Lattice QCD at $\mu \neq 0$

Part II

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Outline :

1. Introduction
2. A Look inside Lattice Gauge Theory
3. Introducing Chemical Potentials
4. Fighting the Complex Measure Problem in Standard LGT
5. Results for Standard LGT
6. LGT-Motivated Effective Models on the Lattice
7. Complex Langevin Simulation
8. Summary and Conclusions

2. 4. Order Parameters for Finite-Temperature Transitions

Confinement/deconfinement and chiral symmetry breaking/restoration are intertwined for quarks (as long as they belong to the fundamental representation of the color group).

Confinement is understood as the absence (in Nature) of free color charges.

In Theory, this is a (somewhat abstract) property of infinitely heavy static, spinless test charges ("heavy quarks") to be forbidden by an infinite (delocalized ?) amount of excess vacuum Free Energy $F_Q = \infty$.

This property can eventually be destroyed through screening by dynamical color charges (sea quarks, or "dense excess quarks").

In other models (with more exotic gauge groups like G_2, for example several (say 3 of the 14) gluons can screen one fundamental quark.

This mechanism is not possible in QCD with gauge group $SU(3)$!

The increase of vacuum Free Energy caused by an isolated heavy quark is defined by the Polyakov loop (is a holonomy, since the path is closed !)

$$P_{\vec{x}} = \mathcal{T}\left[\prod_{\tau=1}^{N_t} U_{\vec{x},\tau,\nu=4}\right]$$

$\mathbb{Z}(N)$ symmetry : flip all $U_{\vec{x},\tau,\nu=4} \to zU_{\vec{x},\tau,\nu=4}$ at one timeslice $\tau = \tau_0$ this changes (at all $\vec{x}$) the Polyakov loop $P_{\vec{x}} \to zP_{\vec{x}}$ with $z \in \mathbb{Z}(N)$

The local thermal expectation value :

$$L_{\vec{x}} = \langle \text{ Re tr } P_{\vec{x}} \rangle = \frac{Z(\textbf{with quark at } \vec{x})}{Z(\textbf{without quark})}$$

The spatial average of it is important : this is the order parameter

$$\overline{L} = \frac{1}{NV_3}\sum_{\vec{x}} L_{\vec{x}} \propto \exp\left(-\frac{F_Q}{T}\right)$$

Definition as an order parameter for confinement :

$$\overline{L} = 0 \quad \textbf{confinement,} \qquad \mathbb{Z}(N) \textbf{ symmetry satisfied}$$

$$\overline{L} \neq 0 \quad \textbf{deconfinement,} \quad \mathbb{Z}(N) \textbf{ symmetry broken}$$

Also if dynamical (sea) quarks are in the model (even at $T = 0$) one finds (no strict order parameter anymore !)

$$\overline{L} \neq 0$$

This means : $\mathbb{Z}(N)$ symmetry is slightly broken by quarks

Order parameter for dynamical fermions : it tests chiral symmetry

Chiral condensate (D_f is the Dirac operator for quark with flavor f)

$$\langle \left(\bar{\psi}\psi\right)_f \rangle = \frac{1}{N_1 N_2 N_3 N_t} \frac{\partial}{\partial m_f} \ln Z = \frac{1}{4} \frac{1}{N_1 N_2 N_3 N_t} \langle \text{ tr } D_f^{-1} \rangle$$

$$\propto \langle \sum_{\text{eigenvalue } i} \frac{1}{i\lambda_i + m} \rangle \propto \langle \sum_{\text{eigenvalue } i} \frac{2m}{\lambda_i^2 + m^2} \rangle$$

$$\langle \left(\bar{\psi}\psi\right)_f \rangle \propto \int d\lambda \; \langle \; \rho(\lambda) \; \rangle \; \frac{2m}{\lambda^2 + m_f^2} \propto \langle \; \rho(\lambda = 0) \; \rangle$$

This is the Banks/Casher criterion in the limit $m \to 0$:

"If the average spectral density of the Dirac operator vanishes near $\lambda = 0$, this 'gap' signals restoration of chiral symmetry."

Definition as an order parameter (in chiral limit $m \to 0$) :

$$\lim_{m \to \infty} \langle \bar{\psi}\psi \rangle \neq 0 \qquad \textbf{chirally broken phase}$$

$$\lim_{m \to \infty} \langle \bar{\psi}\psi \rangle = 0 \qquad \textbf{chirally restored phase}$$

Other observables show dramatic signals at the phase transition, too, although they are not "order parameters" (that means, never vanish just for symmetry reasons) :

- energy density ϵ
- pressure p
- trace anomaly $\epsilon - 3p$

are signals of liberation of sub-hadronic degrees of freedom which are "frozen" at low temperature, in the hadronic (so-called "confinement") phase.

The central quantity is the "trace anomaly" or "interaction measure" ,

$$I(T) = \epsilon(T) - 3p(T) = \langle T^{\mu\mu} \rangle$$

important because its relation to the scaling behavior of the action

$$\frac{I(T)}{T^4} = \frac{1}{T^3 V} \sum_i \frac{db_i}{da} \left\langle \frac{\partial S}{\partial b_i} \right\rangle_{|subtracted}$$

("subtracted" means subtraction of the same lattice expression at $T = 0$)

The $b_i(a)$ are parameters of different parts of the lattice action varying with the lattice spacing a along the "line of constant physics" :

- **inverse coupling β**
- **bare quark masses m**
- **chemical potential μ (later)**

Then the pressure is obtained by the "integral method"

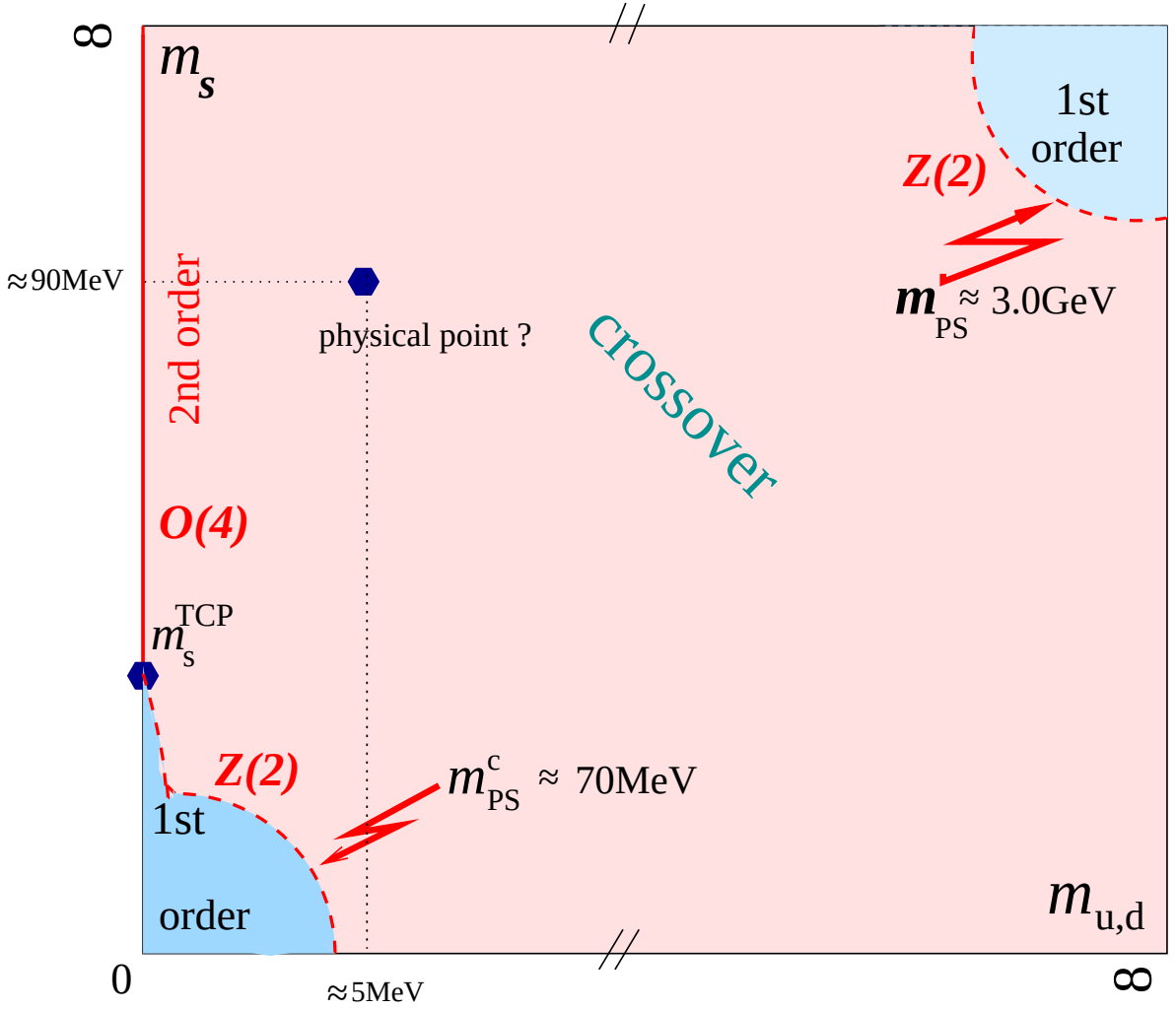
$$\frac{p_{fin}}{T_{fin}^4} - \frac{p_{in}}{T_{in}^4} = \frac{1}{T^3 V} \int_{in}^{fin} \left[d\beta \left\langle \frac{\partial \ln Z}{\partial \beta} \right\rangle + dm \left\langle \frac{\partial \ln Z}{\partial m} \right\rangle + d\mu \left\langle \frac{\partial \ln Z}{\partial \mu} \right\rangle \right]$$

as a line integral along a "line of constant physics" between two points characterizing initial and final state in temperature (or later in the β-μ, i.e. temperature–chemical potential plane).

Later, inside the T-μ phase diagram, each point can be characterized by

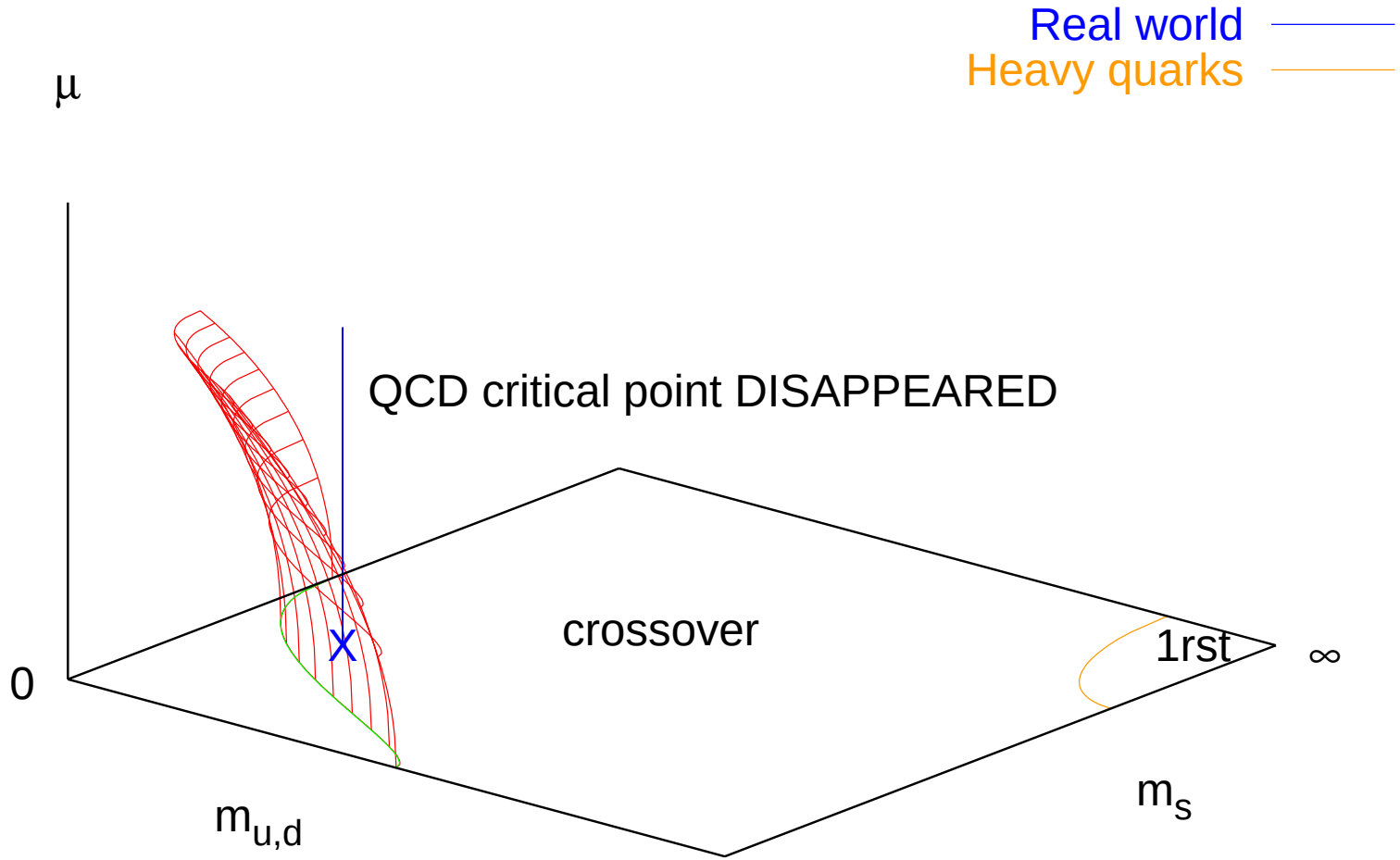
- **trace anomaly (interaction measure)** $(\epsilon - 3p)/T^4$
- **energy density** ϵ
- **pressure** p
- **and other thermodynamical functions.**

The QCD transition at $\mu = 0$ as function of quark masses (Columbia plot) from arXiv:1203.5320 Petreczky

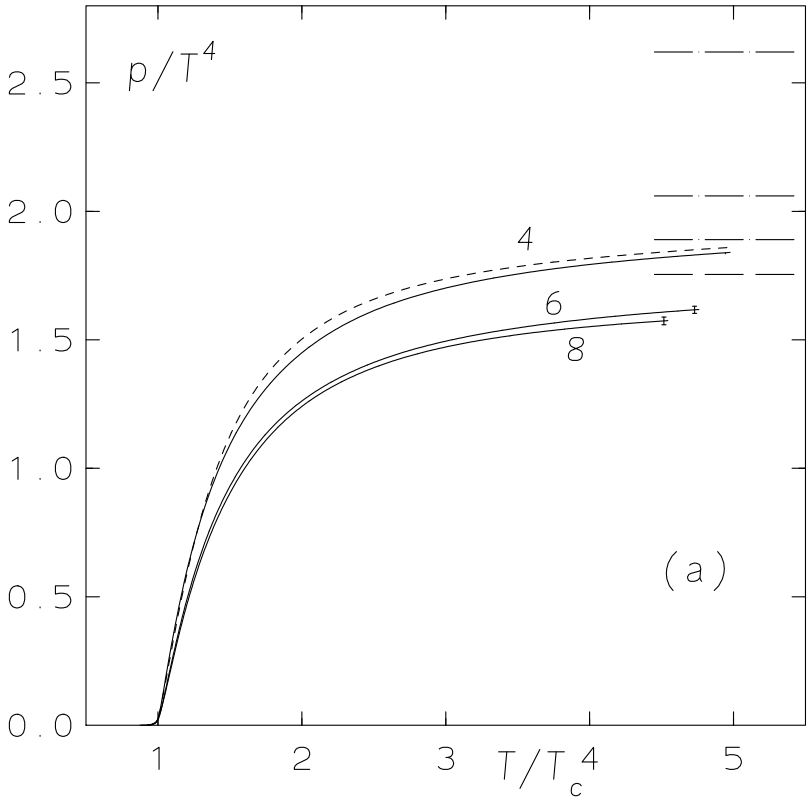


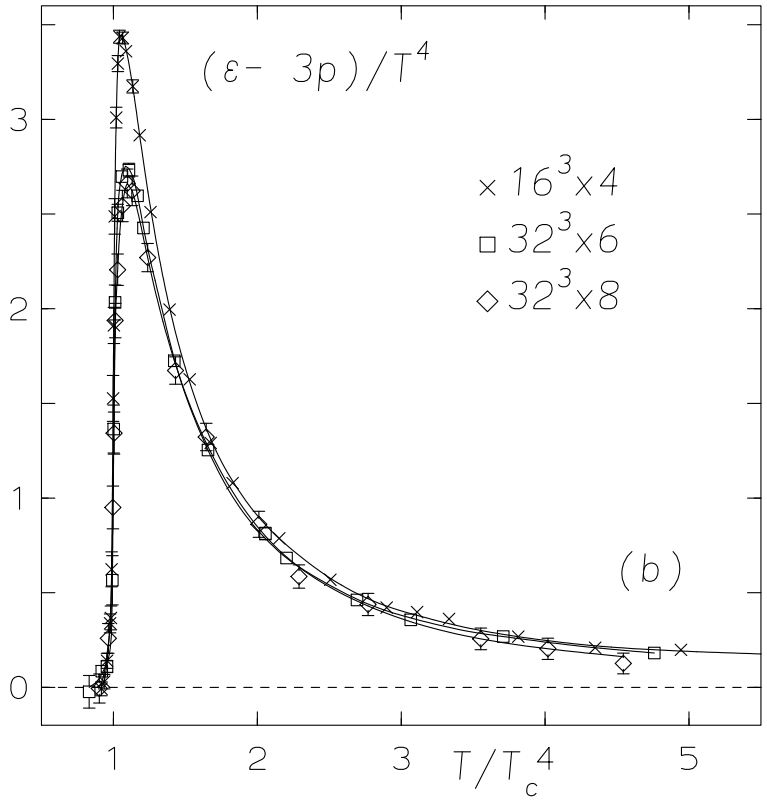
The Columbia plot extended into a third direction μ : will there be a true phase transition (critical point) for physical quark masses ?

from Ph. de Forcrand and O. Philipsen hep-lat/0607017



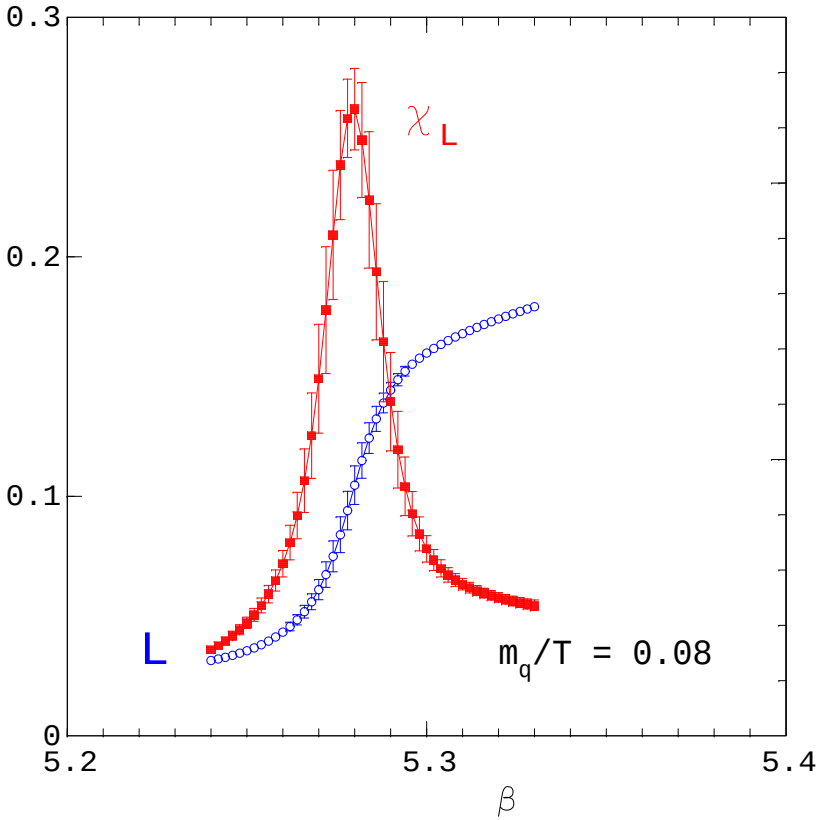
The pressure (left) versus T/T_c for $N_t = 4$, 6 and 8 in pure gluodynamics. The interaction measure of gluons (trace anomaly) $(\epsilon - 3p)/T^4$ (right).
from Boyd et al. 1995

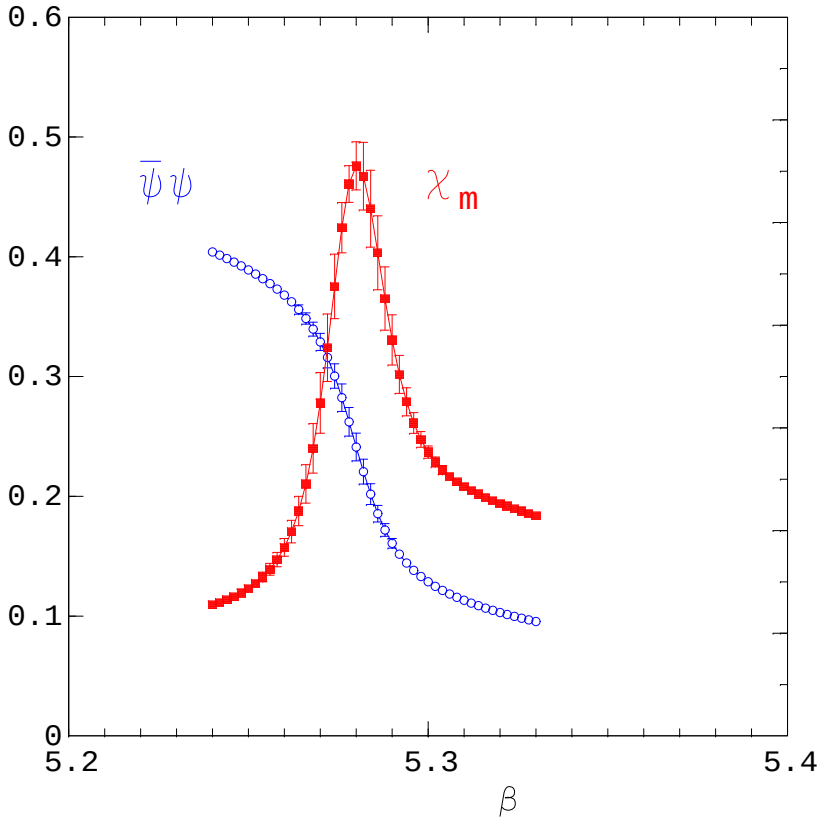




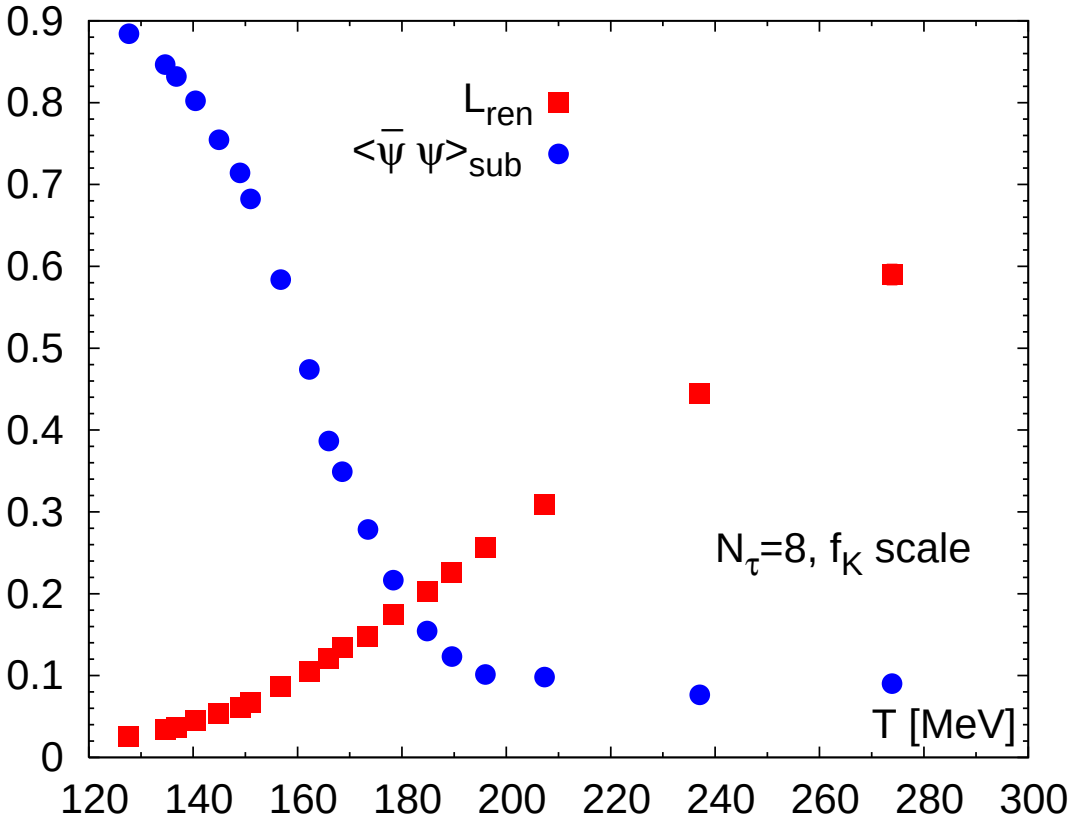
Polyakov loop L (left) and chiral condensate $\langle\bar{\psi}\psi\rangle$ (right) together with their susceptibilities show both transitions in two flavour QCD.

