The QCD Phase Diagram at zero and small Baryon Densities

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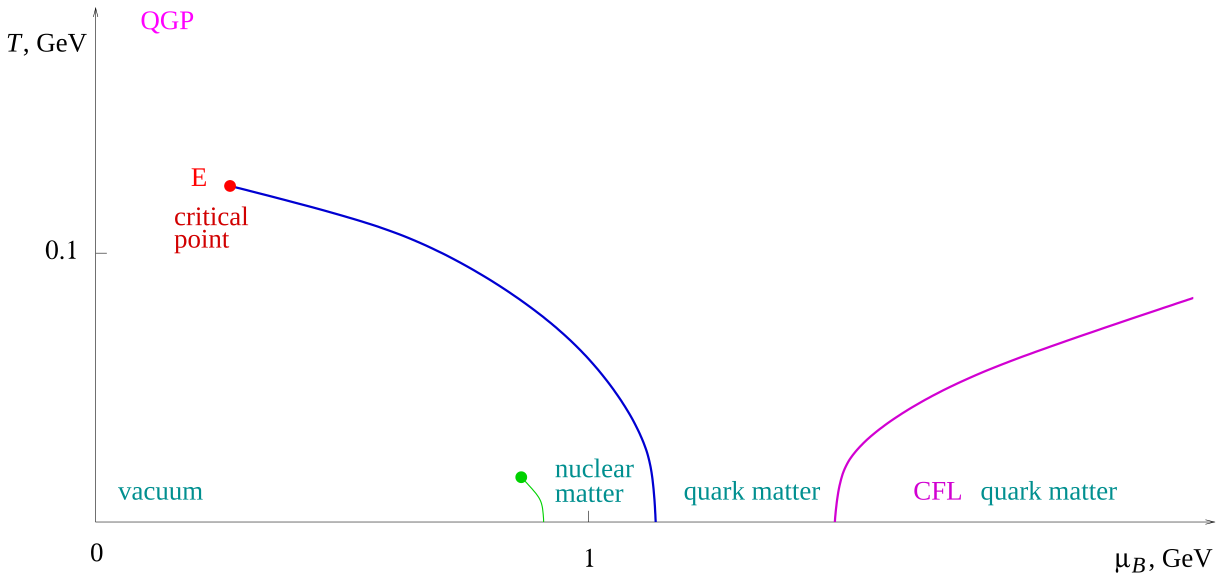
- The expected qualitative picture and computational methods
- The activities in the last year ⇒systematics !
- A non-standard scenario
- Conclusions

The expected phase diagram:



Non-pert. problem ⇒Lattice   1975-2001: $\mu \neq 0$ impossible ⇒sign problem!

Where does this picture come from?

- Simulations on T-axis (light quarks only now)
- models for $T = 0, \mu \neq 0$

Take more general view ⇒parameter space $\{m_{u,d}, m_s, T, \mu\}$

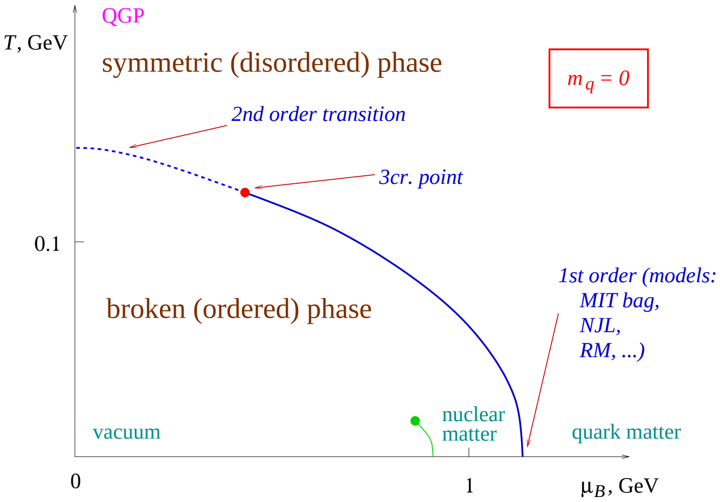
Pisarski, Wilczek

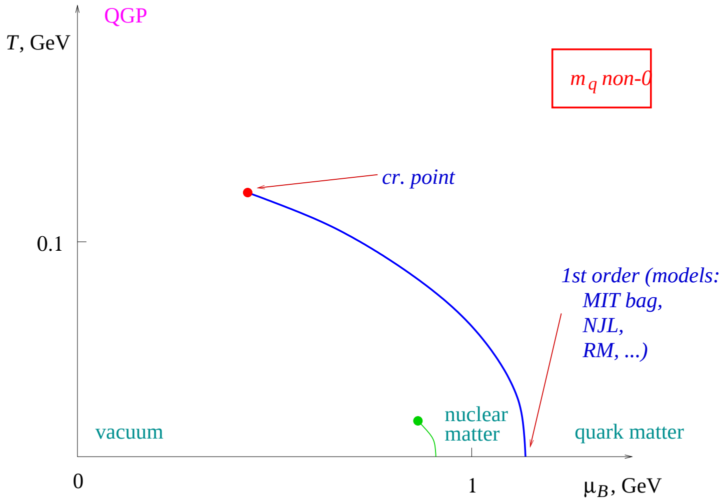
Rajagopal, Wilczek ...

$N_f = 2$:

$\mu, m = 0: \quad SU(2)_V \times SU(2)_A \to SU(2)_V$

true order parameter $\langle \bar\psi \psi \rangle$ $\Rightarrow$separate phases **if** second order **then** $\Rightarrow O(4)$





N.B. m=0: 1.O. all the way also possible

$N_f = 3$:

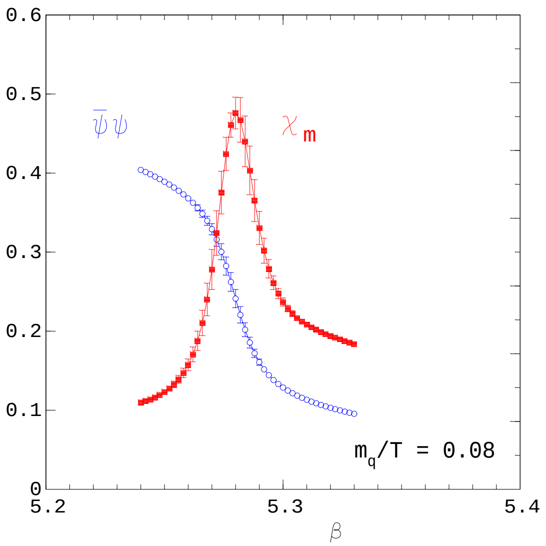
$\mu = 0, m < m_c$ first order

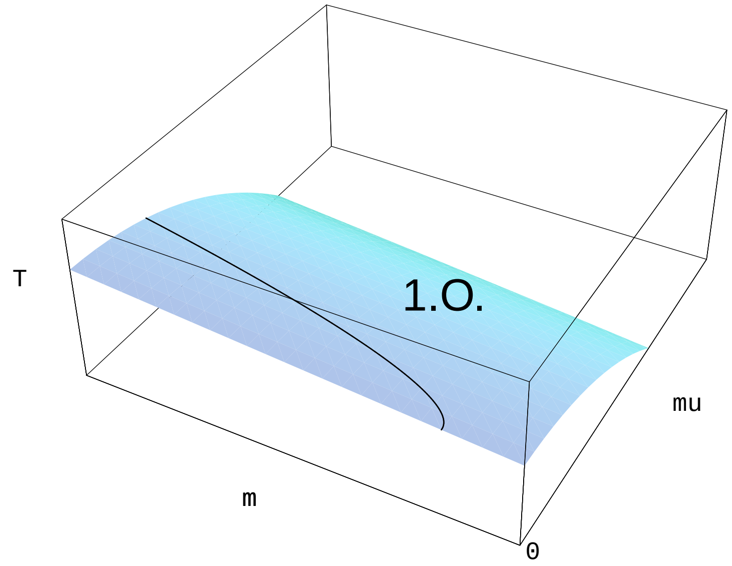
$\mu = 0, m > m_c$ crossover

$\Rightarrow$**standard scenario:** μ_c increases with m ($\mu = 0, T = 0$ transitions connected)

Full phase diagram 3d: $\{m, T, \mu\}$

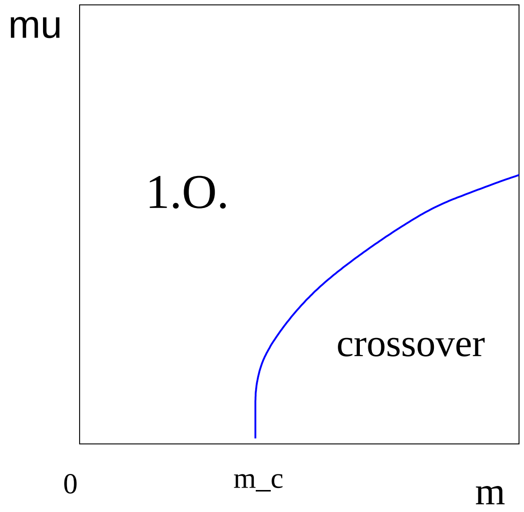
e.g. $N_f = 3$:





●confined/deconfined ⇒pseudo-crit. surface $T_0(\mu, m)$ (from susceptibilities)

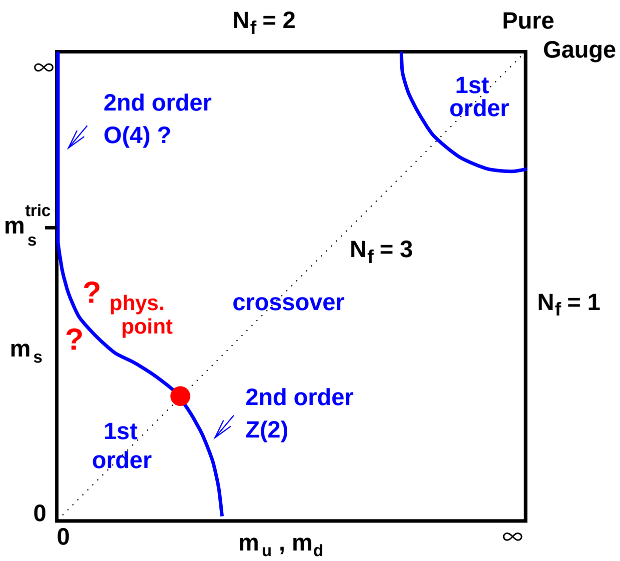
●1.O./crossover ⇒line of crit.points $T^E(\mu) = T_0(\mu, m_c(\mu))$ (from FSS)



Projection onto (pseudo-) critical surface:

⇒$\mu^c(m)$ or $m_c(\mu)$

The case $N_f = 2+1, \mu = 0$:



$\Rightarrow m_c(\mu = 0)$ (unimproved KS)

