The curvature of the critical line from lattice simulations at imaginary μ_B

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Based on work done in collaboration with C. Bonati, M. Mariti, M. Mesiti, F. Negro and F. Sanfilippo

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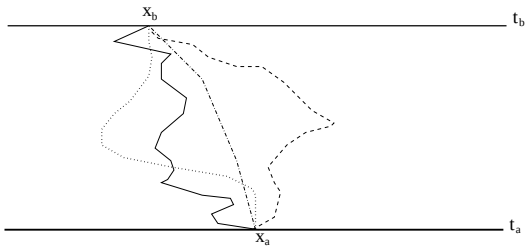
Short introduction to Lattice QCD

The starting point is the path-integral approach to Quantum Mechanics and Quantum Field Theory



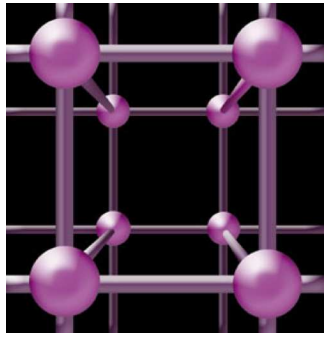
$$\longrightarrow \langle 0|O|0\rangle \Rightarrow \int \mathcal{D}\varphi e^{-S[\varphi]} O[\varphi]$$

The QCD path integral is discretized on a finite space-time lattice

$\Longrightarrow$ **finite number of integration variables**

For QCD, integration variables are 3×3 unitary matrices, $U_\mu(n)$, living on lattice links (elementary parallel transporters)

(K.G. Wilson, 1974)



The path-integral is then computed by Monte-Carlo algorithms which sample field configurations proportionally to $e^{-S[U]}$

$$\langle O\rangle = \frac{1}{Z}\int \mathcal{D}U e^{-S[U]} O[U] \quad \simeq \quad \bar{O} = \frac{1}{M}\sum_{i=1}^{M} O[U^{\{i\}}]$$

The thermal QCD partition function is rewritten in terms of an Euclidean path integral with a compactified temporal extension

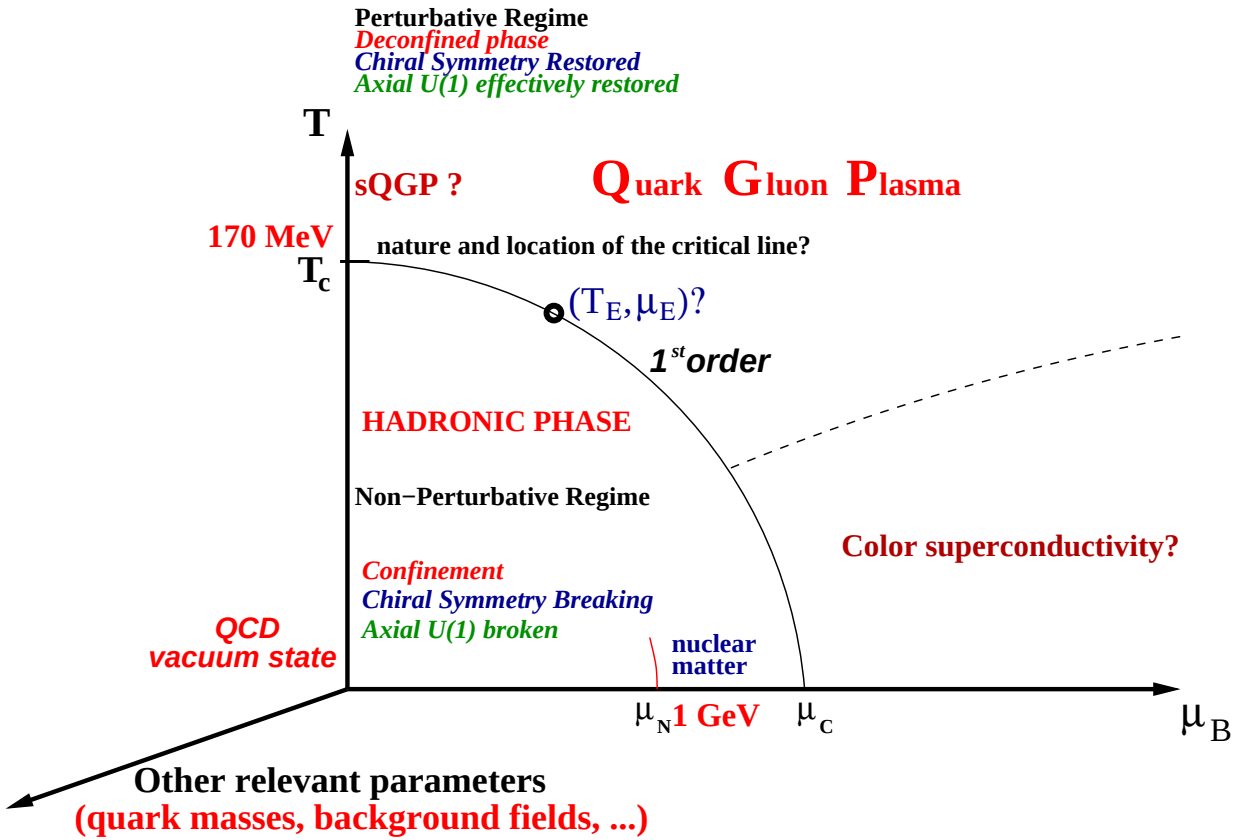
$$S_{QCD} = \int d^4x \left(\sum_f \bar{\psi}_i^f \left(D_{ij}^\mu \gamma_\mu^E + m_f \delta_{ij} \right) \psi_j^f + \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} \right) \rightarrow \bar{\psi} M[U] \psi + S_G[U]$$

$$Z(V,T) = \mathrm{Tr}\left(e^{-\frac{H_{\mathrm{QCD}}}{T}} \right) \Rightarrow \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-(S_G[U] + \bar{\psi} M[U] \psi)} = \int \mathcal{D}U e^{-S_G[U]} \det M[U]$$