from Karsch et al. 2001

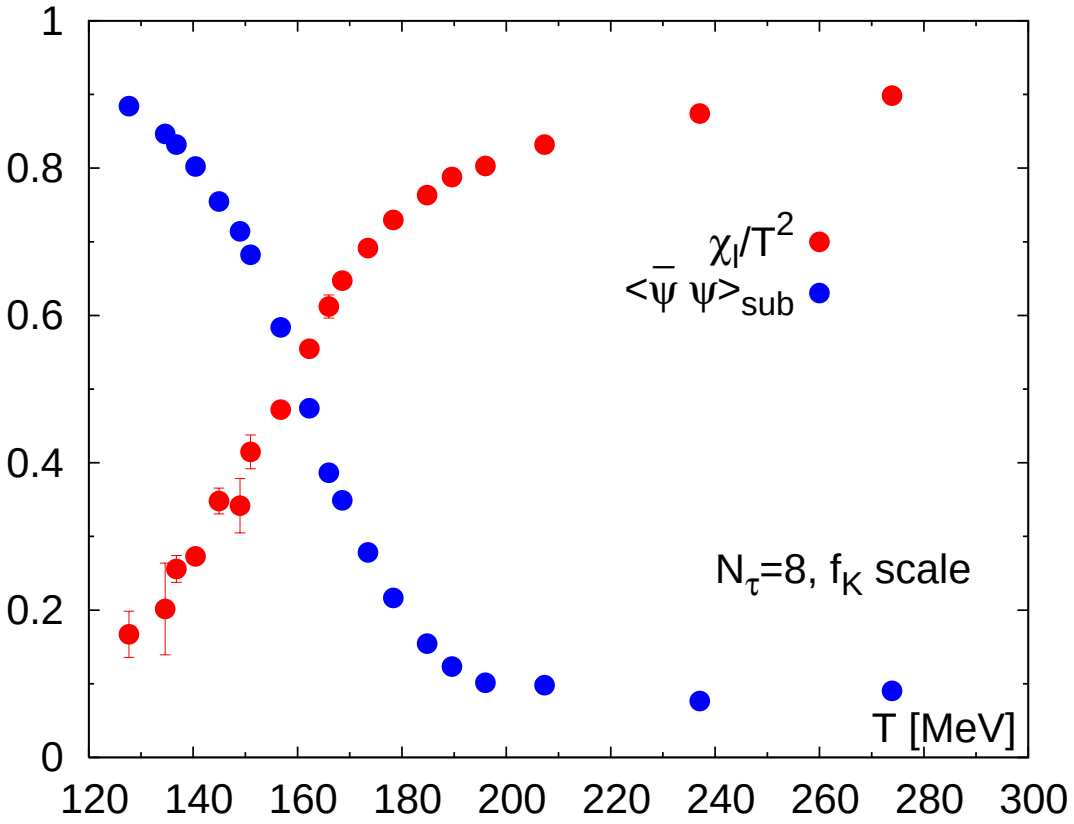




The chiral condensate compared to the renormalized Polyakov loop in full QCD from arXiv:1203.5320 Petreczky

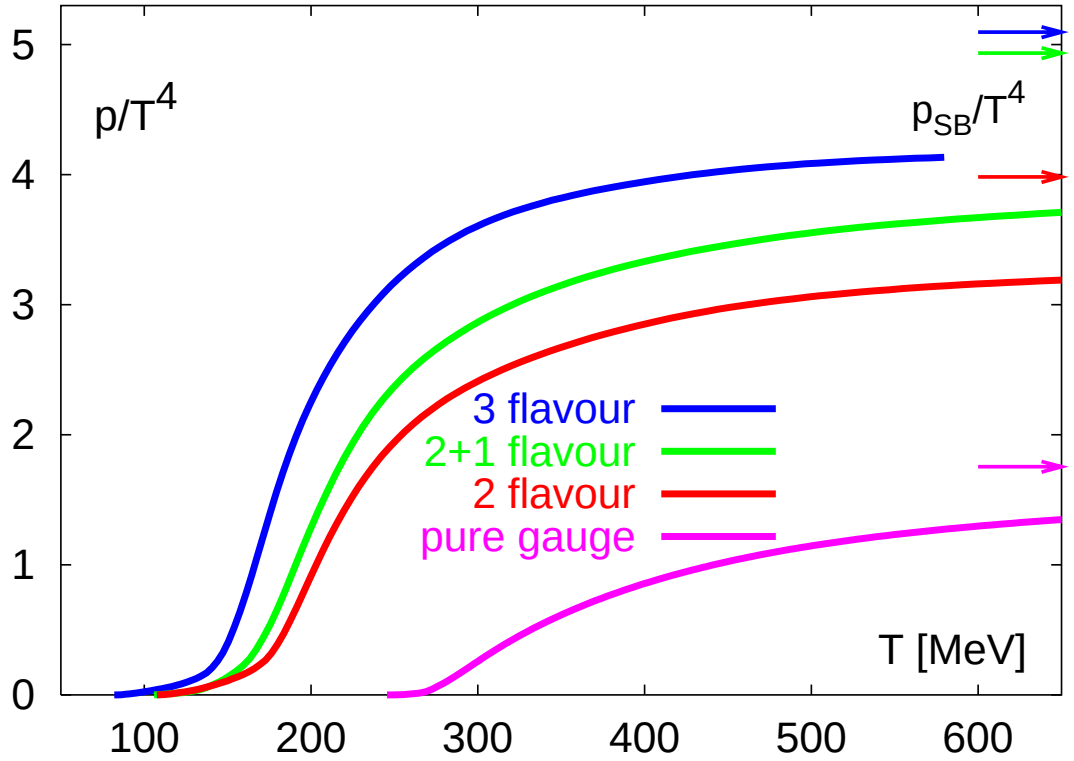


The chiral condensate compared to the light quark number susceptibility in full QCD from arXiv:1203.5320 Petreczky



The pressure : gluons only, 2 light, 2 light + 1 heavy and 3 light flavors

from Karsch, Laermann and Peikert (2000)



3. Introducing Chemical Potentials

- **Chemical Potential for Fermions**
- **Influence of Various $\mu \neq 0$ on the Fermion Determinant**
- **Complex Action for a 4D Complex Scalar Field**

3. 1. Chemical Potential for Fermions

Karsch and Hasenfratz considered this problem first in 1982.

In continuum, the operator of particle minus antiparticle number density $\bar{\psi}(x)\gamma_4\psi(x)$ is the 4-th component of a conserved vector current $\bar{\psi}(x)\gamma_\mu\psi(x)$.

Consider energy density in free case (without external gauge field).

This means : all links put $U_\mu = 1$, $Z = \det D$ (no integration over U_μ !)

$$\epsilon(\mu) = \frac{1}{V_3}\langle\hat{H}\rangle = -\frac{1}{V_3}\frac{\partial}{\partial\beta}\ln Z$$

With $\beta = N_t a_t$, the energy density is obtained by differentiating $\partial/\partial a_t$

$$\epsilon(\mu) = -\frac{1}{(a_s N_s)^3 N_t} \frac{\partial}{\partial a_t} \ln \det D$$

Naively one would be tempted to include the chemical potential term like a mass term.

$$D_{nm} = \sum_{j=1}^{3} \gamma_j \frac{\delta_{n+\hat{j},m} - \delta_{n-\hat{j},m}}{2a_s} + \gamma_4 \frac{\delta_{n+\hat{4},m} - \delta_{n-\hat{4},m}}{2a_t} + m\delta_{nm} + \mu\gamma_4\delta_{nm}$$

Let's see what the consequences would be ?

In the free case, the determinant is solvable by Fourier transform

$$\tilde{D}_{p,q} = \frac{1}{V_4} \sum_{n,m} \mathrm{e}^{-ipn} D_{nm} \mathrm{e}^{iqm} = \delta_{p,q} \tilde{D}_p$$

$$\epsilon(\mu) = C - \frac{4}{N_t N_s^3 a^4} \sum_p F(ap, am, a\mu)$$

$$F(ap, am, a\mu) = \frac{\sum_{j=1}^{3} \sin^2(ap_j) + (am)^2}{\sum_{k=1}^{3} \sin^2(ap_k) + (am)^2 + (\sin(ap_4) - ia\mu)^2}$$

Subtract $\epsilon(0)$, go to zero temperature and to the continuum limit

$$\frac{1}{N_s^3 N_t a^4} \sum_p \to \frac{1}{(2pi)^4} \int_{-\pi}^{\pi} d^4p$$

$$\epsilon(\mu) - \epsilon(0) = -\frac{4}{(2\pi)^4} \int_{-\pi}^{\pi} d^4p \, (F(ap, am, a\mu) - F(ap, am, 0))$$

$$\epsilon(\mu) - \epsilon(0) \propto \left(\frac{\mu}{a}\right)^2$$

$\to$ quadratic divergence with $a \to 0$, appearing as soon as $\mu \neq 0$!

If one defines the quark number density from the beginning as the 4-th component of a $U(1)$ Noether current on the lattice, one directly gets the point-split form of the current, $\bar{\psi}(x)\gamma_\mu\psi(x+\hat{\mu})$.

This dictates the timelike hopping term in the Wilson action :

$$-\frac{1}{2a}\sum_n \Big(f(a\mu)(1-\gamma_4)U_{n,4}\delta_{n+\hat{4},m} + f(a\mu)^{-1}(1+\gamma_4)U^\dagger_{n-\hat{4},4}\delta_{n-\hat{4},m}\Big)$$

For $\mu = 0$ must hold: $f(a\mu) = 1$, $f(a\mu) = 1 + a\mu + \mathcal{O}\left((a\mu)^2\right)$.

Time reflection positivity requires $f(a\mu) = 1/f(-a\mu)$.

This uniquely leads to $f(a\mu) = \mathrm{e}^{a\mu}$.

Moral :

"A chemical potential must enter via the kinetic part of the action like a fourth component A_4 of an Abelian gauge field."

For naive fermion action without gauge field :

$$S_F^{naive}[\bar{\psi},\psi] = a^3 \sum_x \left[ma\bar{\psi}_x\psi_x + \frac{1}{2} \sum_{\nu=1}^{4} \left(\mathrm{e}^{\mu a \delta_{\nu,4}} \bar{\psi}_x \gamma_\nu \ \psi_{x+\hat{\nu}} - \mathrm{e}^{-\mu a \delta_{\nu,4}} \bar{\psi}_{x+\hat{\nu}} \gamma_\nu \psi_x \right) \right]$$

With gauge fields for Kogut-Susskind ("staggered") fermions :

$$S_F^W[\bar{\psi},\psi] = a^3 \sum_x \left[ma\bar{\psi}_x\psi_x - \sum_{\nu=1}^{4} \eta_{x,\nu} \bar{\psi}_x \frac{1}{2} \left(\mathrm{e}^{\mu a \delta_{\nu,4}} U_{x,\nu} \psi_{x+\hat{\nu}} - \mathrm{e}^{-\mu a \delta_{\nu,4}} U^\dagger_{x-\hat{\nu},\nu} \psi_{x-\hat{\nu}} \right) \right]$$

With gauge fields and with the Wilson prescription for fermions :

$$S_F^W[\bar{\psi},\psi] = a^3 \sum_x \left[\bar{\psi}_x\psi_x - \kappa \sum_{\nu=1}^{4} \left(\mathrm{e}^{\mu a \delta_{\nu,4}} \bar{\psi}_x (r-\gamma_\nu) U_{x,\nu} \psi_{x+\hat{\nu}} + \mathrm{e}^{-\mu a \delta_{\nu,4}} \bar{\psi}_{x+\hat{\nu}} (r+\gamma_\nu) U^\dagger_{x,\nu} \psi_x \right) \right.$$

(after rescaling, with κ given by $m_{bare} + 4r = \frac{1}{2\kappa}$)

"This recipe (μ = imaginary Abelian gauge field) can be applied to all other fermion formulation (e.g. overlap fermions) as well."

3. 2. Influence of Various $\mu \neq 0$ on the Fermion Determinant

(a) Remark for $\mu_q = 0$ (counting quarks minus antiquarks)

An important property of the Dirac operator : with $\mu_q = 0$ it fulfills

$$\gamma_5\text{-hermitecity}: \quad \gamma_5 D \gamma_5 = D^\dagger,$$

which implies $\det D = [\det D]^*$. Thus the determinant is real.

"For vanishing μ the determinant is real. If the determinant is negative for some gauge field configurations (sign problem), this can be cured by having two (degenerate) flavors."

(b) The γ_5-hermitecity is spoiled for $\mu_q \neq 0$

Multiplying a hopping term from left and right with γ_5 changes the sign of γ_i; this can be compensated by taking the Hermitean conjugate, thus exchanging U and $U^\dagger$.

The $\mathrm{e}^{+a\mu_q}$ and $\mathrm{e}^{-a\mu_q}$ prevent this to do in the timelike hopping term.

Then, instead

$$\gamma_5 D(\mu_q)\gamma_5 = D^\dagger(-\mu_q)$$

For the determinant written as function of the factor $f = \mathrm{e}^{a\mu_q}$

$$\gamma_5 D(f)\gamma_5 = D^\dagger(1/f^*)$$

with the consequence

$$\det D(f) = [\det D(1/f^*)]^*$$

This establishes real-valuedness only for $f = 1/f^*$.

If f is real, this means $f = 1/f$, in other words $\mu_q = 0$ (see above).

Otherwise holds:

"For nonvanishing real baryonic μ_q the determinant is complex."

A doubling of flavors (which is sometimes physically realistic) would not render the weight factor real.

(c) Imaginary baryonic chemical potential

For imaginary chemical potential $\mu_q = i\eta$, η real, one has $f(a\mu) = f(ia\eta) = 1/f(ia\eta)^* = 1/f(-ia\eta)$ with the consequence:

"For imaginary chemical potential the determinant is real. Therefore, normal importance sampling is applicable ! "

(d) Isospin chemical potential

If one has different chemical potentials for each flavor, adding terms $\sum_f \mu_f \bar{\psi}_f \gamma_4 \psi_f$ to the Lagrangian, one can consider two light flavors u and d with opposite chemical potential :

$\mu_u = \mu_I$ and $\mu_d = -\mu_I$.

This corresponds to the isospin assignment to u and d quarks.

The Dirac operator of both flavors has block-diagonal form

$$\begin{pmatrix} D(\mu_I) & 0 \\ 0 & D(-\mu_I) \end{pmatrix}$$

$$\begin{pmatrix} D(\mu_I) & 0 \\ 0 & \gamma_5 D^\dagger(\mu_I)\gamma_5 \end{pmatrix}$$

The common determinant is

$$\det[D(\mu_I)]\det[\gamma_5 D^\dagger(\mu_I)\gamma_5] = \det[D(\mu_I)]\det[D^\dagger(\mu_I)] = |\det[D(\mu_I)]|^2$$

"For finite isospin chemical potential, the determinantal weight factor in the presence of two flavors (opposite in isospin) is real and positive."

(e) Chiral (or axial) chemical potential μ_5

Creates an imbalance between left handed and right handed matter mimicking the presence of a topologically charged background field :

$$D(\mu_5) = \gamma_\mu D_\mu + m + \mu_5 \gamma_4 \gamma_5$$

$$\begin{aligned}
[D_W(\mu_5)]_{x,y} \;=\; & \delta_{x,y} - \kappa \sum_i \Big[(1-\gamma_i) U_i(x) \delta_{x+\hat{i},y} + (1+\gamma_i) U_i^\dagger (x-\hat{i}) \delta_{x-\hat{i},y} \Big] \\
& - \; \kappa \Big[(1 - \gamma_4 \mathrm{e}^{a\mu_5\gamma_5}) U_4(x) \delta_{x+\hat{4},y} + (1 + \gamma_4 \mathrm{e}^{-a\mu_5\gamma_5}) U_4^\dagger (x-\hat{4}) \delta_{x-\hat{4},y} \Big]
\end{aligned}$$

with

$$\mathrm{e}^{\pm a\mu_5\gamma_5} = \cosh(a\mu_5) \pm \gamma_5 \sinh(a\mu_5)$$

This satifies γ_5-hermitecity : $\gamma_5 D(\mu_5) \gamma_5 = D^\dagger(\mu_5)$

Consequently, the determinant is real-valued !

Result : A current is induced through the chiral magnetic effect (CME) in presence of an external magnetic field $\vec{B}$ acting on electrical charges e

$$\vec{j} = \sigma_\chi \ \vec{B} = \frac{1}{2\pi^2} \ \mu_5 \ e \ \vec{B}$$

(chiral magnetic conductivity σ_χ, Kharzeev and Warringa arXiv:0907.5007)

(f) Gauge group $SU(2)$

This group possesses only real representations.

Pauli-Gürsey symmetry : $ST^aS^{-1} = -(T^a)^\star$ with $S = \sigma^2$

Taking $S = C\gamma_5\sigma^2$ and using $C\gamma_\mu C^{-1} = -\gamma_\mu^T$, one finds

$$SD(\mu)S_{-1} = D(\mu^\star)^\star$$

For real $\mu =$ one has $\det D = (\det D)^\star$, i.e. $\det D =$ real, but not necessarily positive (such models studied mostly by S. Hands and J. Skullerud).

3. 3. Complex Action for a 4D Complex Scalar Field

Finite charge density (finite μ) corresponds to an imaginary Abelian gauge field also in the case of charged (complex valued) scalar fields.

The Noether current has the same point-split form.

The action of a complex scalar field is usually real-valued, but now this is not anymore the case !

$$S_E = \sum_x \left[\kappa |\phi_x|^2 + \lambda |\phi_x|^4 - \sum_{\nu=1}^{4} \left(\mathrm{e}^{\mu a \delta_{\nu,4}} \phi_x^\star \phi_{x+\hat{\nu}} + \mathrm{e}^{-\mu a \delta_{\nu,4}} \phi_x^\star \phi_{x-\hat{\nu}} \right) \right]$$

with $\kappa = 8 + m^2$.

Asymmetric hopping in positive/negative time direction.

If $\mu \neq 0$ this scalar action is explicitly complex-valued, which makes the Boltzmann factor not useful as probability weight in MC simulations !

The problem is overcome by using alternative degrees of freedom, i.e. a flux representation, to be achieved by a duality transformation.

Expansion of the "dangerous " (nearest neighbor) Boltzmann factors :

$$\prod_{x,\nu} \exp\left(e^{\mu\,\delta_{\nu,4}}\phi^{\star}_{x}\phi_{x+\widehat{\nu}}\right)\exp\left(e^{-\mu\,\delta_{\nu,4}}\phi_{x}\phi^{\star}_{x+\widehat{\nu}}\right) =$$

$$\sum_{\{n,\overline{n}\}} = \left(\prod_{x,\nu}\frac{1}{n_{x,\nu}!\,\overline{n}_{x,\nu}!}\right)\left(\prod_{x} e^{\,\mu[n_{x,4}-\overline{n}_{x,4}]}\right)\left(\prod_{x,\nu}\left(\phi^{\star}_{x}\phi_{x+\widehat{\nu}}\right)^{n_{x,\nu}}\left(\phi_{x}\phi^{\star}_{x+\widehat{\nu}}\right)^{\overline{n}_{x,\nu}}\right)$$

$$= \sum_{\{n,\overline{n}\}}\left(\prod_{x,\nu}\frac{1}{n_{x,\nu}!\,\overline{n}_{x,\nu}!}\right)\left(\prod_{x} e^{\,\mu[n_{x,4}-\overline{n}_{x,4}]}\;\phi_{x}^{\star\sum_{\nu}[n_{x,\nu}+\overline{n}_{x-\widehat{\nu},\nu}]}\;\phi_{x}^{\sum_{\nu}[\overline{n}_{x,\nu}+n_{x-\widehat{\nu},\nu}]}\right),$$

From now, "configurations" are not understood as specification of the values of the fields (as before), but as a selected set of (integer, non-negative !) expansion powers $n_{x,\nu}, \overline{n}_{x,\nu} \in [0,\infty)$,....

.... in other words, the multiple sum

$$\sum_{\{n,\overline{n}\}} = \prod_{x,\nu} \sum_{n_{x,\nu}=0}^{\infty} \sum_{\overline{n}_{x,\nu}=0}^{\infty}$$

replaces the integral over configurations of the usual path integral, realized in the usual Monte Carlo algorithm, which now would fail because of the complex measure.

The complex field variables are written in polar form, $\phi_x = r_x\, e^{i\theta_x}$. Splitting the integration measure in polar coordinates one finds for the partition function the form

$$Z = \sum_{\{n,\overline{n}\}} \left(\prod_{x,\nu} \frac{1}{n_{x,\nu}!\, \overline{n}_{x,\nu}!} \right) \left(\prod_x \int_{-\pi}^{\pi} \frac{d\theta_x}{2\pi} e^{-i\theta_x \sum_\nu [n_{x,\nu} - \overline{n}_{x,\nu} - (n_{x-\widehat{\nu},\nu} - \overline{n}_{x-\widehat{\nu},\nu})]} \right)$$
$$\times \left(\prod_x e^{\,\mu[n_{x,4} - \overline{n}_{x,4}]} \int_0^{\infty} dr_x\; r_x^{\,1+\sum_\nu [n_{x,\nu} + n_{x-\widehat{\nu},\nu} + \overline{n}_{x,\nu} + \overline{n}_{x-\widehat{\nu},\nu}]}\; e^{-\kappa r_x^2 - \lambda r_x^4} \right)$$

The integrals over the angular part θ_x of the usual "configuration space have now given rise to Kronecker deltas written as $\delta(n)$.

The integrals over the moduli $|\phi_x|$ (tabulated for MC) are denoted as

$$W(n) \;=\; \int_0^\infty dr\, r^{n+1}\, e^{-\kappa r^2 - \lambda r^4}$$

The partition function now reads :

$$Z = \sum_{\{n,\overline{n}\}} \left(\prod_{x,\nu} \frac{1}{n_{x,\nu}!\, \overline{n}_{x,\nu}!} \right) \left(\prod_x \delta \left(\sum_\nu \left[n_{x,\nu} - \overline{n}_{x,\nu} - (n_{x-\widehat{\nu},\nu} - \overline{n}_{x-\widehat{\nu},\nu}) \right] \right) \right)$$
$$\times \left(\prod_x e^{\,\mu[n_{x,4} - \overline{n}_{x,4}]}\; W \left(\sum_\nu \left[n_{x,\nu} + \overline{n}_{x,\nu} + n_{x-\widehat{\nu},\nu} + \overline{n}_{x-\widehat{\nu},\nu} \right] \right) \right)$$

In this form the complex phase problem is completely eliminated !

All weight factors for configurations of the n and $\overline{n}$ variables are now real and non-negative !

One minute of contemplation :

In all the integrals giving the Kronecker delta symbols all the non-real, non-positive contributions are hidden !

Ths way the model is "decontaminated" from the sign problem !

However, many configurations of n and $\overline{n}$ would have vanishing weight, if the constraints enforced by the Kronecker deltas are violated, i.e., when – at least for one site x – one has

$$(\nabla n)(x) - (\nabla \overline{n})(x) \neq 0.$$

If no intelligent update algorithm would be available, the sampling would be hopelessly inefficient !

