

# Lattice QCD at $\mu \neq 0$

## Part I

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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

Latest review of results contained in :

O. Philipsen “The QCD equation of state from the lattice”

arXiv:1207.5999 (Invited Review Article)

interesting for us :

**EoS for finite baryonic density, from Taylor expansion and imaginary  $\mu$**

See also:

O. Philipsen “Status of the QCD phase diagram from lattice calculations”

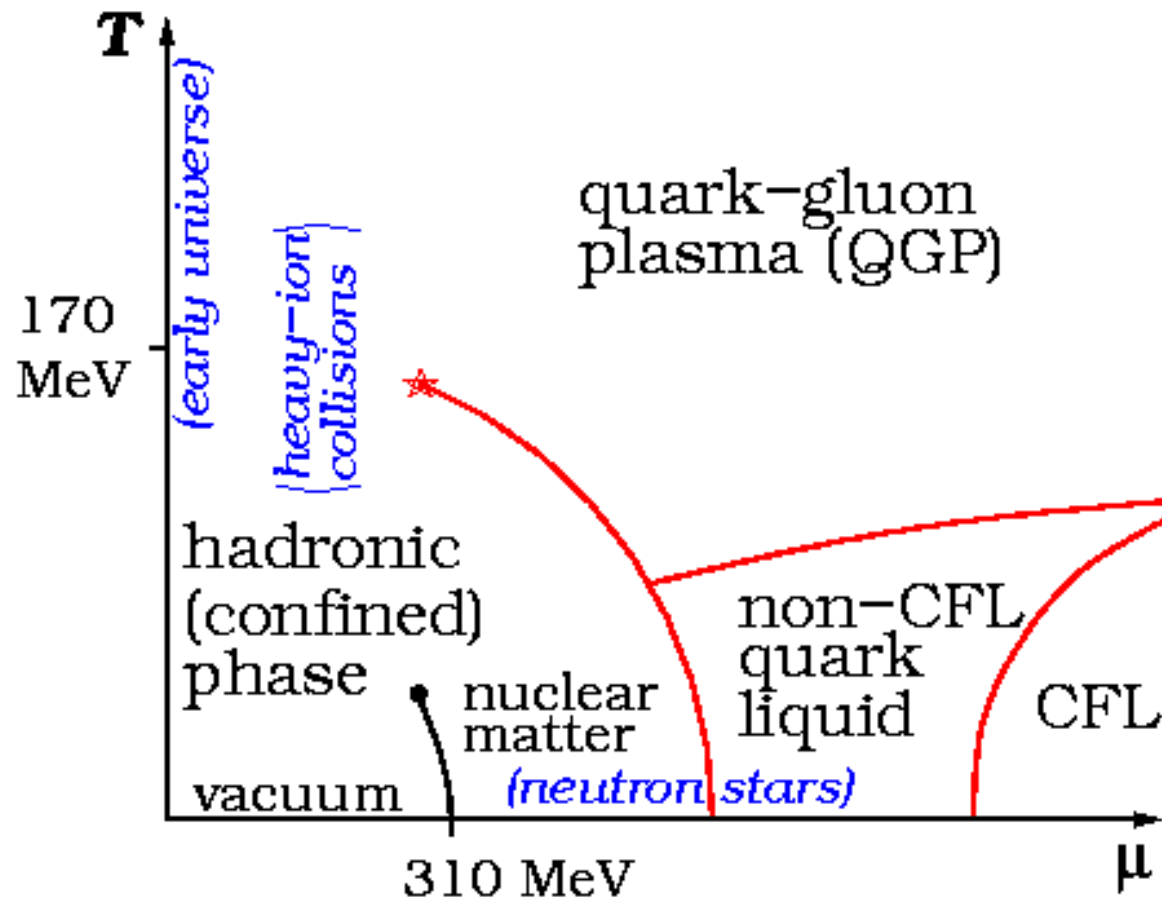
arXiv:1111.5370 (Lecture at HIC for FAIR workshop and XXVIII Max Born Symposium, Wroclaw, May 19-21, 2011)

O. Philipsen “Lattice QCD at non-zero temperature and baryon density”

arXiv:1009.4089 (Lectures given at the Summer School on “Modern perspectives in lattice QCD”, Les Houches, August 3-28, 2009)

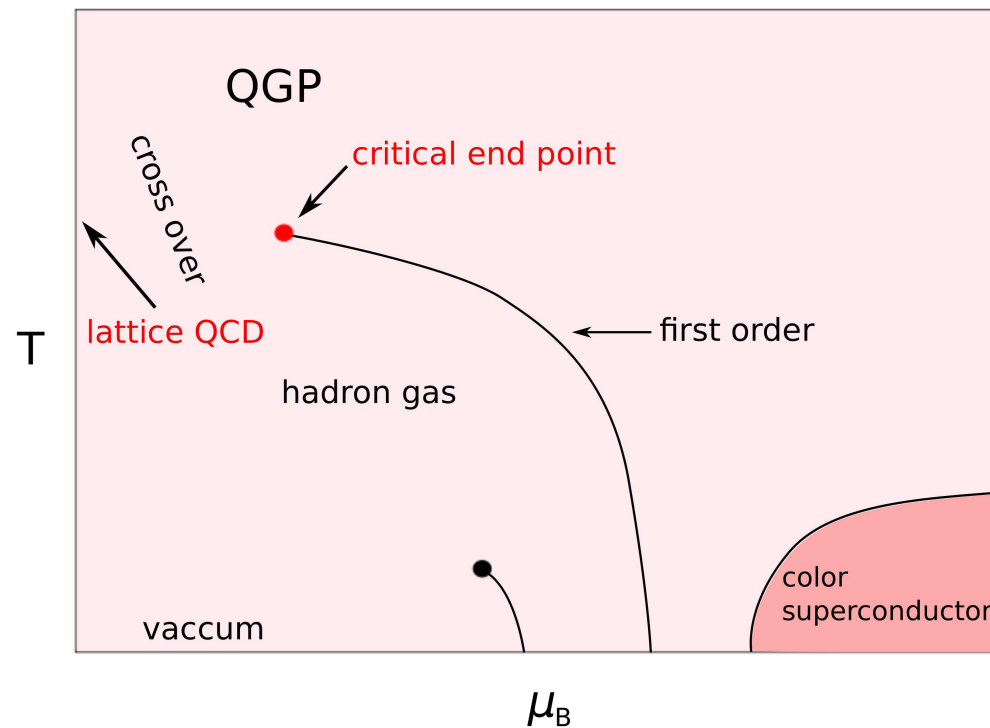
## 1. Introduction

Hypothetic phase diagram of QCD (from Wikipedia)  
after Ph. de Forcrand arXiv:1005.0539



# Crossover vs. First Order Transition in the Phase Diagram of QCD

from Anyi Li arXiv:1002:4459



This is a **School of Dense Matter**, not **Lattice Gauge Theory**.

You will **not hear much about the technical details of LGT**.

I will concentrate on **central questions**: “meta-problems”

This talk is dealing with **relativistic matter with a prescribed number of particles carrying particular charge (baryonic charge)** in a grand canonical formalism.

Surprisingly, this is related to a **number of difficult problems**, as soon as such problems are attacked within Lattice Gauge Theory, known under the names :

- “sign problem”
- “complex action”
- “complex weights”

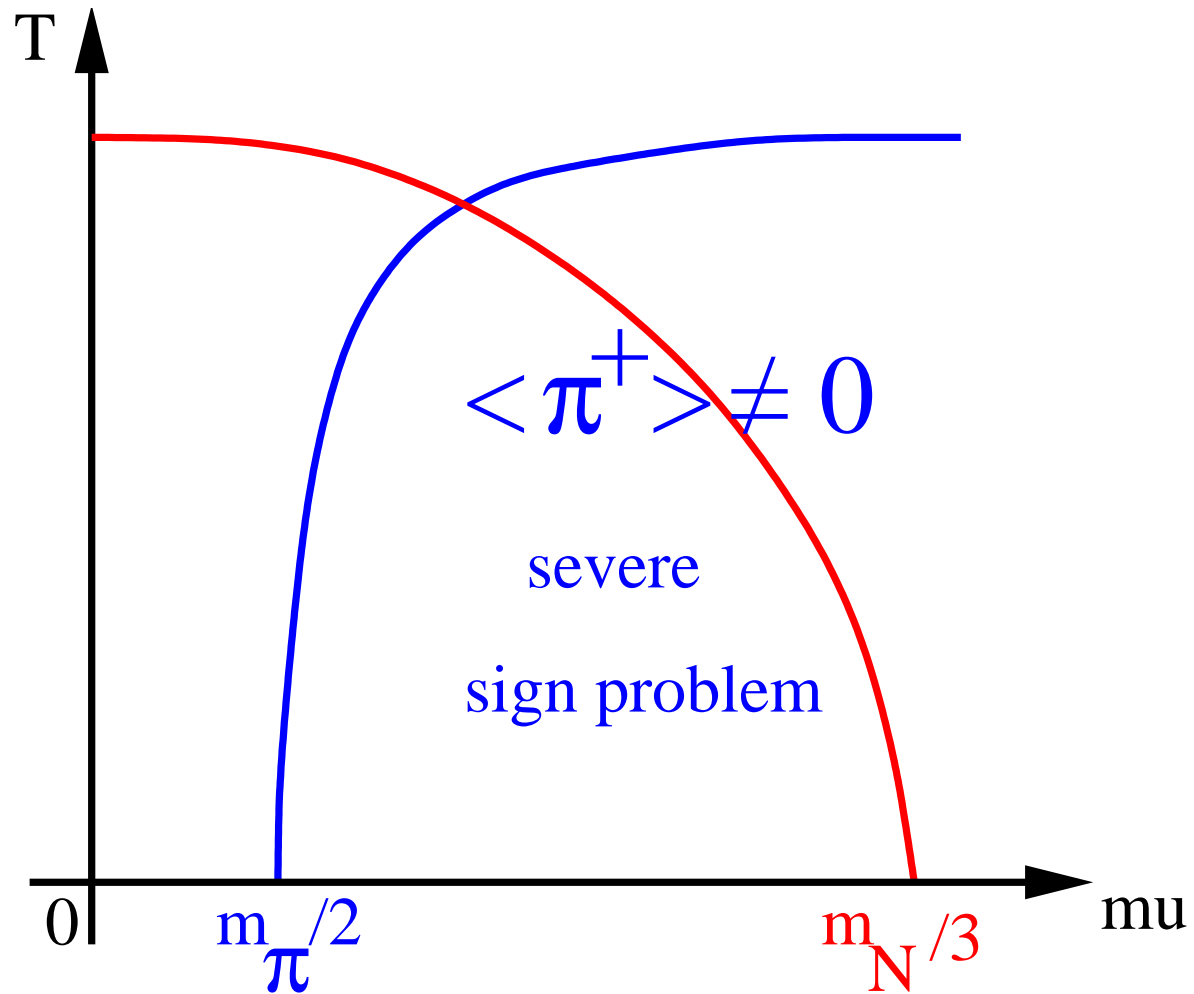
While the first “problems” seem to describe the **technical side** of the problem, the following are closer to **the physical side** :

- **“average phase factor”**; its vanishing in  $\lim_{V \rightarrow \infty}$  discourages the so-called “phase quenching approach” for big volumes
- **“overlap problem”**; a real incompatibility of configurations
- **“silver blaze problem”** (T. D. Cohen after “Sherlock Holmes”)

The latter is a genuine **physical miracle** witnessing big cancellations: **“At low temperature, there are no observables depending on the chemical potential below some threshold (onset) value  $\mu_{onset} = \mathcal{O}(m_p/3)$ .”**

The “premature onset”  $\mu_{onset} \approx m_\pi/2$  (with the “Glasgow method”) has ruled out the first serious attempt to cope with the problem.

Where the quenched and phase-quenched simulation fails  
from Ph. de Forcrand arXiv:1005.0539





This negative result points out, that some kind of arithmetic **cancellation** *must take care to reproduce the right physics.*

Let me explain how (and where) this comes about.

*At the same time, I am trying to give a mini-review of progress in the field addressed to non-experts in LGT, while trying to touch most of the ideas presently around.*

My own lattice activity was not in finite density lattice field theory (rather in confinement mechanisms, vacuum structure and topology). Sorry, my apologies ! This is mostly a compilation ! **However, I have contributed to our field when it was in infancy.**

This was when CERN SPS was preparing for Heavy Ion collisions (NA35, 1986/1987). From 1994 really heavy ions (Pb) at NA49.

- **Dynamical Fermions At Nonzero Chemical Potential And Temperature: Mean Field Approach**, E.-M. I., J. Kripfganz (Leipzig U.)  
Sept. 1984, published in Z. Phys. C29 (1985) 79-82
- **QCD Thermodynamics and Non-Zero Chemical Potential**, E.-M. I., J. Kripfganz (Leipzig U.), in: “Hadronic Matter under Extreme Conditions”, Kiev, Naukova Dumka 1986, part 1, p. 153  
Proceedings of a workshop organized in Kiev by Gennady Zinovjev (that did not take place because of the Chernobyl desaster)
- **Complex Langevin Simulation Of Chiral Symmetry Restoration At Finite Baryonic Density**, E.-M. I. (ICTP, Trieste). Jul. 1986, published in Phys. Lett. B181 (1986) 327

# The paper

## Dynamical Fermions at Non-Zero Chemical Potential and Temperature: Mean Field Approach

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**Abstract.** We derive a strong coupling effective Lagrangian describing Wilson lines coupled to quark bilinears. Wilson line and dynamical quark mass are studied in mean field approximation. A second-order finite-temperature chiral phase transition is found at zero chemical potential  $\mu$ . For  $\mu \neq 0$  this transition becomes a first-order one.

### 1. Introduction

$SU(3)$  pure gauge theory is known to show a 1st order deconfining phase transition [1,2]. The low-temperature phase is characterized by a non-vanishing string tension indicating confinement. In the high-temperature phase the long range part of the static quark potential is Debye screened. The thermodynamic behaviour approaches that of a gas of non-interacting gluons.

As soon as dynamical quarks (in the fundamental representation) are taken into account the static potential is screened anyway, also at low temperature. Therefore, there is no longer an order parameter for a deconfining phase transition.

The deconfining phase transition of the pure gauge theory may also be characterized by the spontaneous breakdown of a global  $Z_3$  symmetry, where  $Z_3$  is the center of the gauge group  $SU(3)$ . The quark Lagrangian explicitly breaks this  $Z_3$  symmetry. Therefore, a possible deconfinement phase transition could no longer be related to the spontaneous breakdown of a global symmetry, i.e. again no order parameter. One might therefore expect [3,4] the deconfinement phase transition of the pure gauge theory (corresponding to quark mass  $m_q = \infty$ ) to be washed out completely below some finite quark mass.

Quantum Chromodynamics however possesses other global symmetries (chiral symmetries) whose spontaneous breakdown or restoration may

characterize phase transitions at finite temperature and/or chemical potential. Indeed, quenched QCD shows a first order chiral phase transition at a temperature close or equal to the deconfinement temperature [5]. This chiral phase transition has a good chance to survive the introduction of dynamical quarks, despite the fact that certain gauge field configurations (e.g. instantons) which break chiral symmetry are suppressed by fermionic zero modes.

Restoration of chiral symmetry at high temperature has been demonstrated rigorously [6] for gauge group  $SU(2)$  and zero-mass quarks. The order of the corresponding phase transition, the precise value of the transition temperature, as well as the behaviour at non-zero quark mass can probably be found out by lattice Monte Carlo calculations only. Interesting Monte Carlo results [7] have become available during the last few months. They do not definitely establish the presence of a phase transition but in any case indicate rapid variations of various thermodynamic quantities.

Although Monte Carlo results will improve more and more it will still be important to have some approximate analytical understanding of chiral dynamics at non-zero temperature and chemical potential  $\mu$ . In particular for  $\mu \neq 0$  this is relevant since the Monte Carlo approach is not easily extendable to this case (because of the complex measure).

For this reason we develop analytical techniques to study the chiral phase transition in the presence of dynamical quarks. We emphasize the dependence on the chemical potential. Our approach is based on standard strong coupling and mean field techniques. These methods have been applied before [8–12] to study chiral dynamics. Strong coupling Hamiltonian approaches [8,9] have established the analogy with the behaviour of an antiferromagnetic Ising model. For  $\mu = 0$  one expects a second-order transition at  $m_q = 0$  which disappears for  $m_q \neq 0$  (the mass acts like a staggered magnetic field). The chemical potential on

# The result

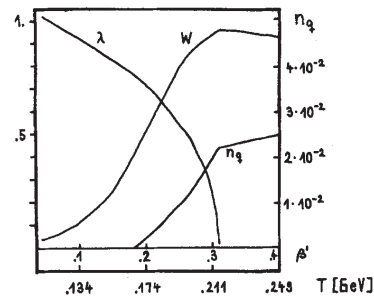


Fig. 1. Chiral order parameter  $\lambda$ , Wilson line  $W$  and quark density  $n_q$  as function of  $\beta'$ , for zero chemical potential. The temperature in physical units is obtained as explained at the end of Sect. 2

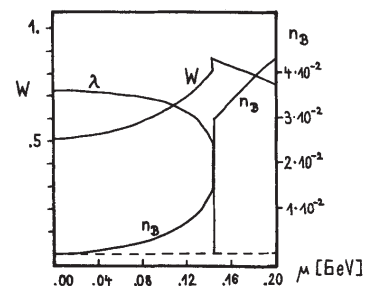


Fig. 2.  $\lambda$ ,  $W$ , and baryon density  $n_b$  as function of the chemical potential at  $\beta' = 0.2$  ( $T \sim 174$  MeV)

At lower temperature the picture is different. For  $\beta' = 0.05$  (corresponding to  $T = 110$  MeV, shown in Fig. 3b) there is a clear local minimum at  $\lambda = 0$  also at  $\mu$  below  $\mu_c \sim 215$  MeV. It remains separated from the minimum at  $\lambda \cong 1.0$  by a potential threshold within some interval in  $\mu$  around  $\mu_c$ .

Our results are reassuring for those interested in high energy heavy ion experiments. Transition phenomena should be even more violent in the fragmentation region at heavy ion collisions. A significant increase in the density of heavy quarks (characterized by the behaviour of the Wilson line, (16)) should however be expected in the central region only.

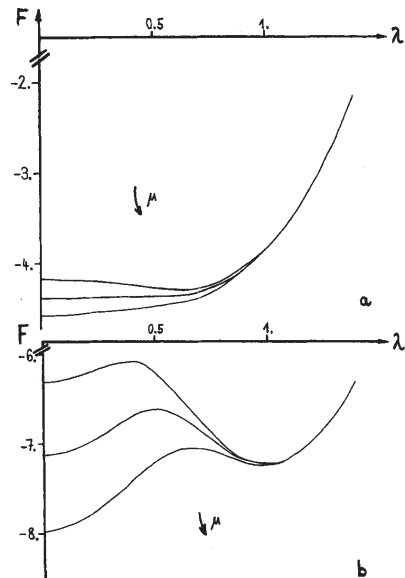


Fig. 3a and b. Mean free energy per site as function of  $\lambda$  for two values of  $\beta'$ : a)  $\beta' = 0.2$ ,  $W = 0.9$ ,  $\mu = 0.12, 0.14, 0.16$  GeV; b)  $\beta' = 0.05$ ,  $W = 0.2$ ,  $\mu = 0.18, 0.21, 0.24$  GeV

## References

1. C. Borgs, E. Seiler: Nucl. Phys. **B215**, 125 (1983); E.T. Tomboulis, L.G. Yaffe: Phys. Rev. **D29**, 780 (1984)
2. H. Satz: Bielefeld-preprint BI-TP 83/20 (1983); B. Svetitsky: Cornell preprint CLNS 84-607 (1984)
3. T. Banks, A. Ukawa: Nucl. Phys. **B225**, 145 (1983)
4. P. Hasenfratz, F. Karsch, I.O. Stamatescu: Phys. Lett. **133B**, 221 (1983)
5. J. Engels et al.: Nucl. Phys. **B205**, 545 (1982); J. Engels, F. Karsch, H. Satz: Phys. Lett. **113B**, 398 (1982); J. Kogut et al.: Phys. Rev. Lett. **50**, 393 (1983)
6. E.T. Tomboulis, L.G. Yaffe: Princeton preprint 1984
7. R.V. Gavai, M. Lev, B. Petersson: Phys. Lett. **140B**, 397 (1984); Bielefeld preprint BI-TP 84/10 (1984); F. Fucito, S. Solomon: Caltech preprint CALT-68-1084 (1984); F. Fucito, C. Rebbi, S. Solomon: Caltech preprints CALT-68-1124, CALT-68-1127 (1984); M. Fischler, R. Roskies: Pittsburgh preprint PITT-18-84 (1984); J. Polonyi et al.: University of Illinois preprint P/84/5/66 (1984); T. Celik, J. Engels, H. Satz: Bielefeld preprint BI-TP 84/09 (1984)
8. A. Patel: Caltech preprint CALT 68-1079 (1984)
9. C.P. van den Doel: Santa Cruz preprint UCSC TH 157-83 (1983), and UCSC preprint 1984
10. V. Alessandrini: Orsay preprint LPHE Orsay 84/14 (1984)
11. A. Gocksch, M. Ogilvie: Brookhaven preprint BNL 34559 (1984)
12. P.H. Damgaard, N. Kawamoto, K. Shigemoto: preprint NORDITA 84/16 (1984)

There are Yang-Mills theories, whose gauge groups do not create a sign problem :

for example

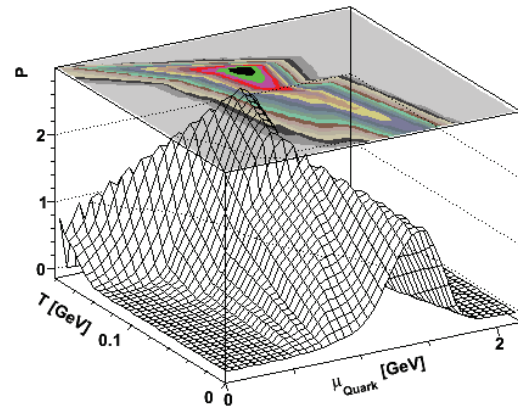
- $SU(2)$
- $G_2$  (worked on mainly by Maas, Wellegehausen [Jena group])
- $SO(2N)$

Also : not all kinds of chemical potentials create a sign problem !

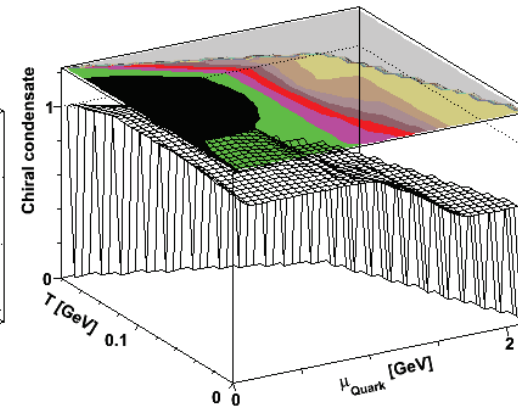
# Phase diagram

[Maas, von Smekal, Wellegehausen, Wipf '12]

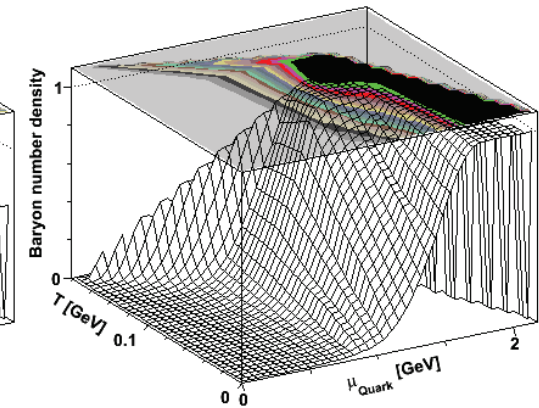
Polyakov loop



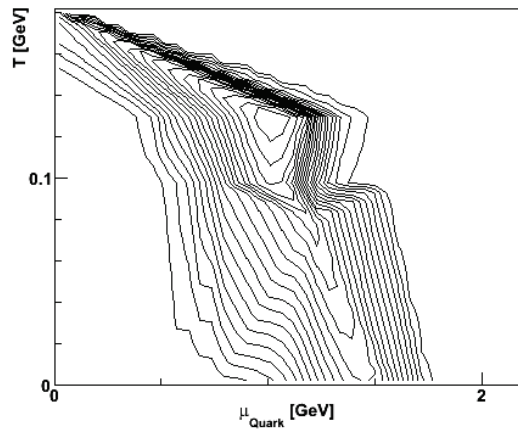
$\langle \bar{\Psi}\Psi \rangle(T, \mu) / \langle \bar{\Psi}\Psi \rangle(0, 0)$



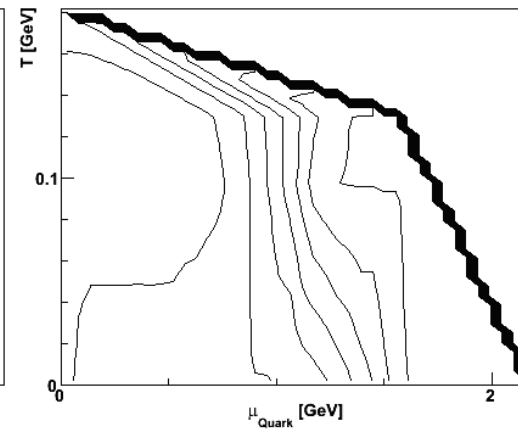
$n_B / n_B^{\text{sat}}$



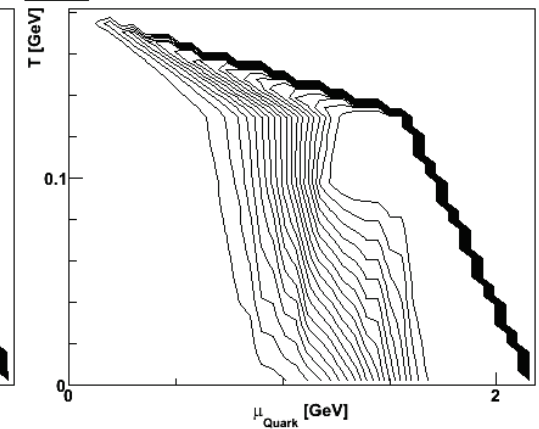
Polyakov loop



$\langle \bar{\Psi}\Psi \rangle(T, \mu) / \langle \bar{\Psi}\Psi \rangle(0, 0)$



$n_B / n_B^{\text{sat}}$



## Finite baryon density in standard Statistical Mechanics,

calculations at finite baryonic density look innocent :

**Grand canonical density operator** ( $\hat{\text{Tr}}$  = trace in Hilbert space)

$$\rho = e^{-\frac{1}{T}(H - \mu_i N_i)}, \quad Z = \hat{\text{Tr}} \rho, \quad \hat{\text{Tr}} (\dots) = \sum_n \langle n | (\dots) | n \rangle$$

Everything is real valued: energy eigenvalues, partition function, extra weighting according to the number of particles.

