Analytic continuation from an imaginary chemical potential

A numerical study in 2-color QCD (hep-lat/0612018, to appear on JHEP)

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Outline

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Introduction and motivation

- Understanding the phase diagram of QCD on the temperature – chemical potential (T, μ) has many important implications in cosmology, in astrophysics and in the phenomenology of heavy ion collisions.

- The discretization of QCD on a space-time lattice and the use of Monte Carlo numerical simulations in the Euclidean space-time provide us with a useful investigation tool.

- However, in QCD with non-zero chemical potential, however, the fermion determinant becomes complex and standard numerical simulations are not feasible – the so-called sign problem.

Introduction and motivation

- Ways out:
  - 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 suitable reweighting;

    [I.M. Barbour et al., 1998]
    [Z. Fodor and S.D. Katz, 2002 $\rightarrow$]

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

    [S.A. Gottlieb, 1988]
    [QCD-TARO coll., 2001]
    [C.R. Allton et al., 2002-2003-2005]
    [R.V. Gavai and S. Gupta, 2003-2005]
    [S. Ejiri et al., 2006]

Introduction and motivation

- Ways out (cont'd)
  - to build canonical partition functions by Fourier transform of the grand canonical function at imaginary chemical potential

[A. Hasenfratz and D. Toussaint, 1992]
[M.G. Alford, A. Kapustin, F. Wilczek, 1999]
[P. de Forcrand and S. Kratochvila, 2004-2005-2006]
[A. Alexandru et al., 2005]

Introduction and motivation

- Ways out (cont'd)
  - to perform numerical simulations at *imaginary* chemical potential, for which the fermion determinant is real, and to analytically continue the results to real μ (method of analytic continuation)

[M.P. Lombardo, 2000]
[A. Hart, M. Laine, O. Philipsen, 2001]
[Ph. de Forcrand and 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 and 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 et al., 2006]
[F. Karbstein and M. Thies, 2006]

Introduction and motivation

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

[O. Philipsen, Lattice 2005]
[C. Schmidt, Lattice 2006]

Introduction and motivation

Method of analytic continuation

- the coupling β and the chemical potential μ can be varied independently
- no limitation from increasing lattice sizes
- the extent of the attainable domain with real μ is limited
  1. by the periodicity and the non-analyticities present for imaginary μ
  2. by the accuracy of the interpolation of data for imaginary μ.

The present work is carried out in a theory which does not suffer the sign problem, 2-color QCD, and aims at

- finding out the optimal way to extract information from data at imaginary chemical potential
- assessing the actual ranges of applicability of the method.

Outline

QCD with finite chemical potential

- On the continuum:

$$\mathcal{L} = \mathcal{L}_{QCD} + \mu J_0 \,, \qquad J_\mu = \overline{\psi}\gamma_\mu\psi$$

$$\int d^3x J_0 = N - \overline{N} \,, \qquad N\,(\overline{N}) \text{ no. of (anti-)particles}$$

- On the lattice:

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

[F. Karsch, P. Hasenfratz, 1983]

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

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

Outline

The "sign" problem

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

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

- In order to perform numerical 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; indeed, 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 $M^\dagger(i\mu) = M(i\mu)$

Outline

QCD with imaginary chemical potential

- SU(N_c) gauge theory with imaginary μ

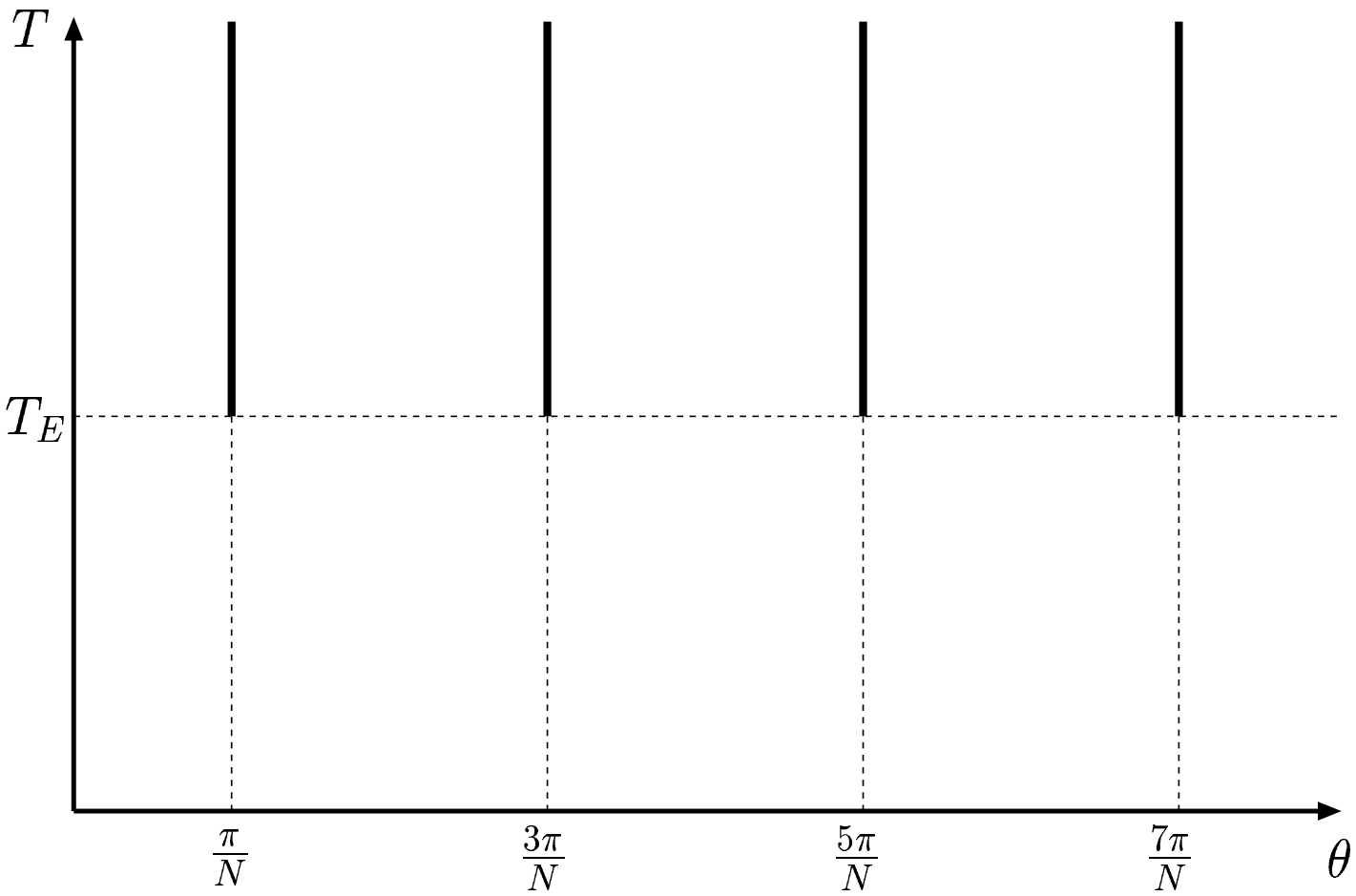
$$\mu \to i\nu, \qquad Z(\theta) = \mathrm{Tr}\left[e^{-\beta H + i\theta \hat{N}}\right], \qquad \theta = \beta\nu$$

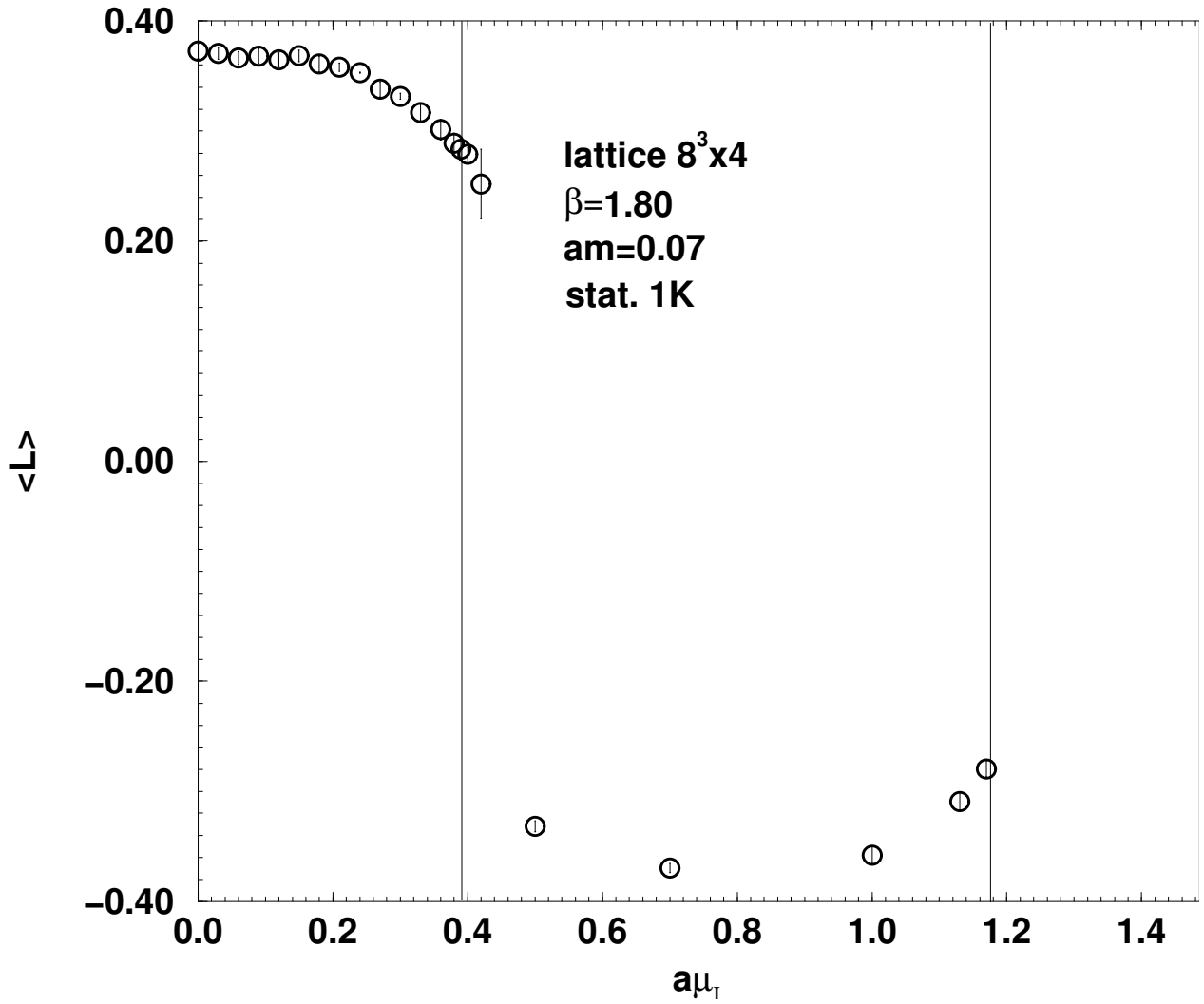
  - Free quarks ($N = 0, 1, 2, \ldots$) $\longrightarrow$ $Z(\theta)$ periodic with 2π
  - Color singlets (N multiple of N_c) $\to$ $Z(\theta)$ periodic with $2\pi/N_c$

- [Roberge and Weiss, 1986] have shown that
  - $Z(\theta)$ is always periodic with $2\pi/N_c$
  - the free energy, $F(\theta) = -\ln Z(\theta)/\beta$,
    is a regular function of θ for $T < T_E$
    is a discontinuous function in $\theta = 2\pi(k + 1/2)/N_c$ for $T > T_E$