The geometric nature of the variables k and l makes geometric updates possible, avoiding configurations with vanishing weight :

Worm algorithm (N. Prokof'ev and B. Svistunov)
for a self-review see arXiv:0910.1393

This way of transformation of the problem and the simulation algorithm is similar/typical for all flux representations of spin systems, also for Abelian gauge systems (e.g. the Abelian $\mathbb{Z}(3)$ Higgs model) !
(A. Schmidt and Ch. Gattringer, talk at LATTICE 2012)

Thus, in many models one can successfully avoid the sign problem !

The representation of the observables of interest differs from case to case.

The worm algorithm has been tested by comparison with

- **the exact solution for $\lambda = 0$ (solvable by Fourier transform)**
- **conventional Monte Carlo simulations for $\mu = 0$.**

The crucial test : reproducing the silver blaze effect at $T = 0$

for some sets of parameters, e.g. $\kappa = 9.0$ $\lambda = 1.0$, one can measure the averages of n and $|\phi|^2$ and its derivatives as function of μ :

- **n vanishes up to $\mu_c = 1.146$ and rises linearly for $\mu > \mu_c$**
- **the derivative χ_n jumps from zero to a finite value at μ_c**
- **χ_n' shows a sharp peak at μ_c with a height growing linearly with the volume (showing a singularity developing in the limit $V \to \infty$)**

- **the average of $|\phi|^2$ and its derivatives behave similarly**

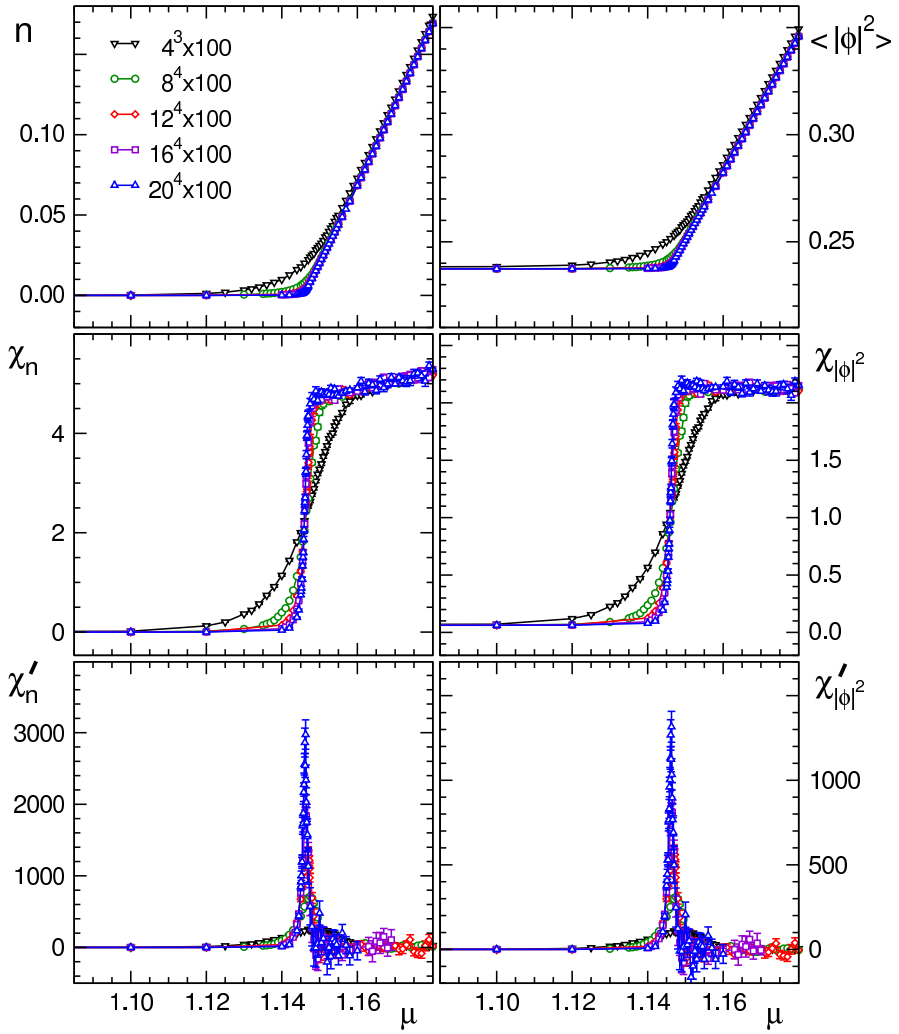
A pseudo silver blaze effect is observed at $T > 0$

At $T > 0$ (shorter lattice in time direction, $N_t < N_s$), a weaker pseudo silver blaze effect is observed :

- **a weak dependence on μ begins below μ_c**
- **there is a "threshold value" μ_{onset} which rises with T relative to μ_c at $T = 0$.**

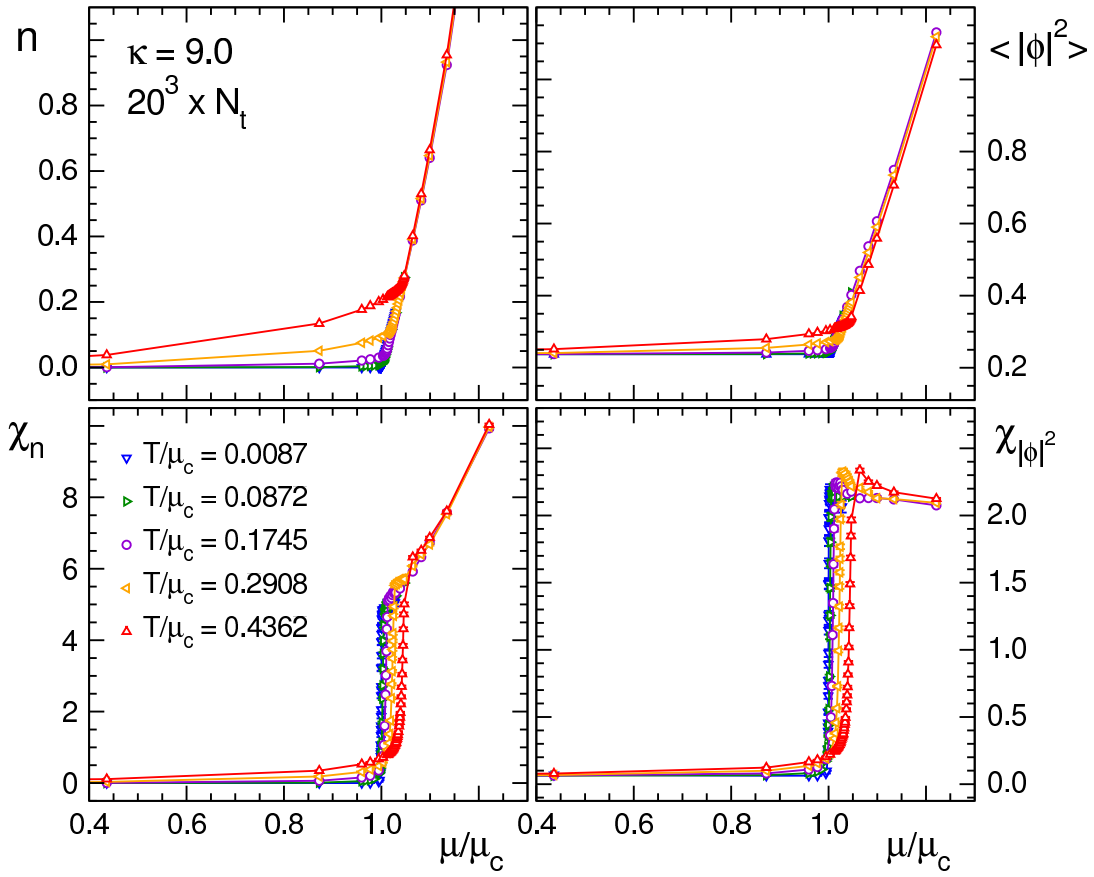
Silver blaze effect at very low temperature

from arXiv:1206.2954 Gattringer and Kloiber



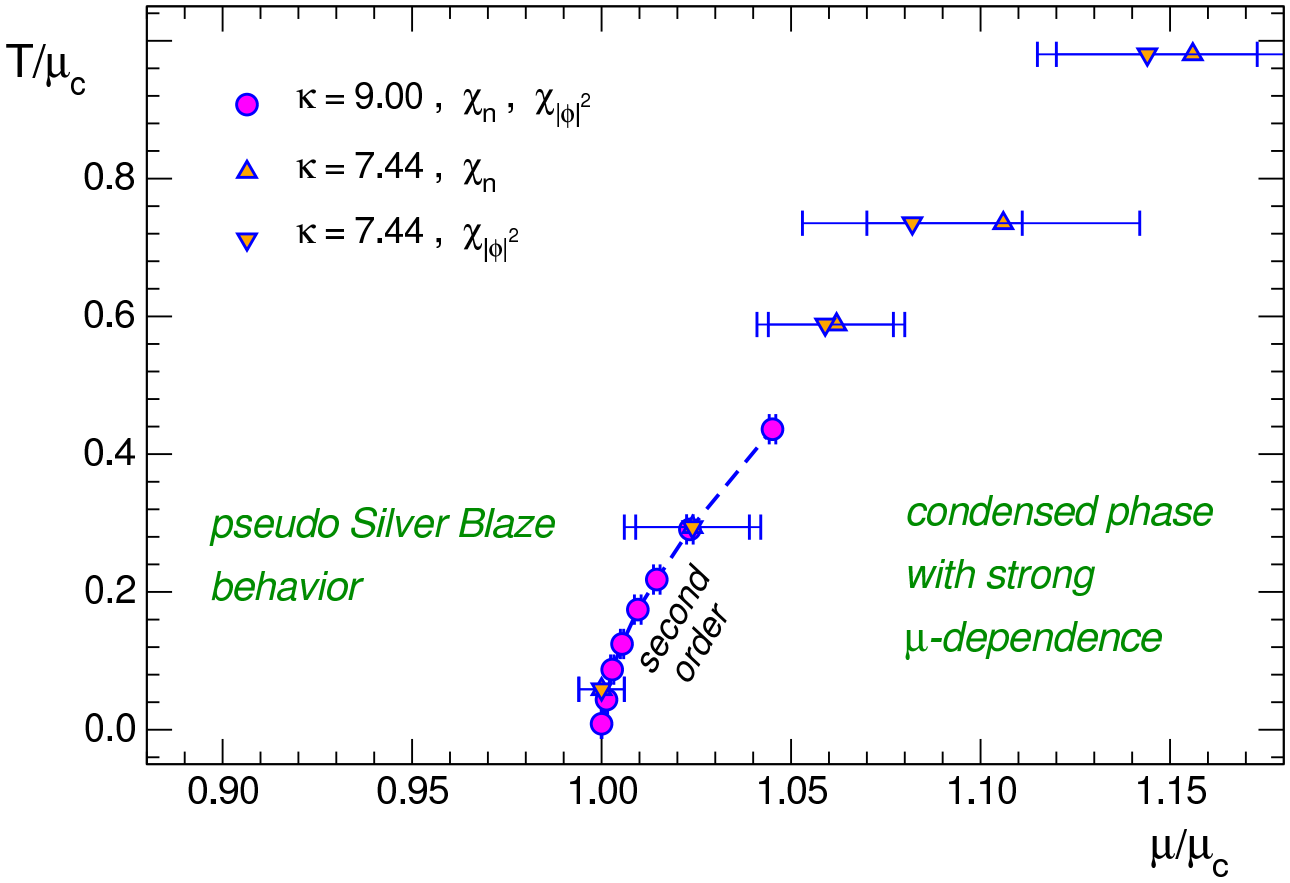
What remains from the Silver blaze effect at higher temperature ?

from arXiv:1206.2954 Gattringer and Kloiber



Phase structure in the T-μ plane

from arXiv:1206.2954 Gattringer and Kloiber



This is a very important observation :

- **the worm algorithm can be applied in a field theory problem, if the lattice formulation is chosen and reformulated by strong coupling methods**
- **silver blaze problem is a more general/ubiquitous phenomenon**
- **silver blaze problem is related to the complex weight problem**
- **silver blaze problem is not specific for fermion problems**

Moral :

"If importance sampling does not work in one representation, use strong coupling methods to go over to another representation, where importance sampling works again, however in other variables and in another environment."

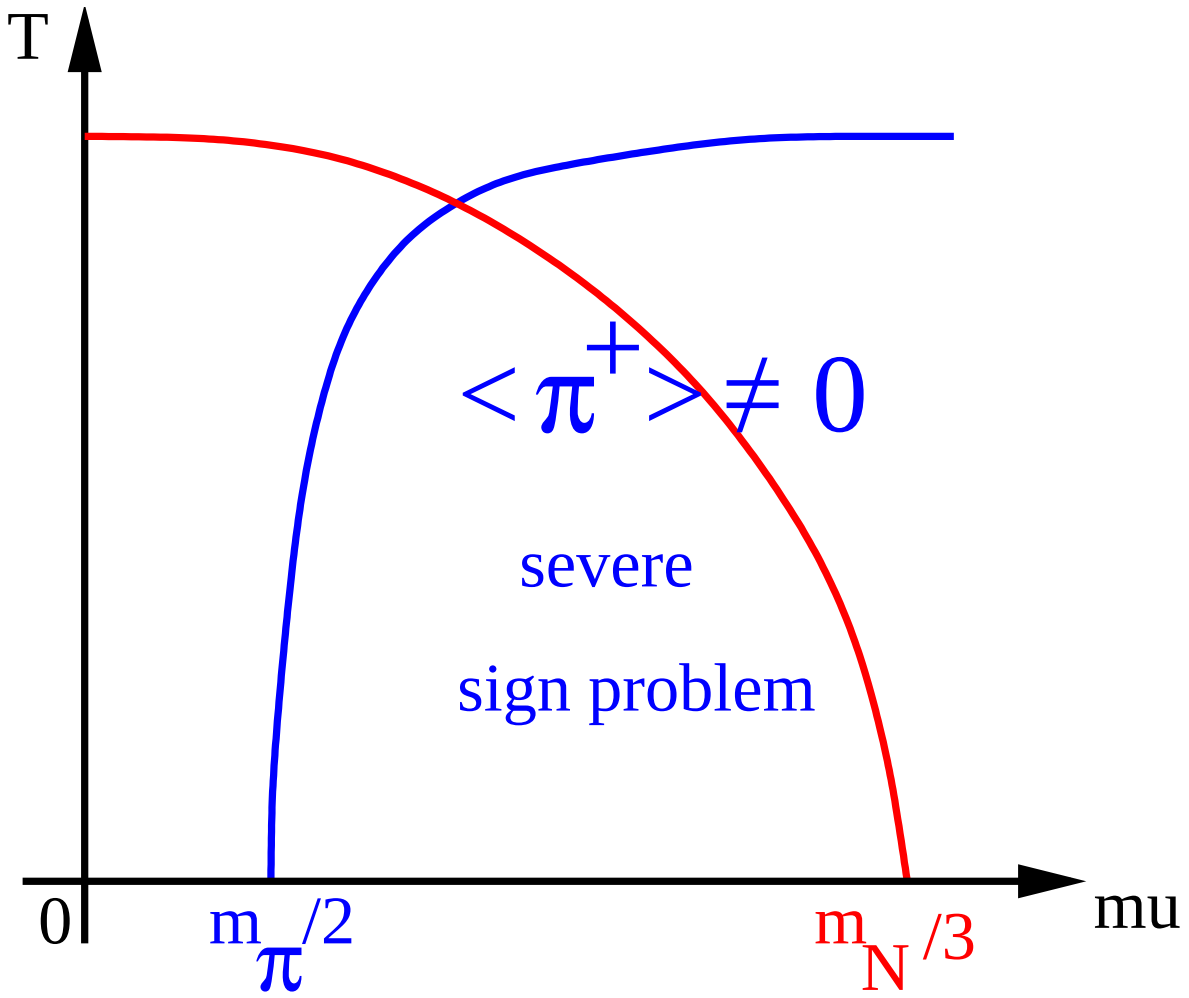
This is sometimes called
"Duality transformation" (from one representation to the other.)

4. Fighting the Complex Measure Problem in Standard LGT

- General Remarks
- Reweighting across the β-μ Plane : Determinants
- Extrapolation by Taylor Expansion
- Continuation from Imaginary Chemical Potential
- Canonical Ensemble Approach

Where the quenched and phase-quenched simulation fails

from Ph. de Forcrand arXiv:1005.0539



4. 1. General Remarks

Quenched simulations have been misleading !

$\mu_{onset} \simeq m_\pi/2$ **(too low, this would vanish in chiral limit !)**

At zero temperature one expects $\mu_{onset} = \mathcal{O}(m_p/3)$

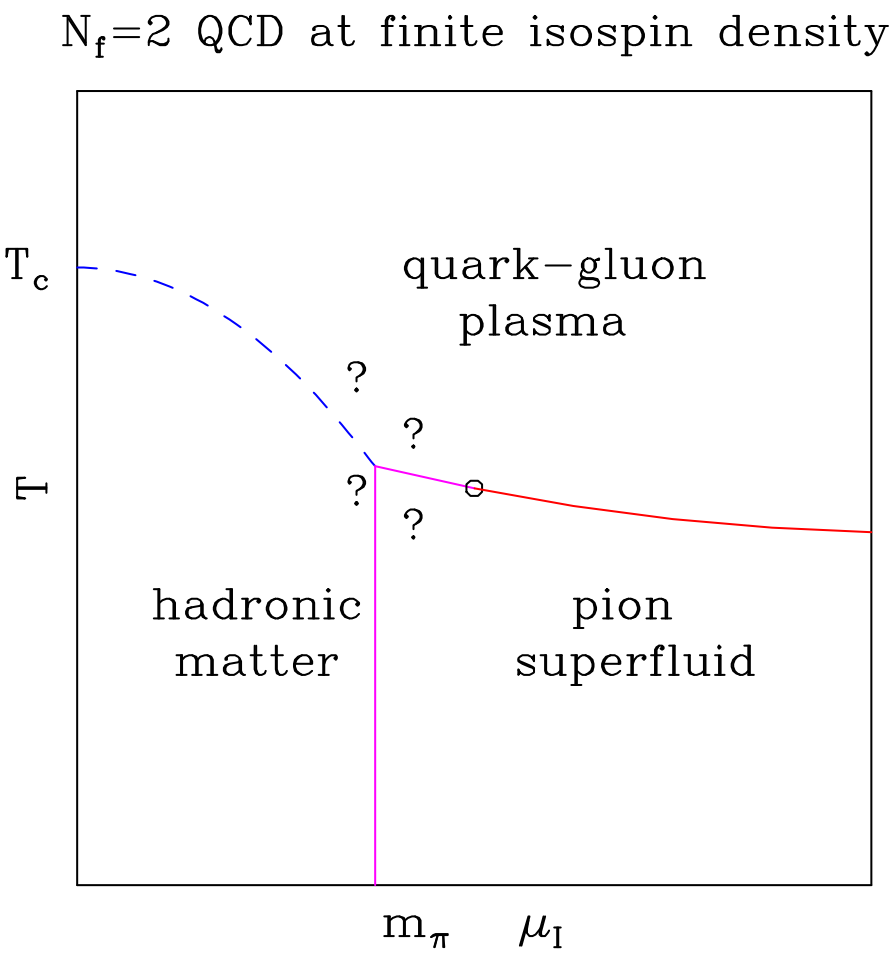
Quenched QCD is not the $N_f \to 0$ **limit of QCD, as soon as** $\mu \neq 0$ **!**
Therefore quenched simulation is not an approximation at all !
There is no way to circumvent the problem by ignoring dynamical quarks, calculating observables in the valence approximation.

But then the phase of the determinant is particularly important !

There is no way to describe real physics by ignoring the phase of the fermion determinant. Ignoring the phase describes an unwanted physical situation governed by π **condensation, where** μ **acts actually as** μ_I**.**

Schematic phase diagram for QCD at finite isospin density

from Philipsen



"The determinant may be complex, and it *must* be complex to produce the physically expected behavior." (Ph. de Forcrand)

Consider the free energy of a static color charge or anti-charge:

Denote by $\det D\ \mathrm{e}^{-S_G}\ D[U]$ **the measure, so it has a real and an imaginary part.**

P **is the Polyakov loop, which has also real and an imaginary part.**

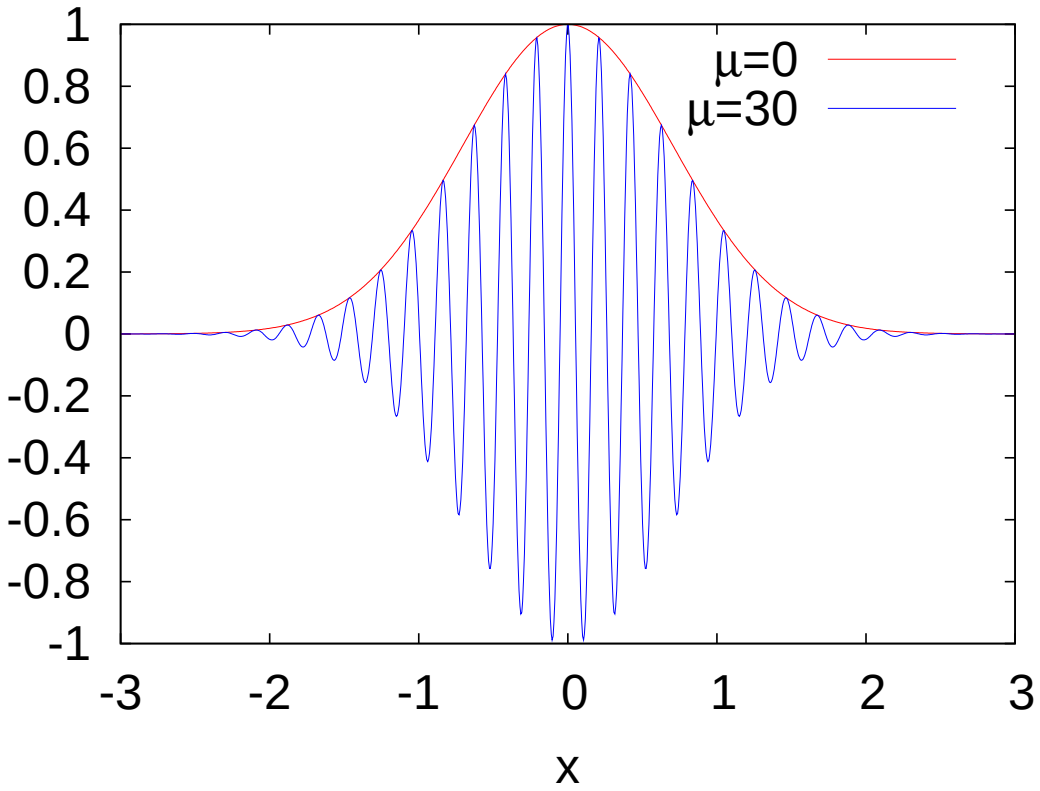
The expectation values are the two real integrals:

$$\langle \mathrm{tr}\ \ P \rangle \ = \ \mathrm{e}^{-\frac{1}{T} F_q} = \int (\mathrm{Re}\ \mathrm{tr}\ \ P \times \mathrm{Re}\ \ \det D - \mathrm{Im}\ \mathrm{tr}\ \ P \times \mathrm{Im}\ \ \det D)\ \ \mathrm{e}^{-S_G}\ \ D[U]$$

$$\langle \mathrm{tr}\ \ P^\dagger \rangle \ = \ \mathrm{e}^{-\frac{1}{T} F_{\bar{q}}} = \int (\mathrm{Re}\ \mathrm{tr}\ \ P \times \mathrm{Re}\ \ \det D + \mathrm{Im}\ \mathrm{tr}\ \ P \times \mathrm{Im}\ \ \det D)\ \ \mathrm{e}^{-S_G}\ \ D[U]$$

Different free energies (very plausible in a dense baryonic medium !) are only possible if the measure has an imaginary part, $\mathrm{Im}\ \ \det D \neq 0$**.**

The toy model



General considerations about modified sampling :

Reweighting for an oscillating measure

Assume a real, but oscillating weight function $f(x)$ that is the "correct" one; it has the correct partition function :

$$Z_f = \int dx \; f(x)$$

Is there any better weight $g(x) \geq 0$ to be taken instead for sampling ?