Bielefeld; Columbia; de Forcrand, O.P.

universality: 3d Ising

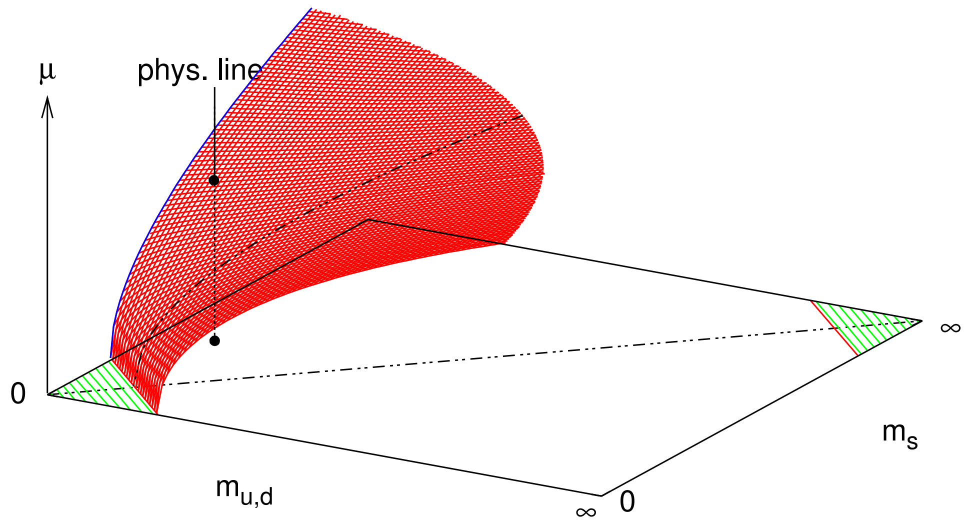
Bielefeld

N.B: m_c has cut-off effects!

(factor 1/4?)

Bielefeld, MILC

Finite density, $\mu \neq 0$:



Lattice QCD at finite temperature and density

Difficult (impossible?): **sign problem of lattice QCD**

$$Z = \int DU \, [\det M(\mu)]^f \mathrm{e}^{-S_g[U]}, \quad S_f = \sum_f \bar{\psi} M \psi$$

$\det(M)$ complex for SU(3), $\mu = \mu_B/3 \neq 0 \Rightarrow$ no Monte Carlo importance sampling

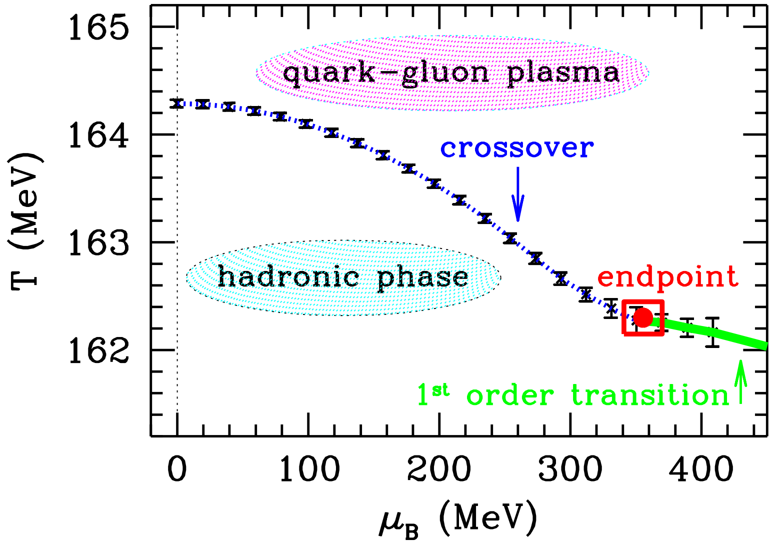
Evading the sign problem:

I. Two-parameter reweighting in (μ, β)

Fodor, Katz

$$Z = \left\langle \frac{\mathrm{e}^{-S_g(\beta)} \det(M(\mu))}{\mathrm{e}^{-S_g(\beta_0)} \det(M(\mu = 0))} \right\rangle_{\mu=0,\beta_0}$$

idea: simulate at $\beta_0 = \beta_c(0)$, better overlap by sampling both phases; errors? ovlp.?



I.a Reweighting + density of states

$\Rightarrow$larger μ, low T Fodor, Katz, Schmidt, Lat05

MILC

Bielefeld-Swansea

Gavai, Gupta

II. Taylor expansion

idea: for small μ/T, compute coeffs. of Taylor series $\Rightarrow$local ops. $\Rightarrow$gain V

convergence?

de Forcrand, O.P.

D'Elia, Lombardo

Azcoiti et al.

Chen, Luo

III.a Imaginary μ + analytic continuation

fermion determinant positive $\Rightarrow$no sign problem

idea: for small μ/T, fit **full** simulation results of imag. μ by Taylor series

- vary **two** parameters (μ, T) $\Rightarrow$controlled continuation?

de Forcrand, Kratochvila

Alexandru et al

III.b Imaginary μ + Fourier transformation

idea: canonical partition function at fixed baryon density

- no analytic continuation, but determinant needed $\Rightarrow$thermodynamic limit?

IV. Theories without sign prob.: finite isospin density

Kogut, Sinclair

idea: no sign problem, reproduces baryon chem. pot. for small μ/T?

All agree on $T_0(m, \mu)$!!! $(\mu/T \lesssim 1)$

$N_f = 2, \mu = 0, m = 0$: is it O(4)?

(or O(2) for finite a)

●previous evidence inconclusive

cf. old proceedings

New investigation:

D'Elia, Di Giacomo, Pica

FSS on $L^3 \times 4, L = 16 - 32$, standard staggered Fermions, R-algorithm, $m/T \gtrsim 0.055$

In critical region:

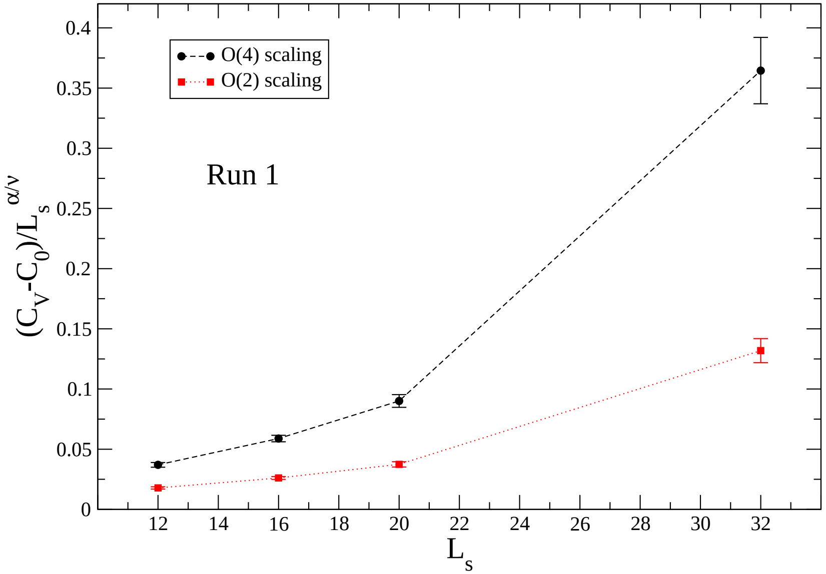
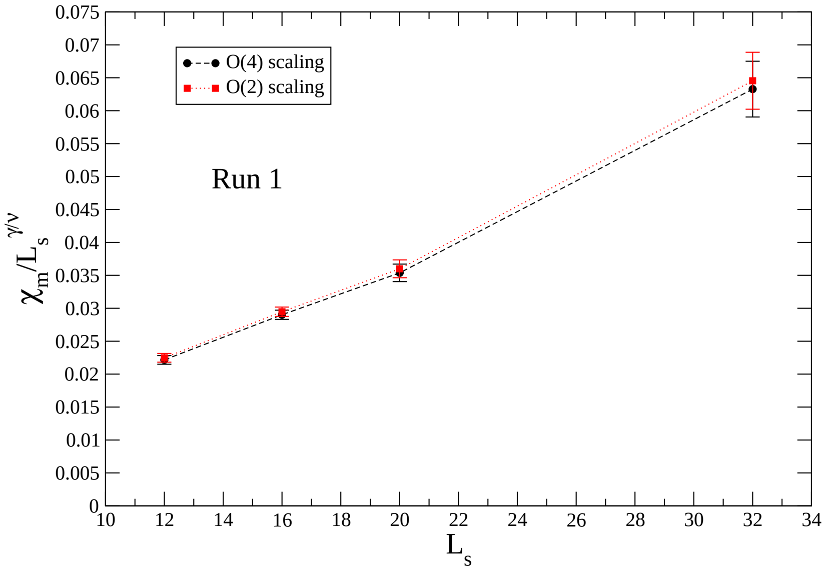
⇒spec. heat : $C_V - C_0 \simeq L^{\alpha/\nu} f_c \left(\tau L^{1/\nu}, am\, L^{y_h}\right) \quad \tau = 1 - T/T_c$

⇒suscept. of order param. : $\chi \simeq L^{\gamma/\nu} f_\chi \left(\tau L^{1/\nu}, am\, L^{y_h}\right)$ and others...

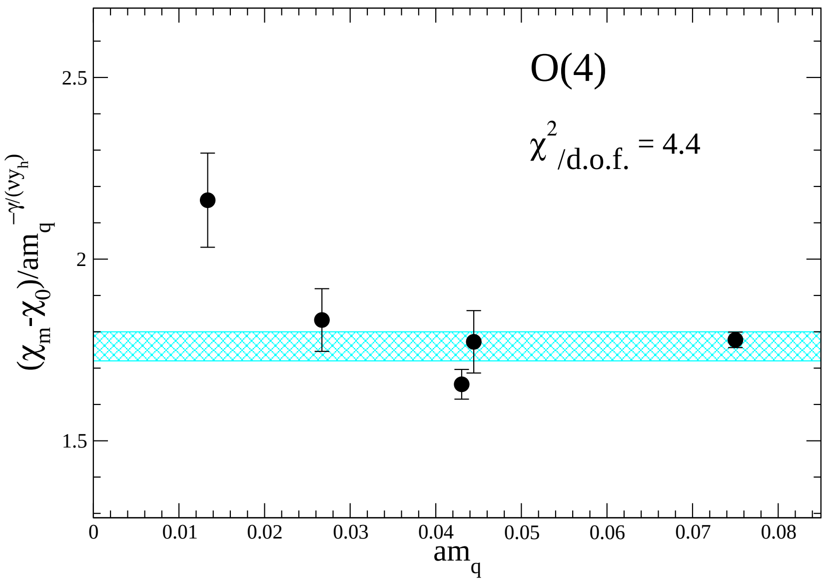
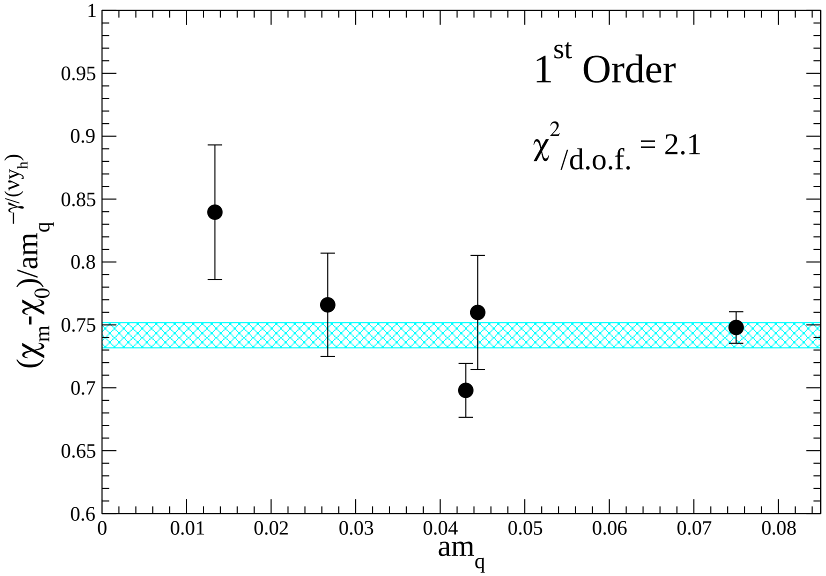
Strategy:

- Fix y_h to O(4) value
- choose L, am to keep $am\, L^{y_h}$ fixed⇒one variable only, inf. V⇒$am = 0$.

