QCD at nonzero chemical potential and the sign problem

INT lectures 2012

IV: strong coupling

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Where are we?

complex weight:

- straightforward importance sampling not possible
- overlap problem

various possibilities:

- preserve overlap as best as possible
- use approximate methods at small μ
- do something radical:
  - rewrite partition function in other dof
  - explore field space in a different way
  - ...

Fermion determinant

- standard approach suffers from sign problem
- complex determinant after integrating out fermions

try something else:

- do not integrate out fermions!
- integrate out gluons first!

$$Z = \int DU D\bar{\psi} D\psi \, e^{-S_{\rm YM}} e^{-S_{\rm F}} \qquad S_{\rm YM} = -\beta \sum \text{plaquettes}$$

how to integrate out gluons? YM theory cannot be solved ...

- instead: 'strong coupling expansion'

  expansion in $\beta \equiv 2N/g^2 \ll 1$

Strong coupling expansion

at leading order: $\beta \equiv 2N/g^2 = 0$

'wrong limit': asymptotic freedom: $g^2 \to 0 \Leftrightarrow \beta \to \infty$

- no continuum limit
- coarse lattice by construction
- no universality

but

- confinement
- formulated in terms of mesons and baryons
- qualitative insight
- (apparent) milder sign problem

illustration how to think differently

Strong coupling limit

$\beta = 0$: no YM action

$$Z = \int D\bar{\psi} D\psi \int DU e^{\bar{\psi} U \psi}$$

do U-integral first: set of independent one-link integrals

Rossi & Wolff 84, Karsch & Mütter 89

Fromm & de Forcrand 08-10, thesis Fromm 10

for definiteness: one flavour of staggered fermion χ

$$S_{\mathrm{F}} = \sum_x \left[\sum_\nu \eta_{\nu x} \left(\bar{\chi}_x U_{\nu x} \chi_{x+\nu} - \bar{\chi}_{x+\nu} U^\dagger_{\nu x} \chi_x \right) + 2 m_q \bar{\chi}_x \chi_x \right]$$

$\eta_{\nu x} = (-1)^{\sum_{\rho<\nu} x_\rho}$ Kawamoto-Smit phases

left-overs from γ-matrices

Strong coupling limit

single-component Grassmann variables $\chi_{ix}, \bar{\chi}_{ix}$
(colour index $i = 1, \ldots, N$)

$$\int d\chi_{ix} d\bar{\chi}_{jy}\, \bar{\chi}_{ix}\chi_{jy} = 1 \qquad \int d\chi_{ix}\, 1 = \int d\bar{\chi}_{ix}\, 1 = 0$$

- introduce different lattice spacing in space and time ($a_s \equiv a, a_\tau$) anisotropy $\gamma = a/a_\tau$ (in weak coupling)

$$Z = \int \prod_x d\chi_x d\bar{\chi}_x\, e^{2m_q \bar{\chi}_x \chi_x} \prod_{\nu=1}^{4} z(x, x+\nu)$$

one-link integral: $z(x, x+\nu) = \int dU_{\nu x}\, e^{\eta_{\nu x}\left[\bar{\chi}_x U_{\nu x} \chi_{x+\nu} - \bar{\chi}_{x+\nu} U^\dagger_{\nu x} \chi_x\right]}$

- introduce chemical potential: $U_{\pm 4x} \to \gamma e^{\pm\mu} U_{\pm 4x}$

One-link integrals

one-link integral: $z(x,y) = \int dU\, e^{\bar{\chi}_{ix} U_{ij} \chi_{jy} - \bar{\chi}_{iy} U^\dagger_{ij} \chi_{jx}}$ $\qquad (y = x + \nu)$

invariant measure for group integrals:

- normalization $\int dU = 1$
- invariance $\int dU\, f(U) = \int dU\, f(UV) = \int dU\, f(VU)$
  (V arbitrary SU(N) matrix)

examples:

$$\int dU\, U_{ij} \qquad \int dU\, U_{ij} U^\dagger_{kl}$$

$$\int dU\, U_{ij} U_{kl} \qquad \int dU\, U_{i_1 j_1} \ldots U_{i_N j_N}$$

all integrals should be proportional to invariants δ_{ij}
and $\epsilon_{i_1 \ldots i_N}$

One-link integrals

$$\int dU\, U_{ij} = \int dU\, U_{ij} U_{kl} = 0 \qquad \int dU\, U_{ij} U^\dagger_{kl} = \frac{1}{N}\delta_{il}\delta_{jk}$$

etc.

