Recent results on QCD thermodynamics from lattice simulations

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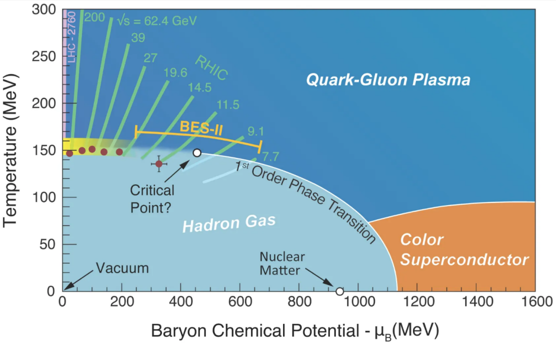
The phase diagram of QCD

What do we know about QCD thermodynamics at finite T, μ_B?

From a combination of approaches (experiment, models, first principle calculations, ...), *we are pretty sure* of some things, and *suspect* others.

- ⋆ Ordinary nuclear matter at $T \simeq 0$, $\mu_B \simeq 922\,\mathrm{MeV}$
- ⋆ Smooth crossover for $\mu_B = 0$ at $T \simeq 155 - 160\,\mathrm{MeV}$
- ⋆ Transition line at finite μ_B is known to some precision (+ freeze-out extraction)
- ⋆ Perturbative regime is under control: high T, μ_B
- ⋆ Compact astronomical objects at low-T, high-μ_B
- ⋆ Critical point? Exotic phases?



Lattice formulation of QCD

In a nutshell, lattice QCD amounts to calculating path integrals like

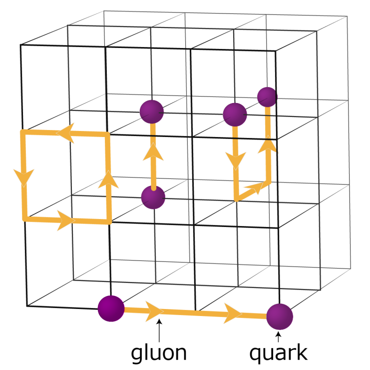
$$\mathcal{Z}[A,\bar{\psi},\psi] = \int \mathcal{D}A^a_\mu(x)\,\mathcal{D}\bar{\psi}(x)\,\mathcal{D}\psi(x)\,e^{-\int d^4x\,\mathcal{L}_E[A,\bar{\psi},\psi]}$$

by defining the theory on a discretized 3+1d lattice with $N_s^3 \times N_\tau$ sites. This allows us to reduce the (otherwise infinite) dimensionality of the problem.

- The quark fields $\bar{\psi},\psi$ are defined on the lattice sites, the gauge fields A_μ are defined on the lattice links as $U_\mu = \exp[iaA_\mu]$
- Now, one can calculate a *finite* number of integrals to evaluate expressions of the like:

$$Z[U,\bar{\psi},\psi] = \int \mathcal{D}U\,\mathcal{D}\bar{\psi}\,\mathcal{D}\psi\,e^{-S_G[U,\bar{\psi},\psi]-S_F[U,\bar{\psi},\psi]}$$

where S_G and S_F are the gauge (gluonic) and fermionic actions

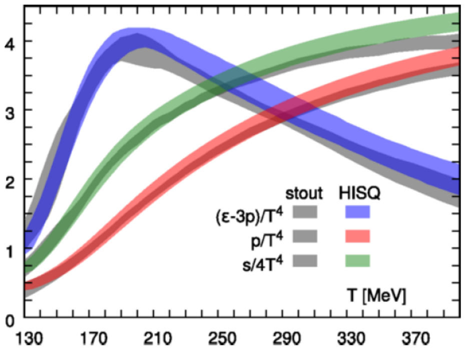


The equation of state of QCD at $\mu_B = 0$

- A crucial input to modeling of heavy-ion collisions (hydro)
- Known at $\mu_B = 0$ to high precision for a few years now (continuum limit, physical quark masses) $\longrightarrow$ Agreement between different calculations

From grancanonical partition function $\mathcal{Z}$

- ⋆ **Pressure**: $p = -k_B T \frac{\partial \ln \mathcal{Z}}{\partial V}$
- ⋆ **Entropy density**: $s = \left(\frac{\partial p}{\partial T}\right)_{\mu_i}$
- ⋆ **Charge densities**: $n_i = \left(\frac{\partial p}{\partial \mu_i}\right)_{T,\mu_{j\neq i}}$
- ⋆ **Energy density**: $\epsilon = Ts - p + \sum_i \mu_i n_i$
- ⋆ More (**Fluctuations**, etc...)