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

Phase diagram on the (T,θ)-plane




0.40
0.20
0.00
−0.20
−0.40
0.0
0.2
0.4
0.6
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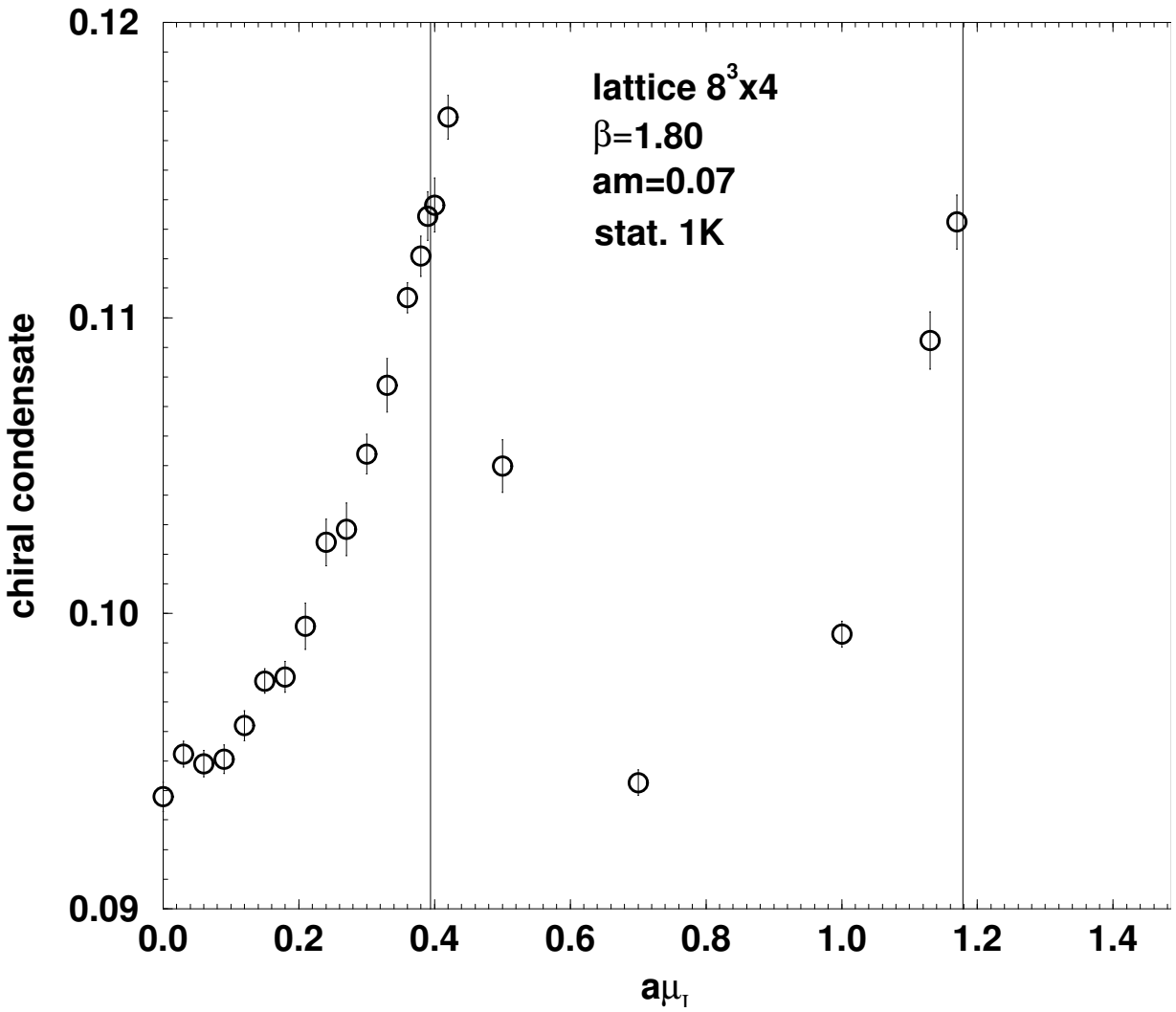
1.4
<L>
aμI
lattice 8^3x4
β=1.80
am=0.07
stat. 1K


lattice 8^3x4
β=1.80
am=0.07
stat. 1K
chiral condensate
aμ_I
0.12
0.11
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0.09
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0.8
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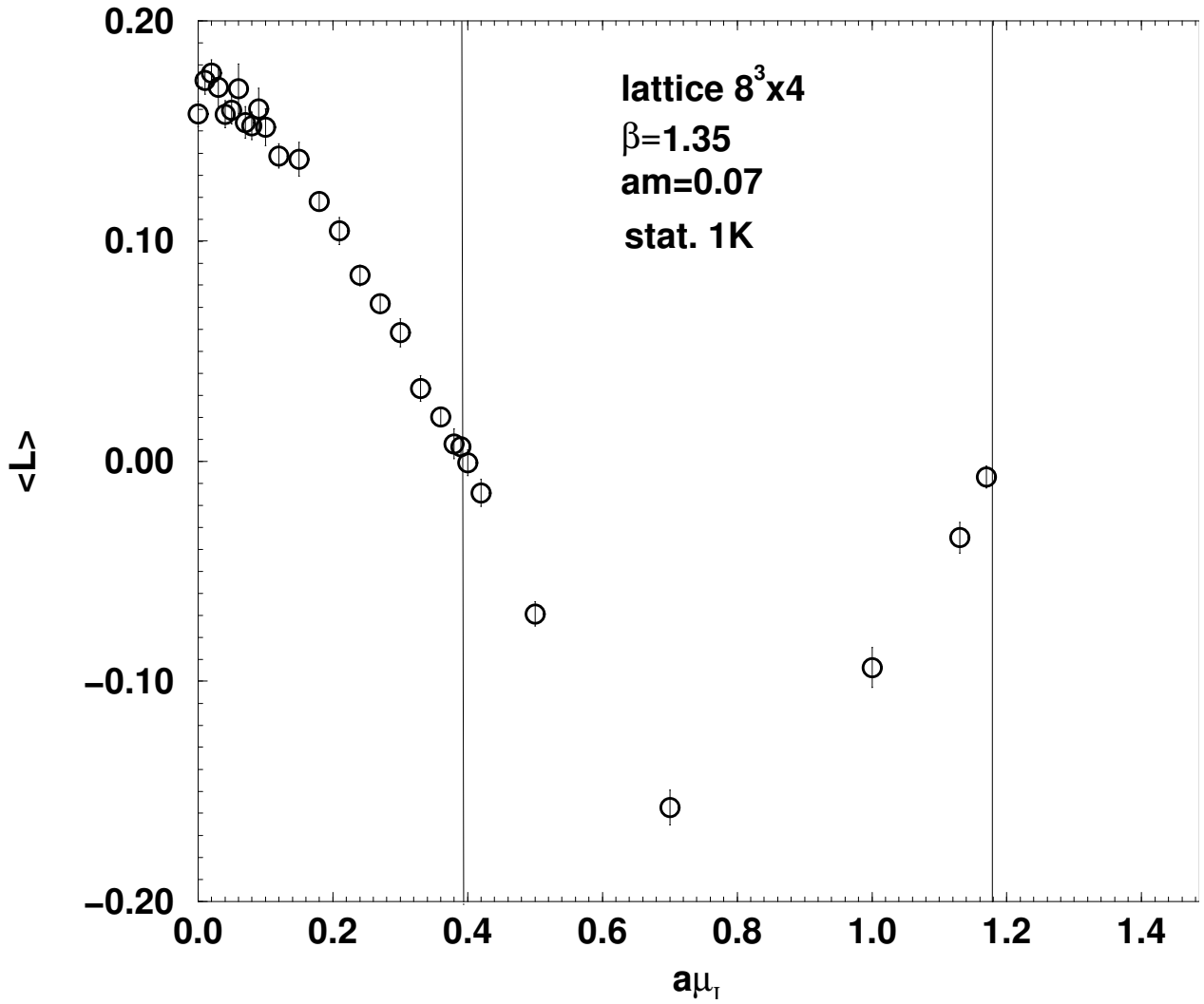
1.4


lattice 8^3x4
β=1.35
am=0.07
stat. 1K
<L>
aμ_I
0.20
0.10
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−0.10
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0.0
0.2
0.4
0.6
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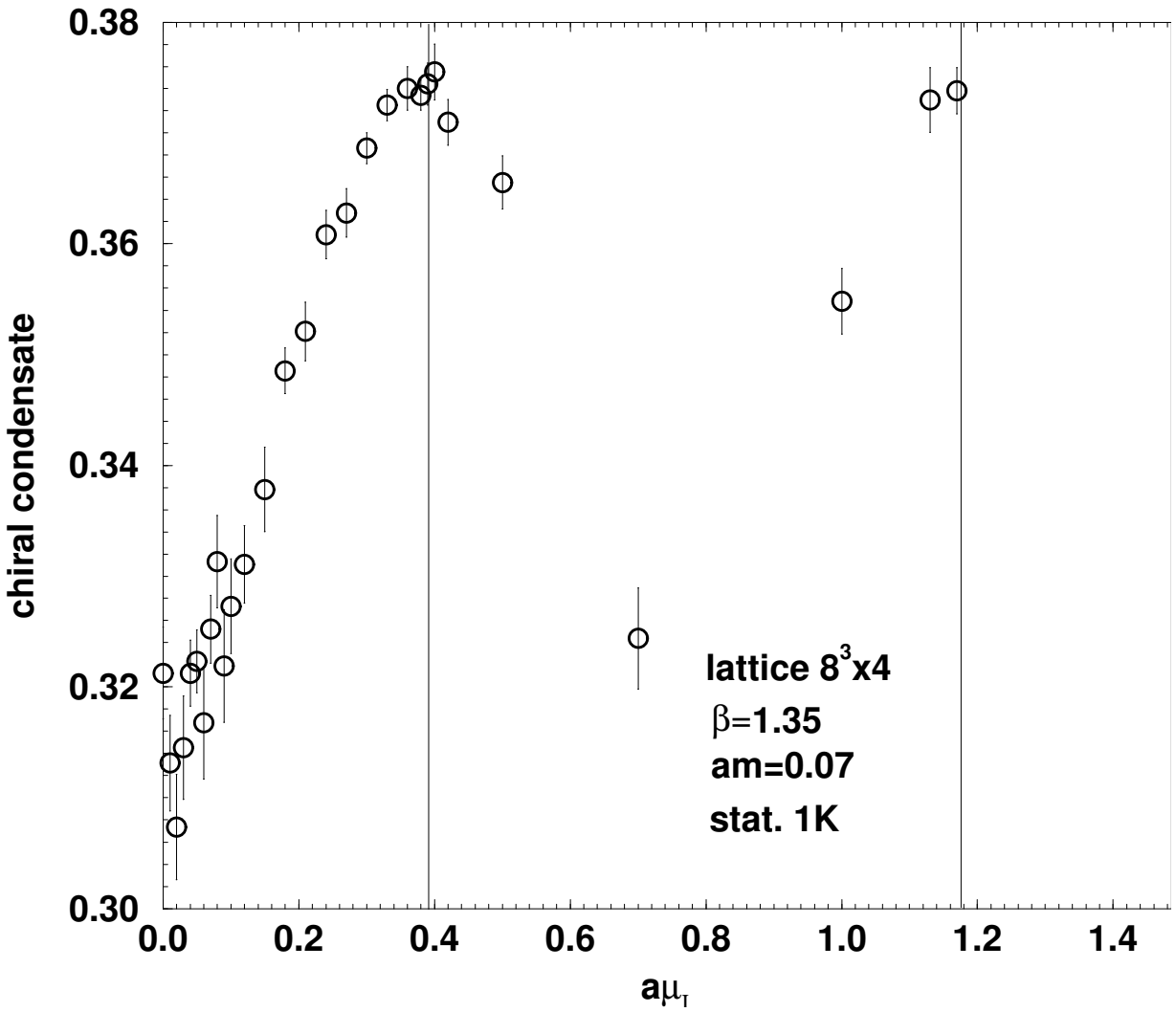
1.0
1.2
1.4