**Usual observables as thermal averages :**

$$\langle O \rangle = Z^{-1} \hat{\text{Tr}} (\rho O)$$

**obtained with the partition function :**

$$Z = \hat{\text{Tr}} (\rho)$$

One can directly derive the **thermodynamic functions** from the partition function  $Z(T, V, \mu)$  :

$$\begin{aligned} F &= -T \ln Z && \text{free energy} \\ p &= \frac{\partial}{\partial V} (T \ln Z) && \text{pressure} \\ S &= \frac{\partial}{\partial T} (T \ln Z) && \text{entropy} \\ \bar{N}_i &= \frac{\partial}{\partial \mu_i} (T \ln Z) && \text{average particle number} \\ E &= -p V + T S + \mu_i \bar{N}_i && \text{energy} \end{aligned}$$

Useful for homogeneous phases : **densities of thermodynamical functions**

$$f = \frac{F}{V}, \quad p = -f, \quad s = \frac{S}{V}, \quad n_i = \frac{\bar{N}_i}{V}, \quad \epsilon = \frac{E}{V}$$



in appropriate units of  $T^4$ ,  $T^3$  or  $T^2$

$$\begin{aligned}\frac{p}{T^4} &= \frac{1}{V T^3} \ln Z && \text{pressure } p \\ \frac{\epsilon}{T^4} &= -\frac{1}{V T^4} \frac{\partial}{\partial(1/T)} \ln Z && \text{energy density } \epsilon \\ \frac{n_q}{T^3} &= \frac{1}{V T^3} \frac{\partial}{\partial(\mu_q/T)} \ln Z && \text{quark density } n_q \\ \frac{\chi_q}{T^2} &= \frac{1}{V T^3} \frac{\partial^2}{\partial(\mu_q/T)^2} \ln Z = \frac{T}{V} (\langle N_q^2 \rangle - \langle N_q \rangle^2) && \text{quark number susceptibility } \chi_q\end{aligned}$$

Once the partition function is known from another formalism (say, from lattice calculation) all these relations remain valid.

Here, in the standard quantum statistical formalism, the addition of any phase factor would eventually also lead to problems similar to those encountered within the lattice formalism.

Example :

**Imaginary chemical potential**  $\mu_B = i\eta_B$  ; this looks a bit artificial !

Periodicity  $\eta_B/T \rightarrow \eta_B/T + 2\pi$  is obvious

(or later  $\eta_q \rightarrow \eta_q + \frac{2\pi}{3}$  for quarks).

Later, just this case will turn out to be the “easy case”, and this “detour” is actually taken, hoping that **analytical continuation** gives the *right answer for the real case of real  $\mu$* .

$$\rho = e^{-\frac{1}{T}(H - i\eta_q N_q)}$$

- The special problems are originating in the lattice technique !
- We are pampered by decades of lattice simulations giving us all results (almost) for free (due to the *ab initio* style of calculation).
- We were used to **blindly rely on importance sampling** techniques. However, sometimes **variance reduction tricks** have been necessary !
- Compared to this comfortable situation, finite baryonic density **creates a complicated situation**. It requires really fresh thought !

**Gives impulses for developing new algorithms/data handling !**

Other chemical potentials (isospin, chiral chemical potential etc.) are (relatively) harmless.

***CP*-violation, so-called  $\Theta$ -vacuum effects, are similarly challenging.**

**This makes life less mundane, more interesting !**

What, after all, is the advantage of the lattice ?

- It gives a **characterization of configurations** by specifying a finite number of degrees of freedom (suitable for simulation).
- We have **many methods to our disposal only on the lattice, two of them assisting each other at finite baryonic density !**

### 1. Importance sampling

- Let an algorithm generate a sequence of configurations, with a frequency of occurrence proportional to a theoretically justified weight (“frequentist’s probability”). This works only if the weight is real/positive (heatbath, Metropolis and Co.)
- Take the arithmetic average of the observable of interest.
- Evaluate the error of deviation from the theoretical average.

## 2. Strong coupling expansion

- Known from statistical mechanics as HTE.
- Expand the (pairwise) interaction of spins  $\exp\left(\frac{1}{T}S_xS_y\right)$  in orders of  $1/T$  (HTE = high temperature expansion).
- Would not be possible without discretization !
- Because there are so many pairs the system, it seems hopeless to keep the overview over all generated terms.
- But integration/summation over spins erases most of the terms, leaving only terms with the structure of closed loops.
- Use diagrammatic/loop/worm algorithms (which perform – on a lattice – discrete updates of loops).

**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.)

**Most lattice results achieved** within standard importance sampling :

- **hadron eigen energies** (inserting sources, relying on  $\Delta\tau \rightarrow \infty$ )
- **structure of the hadrons** (inserting sources plus probes, separated by  $\Delta\tau \rightarrow \infty$  from the sources [relaxation !] )
- **structure of extended systems** (hadronic matter at different temperatures) calculated in all phases within the same set-up
- **no prior knowledge needed about the “relevant” degrees of freedom**

**Limitations only in resources, that are easy/difficult to overcome :**

- **finite volume**  $N_i \rightarrow \infty$  ( $i = 1, 2, 3$ )
- **finite discretization** (lattice spacing  $a \rightarrow 0$ )
- **non-physical fermion and pion masses** ( $m_q \propto m_\pi^2 \rightarrow \text{phys.}, \text{hardest !}$ )

## 2. A Look inside Lattice Gauge Theory

- Path Integral Approach : Euclidean vs. Minkowskian
- Briefly about Gauge Fields
- Coupling Fermions to Gauge Fields
- Order Parameters for Finite-Temperature Transitions



## 2. 1. Path Integral Approach : Euclidean vs. Minkowskian

Success of Lattice Field Theory, in particular Lattice Gauge Theory, rests on the **path integral approach**.

**The whole path integral story is full of sign problems !**

Everything begins with the Lagrangian approach.

Consider first  $0 + 1$  dimensions : Quantum Mechanics :

**Path integral in quantum mechanics** based on the **real time evolution operator**

$$\langle q' | e^{-\frac{i}{\hbar} \hat{H} T} | q \rangle = \langle q' | U(T, 0) | q \rangle$$

The **Feynman path integral** was first proposed to evaluate this as

$$\langle q' | U(T, 0) | q \rangle = \int D[q]_{(0,q)}^{(T,q')} e^{\frac{i}{\hbar} S[q]}$$

with the **“real time”** action in the exponent (M = Minkowski)

$$S_M[q] = \int_0^T dt \left( \frac{m}{2} \dot{q}^2 - V(q(t)) \right) = \int_0^T L[q(t), \dot{q}(t)]$$

$D[q]_{(0,q)}^{(T,q')}$  = **measure of trajectories** running from  $(t = 0, q)$  to  $(t = T, q')$  .

**Discretization** → introduce a **time lattice** (with lattice spacing  $a = \frac{T}{N}$ )

$$t_0 = 0, \dots, t_n = na, \dots, t_{N-1} = (N-1)a, t_N = Na = T$$

Thus, it is possible to give a **precise meaning to the path integral**.

$$\begin{aligned}
\langle q'|U(T,0)|q\rangle &= \int dq_{N-1} \cdots dq_1 \langle q'|T|q_{N-1}\rangle \langle q_{N-1}|T|q_{N-2}\rangle \cdots \langle q_1|T|q\rangle \\
&= \int D[q]_{(0,q)}^{(T,q')} e^{\frac{i}{\hbar} S[q]}
\end{aligned}$$

with **polygon-shaped**, “zig-zag” trajectories and a **discretized action** :

$$\langle q_{n+1}|T|q_n\rangle = \mathcal{N} e^{-\frac{ia}{2\hbar} V(q_{n+1})} e^{\frac{im}{2a\hbar} (q_{n+1}-q_n)^2} e^{-\frac{ia}{2\hbar} V(q_n)}$$

The product of the “transfer matrices”  $\langle q_{n+1}|T|q_n\rangle$  is **not usable as a numerically manageable measure** (it is a complex number !).

The discretized action  $S[q]$  is real-valued, but the exponent purely imaginary:

$$\frac{i}{\hbar} S[q] = \ln \left( \prod_{n=1}^N \langle q_n|T|q_{n-1}\rangle \right)$$

Considering the integral over each of the  $q_i$ , it is over a rapidly **oscillating, complex valued integrand**.

In this stage the path integral is completely governed (i.e. obscured) by the **“complex weight problem”**.

(I put from now  $\hbar = 1$ .)

**Rescue : the Wick rotation** provides a solution !

Do an **analytical continuation** of the time step  $a$  to imaginary time:

$$a = |a|e^{-i \phi} \quad \phi : 0 \rightarrow \frac{\pi}{2}$$

For all  $\phi \in (0, \pi/2]$  the real part of the exponent  $iS[q]$  is non-vanishing and negative (responsible for **suppressing the measure** far away from the **classical trajectories**). The **“time evolution”** is now **“diffusive”**.

With this **analytical continuation to  $\phi = \pi/2$** , the discretized path integral takes the form

$$\langle q' | U_I(T, 0) | q \rangle = \int D[q]_{(0,q)}^{(T,q')} e^{-S_I[q]}$$

$$S_I[q] = |a| \sum_{n=1}^N \left[ \frac{m}{2 |a|^2} (q_n - q_{n-1})^2 + \frac{1}{2} V(q_n) + \frac{1}{2} V(q_{n-1}) \right]$$

This is the **discrete approximation** of the **Euclidean action** :

$$S_E[q] = \int_0^T d\tau \left( \frac{m}{2} \dot{q}^2 + V(q(\tau)) \right) = \int_0^T d\tau L_E[q(\tau), \dot{q}(\tau)]$$

Now, the discretized path integral is convergent !

Matrix elements like the **time-ordered product of Heisenberg operators in real time**

$$\langle T[\hat{q}(t_1) \cdots \hat{q}(t_l)] \rangle$$

can be obtained from the path integral averages (**commuting numbers do not need to be explicitly ordered in [any] time !**)

$$\langle q' | T[\hat{q}(\tau_1) \cdots \hat{q}(\tau_l)] | q \rangle_{QM} = \langle q(\tau_1) \cdots q(\tau_l) \rangle = \int D[q]_{(q,0)}^{(q',T)} q(\tau_1) \cdots q(\tau_l) e^{-S_E[q]}$$

**in imaginary time by analytical continuation back to  $\phi = 0$ .**

Very important advantage/convenience of this formulation :

**“Euclidean correlation functions can be *blindly* calculated by importance sampling due to the positive measure of trajectories.”**

Analysis and interpretation then are the harder part of labor !

## More about the Euclidean measure :

- The **form of the measure** is readable from the partition function, i. e. from the **Euclidean action**.
- Without interaction, it becomes the **Wiener measure** well-known from **Brownian motion**.
- For **thermal averages** (describing quantum statistics) the **Euclidean form is just what is needed !**
- For **thermodynamic functions** no analytical continuation is needed, all is **derivable from the partition function**.
- However: discerning the **spectral density** of a particle (giving mass and width) or current correlator (transport coefficient) requires **analytical continuation** (“Maximal Entropy Method”).

The issue of boundary conditions of the trajectories :

**Density matrix** is now given in the **coordinate representation** :

$$\begin{aligned}\langle q' | \rho | q \rangle &= \frac{1}{Z} \langle q' | e^{-\frac{1}{T} \hat{H}} | q \rangle \\ &= \mathcal{N} \int D[q]_{(q,0)}^{(q',1/T)} e^{-S_E[q]}\end{aligned}$$

Taking the trace  $\int dq \langle q | \rho | q \rangle$  implies integration over **periodic trajectories** (with the identification  $q' = q$ ) at  $t = 0$  and  $t = 1/T = \beta$ .



Single-time expectation values obtained by importance sampling :

1. sample periodic trajectories according to the measure
2. evaluate for each trajectory  $O(q(\tau))$  at fixed time  $\tau = 0$
3. average this “observable” over trajectories

In order to improve statistics, in step 2 one can first average  $O(q(\tau))$  over  $\tau \in [0, 1/T]$ .

This defines a “center of gravity value”  $\bar{O}$  of  $O$  along the trajectory.

Averaging  $\bar{O}$  instead of  $O(q(0))$  over trajectories is equivalent due to the cyclic invariance of the trace (but variance-reduced !).

All this is **applicable also for scalar field theories** (including charged scalars, with complex field) **given in Minkowski space :**

$$S[\phi] = \sum_x \left[ \frac{1}{2} |\phi_{x+\hat{4}} - \phi_x|^2 - \sum_{i=1}^3 \frac{1}{2} |\phi_{x+\hat{i}} - \phi_x|^2 - \frac{m^2}{2} |\phi_x|^2 - V(|\phi_x|) \right]$$

Upon **Wick rotation**, only **the potential part changes sign in the Euclidean version of action :**

$$S_E[\phi] = \sum_x \left[ \frac{1}{2} |\phi_{x+\hat{4}} - \phi_x|^2 + \sum_{i=1}^3 \frac{1}{2} |\phi_{x+\hat{i}} - \phi_x|^2 + \frac{m^2}{2} |\phi_x|^2 + V(|\phi_x|) \right]$$

**These actions** (both in Minkowski or Euclidean space) are **real-valued.**

It seems, the **“oscillatory integrand”** is overcome by going over to **Euclidean space.**

Can the “complex measure problem” never reappear ?

This will happen when one tries to translate the **finite charge density constraint** into the **Lagrangian/Path Integral** formalism (see this later for the  $\phi^4$  theory).

Thus, the “complex measure” or “silver blaze problem” is not at all restricted to QCD !

## 2. 2. Briefly about Gauge Fields

If **gauge invariance** enters the game, such that the action should be invariant under transformations  $\phi_x \rightarrow g_x \phi_x$  with  $g_x \in G$  (gauge group), that may be **independently** chosen at each site  $x$ . One needs to introduce “transporters”  $U_{x\mu}$  between neighboring sites (to form **covariant derivatives**, resp. **covariant finite difference quotients**)

$$S_E[\phi] = \sum_x \left[ \frac{1}{2} |U_{x,4} \phi_{x+\hat{4}} - \phi_x|^2 + \sum_{i=1}^3 \frac{1}{2} |U_{x,i} \phi_{x+\hat{i}} - \phi_x|^2 + \frac{m^2}{2} |\phi_x|^2 + V(|\phi_x|) \right]$$

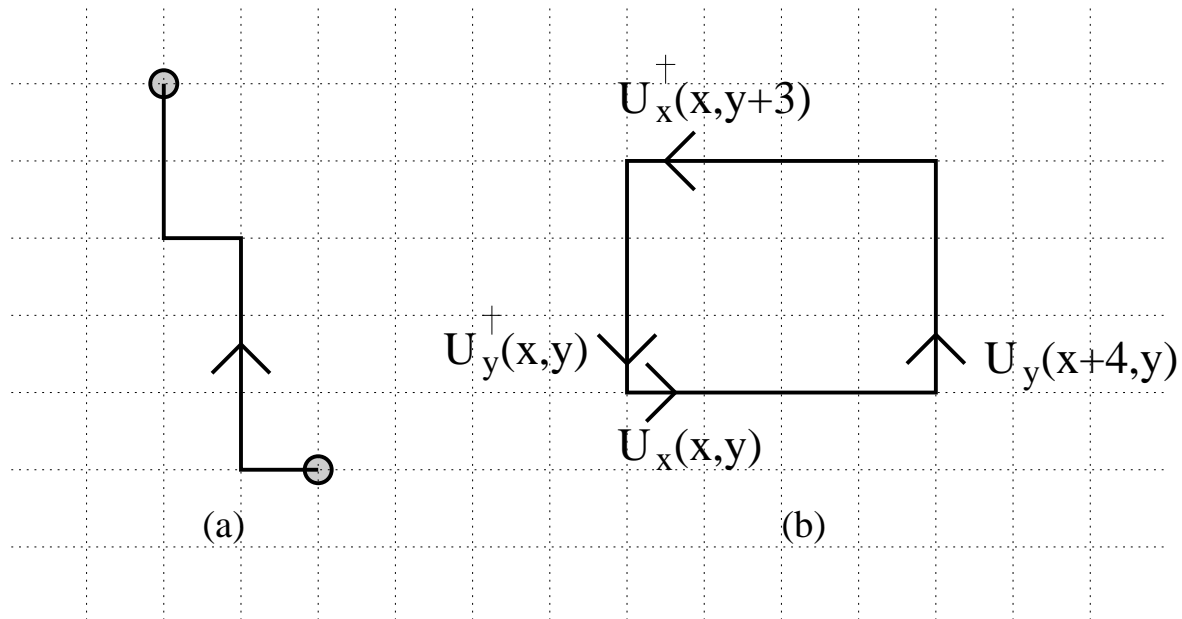
**Transporters have to transform** under gauge transformations accordingly

$$U_{x,\mu} \rightarrow g_x U_{x,\mu} g_{x+\hat{\mu}}^\dagger$$

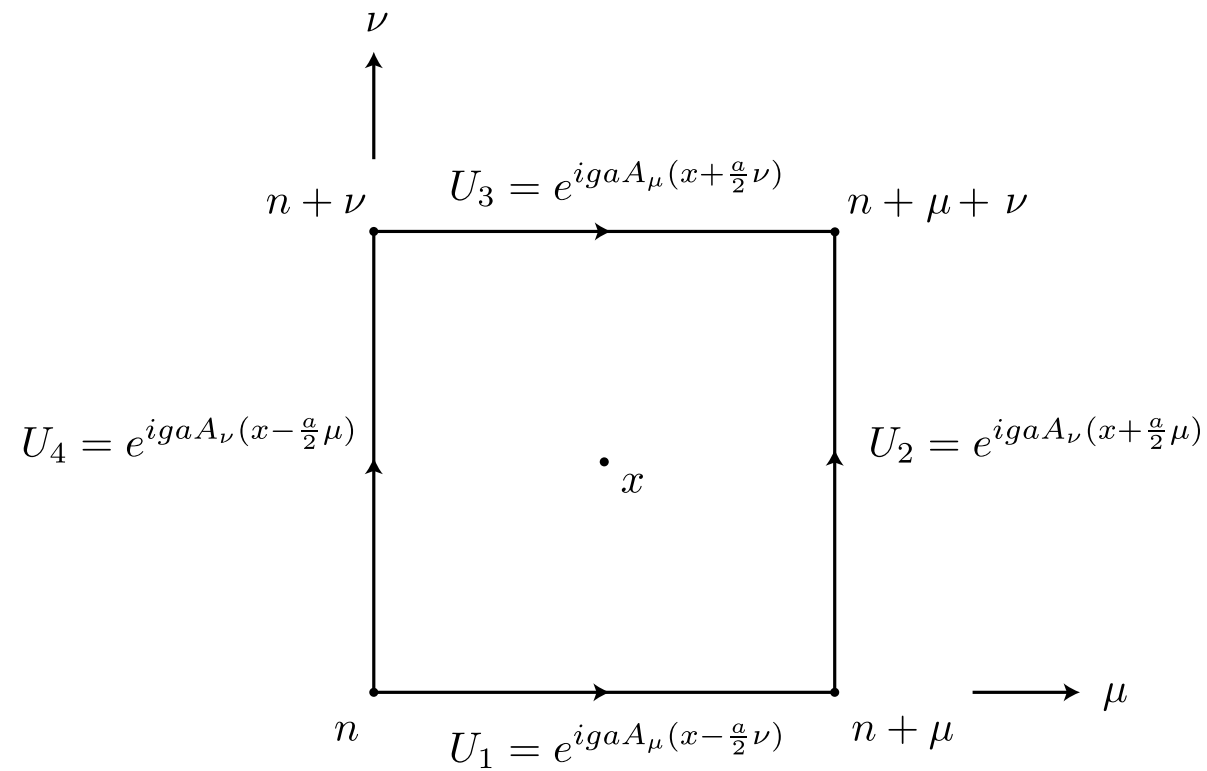
This clarifies **how transporters are defined** in terms of the field  $A_\mu$ :

$$U_{x,\mu} = e^{iaA_{x+\hat{\mu}/2,\mu}}$$

# Labelling of links and the formation of strings and loops



## Construction of a plaquette



The **gauge field acquires an own action**: standard example is **Wilson's action of gluons** (by expressing  $F_{\mu\nu} = A_{\mu;\nu} - A_{\nu;\mu} + [A_\mu, A_\nu]$  as a loop)

$$S_G[U] = \sum_x \sum_{1 \leq \mu < \nu \leq 4} \beta \left( 1 - \frac{1}{3} \text{Re tr } U_p \right) \approx \int_0^{1/T} d\tau \int_V d^3x \frac{1}{2} \text{Tr } F_{\mu\nu}(x) F_{\mu\nu}(x)$$

Here  $U_p = U_{x,\mu} U_{x+\hat{\mu},\nu} U_{x+\hat{\nu},\mu}^\dagger U_{x,\nu}^\dagger$  (4 “links”) is the **elementary plaquette**. Lattice **gauge coupling**  $\beta$  and continuum one are related by  $\beta = 2N/g^2$ .

Since it is **bosonic**, we impose **periodic boundary conditions** in all four directions,  $U_\mu(\tau, \mathbf{x}) = U_\mu(\tau + N_\tau, \mathbf{x})$ ,  $U_\mu(\tau, \mathbf{x}) = U_\mu(\tau, \mathbf{x} + N_s)$ .

Define the transfer matrix between two times slices  $\tau$  and  $\tau + 1$  :

$$T[U_i(\tau + 1), U_i(\tau)] = \langle U_{\tau+1} | e^{-aH} | U_{\tau} \rangle = \int DU_0(\tau) \exp -L[U_i(\tau + 1), U_0(\tau), U_i(\tau)]$$

Here the action is written **grouped in two subsequent timeslices** :

$$S_G = \sum_{\tau} L[U_i(\tau + 1), U_0(\tau), U_i(\tau)]$$

Similar to the **kinetic/potential splitting** in the QM case

$$L[U_i(\tau + 1), U_0(\tau), U_i(\tau)] = \frac{1}{2}L_1[U_i(\tau + 1)] + \frac{1}{2}L_1[U_i(\tau)] + L_2[U_i(\tau + 1), U_0(\tau), U_i(\tau)]$$

with

$$L_1[U_i(\tau)] = -\frac{\beta}{N} \sum_{p(\tau)} \text{Re Tr } U_p$$

containing all **spacelike plaquettes and links at fixed  $\tau$** ,

(“potential energy”, no double-counting) and the inter-slice action ....



$$L_2[U_i(\tau + 1), U_0(\tau), U_i(\tau)] = -\frac{\beta}{N} \sum_{p(\tau, \tau+1)} \text{Re Tr } U_p$$

containing all **timelike plaquettes and links spanned between timeslices** at subsequent times  $\tau$  and  $\tau + 1$  (this is the “kinetic energy”).

**Partition function :**

$$Z = \int \prod_{\tau=1}^{N_\tau} (DU_i(\tau, \mathbf{x}) T[U_i(\tau), U_i(\tau - 1)]) = \hat{\text{Tr}}(T^{N_\tau}) = \hat{\text{Tr}}(e^{-N_\tau a H})$$

**Periodic boundary condition  $U_i(N_\tau) = U_i(0)$  in the temporal direction warrants, that the same (!) states  $|n\rangle = |U_i\rangle$  are taken on the time slices 0 and  $N_\tau$ , in order to take the trace.**

Again, the inverse temperature is  $1/T = aN_\tau$ , the temporal length.

Periodicity in spatial directions is the most unbiased option for **imitating** a proper “environment” for the finite system (made out of mirror systems of the actual system, which is the “central” box).

This construction is sometimes abandoned for particular purposes (e.g. mimicking a **cold environment for the QGP [B. A. Berg et al.]**).  
for instance: Bernd A. Berg and Hao Wu arXiv:1109.0599

**Thermal expectation value of an observable (some operator  $O$ )**

$$\langle O \rangle = Z^{-1} \hat{\text{Tr}}(e^{-\frac{H}{T}} O) = Z^{-1} \sum_n \langle n | T^{N_\tau} O | n \rangle = \frac{\sum_n \langle n | O | n \rangle e^{-a N_\tau E_n}}{\sum_n e^{-a N_\tau E_n}},$$

**otherwise calculated in a (unknown !) basis, can now alternatively be obtained by inserting a function  $O(U_i(\tau))$  related to some time slice (or averaged over all time slices) into the path integral.**

Zero temperature ? This is now not more than a special case !

