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The Critical Line of the QCD phase diagram from Lattice QCD

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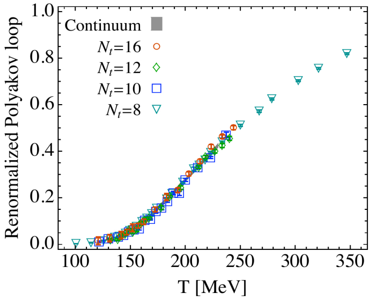
Outline

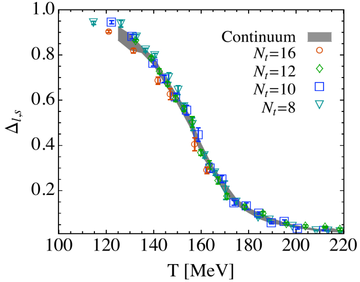
- Introduction
  - The phase diagram for strongly interacting matter
    Theory: the chiral/deconfinement crossovers, Experiments: chemical freeze-out point
  - Theory from first principles: Lattice QCD
    Basics, $T \neq 0$,$\mu_B \neq 0 \rightarrow \ldots$
  - The sign problem and proposed solutions
    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 Discretization used,

    Parameters, Statistics
- Numerical results
  - Effects of $\mu_s \neq 0$
  - Results extrapolated to the continuum
- Comparison with other determinations
- Conclusions and outlooks

QCD at finte T and zero density

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





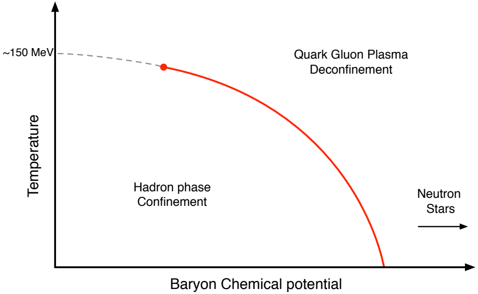
Left: Polyakov loop ($e^{-F_Q/T}$) as a function of temperature.

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)

QCD at finite T and finite baryon density

Conjectured Phase diagram for QCD at finite density



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

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 **Path 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 around

Applied to the theory at the physical point:

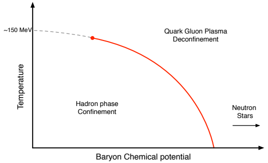
- Analytic Continuation from imaginary μ [Our Choice]
- Taylor expansion from $\mu = 0$ [precision issues with higher order derivatives on the lattice, due to lack of self-averaging]

Other methods: [Huge effort going on]

- 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 [rewriting the partition function in terms of other variables]

The pseudocritical line and analytic continuation

At lowest order in μ, the pseudocritical line can be parameterized 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)

Analytic continuation from imaginary μ_B

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

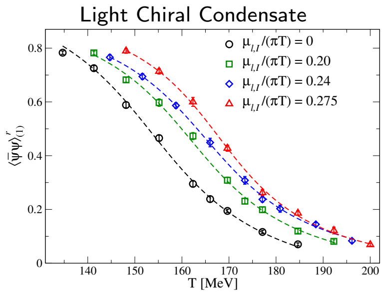
With the transformation $\mu_B = i\mu_{B,I}$, the pseudocritical line parameterization is **modified as follows**:

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

κ can be computed on the lattice.

In order to locate the position of the pseudo transition on the phase diagram, we compute the order parameter for chiral symmetry, the **Light chiral condensate** :

$$\langle \bar{\psi}\psi \rangle_{ud} = \frac{T}{V}\frac{\partial \log Z}{\partial m_{ud}} = \langle \bar{u}u \rangle + \langle \bar{d}d \rangle$$



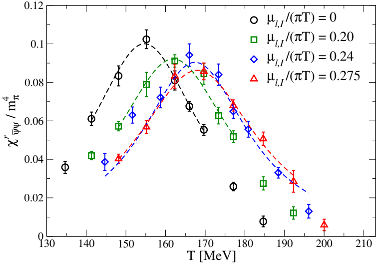
To locate T_c, fit with the function

$$\langle \bar{\psi}\psi \rangle^r = a_1 + b_1 \arctan\left[c_1\left(T - T_c\right)\right]$$

We also compute its susceptibility, the **Light chiral susceptibility** :

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

Light Chiral Susceptibility

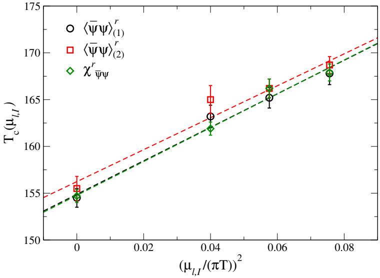


To locate T_c, fit with the function

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

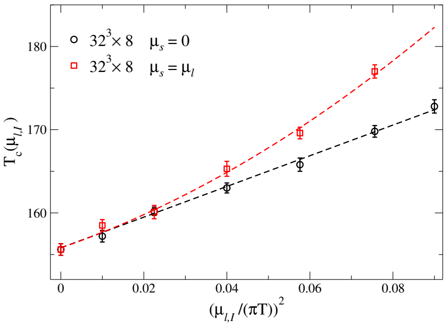
Once we obtained the pseudocritical temperature T_c for each value of $\mu_{B,I}$, we can find the curvature with a simple fit.