⇒check consistency with scaling

similar: keeping $\tau L^{1/\nu}$ fixed, check of 1st order:

But no metastability in plaquette distributions

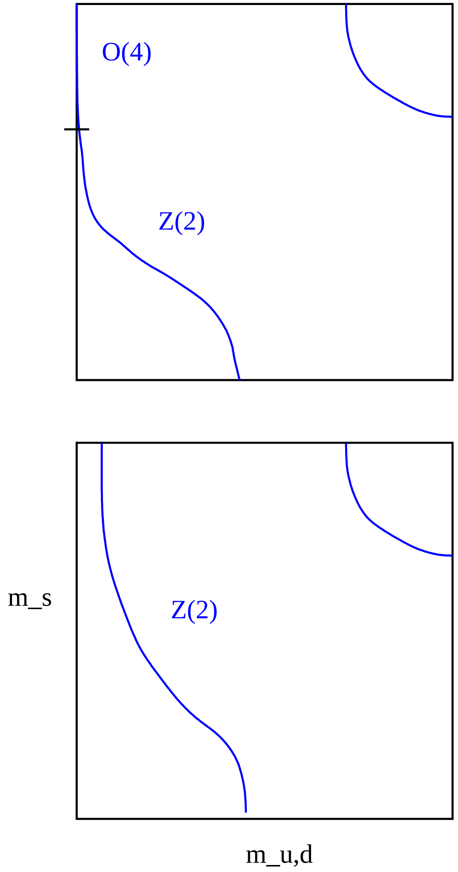
⇒still not conclusive!

- scaling window very small **?**
- fermion formulation**?** (Wilson sees O(4))
- cut-off effects **?**

⇒$N_t = 6$ study promised;

Suggestions:

- FSS at fixed am
- Binder cumulants
- exact algorithm



Finite density by Taylor expansion, $N_f = 2$:

Finite V: $Z(m > 0, \mu, T)$ analytic in entire parameter space

CP-Symmetry: $Z(\mu) = Z(-\mu)$ $\Rightarrow$all observables have Taylor series in $(\mu/T)^2$

pressure density: $p(T,\mu) = \left(\frac{T}{V}\right) \log Z(T,\mu)$, $\quad \frac{p}{T^4} = \sum_{n=0}^{\infty} c_{2n}(T) \left(\frac{\mu}{T}\right)^{2n}$

Coefficients: generalized quark number suscept. at $\mu = 0$ $\Rightarrow$measurable!

$V \to \infty$: phase transitions $\Rightarrow$singularities in pressure

radius of convergence $\equiv$ distance to nearest singularity;

e.g.: $\rho_n = \left|\frac{c_0}{c_{2n}}\right|^{1/2n}$, $\quad r_n = \left|\frac{c_{2n}}{c_{2n+2}}\right|^{1/2}$, $\quad \rho, r = \lim_{n\to\infty} \rho_n, r_n$

if singularity on real axis (asymptotically all coeffs. positive) $\Rightarrow$critical point

Technicalities:

μ-dependence in $\det M \Rightarrow \frac{\partial \ln \det M}{\partial \mu} = \mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial \mu}\right)$ etc.

$\Rightarrow$traces of composite local ops., Gaussian noise vectors $\sim O(10-100)$

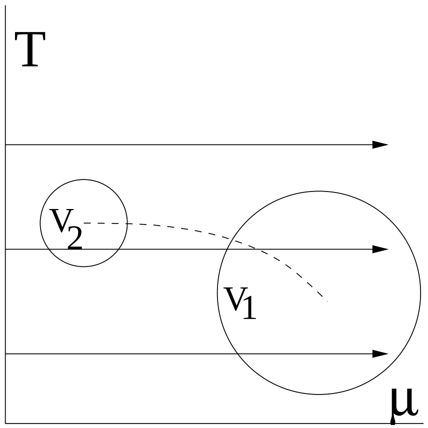
non-trivial FSS of susceptibilities $\Rightarrow$delicate cancellations for large V

Quark number susceptibility to order μ^6

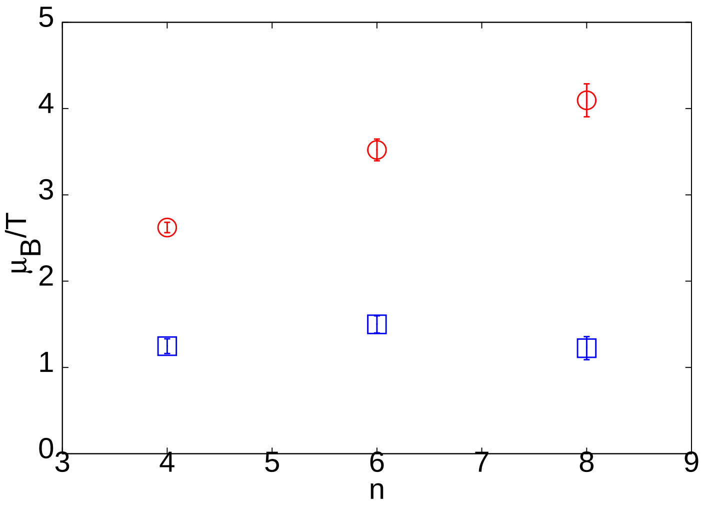
Gavai, Gupta

Lattices $L^3 \times 4, L = 8-24$, standard staggered, R-algorithm, $m/T_0 = 0.1$

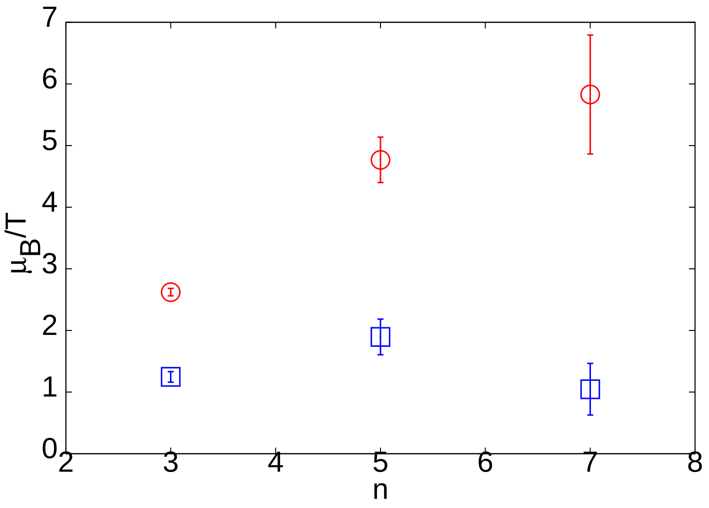
Strategy: compute coeffs. at different $T/T_0 = 0.75 - 2.15$$\Rightarrow$extrapolate to finite μ



$T/T_0 = 0.95$, convergence radius vs. order n:



ρ_n on $8^3, 24^3$



r_n ond $8^3, 24^3$

⇒**strong volume dependence!** need $Lm_\pi \gtrsim 5-6 \quad (L \gtrsim 16-18)$

⇒need more terms for larger V

⇒quoted result:

$$\mu_B^c/T = 1.1 \pm 0.2$$
$$T/T_0 = 0.95$$

The pressure to order μ^6

Bielefeld-Swansea

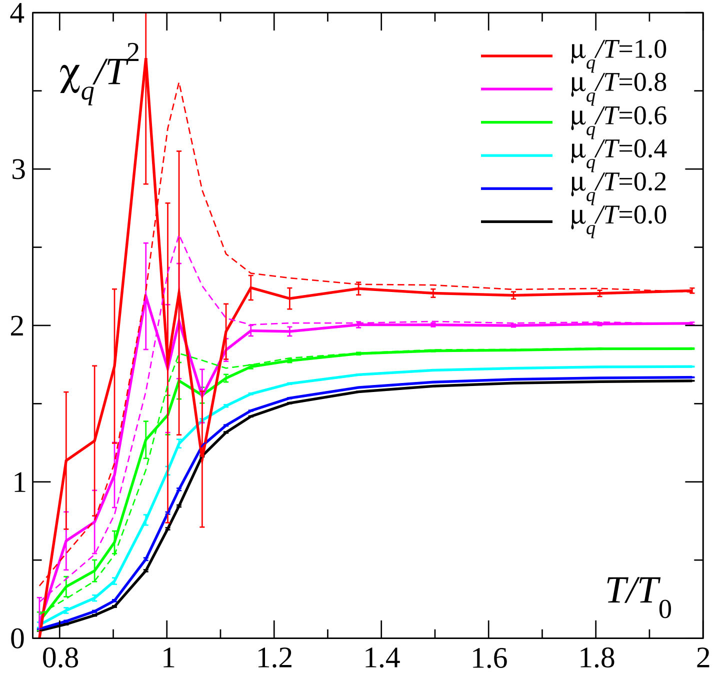
Lattice $16^3 \times 4$, Symanzik improved Wilson, p4-improved staggered fermions, R-algorithm, $m/T_0 \approx 0.4$

Comparisons with (μ/T)-expansions of

- high T pert.theory — Vuorinen
- hadron resonance gas (HRG) model — Karsch, Redlich, Tawfik