$T = 0$  physics is recovered in the limit  $N_\tau \rightarrow \infty$ ,

or, at least, for  $N_\tau \geq N_i \quad i = 1, 2, 3$ .

Why the lattice approach will not be given up :

This calculational scheme is so attractive, such that hard work is going on with the aim **not to abandon it**, despite the problems encountered on the lattice, as soon as **finite density is under study**.

One should rather try to **exploit all the specific opportunities** of lattice gauge field theory, which seem to be not yet fully explored !

## 2. 3. Coupling Fermions to Gauge Fields

Adding fermions (at  $T = 0$  or  $T > 0$ ) means inclusion of a suitable **bilinear action** into the path integral

$$S_F = \sum_{x,y} \bar{\psi}(x) M_{xy}(m_f) \psi(y)$$

There are **many competing choices** to write the fermion action.

The fields are **Grassmann fields**. The integral can be **formally done**,

- with periodic boundary conditions in three spatial directions
- with antiperiodic boundary condition in the temporal direction.

**In contrast to a free complex bosonic field** with a quadratic action  $\sum_{xy} \phi^*(x) Q_{xy} \phi(y)$  and periodic boundary conditions, one gets

- $\det M(m_f)$  (spectrum taken with mixed antiperiodic/periodic b.c.) in the case of fermions, whereas one would get the formal result
- $(\det Q)^{-1}$  (spectrum taken with periodic b.c.) in case of bosons

With fermions included, the **partition function** is now

$$Z(N_s, N_\tau; \beta, m_f) = \int DU \prod_{f=1}^{N_f} \det M(m_f) e^{-S_g[U]}$$

$$U_\mu(\tau, \mathbf{x}) = U_\mu(\tau + N_\tau, \mathbf{x}) \quad \psi(\tau, \mathbf{x}) = -\psi(\tau + N_\tau, \mathbf{x})$$

For example, the **action for so-called “Wilson fermions”** is shown here :

$$S_F^W = \frac{1}{2a} \sum_{x, \mu, f} a^4 \bar{\psi}_f(x) [(\gamma_\mu - r)U_\mu(x)\psi_f(x + \hat{\mu}) - (\gamma_\mu + r)U_\mu^\dagger(x - \hat{\mu})\psi_f(x - \hat{\mu})]$$

$$+ (m + 4\frac{r}{a}) \sum_{x, f} a^4 \bar{\psi}_f(x)\psi_f(x)$$

## One minute of contemplation :

This order of **nested integrations** is probably the root of the sign problem.

**For  $\mu = 0$  it is convenient** to concentrate the fermion dynamics in a single number, the determinant, because of possible **stochastic representations for the determinant** (pseudofermions, Hybrid Monte Carlo Algorithm).

**As soon as  $\mu \neq 0$ , this advantage turns into a problem.**

In order to illustrate **possible ways out**, I will give later reformulations (in the case of **3D bosonic models/effective field theories**), where the **original sign problem (inherited from the fermion determinant)** can be overcome.

For real 4D gauge theory, people have dreamed to **reverse the order of integration : gauge degrees of freedom first, fermions later**. Not easy !

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

The **local thermal expectation value** :

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

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

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



**Definition as an order parameter for confinement :**

$$\bar{L} = 0 \quad \text{confinement,} \quad \mathbb{Z}(N) \text{ symmetry satisfied}$$

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

Also if dynamical (sea) quarks are in the model (even at  $T = 0$ ) one finds

$$\bar{L} \neq 0$$

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  $f$ )

$$\begin{aligned} \langle (\bar{\psi}\psi)_f \rangle &= \frac{1}{N_1 N_2 N_3 N_t} \frac{\partial}{\partial m_f} \ln Z = \frac{1}{4 N_1 N_2 N_3 N_t} \langle \text{tr} D_f^{-1} \rangle \\ &\propto \left\langle \sum_{\text{eigenvalue } i} \frac{1}{i\lambda_i + m} \right\rangle \propto \left\langle \sum_{\text{eigenvalue } i} \frac{2m}{\lambda_i^2 + m^2} \right\rangle \end{aligned}$$

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

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

“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  $m \rightarrow 0$ ) :**

$$\begin{aligned} \lim_{m \rightarrow \infty} \langle \bar{\psi}\psi \rangle &\neq 0 && \text{chirally broken phase} \\ \lim_{m \rightarrow \infty} \langle \bar{\psi}\psi \rangle &= 0 && \text{chirally restored phase} \end{aligned}$$

Other observables show **dramatic signals at the phase transition**, too, **although they are not “order parameters”** (i.e., never vanish just for symmetry reasons) :

- energy density  $\epsilon$
- 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**

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

(“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  $\beta$
- bare quark masses  $m$
- chemical potential  $\mu$  (later)

Then the pressure is obtained by the “integral method”

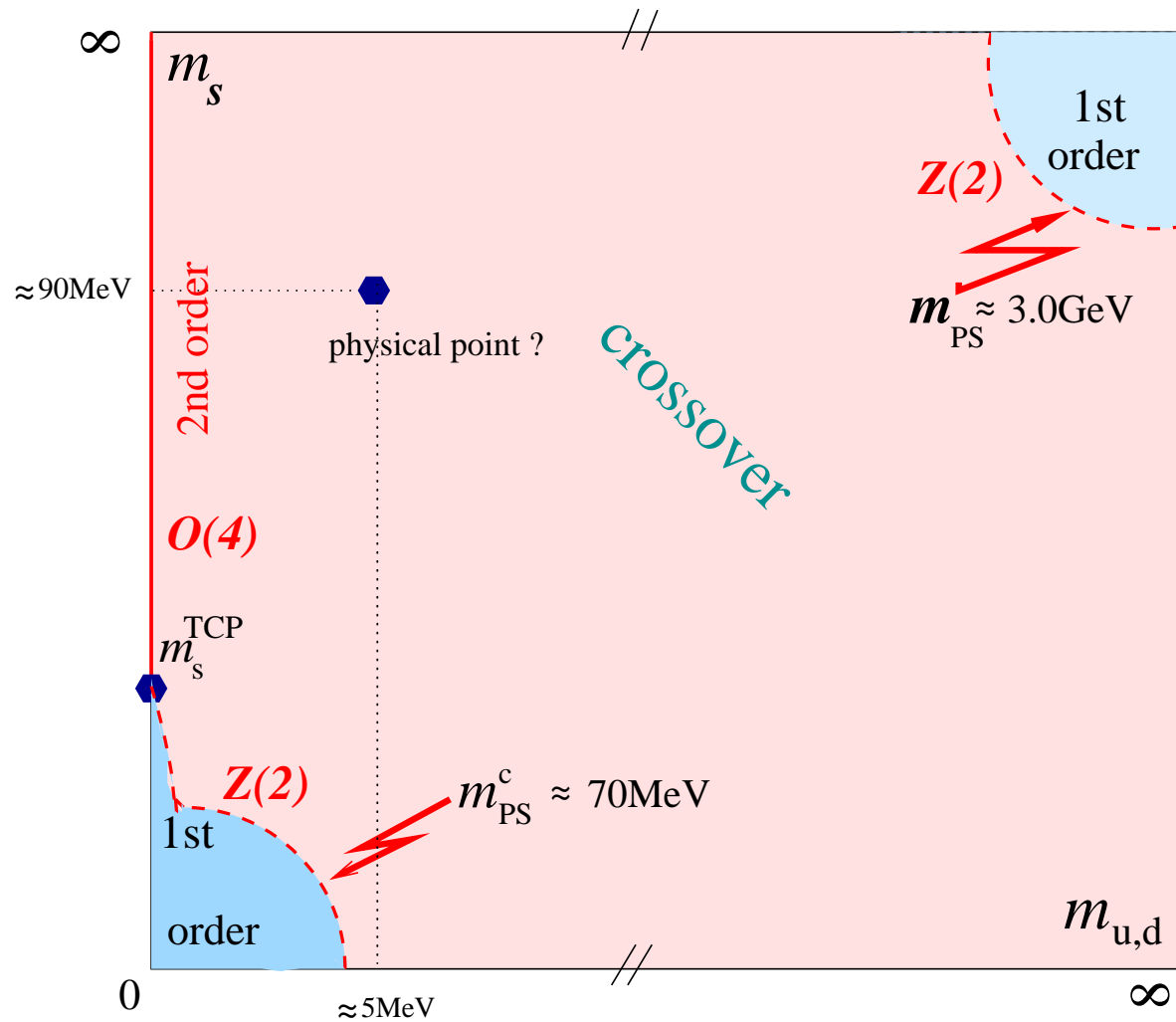
$$\frac{p_{fin}}{T_{fin}^4} - \frac{p_{in}}{T_{in}^4} = \frac{1}{T^3 V} \int_{in}^{fin} \left[ d\beta \left\langle \frac{\partial \ln Z}{\partial \beta} \right\rangle + dm \left\langle \frac{\partial \ln Z}{\partial m} \right\rangle + d\mu \left\langle \frac{\partial \ln Z}{\partial \mu} \right\rangle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

as a line integral along a “line of constant physics” between two points characterizing initial and final state in temperature (or later in the  $\beta$ - $\mu$ , i.e. temperature–chemical potential plane).

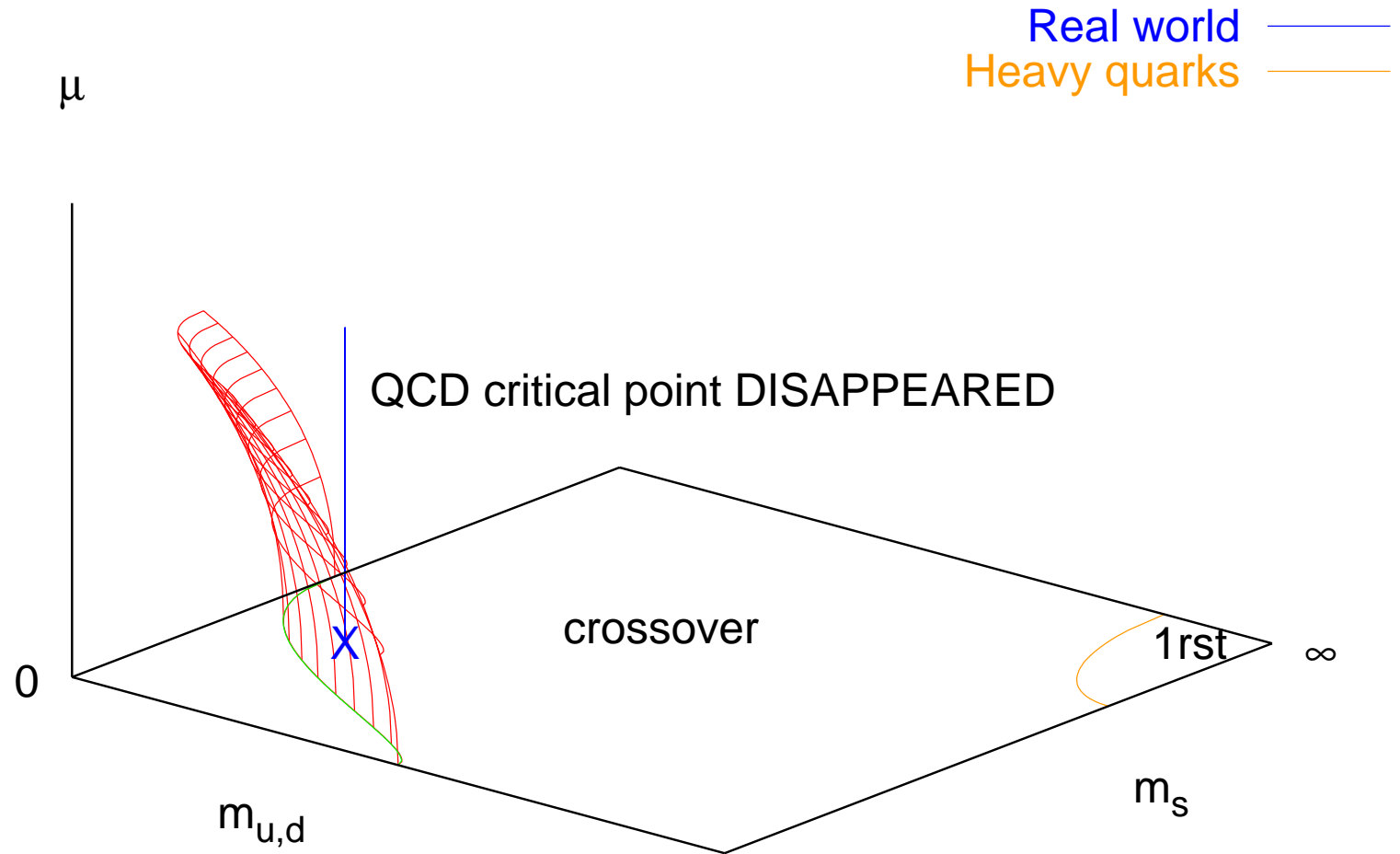
Later, inside the  $T$ - $\mu$  phase diagram, each point can be characterized by

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

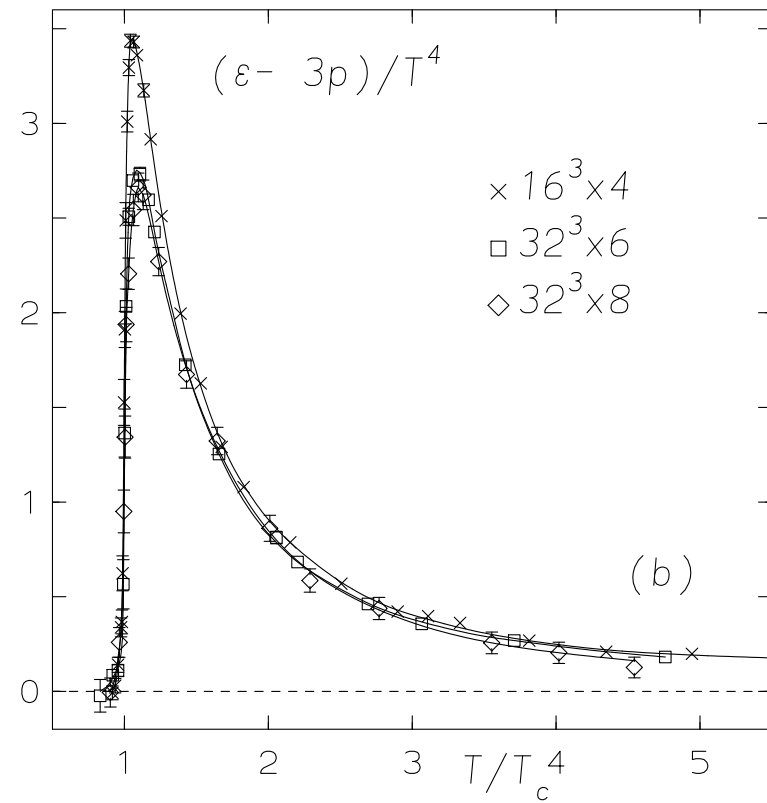
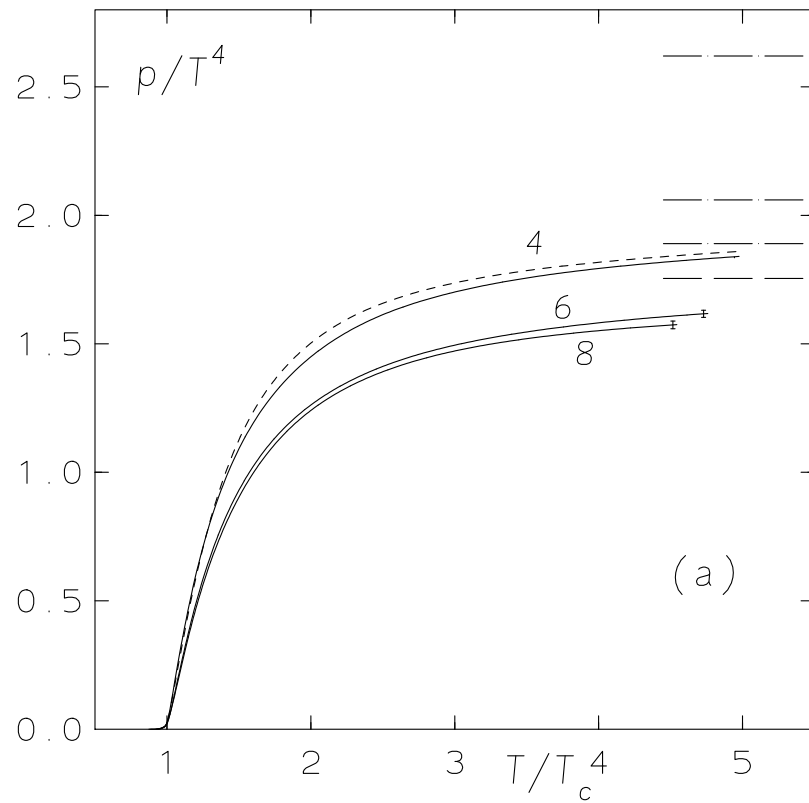
The QCD transition at  $\mu = 0$  as function of quark masses  
 (Columbia plot) from arXiv:1203.5320 Petreczky



The Columbia plot extended into a third direction  $\mu$  : will there be a true phase transition (critical point) for physical quark masses ?  
from Ph. de Forcrand and O. Philipsen hep-lat/0607017

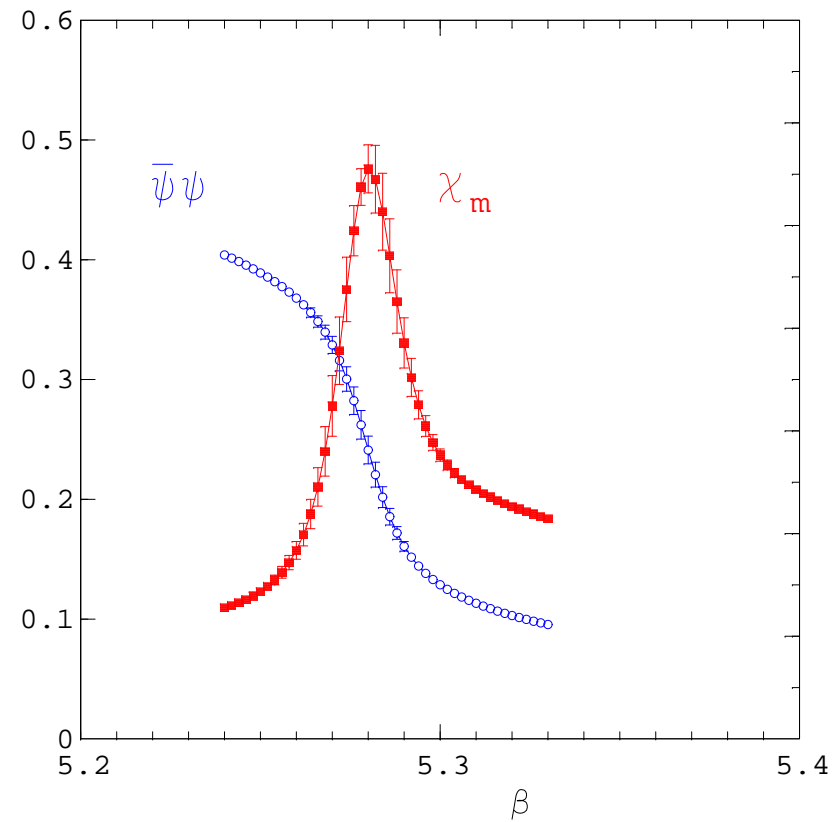
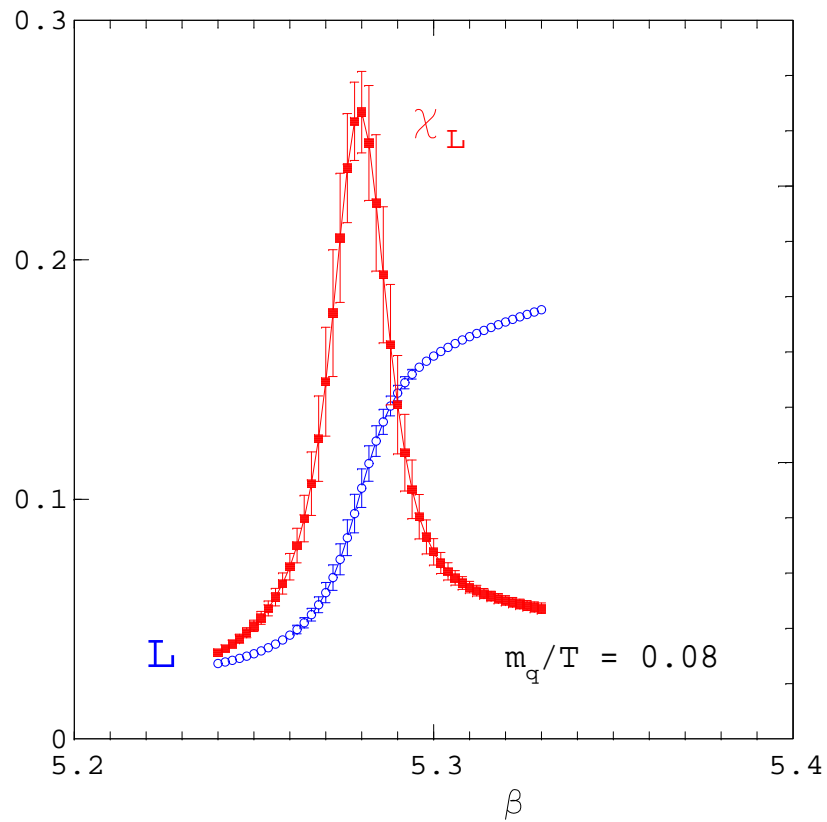


The pressure (left) versus  $T/T_c$  for  $N_t = 4, 6$  and  $8$  in pure gluodynamics.  
The interaction measure of gluons (trace anomaly)  $(\epsilon - 3p)/T^4$  (right).  
from Boyd et al. 1995

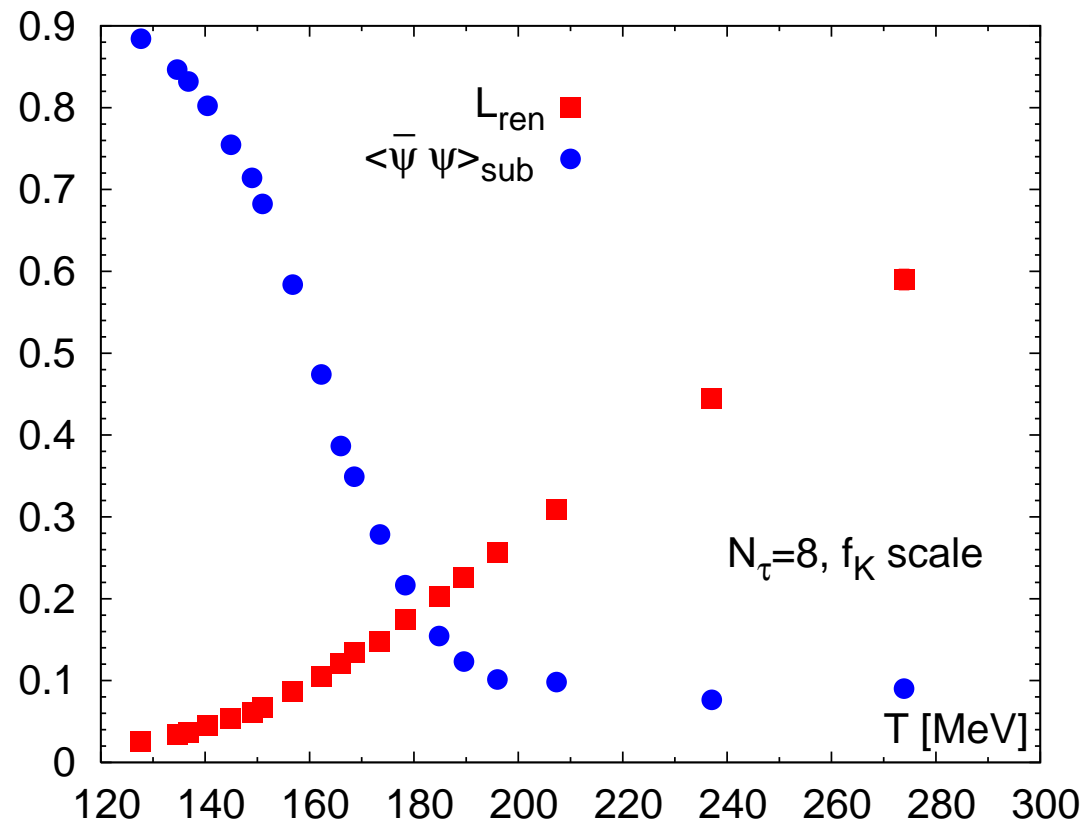




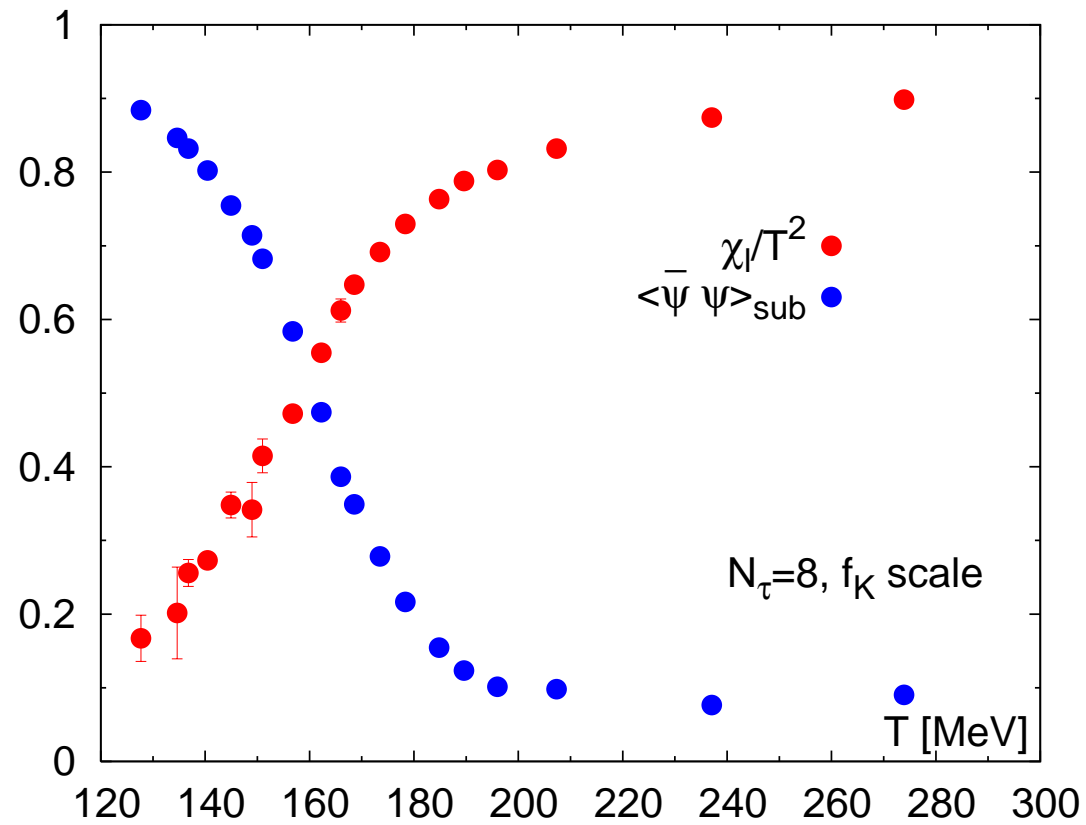
Polyakov loop  $L$  (left) and chiral condensate  $\langle \bar{\psi}\psi \rangle$  (right) together with their susceptibilities show both transitions in two flavour QCD.  
from Karsch et al. 2001