Temperature is the inverse of the temporal extension, which is compactified with periodic (antiperiodic) boundary conditions for bosons (fermions)

As long as $\mathcal{D}U e^{-S_G} \det M[U]$ is positive, it can be interpreted as a probability distribution $\mathcal{D}U \mathcal{P}[U]$ over gauge link configurations, which can be sampled by proper Monte-Carlo algorithms

Lattice QCD is a candidate first principle tool for computing the QCD phase diagram



Unfortunately, the region at non-zero baryon chemical potential μ_B is affected by the so-called sign problem

Problems in lattice QCD at $\mu_B \neq 0$

$$Z(\mu_B, T) = \mathrm{Tr}\left(e^{-\frac{H_{\mathrm{QCD}} - \mu_B N_B}{T}}\right) = \int \mathcal{D}U e^{-S_G[U]} \det M[U, \mu_B]$$

$$\text{at } \mu_B \neq 0: \qquad \gamma_5 M^\dagger \gamma_5 \neq M \implies (\det M)^* \neq \det M$$

$\det M[\mu_B]$ **complex** $\implies$ **Monte Carlo simulations are not feasibile.**

This is usually known as the sign problem

Many algorithms are being explored to completely overcome this problem (Langevin simulations, rewriting the partition function in terms of new variables, etc.).

By now we can just rely on a few approximate methods, which are suitable only for small values of μ_B/T

- **Taylor expansion** of physical quantities around $\mu = 0$, coefficients are computable with a positive measure, but going up with the expansion order is harder and harder. Systematics: truncation error.

  Bielefeld-Swansea collaboration 2002; R. Gavai, S. Gupta 2003

- **Reweighting:** complex phase taken out of the measure and put into observables

$$\int \mathcal{D}U \mathcal{P}[U] O[U] = \int \mathcal{D}U \tilde{\mathcal{P}}[U] \left(\frac{\mathcal{P}[U]}{\tilde{\mathcal{P}}[U]} O[U] \right)$$

  Systematics out of control if phase oscillations explode (unavoidable as $V \to \infty$)

  Barbour et al. 1998; Z. Fodor and S, Katz, 2002

- **Simulations at imaginary chemical potentials:** if $\mu = i\, \mu_I$ the measure is positive again, then analytic continuation to the real plane $\mu^2 < 0 \to \mu^2 > 0$. Be careful about transition crossings. Systematics: choice of interpolation functions

  Alford, Kapustin, Wilczek, 1999; de Forcrand, Philipsen, 2002; M.D'E., Lombardo 2003.

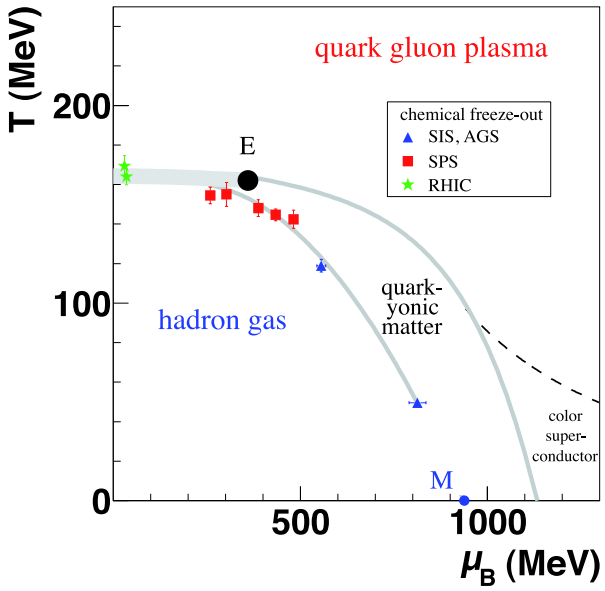
Those methods give the possibility to access many quantities of physical interest, like the pseudo-critical temperature $T_c(\mu_B)$, signalling deconfinement/chiral symmetry restoration, for small values of μ_B/T

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

the coefficient κ defines the curvature of the pseudo-critical line. It can be obtained by:

- **suitable ratios of expectation values computed at $\mu_B = 0$ (Taylor expansion method)**

- **determining T_c for purely imaginary values of μ_B, then fixing the behavior for small and real μ_B by analytic continuation**



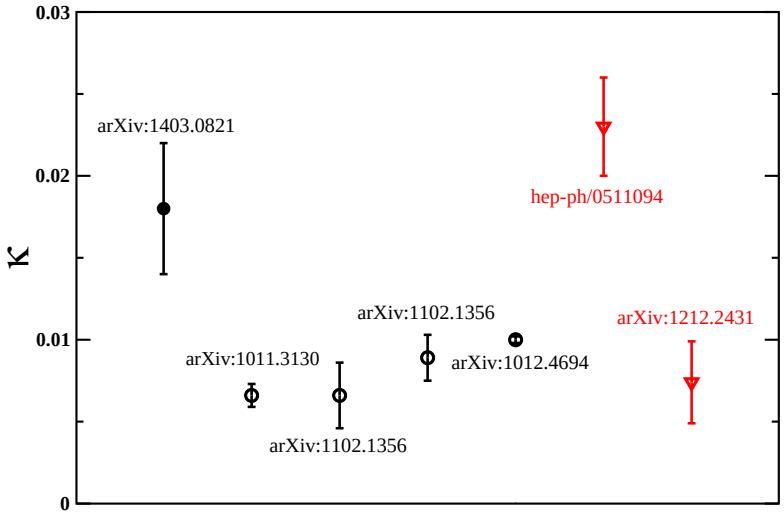
There is a well known discrepancy between the lattice curvature and the standard experimental determinations of freeze-out conditions.

