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The Critical Line of the QCD phase diagram from Lattice QCD

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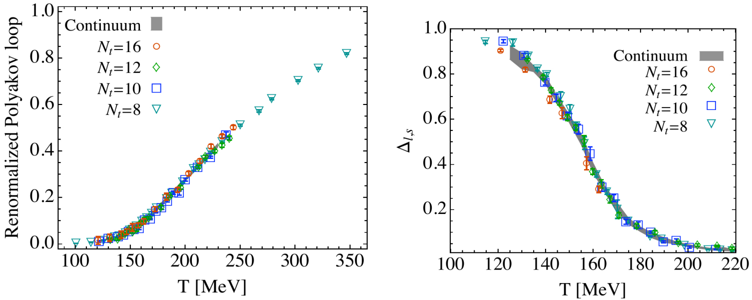
Outline

- Introduction
  - The phase diagram for strongly interacting matter
    Theory: the chiral/deconfinement crossovers, Experiments: chemical freeze-out point
  - Theory from first principles: Lattice QCD
    Basics, $T \neq 0$,$\mu_B \neq 0 \rightarrow \ldots$
  - The sign problem and proposed solutions
    Taylor expansion, Reweighting, Analytic continuation (...)
- Setup
  - The critical line of QCD and Analytic continuation
    Basics, $T \neq 0$,$\mu_B \neq 0 \rightarrow$ the sign problem!
  - Renormalized observables and the definitions of $T_c(\mu)$
    Chiral condensate, renormalization (I) and (II), Chiral susceptibility
  - Numerical setup
    Discretization used, Parameters, Statistics
- Numerical results
  - Results extrapolated to the continuum
  - Effects of $\mu_s \neq 0$
- Conclusions

- Low temperature: Confinement, (spontaneous) chiral symmetry breaking
- High temperature: Deconfinement, chiral symmetry restoration

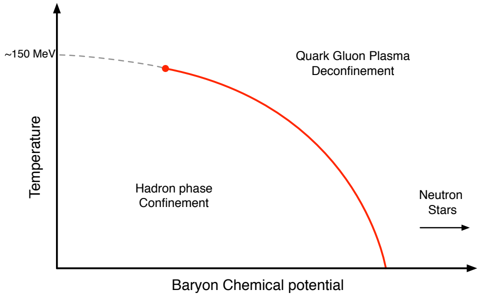


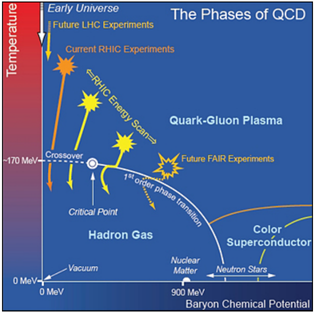
Left: Polyakov loop ($e^{-F_Q/T}$) as a function of temperature.

Right: Chiral condensate ($\sim \langle\bar{\psi}\psi\rangle$) (from JHEP 1009 (2010) 073)

Lattice data indicates no real transitions at "T_c", only crossovers (for physical values of the quark masses)

Conjectured Phase diagrams for QCD at finite density





Goal: Study $T_c(\mu_B)$, in physically relevant conditions (strangeness neutrality and $Z/A = 0.4$).

Lattice QCD and the sign problem at finite density

A Wick rotation + temporal periodic [1] boundary conditions allow us to study QCD at finite temperature:

$$t = -i\tau \quad \Rightarrow \quad \mathrm{Tr} e^{-iHt} = \mathrm{Tr} e^{-H\tau} = \mathrm{Tr} e^{-H/T} \, [\tau = 1/T]$$

Lattice discretization ⇒ Finite number of degrees of freedom ⇒ The functional integral become a *finite dimensional integral*, evaluable with Montecarlo and Importance Sampling methods *if* $S_G[U]$ *and* $\det M$ *are real*:

$$Z = \int DU e^{-S_G[U]} \prod_f \det M_f[\mu_f, U]$$

Various possible choices for the discretized action, for both S_G and M_f

Unfortunately, in the presence of a *real* nonzero chemical potential, $\det M_f$ *is complex*. ⇒ **Importance sampling methods don't work in this situation**

[1] Antiperiodic for Fermion fields

Sign problem: Ways out

Applied to the theory at the physical point:

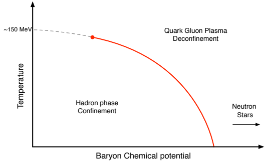
- Analytic Continuation from imaginary μ [Our Choice]
- Taylor expansion from $\mu = 0$ [precision issues with higher order derivatives on the lattice, due to lack of self-averaging]

Other methods:

- Reweighting from the $\mu = 0$ ensemble [scales badly with volume]
- Canonical method [the sign problem is back in a different form]
- Strong coupling methods + Reweighting
- Complex Langevin
- Lefschetz Thimbles
- Density of States methods
- Dual formulations

The pseudocritical line and analytic continuation

At lowest order in μ, the pseudocritical line can be parametrized as:



$$\frac{T_c(\mu_B)}{T_c} = 1 - \kappa \left(\frac{\mu_B}{T_c(\mu_B)} \right)^2 + O(\mu^4)$$

(odd order terms are forbidden by charge conjugation symmetry of QCD)

The sign problem and analytic continuation

For purely imaginary μ, the fermion determinant is real positive, and the sign problem is non existent.

With the transformation $\mu_B = i\mu_{B,I}$, the pseudocritical line parametrization is modified as follows:

$$\frac{T_c(\mu_{B,I})}{T_c} = 1 + \kappa \left(\frac{\mu_{B,I}}{T_c(\mu_{B,I})} \right)^2 + O(\mu_{B,I}^4)$$

Observables: chiral condensate and chiral susceptibility

Light chiral condensate - Definition:

$$\langle\bar{\psi}\psi\rangle_{ud} = \frac{T}{V}\frac{\partial \log Z}{\partial m_{ud}} = 2\frac{T}{V}\langle \mathrm{Tr} M_l^{-1}\rangle = \langle\bar{u}u\rangle + \langle\bar{d}d\rangle$$

Two possible renormalizations:

As in [Cheng *et al.*, 08] :

$$\langle\bar{\psi}\psi\rangle^r_{(1)} \equiv \frac{\langle\bar{\psi}\psi\rangle_{ud}(T) - \frac{2m_{ud}}{m_s}\langle\bar{s}s\rangle(T)}{\langle\bar{\psi}\psi\rangle_{ud}(0) - \frac{2m_{ud}}{m_s}\langle\bar{s}s\rangle(0)}$$

Alternatively [Endrodi *et al.*, 11]:

$$\langle\bar{\psi}\psi\rangle^r_{(2)} \equiv (-)\frac{m_{ud}}{m_\pi^4}\left(\langle\bar{\psi}\psi\rangle_{ud} - \langle\bar{\psi}\psi\rangle_{ud}(T=0)\right)$$

[to make a more significant comparison]

Light chiral susceptibility - Definition:

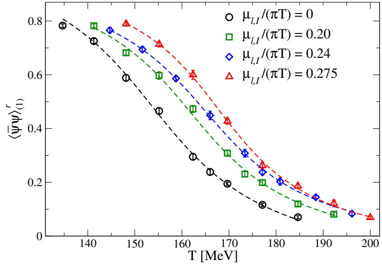
$$\chi_{\bar{\psi}\psi} \equiv \frac{\partial\langle\bar{\psi}\psi\rangle_{ud}}{\partial m_l}$$

We have chosen this renormalization[Y.Aoki *et al.*, 06]:

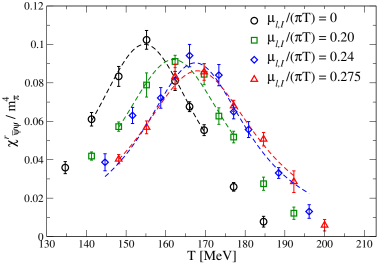
$$\chi^r_{\bar{\psi}\psi}(T) \equiv m_{ud}^2\left[\chi_{\bar{\psi}\psi}(T) - \chi_{\bar{\psi}\psi}(0)\right]$$