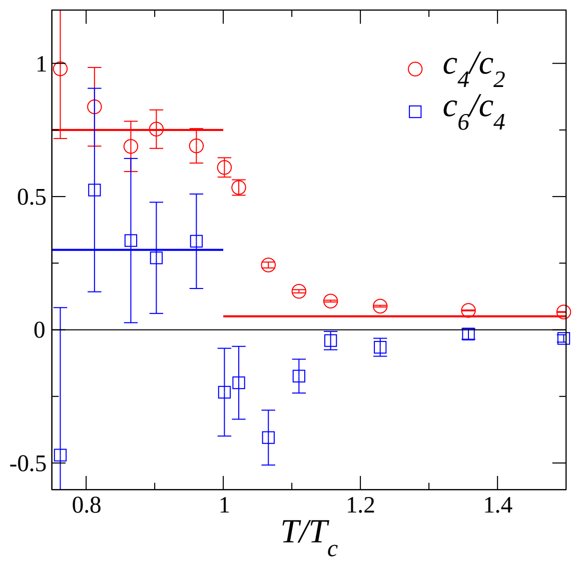
coefficients in different orders:

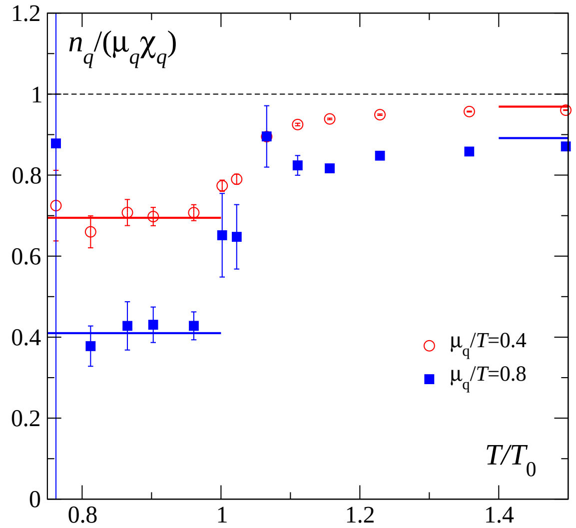
$c_6 \ll c_4 \ll c_2 \Rightarrow$coeffs.$\sim O(1)$ for "natural" expansion parameter $\frac{\mu}{\pi T}$ — de Forcrand, O.P.



radius of convergence:

$n_q/\chi_q = \frac{\partial p}{\partial n_q}$ ($= 0$ for 2.O.)





lines: coeffs. from HRG model: $c_4/c_2 = 3/4$

- consistency with hadron resonance gas
- no evidence for critical point
- Not in conflict with Gavai, Gupta (different action, larger m)
- but different conclusion than at μ^4!
- previous experience (spin models, strong coupling series), use many terms (10-20)

  some work, some fail $\Rightarrow$experiment e.g.Itzykson, Drouffe

Systematics of reweighting and Taylor expansion

$$\langle O \rangle_{(\beta,\mu)} = \frac{\langle O\, e^{\frac{n_f}{4}\Delta \ln \det M} e^{-\Delta S_g} \rangle_{(\beta_0,0)}}{\langle e^{\frac{n_f}{4}\Delta \ln \det M} e^{-\Delta S_g} \rangle_{(\beta_0,0)}} \sim e^{-V\Delta F}$$

$$\det M = |\det M| e^{i\theta}$$

⇒**Breakdown of reweighting** for $\langle \cos\theta \rangle \ll 1$

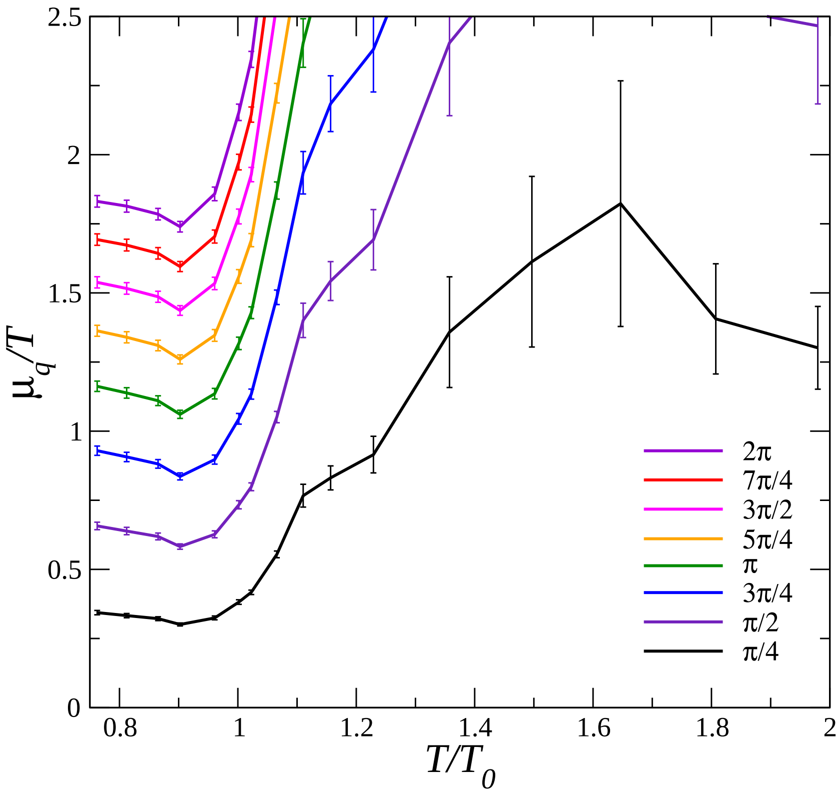
or $\sigma(\theta) = \sqrt{\langle \theta^2 \rangle - \langle \theta \rangle^2} > \pi/2$

⇒compute variance from Taylor coeffs.

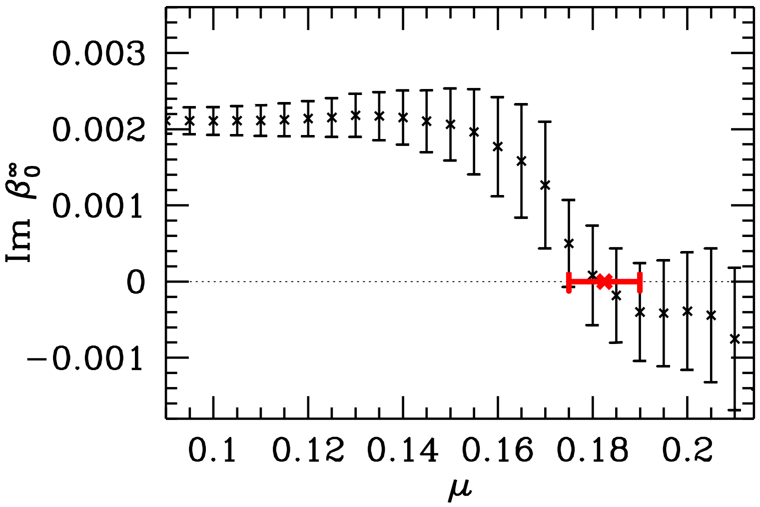
Bielefeld-Swansea

$$\theta^{(n)} = \frac{n_f}{4} \mathrm{Im} \sum_{j=1}^{n} \frac{\mu^{2j-1}}{(2j-1)!} \frac{\partial^{2j-1} \ln \det M}{\partial \mu^{2j-1}}$$

Contours of $\sigma(\theta)$: (fixed $V = 16^3$)



Fodor, Katz:



Observation: LYZ competing with noise of $\det M$

$$\mathcal{Z}_{\rm norm}(\beta_{\rm Re},\beta_{\rm Im},\mu) = \left| \left\langle e^{6i\beta_{\rm Im}N_{\rm site}\Delta P} e^{i\theta} \left| e^{(N_{\rm f}/4)(\ln\det M(\mu) - \ln\det M(0))} \right| \right\rangle_{(\beta_{\rm Re},0,0)} \right|$$

⇒doesn't work at infinite V (not surprising...)

In practice: ●enough statistics for a given volume? ●errors reliable?

QCD at finite isospin density

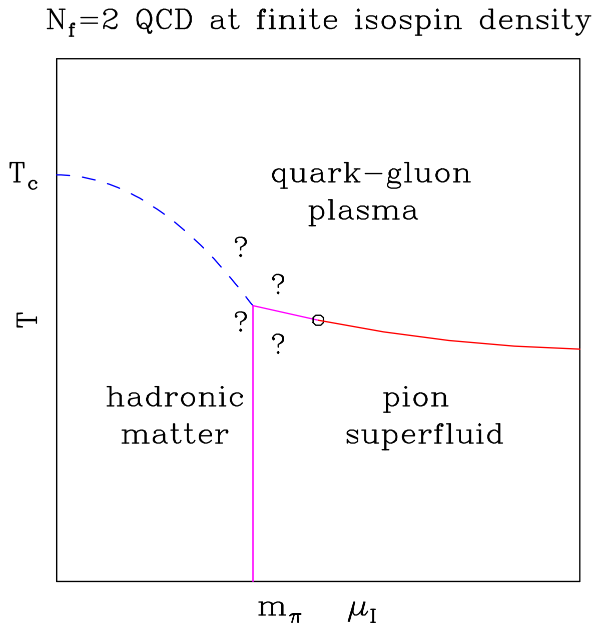
Son, Stephanov

Opposite chemical potentials for u,d-quarks:

$\mu_u = -\mu_d = \mu \Rightarrow \mu_I \equiv (\mu_u - \mu_d) = 2\mu$

$\Rightarrow$phases of determinants cancel

$$Z = \int DU \, |\det M(\mu)|^{N_f} \, \mathrm{e}^{-S_g[U]}$$



Pion condensate $\neq$ QCD, but for $\mu_I < m_\pi$ recover QCD:

$$\langle O \rangle_\mu = \frac{\langle e^{i\theta} O \rangle_{\mu_I = 2\mu}}{\langle e^{i\theta} \rangle_{\mu_I = 2\mu}}$$

consider O probing p.t.

for $\langle \cos\theta \rangle_{\mu_I} \sim 1, O' = e^{i\theta} O$ shows same transition!

Numerically verified for $T_0(\mu, m), \quad N_f = 2, 3$:

- in Taylor expansion (Bielefeld-Swansea)
- simulations at μ_I (Kogut, Sinclair) and μ_i (de Forcrand, O.P.)

