BROOKHAVEN
NATIONAL LABORATORY

The total chiral susceptibility

at finite chemical potential

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Chiral crossover in QCD at zero and non-zero chemical potentials ☆

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Abstract

We present results for pseudo-critical temperatures of QCD chiral crossovers at zero and non-zero values of baryon (B), strangeness (S), electric charge (Q), and isospin (I) chemical potentials $\mu_{X=B,Q,S,I}$. The results were obtained using lattice QCD calculations carried out with two degenerate up and down dynamical quarks and a dynamical strange quark, with quark masses corresponding to physical values of pion and kaon masses in the continuum limit. By parameterizing pseudo-critical temperatures as $T_c(\mu_X) = T_c(0)\left[1 - \kappa_2^X(\mu_X/T_c(0))^2 - \kappa_4^X(\mu_X/T_c(0))^4\right]$, we determined κ_2^X and κ_4^X from Taylor expansions of chiral observables in μ_X. We obtained a precise result for $T_c(0) = (156.5 \pm 1.5)$ MeV. For analogous thermal conditions at the chemical freeze-out of relativistic heavy-ion collisions, *i.e.*, $\mu_S(T, \mu_B)$ and $\mu_Q(T, \mu_B)$ fixed from strangeness-neutrality and isospin-imbalance, we found κ_2^B=0.012(4) and κ_4^B=0.000(4). For $\mu_B \lesssim 300$ MeV, the chemical freeze-out takes place in the vicinity of the QCD phase boundary, which coincides with the lines of constant energy density of 0.42(6) GeV/fm^3 and constant entropy density of 3.7(5) fm^{-3}.

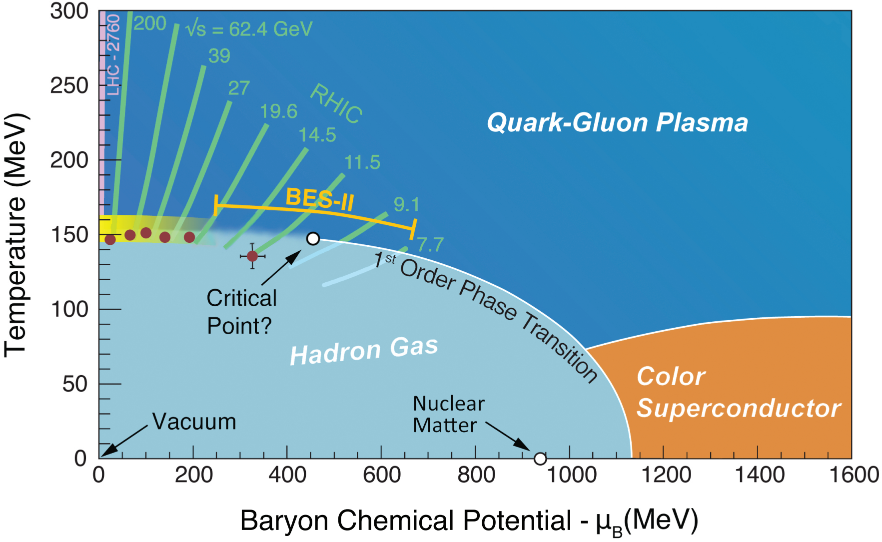
1. Introduction

The spontaneous breaking of the chiral symmetry in quantum chromodynamics (QCD) is a key ingredient for explaining the masses of hadrons that constitute almost the entire mass of our visible Universe. Lattice-regularized QCD calculations have demonstrated (near) restoration of the broken chiral symmetry in QCD at high temperature (T) through a smooth crossover [1]. The chiral crossover temperature of QCD marks the epoch at which massive hadrons were born during the evolution of the early Universe. The chiral crossover in the early Universe took place at vanishingly small baryon chemical potential μ_B, although the electric charge chemical potential μ_Q at that stage might have been non-vanishing [2]. For $\mu_B > 0$, *i.e.*, when QCD-matter is doped with an

the proximity of the chiral crossover phase boundary in the T-μ_B plane [5]. Since the colliding heavy-ions do not carry any net strangeness, the medium formed in the process is strangeness-neutral, *i.e.*, characterized by $n_S = 0$, n_S being the net strangeness-density. Additionally, the proton-to-neutron ratio of the colliding nuclei determines the ratio of net charge-density (n_Q) to net baryon-density (n_B) of the produced medium. For the most common relativistic heavy-ion collisions with Au+Au and Pb+Pb this ratio turns out to be $n_Q/n_B = 0.4$; consequently, the corresponding chemical freeze-out stages also respect the conditions $n_S = 0$ and $n_Q = 0.4n_B$.