The corresponding auxiliary partition function would be :

$$Z_g = \int dx \; g(x)$$

The expectation value of an observable O is :

$$\langle O \rangle_f = \frac{\int dx \; O(x) \; f(x)}{\int dx \; f(x)} = \frac{\int dx \; O(x) \; \frac{f(x)}{g(x)} \; g(x)}{\int dx \; \frac{f(x)}{g(x)} \; g(x)} = \frac{\langle O \; \frac{f}{g} \rangle_g}{\langle \frac{f}{g} \rangle_g}$$

with a reweighting factor function of x

$$R = \frac{f}{g}$$

The average of $\langle \frac{f}{g} \rangle$ is called "average sign" (or "average phase factor" in the more general case of a complex measure).

The optimal choice (de Forcrand, Kim, Takaishi, hep-lat/0209126) is what renders the variance of the reweighting factor $\frac{f}{g}$ minimal.

If the average sign tends to zero, the solution to the problem is given by $g(x) = |f(x)|$. Then the reweighting factor takes only values

$$R = \frac{f}{g} = \pm 1 = \mathbf{sign}(f)$$

.

The ensemble of x generated in such way is called "sign-quenched ensemble" (or "phase quenched ensemble").

The average sign

This is the ratio of two partition functions giving rise to different free energies :

$$\left\langle \frac{f}{g} \right\rangle_g = \frac{Z_f}{Z_g} = \mathrm{e}^{-\frac{V}{T}\Delta f}$$

The difference in free energy densities $\Delta f = f_{ensemble\ f} - f_{ensemble\ g}$ **is multiplied by** V/T **in the exponent. Bad for large** V **and low** T **!**

Therefore the statistics, that is necessary to get the denominator $\left\langle \frac{f}{g} \right\rangle_g \approx 0$ **with sufficient precision, grows exponentially with** V **!**

This is compulsory in order to be able to estimate the expectation value $\langle W \rangle_f$ **itself with sufficient precision.**

"The necessary amount of simulation time decides whether the sign (or phase) quenching approach is feasible or non-feasible."

Another problem of modified sampling : The overlap problem

Reweighting means to give configurations typical for the sampling ensemble (g) a weight different from 1 in order to mimick another target ensemble (f).

If the overlap of the two distributions is satisfactory, the apparent loss in statistics is tolerable.

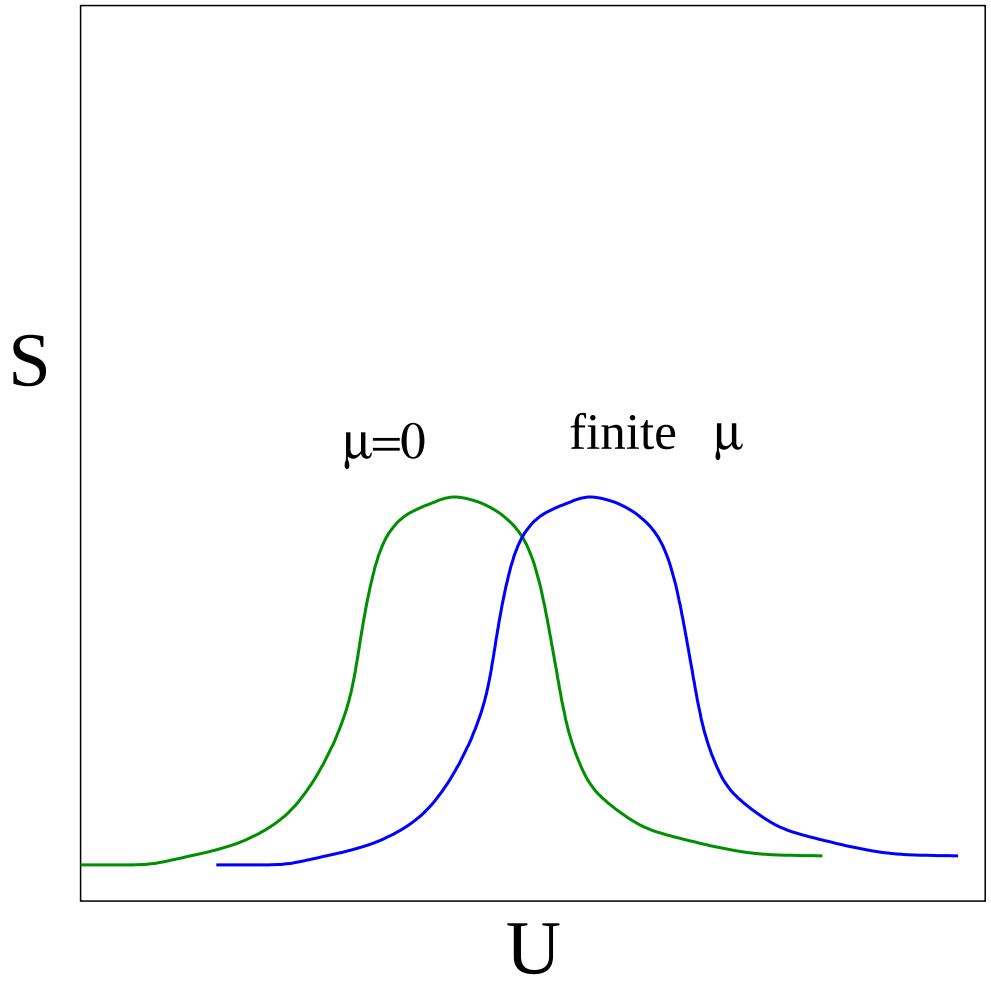
If, however, only the tails overlap, most of the proposed configurations would get a small weight (are produced for waste !).

Then, one needs exponentially large statistics to get reliable results.

The result will be distorted, while the problem may remain unnoticed.

This effect seriously limits the applicability of reweighting.

The overlap problem with "horizontal reweighting" (only in μ)



4. 2. Reweighting across the β-μ Plane : Determinants

Explanation for staggered fermions (taking 4-th root for each flavor)

Exact partition function :

$$Z(\beta,\mu) = \int (\det D(U,\mu))^{\frac{N_f}{4}} \, \mathrm{e}^{-\beta S_G} D[U]$$

Now factorize the determinant into modulus and phase factor :

$$Z(\beta,\mu) = \int |\det D(U,\mu)|^{\frac{N_f}{4}} \, \mathrm{e}^{i\Theta} \mathrm{e}^{-\beta S_G} D[U]$$

According to the previous arguments, the optimal choice would be to change $\beta \to \beta'$ and $\mu \to \mu'$ for sampling (g) and to include the $|\cos(\Theta)|$ factor in the sampling measure :

$$Z_g(\beta',\mu') = \int |\det D(U,\mu')|^{\frac{N_f}{4}} \, |\cos(\Theta)| \mathrm{e}^{-\beta' S_G} D[U]$$

This is very inefficient, since Θ is too expensive to be evaluated in each Molecular Dynamics or Monte Carlo step !

The next best choice is :

$$Z_g(\beta', \mu') = \int |\det D(U, \mu')|^{\frac{N_f}{4}} \, \mathrm{e}^{-\beta' S_G} D[U]$$

This ensemble (sampling) is called "phase quenched ensemble".

It would be exact for an even number of flavors with pairwise opposite isospin, if the chemical potential μ would be considered as isospin chemical potential $\mu = \mu_I$

$$\left|\det D(\mu_I)^{N_f}\right| = \det D(+\mu_I)^{\frac{N_f}{2}} \det D(-\mu_i)^{\frac{N_f}{2}}$$

Standard reweighting approach seems to suggest for sampling :

$$Z_g = Z(\beta', 0)$$

Then the reweighting factor function is :

$$R = \frac{f}{g} = \left|\frac{\det D(\mu)}{\det D(0)}\right|^{\frac{N_f}{4}} \mathrm{e}^{i\Theta} \mathrm{e}^{-(\beta-\beta')S_G}$$

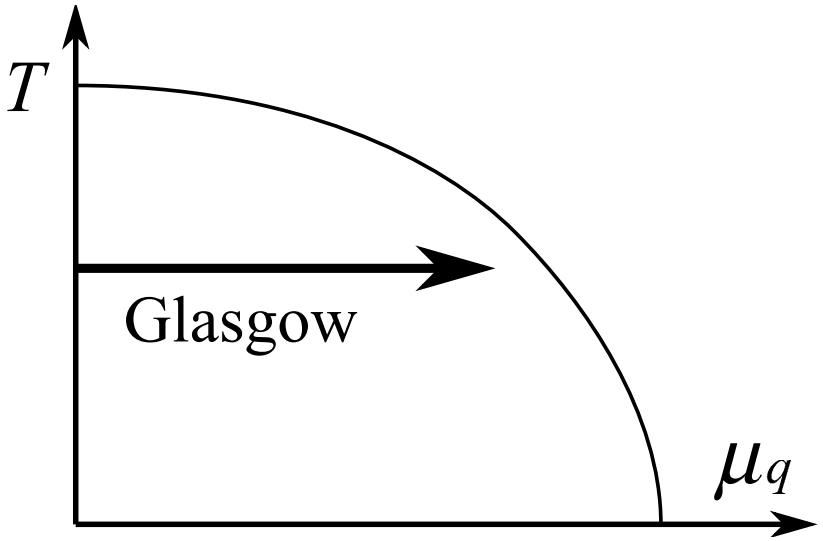
It has to be evaluated together with the evaluation of the observables in order to calculate finally the correlator with O and the average sign :

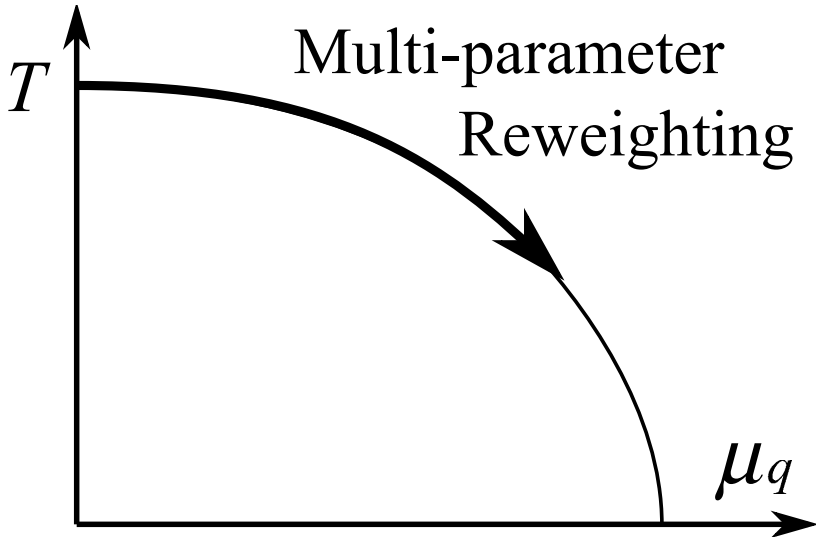
$$\langle O \rangle_f = \frac{\int dx \; O(x) \; f(x)}{\int dx \; f(x)} = \frac{\int dx \; O(x) \; \frac{f(x)}{g(x)} \; g(x)}{\int dx \; \frac{f(x)}{g(x)} \; g(x)} = \frac{\langle O \; \frac{f}{g} \rangle_g}{\langle \frac{f}{g} \rangle_g}$$

Historically, this technique has been practized within two variants :

- **horizontal reweighting ("Glasgow method") at $\beta' = \beta$ fixed**
- **multiparameter reweighting (Budapest Fodor/Katz) : this method actually explores the region in β-μ plane surrounding the finally identified crossover line, starting from the transition point at $\mu = 0$.**

Glasgow (horizontal) vs. Budapest (multiparameter) reweighting





The Glasgow method failed miserably, due to the overlap problem.

In both cases the exact calculation of the fermion determinant at $\mu \neq 0$ is required, but only when a configuration is under examination, not in every update step !

Special method of Fodor and Katz to evaluate determinants :

- **shift the μ-dependence into two time slices**
- **factorization of the μ-dependence**

$$\det D(\mu) = \mathrm{e}^{-3N_s^3 N_t \mu} \det\left(P - \mathrm{e}^{N_t \mu}\right)$$

P is the "reduced fermion matrix" (a $2NN_s^3 \times 2NN_s^3$ matrix) with two time slices.

When all $2NN_s^3$ eigenvalues λ_i of the reduced matrix are known,

$$\det D(\mu) = \mathrm{e}^{-NN_s^3 N_t \mu} \prod_{i=1}^{2NN_s^3} \left(\mathrm{e}^{N_t \mu} - \lambda_i\right)$$

Thus the reweighting factor is evaluated, while the sampling runs with real positive weight $\det D(\mu = 0)$ at $\beta' \neq \beta$!

This reduced fermion matrix technique is broadly applied.

A very useful tool : one can define an "overlap measure" α :

α is defined as the fraction of sampled configurations that contributes the fraction $1-\alpha$ to the total weight (in the target ensemble).

The reweighting step should not be too small and not too far !

Optimal is an overlap $\alpha = 50$ %

The height lines of the overlap measure α in the $\beta - \mu$ plane show clearly, where one can rely on reweighting.

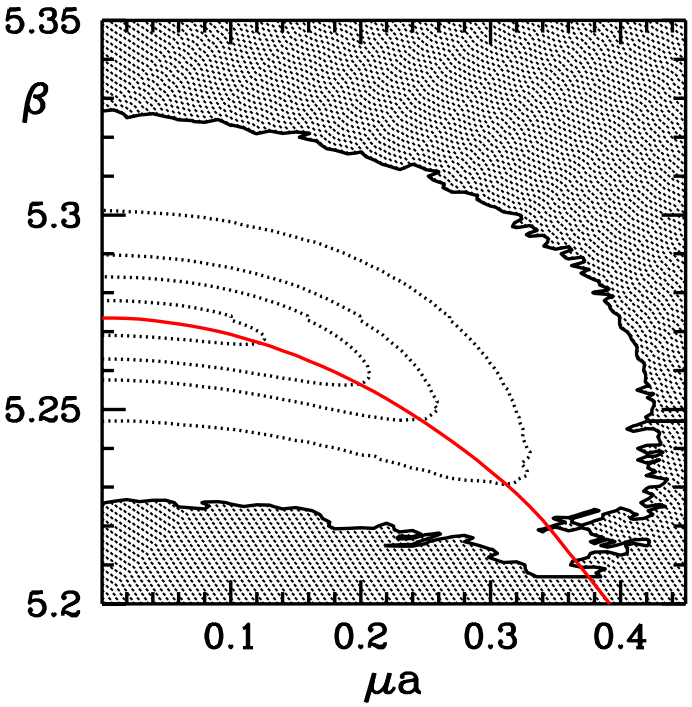
The grey area is not accessible by reweighting from β_c at $\mu = 0$.

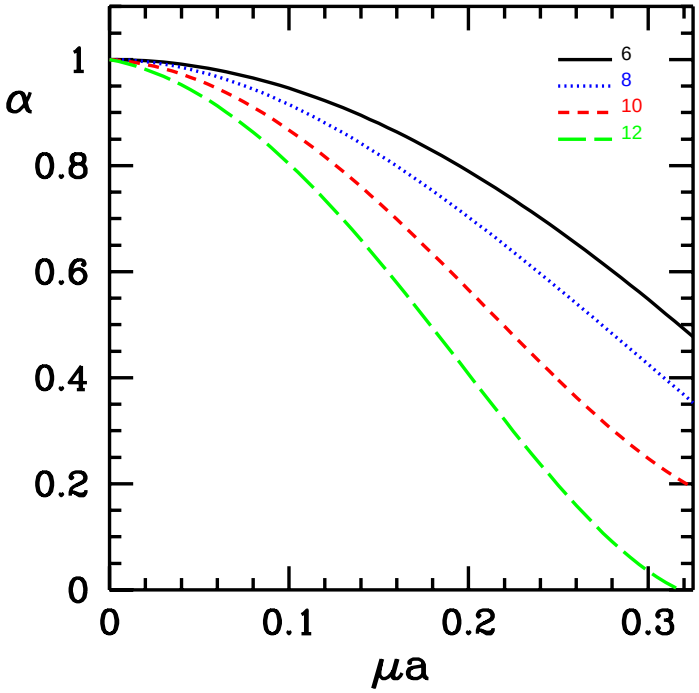
The ridge of the susceptibility (usually locating the crossover line) falls on top of the ridge of the overlap measure α.

This is the way to find the optimal path for reweighting.

Left: Contour plots of the overlap measure; the red line (line of the cross-over) is determined by the peaks of susceptibility. Right: volume and μ dependence of the overlap measure. The half width ($\mu_{1/2}$; defined by $\alpha = 1/2$) shrinks according to: $\mu_{1/2} \propto V^{-\gamma}$ with $\gamma \approx 1/3$.

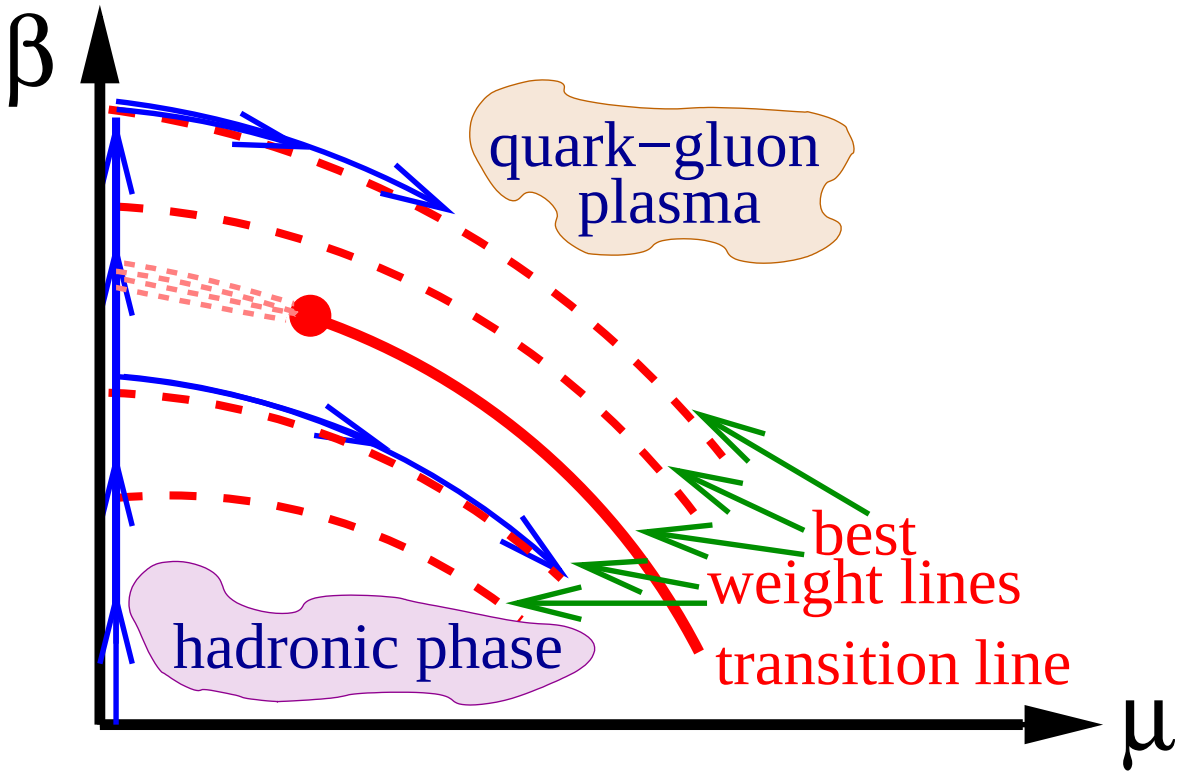
from F. Csikor et al. hep-lat/0401016





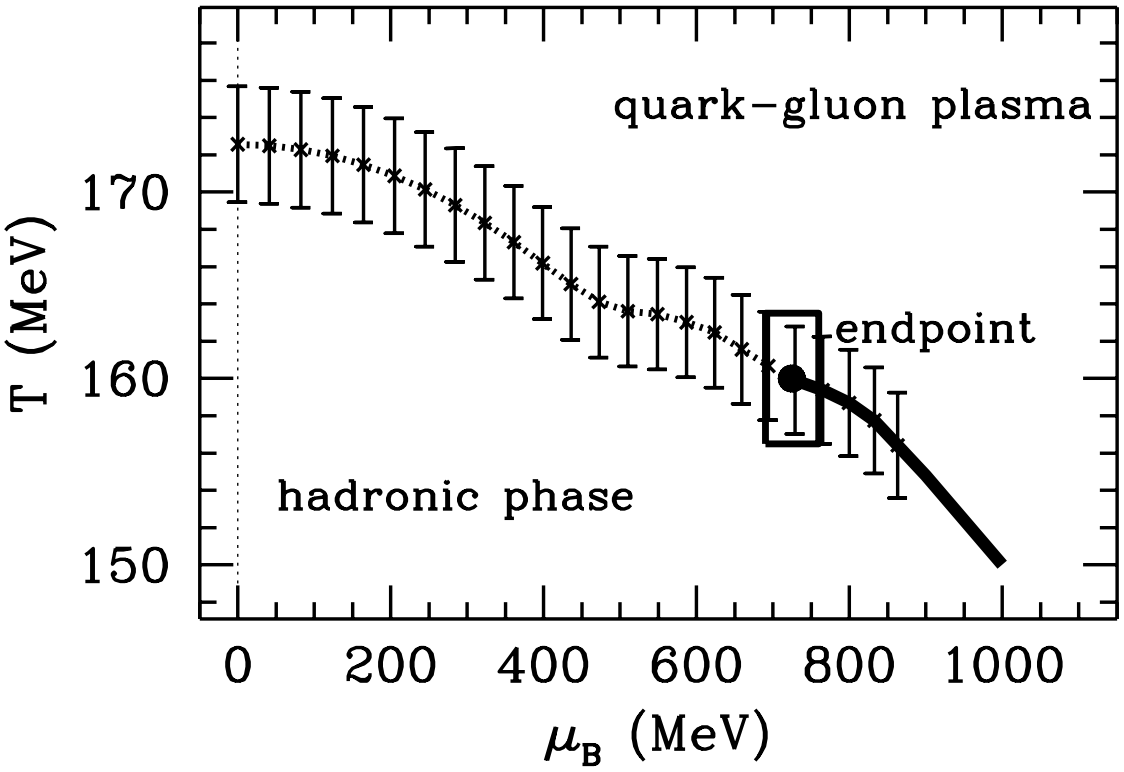
Best pathes for reweighting

from F. Csikor et al. hep-lat/0301027



Finding the Line of the Crossover

from F. Csikor et al. hep-lat/0301027



Where along the crossover line the endpoint is finally found ?

Adding an imaginary part to β allows to study the Lee-Yang zeroes of the theory : these are the zeroes of the partition function.

When the Lee-Yang zeroes in the limit $V \to \infty$ approach the real axis this signals that a real singularity (phase transition) appears.