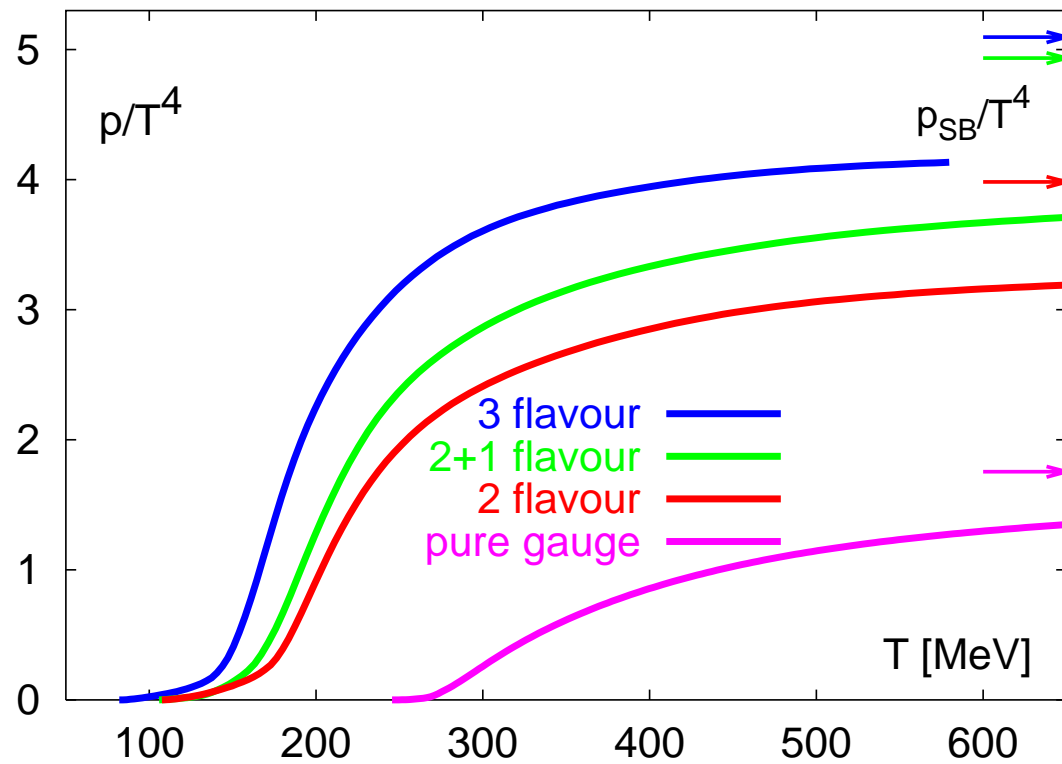
The chiral condensate compared to the renormalized Polyakov loop  
in full QCD from arXiv:1203.5320 Petreczky



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  $U_\mu$  !)

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

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

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

$$\tilde{D}_p = \frac{1}{a_t} \left[ i \frac{a_t}{a_s} \sum_{j=1}^3 \gamma_j \sin(p_j a_s) + i \gamma_4 \sin(p_4 a_t) + a_t m + a_t \mu \gamma_4 \right]$$

$$\ln \det D = \sum_p \text{tr}_{Dirac} \ln \tilde{D}_p$$

$$\frac{\partial}{\partial a_t} \ln \det D_{|\mu a_t = const} = \sum_p \text{tr}_{Dirac} \left[ \frac{\partial}{\partial a_t} \ln \tilde{D}(p) \right]_{|\mu a_t = const}$$

$$\rightarrow C + \sum_p \text{tr}_{Dirac} \left[ (a_t \tilde{D}(q))^{-1} \left( \frac{i}{a_s} \sum_j \gamma_j \sin(p_j a_s) + m \right) \right]$$

with a geometric constant

$$C = -4N_t N_s^3 / a_t$$

Putting finally  $a_t = a_s = a$  , one gets :



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

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

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

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

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

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

→ quadratic divergence with  $a \rightarrow 0$ , 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 :

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

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

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

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

**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 :**

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

**With gauge fields for Kogut-Susskind (“staggered”) fermions :**

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

**With gauge fields and with the Wilson prescription for fermions :**

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

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

“This recipe ( $\mu =$  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

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

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

“For vanishing  $\mu$  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 $\gamma_5$ -hermiticity is spoiled for $\mu_q \neq 0$

Multiplying a hopping term from left and right with  $\gamma_5$  changes the sign of  $\gamma_i$ ; this can be compensated by taking the Hermitean conjugate, thus exchanging  $U$  and  $U^\dagger$ .

The  $e^{+a\mu_q}$  and  $e^{-a\mu_q}$  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  $f = e^{a\mu_q}$

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

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  $\mu_q$  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  $\mu_q = i\eta$ ,  $\eta$  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 :

$$\mu_u = \mu_I \text{ and } \mu_d = -\mu_I.$$

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  $\mu_5$**

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

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

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

with

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

**This satisfies  $\gamma_5$ -hermiticity :  $\gamma_5 D(\mu_5) \gamma_5 = D^\dagger(\mu_5)$**



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  $e$

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

**(f) Gauge group  $SU(2)$**

This group possesses only real representations.

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

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

$$SD(\mu)S^{-1} = D(\mu^*)^*$$

For real  $\mu = \text{one}$  has  $\det D = (\det D)^*$ , i.e.  **$\det D = \text{real}$ , 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  $\mu$ ) **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 !

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

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 :

$$\begin{aligned}
 & \prod_{x,\nu} \exp\left(e^{\mu\delta_{\nu,4}}\phi_x^*\phi_{x+\hat{\nu}}\right) \exp\left(e^{-\mu\delta_{\nu,4}}\phi_x\phi_{x+\hat{\nu}}^*\right) = \\
 & \sum_{\{n,\bar{n}\}} \left( \prod_{x,\nu} \frac{1}{n_{x,\nu}! \bar{n}_{x,\nu}!} \right) \left( \prod_x e^{\mu[n_{x,4}-\bar{n}_{x,4}]} \right) \left( \prod_{x,\nu} \left( \phi_x^*\phi_{x+\hat{\nu}} \right)^{n_{x,\nu}} \left( \phi_x\phi_{x+\hat{\nu}}^* \right)^{\bar{n}_{x,\nu}} \right) \\
 & = \sum_{\{n,\bar{n}\}} \left( \prod_{x,\nu} \frac{1}{n_{x,\nu}! \bar{n}_{x,\nu}!} \right) \left( \prod_x e^{\mu[n_{x,4}-\bar{n}_{x,4}]} \phi_x^{\sum_{\nu}[n_{x,\nu}+\bar{n}_{x-\hat{\nu},\nu}]} \phi_x^* \phi_x^{\sum_{\nu}[\bar{n}_{x,\nu}+n_{x-\hat{\nu},\nu}]} \right),
 \end{aligned}$$

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**  $n_{x,\nu}, \bar{n}_{x,\nu} \in [0, \infty), \dots$

.... in other words, the multiple sum

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

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

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

The integrals over the **angular part**  $\theta_x$  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 :

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

**In this form the complex phase problem is completely eliminated !**

All weight factors for configurations of the  $n$  and  $\bar{n}$  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 !

This way the model is “decontaminated” from the sign problem !

However, many configurations of  $n$  and  $\bar{n}$  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

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

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

In the current representation the **constraints mix  $n$  and  $\bar{n}$  variables.**

The structure of the constraints can be simplified by **introducing new variables**  $k_{x,\nu} \in (-\infty, \infty)$  and  $l_{x,\nu} \in [0, \infty)$  which are related to the old variables by

$$n_{x,\nu} - \bar{n}_{x,\nu} = k_{x,\nu} \quad (\text{net current}) \quad \text{and} \quad n_{x,\nu} + \bar{n}_{x,\nu} = |k_{x,\nu}| + 2l_{x,\nu}$$

**The partition function turns into**

$$Z = \sum_{\{k,l\}} \left( \prod_{x,\nu} \frac{1}{(|k_{x,\nu}| + l_{x,\nu})! l_{x,\nu}!} \right) \left( \prod_x \delta \left( \sum_{\nu} [k_{x,\nu} - k_{x-\hat{\nu},\nu}] \right) \right) \\ \times \left( \prod_x e^{\mu k_{x,4}} W \left( \sum_{\nu} [ |k_{x,\nu}| + |k_{x-\hat{\nu},\nu}| + 2(l_{x,\nu} + l_{x-\hat{\nu},\nu}) ] \right) \right)$$

**This is the suitable flux representation for the  $\phi^4$  theory !**

The constraints no longer mix the two types of flux variables.

Obviously **only the  $k$ -fluxes** (net charge) are subject to **conservation of flux**, i.e., only these variables must **obey the absence of divergence**

$$(\nabla k)(x) = \sum_{\nu} (k_{x,\nu} - k_{x-\hat{\nu},\nu}) = 0$$

for all sites  $x$ .

**The Monte Carlo update should consist of simultaneous moves**

$$n_{x,nu} \rightarrow n'_{x,\nu} \quad \text{and} \quad \bar{n}_{x,\nu} \rightarrow \bar{n}'_{x,\nu}$$

such the constraints are respected. The product

$$\prod_x (e^{\mu k_x} W(\dots))$$

over all sites  $x$ , where an update is attempted, is then subject to the **Metropolis check**.



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.

A suitable algorithm for the  $\phi^4$  theory is the following :

In the present model we have two different sets of variables (integer-valued), that can be updated in alternating order :

1. step : update of  $l_{x,\nu}$  has no constraints :

simple Metropolis algorithm

- visit each link  $(x, \nu)$ ;
- increase or decrease  $l_{x,\nu}$  by  $\pm 1$  with equal probability;
- accept (or reject) the change according to the usual Metropolis probability (the ratio of the weights of new and old configuration);
- negative  $l_{x,\nu}$  is always rejected.

## 2. step : update of $k_{x,\nu}$ with account of the local constraints

$\sum_{\nu}[k_{x,\nu} - k_{x-\hat{\nu},\nu}] = 0$  : by a generalization of the PS worm algorithm

- start the worm at a randomly chosen site of the lattice;
- let the worm grow by a random walk to form a chain of links: at given position  $x$  the worm chooses randomly the next link among the 8 links attached to  $x$ ;
- for the chosen link the algorithm proposes to change the old variable  $k$  by  $\pm 1$ , which is accepted (or not) through a Metropolis check;
- since at the starting point (tail) and at the head of the worm the constraint is violated, the worm must continue until its head reaches (“bites”) the tail;
- only then, along the closed contour of changed links, the constraints are intact again (as before the sweep).

- A possible **initial configuration** for the  $k_{x,\nu}$  is to set  $k_{x,\nu} = 0$  at all links, a configuration that obviously satisfies the constraints.

The local weight for a variable  $k_{x,\nu}$  depends on variables that are defined

- **on the link:** the factorials in  $1/(|k_{x,\nu}| + l_{x,\nu})!$  and the contribution from the chemical potential (before and after update);
- **on the endpoints:**  $W(f_x)$  and  $W(f_{x+\hat{\nu}})$  (where again  $f_x = \sum_{\nu} [ |k_{x,\nu}| + |k_{x-\hat{\nu},\nu}| + 2(l_{x,\nu} + l_{x-\hat{\nu},\nu}) ]$ ). These arguments of the factors  $W$  at the endpoints of the link have to be updated as well (the functions  $W$  are precalculated and tabulated).

## A typical example of practical run parameters

- A full sweep includes :
  - one sweep for  $l_{x,\nu}$
  - one worm growing until it bites the tail
- Number of full sweeps between measurements : 5
- Number of measurements : 500.000 to 1.000.000
- Number of additional equilibration sweeps : 25.000

## Observables

$$n = \frac{T \partial \ln Z}{V \partial \mu} = \frac{1}{N_s^3 N_t} \frac{\partial \ln Z}{\partial \mu}, \quad \chi_n = \frac{\partial n}{\partial \mu}, \quad \chi'_n = \frac{\partial \chi_n}{\partial \mu}$$
$$\langle |\phi|^2 \rangle = \frac{-T \partial \ln Z}{V \partial \kappa} = \frac{-1}{N_s^3 N_t} \frac{\partial \ln Z}{\partial \kappa}, \quad \chi_{|\phi|^2} = \frac{-\partial \langle |\phi|^2 \rangle}{\partial \kappa}, \quad \chi'_{|\phi|^2} = \frac{\partial \chi_{|\phi|^2}}{\partial \mu}$$

The primary observables  $n$  and  $\langle |\phi|^2 \rangle$  can be easily expressed directly by flux variables or assessed through (ratios of) the weight function :

$$n = \frac{1}{N_s^3 N_t} \left\langle \sum_x k_{x,4} \right\rangle$$
$$\langle |\phi|^2 \rangle = \frac{1}{N_s^3 N_t} \left\langle \sum_x \frac{W(f_x + 2)}{W(f_x)} \right\rangle$$

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  $\mu$  :

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

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

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

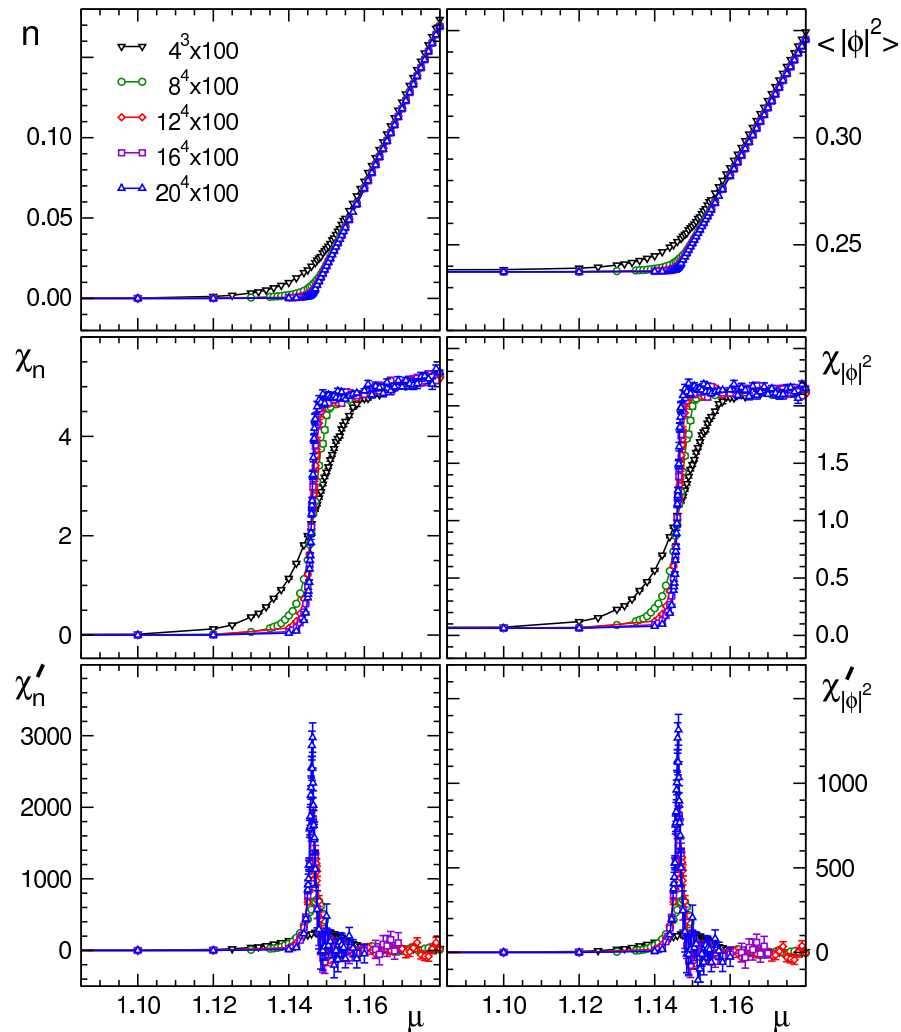
At  $T > 0$  (shorter lattice in time direction,  $N_t < N_s$ ),  
a weaker **pseudo silver blaze effect** is observed :

- a weak dependence on  $\mu$  begins below  $\mu_c$
- there is a “threshold value”  $\mu_{onset}$  which rises with  $T$   
relative to  $\mu_c$  at  $T = 0$ .



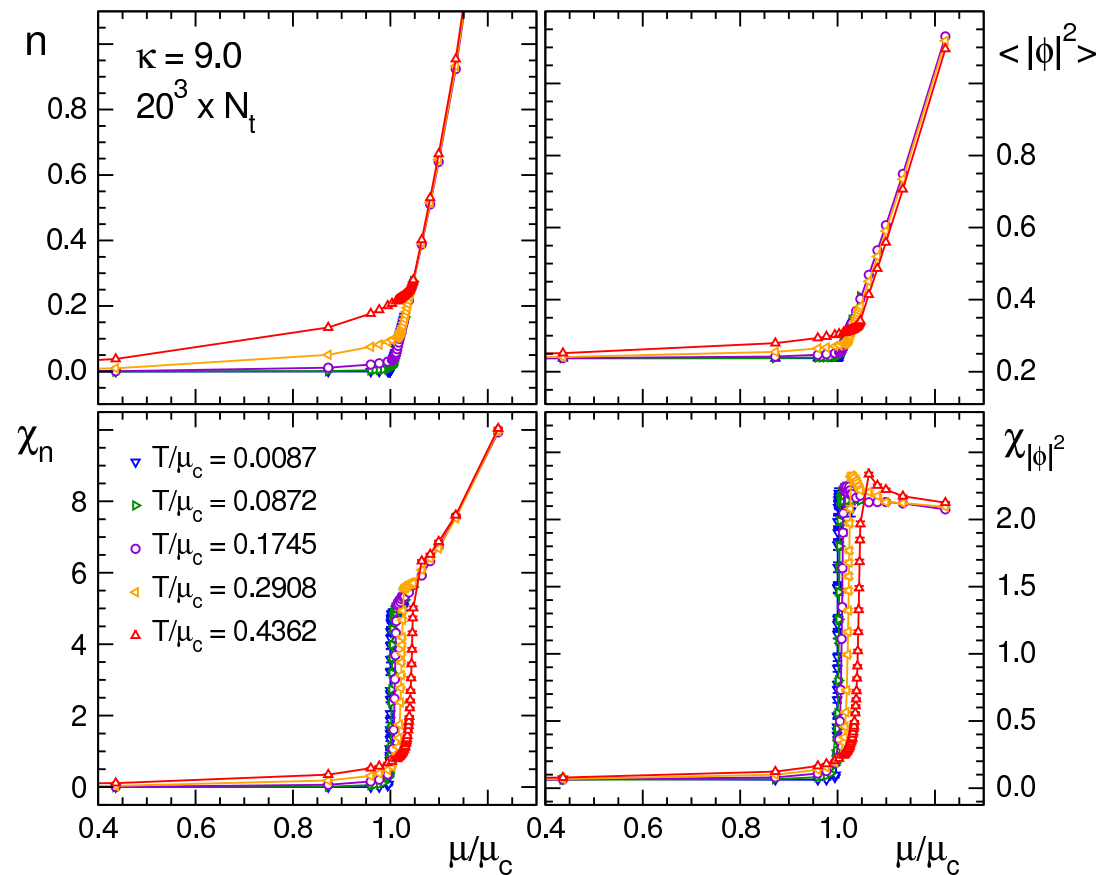
# Silver blaze effect at very low temperature

from arXiv:1206.2954 Gattringer and Kloiber



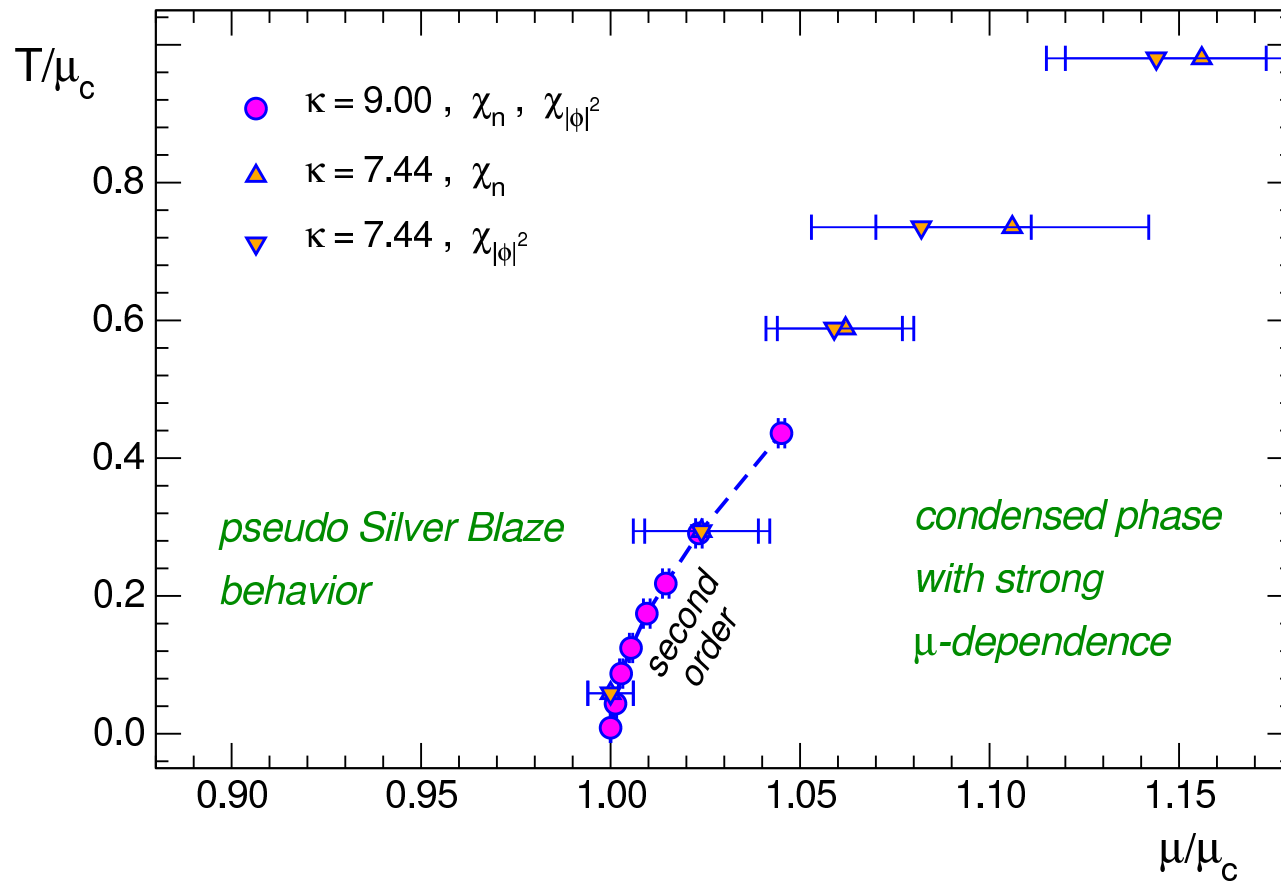
What remains from the Silver blaze effect at higher temperature ?