Phase of the determinant and phase-quenched QCD

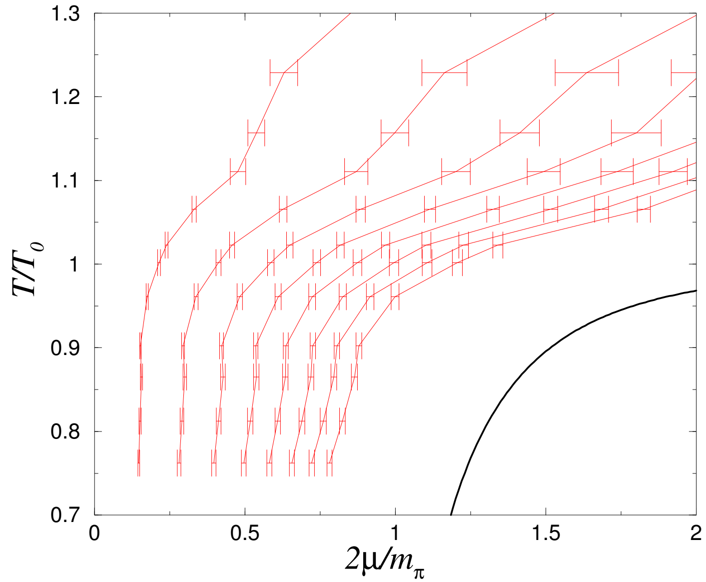
Splittorff

$\sigma(\theta)$ and the transition to a pion condensate at finite isospin:

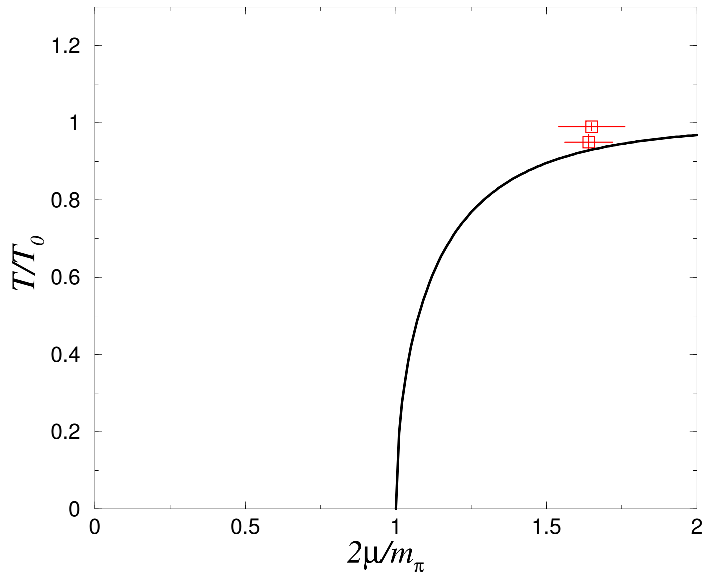
$\Rightarrow$related, since

phase of $\det M$ "destroys" pion condensate

boundary for reweighting?



Fodor, Katz endpoints, different m



observation:

FK-points both lie on boundary $\Rightarrow$...?

similarly for Taylor exp.

QCD at complex μ: general properties

$$Z(V,\mu,T) = \mathrm{Tr}\left(\mathrm{e}^{-(\hat{H}-\mu\hat{Q})/T}\right); \quad \mu = \mu_r + \mathrm{i}\mu_i; \quad \bar{\mu} = \mu/T$$

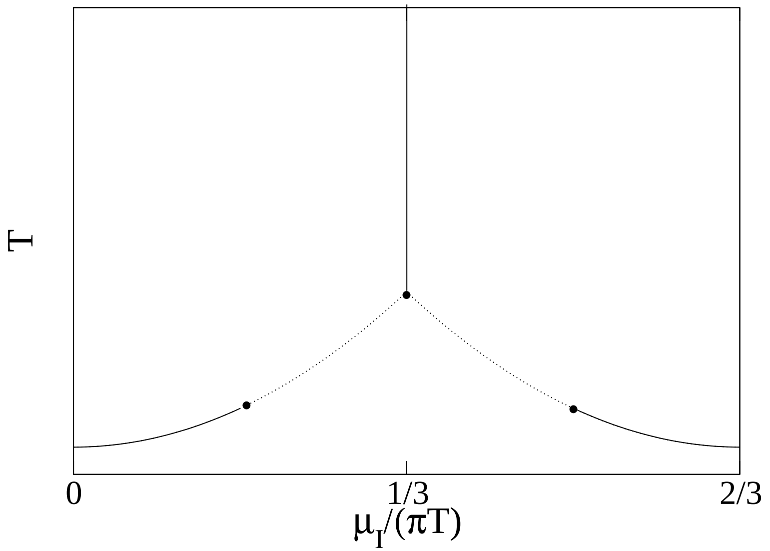
exact symmetries: μ-reflection and μ_i-periodicity — Roberge, Weiss

$$Z(\bar{\mu}) = Z(-\bar{\mu}), \qquad Z(\bar{\mu}_r,\bar{\mu}_i) = Z(\bar{\mu}_r,\bar{\mu}_i + 2\pi/N_c)$$

Imaginary μ phase diagram:

Z(3)-transitions: $\bar{\mu}_i^c = \frac{2\pi}{3}\left(n+\frac{1}{2}\right)$

1rst order for high T, crossover for low T



analytic continuation within arc:

$$|\mu|/T \leq \pi/3 \Rightarrow \mu_B \lesssim 550\mathrm{MeV}$$

$$\langle O \rangle = \sum_n^N c_n \bar{\mu}_i^{2n} \Rightarrow \mu_i \longrightarrow \mathrm{i}\mu_i$$

Pade approximants? (Lombardo, Lat05)

A generalized imaginary μ-approach

Azcoiti, Di Carlo, Galante, Laliena

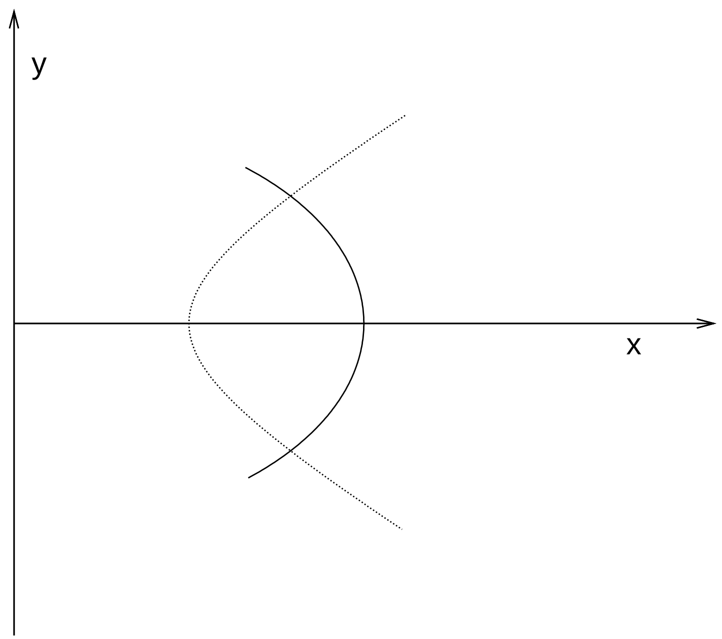
Reformulation of staggered action, chemical potential term

$$\frac{1}{2}\sum_n \bar{\psi}_n \eta_0(n) \left(e^{\mu a} U_{n,0}\psi_{n+0} - e^{-\mu a} U^\dagger_{n-0,0}\psi_{n-0} \right)$$

Hasenfratz, Karsch

$$\rightarrow \quad x\frac{1}{2}\sum_n \bar{\psi}_n \eta_0(n) \left(U_{n,0}\psi_{n+0} - U^\dagger_{n-0,0}\psi_{n-0} \right)$$

$$+ \quad y\frac{1}{2}\sum_n \bar{\psi}_n \eta_0(n) \left(U_{n,0}\psi_{n+0} + U^\dagger_{n-0,0}\psi_{n-0} \right), \qquad x = \cosh(a\mu), y = \sinh(a\mu)$$



solid line: phase transitions

dotted line: physical line $x^2 - y^2 = 1$

Sign problem $\Rightarrow$simulations at imaginary $y = i\bar{y}$

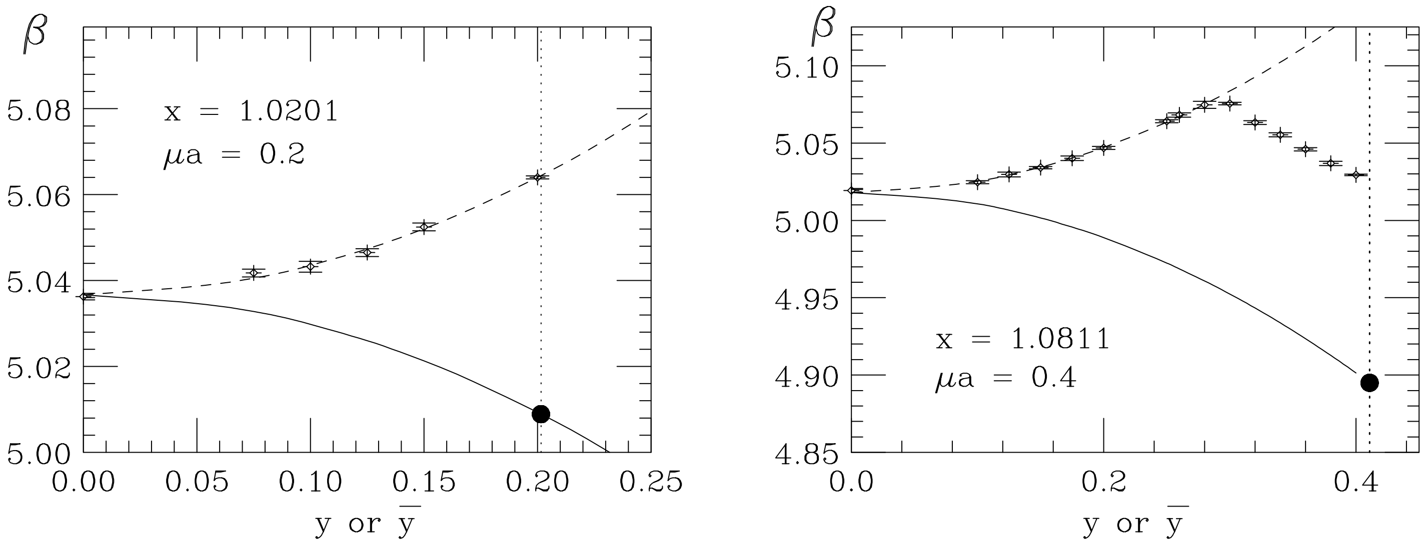
possible improvement: simulations at different x, y, lower temperatures

better control of continuation?

Numerical results, $N_f = 4$

$8^3 \times 4$, standard staggered, R-algorithm, $m/T \approx 0.2$

Fitting to $\beta_c(\bar{y}) = \beta_0 + \beta_1 \bar{y}^2$ plus continuation:



- works at least as well as standard imag. μ, more expensive
- can it be made to work better? control of errors beyond $\mu/T \gtrsim 1$?
- $N_f = 2$ in progress, preliminary evidence for critical point — Laliena, Lat05
- point of departure for reweighting, improved range?

