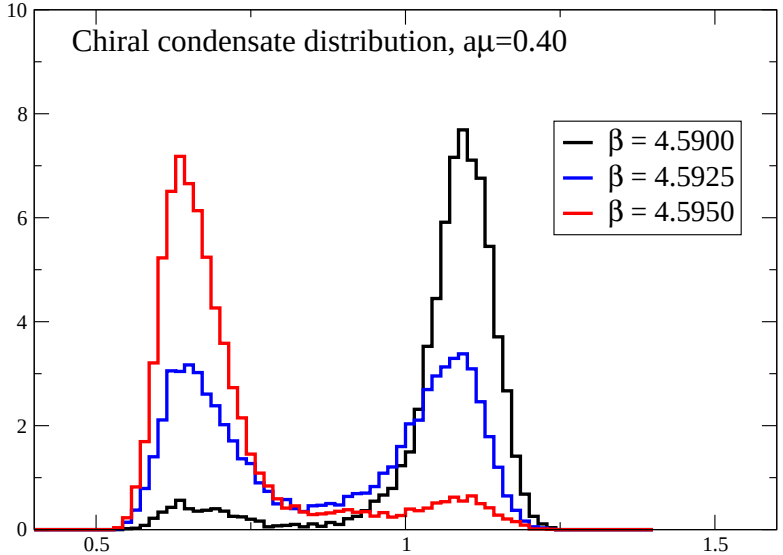
Data are $\mu^2 > 0$ are taken from
[S. Conradi, A. D'Alessandro, M. D'Elia, 2006]





SU(3) isospin, $8^3 \times 4$, am=0.1 (preliminary)





$\hat{\mu}$	peak
0.48 *i*	4.8420(25)
0.40 *i*	4.7915(25)
0.30 *i*	4.750(2)
0.20 *i*	4.721(3)
0.10 *i*	4.702(3)
0.	4.695(3)
0.20	4.6700(25)
0.30	4.6415(15)
0.40	4.5925(20)
0.45	4.5575(20)

The analysis of the RW phase structure at imaginary chemical potential is being done by [M. D'Elia, Manneschi, in progress].

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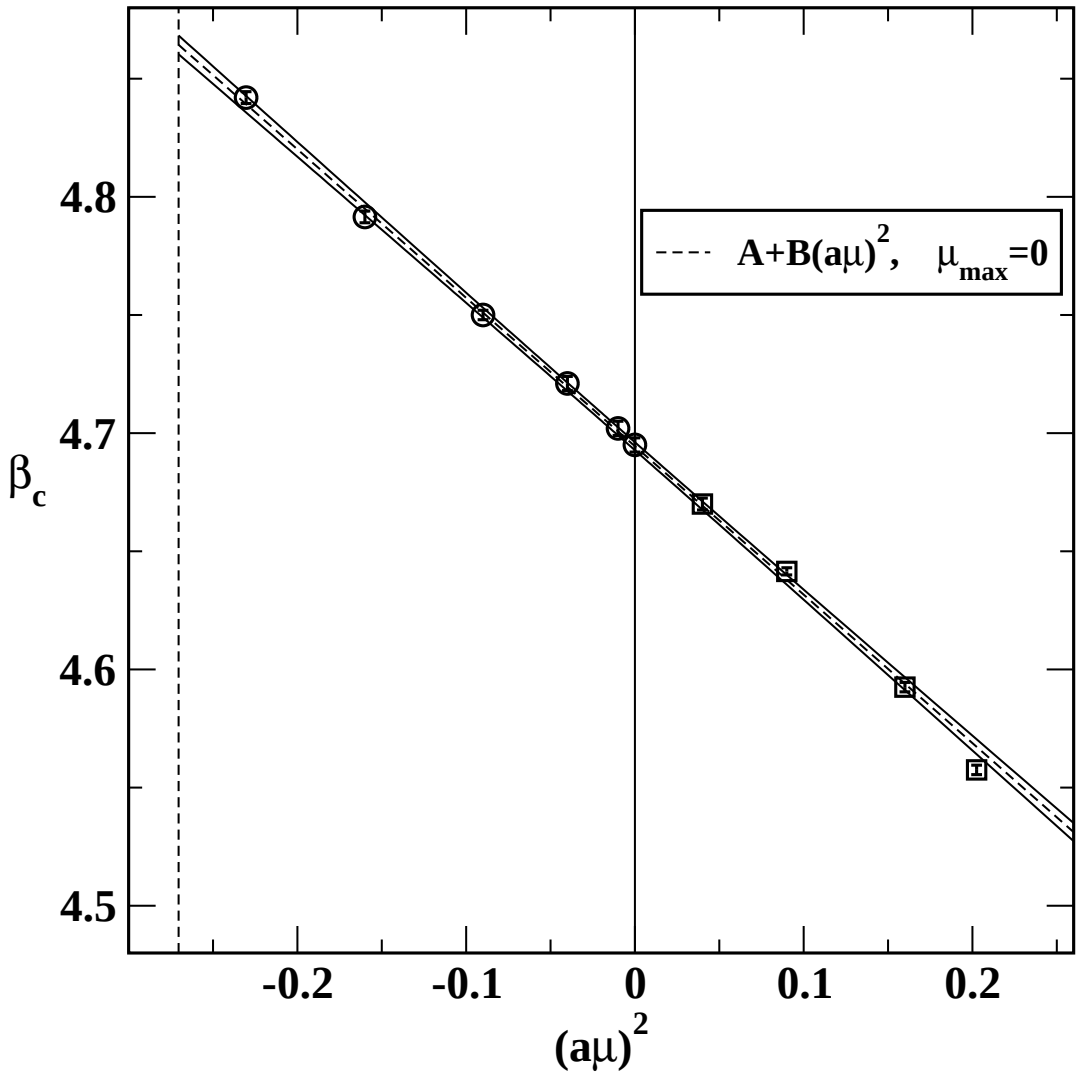