from arXiv:1206.2954 Gattringer and Kloiber



# Phase structure in the $T$ - $\mu$ 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.”

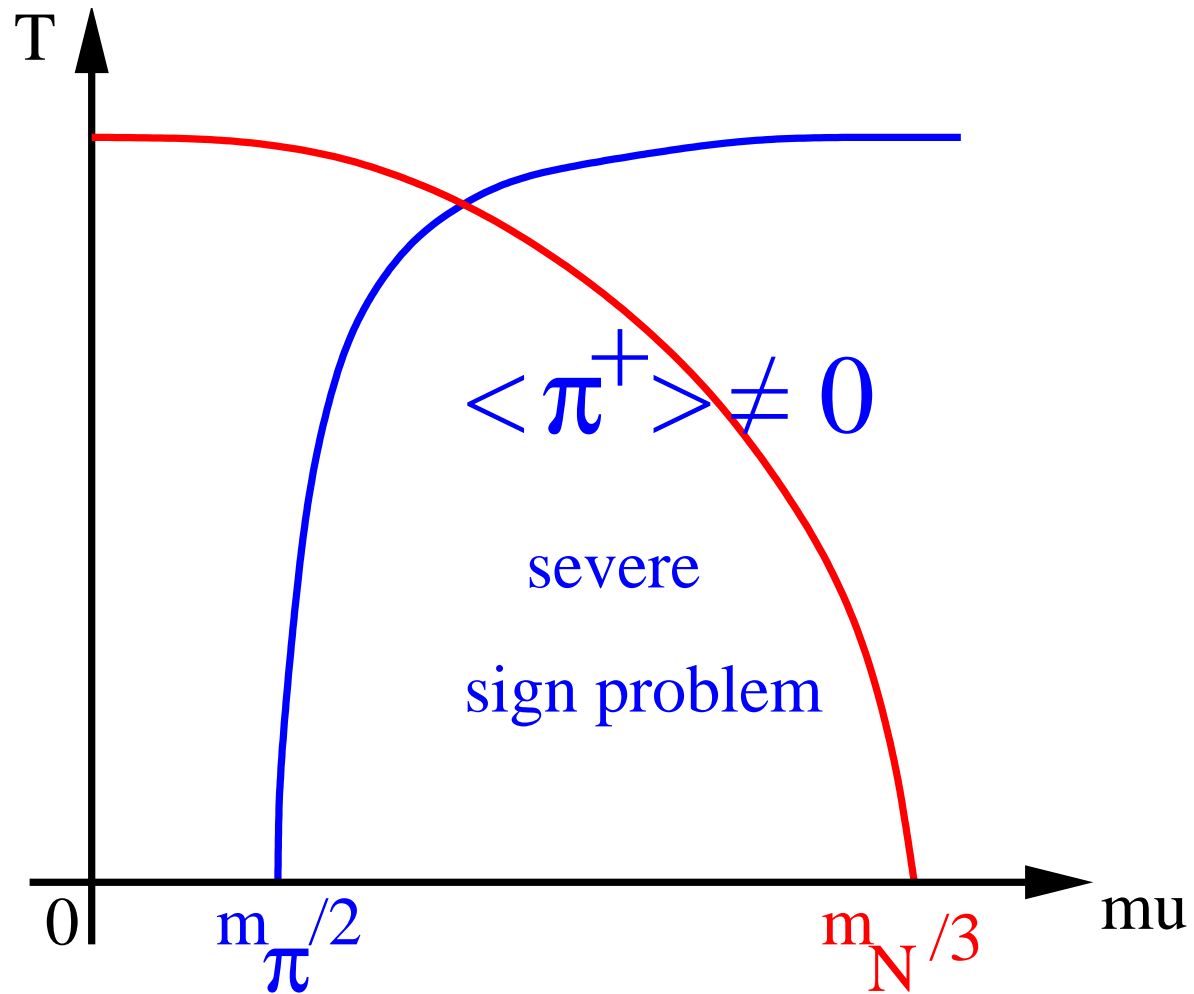
This is sometimes called

**“Duality transformation”** (from one representation to the other.)

## 4. Fighting the Complex Measure Problem in Standard LGT

- General Remarks
- Reweighting across the  $\beta$ - $\mu$  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  $N_f \rightarrow 0$  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.

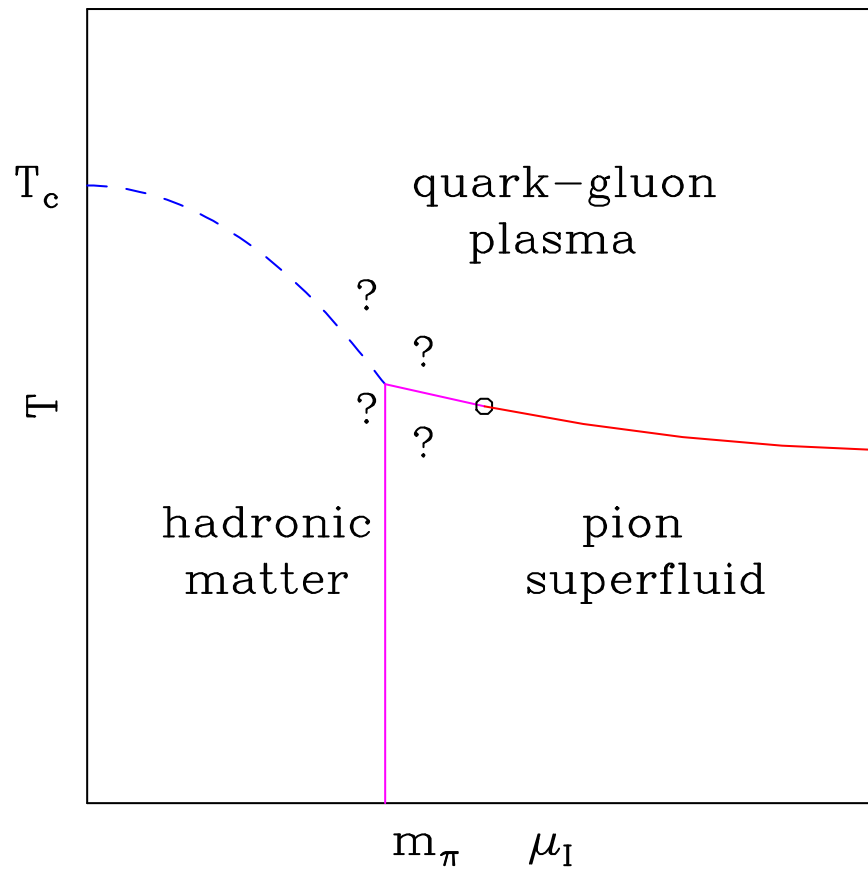
But the phase of the determinant is particularly important !

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  $\pi$  condensation**, where  $\mu$  acts actually as  $\mu_I$ .



# Schematic phase diagram for QCD at finite isospin density from Philipsen

$N_f=2$  QCD at finite isospin density



“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  $\det D e^{-S_G} D[U]$  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:

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

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

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

Consider a toy model of an oscillating measure :

$$Z(\lambda) = \int_{-\infty}^{+\infty} dx e^{-x^2+i\lambda x}$$

Since the result is real, consider also the real part of the integrand,

$$e^{-x^2} \cos(\lambda x)$$

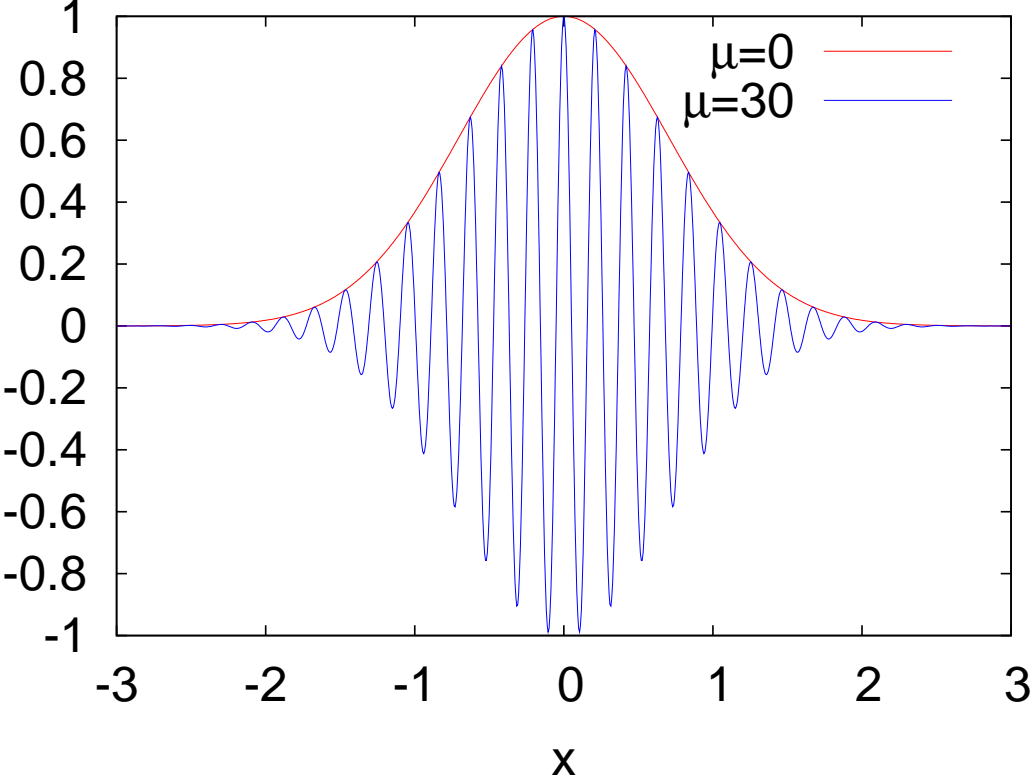
As soon as  $\lambda \neq 0$ , important values of  $x$  are not only those  $x \approx 0$ .

**The size of the important region is dictated by  $\lambda$ , not alone by the Gaussian's width.**

Restricting the integral to a finite interval  $x \in [-\lambda, \lambda]$  will give  $\mathcal{O}(100\%)$  error. The integral must be extended into the tail region in order to reproduce the result  $Z(\lambda)/Z(0) = e^{-\lambda^2/4}$  with reasonable accuracy.

**“In simulations at  $\mu \neq 0$  all configurations are potentially important !”**

# 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

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

.

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** :

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

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 !).

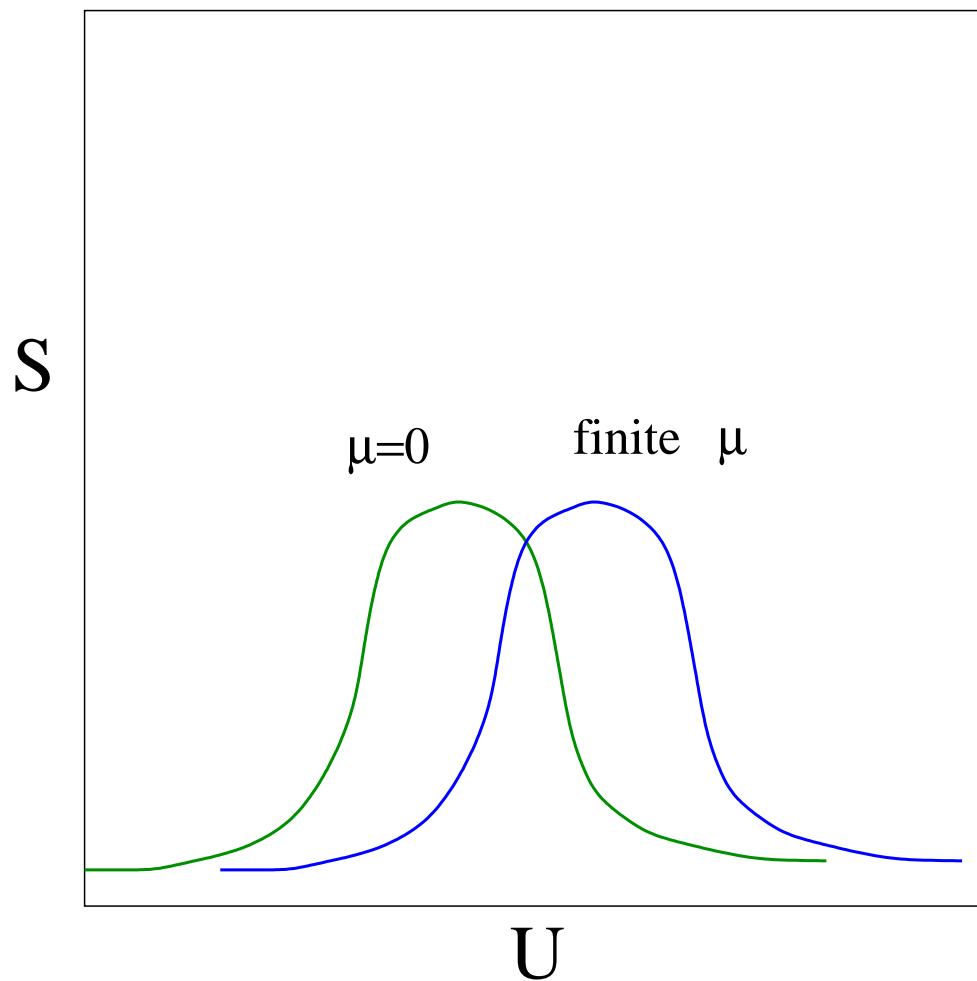
Then, one needs **exponentially large statistics** to get reliable results.

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  $\mu$ )



## 4. 2. Reweighting across the $\beta$ - $\mu$ Plane : Determinants

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

**Exact partition function :**

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

Now factorize the determinant into **modulus and phase factor :**

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

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

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

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

The next choice is :

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

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  $\mu$  would be considered as isospin chemical potential  $\mu = \mu_I$**

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

Standard reweighting approach seems to suggest for sampling :

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

Then the reweighting factor function is :

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

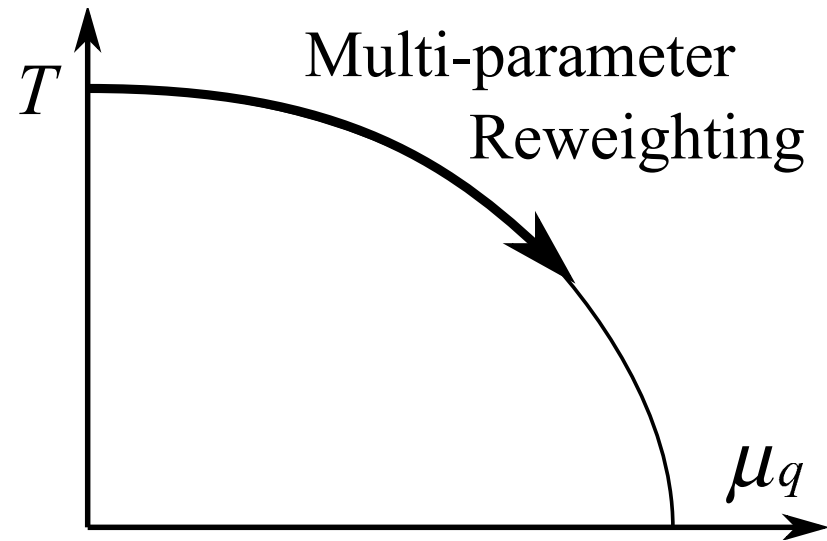
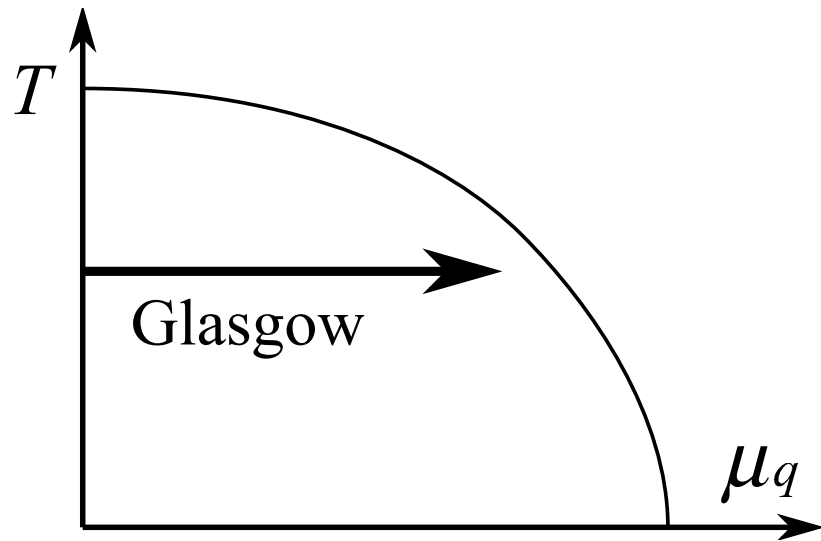
It has to be **evaluated together with the evaluation of the observables** in order to calculate finally the correlator with  $O$  and the average sign :

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

Historically, this technique has been practiced within two variants :

- **horizontal reweighting** (“Glasgow method”) at  $\beta' = \beta$  fixed
- **multiparameter reweighting** (Budapest Fodor/Katz) : this method actually explores the region in  $\beta$ - $\mu$  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  $\mu$ -dependence into two time slices
- factorization of the  $\mu$ -dependence

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

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

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

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

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”  $\alpha$  :

$\alpha$  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  $\alpha$  in the  $\beta - \mu$  plane show clearly, where one can rely on reweighting.

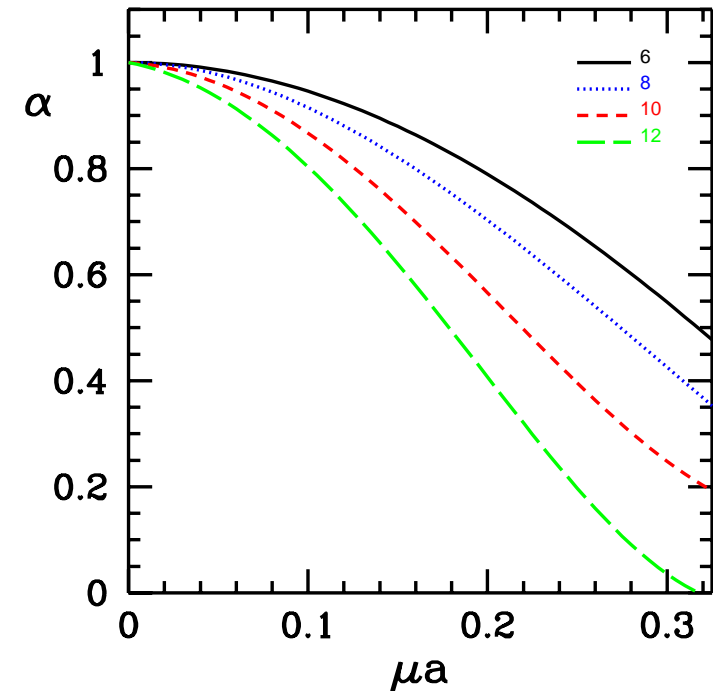
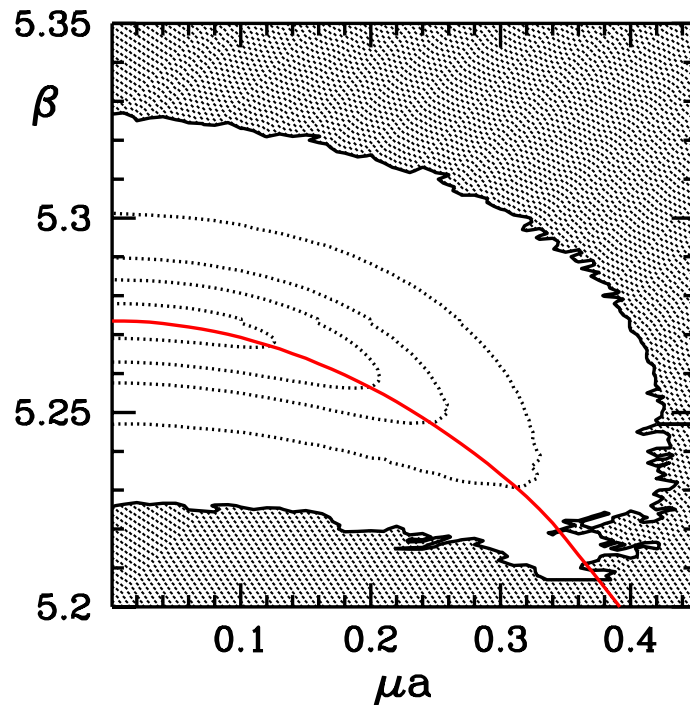
The grey area is not accessible by reweighting from  $\beta_c$  at  $\mu = 0$ .

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

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

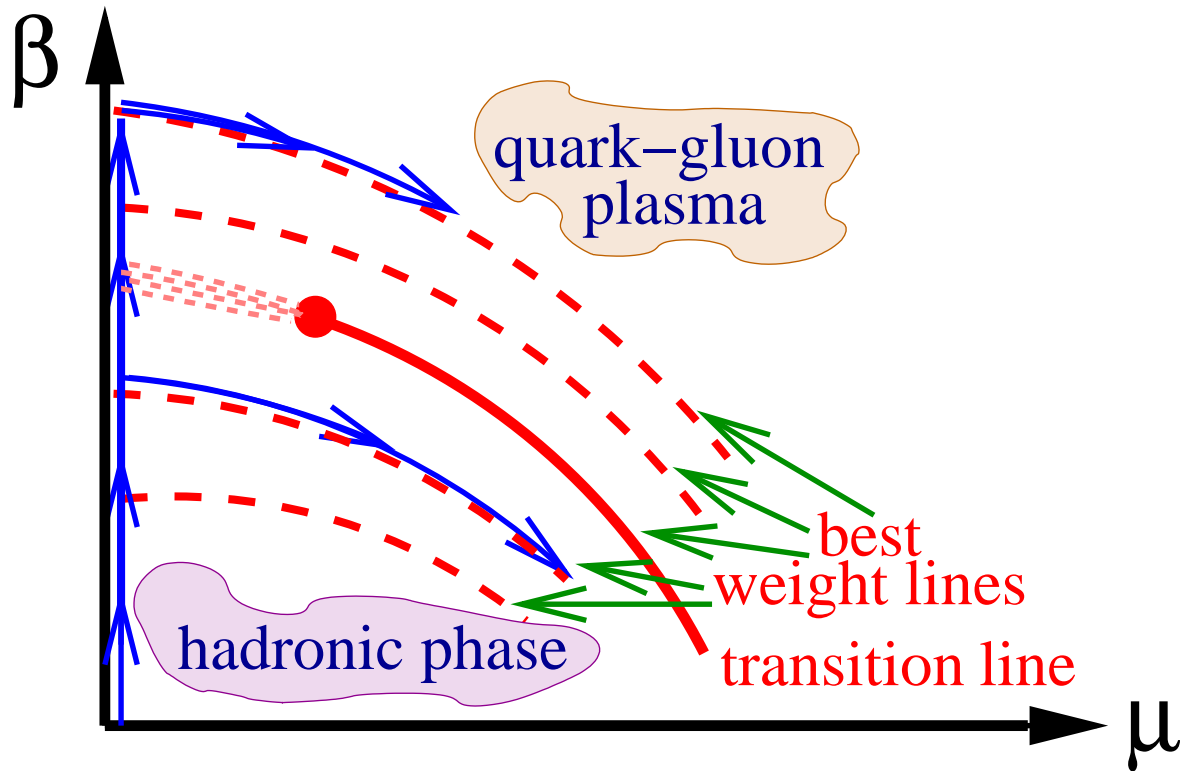


Left: Contour plots of the overlap measure; the red line (line of the cross-over) is determined by the peaks of susceptibility. Right: volume and  $\mu$  dependence of the overlap measure. The half width ( $\mu_{1/2}$ ; defined by  $\alpha = 1/2$ ) shrinks according to:  $\mu_{1/2} \propto V^{-\gamma}$  with  $\gamma \approx 1/3$ .  
 from F. Csikor et al. hep-lat/0401016



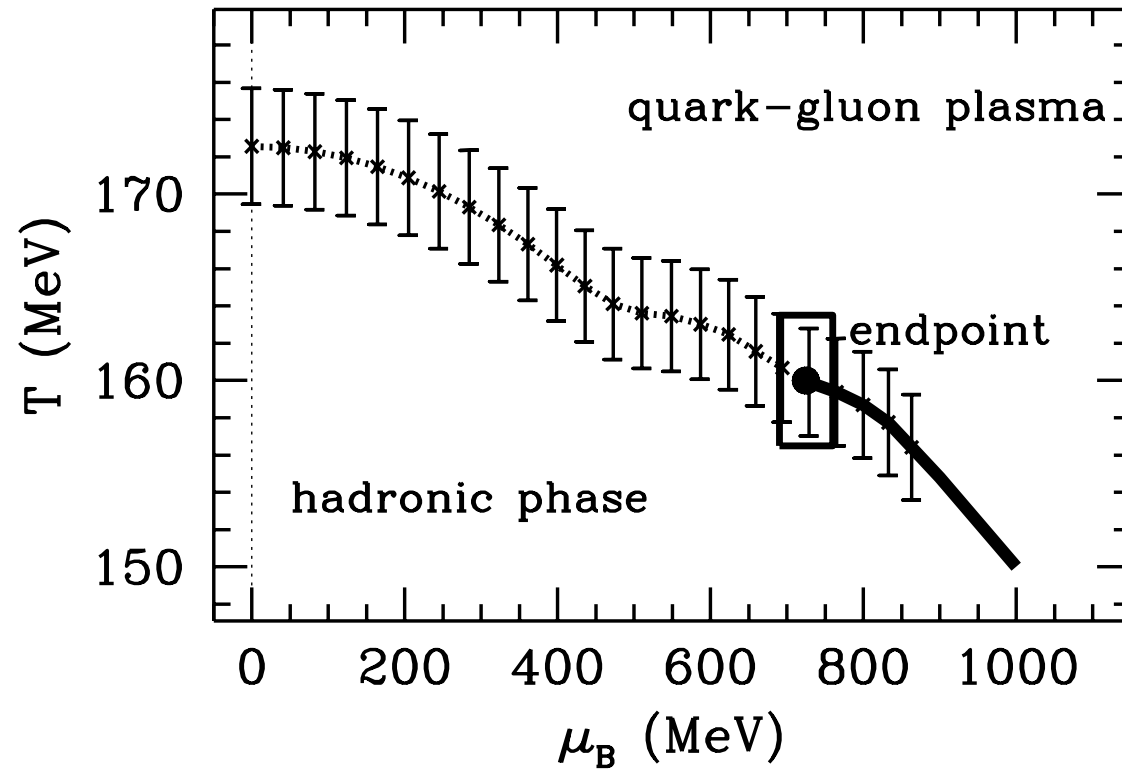
## Best paths for reweighting

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



## Finding the Line of the Crossover

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



Adding an imaginary part to  $\beta$  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  $V \rightarrow \infty$  approach the real axis this signals that a real singularity (phase transition) appears.