Defining T_c and κ using computed observables - Our method

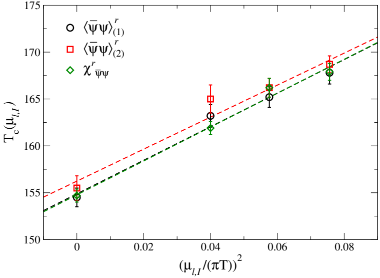
Light Chiral Condensate



Light Chiral Susceptibility



Critical line in the $T - \mu_{l,I}^2$ plane



- Fit for the **chiral condensate(s)**:

$$a_1 + b_1 \arctan\left[c_1\,(t - t_c)\right]$$

- Fit at the peak for the chiral susceptibility:

$$\chi^{r}_{\bar\psi\psi}(T)/m_\pi^4 = \frac{A_2}{(T - T_c)^2 + B_2^2}$$

- Fit for the critical line:

$$\frac{T_c(\mu_{B,I})}{T_c} = 1 + \kappa \left(\frac{\mu_{B,I}}{T_c(\mu_{B,I})}\right)^2$$

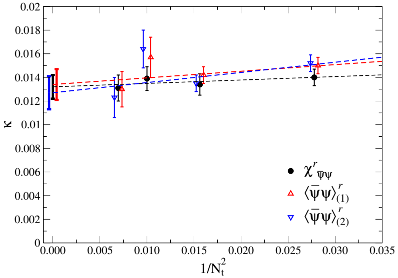
Numerical setup

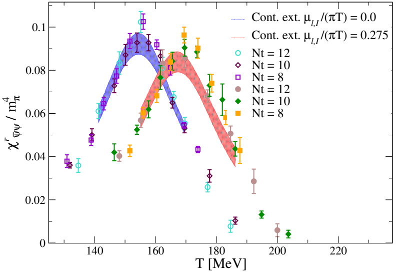
- At the physical point (line of constant physics, parameters taken from [Aoki *et al.*, 09]) $N_t = 6, 8, 10, 12$ lattices.
- Study of the $\mu_s = \mu_l \neq 0$ (32^3x8 only) and $\mu_s = 0$ cases.
- Tree level Symanzik improved gauge action with $N_f = 2 + 1$ flavours of twice-stouted staggered fermions.
- Used lattices with aspect ratio = 4
- Also performed simulations at zero temperature for subtractions (32^4,48^3x96).
- Observables evaluated with noisy estimators, with 8 random vectors per quark.

Simulations run on IBM BG-Q at CINECA (Bologna, Italy) and on the Zefiro Cluster (INFN - Pisa).

Lattice	$16^3 \times 6$	$24^3 \times 6$	$32^3 \times 6$
$i\mu/(\pi T)$	0.00 0.20 0.24 0.275	0.00 0.24 0.275	0.00 0.24 0.275
Lattice	$32^3 \times 8$	$40^3 \times 10$	$48^3 \times 12$
$i\mu/(\pi T)$	0.00 0.10 0.15 0.20 0.24 0.275 0.30	0.00 0.20 0.24 0.275	0.00 0.20 0.24 0.275

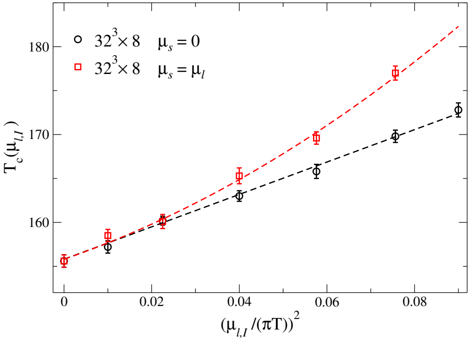
Critical line and continuum Limit of κ





First method: We evaluated the curvature κ for each N_t (6,8,10,12) and then performed the continuum limit extrapolation on κ itself, assuming finite lattice spacing corrections are of the form $const/N_t^2$.

Second method: We extrapolated the values of the observables to the continuum limit (taking data from $N_t = 8,10,12$), obtaining $\lim_{a\to 0} T_c(\mu_B)$. We then obtained κ by fitting $T_c(\mu_B)$ data.



Critical line in the Temperature/Imaginary Baryon chemical potential plane, from the renormalized chiral susceptibility [Bonati *et al.*, 15]

In Heavy Ion Collisions: $Z/A = 0.4$, $S = 0$.