κ from freeze-out is 2-3 times bigger

(picture from F. Becattini *et al*, arXiv:1201.6349)

– **no apriori reason for the two lines to coincide: hadrons interact even after the parton$\longrightarrow$hadron transition. However, the gap leaves space for speculations about new possible phases, like the so-called "Quarkyonic Phase" (McLerran, Pisarsky, 2007)**

– **a recent reanalysis of freeze-out data, taking into account inelastic collisions after freeze-out, seems to bring to a significant reduction of such a discrepancy (F. Becattini *et al*, arXiv:1212.2431)**



Most lattice determinations have been obtained by Taylor expansion

A recent lattice determination claims a somewhat larger value of κ

FROM LEFT TO RIGHT:

- arXiv:1403.0821: **P. Cea, L. Cosmai and A. Papa, $N_f = 2 + 1$ QCD with HISQ staggered tree level action, analytic continuation, $\mu_s = \mu_u = \mu_d$**

- arXiv:1011.3130: **O. Kaczmarek *et al.*, $N_f = 2+1$ QCD, p4 staggered action, Taylor expansion, $\mu_s = 0$**

- arXiv:1102.1356: **G. Endrodi *et al.*, $N_f = 2 + 1$ QCD, stout staggered fermions, Taylor expansion, $\mu_s = 0$**

- arXiv:1012.4694: **R. Falcone, E. Laermann, M. Lombardo, $N_f = 2 + 1$, p4 staggered action, analytic continuation, $\mu_s = \mu_u = \mu_d$**

- hep-ph/0511094: **J. Cleymans *et al*, standard freeze-out analysis**

- arXiv:1212.2431: **F. Becattini *et al*, reanalysis of freeze-out data**

The spread of lattice determinations opens a number of question on the possible sources of systematic effects:

- **Different methods and observables to locate T_c (there is no real transition, so the question is non-trivial)**

- **Different methods to define the variation of T_c with μ_B (in particular Taylor vs analytic continuation)**

- **Different discretizations of QCD**

- **Different setup of chemical potentials ($\mu_s = 0$ vs $\mu_s \neq 0$)**

The purpose of this study

- **Determine the curvature of the pseudo-critical line by analytic continuation, for $N_f = 2 + 1$ QCD discretized at the physical point**

- **Consider a stout-smeared staggered action, and two different lattice spacings ($N_t = 6$ and $N_t = 8$)**

- **Chiral condensate and chiral susceptibility as probes of the transition**

- **Two different setups of chemical potential, in order to estimate the effect of $\mu_s \neq 0$**

Numerical Setup

We consider a lattice discretization of

$$Z(\mu_u, \mu_d, \mu_s, T) = \mathrm{Tr}\left(e^{-\frac{H_{\mathrm{QCD}} - \sum_i \mu_i n_i}{T}}\right) \qquad \sum_i \mu_i n_i = \mu_u n_u + \mu_d n_d + \mu_s n_s$$

n_i are the quark number operators. The relation with the other standard convention in terms of conserved charges is:

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

We consider two different setups:

- $\mu_u = \mu_d \equiv \mu_l \; ; \quad \mu_s = 0$ **matches initial conditions in heavy ion collisions**
- $\mu_u = \mu_d \equiv \mu_l \; ; \quad \mu_s = \mu_l$ **to test the contribution from μ_s**

In both cases, $\mu_B = 3\mu_l$

On the lattice, considering purely imaginary chemical potentials, the partition function is discretized as follows

$$\mathcal{Z} = \int \mathcal{D}U \, e^{-\mathcal{S}_{YM}} \prod_{f=u,\,d,\,s} \det\left(M^f_{\text{st}}[U, \mu_{f,I}]\right)^{1/4}$$

$$\mathcal{S}_{YM} = -\frac{\beta}{3} \sum_{i,\mu\neq\nu} \left(\frac{5}{6} W^{1\times1}_{i;\,\mu\nu} - \frac{1}{12} W^{1\times2}_{i;\,\mu\nu} \right)$$

$$(M^f_{\text{st}})_{i,\,j} = a m_f \delta_{i,\,j} + \sum_{\nu=1}^{4} \frac{\eta_{i;\,\nu}}{2} \left[e^{i\mu_{f,I}\delta_{\nu,4}} U^{(2)}_{i;\,\nu} \delta_{i,j-\hat{\nu}} - e^{-i\mu_{f,I}\delta_{\nu,4}} U^{(2)\dagger}_{i-\hat{\nu};\,\nu} \delta_{i,j+\hat{\nu}} \right]$$

- $\mathcal{S}_{YM}$ **is the tree level improved Symanzik action**
- $(M^f_{\text{st}})_{i,\,j}$ **is the staggered Dirac operator built up with two times stout-smeared links** $U^{(2)}_{i;\,\nu}$

$\mu_{f,I}$ **is the imaginary chemical potential assigned to each flavor**

At fixed N_t**, the temperature** $T = 1/(aN_t)$ **is changed by varying the value of the bare coupling constant** β **on a line of constant physics (**$m_\pi \simeq 135\,\text{MeV}$ **and** $m_s/m_l = 28.15$**)**

Critical line and analytic continuation

The most general parametrization, compatible with isospin symmetry, is

$$T_c(\mu_u,\mu_d,\mu_s) = T_c(0,0,0) - A(\mu_u^2+\mu_d^2) - B\mu_s^2 - C\mu_u\mu_d - D\mu_s(\mu_u+\mu_d) + O(\mu^4)$$

$$\mu_u = \mu_d = \mu_l \; ; \; \mu_s = 0 \implies T_c(\mu_l) = T_c(0) - (A+C)\mu_l^2 + O(\mu_l^4)$$