Roberge, Weiss

Hasenfratz, Toussaint

Alford, Kapustin, Wilczek

de Forcrand, Kratochvila

QCD at fixed baryon number

Fix baryon number B: $\Rightarrow \delta(3B - \int d^3x\, \bar{\psi}\gamma_0\psi)$

$$Z_C(B) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\left(\frac{\mu_i}{T}\right)\ e^{-i3B\frac{\mu_i}{T}}\, Z_{GC}(\mu = i\mu_i)$$

canonical ensemble

- Sample $Z_{GC}(\mu = i\mu_{MC})$

$$\Rightarrow \frac{Z_C(B)}{Z_{GC}(i\mu_{MC})} = \left\langle \frac{1}{\det(i\mu_{MC})} \int d\mu_i \exp\left(i3B\frac{\mu_i}{T}\right) \det(i\mu_i) \right\rangle$$

- Fourier transform each determinant exactly (work $\propto L_s^9 L_t$) $\Longleftarrow$ low T
- Sign problem $\leftrightarrow$ noise in $Z_C(B)$ $\Longleftarrow$ governed by B (not V)
- Study few-baryon system at low temperature: Nuclear Physics!

preliminary results, Wilson fermions: Alexandru et al, Lat05

Numerical results, $N_f = 4$

de Forcrand, Kratochvila

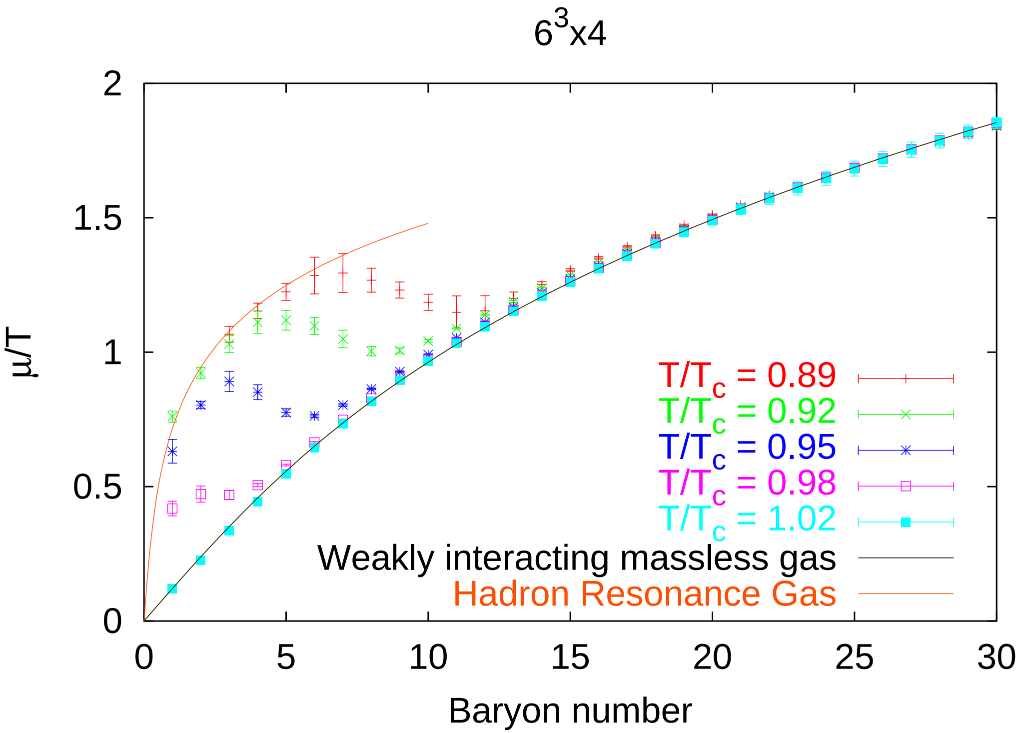
$6^3 \times 4$, standard staggered, HMC-algorithm, $m/T \approx 0.2$ (p.t. first order $\forall \mu$)

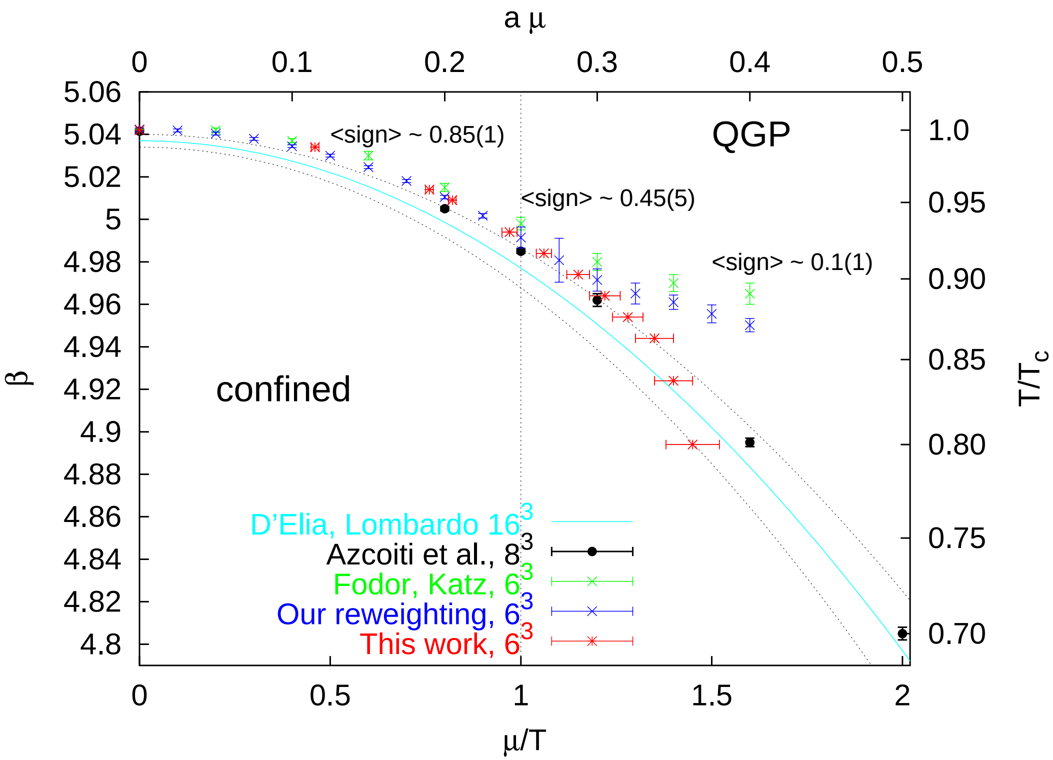
Chemical potential versus baryon density

$F(B) \rightarrow \mu$ transformation via saddle point approximation:

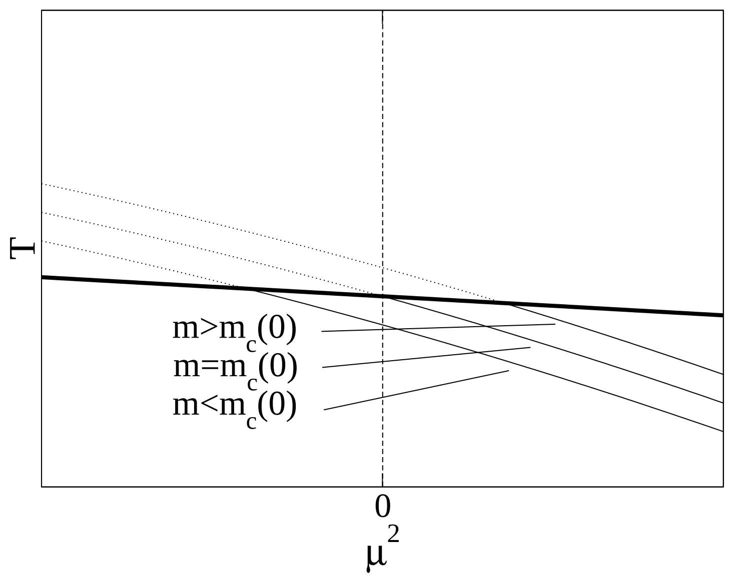
$$Z_{GC}(\mu) = \int d\rho \exp(-\frac{V}{T}(f(\rho)) + \mu\rho)) \Longrightarrow \mu \approx f'(\rho) \approx \frac{F(B+1)-F(B)}{3}$$

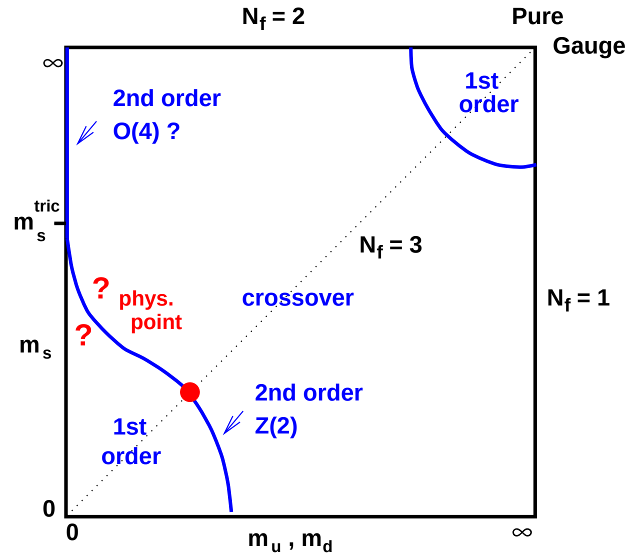
Comparison of methods:



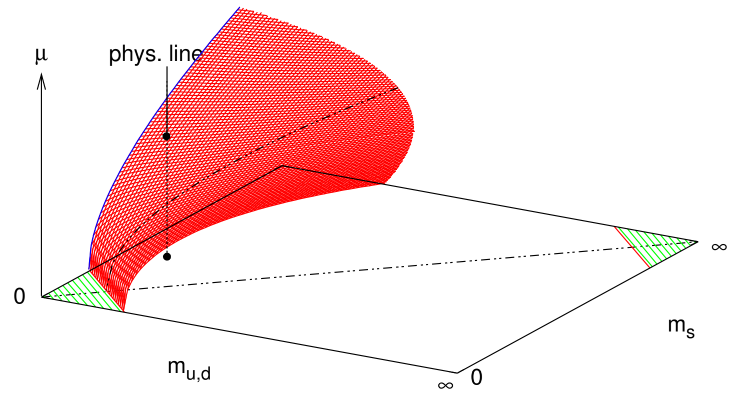


The critical endpoint and its quark mass dependence in $N_f = 3$





Expect: $$\frac{m_c(\mu)}{m_c(\mu=0)} = 1 + c_1 \left(\frac{\mu}{\pi T}\right)^2 + \ldots$$