At finite volume, the pattern of the n^{th} Lee-Yang zeroes β_{LY}^n is $\mathrm{Im}\ \beta_{LY}^{(n)} = C(2n+1)$**.**

When the crossover turns into a first order transition, the location of the (extrapolated) lowest Lee-Yang zero touches the real axis, $C \to 0$**.**

This fixes the critical endpoint : F. Csikor et al. hep-lat/0301027

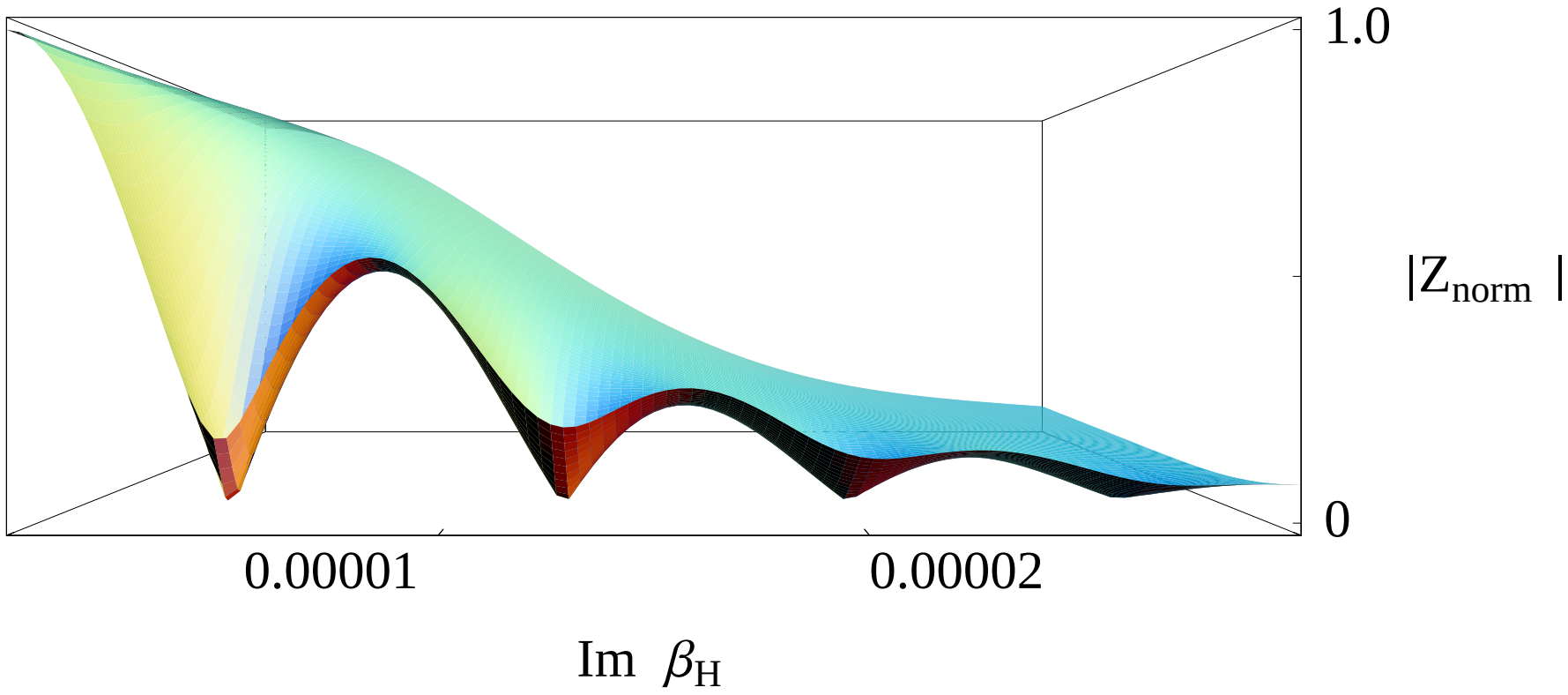
For $2+1$ flavors the Wuppertal-Budapest group has obtained

$\mu_B^E = 725 \pm 35$ MeV $\qquad T^E \approx 160 \pm 3.5$ MeV $\qquad T_c(\mu = 0) = 172 \pm 3$ MeV

(this result has been later updated !)

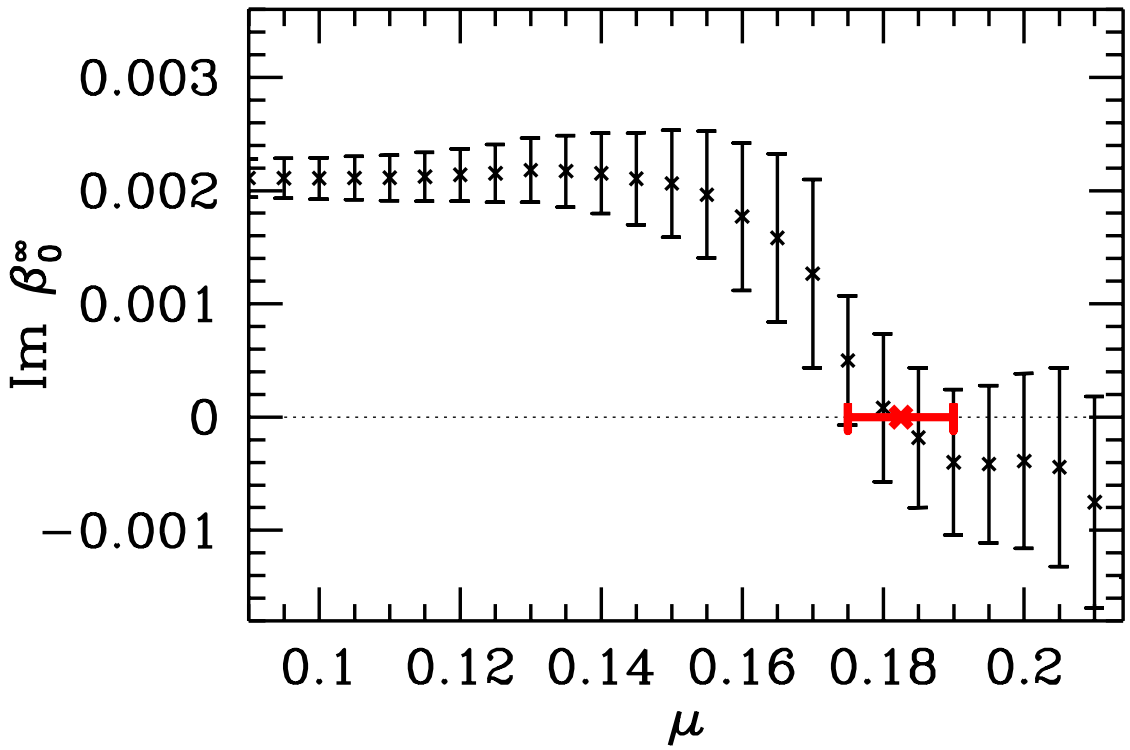
The zeroes of the partition function near to the endpoint of the first order electroweak phase transition ($m_{Higgs} \approx 70$ GeV)

from hep-lat/9704013 Gürtler, Ilgenfritz, Schiller



Locating the Critical Endpoint by the lowest Lee-Yang zero (extrapolated to $V \to \infty$) ($\mathrm{Im}\ \beta_{LY}^{(0)}$) in the complex β plane.

from Z. Fodor and S. D. Katz hep-lat/0111064



An important cross-check for the different methods :

At imaginary μ, where direct simulation is possible, the Glasgow (horizontal) and Budapest (multiparameter) reweighting can be compared with direct simulation, "on the spot" $(\beta, \mu = i\eta)$.
($N_f = 4$ staggered fermions)

Even though all determinants are positive (at $\mu = 0$ and $\mu = i\eta$), Glasgow reweighting fails.

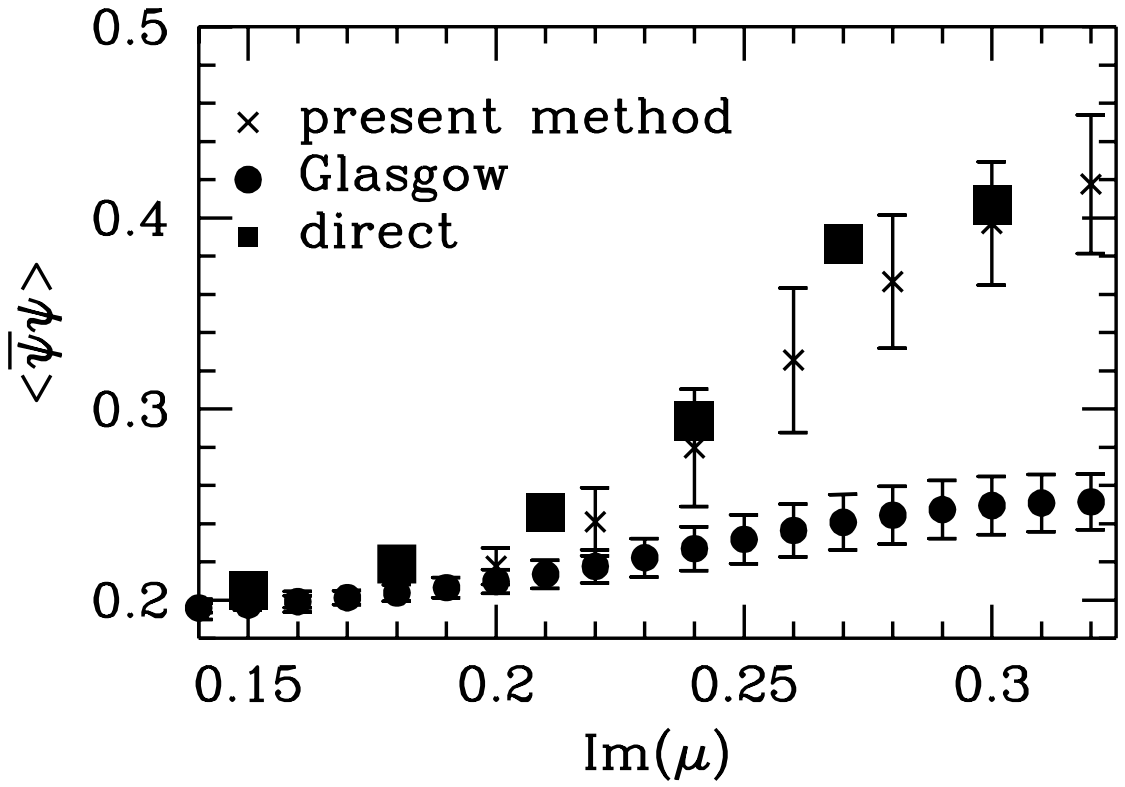
There exists a quasi-physical prediction :

For imaginary μ the chiral condensate $\langle\bar{\psi}\psi\rangle$ should grow !

The Glasgow reweighting fails to reproduce this result of the other two methods (the rise is insufficient !).

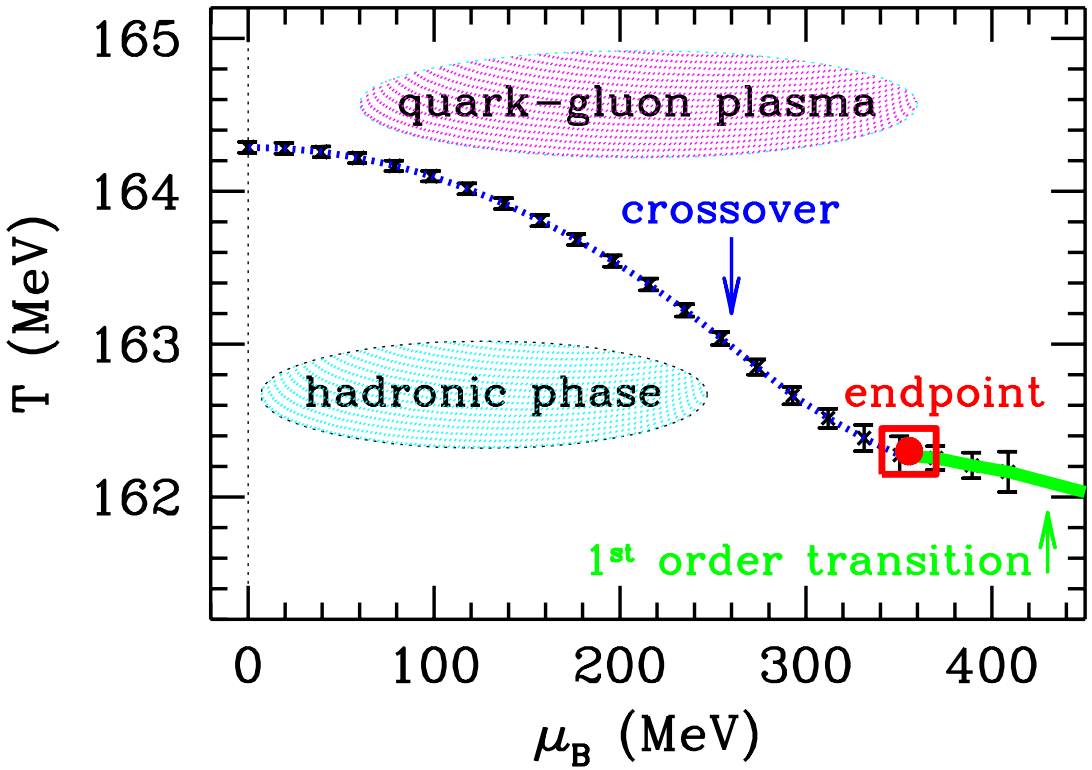
Testing the Method at Imaginary μ by Comparison with Direct Simulation. Failure of the Glasgow method due to the Overlap Problem.

from Z. Fodor and S. D. Katz hep-lat/0111064



Update of the critical point (small square) in physical units. Dotted line for the crossover, solid line for the first order phase transition. The small square shows the endpoint. Combining all uncertainties one obtains $T_E = 162 \pm 2$ MeV and $\mu_E = 360 \pm 40$ MeV.

from Z. Fodor and S. D. Katz hep-lat/0402006



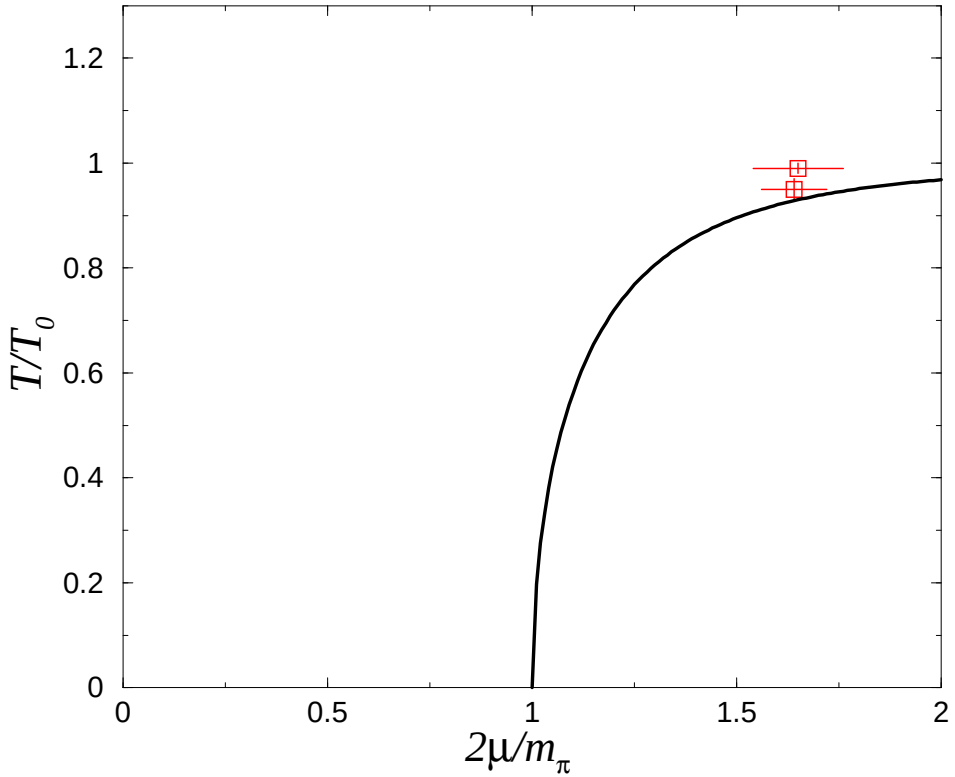
Compared to the previous finding, the light quark masses had been reduced by a factor three, while the largest volume has been increased by a factor three.

This simulation is still far from the continuum limit $N_t = 4$:

$$a = \frac{1}{4T_c} \sim \mathcal{O}(0.25 \text{ fm})$$

Doubts are still allowed : The critical endpoint lies too close to the critical line for pion condensation (in phase-quenched simulations).

from Splittorff hep-lat/0505001



Systematic investigations of the average phase factor are needed (and done) to assess the reliability of reweighting

How good/bad reweighting by phase quenching works can be monitored by evaluation of the average phase factor :

$$\langle \exp(2i\theta) \rangle = \frac{Z(+\mu,+\mu)}{Z(+\mu,-\mu)} = \left\langle \frac{\det(\mu)^2}{|\det(\mu)|^2} \right\rangle_{|phase\ \ quenched}$$

The reference ensemble is the isospin-μ ensemble with real and positive determinant weight (effectively $\mu_I = \mu$).

Here, the phase factor is the observable of interest.

Let's recall the physical background for this "observable" !

With $N_f = 2$ the physically true partition function at $\mu \neq 0$ is

$$Z_B = \int D[U] \ \left(\det D(\mu)\right)^2 \ \mathrm{e}^{-S_{YM}}$$

B stands for "baryonic chemical potential" μ.

The phase quenched partition function (subscript I, since this would be correct for the "isospin chemical potential" μ)

$$Z_I = \int D[U] \ \left|\det D(\mu)\right|^2 \ \mathrm{e}^{-S_{YM}}$$

Distinguish the two "expectation values" of $\mathcal{O}$:

$$\langle \mathcal{O} \rangle_B \ = \ \frac{1}{Z_B} \int D[U] \ \mathcal{O} \ \left(\det D(\mu)\right)^2 \ \mathrm{e}^{-S_{YM}}$$

$$\langle \mathcal{O} \rangle_I \ = \ \frac{1}{Z_I} \int D[U] \ \mathcal{O} \ \left|\det D(\mu)\right|^2 \ \mathrm{e}^{-S_{YM}}$$

Each of the two determinants involved have the decomposition :

$$\det D(\mu) = |\det D(\mu)| \ \mathrm{e}^{i\Theta}$$

Θ is the phase of the determinant; it fluctuates strongly with the configuration $\{U\}$ (fluctuations growing with the volume of the system) !

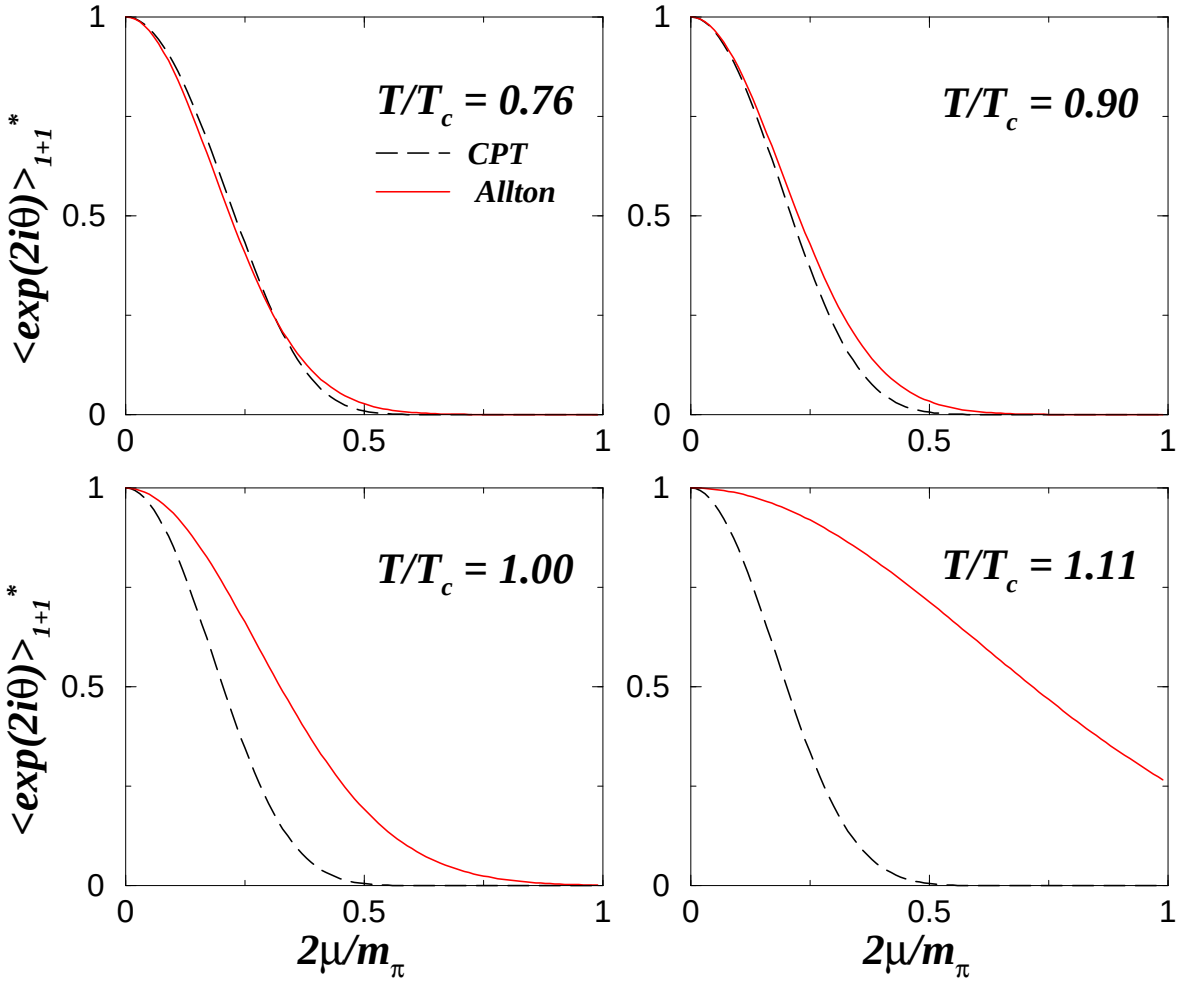
Although $\langle \mathcal{O} \rangle_B$ cannot be directly calculated by importance sampling, it can be estimated as follows (with $N_f = 2$)

$$\langle \mathcal{O} \rangle_B = \frac{\langle \mathcal{O}\ \mathrm{e}^{2i\Theta} \rangle_I}{\langle \mathrm{e}^{2i\Theta} \rangle_I}$$

Numerator and denominator are both based on a phase-quenched simulation (subscript I). The phase factor $\mathrm{e}^{2i\Theta}$ is handled like an observable and must be evaluated for each configuration encountered. It is a global quantity and fluctuates very strongly !

Both numerator and denominator will become very small for realistic volumes. "The smallness of the denominator quantifies the severity of the sign problem."

Comparison of values of the "average phase factor" $\langle \exp(2i\theta) \rangle$ measured in lattice simulations with predictions from one-loop chiral perturbation theory (Splittorff, Verbaarschot 2007). Good agreement persists up to $T/T_c \sim 0.90$.



Analytic results from chiral perturbation theory :

$$\langle \exp(2i\theta) \rangle = \left(1 - \frac{4\mu^2}{m_\pi^2}\right)^{N_f+1}$$

Results of the comparison :

- **The sign problem is not severe for $\mu < \frac{m_\pi}{2}$**
- **Large differences exist between the free energy densities of the phase-quenched and full theory for $\mu > \frac{m_\pi}{2}$.**
- **The method becomes problematic for large volumes.**
- **For high temperature the average phase factor doesn't drop as fast as for $T \leq T_c$**

"Reweighting is problematic at low temperature and high density"

4. 4. Extrapolation by Taylor Expansion

- The chemical potential enters always in the combination μ/T.
- Reweighting gives μ-dependence (in principle, at least).
- In fact, reweighting is restricted to small μ/T and small V.
- The error analysis of results of reweighting is difficult, a breakdown might even not be noticed (Glasgow method).

Rescue : Observables can be obtained as power series in μ/T.