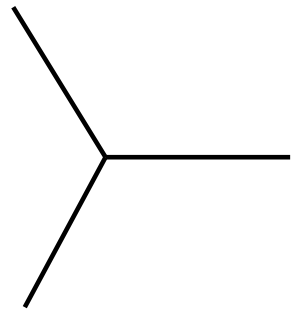
$$\mu_s = \mu_u = \mu_d = \mu_l \implies T_c(\mu_l) = T_c(0) - (A+B+C+2D)\mu_l^2 + O(\mu_l^4)$$

Such leading order behaviors can be continued to purely imaginary $\mu_l = i\mu_{l,I}$ and fitted to determinations of T_c obtained by numerical simulations.

$$T_c(\mu_{l,I}) = T_c(0) + \text{const} \times \mu_{l,I}^2 + O(\mu_{l,I}^4)$$

The range of available values of $\mu_{l,I}$ is limited by the presence of non-physical phase transitions in the $T - \mu_{l,I}$ plane, known as Roberge-Weiss transition. However the range is different for $\mu_s = 0$ and $\mu_s = \mu_l$.

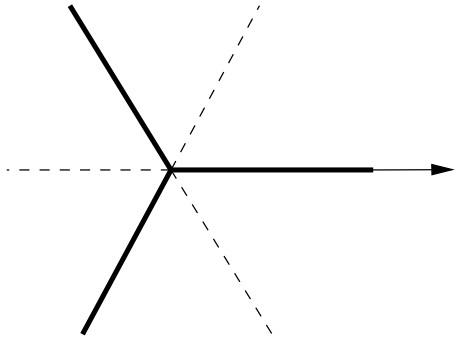
The $T-\mu_I$ phase structure is dictated by center symmetry. Assume flavor symmetric chemical potentials at first. $\mu = i\mu_I$ rotates fermion temporal b.c. by μ_I/T



Pure gauge theory: Exact Z_3 center symmetry

Spontaneously broken at $T > T_c$

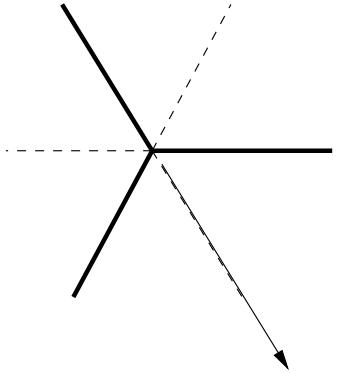
Order parameter: Polyakov loop



Full QCD, $\mu = 0$

Determinant breaks $Z_3 \to Z_2$

No further spontaneous breaking



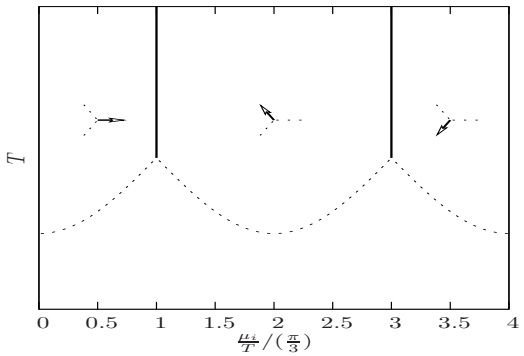
Full QCD, $\mu_I/T = (2k+1)\pi/3$

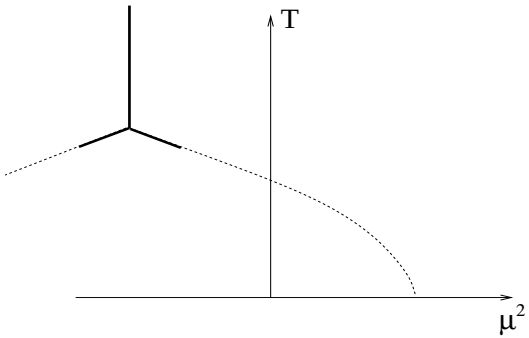
Determinant breaks $Z_3 \to Z_2$

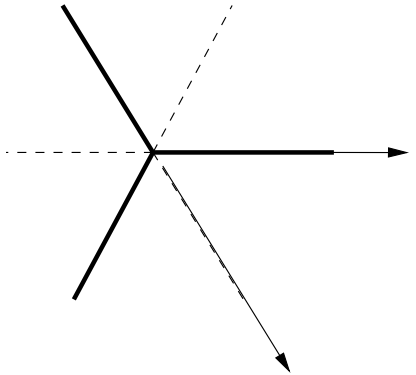
Z_2 breaks spontaneously at $T > T_{RW}$

For $\mu_I/T = (2k+1)/3\pi$ an exact residual Z_2 symmetry exist, which breaks spontaneouly at high T: Roberge-Weiss transition lines

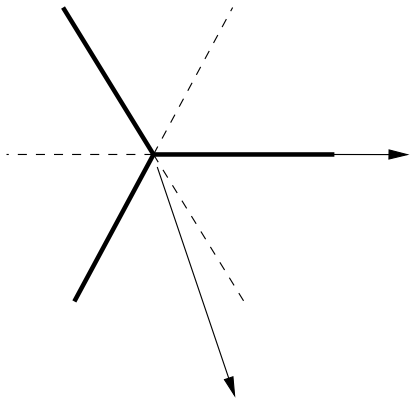
That limits, in the high T regime and for the critical line itself, the region around $\mu = 0$ available for analytic continuation to $\theta_l \equiv \mu_I/T \leq \pi/3$