With the aid of state-of-the-art lattice-regularized QCD calculations this work aims at determining chiral pseudo-critical temperatures in QCD at zero and non-zero chemical potentials $\mu_{B,Q,S}$, as well as for the situation analo-

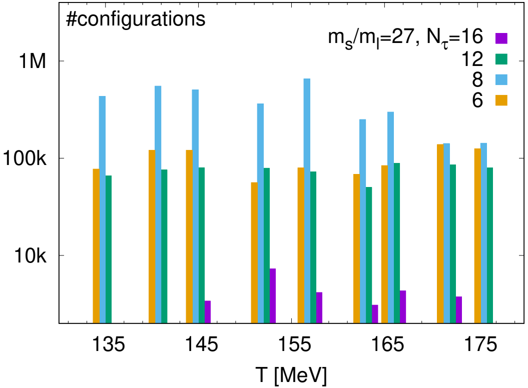
The QCD phase diagram



Quantum Chromodynamics

from first principles

- Lattice QCD
  - HISQ action
  - $N_\sigma = 4N_\tau$
  - sim. at $\mu = 0$
- physical quarks
  - 2 light quarks
  - 1 strange quark
  - $m_s/m_l = 27$
- $m_\pi \simeq 138\ \mathrm{MeV}$



everything continuum extrapolated

Chiral observables in two-flavor formulation

- subtracted condensate

$$\Sigma_{\text{sub}} \equiv m_s(\Sigma_u + \Sigma_d) - (m_u + m_d)\Sigma_s$$

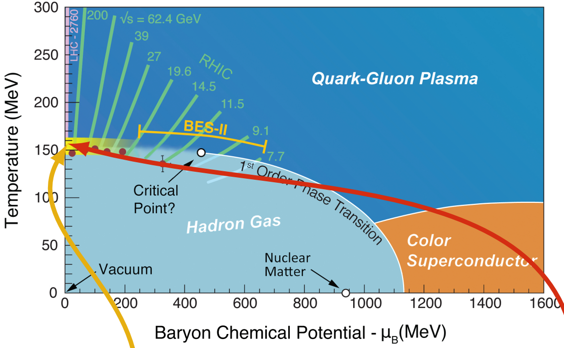
with $\qquad \Sigma_f = \frac{T}{V}\frac{\partial}{\partial m_f} \ln Z$

- total subtracted susceptibility

$$\chi_{\text{sub}} \equiv \frac{T}{V} m_s \left(\frac{\partial}{\partial m_u} + \frac{\partial}{\partial m_d} \right) \Sigma_{\text{sub}}$$

- χ_{disc} is defined as χ_{sub} without connected part

Start of the QCD crossover line: T_0



$$\frac{d^2}{dT^2}\frac{\Sigma_{\rm sub}}{f_K^4} \equiv 0 \qquad \text{and} \qquad \frac{d}{dT}\frac{\chi_{\rm sub}}{f_K^4} \equiv 0$$

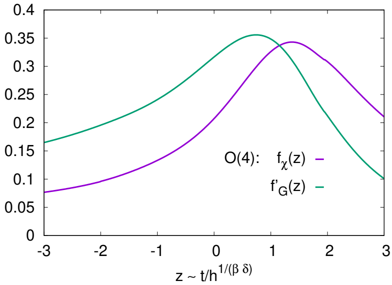
two crossover temperatures: $T_0\left(\Sigma_{\rm sub}\right)$ and $T_0\left(\chi_{\rm sub}\right)$

Pseudo-critical temperatures

- for $m_l \to 0$: pseudo-critical temperatures converge to the chiral transition temperature $T_c^0 = 132^{+3}_{-6}\,\mathrm{MeV}$

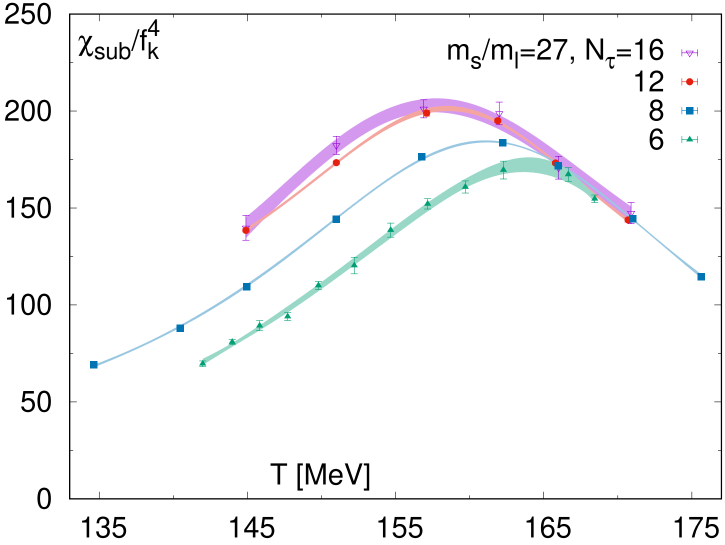
- at finite quark mass T_0 is given by maximum of $O(4)$ universal scaling functions + corrections from regular terms

$$\chi_m = h^{1/\delta-1} \quad f_\chi(z) + \mathrm{reg.}$$
$$\chi_t = h^{(\beta-1)/\beta\delta} f'_G(z) + \mathrm{reg.}$$