Inverted: curvature of critical surface $\mu_c(m)$

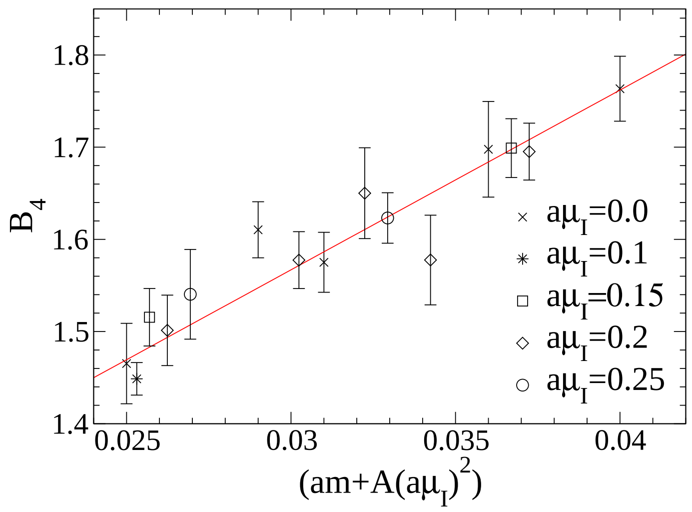
Criticality: cumulant ratios

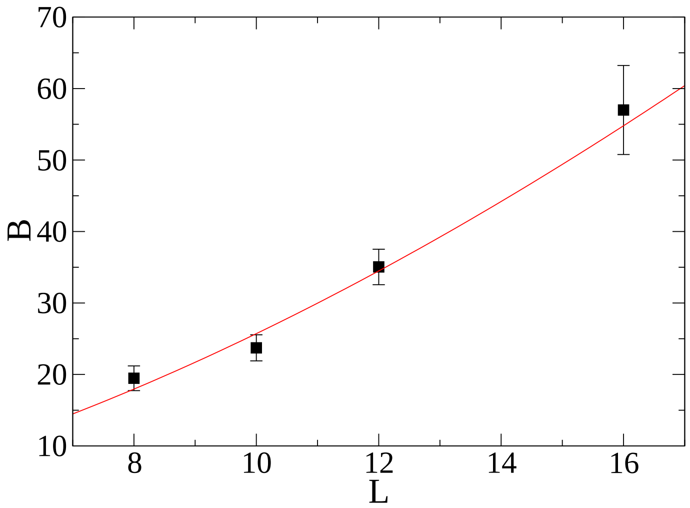
3d Ising universality : $$B_4(m_c,\mu_c) = \frac{\langle(\delta\bar\psi\psi)^4\rangle}{\langle(\delta\bar\psi\psi)^2\rangle^2} \to 1.604, \quad V\to\infty$$

($B_4 = 1$ (first-order), 3 (crossover) for $V=\infty$)

$$B_4(am,a\mu) = 1.604 + B\left(am - am_c(0) + A(a\mu)^2\right) + \ldots$$

de Forcrand, O.P.





FSS:

$\nu = 0.62(3)$

$\nu(Ising) = 0.63$

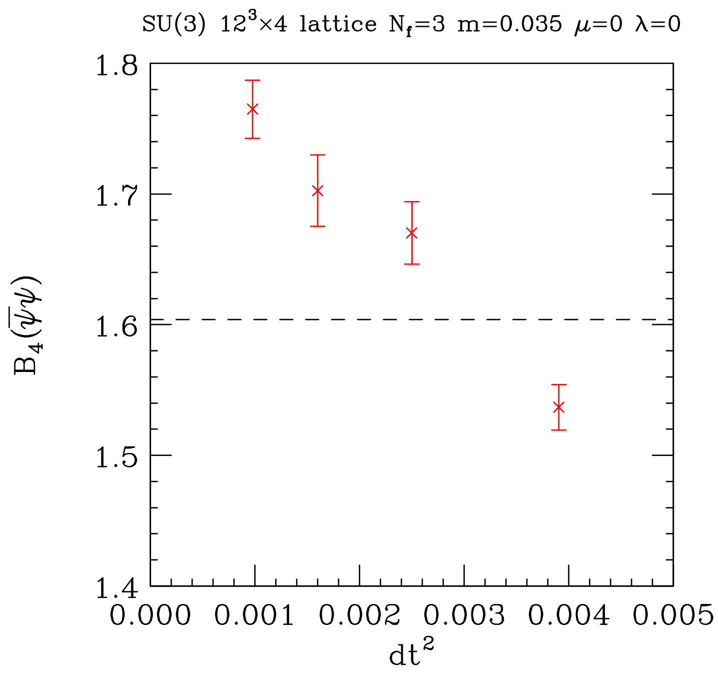
$$\Rightarrow \frac{m_c(\mu)}{m_c(\mu=0)} = 1 + 0.84(36)\left(\frac{\mu}{\pi T}\right)^2 + \ldots$$

$N_f = 3$ at finite isospin density

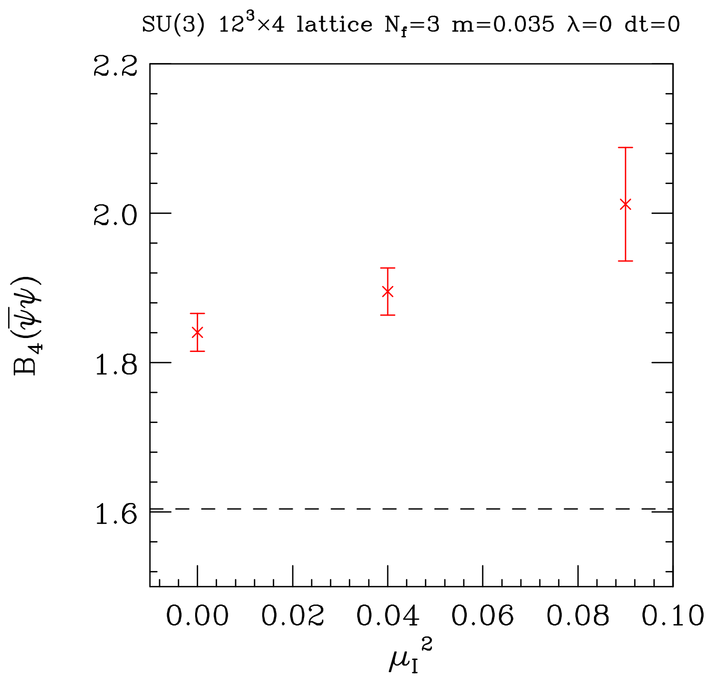
Kogut, Sinclair

Lattices $L^3 \times 4, L = 8, 12, 16$, standard staggered, R-algorithm, $m \gtrsim m_c(0)$

Finite stepsize effects change order:



Extrapolated results:



• $dB_4/d\mu_I^2 \gtrsim 0$, more crossover with μ??

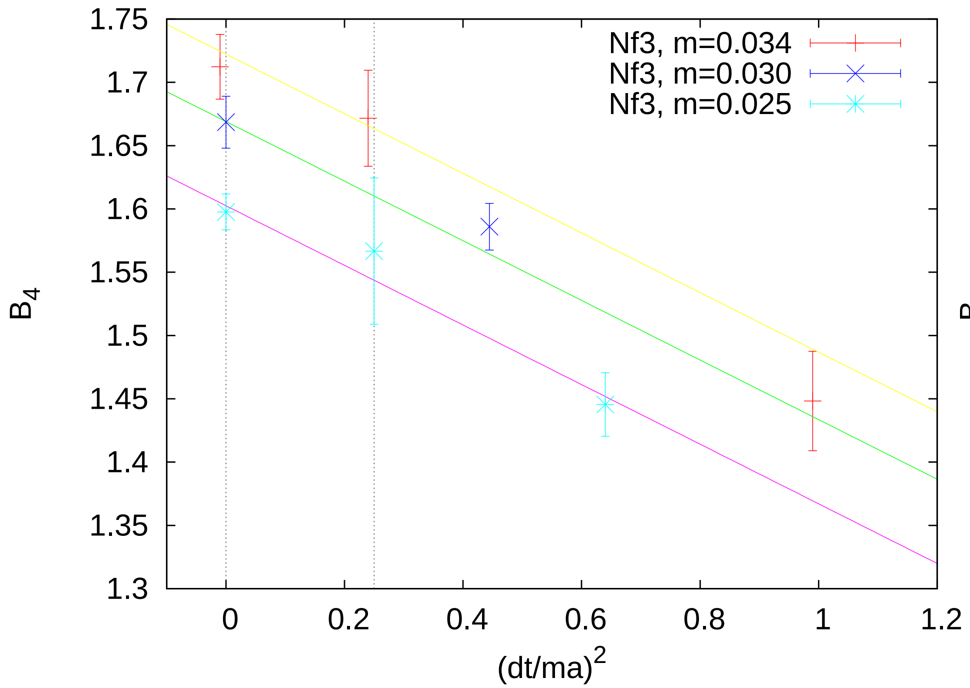
Redoing $N_f = 3$ with an exact algorithm

de Forcrand, O.P.

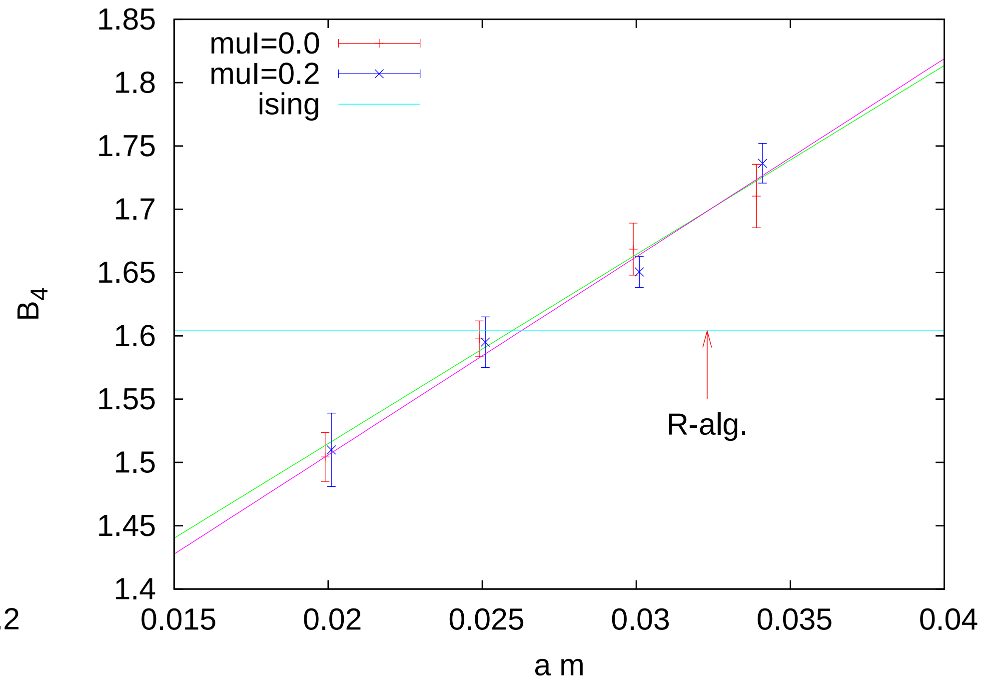
Extrapolations $dt^2 \to 0$ prohibitively expensive for small m