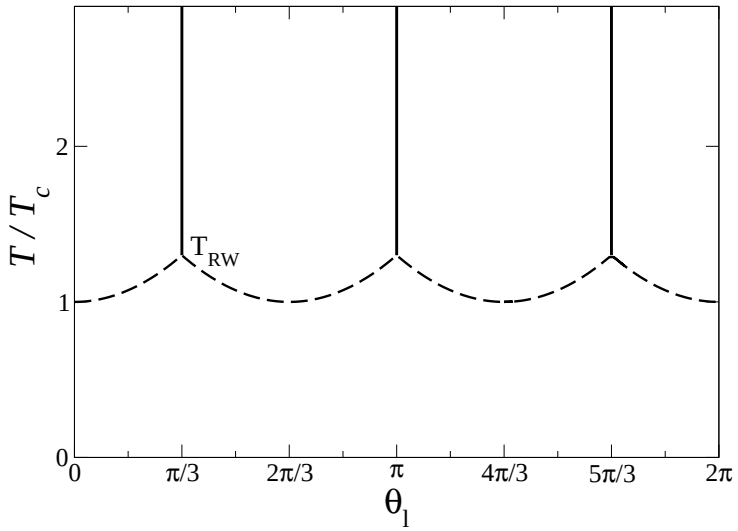


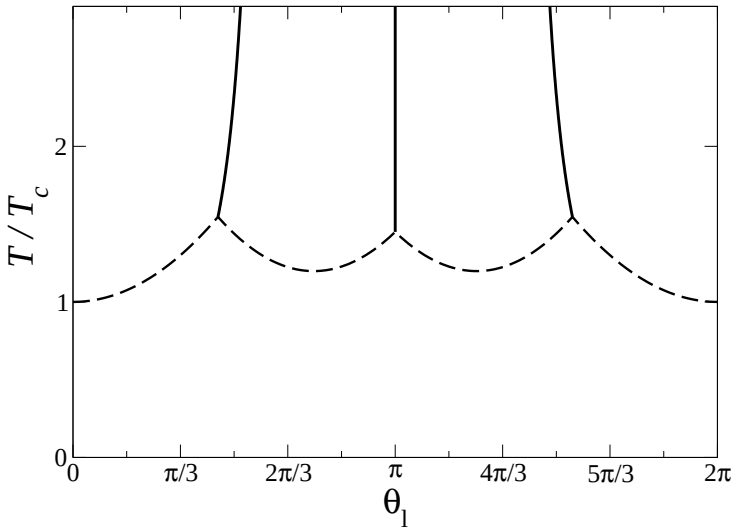
$\mu_{s,I} = 0$ **breaks** Z_2
explicitly, $\mu_{l,I}/T = \pi/3$
still within the analyticity range



For larger $\mu_{l,I}/T$**, finally, the transition to a different center sector take place**

When $\mu_s = 0$**, the situations is different.** $\theta_l = \pi/3$ **is still within the analyticity range. The center sector jump happens for larger** $\theta_l \sim 0.45\,\pi$





LEFT: $T - \theta_l$ **plane for** $\mu_s = \mu_l$

RIGHT: $T - \theta_l$ **plane for** $\mu_s = 0$**: range available for analytic continuation is larger**

Numerical Results

We consider the chiral condensate and its susceptibility as probes for the location of the pseudo-critical temperature:

$$\langle\bar{\psi}\psi_f\rangle = \frac{T}{V}\frac{\partial \log Z}{\partial m_f} \qquad \chi^f_{\bar{\psi}\psi} = \frac{\partial\langle\bar{\psi}\psi_f\rangle}{\partial m_f} = \chi^{disc}_{\bar{\psi}\psi} + \chi^{conn}_{\bar{\psi}\psi}$$

$$\chi^{disc}_{\bar{\psi}\psi} \equiv \frac{T}{V}\left(\frac{N_f}{4}\right)^2\left[\langle(M_f^{-1})^2\rangle - \langle M_f^{-1}\rangle^2\right] \qquad \chi^{conn}_{\bar{\psi}\psi} \equiv -\frac{T}{V}\frac{N_f}{4}\langle M_f^{-2}\rangle\,.$$

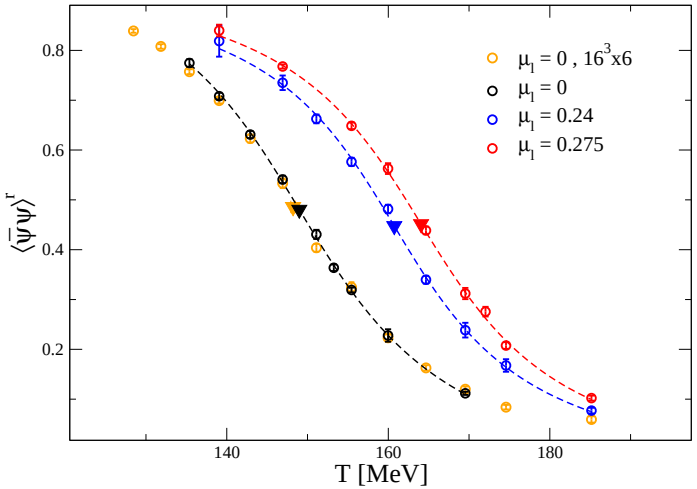
which need proper subtraction of additive and multiplicative renormalizations

$$\langle\bar{\psi}\psi\rangle^r_l(T) \equiv \frac{\left[\langle\bar{\psi}\psi\rangle_l - \frac{2m_l}{m_s}\langle\bar{s}s\rangle\right](T)}{\left[\langle\bar{\psi}\psi\rangle_l - \frac{2m_l}{m_s}\langle\bar{s}s\rangle\right](T=0)}\,,$$