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

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

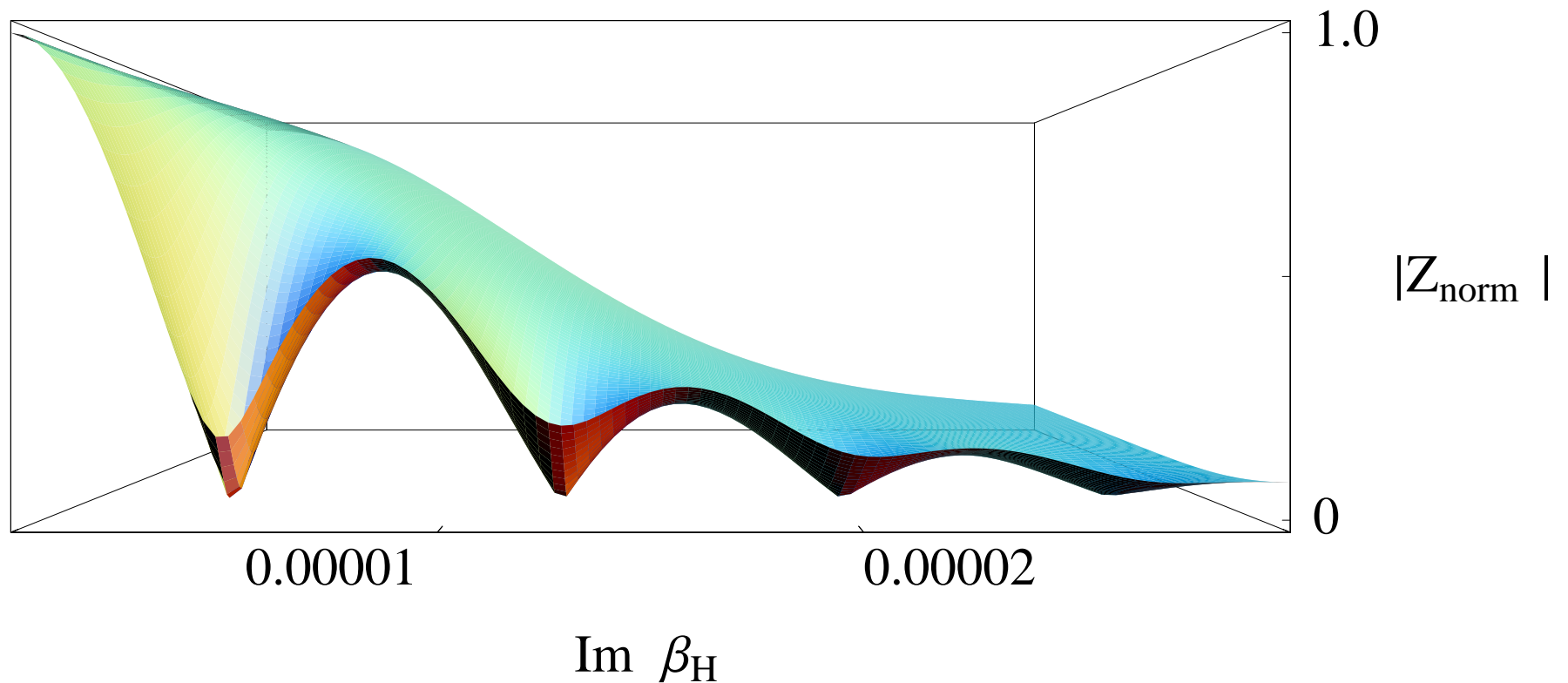
**This fixes the critical endpoint : F. Csikor et al. hep-lat/0301027**

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

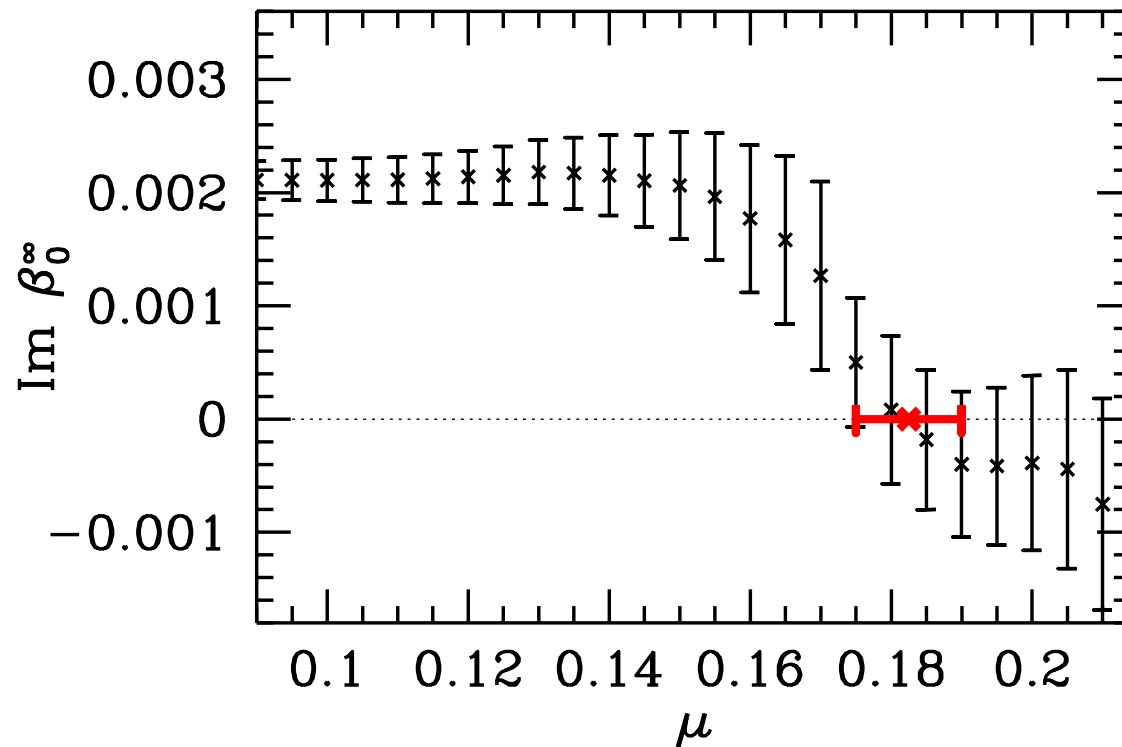
$$\mu_B^E = 725 \pm 35 \text{ MeV} \quad T^E \approx 160 \pm 3.5 \text{ MeV} \quad T_c(\mu = 0) = 172 \pm 3 \text{ MeV}$$

**(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  $V \rightarrow \infty$ ) ( $\text{Im } \beta_{LY}^{(0)}$ ) in the complex  $\beta$  plane.  
from Z. Fodor and S. D. Katz hep-lat/0111064



**An important cross-check for the different methods :**

At **imaginary  $\mu$ , 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 :**

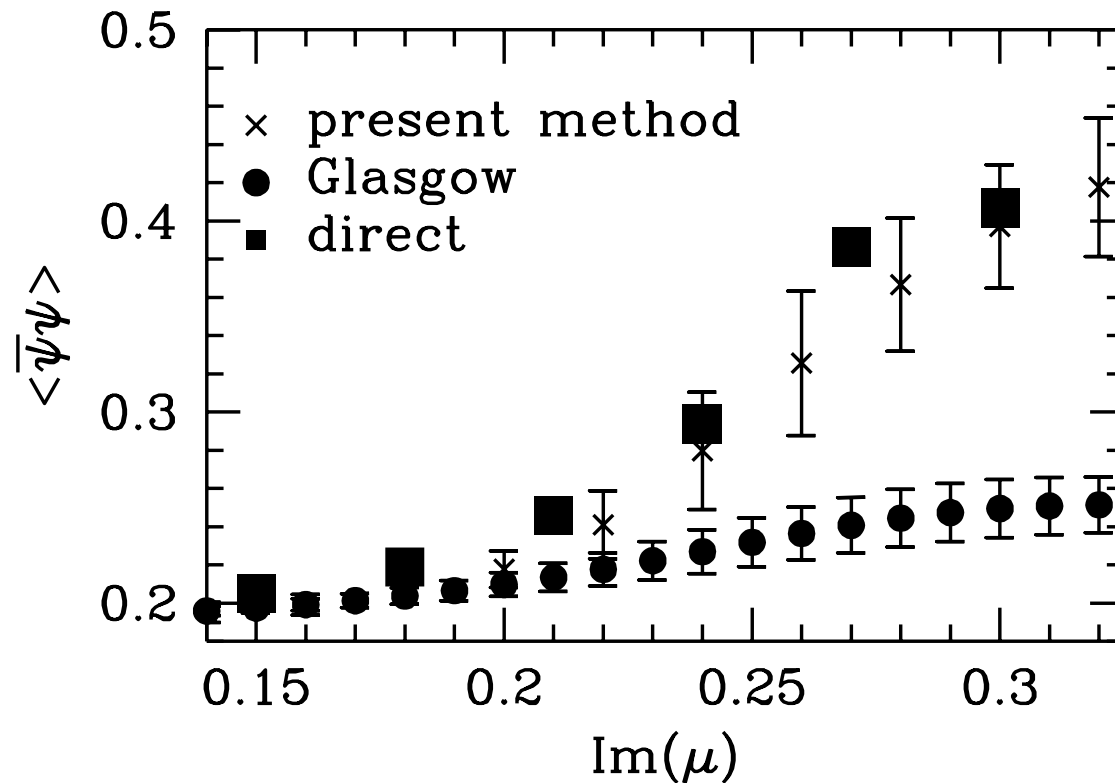
**For imaginary  $\mu$  the chiral condensate  $\langle \bar{\psi}\psi \rangle$  should grow !**

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



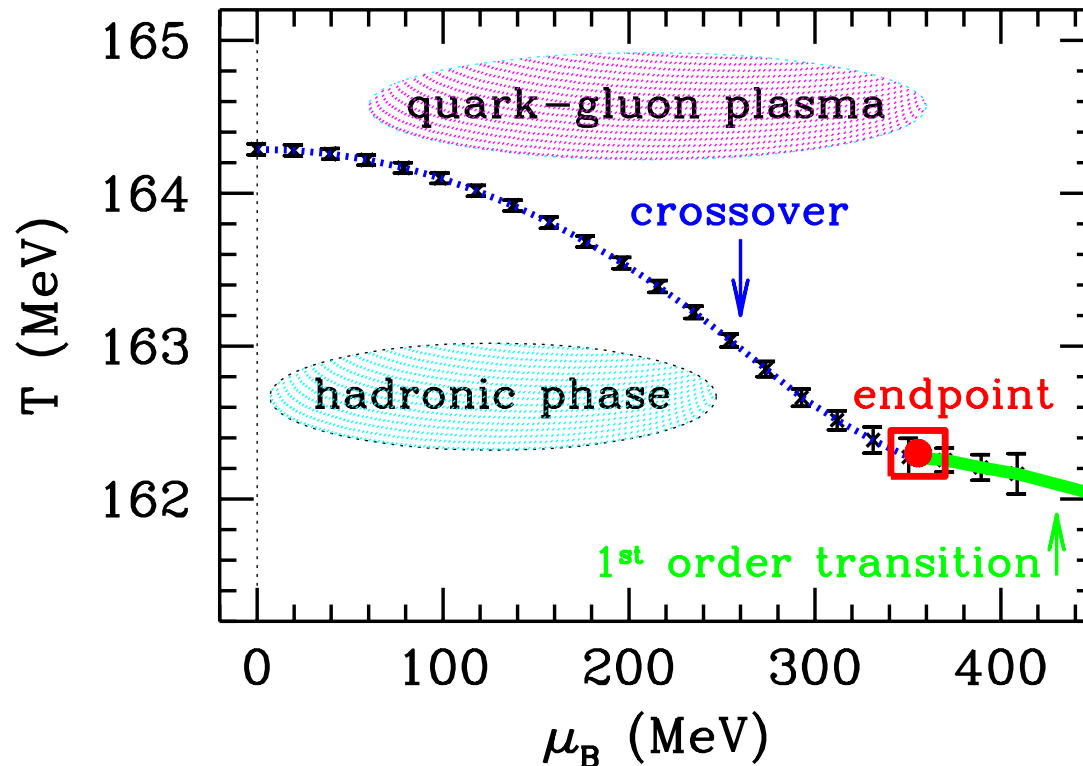
# Testing the Method at Imaginary $\mu$ by Comparison with Direct Simulation. Failure of the Glasgow method due to the Overlap Problem.

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

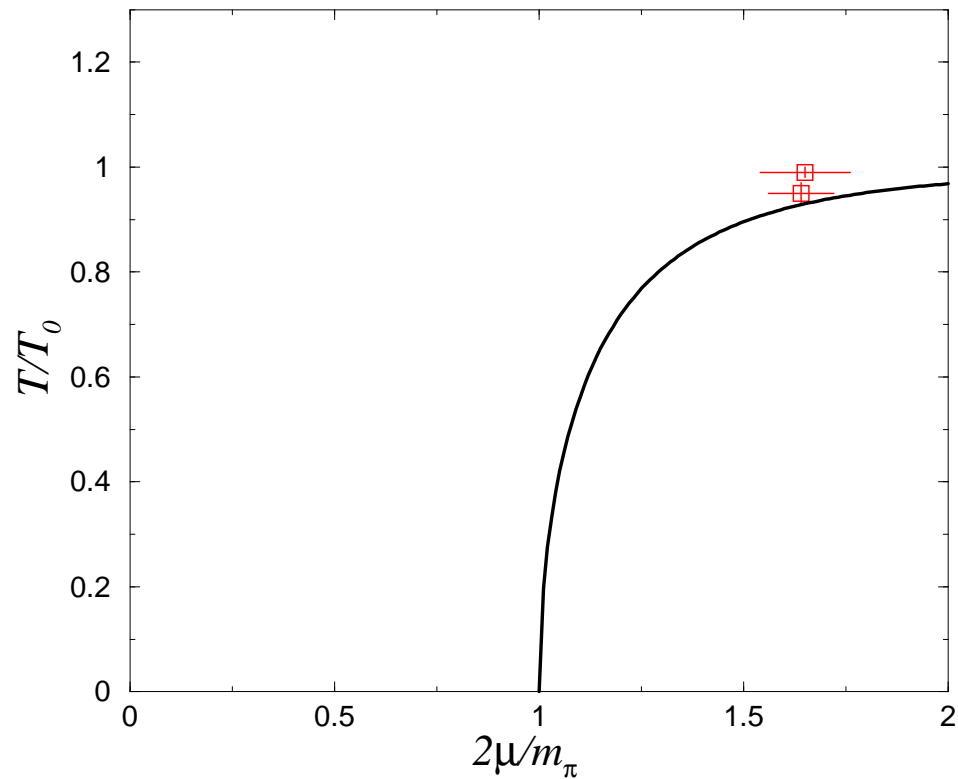


Compared to the previous finding, the light quark masses had been reduced by a factor three, while the largest volume has been increased by a factor three.

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 :

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

The reference ensemble is the isospin- $\mu$  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

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

$B$  stands for “baryonic chemical potential”  $\mu$ .

The **phase quenched partition function** (subscript  $I$ , since this would be correct for the “isospin chemical potential”  $\mu$ )

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

Distinguish the **two “expectation values” of  $\mathcal{O}$**  :

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

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

Each of the **two determinants involved have the decomposition** :

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

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

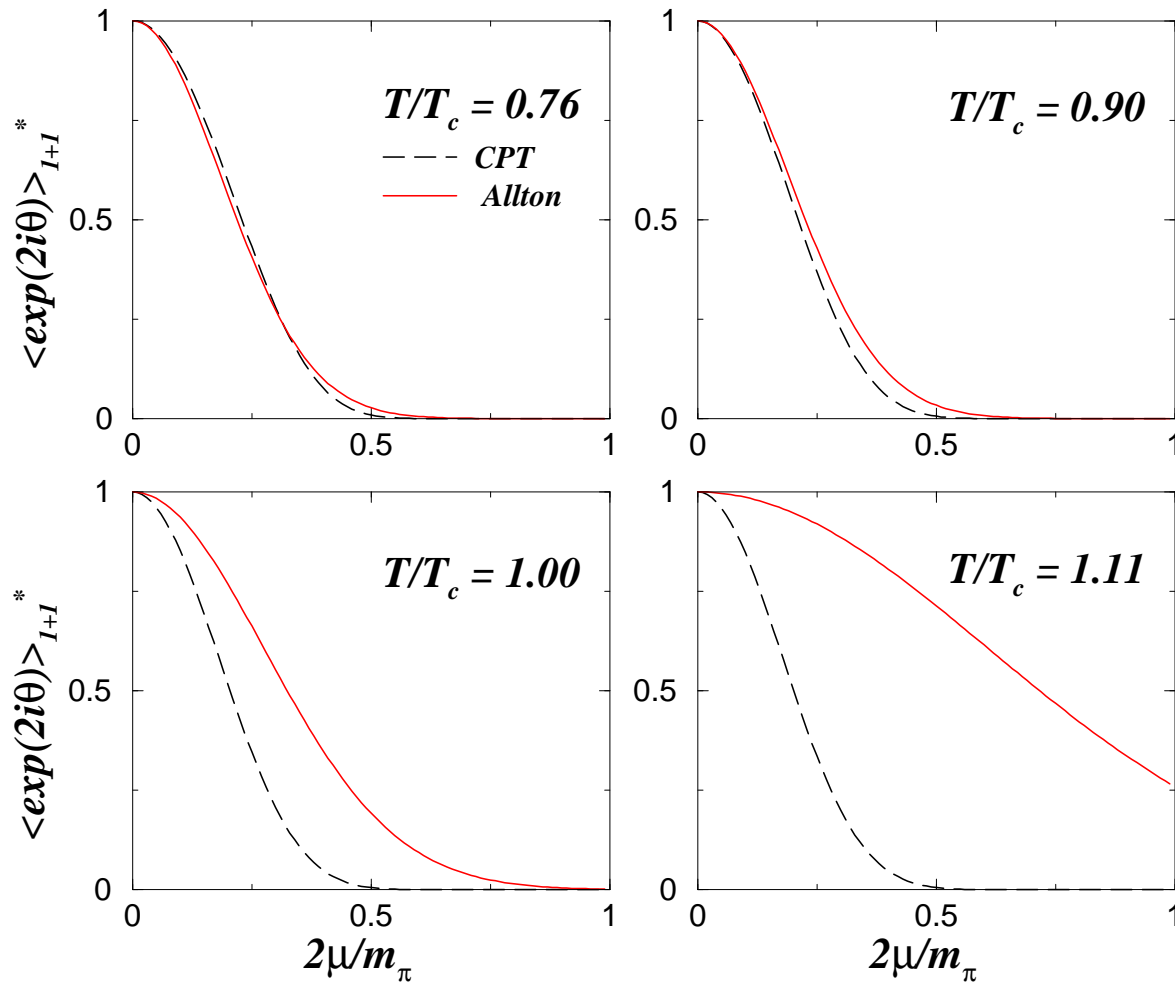
Although  $\langle \mathcal{O} \rangle_B$  **cannot be directly calculated** by importance sampling, it **can be estimated as follows** (with  $N_f = 2$ )

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

**Numerator and denominator are both based on a phase-quenched simulation (subscript  $I$ )**. The phase factor  $e^{2i\Theta}$  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”  $\langle \exp(2i\theta) \rangle_{I+1}^*$  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  $\mu/T$ .
- Reweighting gives  $\mu$ -dependence (in principle, at least).
- In fact, reweighting is **restricted to small  $\mu/T$  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  $\mu/T$ .**

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

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

$\Delta p$  is an even function of  $\mu/T$  (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.  $\mu$  of the determinant, more precisely

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

Therefore

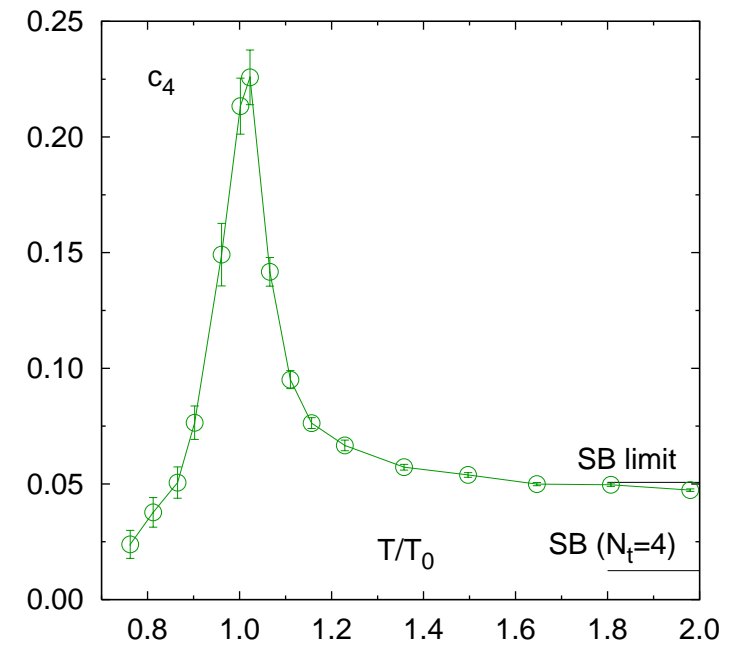
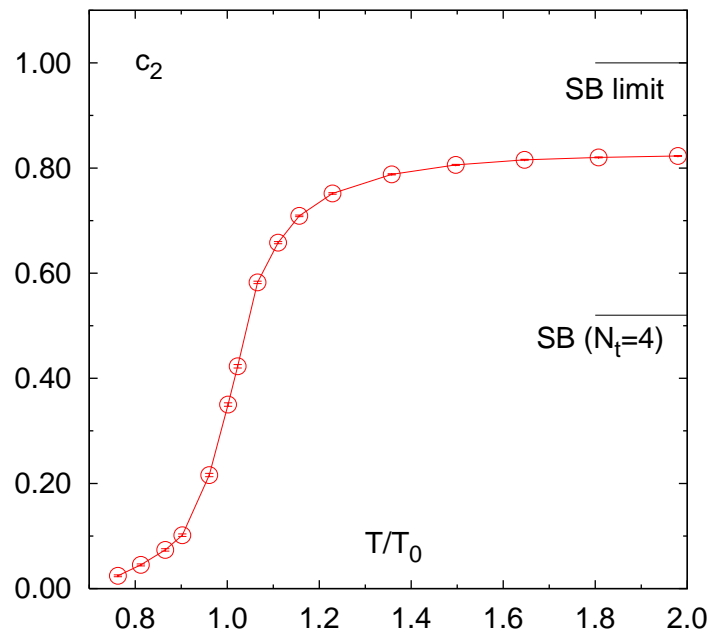
$$c_{2k} = \left\langle \text{tr} \left( \text{polynomial of order } 2k \text{ in } D^{-1} \text{ and } \frac{\partial D}{\partial \mu} \right) \right\rangle_{|\mu=0}$$

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

These observables become increasingly noisy with larger  $k$ .