- what about $\int dU\, U_{i_1 j_1} \ldots U_{i_N j_N}$?
- use

$$\det U = \epsilon_{i_1 \ldots i_N} U_{i_1 1} U_{i_2 2} \ldots U_{i_N N} = 1$$

or $$\epsilon_{i_1 \ldots i_N} U_{i_1 j_1} U_{i_2 j_2} \ldots U_{i_N j_N} = \epsilon_{j_1 \ldots j_N}$$

- result

$$\int dU\, U_{i_1 j_1} \ldots U_{i_N j_N} = \frac{1}{N!}\epsilon_{i_1 \ldots i_N}\epsilon_{j_1 \ldots j_N}$$

One-link integrals

what should we get? $$z(x,y) = \int dU\, e^{\bar{\chi}_x U \chi_y - \bar{\chi}_y U^\dagger \chi_x}$$

two ingredients:

- gauge invariance $$\chi_x \to \Omega_x \chi_x \quad \bar{\chi}_x \to \bar{\chi}_x \Omega_x^\dagger$$

  gauge invariant combinations

$$M_x = \bar{\chi}_{ix}\chi_{ix} \qquad \text{meson}$$

$$B_x = \frac{1}{N!}\epsilon_{i_1 \ldots i_N}\chi_{i_1}\cdots\chi_{i_N} \qquad \text{baryon}$$

$$\bar{B}_x = \frac{1}{N!}\epsilon_{i_1 \ldots i_N}\bar{\chi}_{i_N}\cdots\bar{\chi}_{i_1} \qquad \text{anti-baryon}$$

- Grassmann variables: at most N χ_{ix}'s at one site
  ($\chi_{ix}^2 = 0$ for fixed colour index i)

One-link integrals

- gauge invariance and Grassmann nature:

$$z(x,y) = \sum_{k=0}^{N} \alpha_k \left(M_x M_y\right)^k + \tilde{\alpha}\left(\bar{B}_x B_y + (-1)^N \bar{B}_y B_x\right)$$

combination of meson and baryon fields

$$M_x = \bar{\chi} i x \chi i x \qquad \text{meson}$$

$$B_x = \frac{1}{N!}\epsilon_{i_1 \ldots i_N} \chi i_1 \cdots \chi i_N \qquad \text{baryon}$$

$$\bar{B}_x = \frac{1}{N!}\epsilon_{i_1 \ldots i_N} \bar{\chi} i_N \cdots \bar{\chi} i_1 \qquad \text{anti-baryon}$$

determine coefficients $\alpha_k, \tilde{\alpha}$

Full partition function

- one-link partition function:

$$z(x,y) = \sum_{k=0}^{N} \frac{(N-k)!}{N!k!} \left(M_x M_y\right)^k + \bar{B}_x B_y + (-1)^N \bar{B}_y B_x$$

- to do: remaining Grassmann integrals:

$$Z = \int \prod_x d\chi_x d\bar{\chi}_x \, e^{2m_q \bar{\chi}_x \chi_x} \prod_\nu z(x, x+\nu)$$

- for every site not yet fully occupied with mesons:

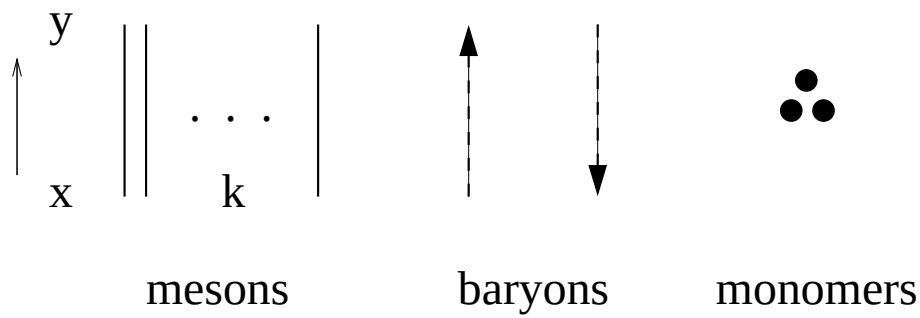
  expand $e^{2m_q \bar{\chi}\chi}$, e.g.