0.38
0.36
0.34
0.32
0.30
chiral condensate
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
aμ_I
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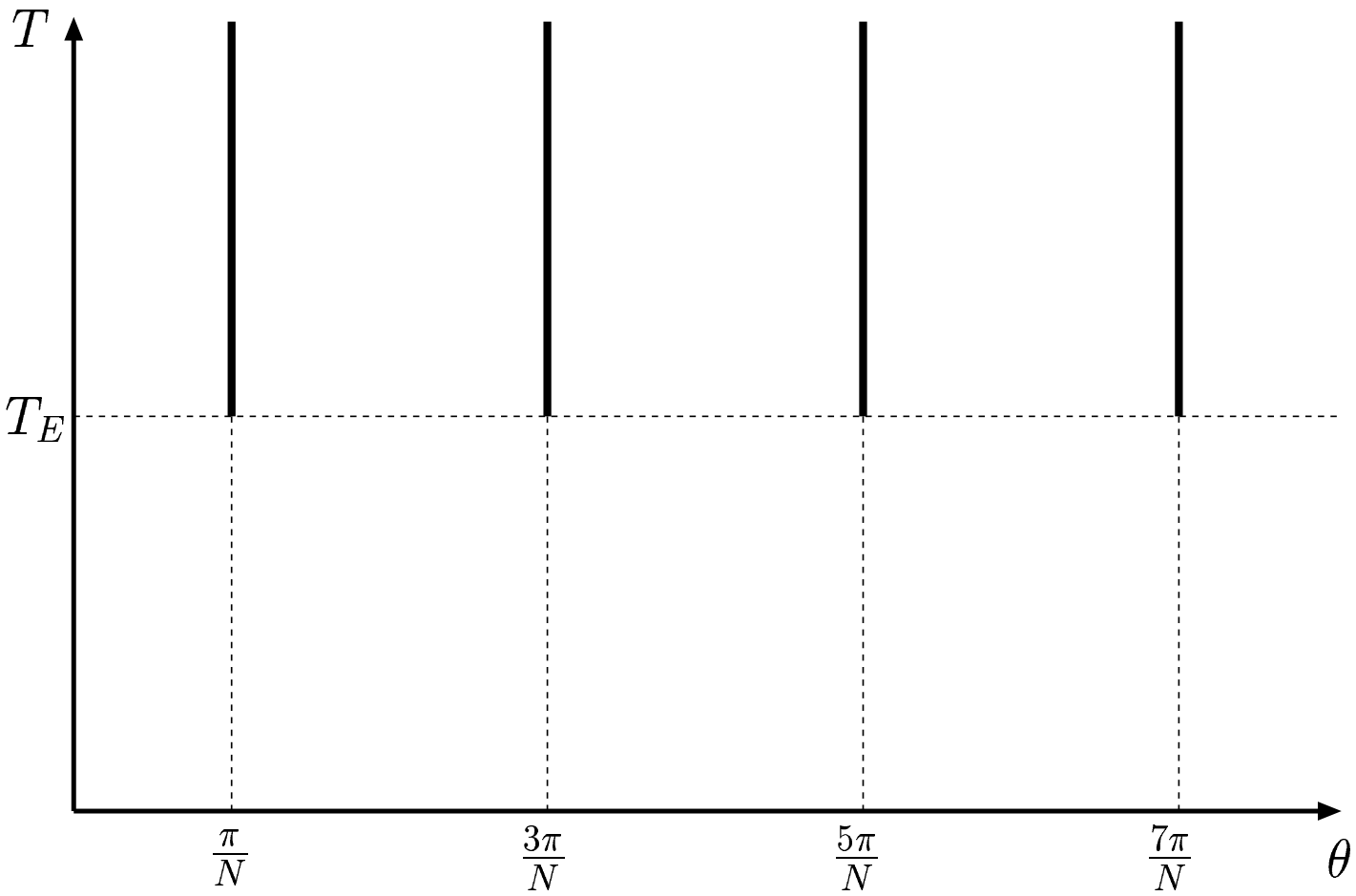
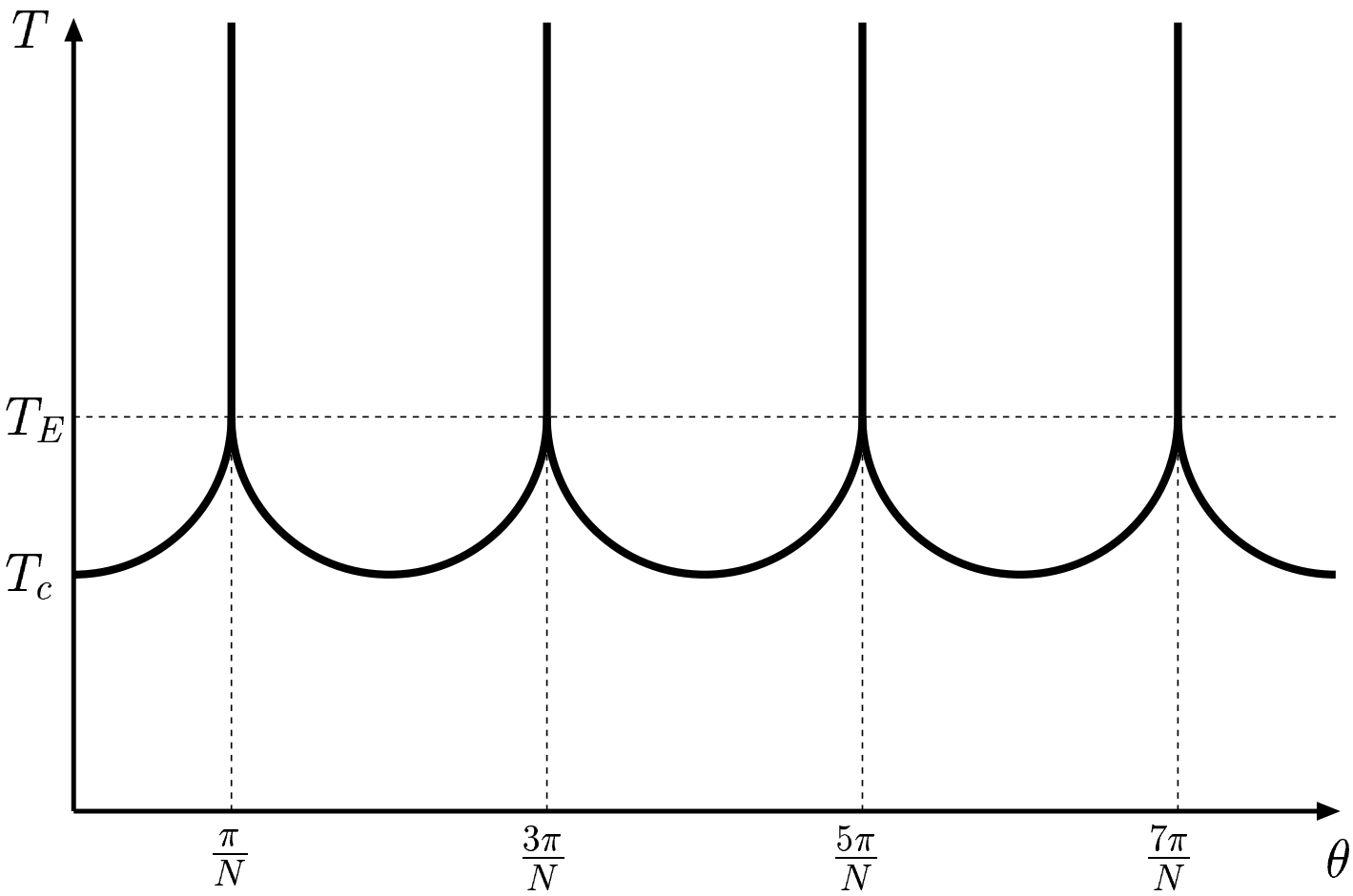
Phase diagram on the (T,θ)-plane



Phase diagram on the (T,θ)-plane



Outline

Description and state-of-the-art

- Strategy of the method of analytical continuation [M.P. Lombardo, 2000]
  - 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), $n_f = 3$ [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 and X.-Q. Luo, 2005]

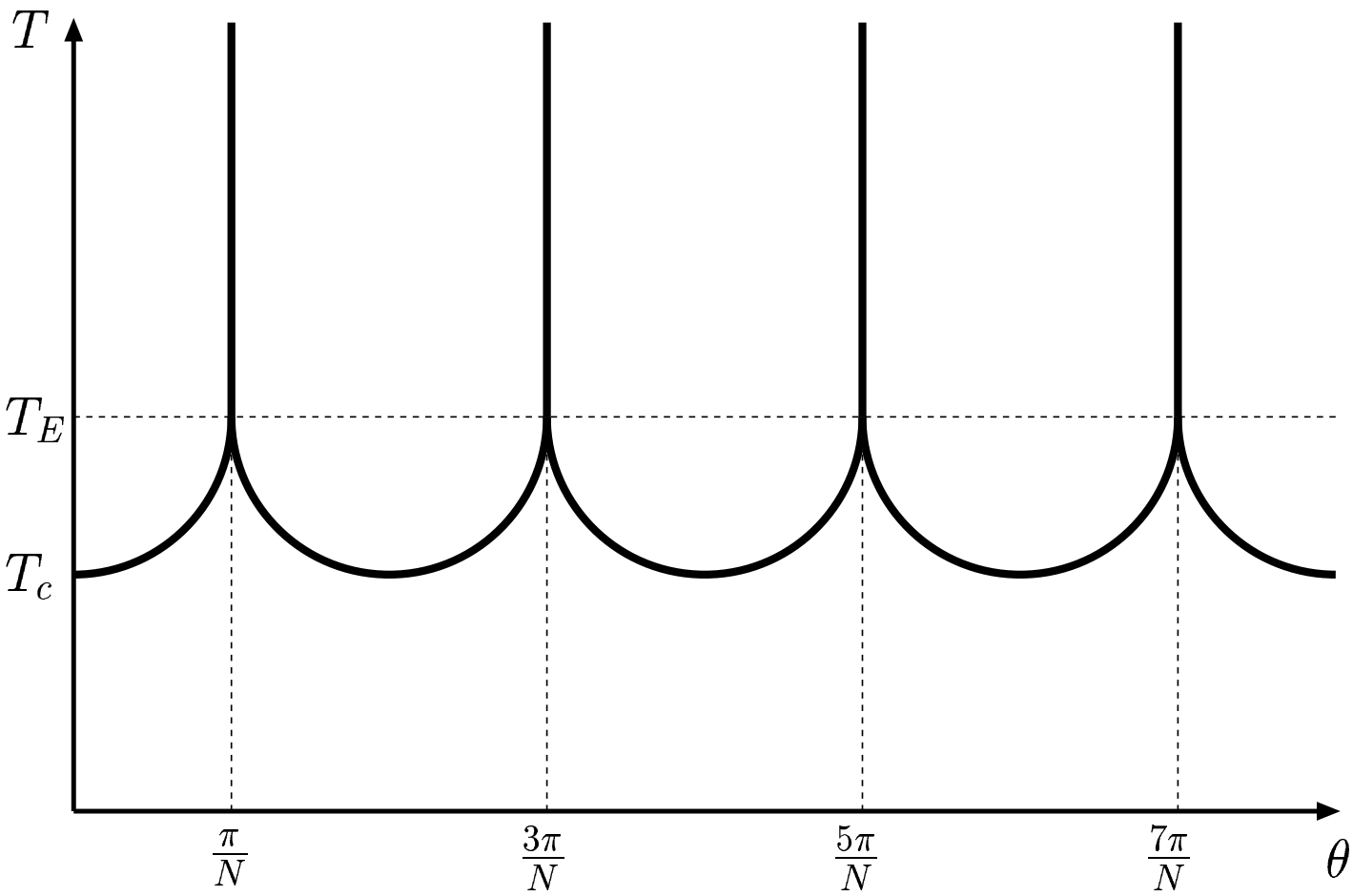
Description and state-of-the-art

- 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]
  - $3d$ 3-state Potts model [S. Kim et al., 2005]
  - 2d Gross-Neveu at large N [F. Karbstein and M. Thies, 2006]

- In most of these applications a truncated Taylor series has been used as interpolating function; sometimes a Fourier sum for the low-temperature regime [M. D'Elia, M.P. Lombardo, 2002].