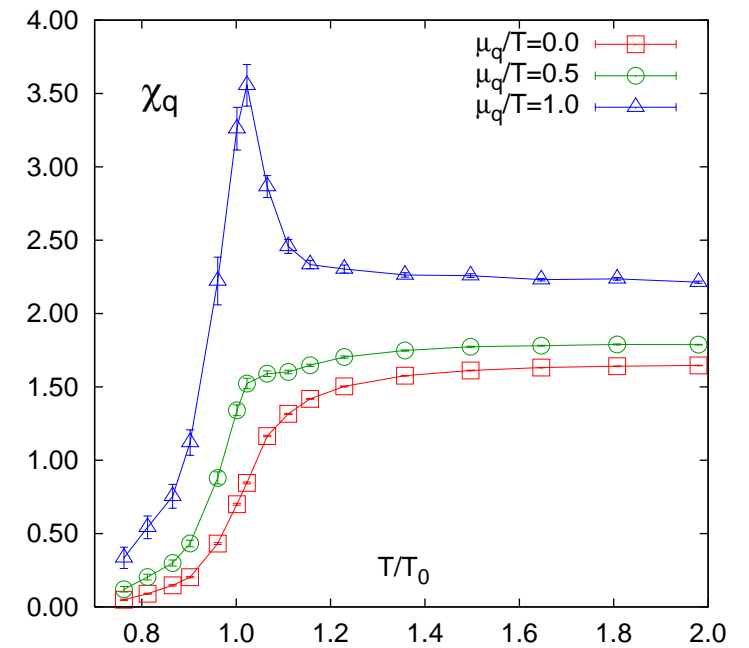
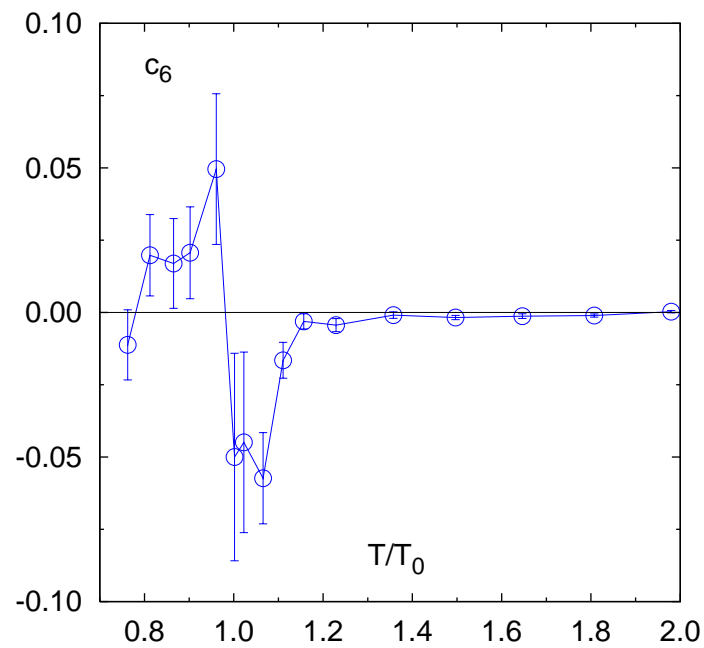
The first two Taylor coefficients  $c_2$  and  $c_4$  as functions of temperature look very nice.

from Ch. Schmidt hep-lat/0610116



The Taylor coefficient  $c_6$  and the quark number susceptibility  $\chi_q$  (for three values of  $\mu$ ), 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  $(\mu_c^E, T_c^E)$

For **all bulk quantities similar** series expansions exist :

$$\frac{n_q}{T^3} = 2c_2 \frac{\mu}{T} + 4c_4 \left(\frac{\mu}{T}\right)^3 + 6c_6 \left(\frac{\mu}{T}\right)^5 + \dots$$
$$\frac{\chi_q}{T^2} = 2c_2 + 12c_4 \left(\frac{\mu}{T}\right)^2 + 30c_6 \left(\frac{\mu}{T}\right)^4 + \dots$$

Going to higher density (higher  $\mu/T$ ) 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:

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

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

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

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

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



Meaning of the first two expansion coefficients for some charge  $X$  :

$$2c_2^X = \frac{1}{VT^3} \langle N_X^2 \rangle$$
$$24c_4^X = \frac{1}{VT^3} (\langle N_X^4 \rangle - 3\langle N_X^2 \rangle^2)$$

This is variance and kurtosis.

## 4. 5. Continuation from Imaginary Chemical Potential

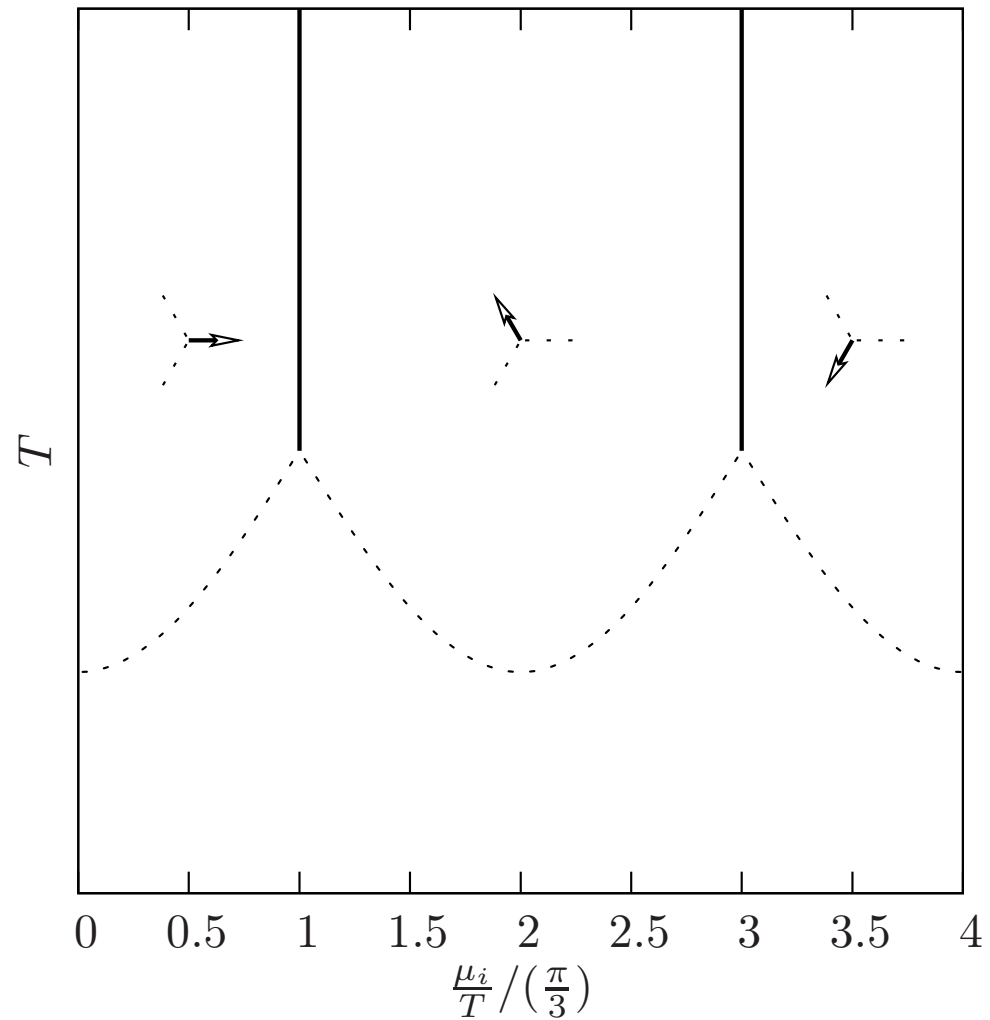
This case is **accessible for normal importance sampling**.

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 from  $\mu = 0$ , the phase transition line (dotted line) bends upward (contrary to downward at real  $\mu$ ).
- The nature of this phase transition is a “continuation” of the physical phase transition at real  $\mu$ .
- For quark masses  $> \mathcal{O}(3 \text{ GeV})$  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  $\mu$ , 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  $\Theta = i\eta_Q$**

through a factor

$$\text{weight} \propto \exp(\eta_Q Q)$$

with the topological charge

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

causes considerable **squeezing of topological charge**.

**Simulations at imaginary  $\Theta$  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  $\eta/T$  with a period of  $2\pi/3$ .

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

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

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

(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** :

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

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  $Z_C(T, n)$ .**

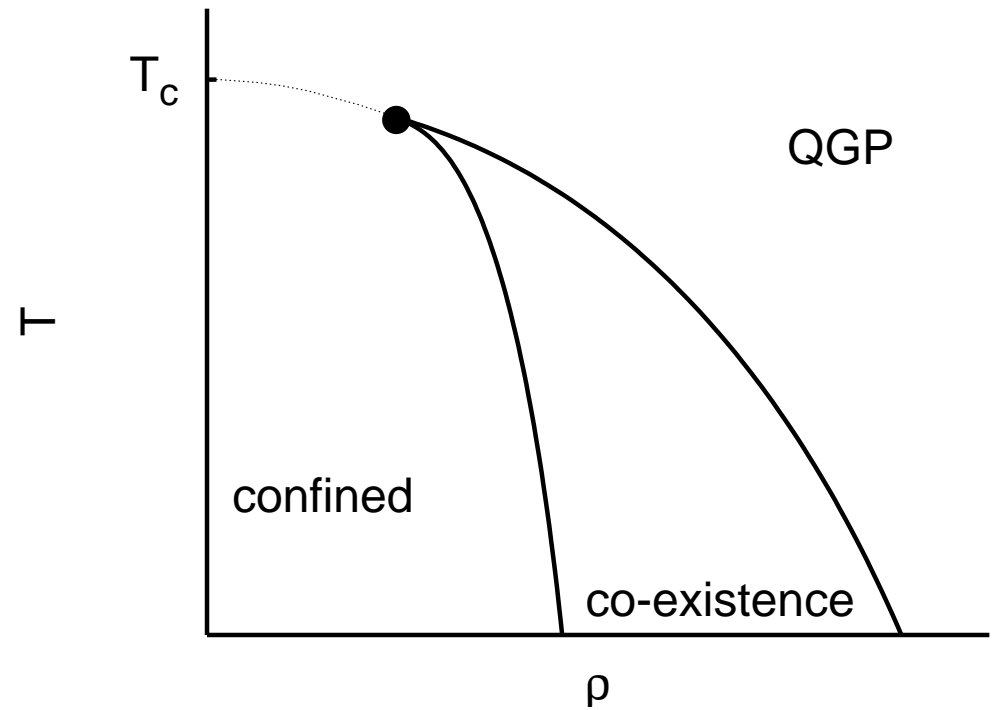
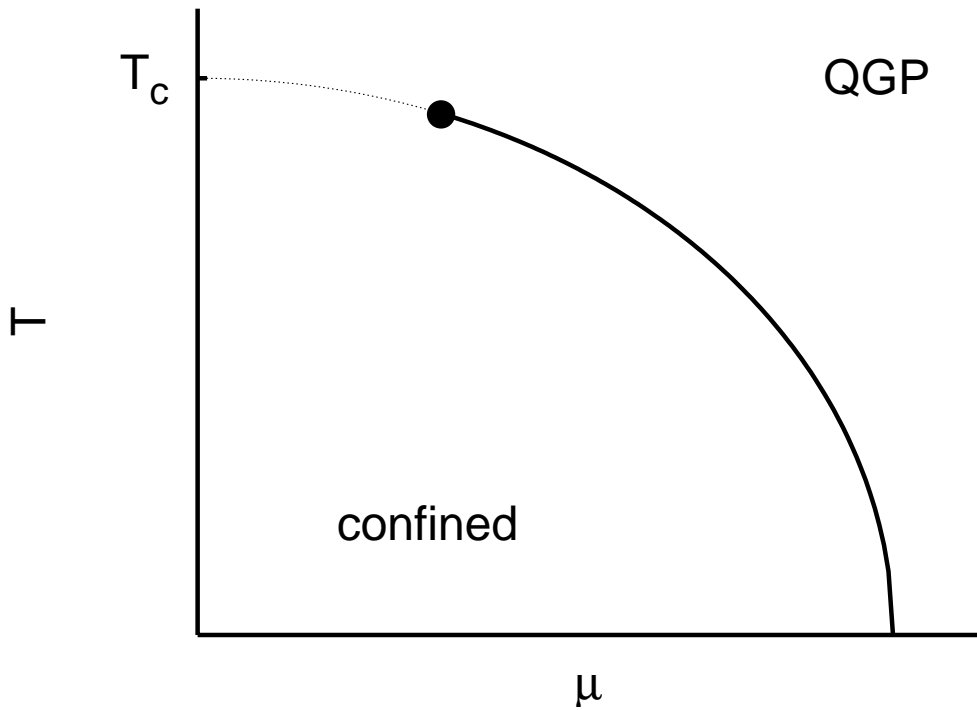
Problem : at higher baryon number  $B = n/3$ , the ratio needs to be evaluated for **very many ( $i_{max}$ ) integration points** ( $i = 1, \dots, i_{max}$ )

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

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  $\rho$  :

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

Then

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

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

Finally,  $\mu$  can be expressed as function of the baryon density  $\rho$  :

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

i

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  $(1.8 \text{ fm})^3$

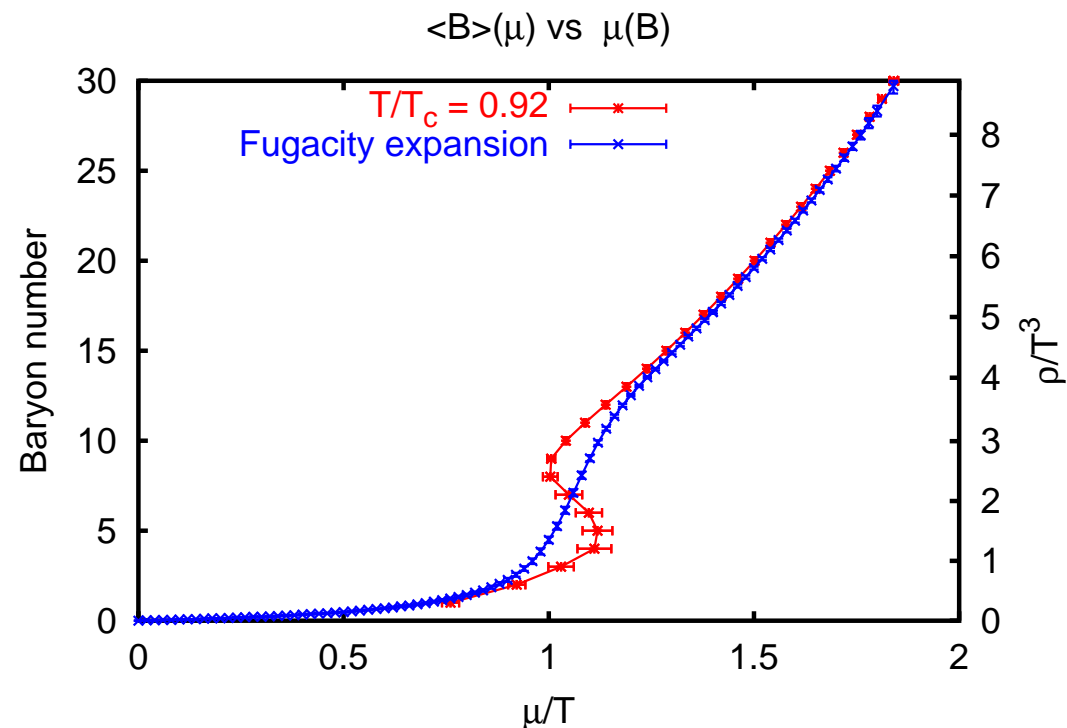
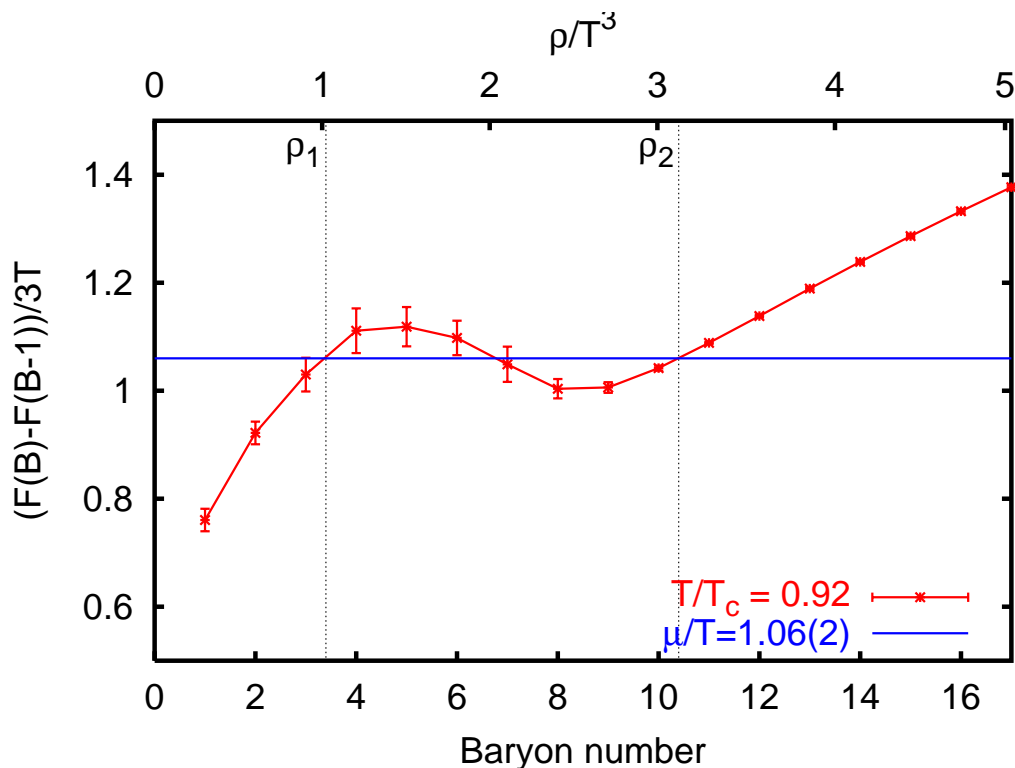
A. Alexandru, M. Faber, I. Horvath and K. F. Liu, hep-lat/0507020

Kentucky group :

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

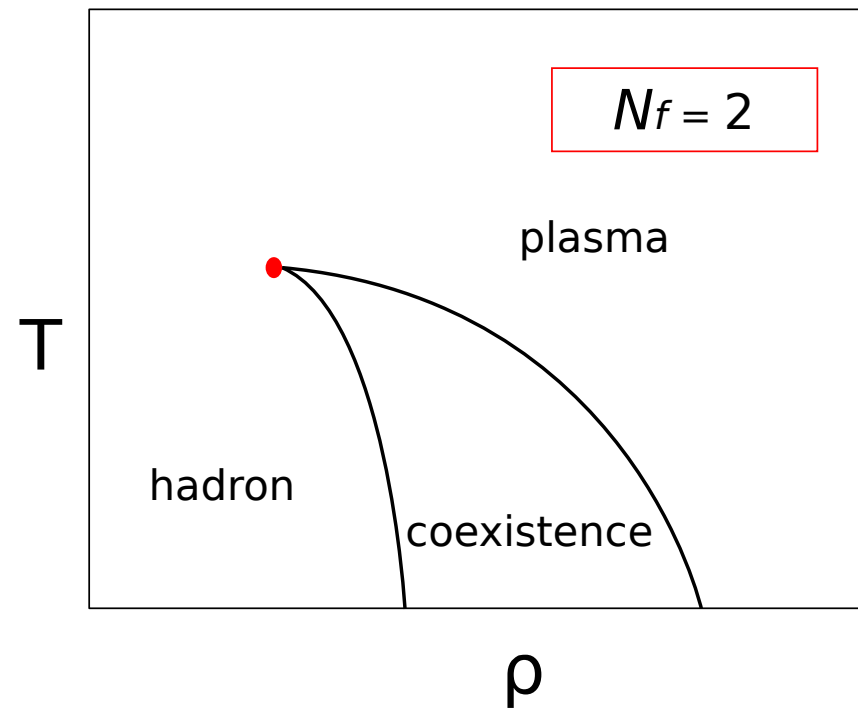
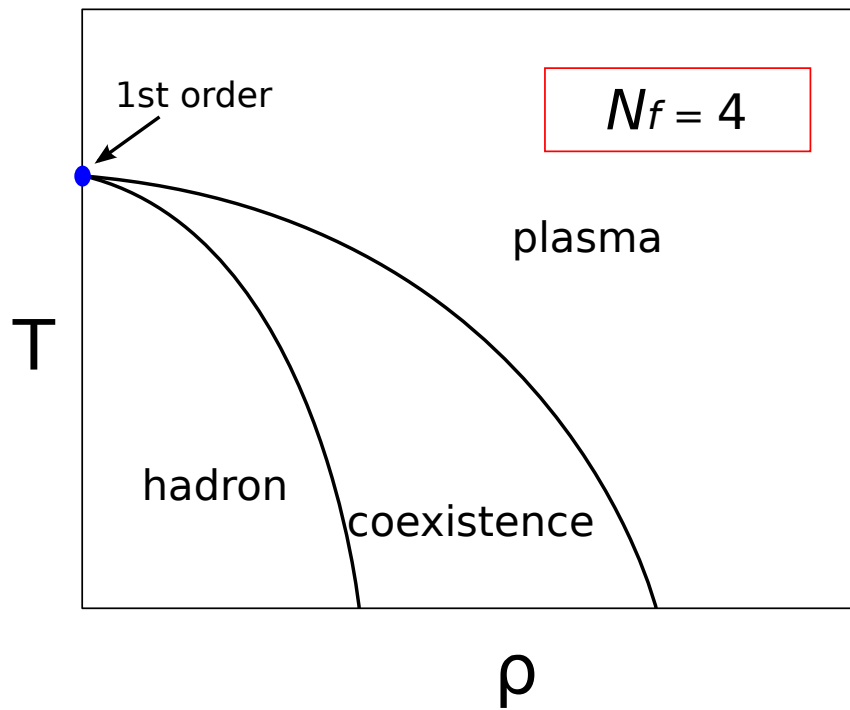
Left: The Maxwell construction allows to extract the critical chemical potential and the boundaries of the co-existence region. Right: Comparing the saddle point approximation (red) with the fugacity expansion (blue). Strong finite-size effects in the latter obscure the first-order transition.