$$\int d\chi_x d\bar{\chi}_x \, e^{2m_q \bar{\chi}_x \chi_x} (\bar{\chi}_x \chi_x)^k = \frac{N!}{n_x!} (2m_q)^{n_x} \qquad n_x = N - k$$

Full partition function

final result: all N_c quarks and anti-quarks below to either:

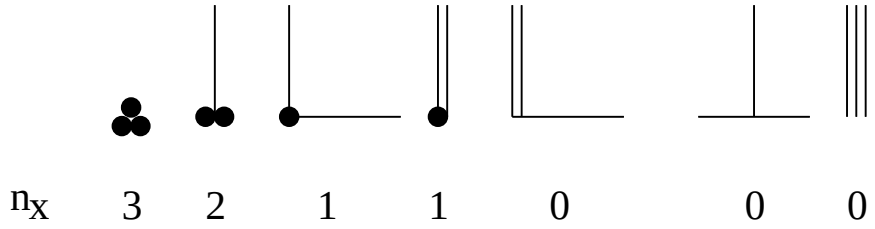
- hopping mesons $(M_x M_y)^k$ dimers
  $k = 0, \ldots, N$ non-oriented
- hopping (anti-)baryons $\bar{B}_x B_y$ oriented
- left-over quarks $(M_x)^{n_x}$ monomers



- baryon loops: all χ_i are involved
  - closed
  - self-avoiding

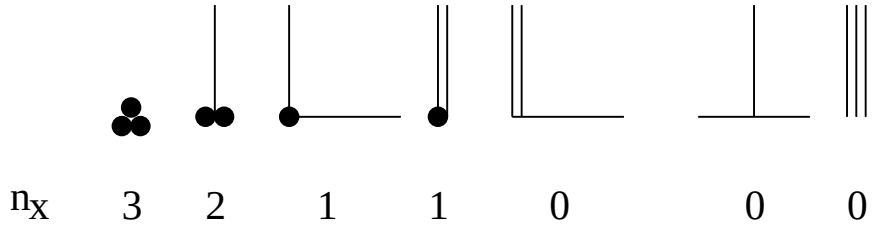
Full partition function

- closed baryon loops
- monomer/dimer system: every site occupied by $N_c = 3$ (anti)quarks

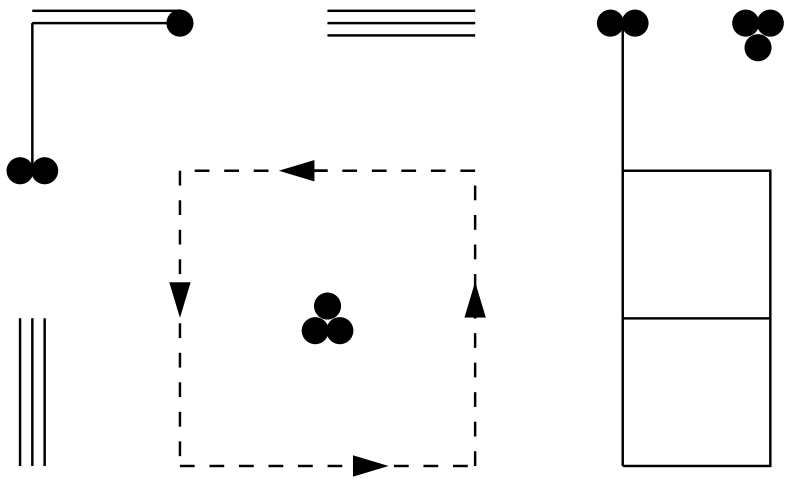


Full partition function

- closed baryon loops
- monomer/dimer system: every site occupied by $N_c = 3$ (anti)quarks



- example configuration ($N_c = 3$):



Ensemble

sum over all these configurations, with proper weight:

- k_b dimers, n_x monomers, l_B baryon loops

$$Z = \sum_{[k_b,n,l_B]} \prod_{\text{links } b=(x,\nu)} \frac{(N-k_b)!}{N!k_b!} \prod_x \frac{N!}{n_x!} (2m_q)^{n_x} \prod_{l_B} w(l_B)$$