- Here we want to consider different Ansätze for the interpolating functions and to directly test the range of reliability of the method itself, by using 2-color QCD as a test-field.

Phase diagram on the (T,θ)-plane



Different temperature regimes

- **Regime (a)**: $T > T_E$ (or $\beta > \beta_E$)
  - the RW transition line is the only expected non-analyticity at imaginary chemical potential
  - no transition line expected on the side of real chemical potential
- **Regime (b)**: $T_c < T < T_E$ (or $\beta_c < \beta < \beta_E$).
  - a non-analyticity is expected at imaginary chemical potential *before* the RW transition line
  - no transition line expected on the side of real chemical potential
- **Regime (c)**: $T < T_c$ (or $\beta < \beta_c$).
  - no non-analyticities expected at imaginary chemical potential, the only limitation coming from periodicity
  - a transition is expected here for a certain *real* value of the chemical potential

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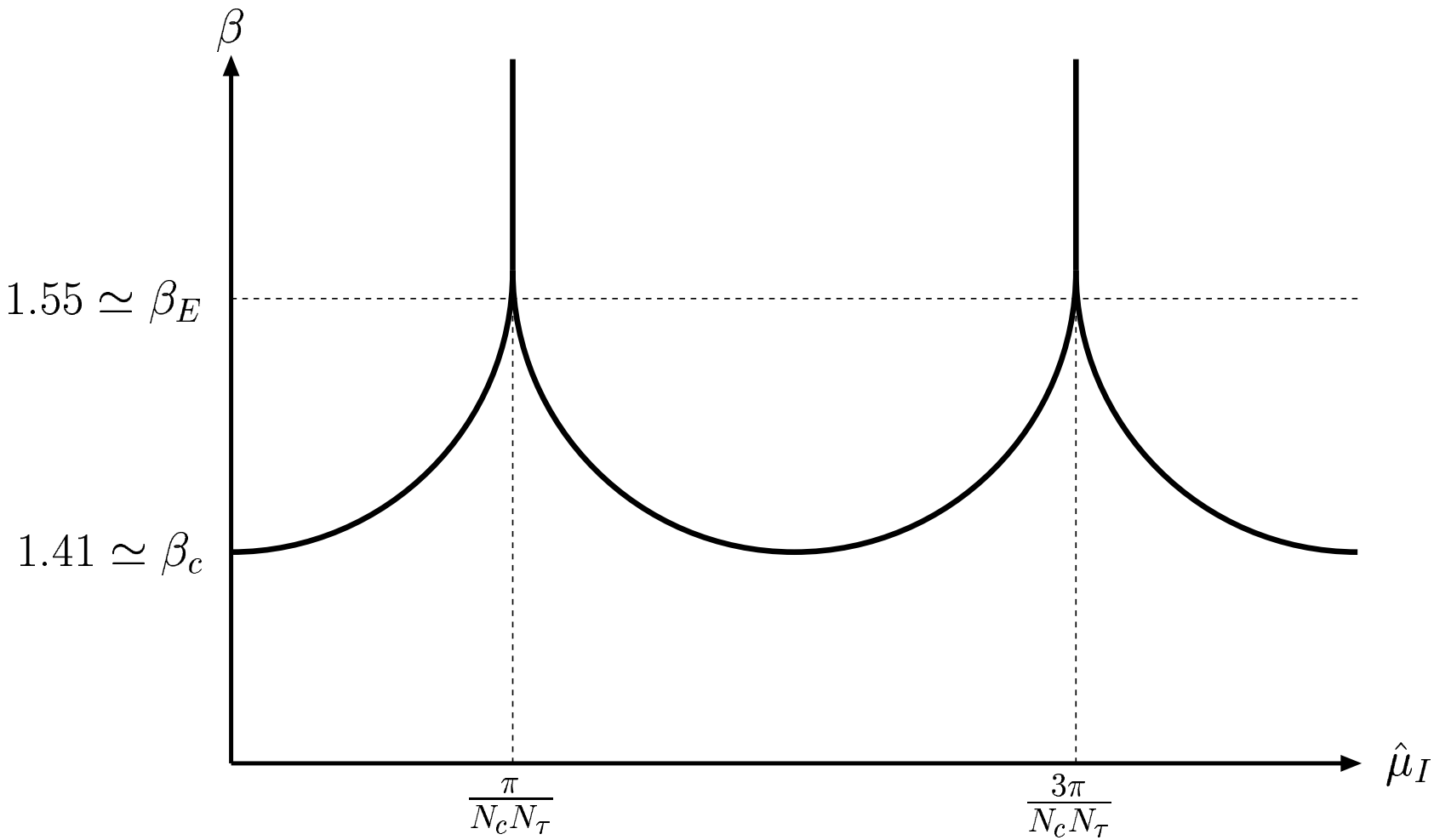
Outline

Numerical results - Details on the lattice simulations

- SU(2) gauge theory with n_f=8 staggered fermions, fermion mass am=0.07, on a $16^3 \times 4$ lattice
- hybrid Monte Carlo algorithm, with dt=0.01 (*exact* ϕ algorithm [S.A. Gottlieb et al., 1987]).
- observables (statistics 1000-9000, errors $\lesssim$1%):
  - chiral condensate $\langle \bar{\psi}\psi \rangle$
  - Polyakov loop
  - fermion number density
- simulations at $\beta = 1.90$ (regime (a)), $\beta = 1.45$ (regime (b)), $\beta = 1.30$ (regime (c)).
- simulations on the APE100 and APEmille crates in Bari and on the computer facilities at the INFN APEnext Computing Center

Phase diagram on the (β,μ_I)-plane



Numerical results: Interpolating functions - regime (a)

- Polyakov loop, chiral condensate
  - second order polynomial in μ^2:

$$A + B\hat{\mu}_I^2 + C\hat{\mu}_I^4$$

  - ratio of two first order polynomials in μ^2:

$$\frac{A + B\hat{\mu}_I^2}{1 + C\hat{\mu}_I^2}$$

- fermionic number density
  - polynomial:

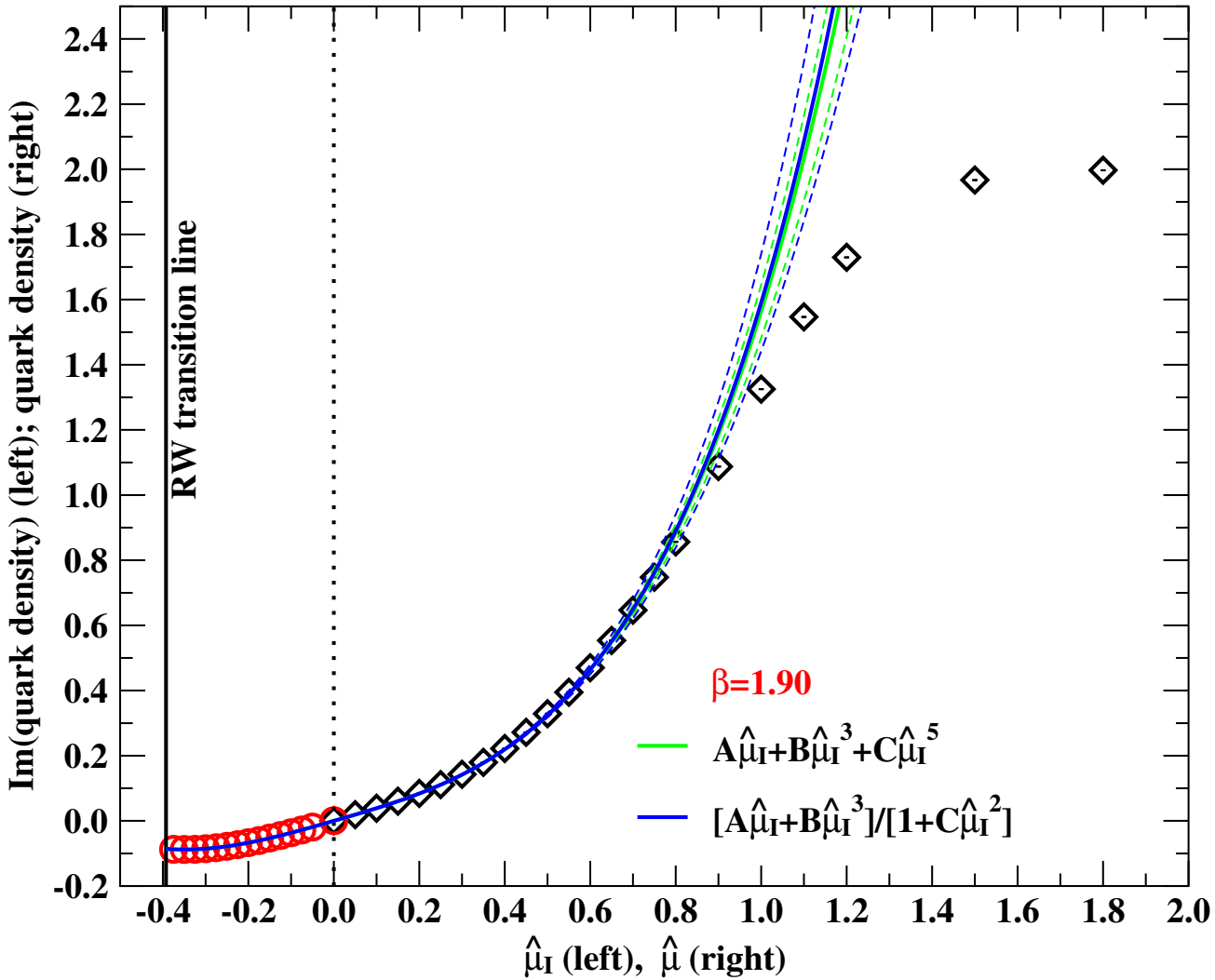
$$A\hat{\mu}_I + B\hat{\mu}_I^3 + C\hat{\mu}_I^5$$

  - ratio of polynomials:

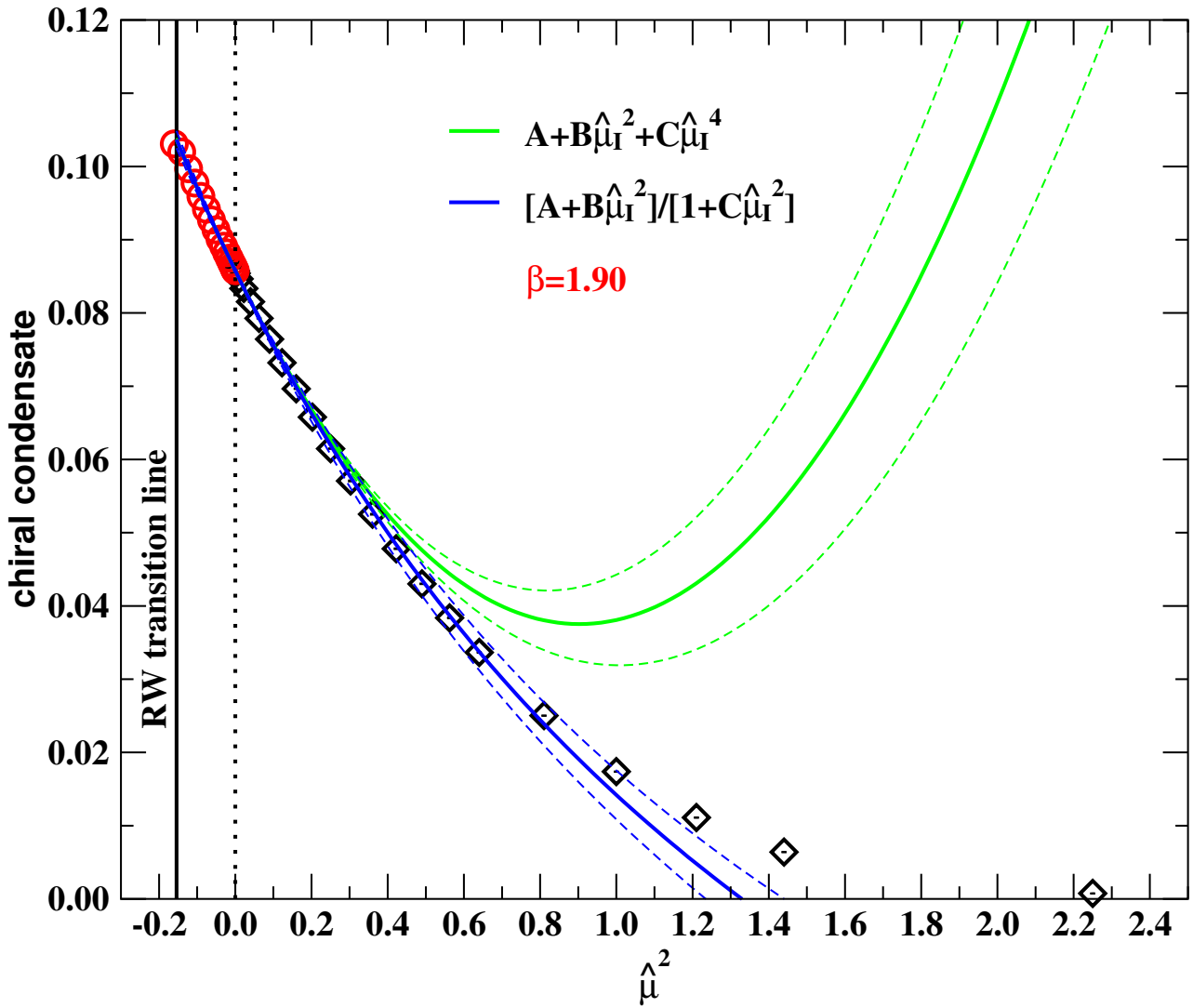
$$\frac{A\hat{\mu}_I + B\hat{\mu}_I^3}{1 + C\hat{\mu}_I^2}$$

The use of Padé approximants as interpolating functions has been suggested by [M.P. Lombardo, 2005].

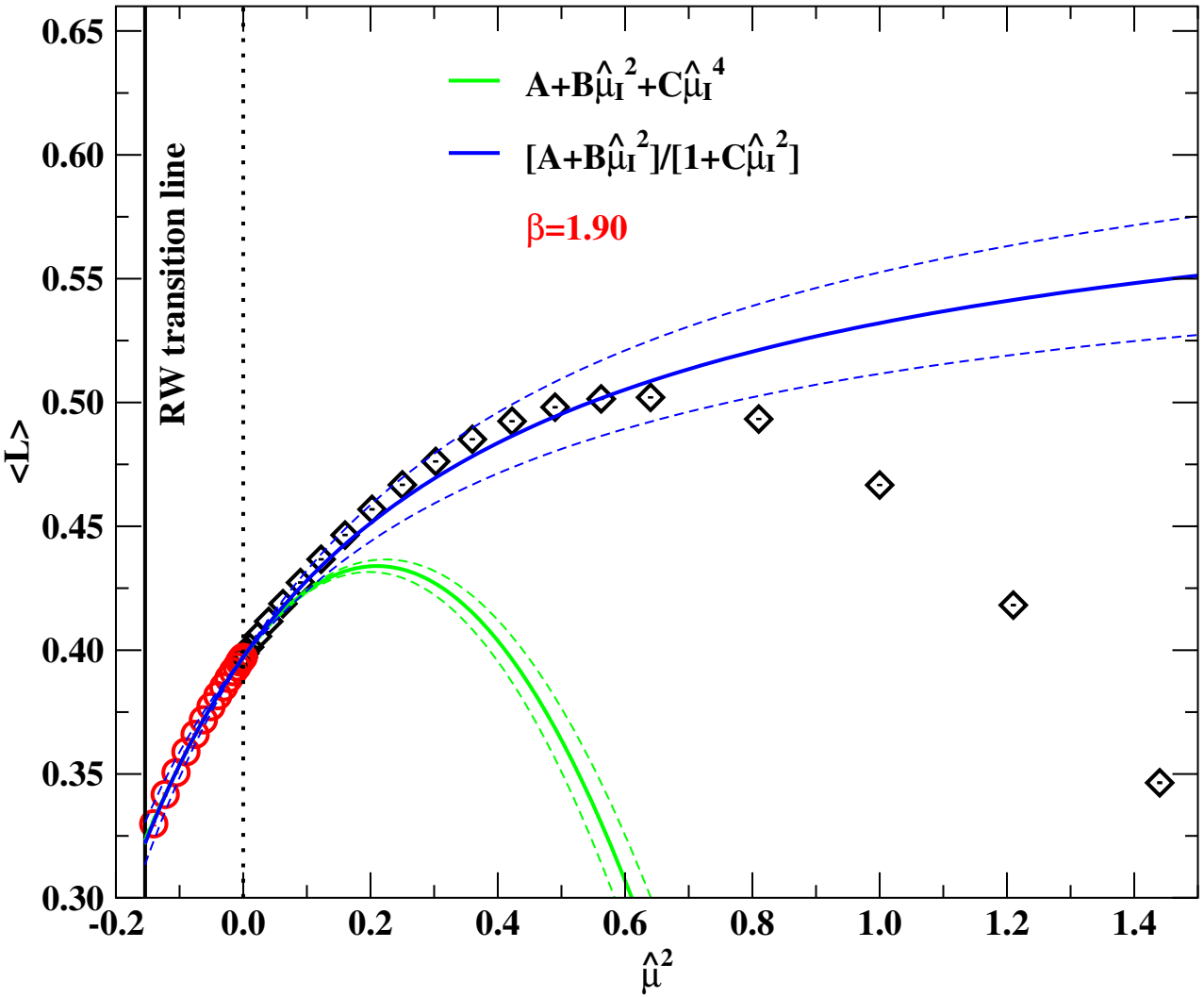
Numerical results: Fermion number density - β=1.90



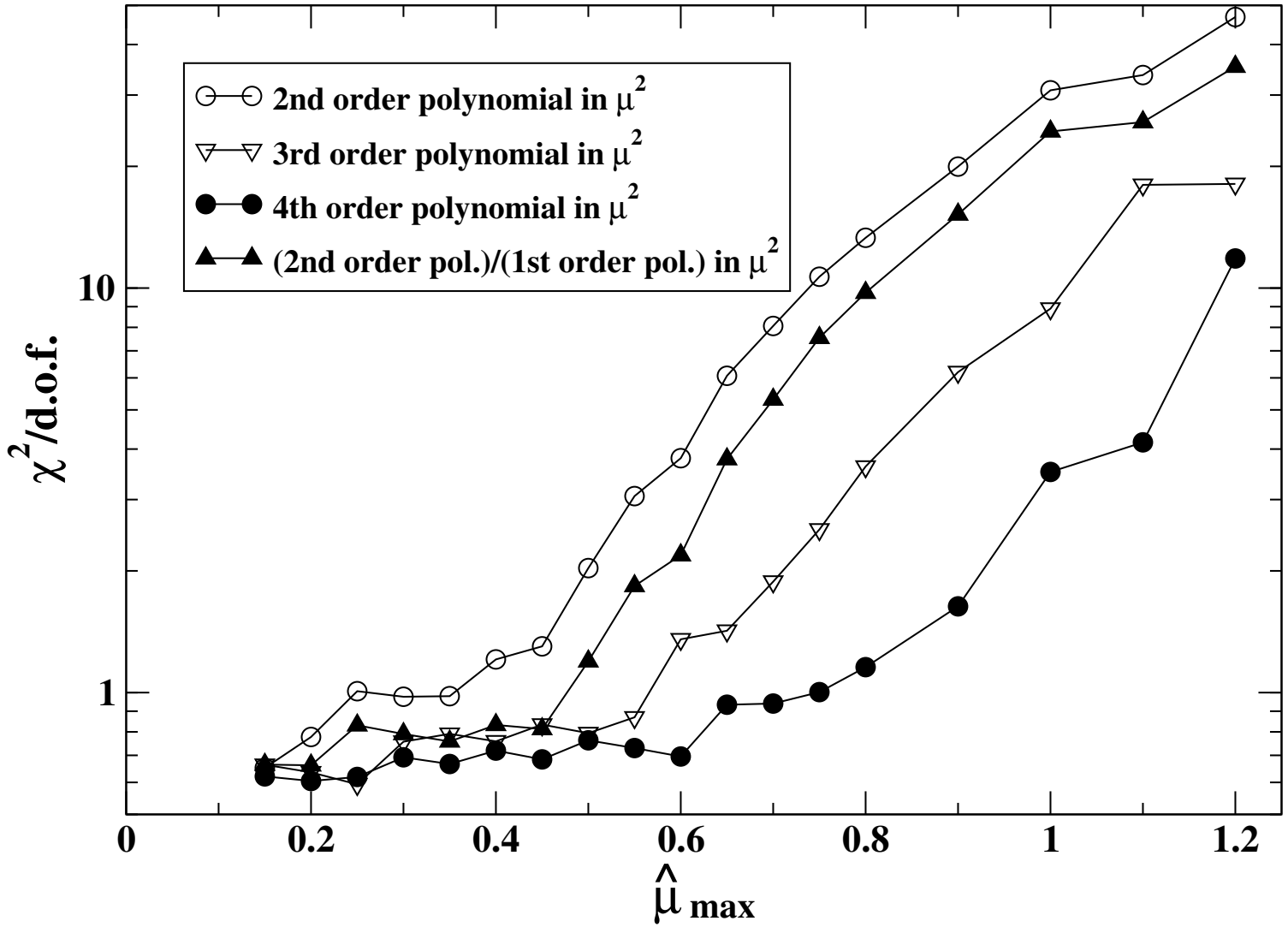
Numerical results: Chiral condensate - β=1.90



Numerical results: Polyakov loop - β=1.90



Numerical results: Global fits, Polyakov loop - β=1.90



Numerical results: Interpolating functions - regime (b)