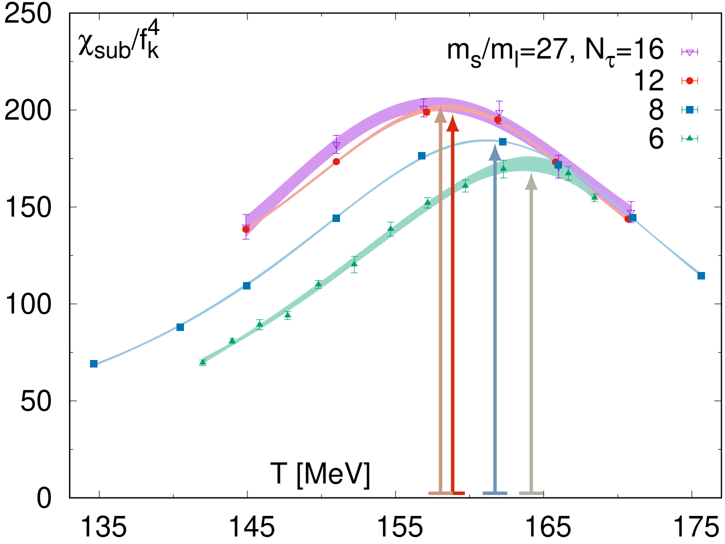


- for $m_l \to 0$
  - $\chi_t \sim \partial_T \Sigma_{\mathrm{sub}}$ and $\chi_t \sim \partial^2_{\mu_B} \Sigma_{\mathrm{sub}}$
  - $\chi_m \sim \chi_{\mathrm{sub}}$ and $\chi_m \sim \chi_{\mathrm{disc}}$