- chemical potential dependence?
- only in baryon loops winding around time direction!

$$w(l_B) \sim \sigma(l_B) e^{r_{l_B} N_c N_\tau \mu}$$

r_{l_B}: winding in temporal direction

Ensemble

baryon loop weight:

$$w(l_B) \sim \sigma(l_B) e^{r_{l_B} N_c N_\tau \mu}$$

- r_{l_B}: winding in temporal direction
- natural combination $r_{l_B} \times N_c \times N_\tau \times \mu = r_{l_B} \mu_B / T$
- $\sigma(l_B) = \pm 1$: geometrical factor, depends on loop

weight not positive-definite even at $\mu = 0$!

Ensemble

aside: observables

- condensate

$$\langle \bar{\chi}\chi \rangle = \frac{1}{\Omega} \frac{\partial}{\partial m_q} \ln Z \sim \frac{1}{\Omega} \left\langle \sum_x n_x \right\rangle$$

  monomer density

- baryon number

$$\langle n_B \rangle = \frac{T}{V} \frac{\partial}{\partial \mu_B} \ln Z \sim \frac{1}{V} \left\langle \sum_{l_B} r_{l_B} \right\rangle$$

  winding number density of baryon loops

Sign problem

- even at $\mu = 0$, baryon weight not positive-definite: geometric loop-dependent sign
- worse off?

general strategy: combine various contributions

- when summed analytically: positive contribution

task: identify proper configurations to sum analytically

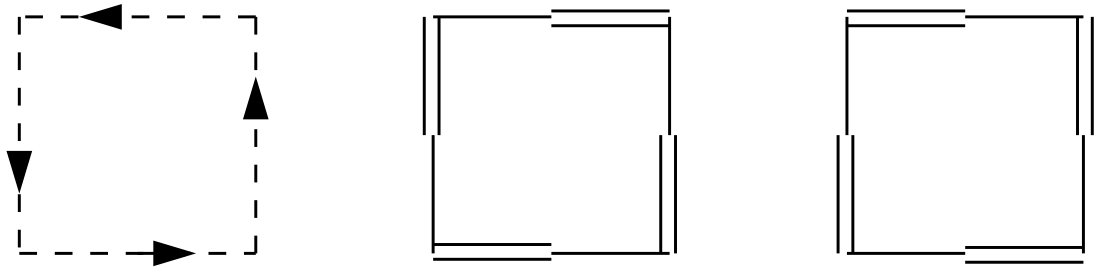
Karsch & Mütter 88

note:

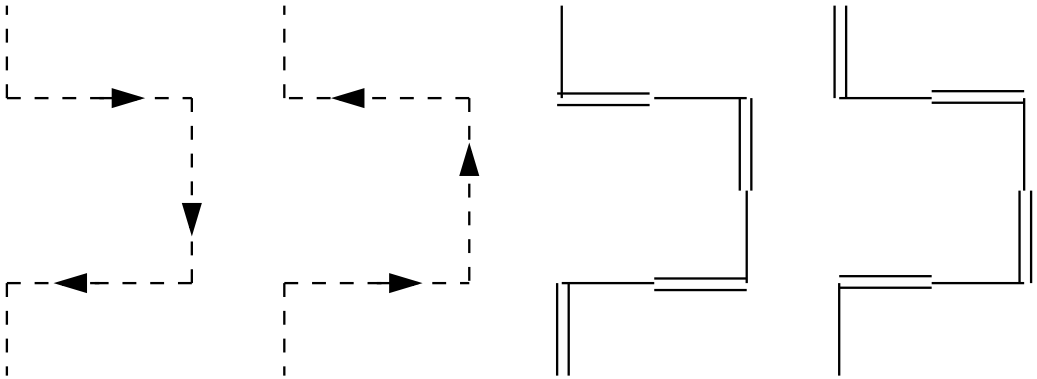
- useful strategy in wide set of models
- but: what contributions to sum?