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

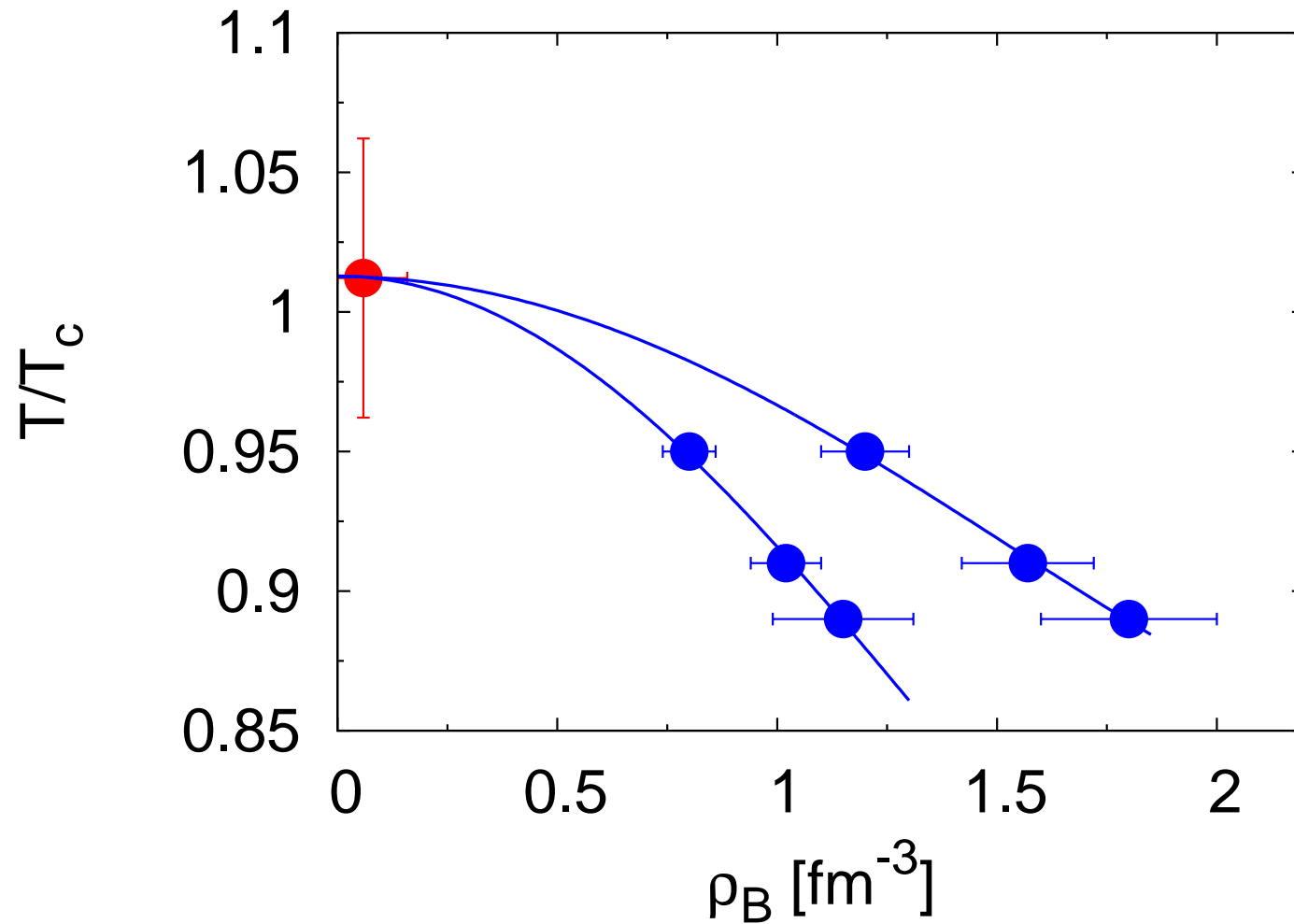


The number of flavors is decisive :  $N_f = 4$  vs.  $N_f = 2$

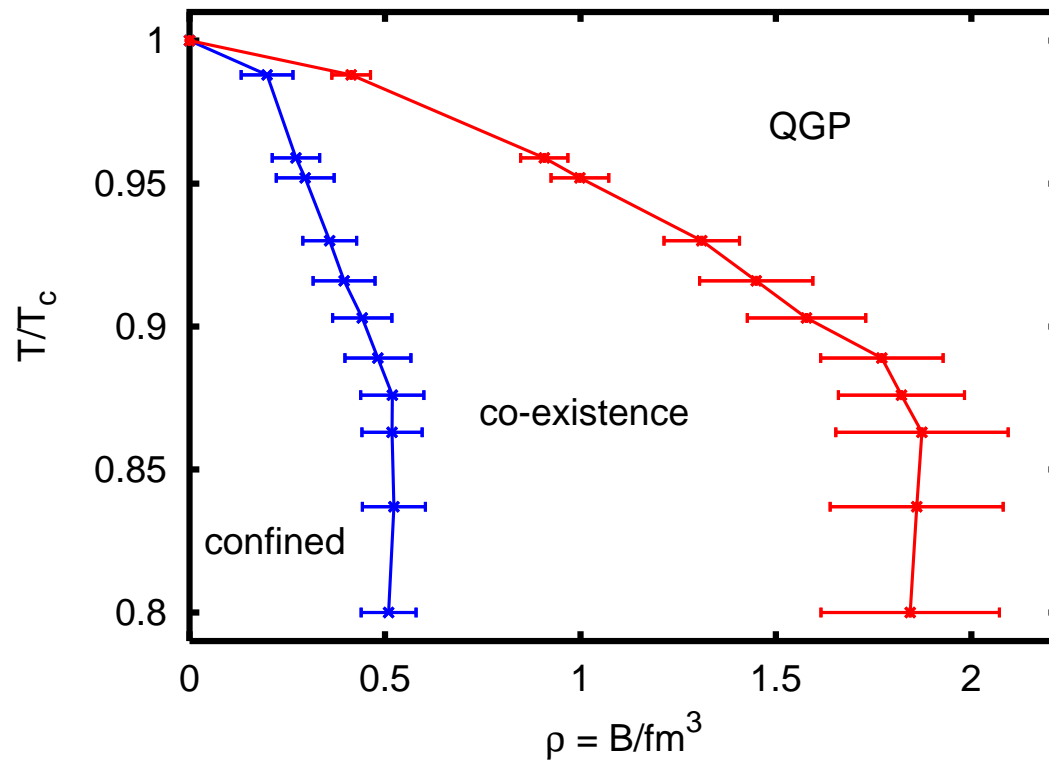
from Anyi Li arXiv:1002:4459



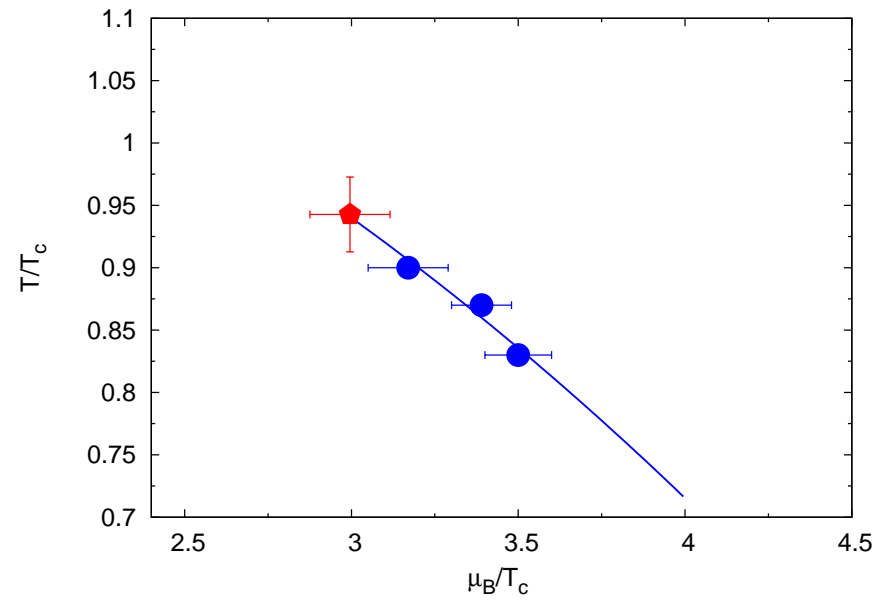
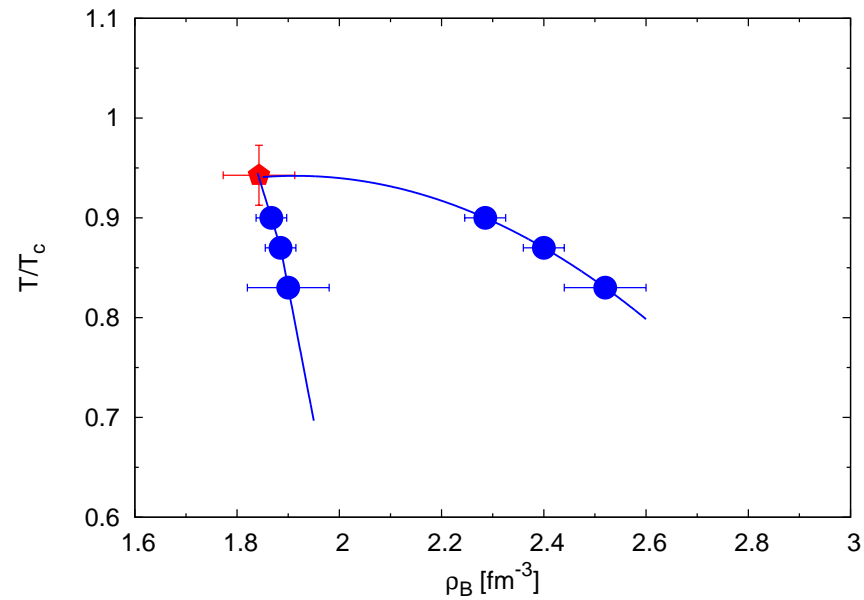
Phase boundaries in the temperature vs. density plot for  $N_f = 4$ .  
from Anyi Li arXiv:1002:4459



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 verify 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  $\mu_B$  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 :

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

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

This has motivated the interest in lattice results for the  $\mu$  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  $\mu$  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 :

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

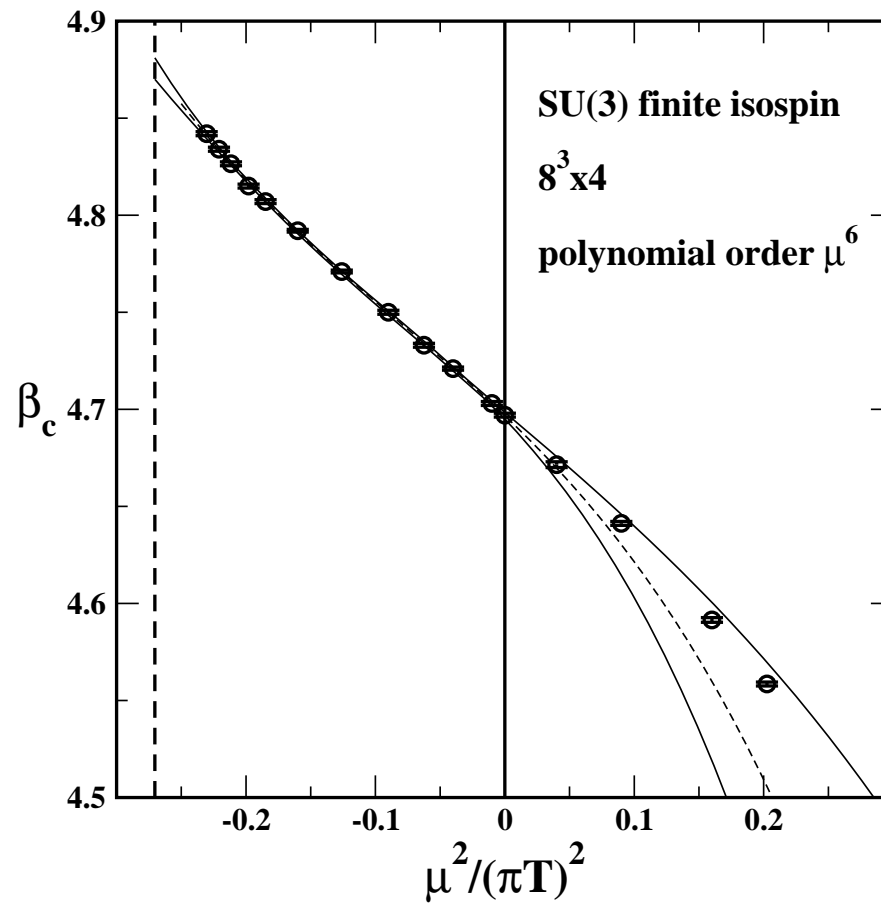
Similarly

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

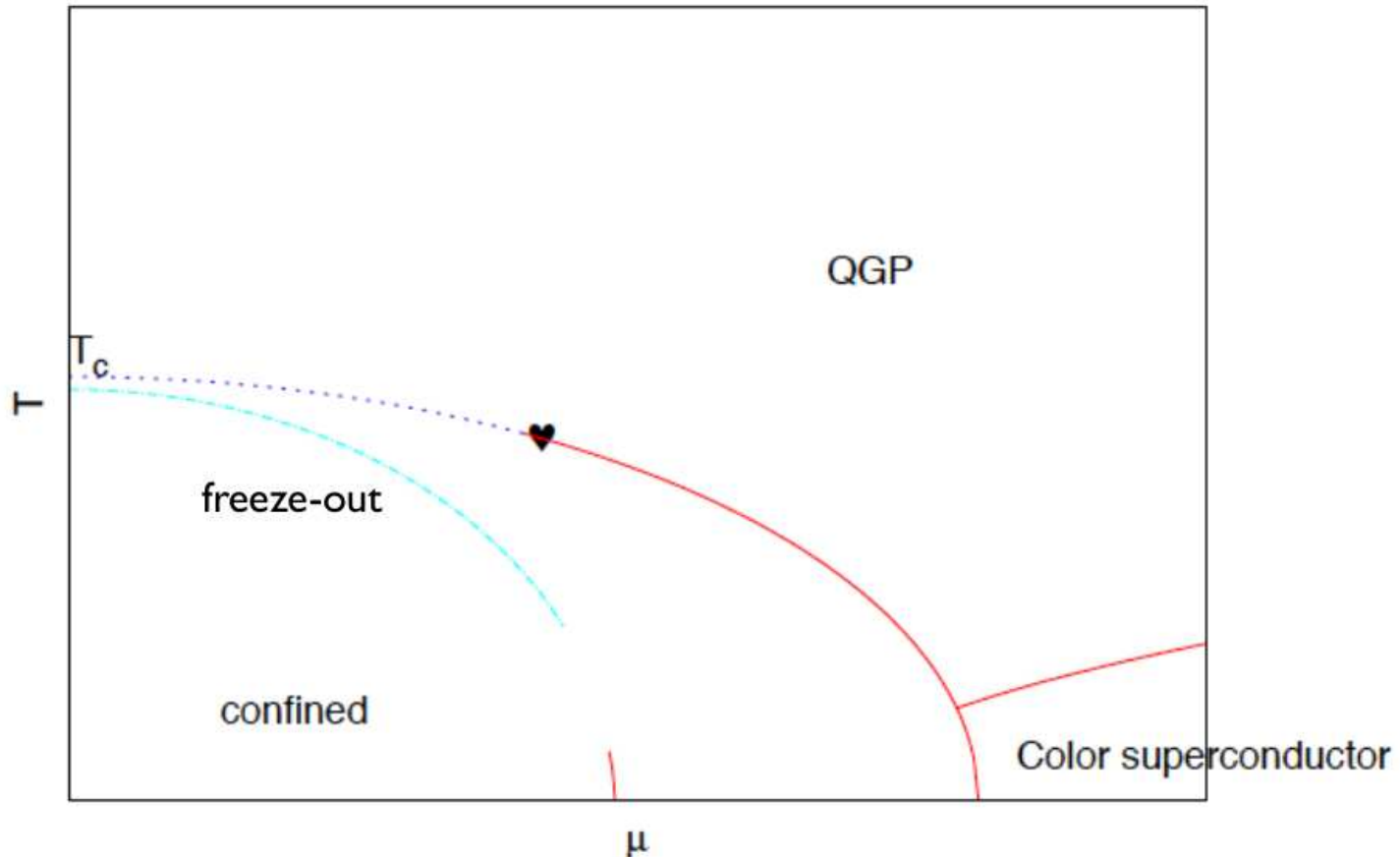
The coefficients must be determined at imaginary  $\mu = i\eta$ .

- It turns out, that the freeze-out temperature is three 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- $\mu$  data :  
The coefficients at imaginary  $\mu$  are alternating in sign and can be determined only with large uncertainty.

Continuation of  $\beta_c$  from negative  $\mu^2$  to positive  $\mu^2$   
from Ph. de Forcrand arXiv:1005.0539

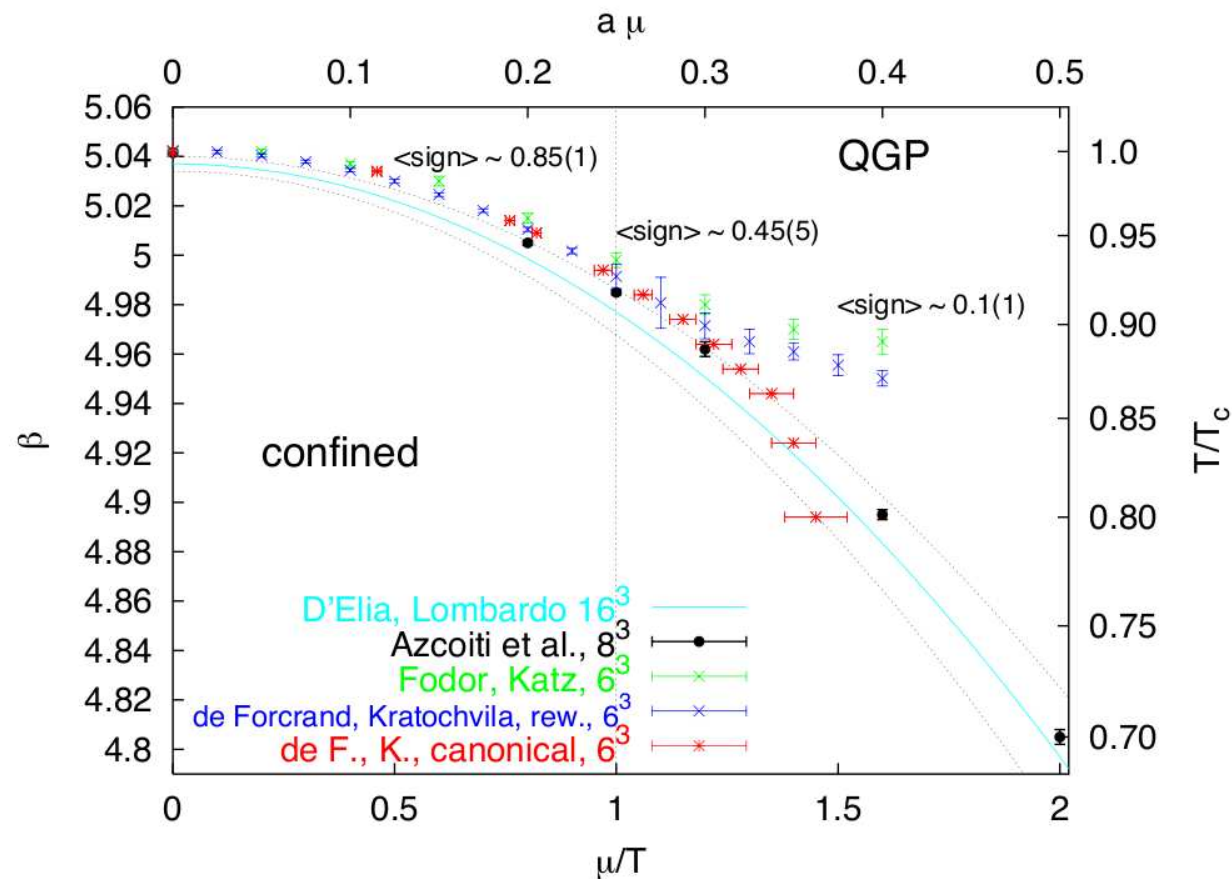


Sketch of the QCD crossover line  $T_c(\mu)$  vs. the experimental freeze-out curve, which has a larger curvature, near  $T_c(0)$ .  
from Ph. de Forcrand arXiv:1005.0539



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

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

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  $\mu$  :

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

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

Ph. de Forcrand and O. Philipsen (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  $p/T^4$ .

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

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  $\mu_l$  and  $\mu_s$

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

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

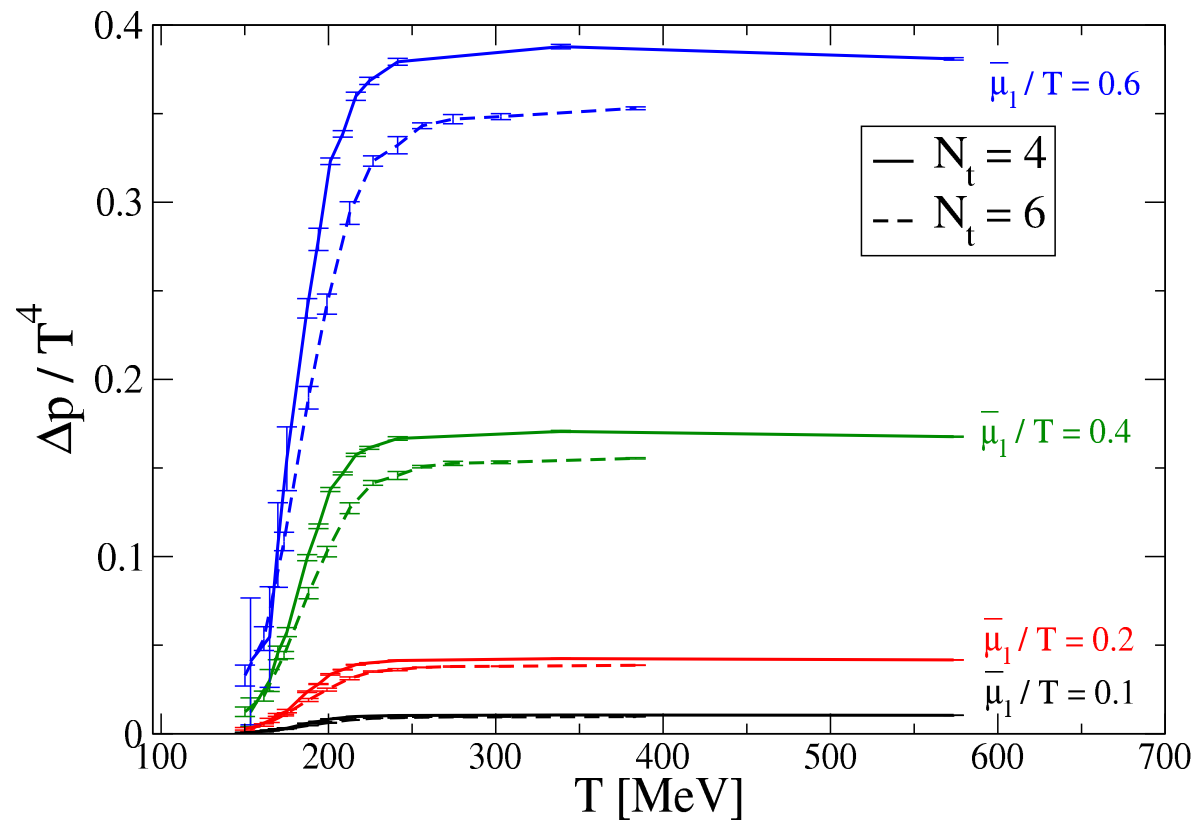
Comparison with HRG (Hadron Resonance Gas, taking the empirical hadron masses [to several GeV] with their baryonic charge into account)

#### 2) BMW collaboration, light and strange quarks

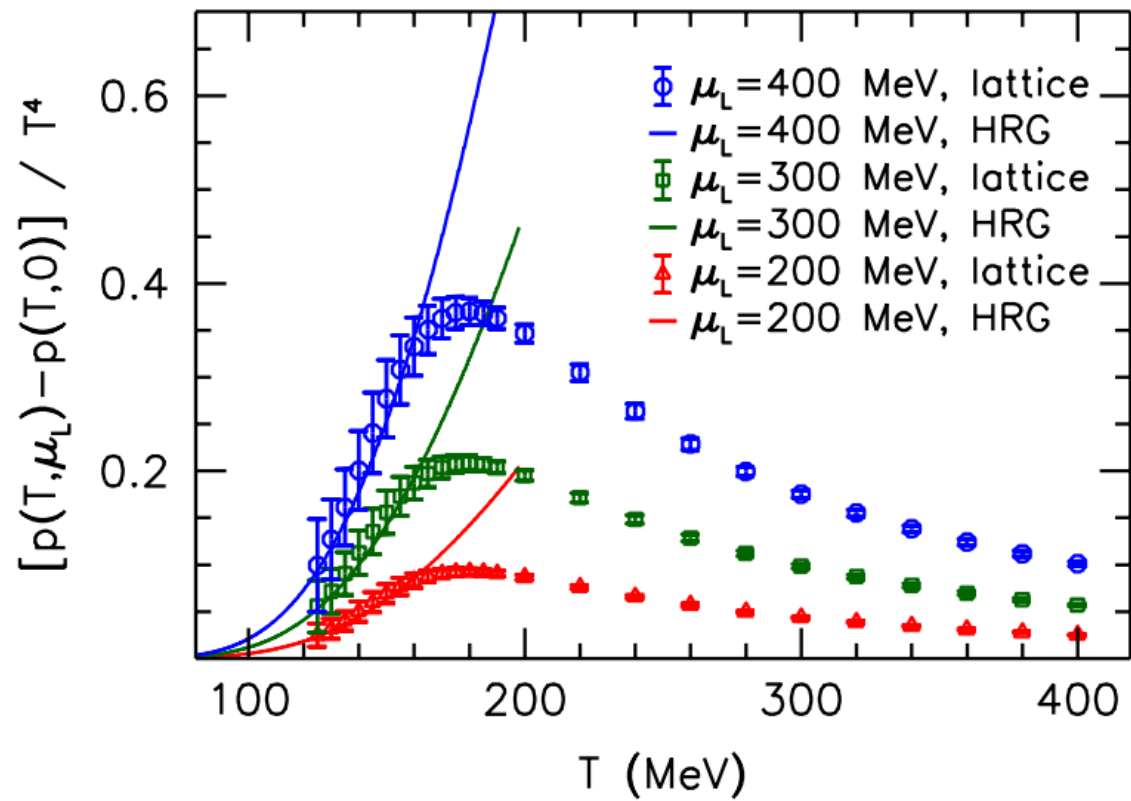
Calculations up to  $\mathcal{O}(\mu^2)$  (up to  $c_2$ )

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

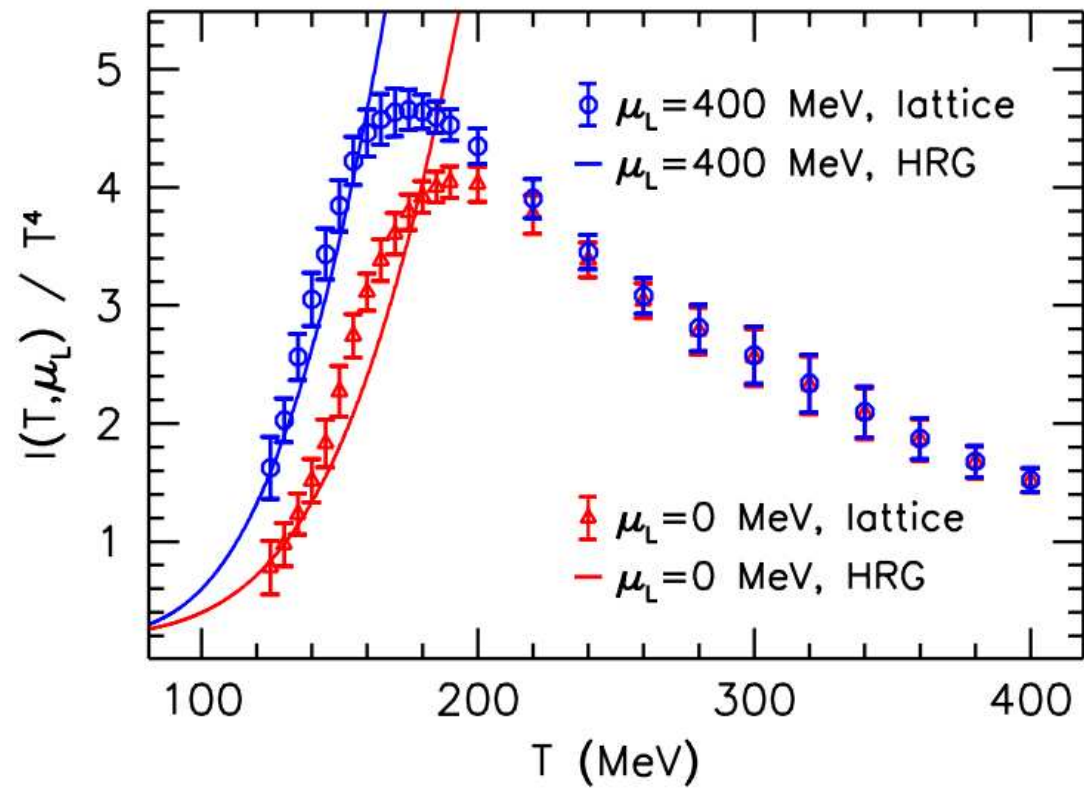
# Change in the pressure due to $\mu \neq 0$ (MILC+hotQCD)



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



The trace anomaly for non-zero  $\mu_L$  (BMW, compared with HRG)



## What else might be interesting ?

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

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

see: A. Hart, M. Laine, and O. Philipsen,

hep-lat/0010008 hep-ph/0004060