WB: Borsányi *et al.*, PLB 370 (2014) 99-104; HotQCD: Bazavov *et al.*, PRD 90 (2014) 094503

Finite density: the sign/complex action problem

Euclidean path integrals on the lattice are calculated with Monte Carlo methods using importance sampling, interpreting the factor $\det M[U]\, e^{-S_G[U]}$ as the Boltzmann weight for the configuration U

$$
\begin{aligned}
Z(V,T,\mu) &= \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi}\; e^{-S_F(U,\psi,\bar{\psi})-S_G(U)} \\
&= \int \mathcal{D}U\; \det M(U) e^{-S_G(U)}
\end{aligned}
$$

- When there is particle-antiparticle-symmetry, i.e. $\mu = 0$, $\det M(U)$ is real
- For real chemical potential ($\mu^2 > 0$), $\det M(U)$ becomes complex (**complex action problem**) and has wildly oscillating phase (**sign problem**)
- Then, it cannot serve as a statistical weight, importance sampling cannot be used, and simulations are unfeasible
- For *purely imaginary* chemical potential ($\mu^2 < 0$) $\rightarrow$ $\det M(U)$ is real again, simulations can be made!

Lattice investigations of the phase diagram

I. QCD transition temperature

Study of the volume and μ_B dependence of T_c

Borsànyi, PP *et al*, 2405.12320

II. Search for critical point with baryon fluctuations

Large-statistics study of Lee-Yang edge singularities

Adam, PP *et al*, coming soon

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Deconfinement and chiral symmetry restoration

The QCD transition is characterized by the spontaneous breaking of two approximater symmetries (SSB)

- **Chiral symmetry restoration**: $SU(2) \times SU(2)$ symmetry (exact for $m_q \to 0$). Order parameter is **chiral condensate**

$$\langle \bar{\psi}\psi \rangle = \frac{T}{V} \frac{\partial \log \mathcal{Z}}{\partial m_{ud}}$$

  Symmetric phase $\langle \bar{\psi}\psi \rangle = 0$ at high-T, and SSB $\langle \bar{\psi}\psi \rangle \neq 0$ at low-T

- **Deconfinement**: $\mathbb{Z}(3)$ center symmetry (exact for $m_q \to \infty$). Order parameter is **Polyakov loop**

$$P(\vec{x}) = \prod_{x_4=0}^{N_\tau - 1} U_4(\vec{x}, x_4) \sim e^{-F/T}$$

  Symmetric phase $P = 0$ ($F \to \infty$) at low-T and SSB $P = 1$ ($F \to 0$) at high-T

A study of T_c

We wish to study the dependence of T_c on the volume V and the chemical potential μ_B

We employ our 4stout staggered action (**Bellwied, PRD 114505 (2015)**) with:

- $N_f = 2 + 1 + 1$ with physical quark masses
- Simulations at $\mu_B = 0$ on $N_\tau = 12$ lattices with $N_s = 20, 24, 28, 32, 40, 48, 64$
- Simulations at imaginary chemical potential with Im $(\mu_B) = i\frac{\pi}{8}n$ with $n = 0, 3, 4, 5, 6, 6.5, 7,$ on $N_\tau = 12$ lattices with $N_s = 32, 40, 48$
- We consider the strangeness neutral case $\langle n_s \rangle = 0$ relevant for heavy ion physics

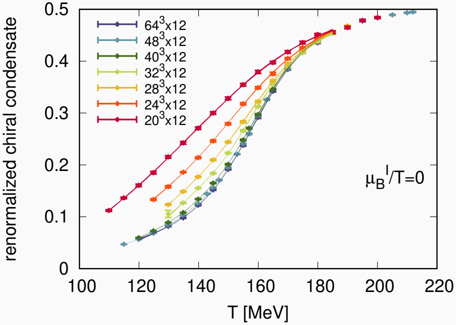
We investigate the behaviour of T_c related to both chiral symmetry restoration and deconfinement, looking for analogies and differences

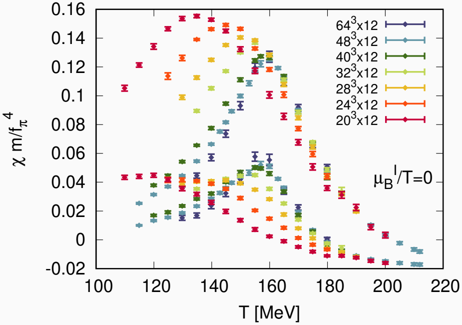
A study of T_c: chiral symmetry

Besides $\langle\bar\psi\psi\rangle$, we look at the chiral susceptibility, as well as its disconnected part:

$$\chi = \frac{T}{V}\frac{\partial^2 \log \mathcal{Z}}{\partial m_{ud}^2} \qquad \chi_{disc} = \frac{T}{V}\left.\frac{\partial^2 \log \mathcal{Z}}{\partial m_u \partial m_d}\right|_{m_u=m_d}$$