Sum contributions

every baryon loop can be combined with two chains of dimer loops

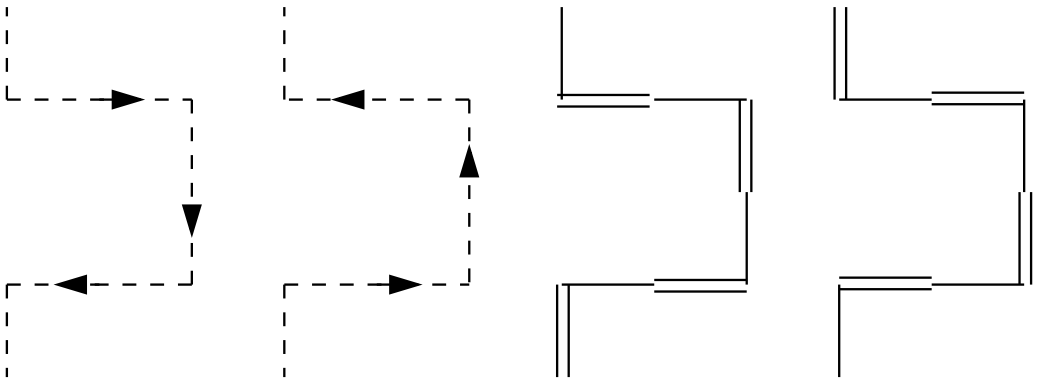


also in temporal direction



Sum contributions

separate weights: $w(l_B)$ $w(l_{B'})$ $w(l_D)$ $w(l_{D'})$



combine the weights in clever combinations: 'polymers'

$$w(l_P) = w(l_D) + \frac{1}{2}\left[w(l_B) + w(l_{B'})\right]$$

$$w(l_{P'}) = w(l_{D'}) + \frac{1}{2}\left[w(l_B) + w(l_{B'})\right]$$

exactly same configurations

Sum contributions

combine the weights: polymer weights (recall $\sigma(l_B) = \pm 1$)

monomer-dimer-polymer (MDP) system

- closed baryon loop: no μ dependence

$$w(l_P) = 1 + \sigma(l_B) \geq 0$$

- temporal loops: baryons $e^{+\mu}$ anti-baryons $e^{-\mu}$ combine

$$w(l_P) = 1 + \sigma(l_B) \cosh\left(\frac{r_{l_B}\mu_B}{T}\right)$$

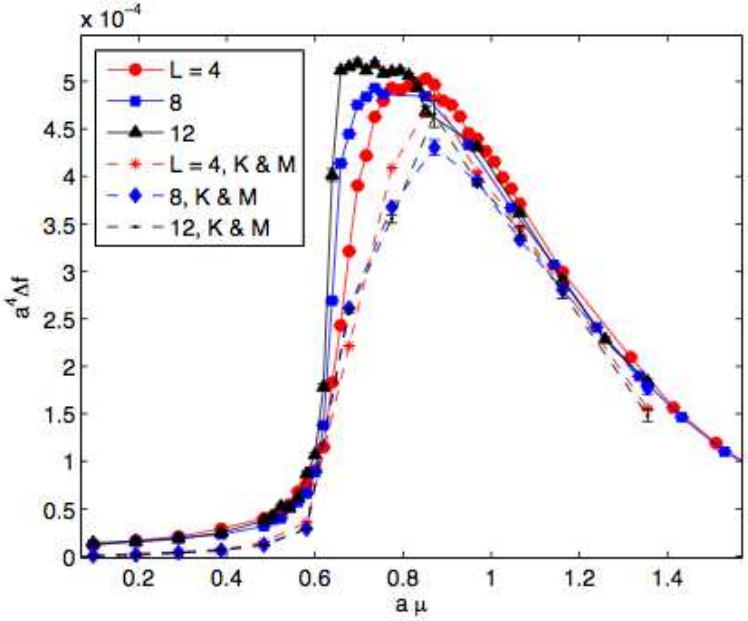
non-negative when $\mu = 0$: new sign problem solved