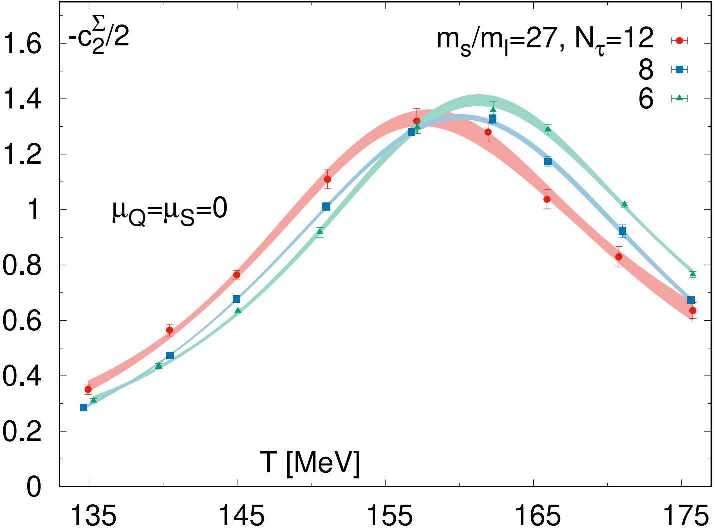
The subtracted chiral susceptibility



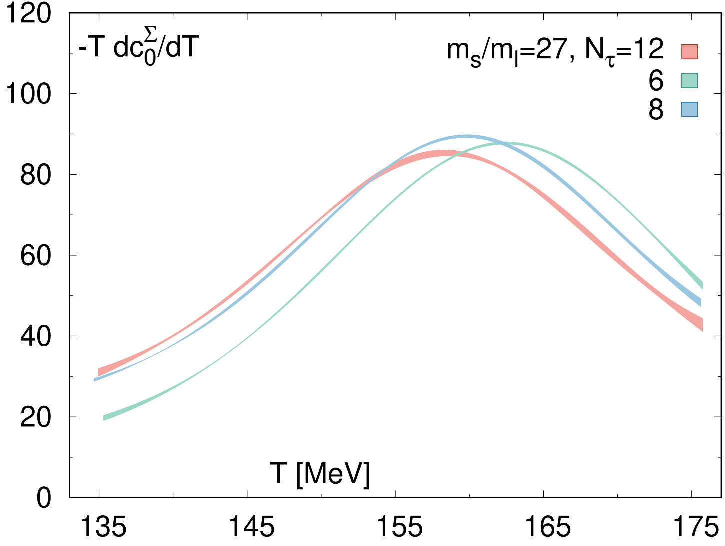
The subtracted chiral susceptibility



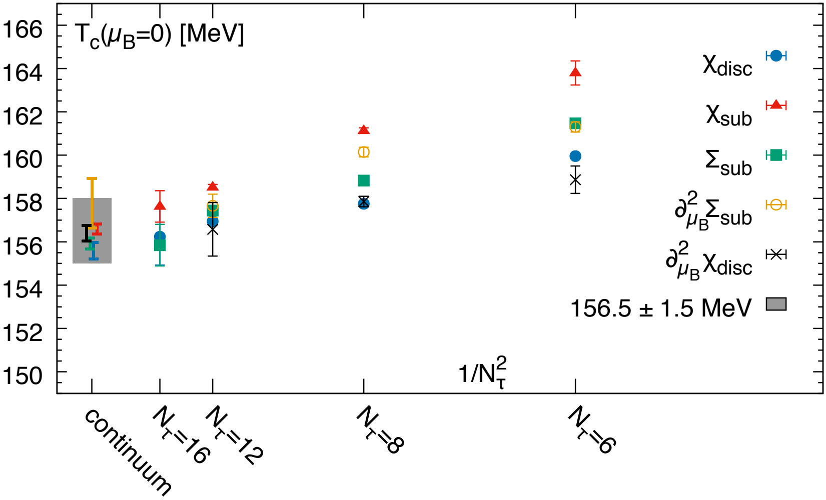
The 2nd μ_B derivative of chiral condensate Σ_{sub}



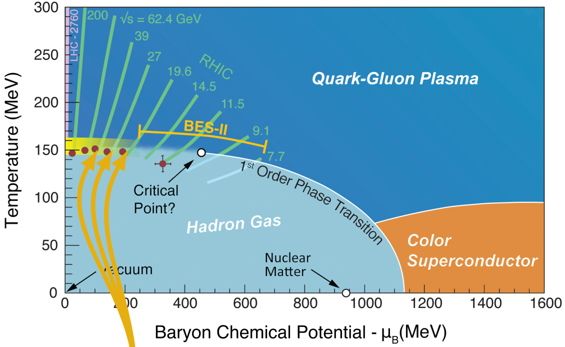
The 1st T derivative of chiral condensate $\Sigma_{\rm sub}$



The T_0 continuum extrapolation



The QCD crossover at $\mu \neq 0$



$$\frac{d^2}{dT^2}\frac{\Sigma_{\rm sub}(T,\mu_B)}{f_K^4} \equiv 0 \qquad \text{and} \qquad \frac{d}{dT}\frac{\chi_{\rm disc}(T,\mu_B)}{f_K^4} \equiv 0$$

need Taylor expansion in T and μ_B around $(T_0, 0)$

1. Taylor expansion in chemical potentials

- subtracted condensate for $\mu_Q = \mu_S = 0$

$$\frac{\Sigma_{\rm sub}}{f_K^4} = \sum_{n=0}^{\infty} \frac{c_n^\Sigma}{n!} \hat{\mu}_B^n \qquad \text{with} \qquad c_n^\Sigma = \left. \frac{\partial \Sigma_{\rm sub}/f_K^4}{\partial \hat{\mu}_B^n} \right|_{\mu=0}$$

- analysis of convergence radius can determine bound on the location of a critical point:

$$r_{2n}^\Sigma = \left| (2n+2)(2n+1) \frac{c_{2n}^\Sigma}{c_{2n+2}^\Sigma} \right|^{1/2}$$

- only if coefficients are positive for all $n \geq n_0$
  - if not $\rightarrow$ no critical point on real axis

Radius of convergence

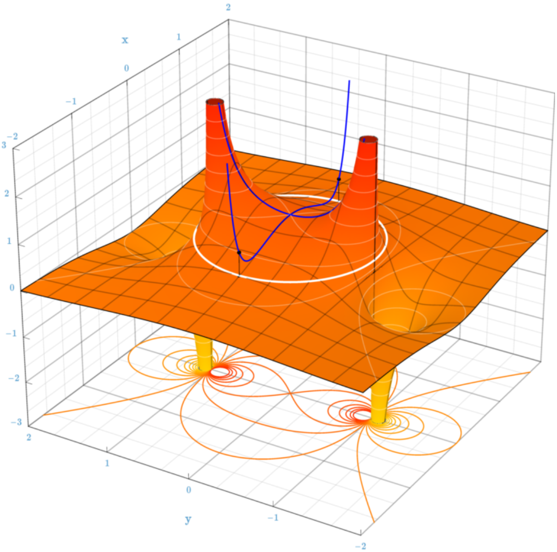
- complex function

  $$f(z) = \frac{1}{1+z^2}$$

- series expansion

  $$f(z) = \sum_n^{\infty} (-1)^n z^{2n}$$

- convergence determined by nearest singularity from the origin



2. Random noise method

condition:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \eta_{ki}^{*} \eta_{kj} = \delta_{ij}$$