Only by Taylor expansion a reliable $V \to \infty$ behavior can be determined.

$$p(T, \mu) = p(T, \mu) + \Delta p(T, \mu)$$

Δp is an even function of μ/T (since $Z(\mu/T) = Z(-\mu/T)$)

$$\frac{\Delta p(T,\mu)}{T^4} = \sum_{k=1}^{\infty} c_{2k}(T) \left(\frac{\mu}{T}\right)^{2k}$$

The Taylor coefficients stem from derivatives w.r.t. μ of the determinant, more precisely

$$\frac{\partial \ln \det D}{\partial \mu} = \mathrm{tr}\left[D^{-1}\frac{\partial D}{\partial \mu}\right]$$

Therefore

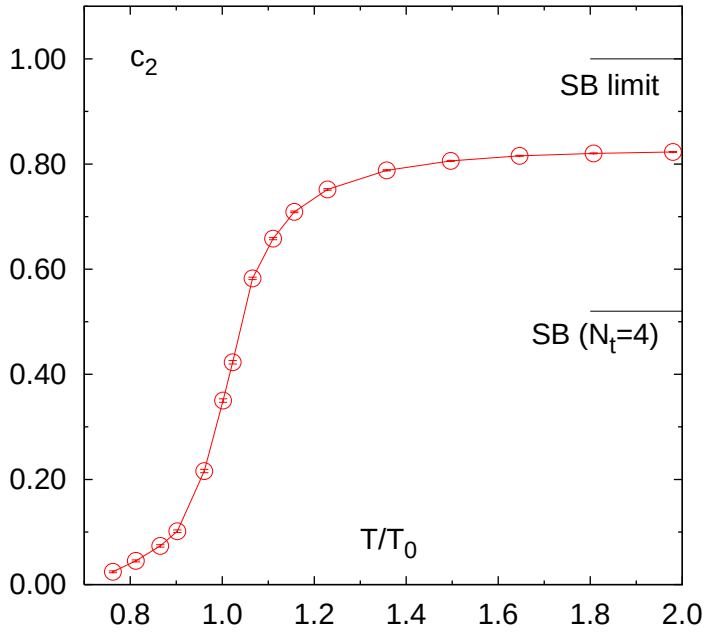
$$c_{2k} = \left\langle \mathrm{tr}\,(\ \textbf{polynomial of order } 2k \textbf{ in } D^{-1} \textbf{ and } \frac{\partial D}{\partial \mu}) \right\rangle_{|\mu=0}$$

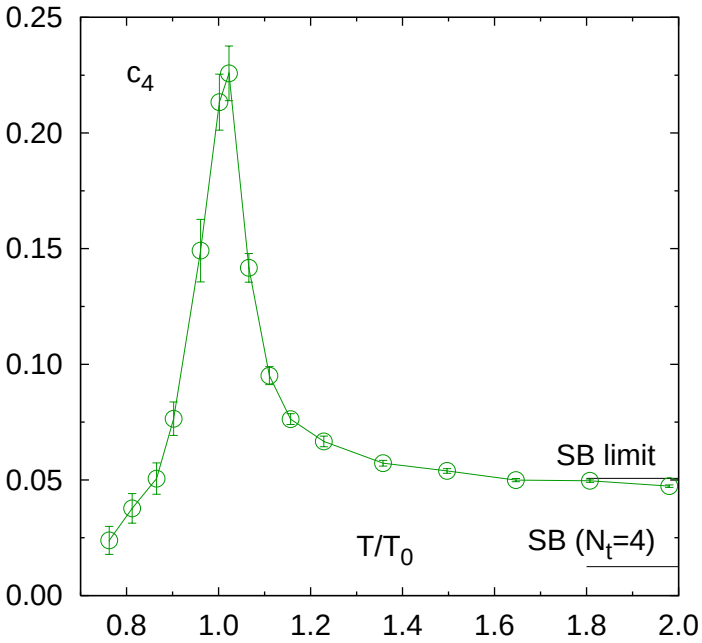
Taylor coefficients are easily calculable (in principle !) in simulations at $\mu = 0$, practically by means of of stochastic estimators.

These observables become increasingly noisy with larger k.

The first two Taylor coefficients c_2 and c_4 as functions of temperature look very nice.

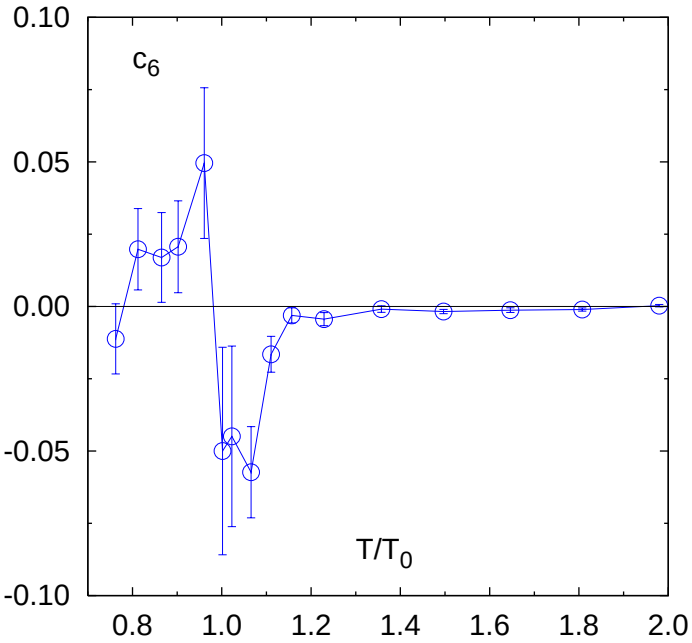
from Ch. Schmidt hep-lat/0610116

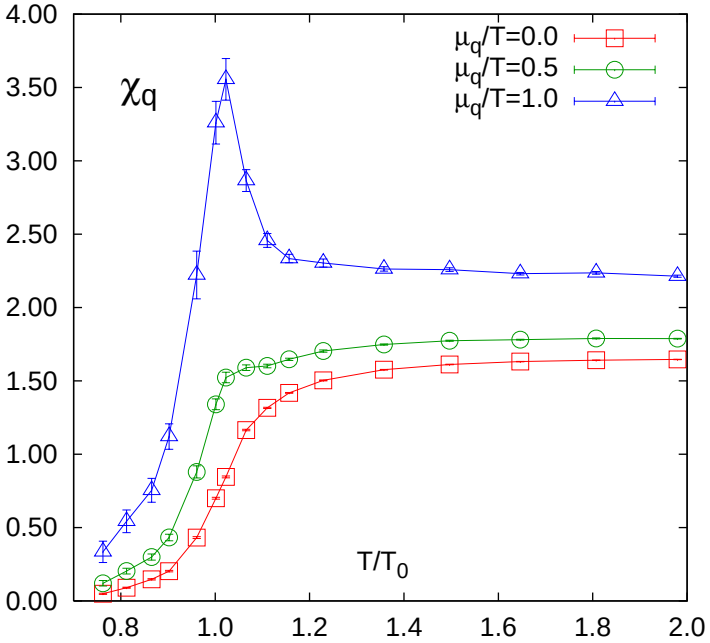




The Taylor coefficient c_6 and the quark number susceptibility χ_q (for three values of μ), all as functions of temperature.

from Ch. Schmidt hep-lat/0610116





In principle, knowledge of c_{2k} should give all thermodynamics :

- **The equation of state (EoS)**
- **The transition line $T_c(\mu)$**
- **The critical endpoint (μ_c^E, T_c^E)**

For all bulk quantities similar series expansions exist :

$$\frac{n_q}{T^3} = 2c_2\frac{\mu}{T} + 4c_4\left(\frac{\mu}{T}\right)^3 + 6c_6\left(\frac{\mu}{T}\right)^5 + \ldots$$

$$\frac{\chi_q}{T^2} = 2c_2 + 12c_4\left(\frac{\mu}{T}\right)^2 + 30c_6\left(\frac{\mu}{T}\right)^4 + \ldots$$

Going to higher density (higher μ/T) meets difficulties :

- **higher order k is required**
- **the coefficients become more noisy**
- **the computation needs large volumes**

A better way by simulations at

- **imaginary baryonic chemical potential ($\mu_q = i\eta_q$)**
- **imaginary isospin chemical potential ($\mu_I = i\eta_I$)**

has been proposed/explored.
(see M. D'Elia and F. Sanfilippo arXiv:0904.1400)

For the prediction of quantum number fluctuations it is important to discriminate between different quarks:

$$\frac{p}{T^4} = \frac{1}{VT^3}\ln Z(T,\mu_u,\mu_d,\mu_s) = \sum_{ijk}\frac{1}{i!j!k!}\chi^{uds}_{ijk}\left(\frac{\mu_u}{T}\right)^i\left(\frac{\mu_u}{T}\right)^i\left(\frac{\mu_d}{T}\right)^j$$

$$\chi^{uds}_{ijk} = \frac{\partial^{i+j+k}p/T^4}{\partial(\mu_u/T)^i\partial(\mu_d/T)^j\partial(\mu_s/T)^k}$$

or quantum numbers (baryon charge, strangeness, electric charge) ;

$$\frac{p}{T^4} = \frac{1}{VT^3}\ln Z(T,\mu_B,\mu_S,\mu_Q) = \sum_{ijk}\frac{1}{i!j!k!}\chi^{uds}_{ijk}\left(\frac{\mu_u}{T}\right)^i\left(\frac{\mu_u}{T}\right)^i\left(\frac{\mu_d}{T}\right)^j$$

$$\chi^{BQS}_{ijk} = \frac{\partial^{i+j+k}p/T^4}{\partial(\mu_B/T)^i\partial(\mu_Q/T)^j\partial(\mu_S/T)^k}$$

Meaning of the first two expansion coefficients for some charge X ?

$$
\begin{aligned}
2c_2^X &= \frac{1}{VT^3}\langle N_X^2\rangle \\
24c_4^X &= \frac{1}{VT^3}\left(\langle N_X^4\rangle - 3\langle N_X^2\rangle^2\right)
\end{aligned}
$$

This is variance and kurtosis.

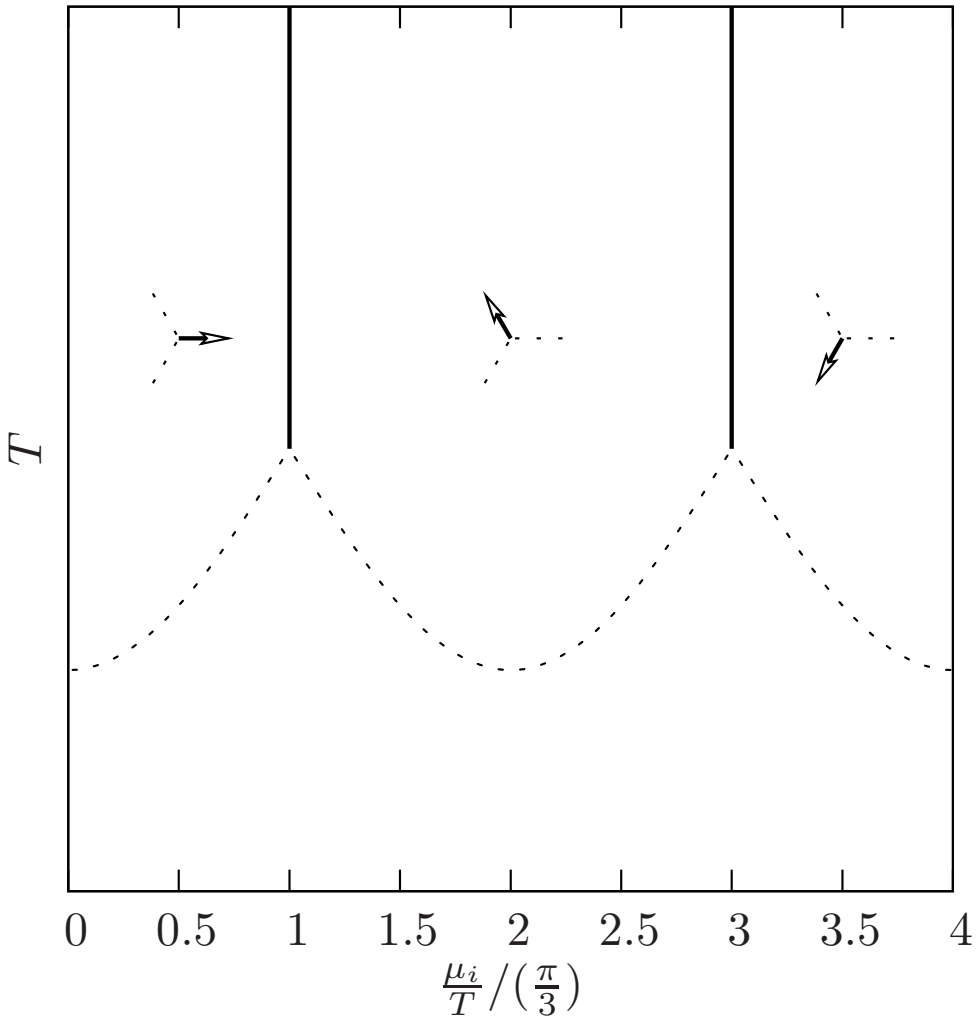
4. 5. Continuation from Imaginary Chemical Potential

This case is accessible for normal importance sampling.
A Taylor expansion is not needed, except (as a fit) for continuation purposes from imaginary to real chemical potential.

Phase diagram for imaginary $\mu = i\eta$:

- **Characterized by periodicity $\frac{\eta}{T} \rightarrow \frac{\eta}{T} + \frac{2\pi}{3}$ (Roberge and Weiss)**
- **Starting fom $\mu = 0$, the phase transition line (dotted line) bends upward (contrary to downward at real μ).**
- **The nature of this phase transition is a "continuation" of the physical phase transition at real μ.**
- **For quark masses $> \mathcal{O}(3$ GeV$)$ it might be first order transitions which then meet in a triple point with the vertical transition.**

Roberge-Weiss diagram : the vertical lines are first order phase transitions between sectors with different $\mathbb{Z}(3)$ orientations of the Polyakov loop.



The power expansion in orders of $\left(\frac{\mu}{T}\right)^{2k}$ for any observable O,

$$\langle O\rangle(\mu = i\eta) = \sum_k g_k \left(\frac{\mu}{T}\right)^{2k}$$

can be read off from many real measurements "on the spots" $(T, \mu = i\eta)$**.**

Each ensemble is really sensitive to the presence of a chemical potential.

In order to conform with real μ, the data should be taken, however, in the first sector with $|\arg L| < \frac{\pi}{3}$.

This implies $\left|\frac{\eta}{T}\right| < \frac{\pi}{3}$.

There might be interesting microscopic properties of configurations (like topological structure) that differ, in the same way as an

imaginary vacuum angle $\Theta = i\eta_Q$,

that, through a factor

$$\textbf{weight} \ \propto \exp\left(\eta_Q \ Q\right)$$

with the topological charge

$$Q \propto \int d^4x \ \mathrm{tr} \ \left(F_{\mu\nu}\tilde{F}_{\mu\nu}\right)$$

causes a considerable squeezing of topologcal charge.

Simulations at imaginary Θ angle are used in order to determine the neutron's electrical dipole moment
(NEDM, G. Schierholz et al., QCDSF/UKQCD Collaboration).

4. 6. Canonical Ensemble Approach

This does not immediately suffer from the complex measure problem.

For imaginary chemical potential $\mu = i\eta$, let's consider the fugacity expansion of the grand canonical partition function.

This is a Fourier sum and is periodic in η/T with a period of $2\pi/3$.

$$Z_{GC}(T, i\eta) = \sum_n \mathrm{e}^{in\eta/T} Z_C(T, n)$$

The canonical partition functions $Z_C(T, n)$ can be obtained from the grand canonical partition function at imaginary chemical potential

$$\begin{aligned} Z_C(T, n) &= \frac{1}{2\pi} \int_{-\pi}^{+\pi} d(\eta/T) \mathrm{e}^{-in\eta/T} Z_{GC}(T, i\eta) \\ &= \frac{3}{2\pi} \int_{-\pi/3}^{+\pi/3} d(\eta/T) \mathrm{e}^{-in\eta/T} Z_{GC}(T, i\eta) \end{aligned}$$

(last step because of the periodicity with restricted period $2\pi/3$)

This is the Roberge-Weiss symmetry

$$Z(\eta/T) = Z(\eta/T + 2\pi/3)$$

One consequence is the triality constraint :

$$Z_C(T, n) = 0 \text{ if not } n = 0 \text{ mod } N$$

Simulations at imaginary chemical potential can give

$$\frac{Z_{GC}(T, i\eta)}{Z_{GC}(T, 0)}$$

enabling the calculation of the canonical partition functions $Z_C(T, n)$.

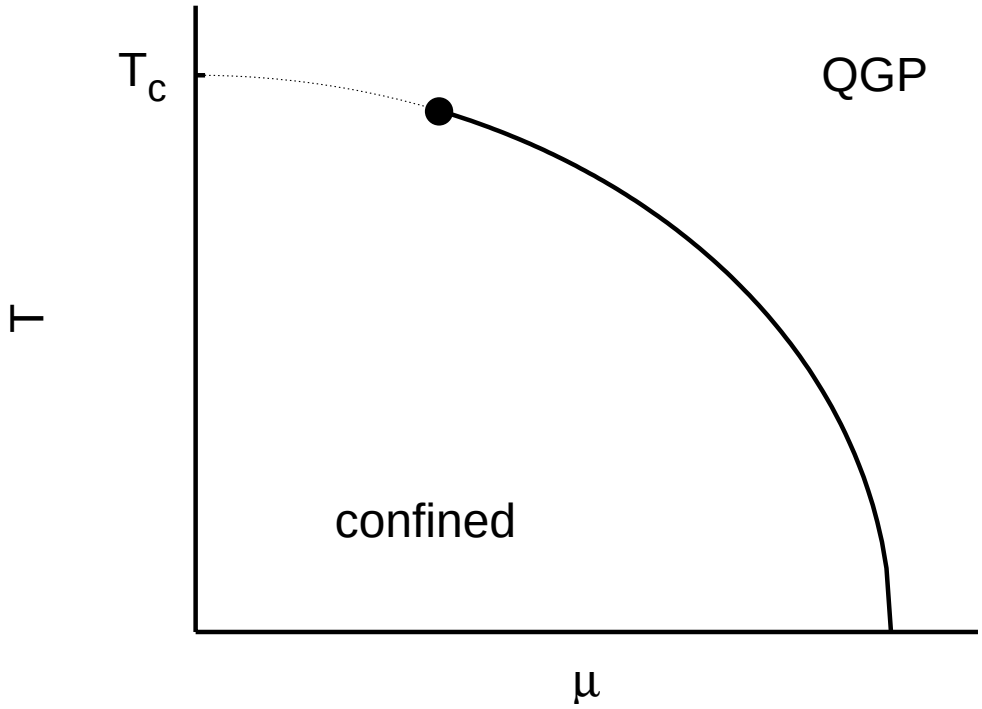
Problem : at higher baryon number $B = n/3$, the ratio needs to be evaluated for very many (i_{max}) integration points ($i = 1, \ldots, i_{max}$)

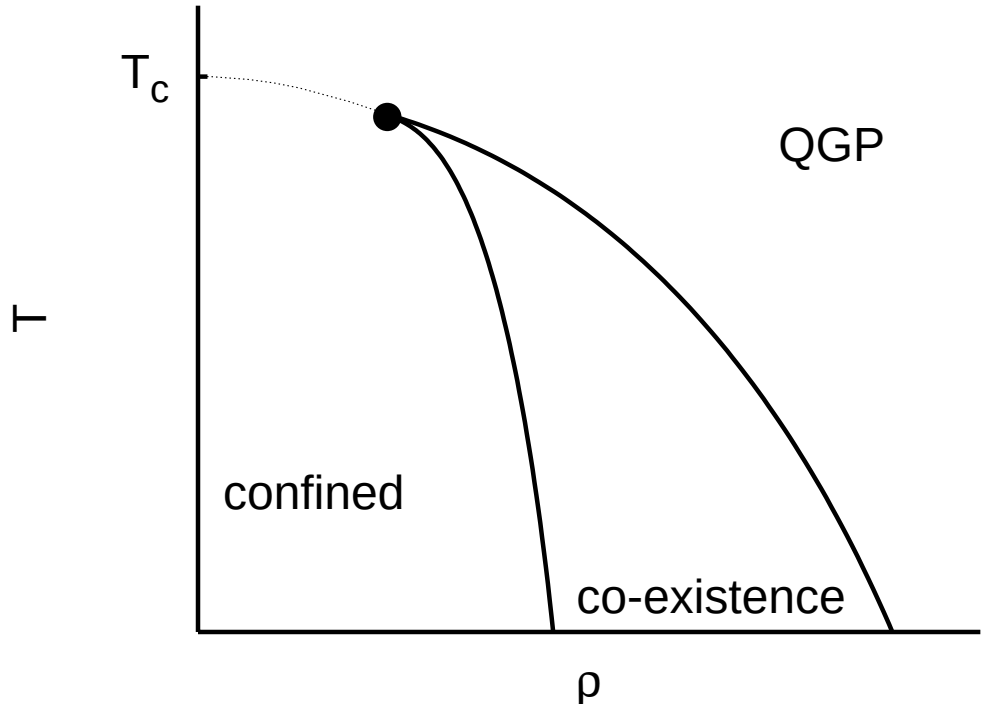
$$\frac{\eta_i}{T} \in [-\pi/3, +\pi/3] \tag{1}$$

in order to get a reliable numerical evaluation of the Fourier transform. Here the sign problem appears again in disguise.

The QCD Phase Diagram: Grand Canonical and Canonical View

from S. Kratochvila and Ph. de Forcrand hep-lat/0509143





Both thermodynamic ensembles should be equivalent in the infinite volume limit. However, this limit is difficult to achieve.

For large, quasi-continuous baryon number B, Z_C becomes a function of the baryon density ρ :

$$Z_C^{(q)}(V,T,n=NB) = Z_C^{(B)}(V,T,B) = Z_C^{(dens)}(V,T,\rho)$$

Then

$$\begin{aligned} Z(V,T,\mu) &= \int_{-\infty}^{+\infty} d\rho \; \mathrm{e}^{VN\rho\mu/T} Z_C^{(dens)}(V,T,\rho) \\ &= \lim_{V\to\infty} \int_{-\infty}^{+\infty} d\rho \mathrm{e}^{-\frac{V}{T}(f(\rho)-\mu\rho)} \end{aligned}$$

with $f(\rho)$ as the free energy density in canonical ensemble.

Finally, μ can be expressed as function of the baryon density ρ :

$$\mu(\rho) = \frac{1}{N}\frac{\partial f(\rho)}{\partial \rho}$$

This function shows a behavior resembling the van der Waals gas.