An estimate of T_c is obtained from **i.** $\langle\bar\psi\psi\rangle = \text{const}$ or **ii.** the peak of χ





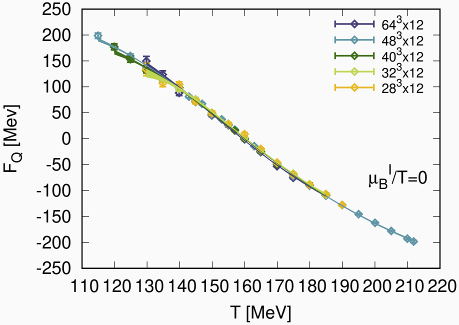
Volume effects are small at high-T, large at small-T, and T_c goes up with V

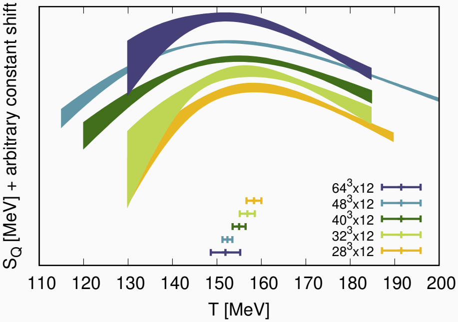
A study of T_c: deconfinement

Starting from the Polyakov loop $P \sim e^{-F/T}$, we study the static quark free energy F_Q and its derivative $S_Q = -\frac{\partial F_Q}{\partial T}$:

$$F_Q = -T \log\left(\frac{1}{\Lambda}\sum_{\vec{x}} \left|\langle P(\vec{x})\rangle_T\right|\right) + T_0 \log\left(\frac{1}{\Lambda}\sum_{\vec{x}} \left|\langle P(\vec{x})\rangle_{T_0}\right|\right)$$

An estimate of T_c is obtained from **i.** $F_Q = \text{const}$ or **ii.** the peak of S_Q



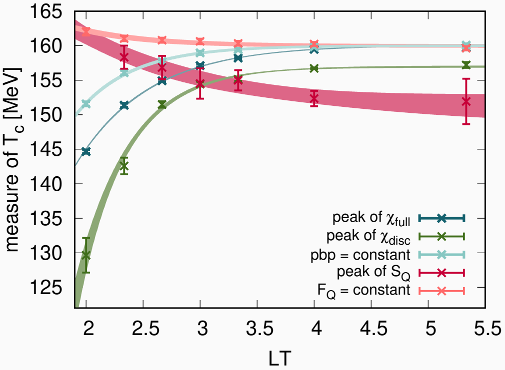


Volume effects much milder than for chiral observables, and T_c goes down with V

Measures of T_c vs V

Combining the estimates of T_c from different observables and volumes we can draw some conclusions:

- Chiral transition T_c estimates have larger V-dependence and decrease with the volume
- Deconfinement T_c estimates have milder V-dependence and increase with the volume
- The spread is ~ 10 MeV for $LT > 2.5$
- Clear ordering $T_c^{\chi} > T_c^{S_Q}$ appears above $LT = 3$

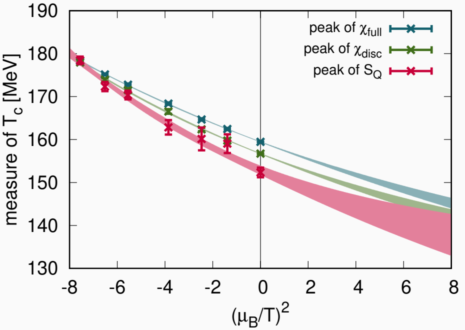


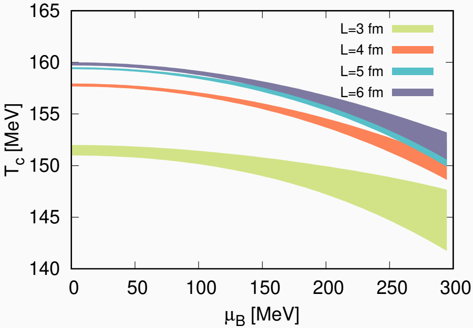
This suggests that studies of T_c can be performed on lattice with smaller volumes based on deconfinement-related observables (ongoing work)

Measures of T_c vs μ_B

Exploiting simulations at imaginary μ_B (no sign problem), we can study the μ_B dependence of T_c too, and extrapolate to real μ_B (here at $LT = 4$)

We find a similar slope in $T(\mu_B)$ at $\mu_B = 0$, although the ordering disappears at larger imaginary μ_B (sensitivity to Roberge-Weiss transition?)