99% of runtime

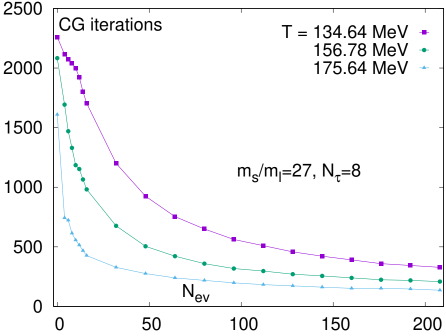
$$\mathrm{Tr}\, M^{-1} = \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \eta_k^{\dagger} M^{-1} \eta_k$$

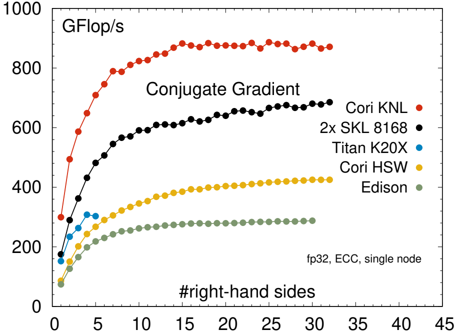
- evaluate traces using N random noise vectors η

  up to 2000 η per gauge field configuration

- Taylor expansion requires more complicated traces
  - e.g. $\mathrm{Tr}\left(M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1}\right)$

3. Conjugate Gradient





- improved CG using deflation and multiple right-hand sides

4. The curvature of the crossover line

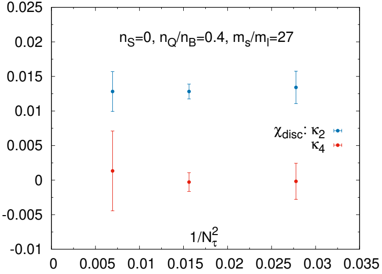
$$\frac{T_c(\mu_B)}{T_0} = 1 - \kappa_2 \left(\frac{\mu_B}{T_0}\right)^2 - \kappa_4 \left(\frac{\mu_B}{T_0}\right)^4 + \mathcal{O}(\mu_B^6)$$

- Taylor expansion in μ and T of:

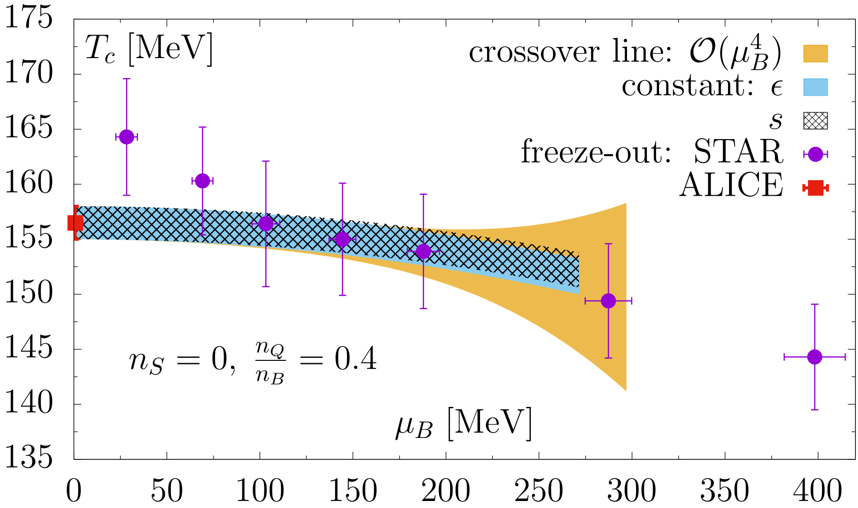
$$\frac{d}{dT}\frac{\chi_{\rm disc}(T,\mu_B)}{f_K^4} = (\ldots)\mu_B^2 + (\ldots)\mu_B^4 + \ldots = \mathbf{0}$$

- has to be zero order by order

$$\kappa_2 = \frac{1}{2T_0^2}\frac{T_0 \left.\frac{\partial c_2^\chi}{\partial T}\right|_{(T_0,0)} - 2\, c_2^\chi\big|_{(T_0,0)}}{\left.\frac{\partial^2 c_0^\chi}{\partial T^2}\right|_{(T_0,0)}}$$