This approach has been pursued numerically :

S. Kratochvila and Ph. de Forcrand, hep-lat/0509143

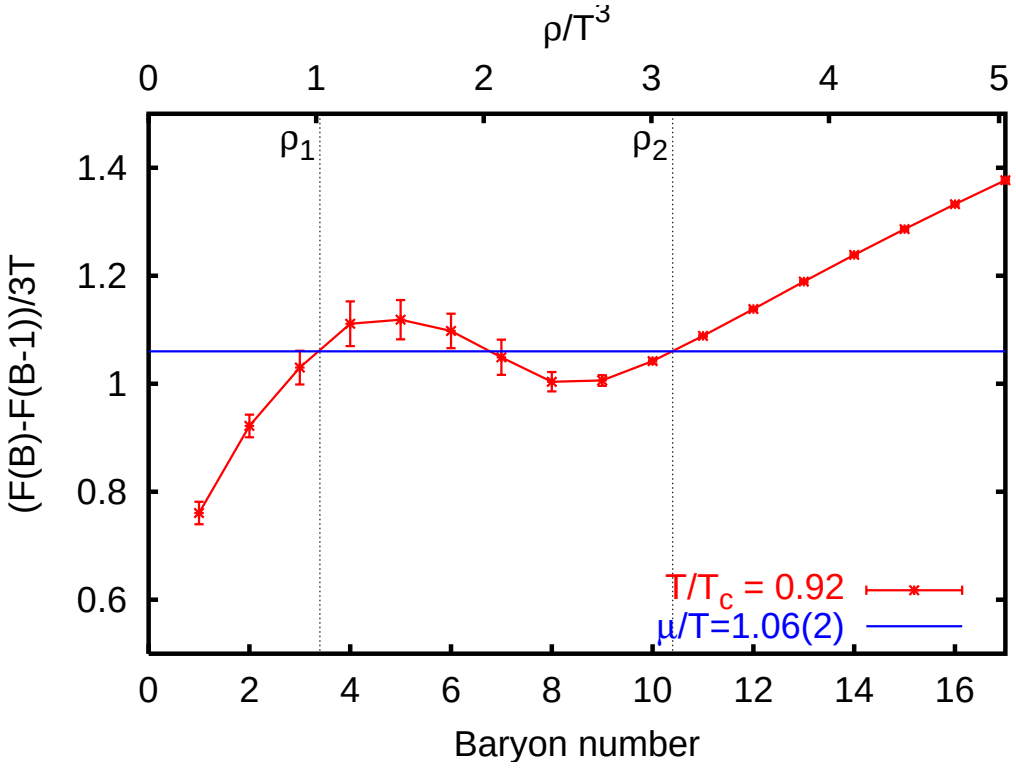
$6^3 \times 4$ **lattice, four degenerate staggered quarks, volume** $(1.8$ **fm**$)^3$

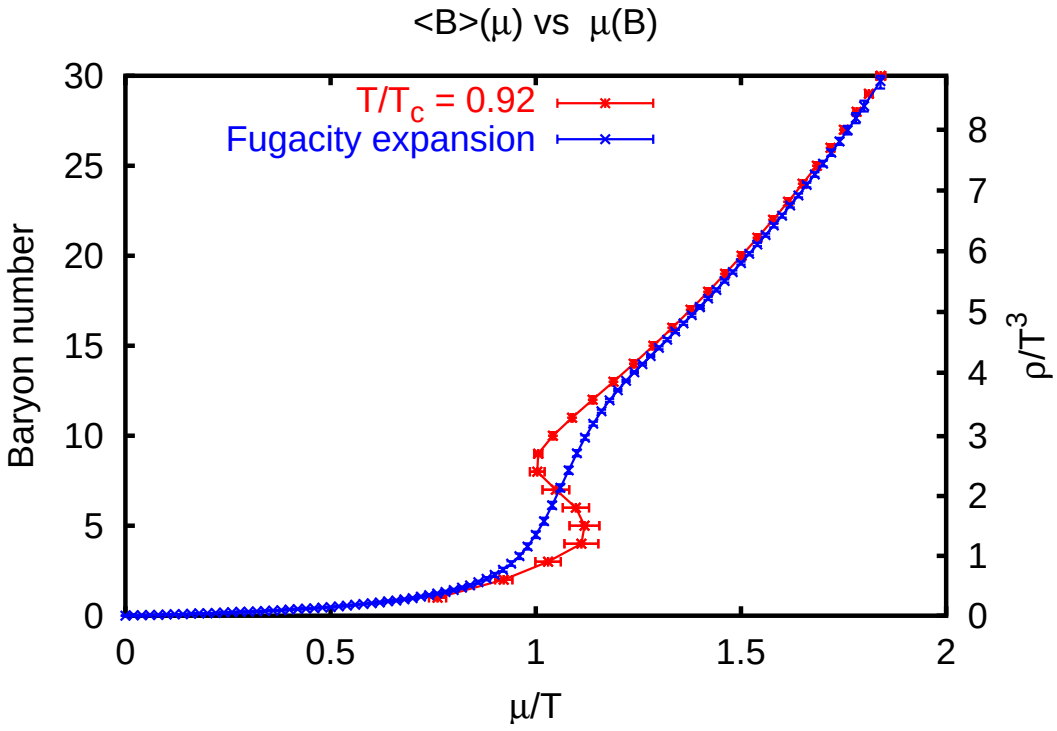
A. Alexandru, M. Faber, I. Horvath and K. F. Liu, hep-lat/0507020

Kentucky group :

$6^3 \times 4$ **lattice, clover-improved Wilson fermions** $N_f = 2$**, 3 and 4.**

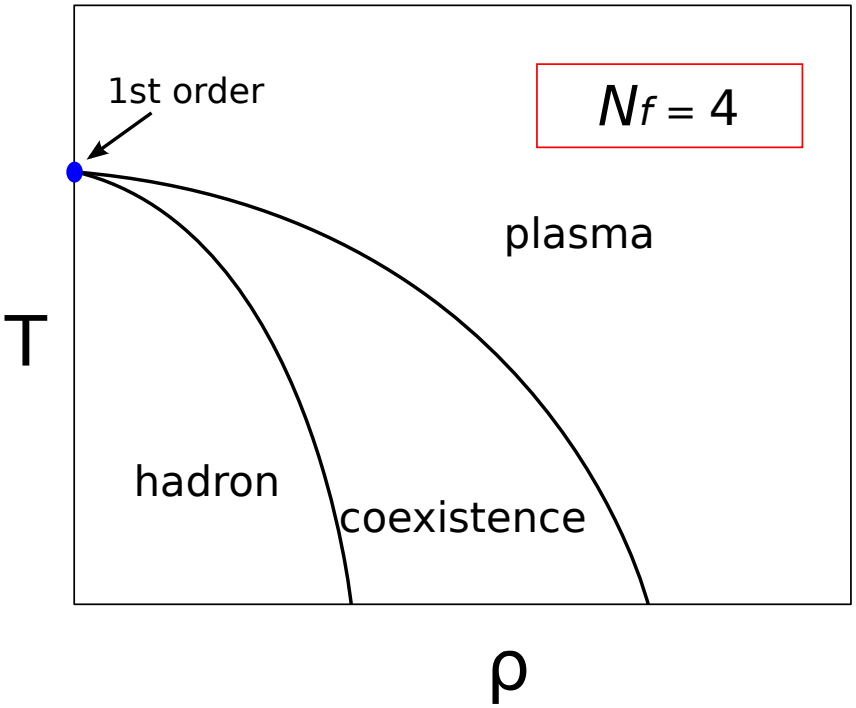
Left: The Maxwell construction allows to extract the critical chemical potential and the boundaries of the co-existence region. Right: Comparing the saddle point approximation (red) with the fugacity expansion (blue). Strong finite-size effects in the latter obscure the first-order transition.
from S. Kratochvila and Ph. de Forcrand hep-lat/0509143

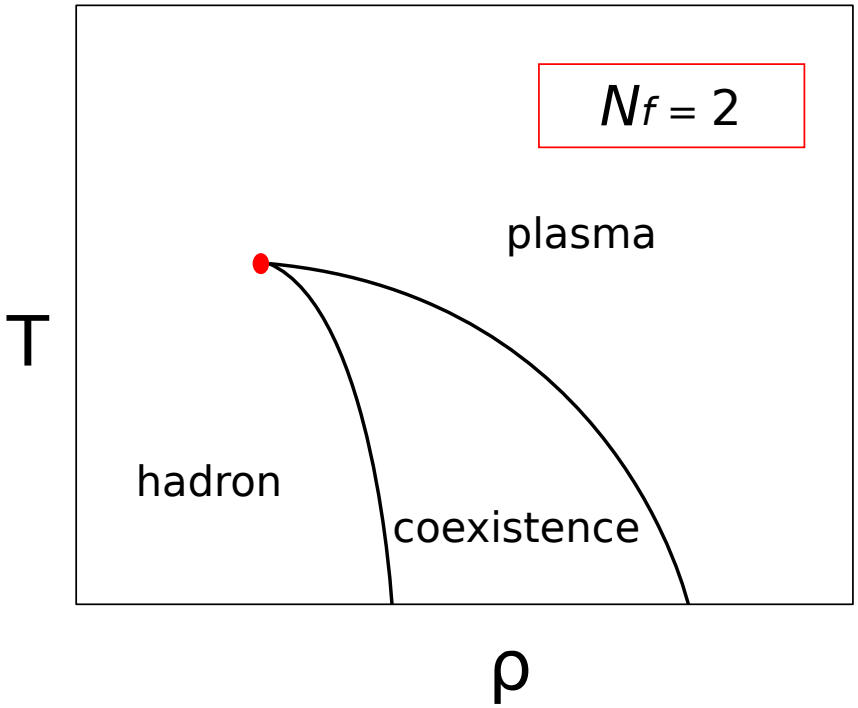




The number of flavors is decisive : $N_f = 4$ vs. $N_f = 2$

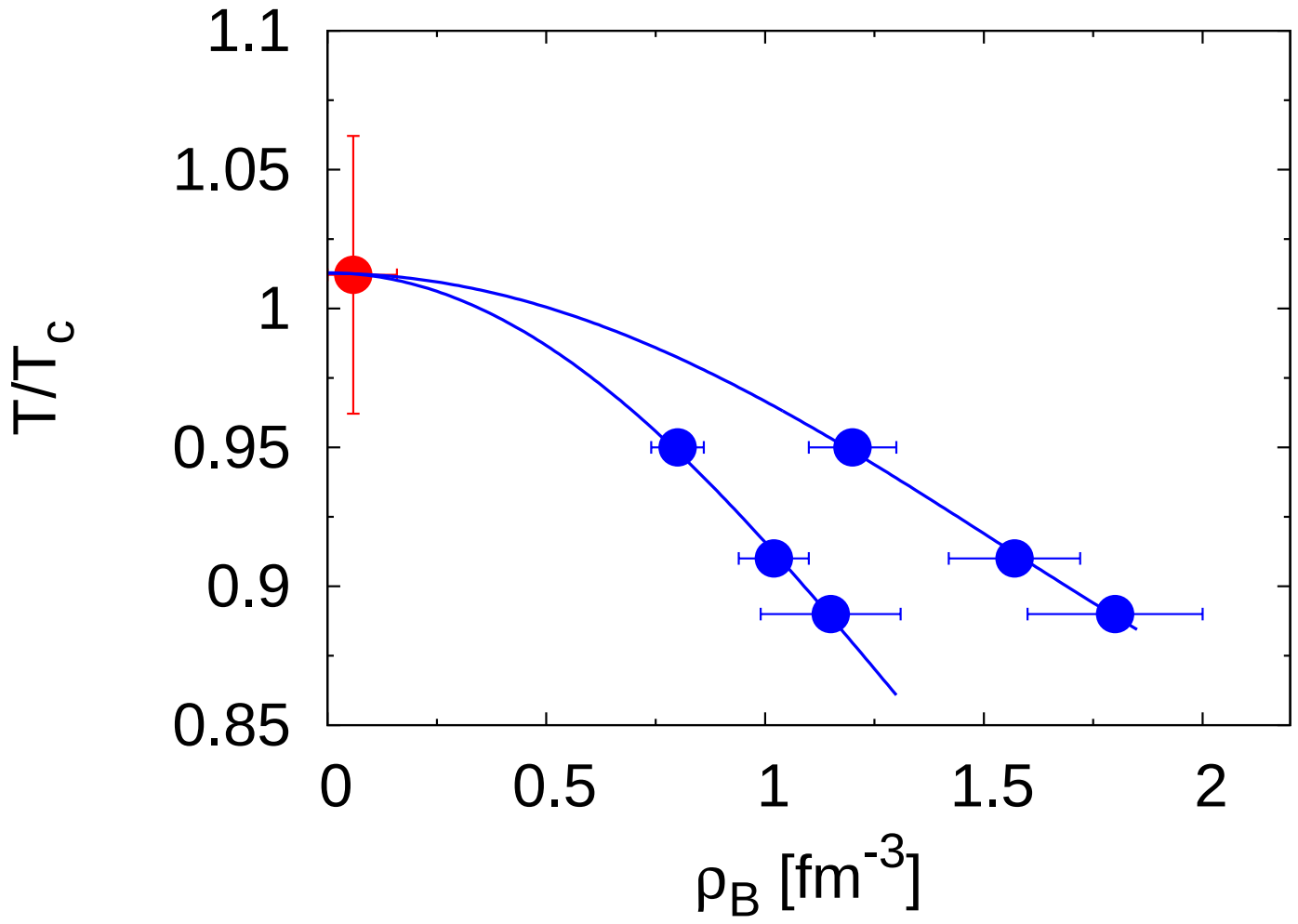
from Anyi Li arXiv:1002:4459





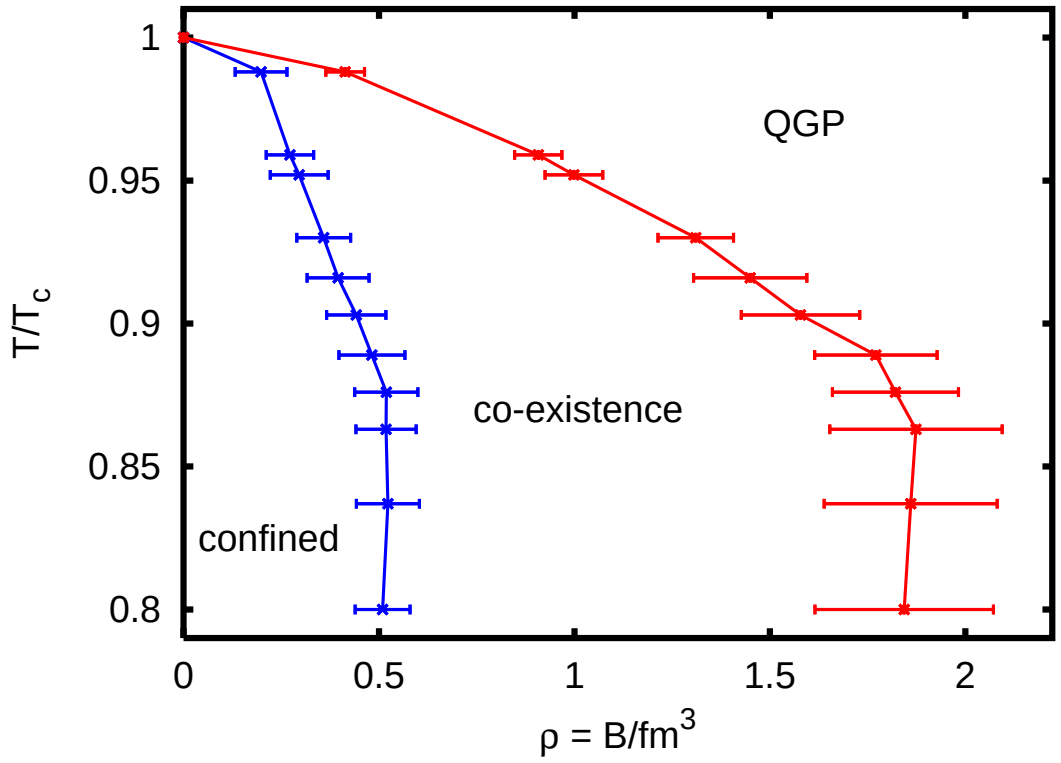
Phase boundaries in the temperature vs. density plot for $N_f = 4$.

from Anyi Li arXiv:1002:4459



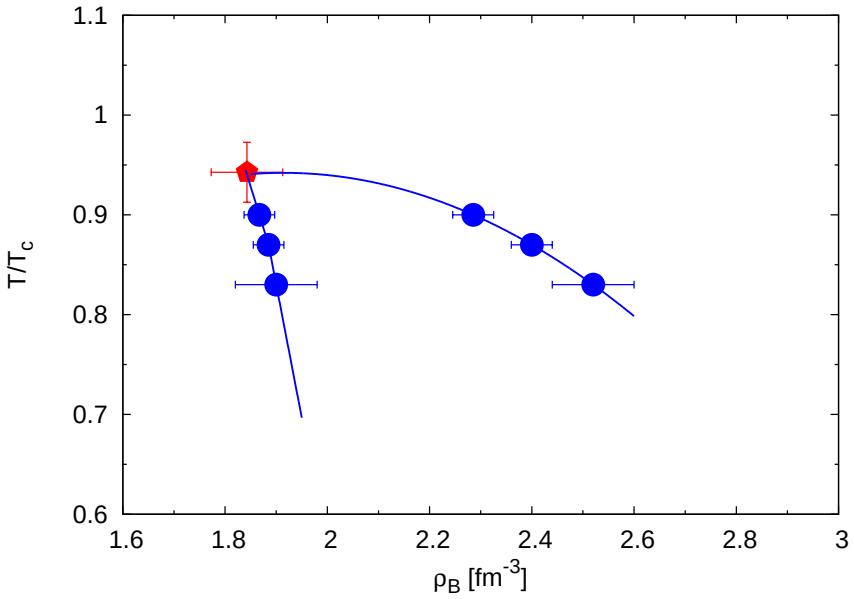
Phase boundaries in the temperature vs. density plot for $N_f = 4$.

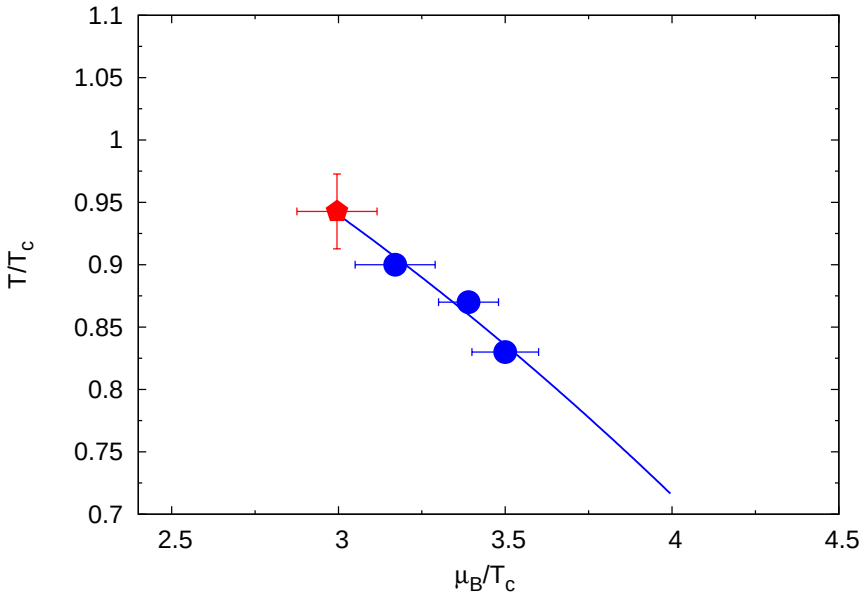
from S. Kratochvila and Ph. de Forcrand hep-lat/0509143



Left: Phase boundaries in the temperature vs. density plot for $N_f = 3$. Right: Transition line in the temperature vs. chemical potential plot.

from Anyi Li arXiv:1002:4459





This looks rather systematic, however the lattices are too small.

There are possible systematic effects of the canonical ensemble method.

One would like to confirm this in a more robust way, that works also for large lattices (Taylor expansion), in order to veryfy the first order character of the transition.

5. Results for Standard LGT

- Results: Getting the Phase Diagram
- Results: Inside the Phase Diagram

5. 1. Results : Getting the Phase Diagram

From central Pb+Pb (Au+Au) collisions at SIS, AGS, SPS and RHIC the collision energy dependence of temperature and baryonic chemical potential (entering the particle yields, say via THERMUS) has been found in the form (s_{NN} is the center of mass energy of a single nucleon pair) ;

$$\mu_B = \frac{1.308}{1 + 0.273\sqrt{s_{NN}}}$$

This μ_B enters the chemical "freeze-out" temperature $T_{freeze}(\mu_B)$ close to the phase transition (crossover) temperature at vanishing baryon density, $T_c(\mu = 0) = 0.166$ GeV parametrized as follows :

$$\frac{T_{freeze}(\mu)}{T_c(\mu = 0)} = 1 - 0.023 \left(\frac{\mu_B}{T}\right)^2 - \mathcal{O}(\left(\frac{\mu}{T}\right)^4)$$

J. Cleymans, Phys. Rev. C 63 (2006) 034905

This has motivated the interest in lattice results for the μ dependence of the phase transition temperature $T_c(\mu)$ near $T_c(0)$ (it is not too hard).

$T_c(\mu)$ must be an even function of μ near $\mu = 0$.

$$\frac{T_c(\mu)}{T_c(\mu=0)} = 1 - \sum_k t_{2k} \left(\frac{\mu}{T}\right)^{2k}$$

The curvature found on the lattice is much smaller than that of the freeze-out curve :

$$\frac{T_c(\mu)}{T_c(\mu=0)} = 1 - 0.0066(7) \left(\frac{\mu}{T}\right)^{2}$$

Similarly

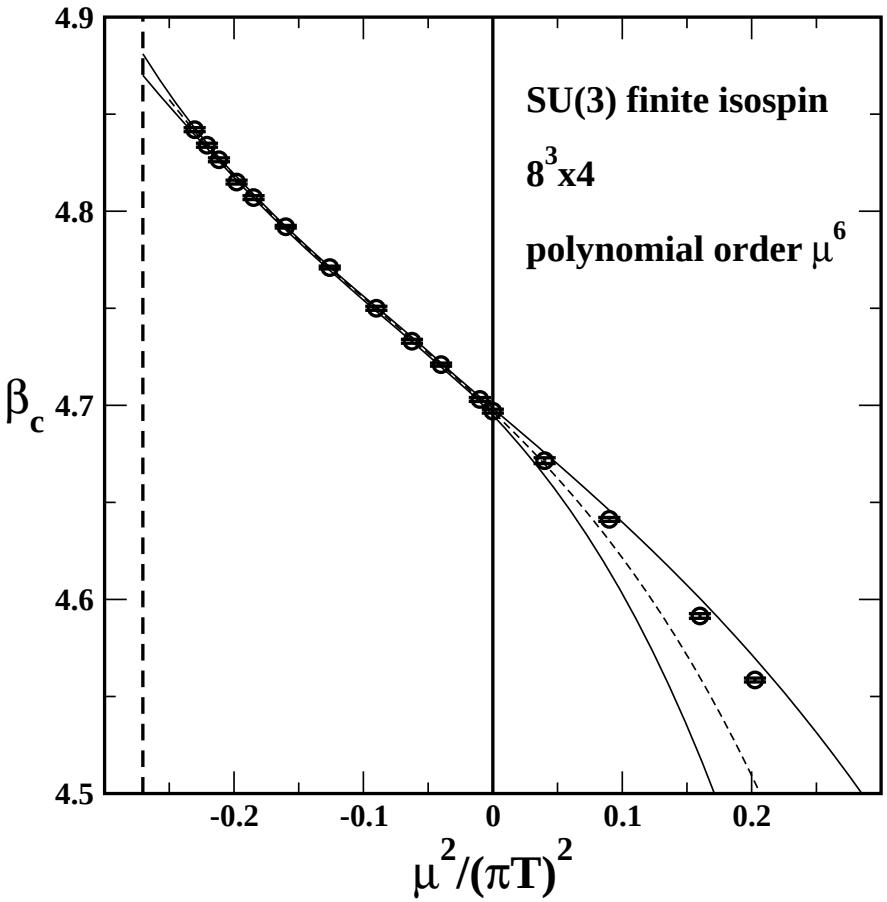
$$\frac{\beta_c(\mu)}{\beta_c(\mu=0)} = 1 - \sum_k b_{2k} \left(\frac{\mu}{T}\right)^{2k}$$

The coefficients must be determined at imaginary $\mu = i\eta$.

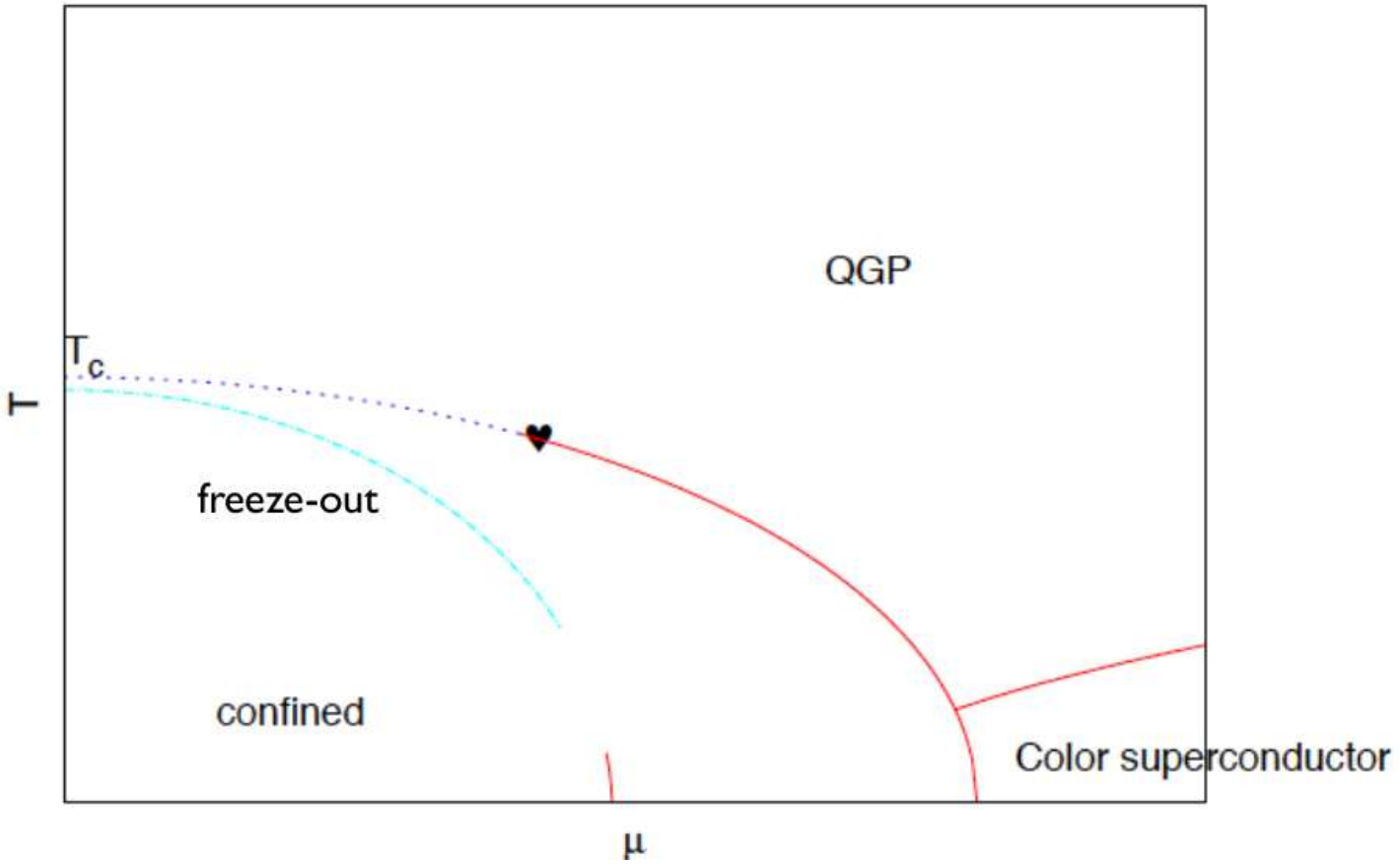
- **It turns out, that the freeze-out temperature is thre times more curved than $T_c(\mu)$.**
- **Moreover, the curvature seems to decrease in the continuum limit !**
- **However, the method is sensitive to the order of the series that is fitted to the imaginary-μ data :**
  The coefficients at imaginary μ are alternating in sign and can be determined only with large uncertainty.