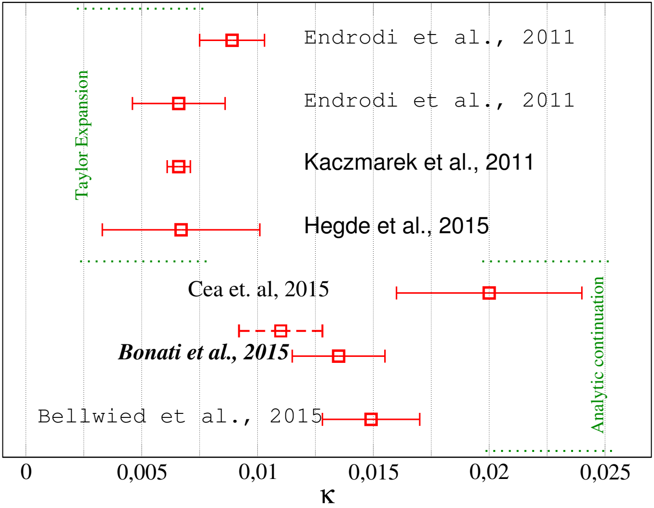
$\Downarrow$

This entails $\mu_u \simeq \mu_d = \mu_l$, and (due to interactions) $\mu_s \simeq 0.25\mu_l$ (for $T = T_c$). [Bazavov et al., 14] [Borsanyi et al.,13] [Bellwied et al.,15]

We **mainly** studied $\mu_s = 0$, and checked the setup $\mu_s = \mu_l$

Result: κ estimated in the two setups are compatible, IF a quartic term is included (or if the fit range is reduced)

Comparison with other determinations



Comparison with other lattice determinations.

Conclusions

- We located the critical line $T_c(\mu_{I,B})$ with a fitting procedure using chiral observables, and obtained an estimate for its curvature at $\mu_B = 0$
- We performed an extensive check to compare our determinations with the ones of other groups.
- We investigated the effects of including a nonzero strange quark potential ($\mu_s = \mu_l = \mu$). We have confirmed the presence of a quartic contribution. Considering such contribution, the curvature of the critical line for $\mu_s = \mu_l$ or $\mu_s = 0$ is compatible within errors.
- We performed a continuum scaling analysis in two ways, directly on κ and on the observables. The resulting estimates of κ are in agreement. Our estimate is $\kappa = 0.0135(20)$.


"That's all Folks!"
I s b e r g©

Chemical potential and sign problem

In the **continuum theory**, a chemical potential coupled with quark number can be introduced:

$$\mu_f N_f = \mu_f \int d^3x \; \bar{\psi}_f \gamma_0 \psi_f$$

On the lattice, the quark chemical potential associated to the flavour f is introduced by multiplying the gauge links in the fermion matrix $M_f[U]$ in the temporal direction by $e^{-a\mu_f}$.
Unfortunately, this causes the so called **sign problem**. When $\mu_f = 0$,

$$\left(\not{D} + m\right)^\dagger = \gamma_5 \left(\not{D} + m\ \right) \gamma_5 \ \rightarrow \det\left(\not{D} + m\right) \in \mathbb{R}$$

When $\mu_f \neq 0$ this is not true any more:

$$\gamma_5 \left(\not{D} + m - \gamma_0 \mu\right) \gamma_5 = \left(-\not{D} + m + \gamma_0 \mu\right) = \left(\not{D} + m + \gamma_0 \mu^*\right)^\dagger$$

$\Rightarrow$ **The fermion determinant is complex!**[2]

[2] Notice that this is not the case if $\Re\mu = 0$

Path Integral formulation: $Z = \int DAD\bar{\psi}D\psi e^{-i\int d^4x\mathcal{L}[A,\bar{\psi},\psi]}$

$$D_\mu = \partial_\mu - ig\hat{A}_\mu,\ (\hat{F}_{\mu\nu} = [D_\mu, D_\nu])$$

$$\mathcal{L} = -\frac{1}{2g^2}\mathrm{Tr}\left\{\hat{F}_{\mu\nu}\hat{F}^{\mu\nu}\right\} + \sum_f \bar{\psi}_f\left(i\gamma^\mu D_\mu - m_f\right)\psi_f$$

Chiral Symmetry: In the vanishing mass limit the Lagrangian is invariant under the transformations

$$\psi'_L = U\psi_L,\ \psi'_R = U^\dagger\psi_R$$

Where ψ_L and ψ_R represent the left- and right-handed parts of all the spinors, and U is a $SU(N_f)$ matrix which mix different flavours. The light quark condensate $\langle\bar{u}u + \bar{d}d\rangle$ is an order parameter for chiral symmetry breaking.