- Polyakov loop, chiral condensate
  - second order polynomial in μ^2:

$$A + B\hat{\mu}_I^2 + C\hat{\mu}_I^4$$

  - ratio of two first order polynomials in μ^2:

$$\frac{A + B\hat{\mu}_I^2}{1 + C\hat{\mu}_I^2}$$

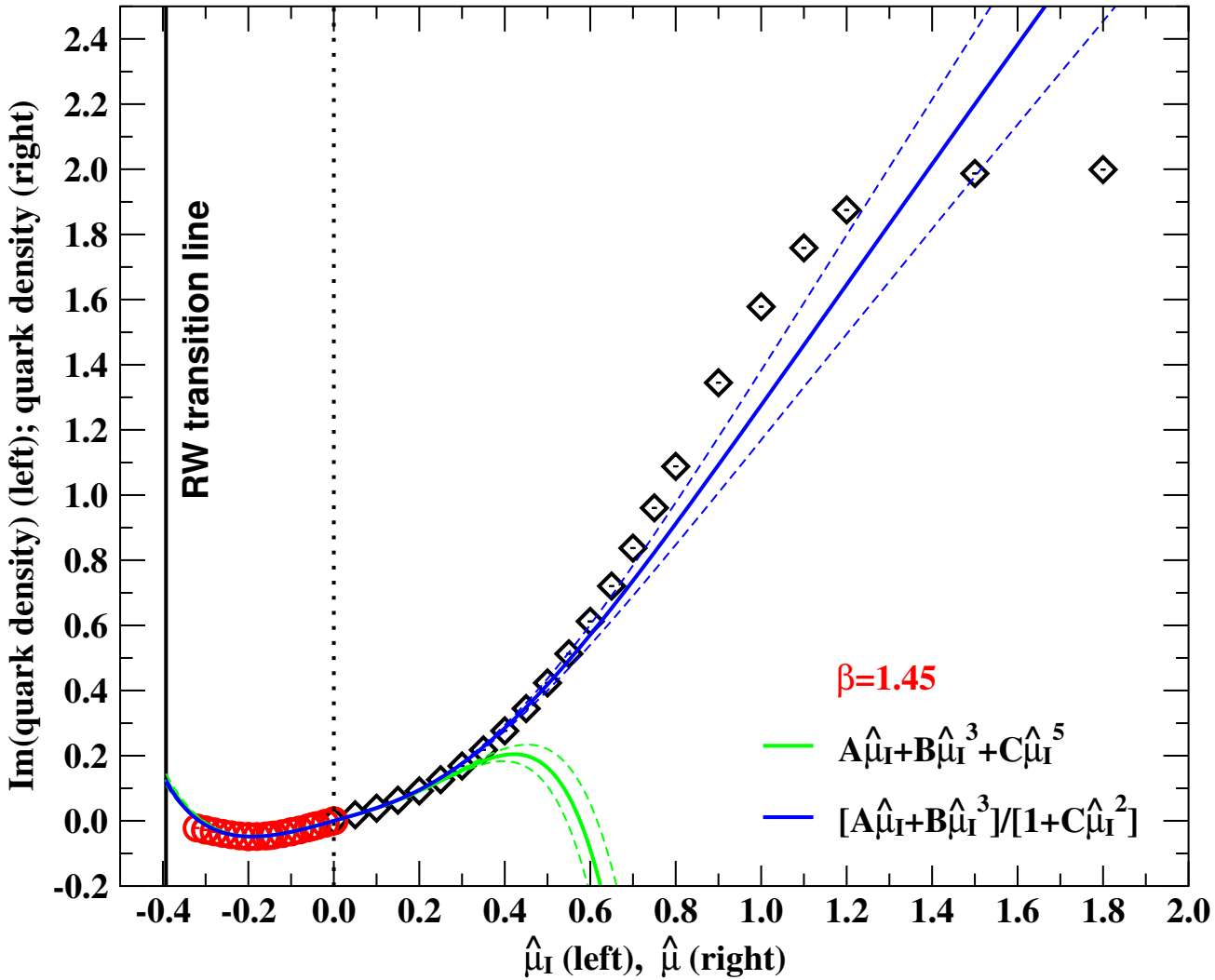
- fermionic number density
  - polynomial:

$$A\hat{\mu}_I + B\hat{\mu}_I^3 + C\hat{\mu}_I^5$$

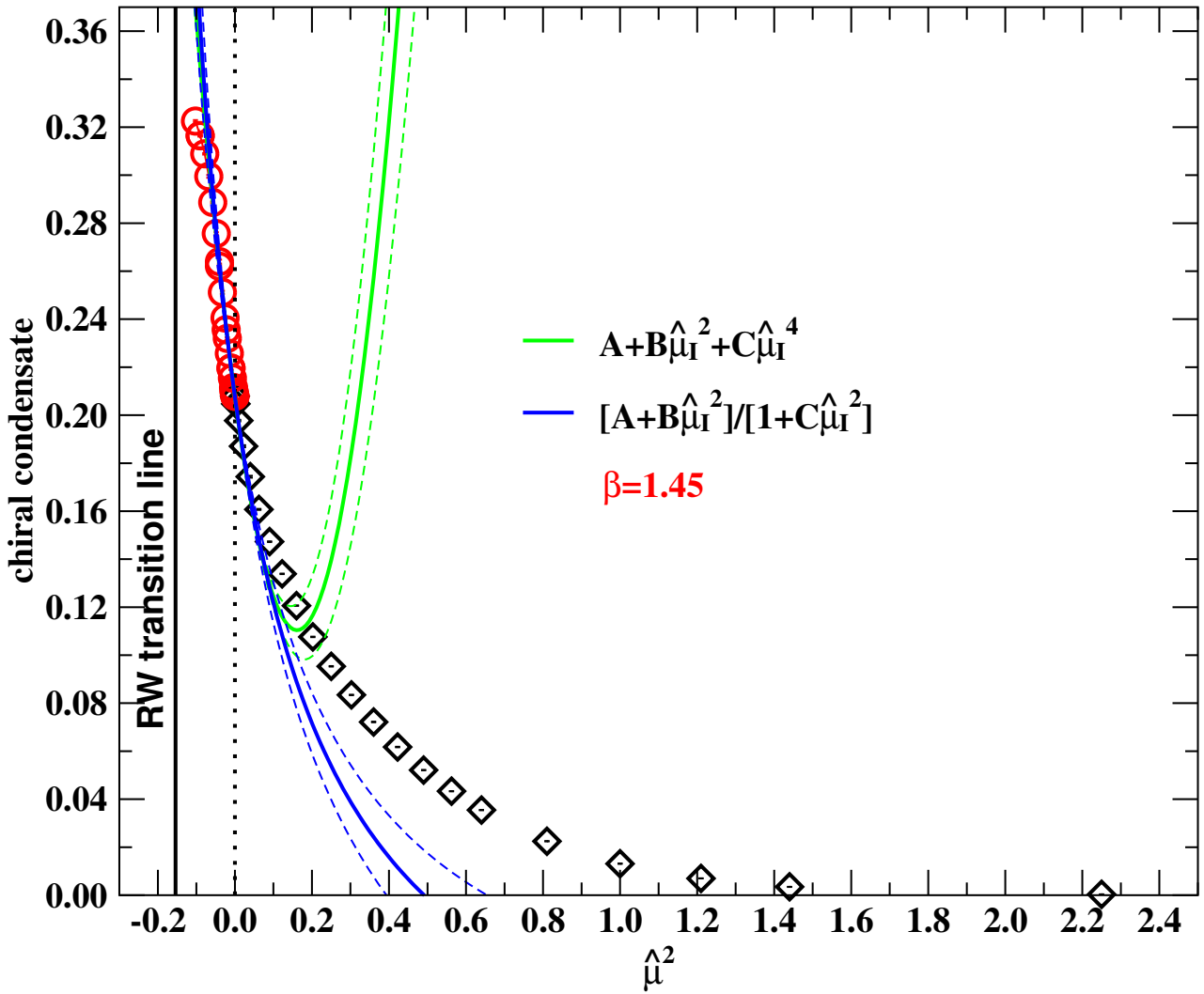
  - ratio of polynomials:

$$\frac{A\hat{\mu}_I + B\hat{\mu}_I^3}{1 + C\hat{\mu}_I^2}$$

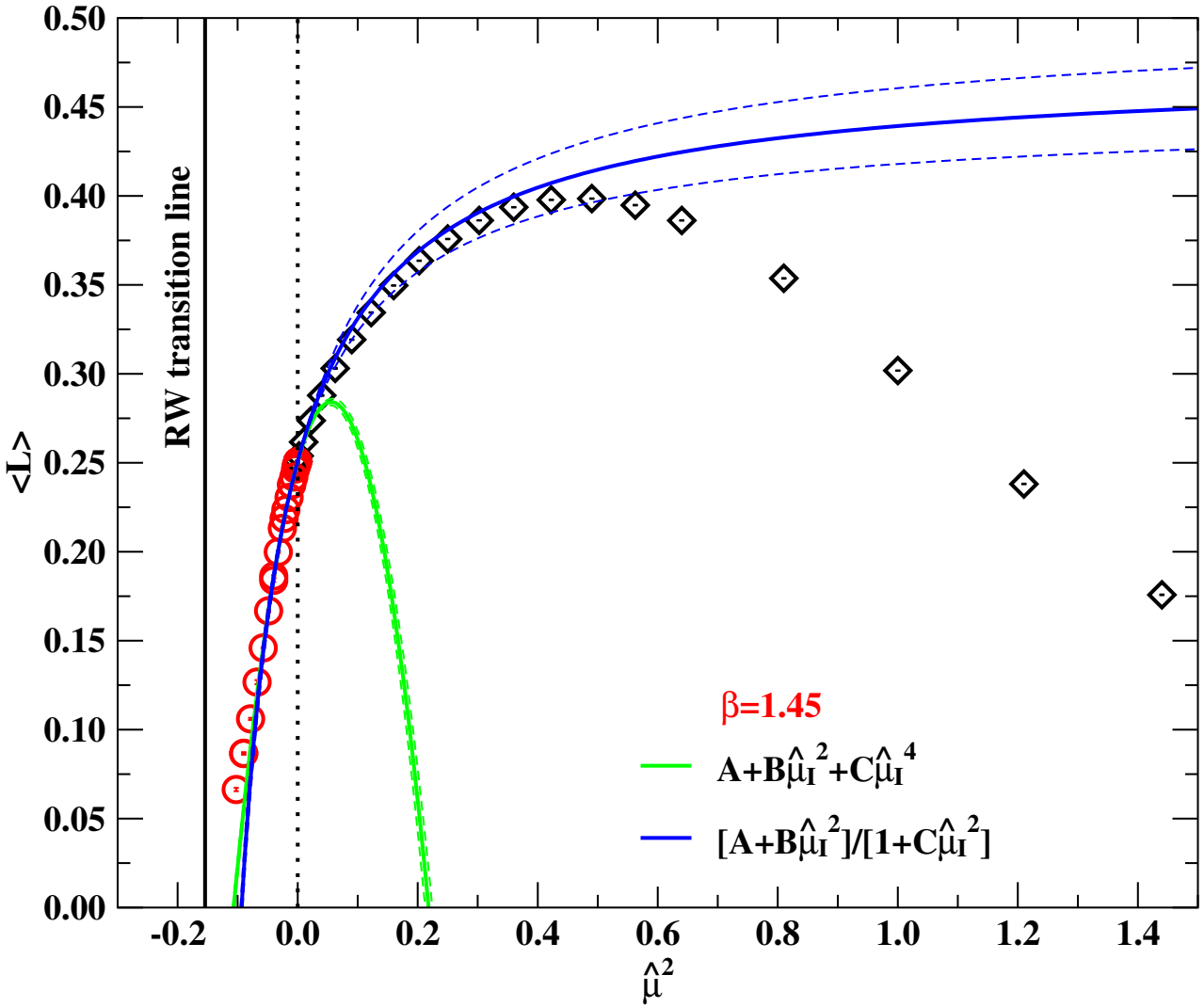
Numerical results: Fermion number density - β=1.45