→ transition line $T(\mu_B)$ at different physical volumes (here from peak of χ)

To summarize

- We looked at chiral observables $\langle\bar{\psi}\psi\rangle$, χ, and deconfinement-related observables F_Q, S_Q to study volume and chemical potential dependence
- Chiral symmetry restoration and deconfinement in the thermodynamic limit take place roughly at the same temperature
- However, the dependence on the volume is quite different: large volume effects for chiral symmetry restoration, much milder for deconfinement; and in opposite directions
- Similar dependence on the chemical potential (at large volume), with almost parallel transition lines $T(\mu_B)$

Lattice investigations of the phase diagram

QCD transition temperature

Study of the volume and μ_B dependence of T_c

Borsànyi, PP *et al*, 2405.12320

II. Search for critical point with baryon fluctuations

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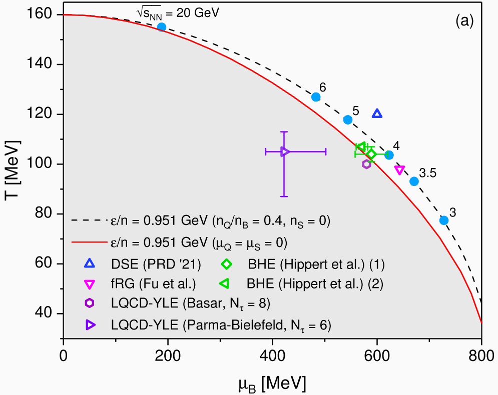
The QCD critical point

The crossover is "expected" to turn first order at larger μ_B, and the critical point would be in the same universality class as the 3D Ising model



Vovchenko, 2408.06473

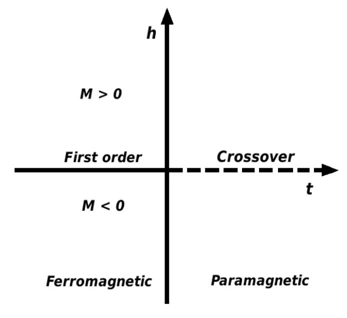
→ recent estimates from different methods seem to "converge"

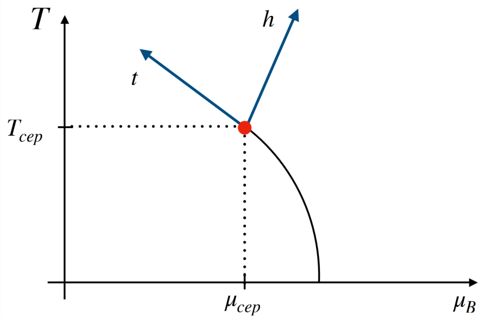
Critical point and universality

In the Ising model, scaling fields are the reduced temperature $t = \frac{T-T_c}{T_c}$ and the magnetic field h. They can be mapped onto QCD coordinates as:

$$t = A_t \Delta T + B_t \Delta \mu_B$$
$$h = A_h \Delta T + B_h \Delta \mu_B$$

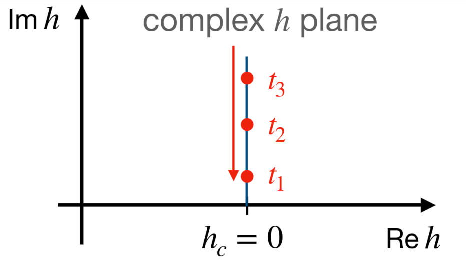
with $\Delta T = T - T_c$, $\Delta \mu_B = \mu_B - \mu_{BC}$.