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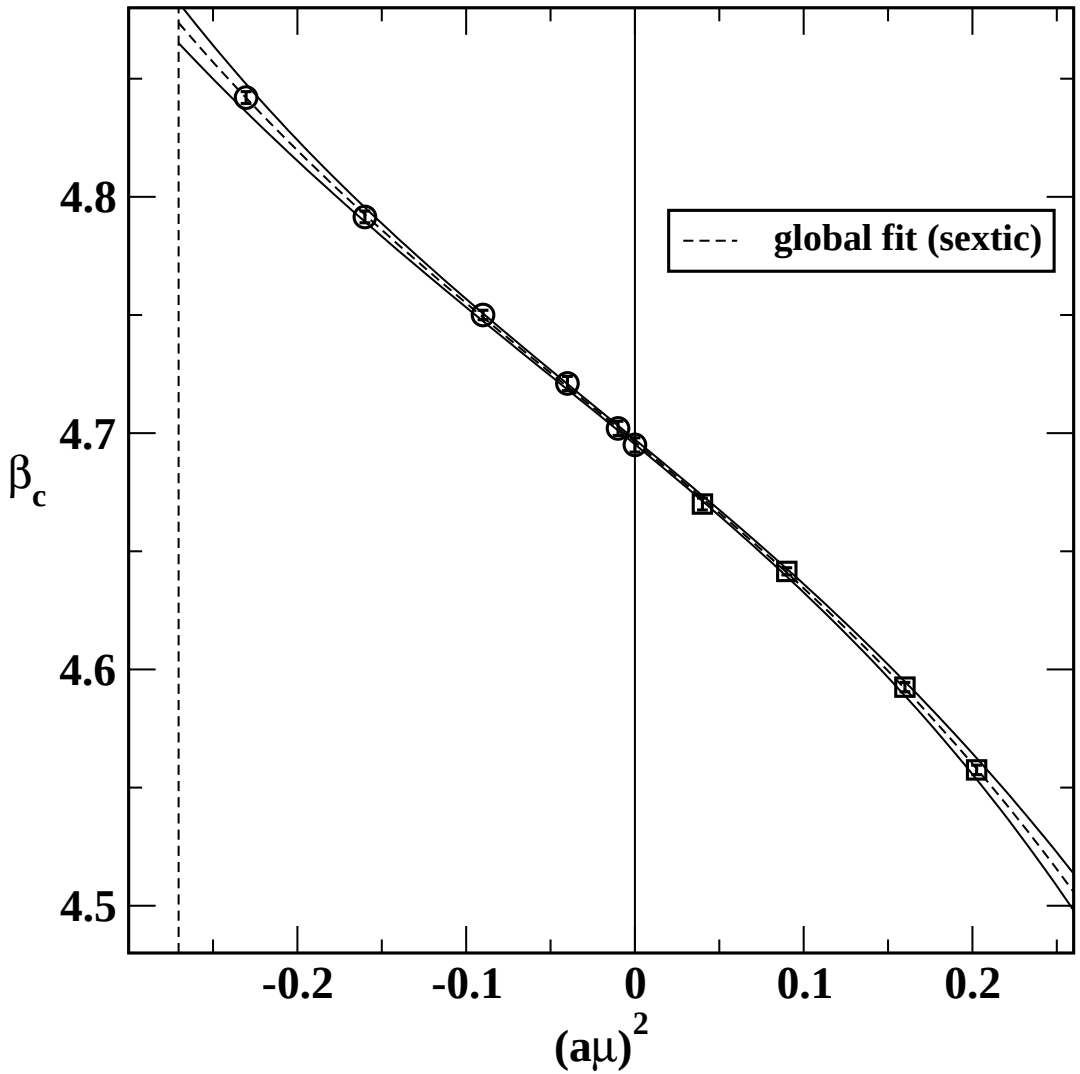

Conclusions

- We have tested the analytic continuation of the critical line in the (T, μ)-plane from imaginary to real chemical potential in 2-color QCD and, preliminarly, in SU(3) with finite isospin density.
- We have found that the critical line around $\mu = 0$ can be described by an analytic function.
- However, when trying to infer the behavior of the critical line at real μ from the extrapolation of its behavior at imaginary μ, a very large precision is needed to get the correct result.
- In the case of polynomial interpolations, there is a clear indication that terms of order μ^4 or even μ^6 play a relevant role at $\mu^2 > 0$, but are less visible at $\mu^2 < 0$, this calling for an accurate knowledge of the critical line in all the first RW sector.
- We have preliminary indications that in 2-color QCD this effect is strongly dependent on the fermionic mass and is more pronounced toward the chiral limit; in SU(3) with finite isospin density it seems to be less severe, but further investigations are needed.

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Roberge-Weiss' proof I

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

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

- change of variables I

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

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

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

Roberge-Weiss' proof II

- change of variables II

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

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

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

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

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

Roberge-Weiss' proof III

- V.e.v.'s of observables which are not modified by the above changes of variables (e.g. chiral condensate, fermionic number density) have the same periodicity of the partition function, $2\pi/N_c$

- The v.e.v. of the Polyakov loop is $2\pi/N_c$ periodic up to an element of $Z(N_c)$:

$$\langle L \rangle_{\theta + 2\pi k/N_c} = \exp(2\pi i k/N_c) \langle L \rangle_\theta$$

$$k = 0, 1, \ldots, N_c - 1$$

so, in fact, the periodicity is 2π