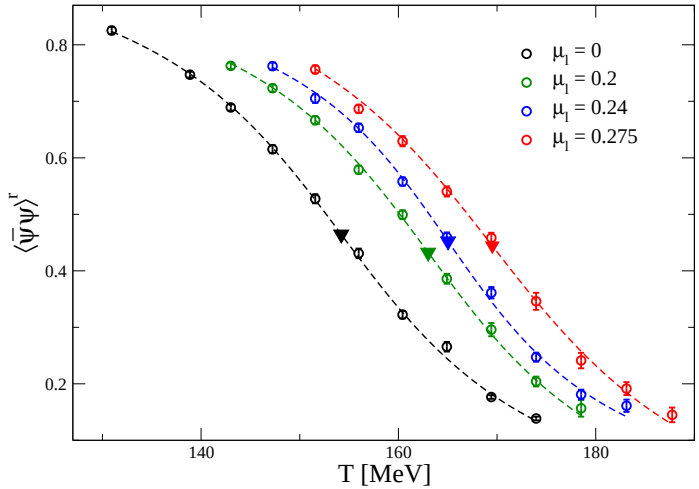
$\langle\bar{s}s\rangle$ **is the strange quark condensate,** $\langle\bar{\psi}\psi\rangle = \langle\bar{u}u\rangle + \langle\bar{d}d\rangle$ **is the light quark one.**

$$\chi^r_{\bar{\psi}\psi} = m_l^2\left[\chi_{\bar{\psi}\psi}(T) - \chi_{\bar{\psi}\psi}(T=0)\right]\,.$$

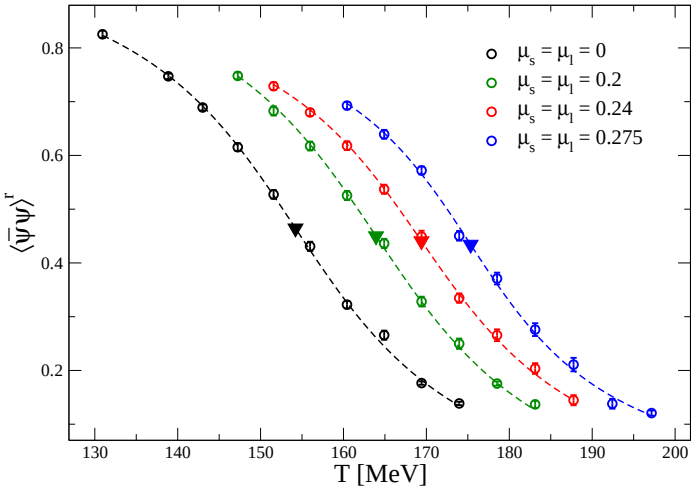
Results for the renormalized chiral condensate



$N_t = 6\,, \;\; \mu_s = 0$



$N_t = 8\,, \;\; \mu_s = 0$

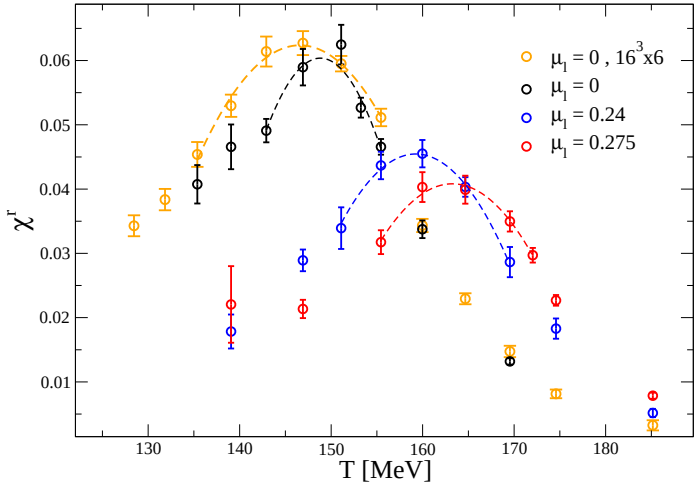


$N_t = 8\,, \;\; \mu_s = \mu_l$

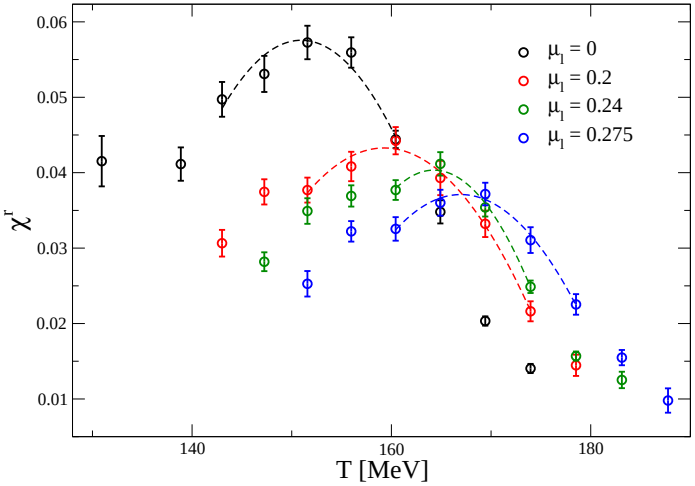
We locate T_c, for each setup of chemical potentials, as the point of maximum slope of the chiral condensate. This is fitted, e.g., by

$$\langle\bar{\psi}\psi\rangle_l^r(T) = A + B\arctan\left(C(T - T_c)\right)$$

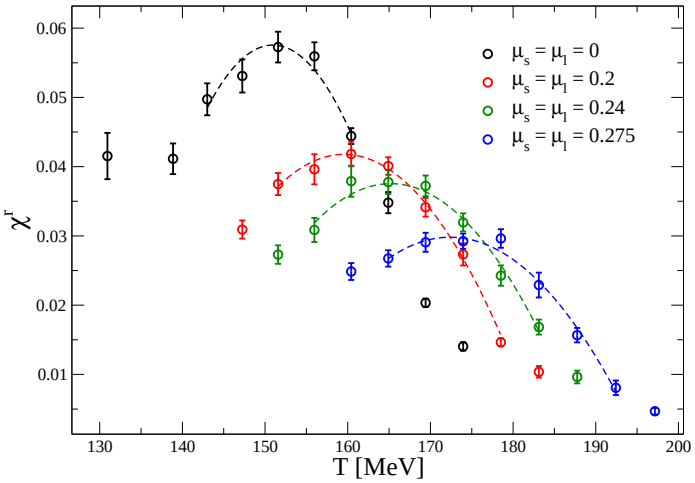
Results for the renormalized chiral susceptibility