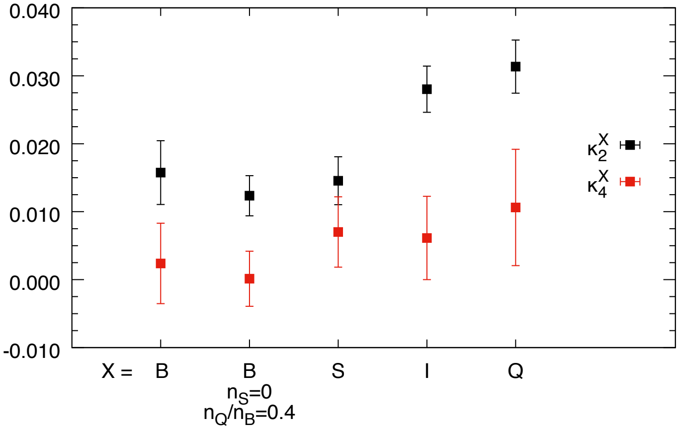


The QCD crossover line

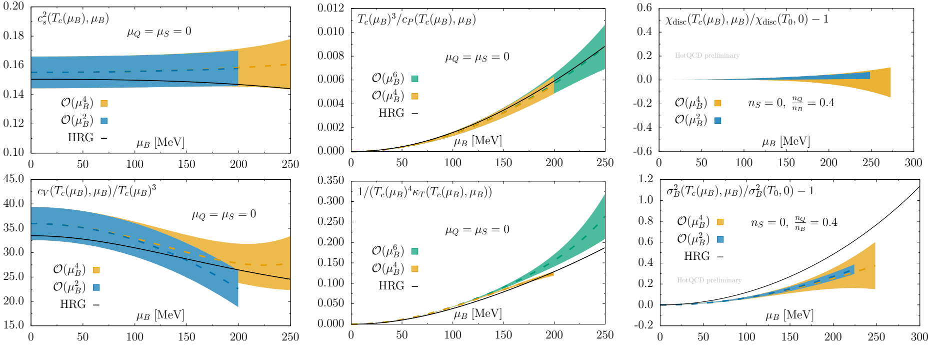


The QCD crossover surface

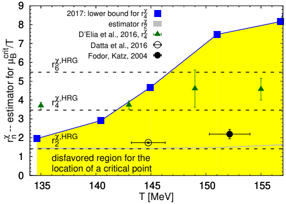
$$\frac{T_c(\mu_X)}{T_0} = 1 - \kappa_2^X \left(\frac{\mu_X}{T_0}\right)^2 - \kappa_4^X \left(\frac{\mu_X}{T_0}\right)^4 + \mathcal{O}(\mu_X^6)$$

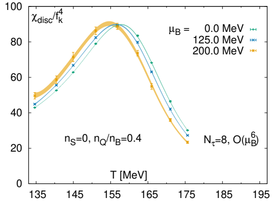


No signs for a QCD critical point along $T_c(\mu_B)$



- no deviations from HRG
- no increased fluctuations
- no narrowing crossover





USQCD Proposal

Motivation

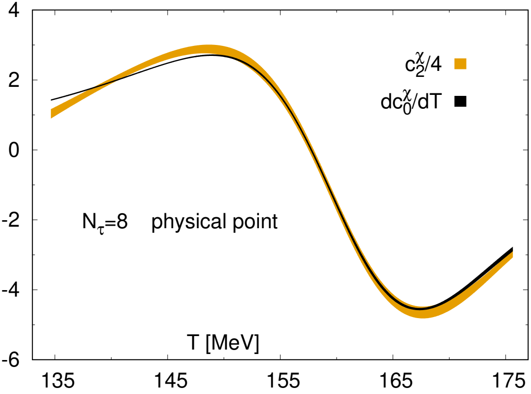
Is $\partial^2/\partial\mu_B^2$ proportional to $\partial/\partial T$ at the physical point?

- χ_{disc} might be described by universal scaling function if corrections from regular terms are small

- if so, χ_{disc} must obey:

$$\kappa_2 = \frac{1}{2T_0}\frac{c_2^\chi}{\frac{\partial c_0^\chi}{\partial T}}$$

$$\kappa_2 \simeq 0.0126 \qquad \Longleftarrow$$



- excellent agreement to our value

2019 Proposal

- logical extension of our crossover paper
  - χ_{disc} is only a proxy for χ_{sub}
  - no full understanding of regular part contributions

- compute Taylor expansion of χ_{sub} up to $\mathcal{O}(\mu_B^2)$
  - extract curvature κ_2

- in combination with our crossover paper
  - unambiguous determination of the QCD crossover line

- scaling analysis
  - comparison to $O(4)$ model predictions
  - determine if physical point is close to scaling regime

Scaling Analysis

- comes as a by-product from Taylor expansion

$$\frac{\chi_{\mathrm{sub}}}{f_K^4} = \sum_{n=0}^{\infty} \frac{c_n^\chi}{n!} \hat{\mu}_B^n \qquad \text{with} \qquad c_n^\chi = \left. \frac{\partial \chi_{\mathrm{sub}}/f_K^4}{\partial \hat{\mu}_B^n} \right|_{\mu=0}$$

- second order c_2^χ requires to compute $\mathrm{Tr}\left(M^{-1} M^{-1} M^{-1}\right)$
  - needed for computing $\partial_{m_s} \chi_{\mathrm{sub}}$ and $\partial_{m_{u,d}} \chi_{\mathrm{sub}}$
  - compare to known $O(4)$ ratios e.g. $\frac{h\,\partial_{m_{u,d}} \chi_{\mathrm{sub}}}{\Sigma_{\mathrm{sub}}}$, $\frac{h\,\partial_{m_{u,d}} \chi_{\mathrm{sub}}}{\chi_{\mathrm{sub}}}$, ...