$\Rightarrow$**use exact algorithm** here: Rational Hybrid MC Clark, Kennedy, Lat05

Testing RHMC against $dt^2 -> 0$:



The critical mass $m_c(0)$ with RHMC:

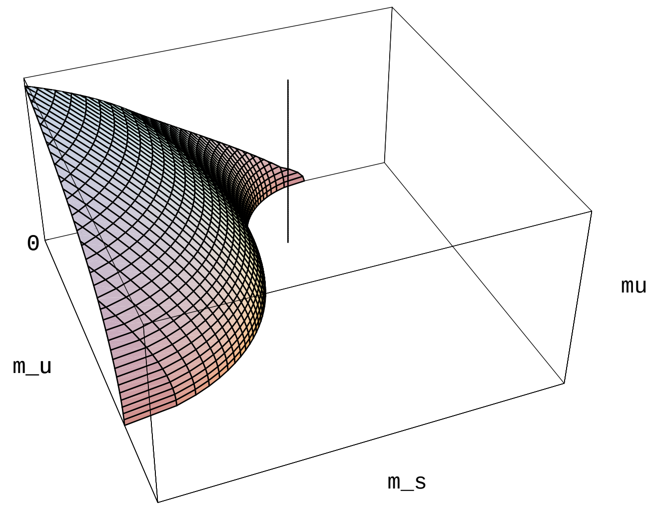


leftmost data: RHMC

- 25% change in $m_c(0)$
- $dB_4/d\mu_I^2 \approx 0$
- consistent with finite isospin!

A non-standard scenario:

no critical point at all?

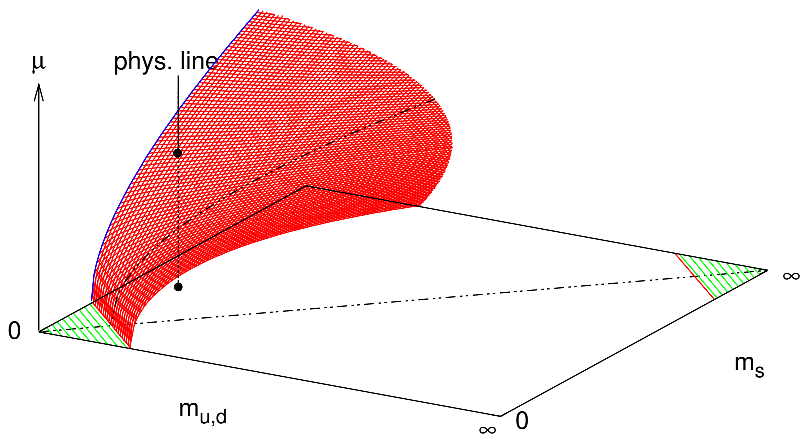


continuum conversion:

$$\Rightarrow \frac{m_c(\mu)}{m_c(\mu=0)} = 1 - 0.6(2)\left(\frac{\mu}{\pi T}\right)^2$$

Positive or negative curvature:

very high quark mass sensitivity of μ_c!!



Can one expect a critical point at "small" μ?

$\mu_B^c \sim 360$ MeV (FK) requires

$$1 < \frac{m}{m_c(\mu=0)} \lesssim 1.05$$

fine tuning of quark masses!!

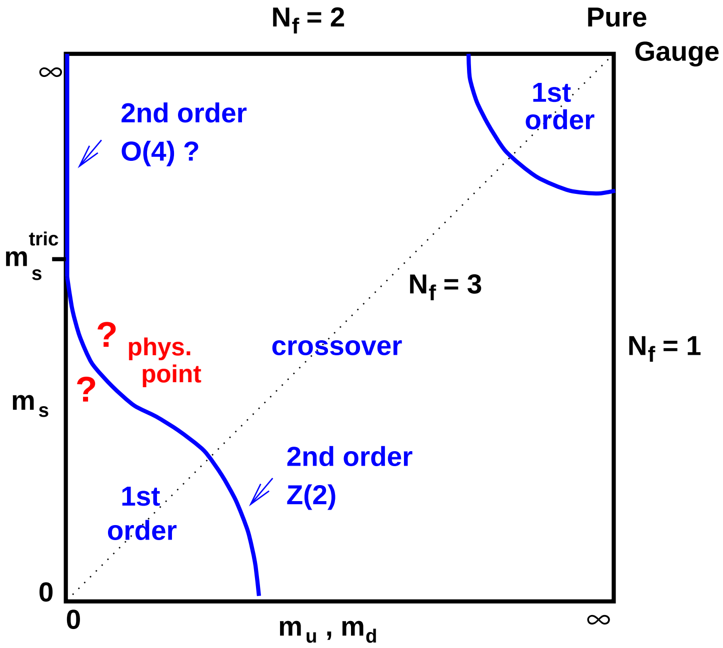
Outlook: $N_f = 2+1$

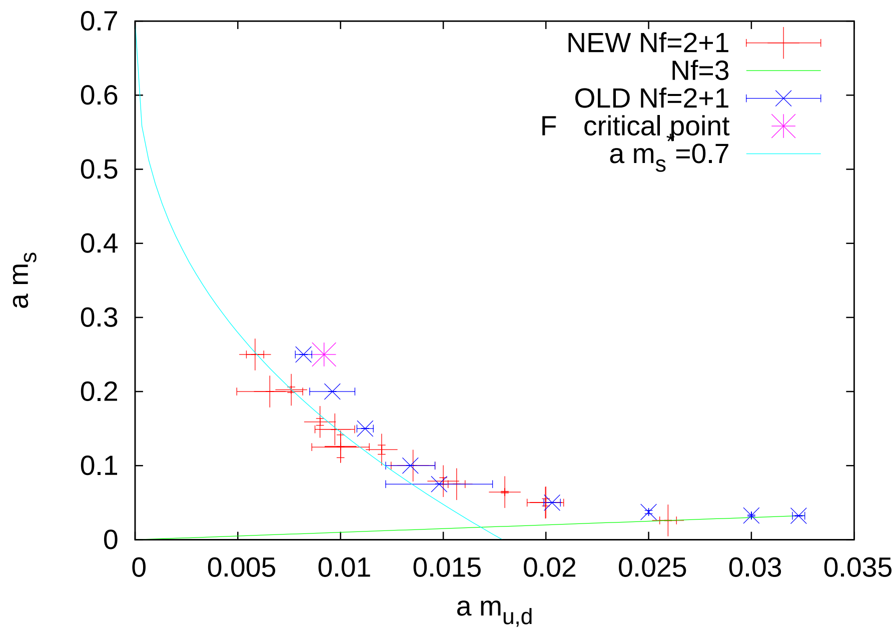
de Forcrand, O.P.

Two-step procedure:

I. $(m_s, m_{u,d})$ phase-diagram at $\mu = 0$ $\Rightarrow m_s^c(m_{u,d})$

II. repeat for $\mu \neq 0$





If there is a tricritical point: $m_s^{tric}/T_0 \approx 2.8$

The quenched limit: Potts model

$m \longrightarrow \infty$: QCD$\longrightarrow$ theory of Polyakov lines $\longrightarrow$ universality class of 3d 3-state Potts model

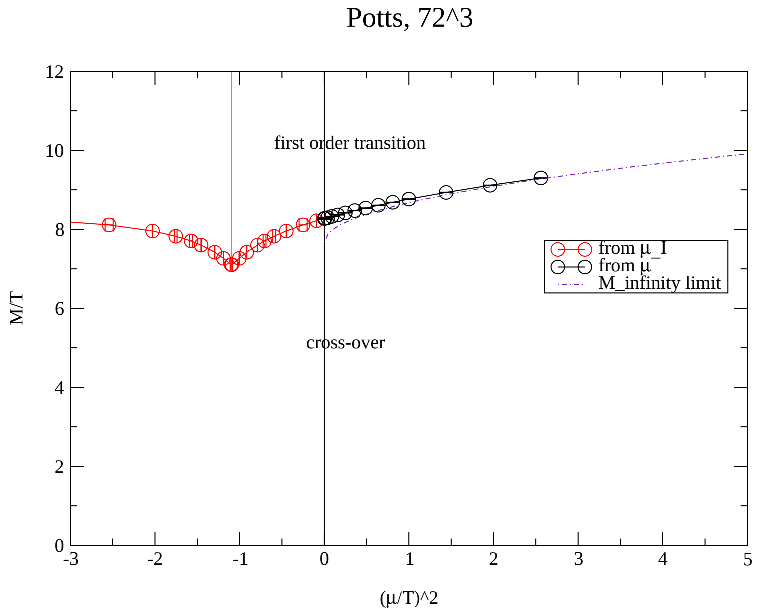
(3d Ising)

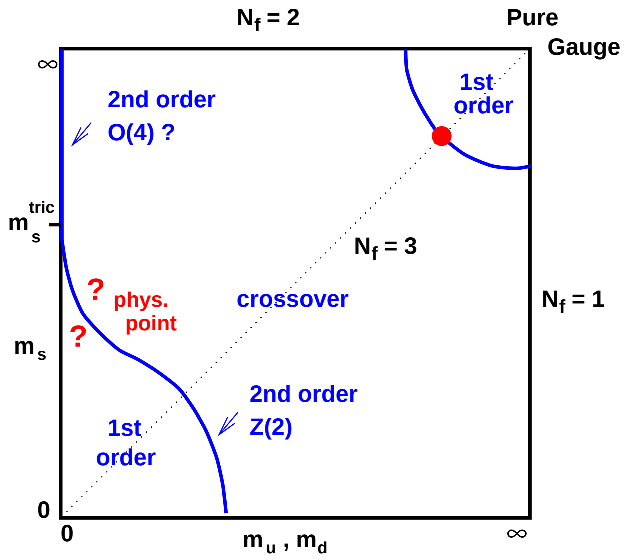
large μ: cluster algorithms — Alford, Chandrasekharan, Cox, Wiese

small μ/T: sign problem mild, doable for real μ**!** — de Forcrand, Kim, Kratochvila, Takaishi

$\Rightarrow$Testing ground for real vs. imaginary μ:

Information on upper right corner:





$\Rightarrow$First order region shrinks with μ !

Conclusions

Physics:

- $N_f = 2$: O(4) vs. 1st order remains open
- several groups tackling critical endpoint at finite μ, no convergence yet
- **strong quark mass sensitivity of μ_c**

Systematics:

- more methods available, more cross checks
- beginning to understand phase of $\det$, finite V
- **use exact algorithms !!!**

$\Rightarrow$qualitative picture in reach

$\Rightarrow$physics in the continuum still a long way.......(we are at $a \sim 0.3 fm$) $\Rightarrow$surprises?