$N_t = 6\,, \quad \mu_s = 0$



$N_t = 8\,, \quad \mu_s = 0$



$N_t = 8\,, \quad \mu_s = \mu_l$

We locate T_c, for each setup of chemical potentials, as the point where the susceptibility reaches a maximum This is fitted, e.g., by

$$\chi^r_{\bar{\psi}\psi} = A + B(T - T_c)^2$$

Lattice	$\mu_{l,I}/(\pi T)$	$\mu_{s,I}/(\pi T)$	$T_c(\bar{\psi}\psi)$	$T_c(\chi^r)$
$16^3 \times 6$	0.00	0.00	148.2(3)	146.6(8)
$16^3 \times 6$	0.20	0.00	155.0(4)	152.5(8)
$16^3 \times 6$	0.24	0.00	158.9(4)	155.9(7)
$16^3 \times 6$	0.275	0.00	161.2(4)	157.9(7)
$24^3 \times 6$	0.00	0.00	149.0(6)	148.7(4)
$24^3 \times 6$	0.24	0.00	160.8(7)	158.9(8)
$24^3 \times 6$	0.275	0.00	164.1(4)	163.3(5)
$32^3 \times 8$	0.00	0.00	154.2(4)	150.9(1.1)
$32^3 \times 8$	0.20	0.00	162.9(8)	159.3(1.3)
$32^3 \times 8$	0.24	0.00	165.0(5)	164.3(8)
$32^3 \times 8$	0.275	0.00	169.5(9)	166.8(1.0)
$32^3 \times 8$	0.20	0.20	163.9(6)	159.7(1.2)
$32^3 \times 8$	0.24	0.24	169.4(7)	165.3(7)
$32^3 \times 8$	0.275	0.275	175.4(6)	172.5(9)

This is a collection of results for T_c in the various setups.

We have different spatial volumes in some cases, in order to check that finite size effects are not large.

Small errors on T_c do not take into account uncertainties on the physical scale (2-3%), which cancels in the ratio of temperatures

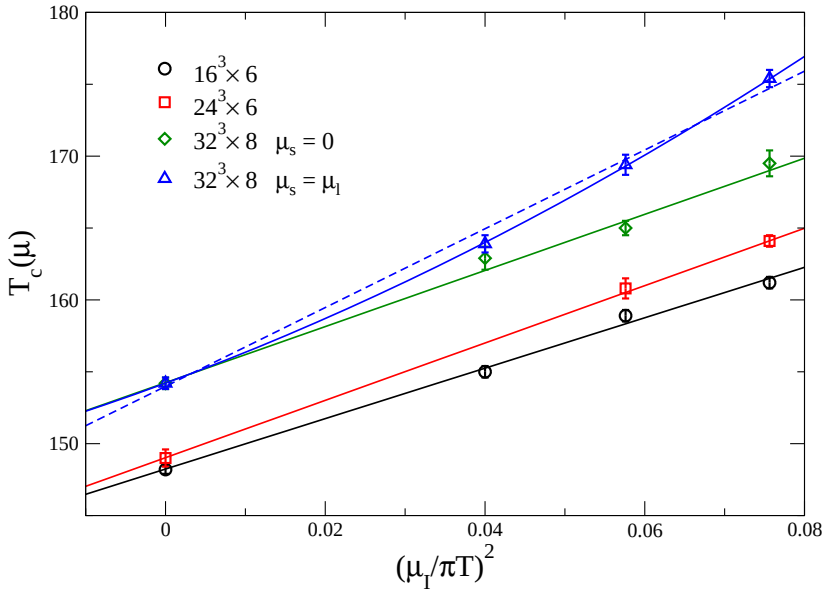
Once $T_c(\mu_{l,I})$ is found, we can fit it according to

$$T_c(\mu_{l,I}) = T_c(0)(1 + 9\kappa(\theta_l^2 + b\theta_l^4))$$

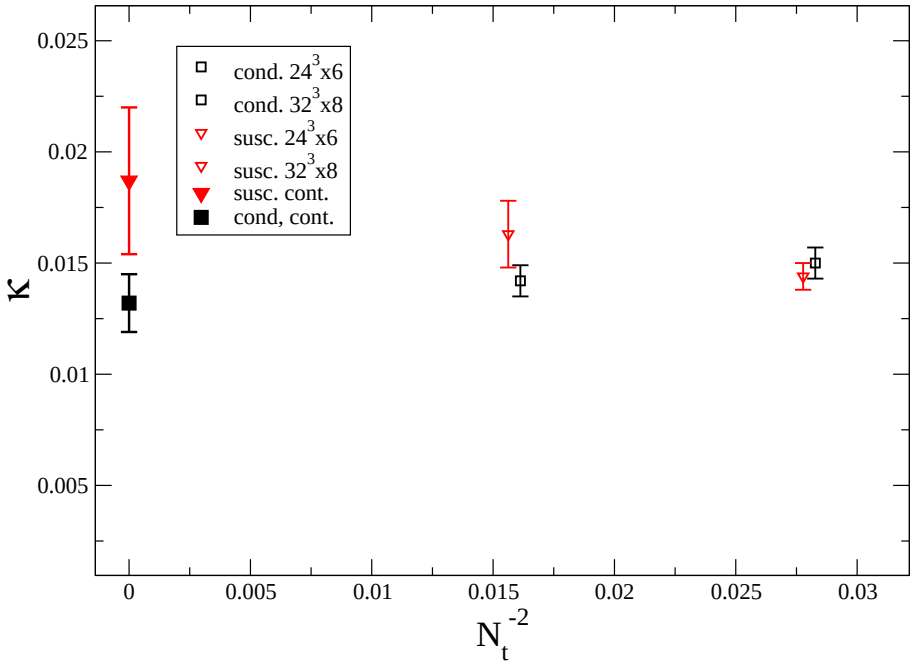
where $\theta_l = \mu_{l,I}/T$. The quartic term is needed in some cases to fit data.