- is $\partial^2/\partial\mu_B^2 \sim \partial/\partial T \sim \partial/\partial m$ at the physical point?
  - test if $\partial_T \chi_{\mathrm{sub}} \sim \partial^2_{\mu_B} \chi_{\mathrm{sub}} \sim \partial_{m_s} \chi_{\mathrm{sub}} \sim \partial^6_{\mu_B} P$

Requested computing time

- measure Taylor expansion of total susceptibility up to $\mathcal{O}(\mu_B^2)$
- re-use existing $32^3 \times 8$ HISQ ensembles
- temperature range: 135 MeV - 175 MeV
- physical quark masses $\rightarrow m_\pi \simeq 138\ \mathrm{MeV}$

	$\#T$	#conf./T	KNL core-h
total request	9	170k	**97.9 M**

Thank you for your attention!

Akaike Information Criterion (AIC)

- need Σ_{sub} and χ_{sub} as continuous function of T
- fit data with several Padé $P_i(T)$ using AIC

$$\overline{P}(T) = \sum_{i=0}^{R} w_i P_i(T)$$

i-th Padé $[m, n]$

model mean

Akaike weight:

- function of χ^2 and #param.

- statistical and systematic error

$$\mathrm{var}\left(\overline{P}(T)\right) = \left(\sum_{i=0}^{R} w_i \sqrt{\mathrm{var}(P_i(T)) + \left(P_i(T) - \overline{P}(T)\right)^2}\right)^2$$

Let's test the Padé AIC method

1. create fake data using Ansatz

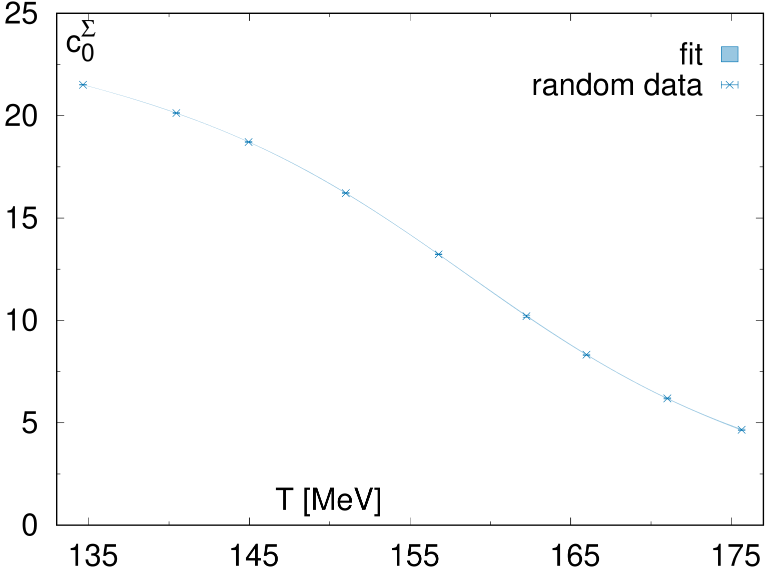
$$\frac{\Sigma_{\mathrm{sub}}}{f_K^4} \equiv c_0^{\Sigma}(T) = A + B\arctan(C(T - T_0))$$