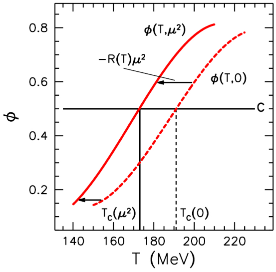


Figure from [Endrodi *et al.*, 11]

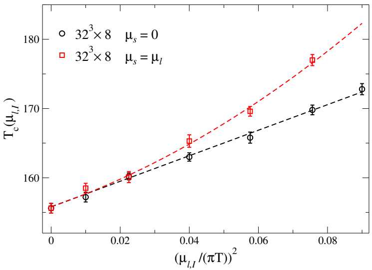
In order to better compare our results with those of [Endrodi *et al.*, 11] (same lattice action, but using the Taylor expansion method), we have located $T_c(\mu_B)$ using the chiral condensate (II), using the following equation

$$\langle\bar{\psi}\psi\rangle^r_{(2)}(T_c(\mu_B),\mu_B) = \langle\bar{\psi}\psi\rangle^r_{(2)}(T_c(0),0)$$

Our result for the curvature using this method is $\kappa = 0.0110(18)$, to be compared with $\kappa = 0.0066(20)$.

Taylor expansion:

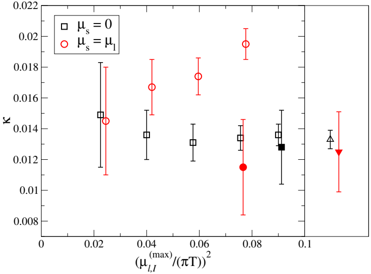
$$\frac{\partial T_c}{\partial \mu^2} = -\left.\frac{\partial^2\langle\bar{\psi}\psi\rangle^r_{(2)}}{\partial\mu^2}\right|_{T=T_c,\mu=0}\left.\left(\frac{\partial\langle\bar{\psi}\psi\rangle^r_{(2)}}{\partial T}\right)^{-1}\right|_{T=T_c,\mu=0} \quad (1)$$



(Renormalized chiral susceptibility)

(From [Bonati *et al.*, 15])

Results for κ varying the μ fit range:



Empty Red: κ, linear fit ($\mu_s = \mu_l$ data)

Full Red: κ, lin+quad fit ($\mu_s = \mu_l$)

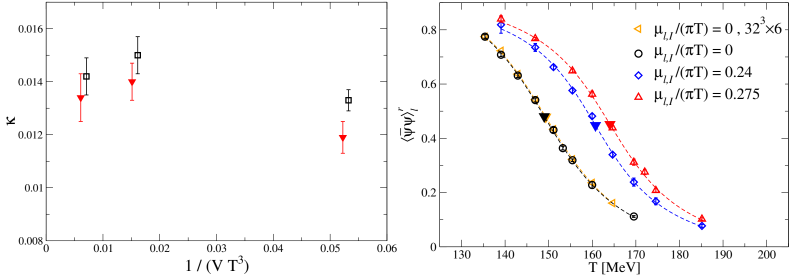
Empty Black: κ, linear fit ($\mu_s = 0$)

Empty Black: κ, lin+quad fit ($\mu_s = 0$)

Right: κ from combined (lin+quad) fit

Finite size effects
On $N_t = 6$ lattices

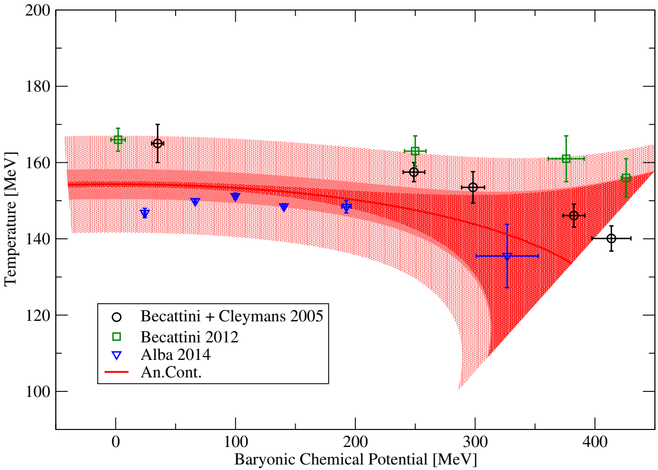
From [Bonati *et al.*, 14] (16^3x6, 24^3x6 and 32^3x6 lattices)