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



To evaluate κ, fit for the critical line:

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



Critical line in the Temperature/Imaginary Baryon chemical potential plane, from the renormalized chiral susceptibility

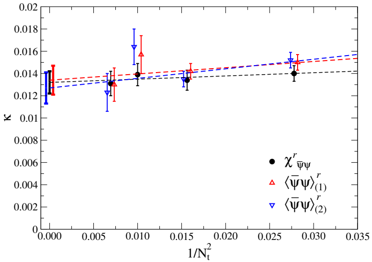
[Bonati *et al.*, 15]

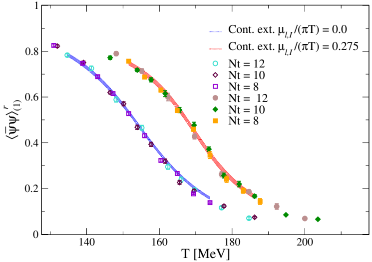
We studied the setups $\mu_s = 0$ and $\mu_s = \mu_l$.

Physical conditions lie between these two cases

Result: κ estimates from the two setups are compatible, if a quartic term is included (or if the fit range is reduced) in the $\mu_s = \mu_l$ case

Conclusion: results for κ with $\mu_s = 0$ are relevant for heavy ion collisions.

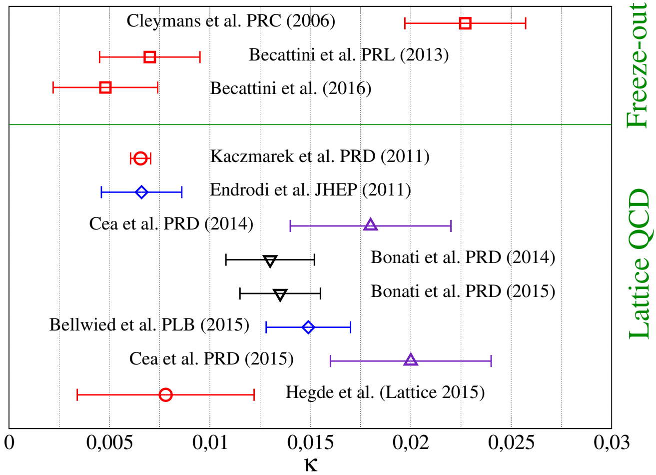




Method I: We evaluated the curvature κ for each N_t (6,8,10,12) and then performed the continuum limit extrapolation on κ itself, assuming finite lattice spacing corrections are of the form $const/N_t^2$.

Method II: 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.

Comparison with other determinations



Comparison with other determinations of the curvature of the critical line.

Conclusions and outlooks

Our results:

- 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 investigated the effects of including a nonzero strange quark potential ($\mu_s = \mu_I = \mu$). Considering a quartic term, the curvature of the critical line for $\mu_s = \mu_I$ or $\mu_s = 0$ is compatible within errors. Our continuum extrapolated value for the curvature of the critical line is

$$\kappa = \mathbf{0.0135(20)}.$$

Comments and outlooks:

- General consensus among the latest lattice determinations
- How to compare with experimental/phenomenological data more precisely? [Lattice Simulations are performed at equilibrium]

Backup slides

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]

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

QCD

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.

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

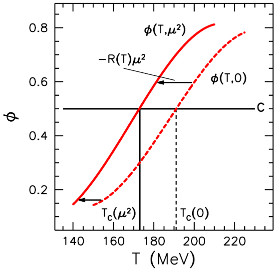


Figure from [Endrodi *et al.*, 11]

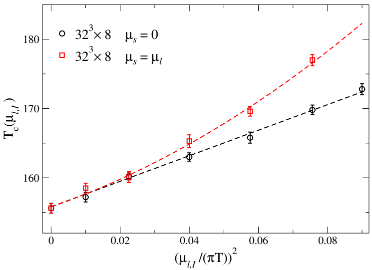
In order to better compare our results with those of [Endrodi *et al.*, 11] (same lattice action, but using the Taylor expansion method), we have located $T_c(\mu_B)$ using the chiral condensate (II), using the following equation

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

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

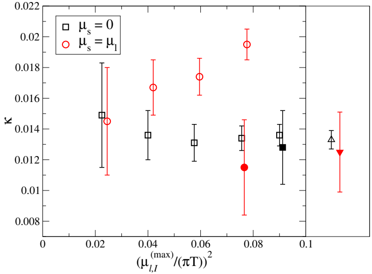
Taylor expansion:

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



(Renormalized chiral susceptibility)

Results for κ varying the μ fit range:



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

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

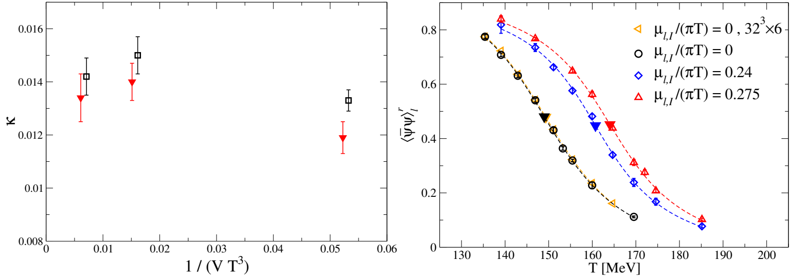
Empty Black: κ, linear fit ($\mu_s = 0$)

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

Right: κ from combined (lin+quad) fit

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

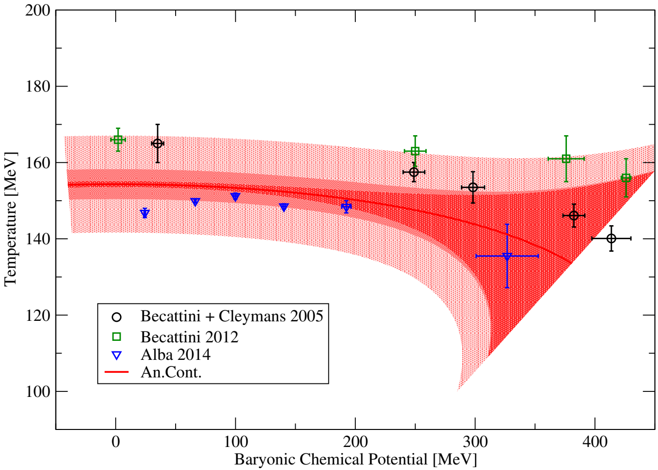
From [Bonati *et al.*, 14] (16^3x6, 24^3x6 and 32^3x6 lattices)



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

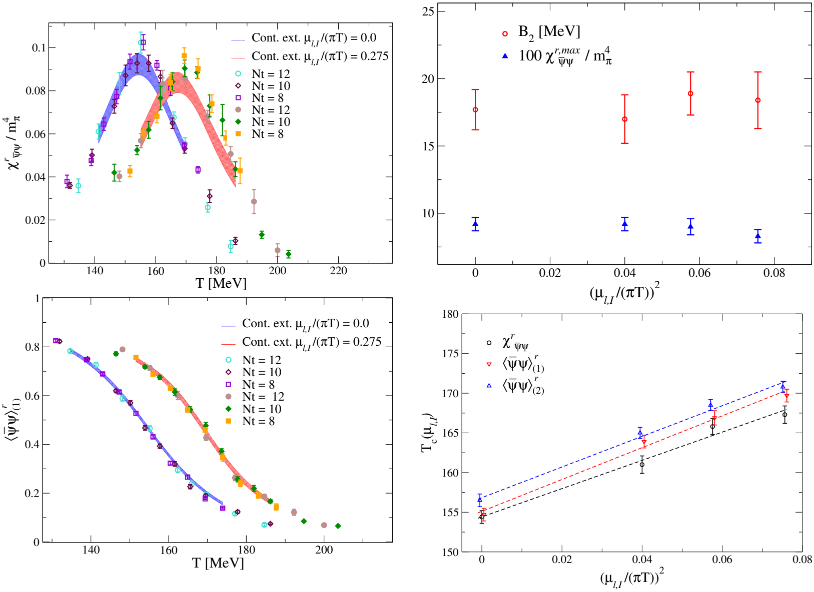
$$\langle\bar{\psi}\psi\rangle^r(T) = A_1 + B_1 \arctan\left[C_1\left(T - T_c\right)\right]$$

  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



Values of the curvature

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 $T_c(\mu_{B,I})/T_c = 1 + \kappa[\mu_{B,I}/\pi T_c(\mu_{B,I})]^2$.

Relation between μ_u, μ_d, μ_s and μ_B, μ_Q, μ_S

Key idea:

$$\mu_u N_u + \mu_d N_d + \mu_s N_s = \mu_B B + \mu_Q Q + \mu_S S$$

Relation between conserved quantities:

$$\begin{aligned} B &= n_u/3 + n_d/3 + n_s/3 \\ Q &= 2n_u/3 - n_d/3 - n_s/3 \\ S &= -n_s \end{aligned}$$

Relations between chemical potentials:

$$\begin{aligned} \mu_B &= \mu_u + 2\mu_u & \qquad \mu_u &= \mu_B/3 + 2\mu_Q/3 \\ \mu_Q &= \mu_u - \mu_d & \qquad \mu_d &= \mu_B/3 - \mu_Q/3 \\ \mu_S &= \mu_d - \mu_s & \qquad \mu_s &= \mu_B/3 - \mu_Q/3 - \mu_S \end{aligned}$$

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]:

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

the role of the strange quark chemical potential μ_s

experimental conditions = strangeness neutrality ($\langle n_s \rangle = 0$), $z = 0.4a$.
note that this **does not** imply $\mu_s = 0$, because in general, e.g. $\partial n_s / \partial \mu_u \neq 0$.
this means μ_u, μ_d, μ_s should be tuned (for each each temperature) to reproduce experimental conditions.

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]

more basic question:
what is the effect of a nonzero strange quark chemical potential?