Continuation of β_c from negative μ^2 to positive μ^2

from Ph. de Forcrand arXiv:1005.0539

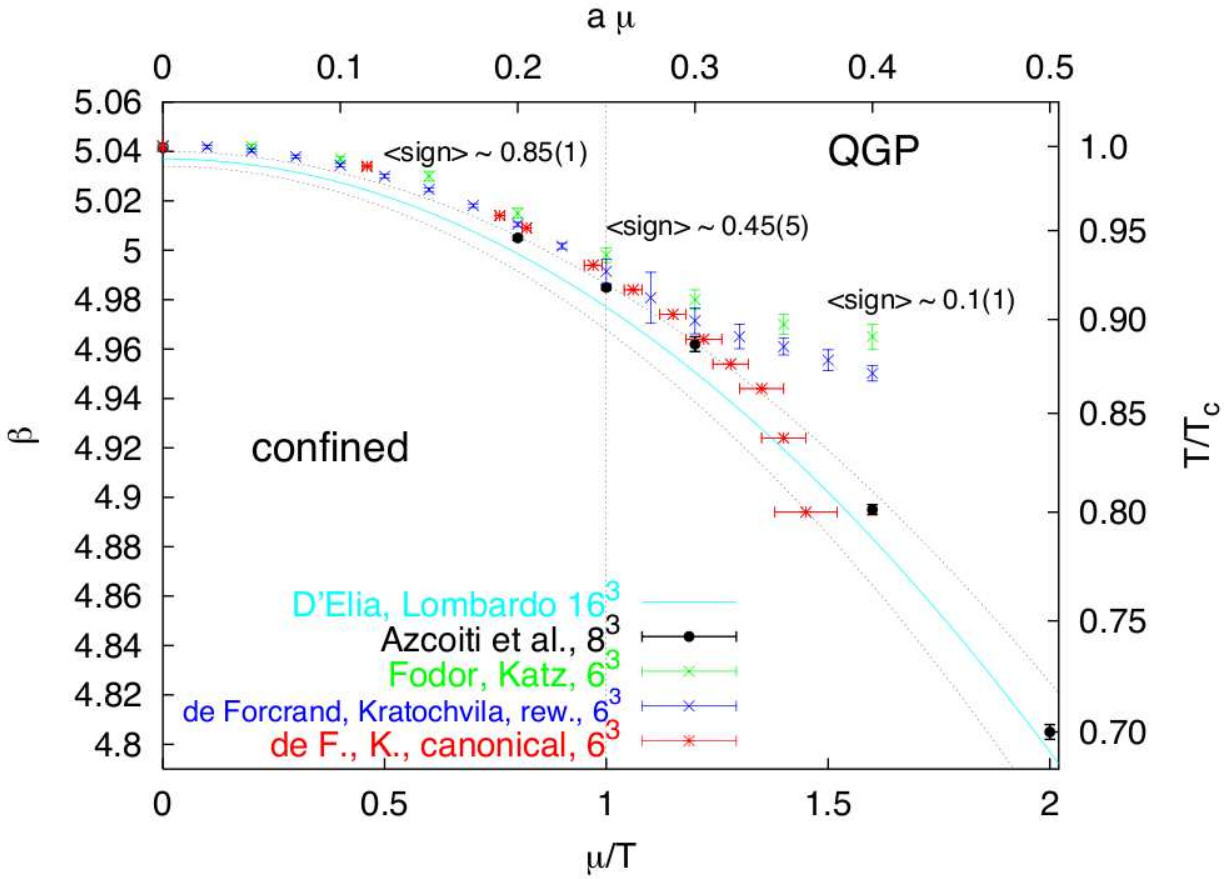


Sketch of the QCD crossover line $T_c(\mu)$ vs. the experimental freeze-out curve, which has a larger curvature, near $T_c(0)$.
from Ph. de Forcrand arXiv:1005.0539



Comparison of the phase boundary for QCD with $N_f = 4$ staggered quarks on $N_t = 4$ lattices.

from S. Kratochvila and Ph. de Forcrand hep-lat/0509143



Is there a critical endpoint ? Is there somewhere a first order phase transition for physical quark masses ?

Look back at the Columbia plot !

One can analyze

$$\frac{m_c(\mu)}{m_c(\mu=0)} = 1 + \sum_k h_k \left(\frac{\mu}{T}\right)^{2k} \tag{2}$$

for imaginary chemical potential.

Then, for real chemical potential, the area in the $m_{u,d}$-m_s plane, where a first order transition will be realized, shrinks with real μ :

$$\frac{m_c^{u,s}(\mu)}{m_c^{u,s}(\mu=0)} = 1 - 39(8)\left(\frac{\mu}{T}\right)^2 \tag{3}$$

Therefore, an intersection with the actual quark masses is unlikely.

Ph. de Forcrand and O. Philpsen (2002-2008).

Can the Taylor coefficients for the pressure constrain an eventual critical endpoint ? This is the recipe :

- **Find the largest temperature where all c_{2k} positive. This is a candidate for T_c^E**
- **Determine the radius of convergence of the Taylor series for p/T^4.**

$$\frac{\mu_E}{T_E} = \lim_{n\to\infty} \sqrt{\left|\frac{c_{2n}}{c_{2n+2}}\right|}\,(T_E)$$

However, low orders are not sufficient !

An independent confirmation of the critical endpoint is still lacking.

5. 2. Results : Inside the Phase Diagram

Results of two collaboration for the Equation of State (EoS)

1) MILC and hotQCD collaborations,
light and strange quarks at almost physical quark masses μ_l and μ_s

Temporal extent $N_t = 4$ and 6 (distance from continuum limit): differences are visible

Calculations up to $\mathcal{O}(\mu^6)$ (up to c_6)

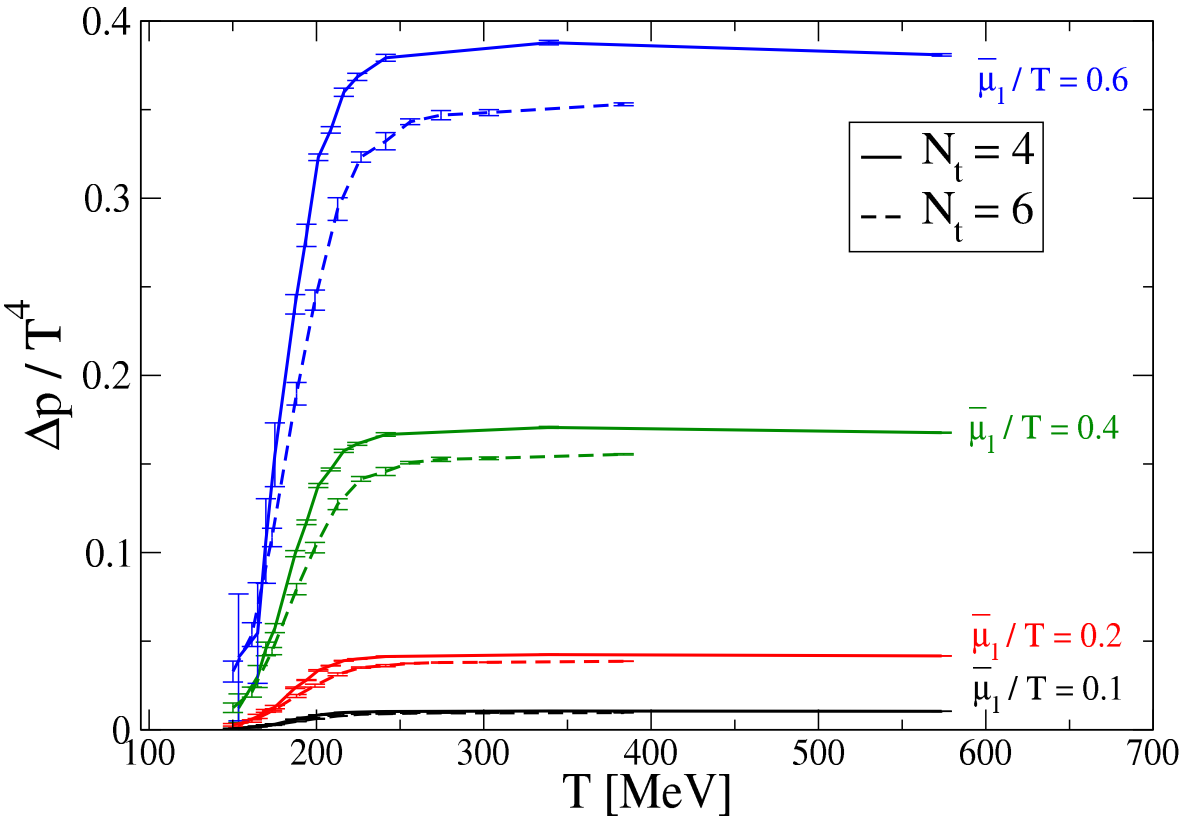
Comparison with HRG (Hadron Resonance Gas, taking the empirical hadron masses [to several GeV] with their baryonic charge into account)

2) BMW collaboration, light and strange quarks

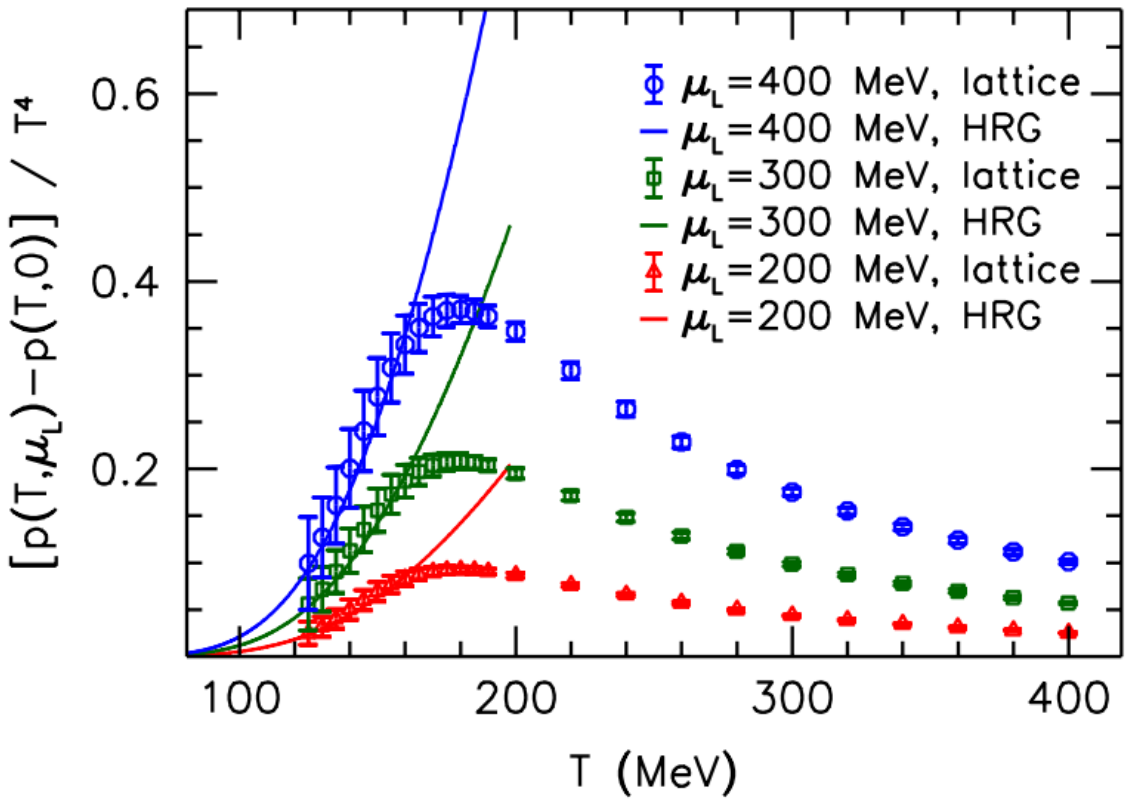
Calculations up to $\mathcal{O}(\mu^2)$ (up to c_2)

Data for $N_t = 6, 8, 10, 12$, quantities can be extrapolated to continuum limit

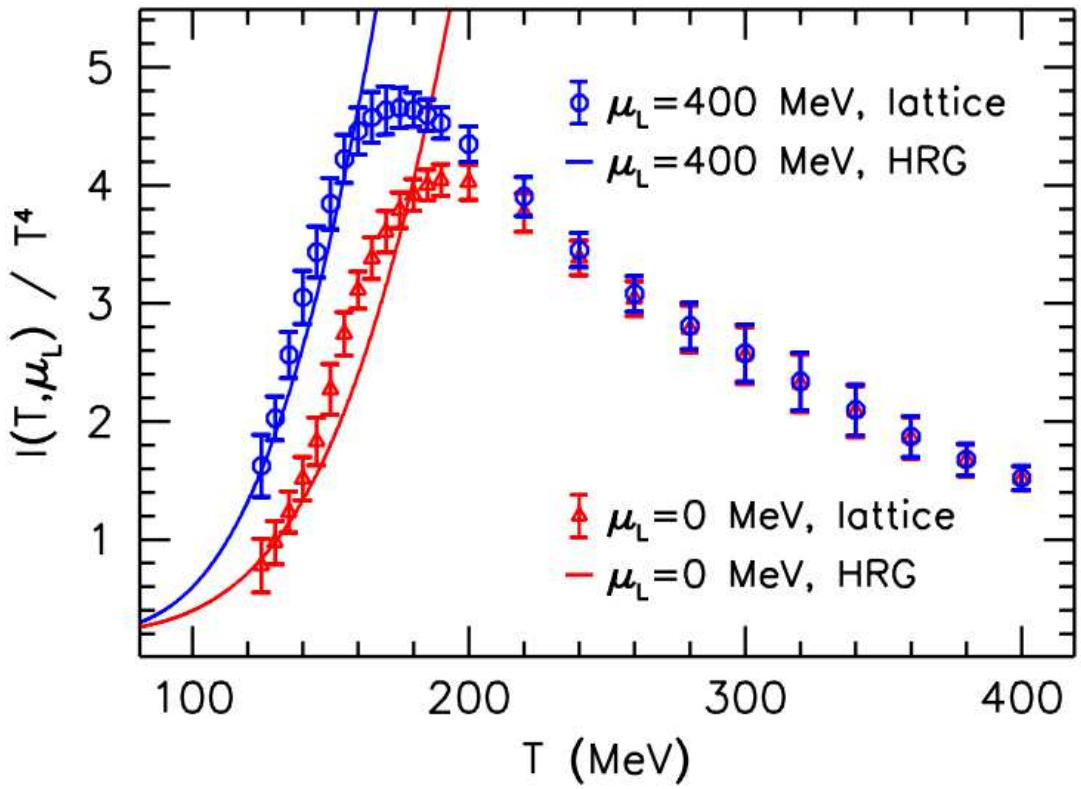
Change in the pressure due to $\mu \neq 0$ (MILC+hotQCD)



Difference between the pressure at $\mu > 0$ and $\mu = 0$ (BMW)



The trace anomaly for non-zero μ_L (BMW, compared with HRG)



What else might be interesting inside the phase diagram ?

For the hadronization process on top of the freeze-out curve (inside the "hadronic phase") the following observables will be of interest:

- screening lengths
- quark condensate $\langle \bar{q} q \rangle$, other condensates ...
- hadron masses
- hadron radii

for screening lengths (by imaginary chemical potential) see:
A. Hart, M. Laine, and O. Philipsen,
hep-lat/0010008
hep-ph/0004060

6. LGT-Motivated Effective Models on the Lattice (N colors)

Heuristic models or models derived from the hopping parameter expansion (heavy quarks) in 3D :

- **Flux tube models**

$$Z_{XY} = \int_{-\pi}^{+\pi} \prod_x d\vartheta_x \exp\left[J \sum_{x,\nu} \cos(\vartheta_{x+\hat{\nu}} - \vartheta_x) + h \sum_x \cos(\vartheta_x) + w \sum_x \cos(N\vartheta_x) \right]$$

- $\mathbb{Z}(N)$ **spin models and** $SU(N)$ **spin models**

$$S^{eff}[P] = -\frac{\beta'}{2} \sum_{<\vec{x},\vec{y}>} \left(\text{ tr } P_{\vec{x}} \cdot \text{tr } P^{\dagger}_{\vec{y}} \right) + S_F^{eff}[P]$$

$$S_F^{eff}[P] = 4\ (2\kappa)^{N_t} \sum_{\vec{x}} \left(\mathrm{e}^{\mu/T} \text{ tr } P_{\vec{x}} + \mathrm{e}^{-\mu/T} \text{ tr } P^{\dagger}_{\vec{x}} \right)$$

These models allow for

- **mean field solutions**
- **exact solutions (worm algorithm)**
- **solution by Complex Langevin simulation,**

for the confinement/deconfinement problem at $\mu \neq 0$.

No first order transition will be found !
They do not cover chiral properties throughout the phase diagram !

But the recently found Flux Representation solution is interesting !

Models derived for light (chiral) fermions :

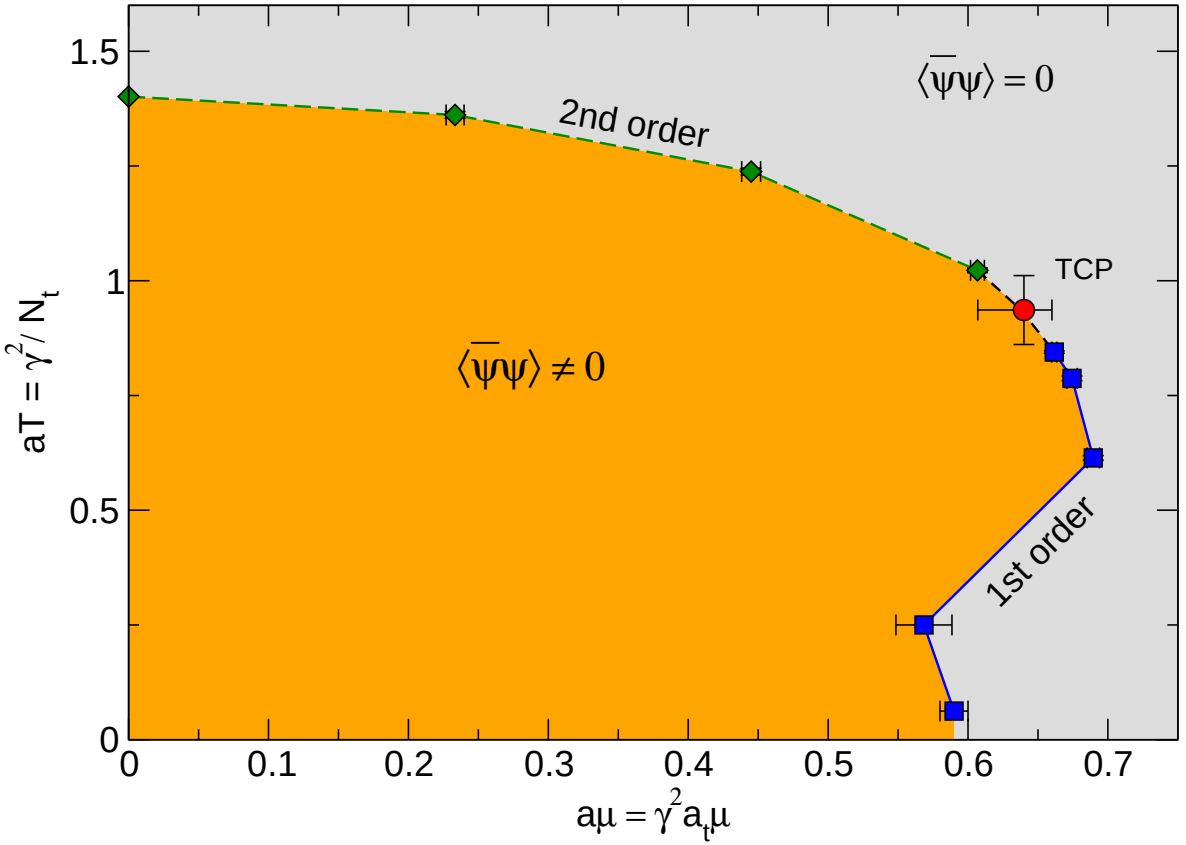
In strong coupling for gluons, local expressions for the fermion determinant can be found.

Solved by monomer/dimer methods or mean field methods.

More interesting phase diagrams can be found in these models !

The phase diagram for $N_f = 1$ QCD in the strong coupling and chiral limit on an $N_t = 4$ lattice contains 2nd and 1st order transitions and a tricritical point !

from arXiv:1111.4677 (talk by O. Philipsen at LATTICE 2011)



8. Summary and Conclusions

Lattice gauge theory at baryonic $\mu \neq 0$ is still an exceptionally difficult field.

- **Direct simulations are impossible because of the complex weight.**
- **Only part of the phase diagram is indirectly accessible for simulations, due to**
  - **the sign problem,**
  - **the overlap problem.**
- **This hampers the reweighting technique, with limitations that are partly under control by the following diagnostic tools**
  - **the average phase factor,**
  - **the overlap parameter.**

- **What causes the overlap problem is not understood in detail.**
- **One would like to inspect configurations of the simulating ensemble (together with their reweighting factor) and confront them with configurations of the genuine target ensemble for inspection.**
- **This is only possible with imaginary chemical potential where the overlap problem, after all, still exists.**
- **Standard methods of extrapolation (diagnostic quantities) are**
  - **reweighting (average phase factor, overlap parameter),**
  - **analytical continuation (requires series expansion at $\mu^2 < 0$), for the transition temperature, for screening lengths etc.**
  - **Taylor expansion (limited by radius of convergence in μ/T).**

- **The reconstruction of the Canonical Ensemble is very costly for realistic baryon numbers and volumes because of the Fourier transformation involved.**
- **Effective field theories obtained by strong coupling methods (applied to the gauge part) are useful, because the sign problem is there partly ameliorated :**
  - **they may be studied on 3D lattices by mean field methods,**
  - **in special cases, their sign problem can be solved in the Flux Representation,**
  - **they may be eventually studied by Complex Langevin simulation.**
- **Such models are useful for obtaining qualitative results (say, connecting chiral vs. confinement aspects), but cannot replace a solution for the real 4D lattice gauge theory.**

An ambitious program has been outlined for LGT in the paper by M. Cristoforetti, F. Di Renzo, and L. Scorzato, "High density QCD on a Lefschetz thimble ?" arXiv:1205.3996

- **searching for stationary points of action,**
- **methods of integration along contours in complex plane,**
- **identifying an optimal integration domain associated with each stationary point (the "thimble"),**
- **evaluating the path integral as sum over integrals over thimbles.**
- **This program was motivated by E. Witten and Morse theory.**

It will be interesting to see first results.