2. generate N data points and add noise

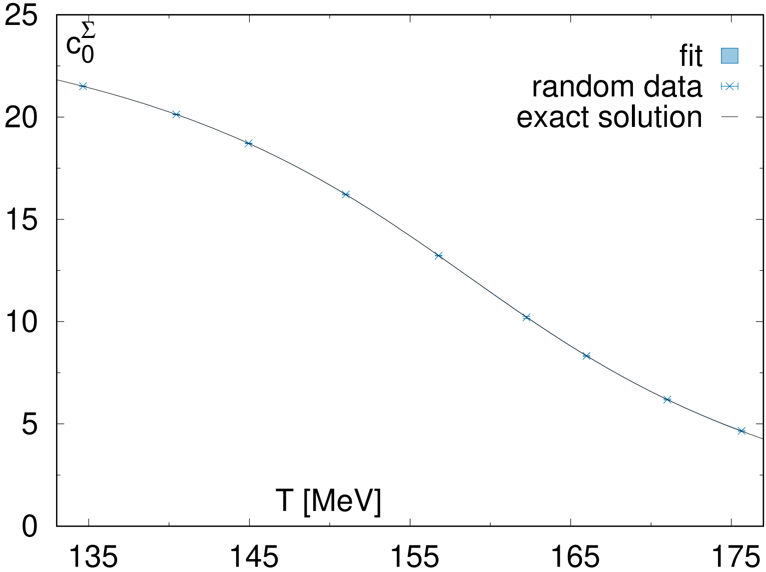
3. fit data with the Padé AIC method

4. compare to exact solution

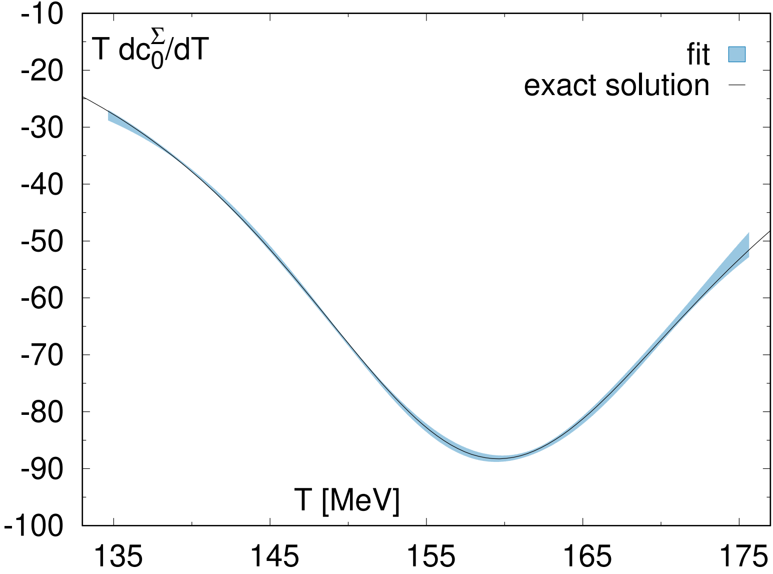
Let's compare...



Let's compare...



Let's compare...



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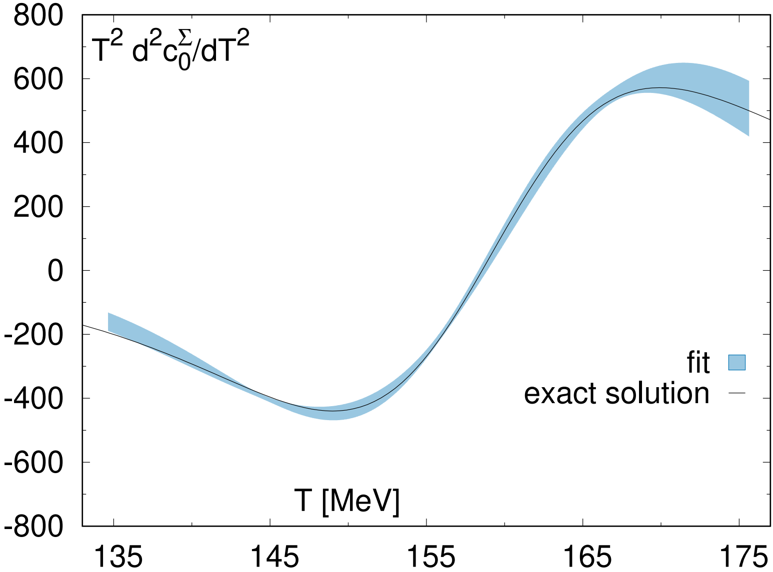
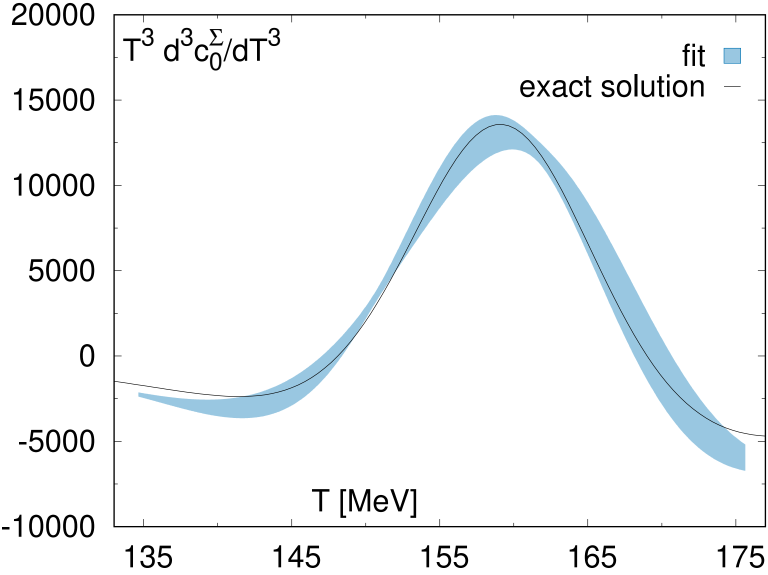


Let's compare...



Let's compare...