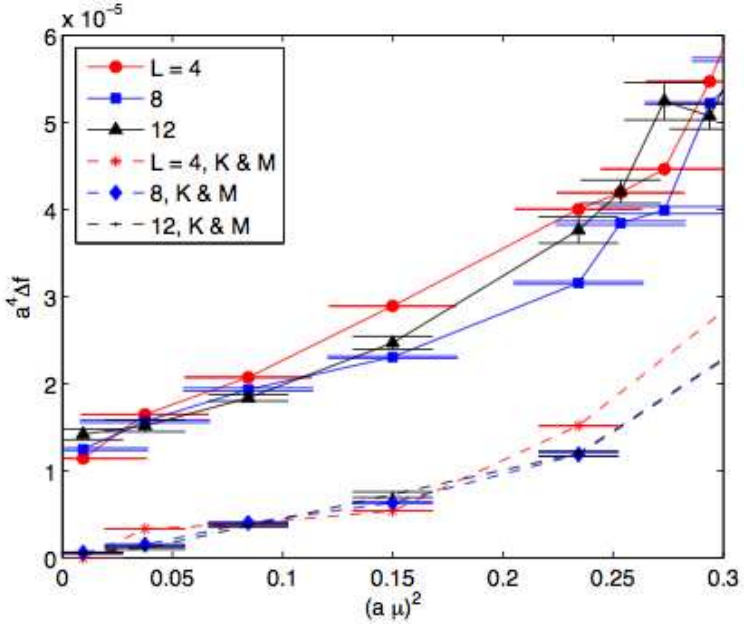
still sign problem remaining at $\mu \neq 0$

Sign problem

in practice: sign problem is mild de Forcrand & Fromm 08-10

recall $$\langle e^{i\varphi}\rangle_{\rm pq} = \frac{Z}{Z_{\rm pq}} = e^{-\Omega\Delta f}$$





- in this model: $a^4\Delta f \lesssim 10^{-4}$
- sign problem under control on small volumes:
  $\Omega = 8^3 \times 4 \quad \Leftrightarrow \quad \Omega\Delta f \sim 0.2$

Simulations

- sign problem present but mild
- simulations on small volumes: can use reweighting

why mild?

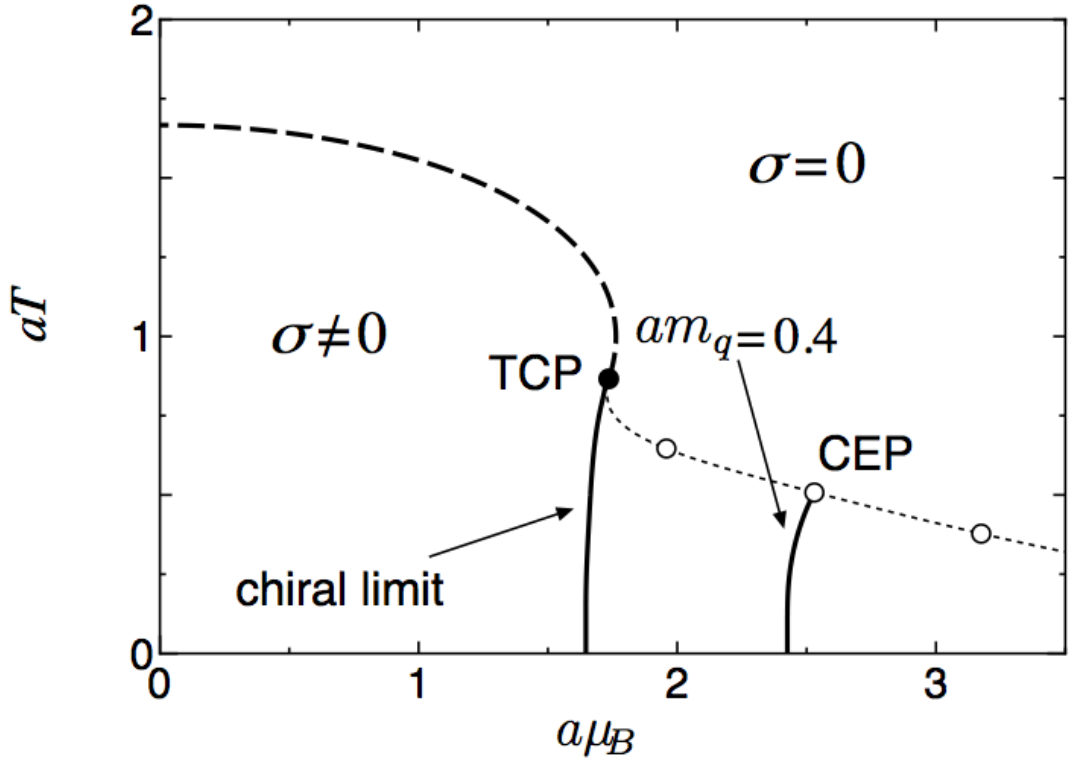
- fluctuating gauge fields integrated out first ($\beta = 0$)
- different sampling of configuration space
- . . . but not completely understood