Results from the chiral condensate

Lattice	μ_s	$T_c(0)$	κ	b	$\tilde{\chi}^2$
$16^3 \times 6$	0.00	148.2(3)	0.0133(4)	-	1.4
$24^3 \times 6$	0.00	149.1(6)	0.0150(7)	-	0.17
$32^3 \times 8$	0.00	154.2(4)	0.0142(7)	-	1.2
$32^3 \times 8$	μ_l	154.0(4)	0.0200(6)	-	2.5
$32^3 \times 8$	μ_l	154.2(4)	0.0149(24)	0.0008(4)	0.04



- A linear behavior in μ_l^2 fits well data, apart from the case $\mu_s = \mu_l$, where a non-linear correction is needed
- Setting $\mu_s = \mu_l$ increases the change in T_c considerably, but that seems mostly due to non-linear corrections. The different phase structure in the $T - \mu_{l,I}$ plane may explain such increased non-linear corrections.
- The linear term (curvature) shows very small finite size and finite lattice spacing corrections (much less than T_c itself)
- Data from the chiral susceptibilty show a similar behavior



We have tried a continuum extrapolation

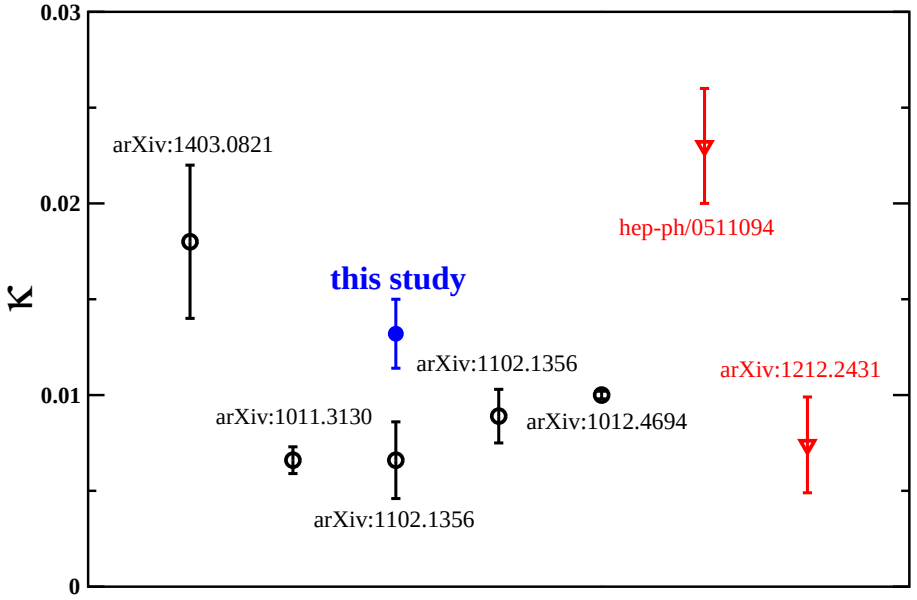
$$\kappa(N_t) = \kappa_{cont} + A/N_t^2$$

but we still have only two lattice spacings, so this is very preliminary.

$$\kappa_{cont}^{cond} = 0.132(18)$$

$$\kappa_{cont}^{susc} = 0.185(37)$$

We can compare our determination (from $\langle\bar{\psi}\psi\rangle_l^r$) to other lattice determinations



Main observations:

- **compatible with results from analytic continuation and a different discretization (arXiv:1403.0821, HISQ action)**
- **generally larger than estimates by Taylor expansion. Especially relevant is comparison with arXiv:1102.1356: same discretization, same observable (chiral condensate)**

Possible systematics?

– **Different observables: renormalized susceptibility vs disconnected susceptibility, or different prescriptions for renormalization: checked, not significant**

– **Different ways to monitor $T_c(\mu_B)$. A strategy adopted in Taylor expansion (arXiv:1102.1356) is to monitor the behavior of some observable ϕ (e.g., order parameter), and define $T_c(\mu_B)$ by**

$$\phi(T_c(\mu_B), \mu_B) = \phi(T_c(0), 0) \; .$$

so that

$$\kappa \equiv -T_c(0) \left. \frac{\mathrm{d}T_c(\mu_B)}{\mathrm{d}\mu_B^2} \right|_{\mu_B=0} = T_c(0) \left. \frac{\partial\phi/\partial\mu_B^2}{\partial\phi/\partial T} \right|_{\mu_B=0, T=T_c} ,$$

If we adopt a similar prescription (line of constant condensate instead of maximum slope) we obtain a decrease in κ by about 10%, bringing the deviation within 2 σ

Conclusions

- **We have determined the curvature of the pseudocritical line for $N_f = 2 + 1$ QCD at the physical point, by analytic continuation from imaginary chemical potentials**

- **Curvature generally larger (2σ) than previous determinations by Taylor expansion. Continuum extrapolation still needed**

- **The inclusion of non-zero μ_s leads to a change of $T_c(\mu)$, but mostly regarding non-linear terms, the curvature itself does not change much within present errors.**

- **In the future we plan to repeat our analysis by considering quark number susceptibilities.**