Left: Estimates of κ. Black : Renormalized Chiral Condensate (1), Red : Renormalized Chiral Susceptibility ; Right: The chiral condensate on the $24^3 \times 6$ lattice, with the data for $\mu_I = 0$ on the $32^3 \times 6$ lattice

$\Rightarrow$ **Aspect ratio 4 is enough.**

Tentative extrapolation at real μ_b



Tentative continuation to real chemical potential, and comparison to the experimental data from chemical freezeout. Note: some assumptions about the higher orders in μ_B have been made.

Continuum limit of Observables

- For the **renormalized chiral condensates**, we used the formula

$$\langle\bar{\psi}\psi\rangle^r(T) = A_1 + B_1 \arctan\left[C_1\left(T - T_c\right)\right]$$

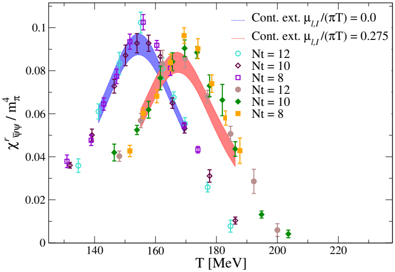
to fit the data from all values of N_t simultaneously. We added a N_t dependency to T_c ($T_c(N_t) = T_c(N_t = \infty) + const./N_t^2$) and a similar one to C_1.

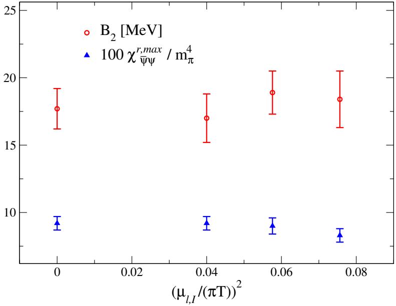
- For the **renormalized chiral susceptibility**, we used the formula

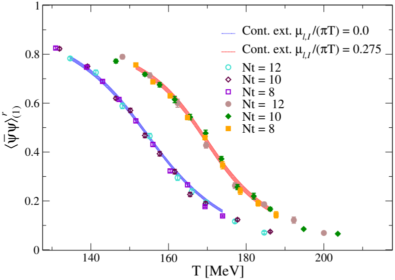
$$\chi^r_{\bar{\psi}\psi}(T) = \frac{A_2}{(T - T_c)^2 + B_2^2}$$

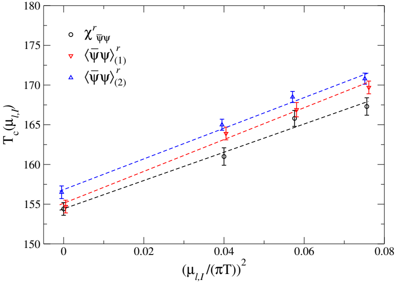
where we added a dependency on N_t similar to $T_c(N_t) = T_c(N_t = \infty) + const./N_t^2$ for all parameters.

Continuum limit of Observables









Numerical values

1st method (continuum limit of κ):

$$\begin{aligned}\kappa_{\bar{\psi}\psi,1} &= 0.0134(13)\\ \kappa_{\bar{\psi}\psi,2} &= 0.0127(14)\\ \kappa_{\chi} &= 0.0132(10)\end{aligned}$$

2nd method (continuum limit of observables):

$$\begin{aligned}\kappa_{\bar{\psi}\psi,1} &= 0.0145(11)\\ \kappa_{\bar{\psi}\psi,2} &= 0.0138(10)\\ \kappa_{\chi} &= 0.0131(12)\end{aligned}$$

Values of T_c obtained with the continuum limit of the observables, fit with the form $T_c(\mu_{B,I})/T_c = 1 + \kappa[\mu_{B,I}/\pi T_c(\mu_{B,I})]^2$.