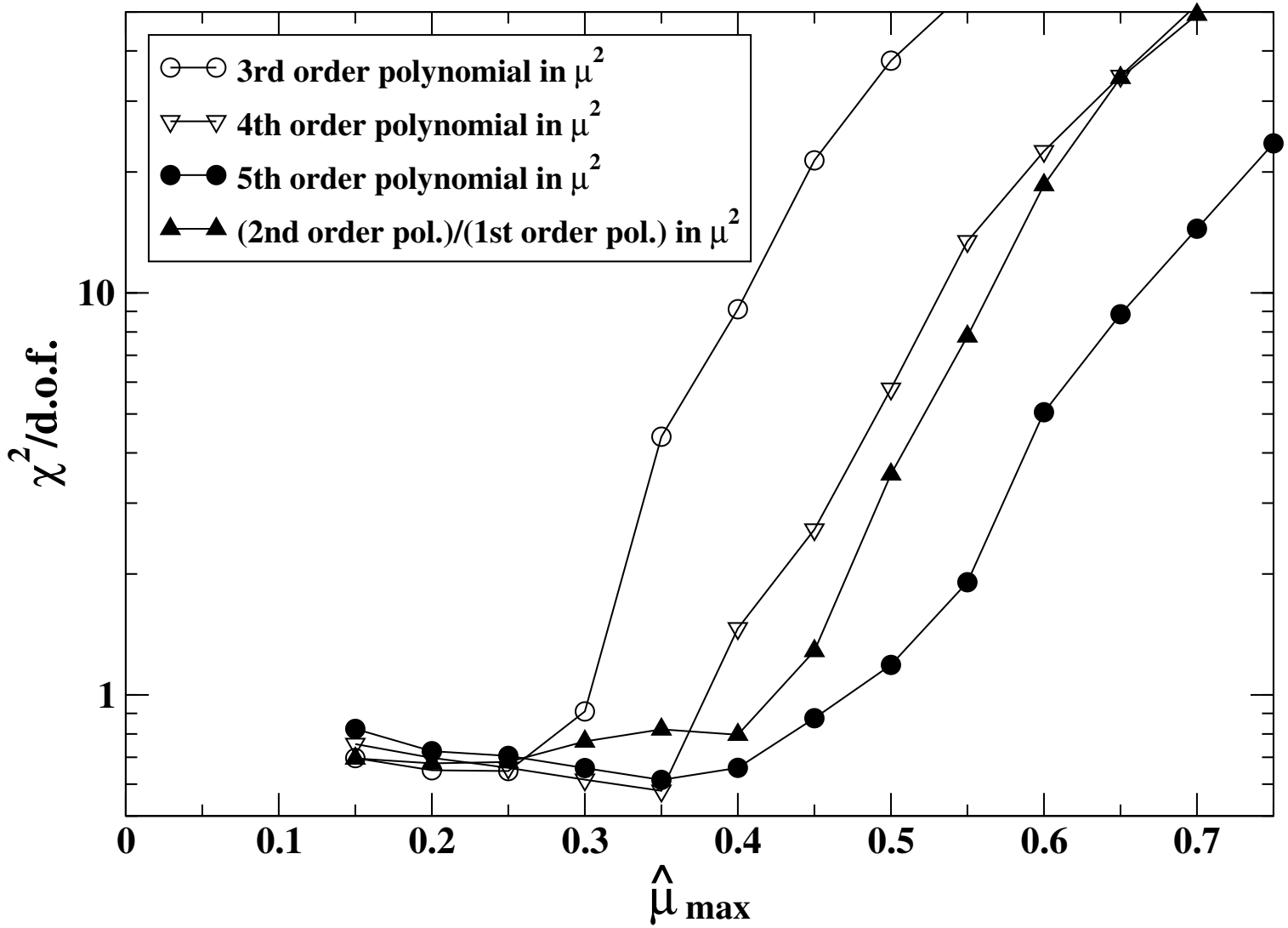
Numerical results: Chiral condensate - β=1.45



Numerical results: Polyakov loop - β=1.45



Numerical results: Global fits, Polyakov loop - β=1.45



Numerical results: Interpolating functions - regime (c)

- chiral condensate (periodicity in $\hat{\mu}_I$ equal to $\pi/4$):

$$A + B\cos(8\hat{\mu}_I) + C\cos(16\hat{\mu}_I)$$

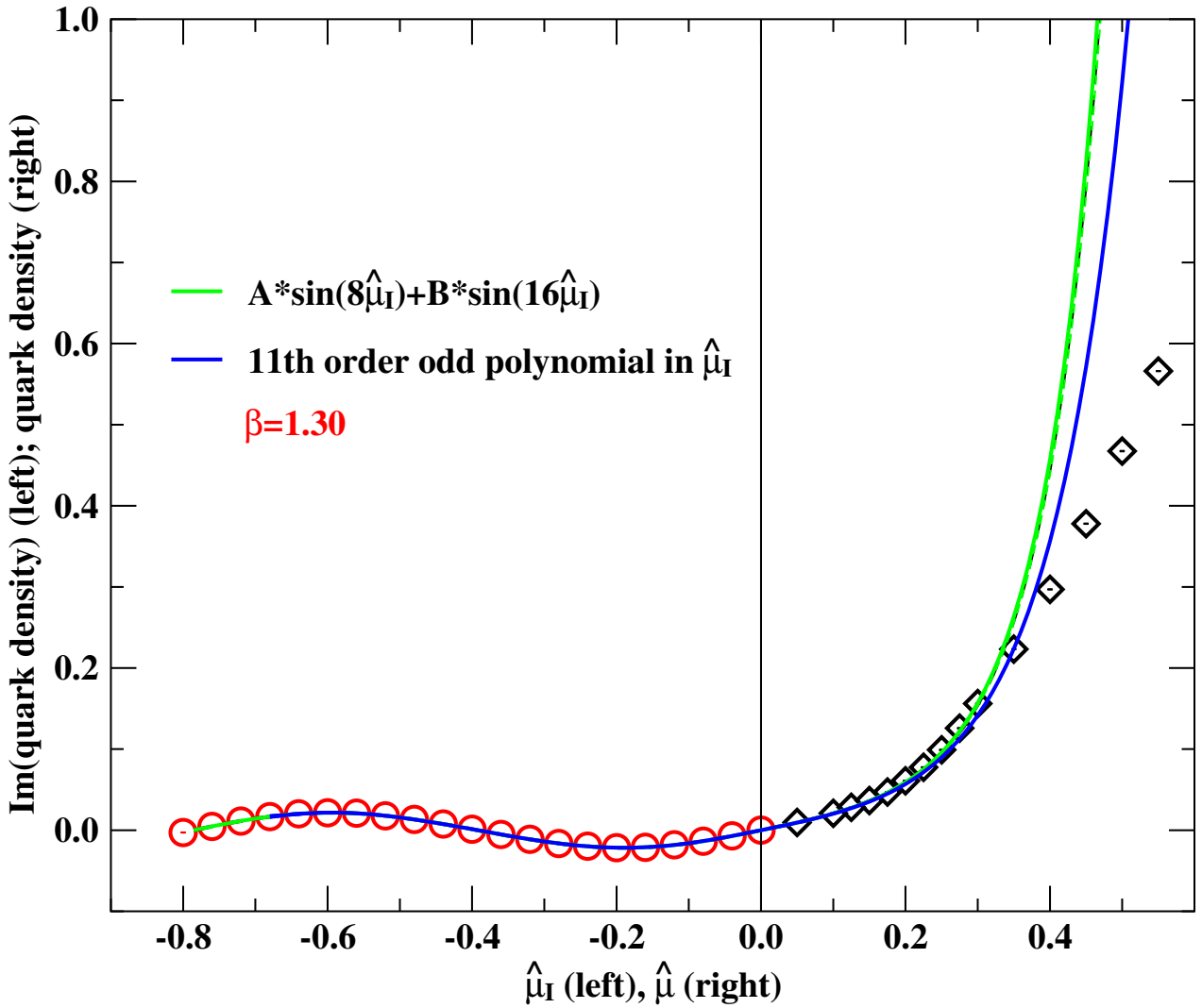
- Polyakov loop (periodicity in $\hat{\mu}_I$ equal to $\pi/2$):

$$A\cos(4\hat{\mu}_I) + B\cos(12\hat{\mu}_I)$$

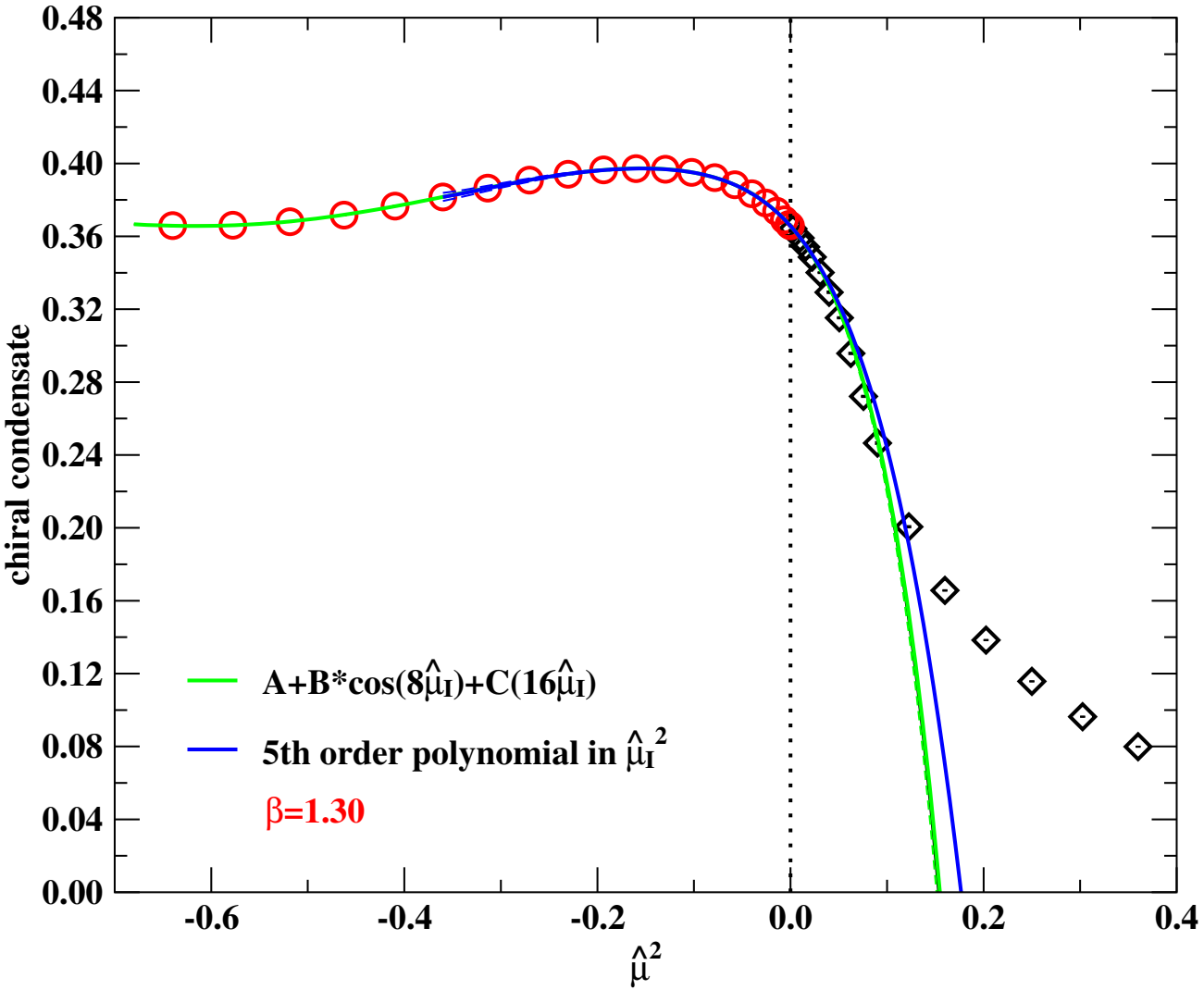
- fermionic number density (periodicity in $\hat{\mu}_I$ equal to $\pi/4$):