aside

- other algorithmic improvement: worm algorithm

Strong coupling phase diagram

mean field prediction Y. Nishida 04, Ohnishi et al 05-now



- $m_q = 0$: $1^{\rm st}$ order at low T, $2^{\rm nd}$ order at higher T separated at tricritical point (TCP)
- $m_q > 0$: crossover at higher T, critical endpoint (CEP)

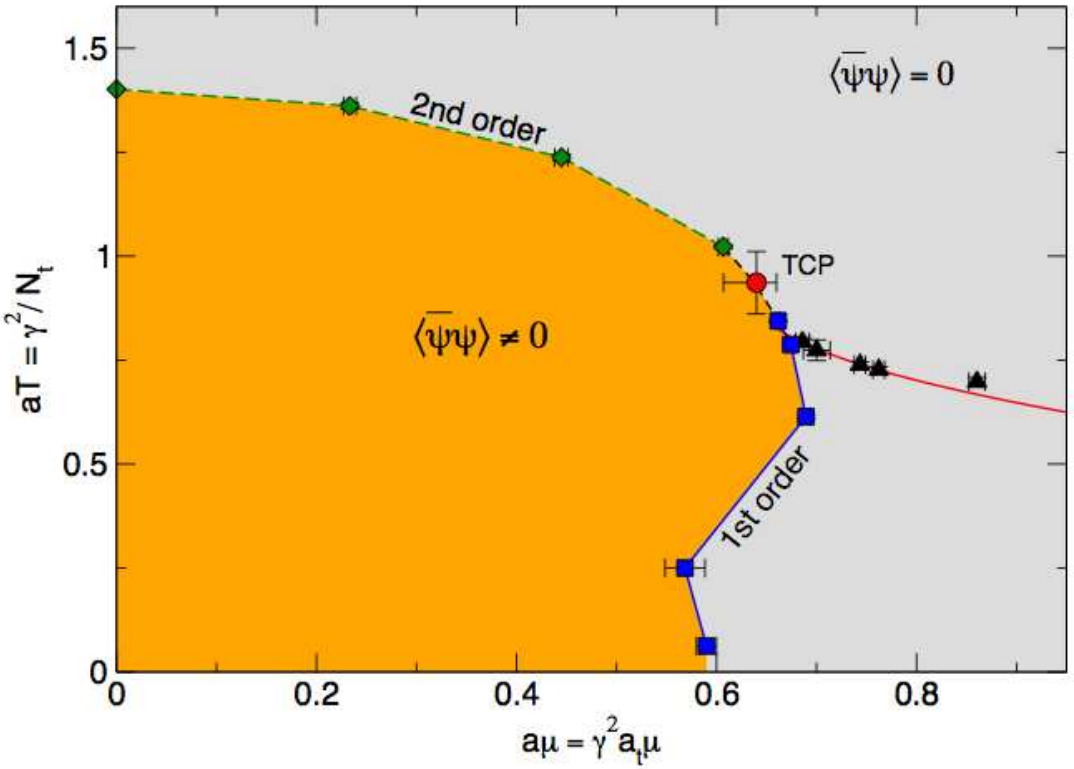
Strong coupling phase diagram

simulations

de Forcrand & Fromm 08

$am_q = 0$

CEP for $am_q > 0$



qualitative agreement / quantitative deviation from MF

note:

- Silver Blaze: $\langle n_B \rangle = 0/1 \quad (\mu < \mu_c)/(\mu > \mu_c)$
- immediate saturation

Ongoing research

- take $a_\tau \to 0$ (continuous time): arXiv:1111.1434
  - sign problem absent even when $\mu \neq 0$
  - reduced discretization (finite N_τ) effects

- corrections to strong-coupling limit: arXiv:1111.4677
  - gluonic observables: Polyakov loop
  - $\mathcal{O}(\beta)$ correction

Summary

strong coupling

- insight in QCD phase diagram
- test ground for alternative algorithms
- sign problem milder than in full QCD