$$A\sin(8\hat{\mu}_I) + B\sin(16\hat{\mu}_I)$$

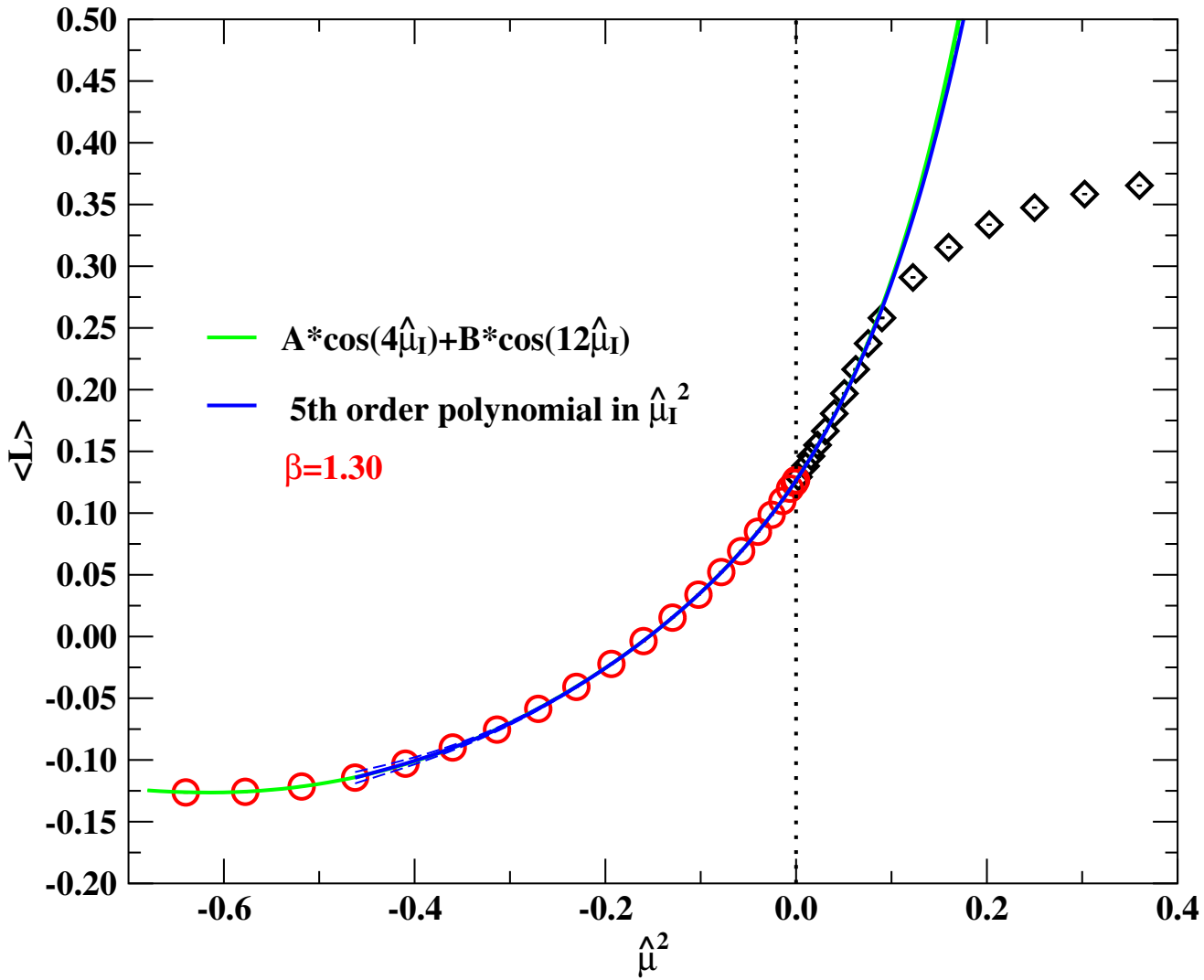
Numerical results: Fermion number density - β=1.30



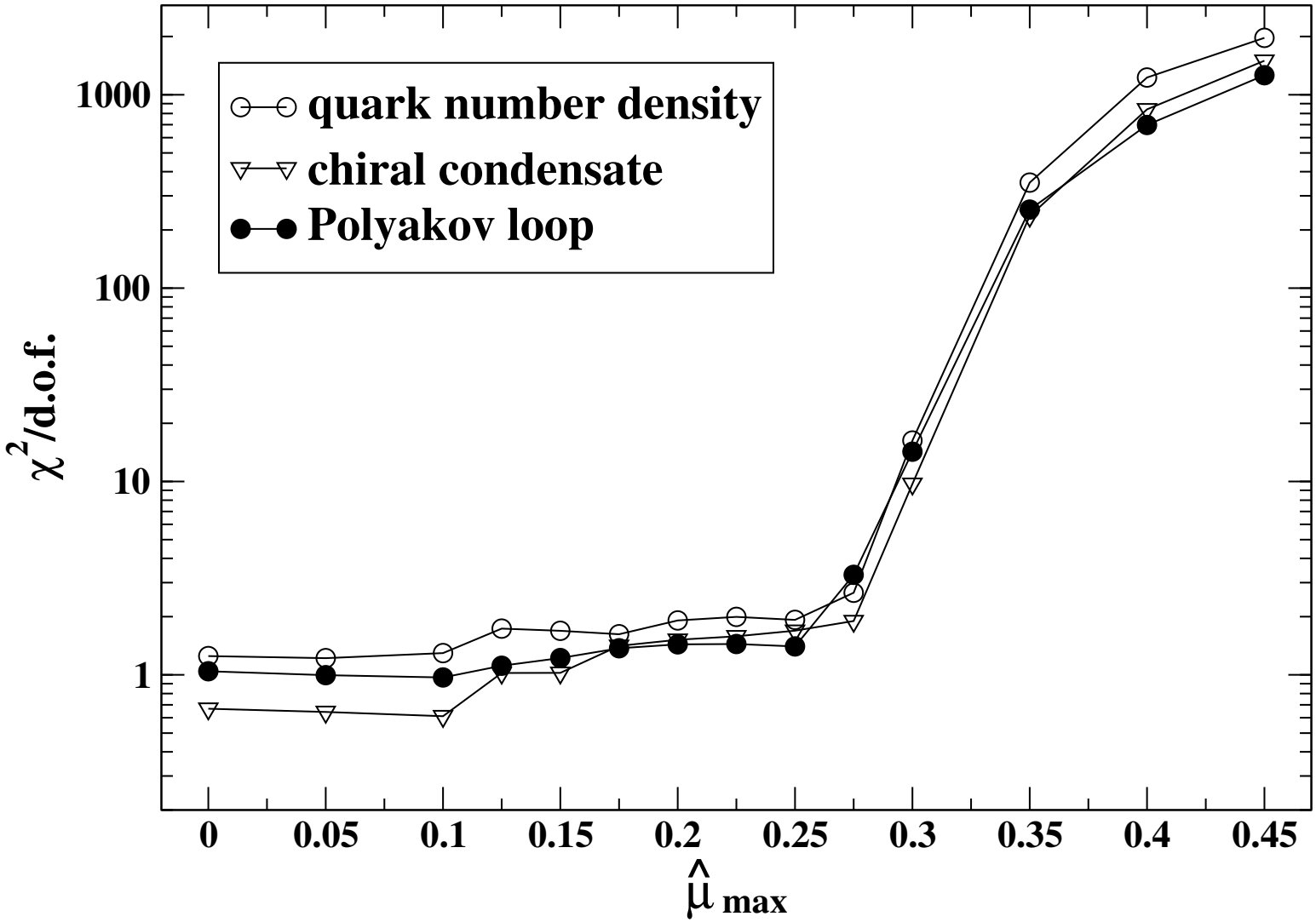
Numerical results: Chiral condensate - β=1.30



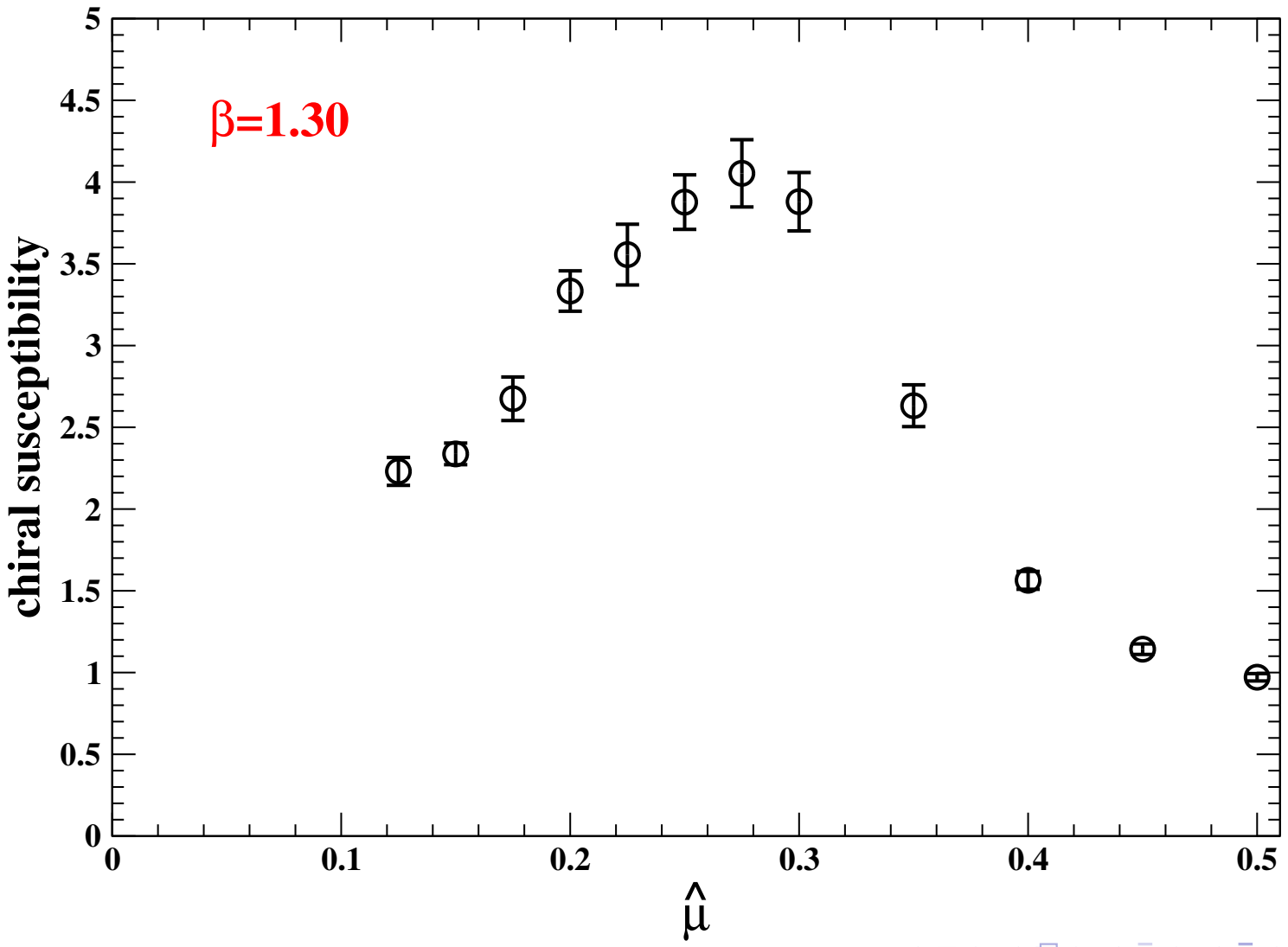
Numerical results: Polyakov loop - β=1.30



Numerical results: Global fits - β=1.30



Numerical results: chiral susceptibility - β=1.30



Conclusions

- By means of accurate Monte Carlo determinations in a theory which does not suffer from the sign problem, we have verified that the method of analytic continuation from an imaginary chemical potential is *well founded* and works fine within the limitations posed by the presence of non-analyticities and by the Roberge-Weiss transition lines.
- Data at real and imaginary chemical potential can be well described by common suitable analytic functions.
- A considerable improvement can be achieved, when extrapolating data from imaginary to real chemical potentials, if ratios of polynomials are used at temperatures larger than the pseudo-critical one at zero chemical potential. Deviations at very large values of the chemical potential could be due to unphysical saturation of the fermionic density (“Pauli blocking”).

Conclusions - cont'd

- The presence of the Roberge-Weiss transition has no influence on the analyticity of the partition function at real values of μ.
- At low temperatures Fourier sums seem to be the best Ansatz.
- These results can represent useful guidelines for the applications to real QCD.
- Numerical data in 2-color QCD at real chemical potential provide a reference for comparisons with analytical results in strong coupling and in μ/T expansions.

Outlook

- Analytical continuation of the critical line in 2-color QCD
- Application to SU(3) with finite isospin density