Critical point from Lee-Yang edge singularities

- The partition function of a thermodynamic system has in general complex zeroes called Lee- Yang zeroes
- When the critical point is approached, these zeroes approach the real μ_B axis
- Zeroes of $\mathcal{Z}$ are singularities of the free energy $f \sim \log \mathcal{Z}$, and they accumulate at the so-called Lee-Yang edge (LYE) singularities



- The idea is to estimate the (complex) location of these singularities, then extrapolate to the critical point exploiting universality:

$$\mathrm{Im}(\mu_{LY})(T) = A(T - T_c)^{\beta\delta}$$

- There are important caveats, mostly the assumption that we are in the scaling regime
- We will see that such an analysis suffers from large systematics

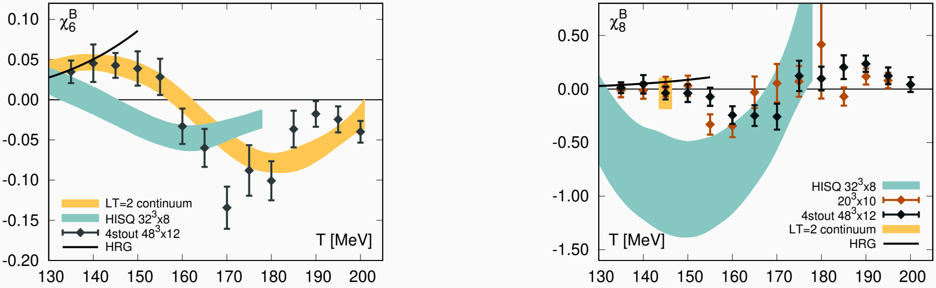
Starting point: fluctuations

Derivatives of the free energy wrt the associated chemical potentials:

$$\chi_{ijk}^{BQS}(T,\mu_B,\mu_Q,\mu_S) = \frac{1}{VT^3}\frac{\partial^{i+j+k}\ln Z\left(T,\mu_B,\mu_Q,\mu_S\right)}{\partial\left(\mu_B/T\right)^i\partial\left(\mu_Q/T\right)^j\partial\left(\mu_S/T\right)^k}$$

- promising signatures of critical point, provide a connection to experiment
- Taylor coefficients of equation of state → basis for expansions/extrapolations

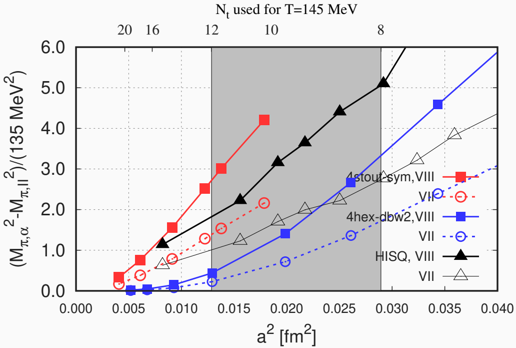
Orders 6,8 have never been continuum extrapolated only recently, in a small volume



Borsanyi, PP *et al.*, PRD 11, L011501 (2024)

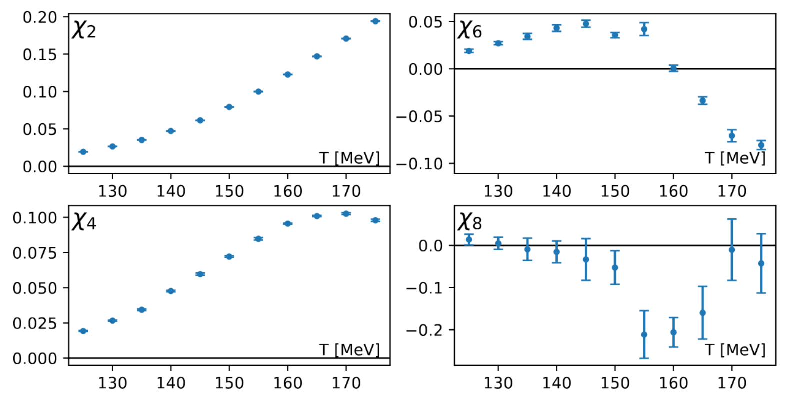
New 4HEX action

- New staggered action, with $N_f = 2+1$ and physical quark masses
- Four steps of HEX smearing, DBW2 gauge action
- The new action has much improved taste breaking over other discretizations $\rightarrow$ much better handle on pion physics and interaction-heavy observables



Our study

- Simulated the temperature range $T = 125 - 175\,\text{MeV}$ on a $16^3{\times}8$ lattice
- Very large statistics ensemble ($\sim$ 500000 configurations per temperature)



We want to carry out a study of LYE singularities with proper *systematic* uncertainties

Our strategy

- Model the μ_B dependence of the free energy (pressure), and search for singularities. We will use a Padé model (in μ_B^2 b/c of charge conjugation symmetry):

$$\text{Pade}[n,m](\mu_B^2) = \frac{P_n(\mu_B^2)}{1+Q_m(\mu_B^2)} = \frac{\sum_{i=0}^n a_n \mu_B^{2i}}{1+\sum_{j=1}^m b_n \mu_B^{2j}}$$

  Systematics # 1: repeat the procedure for related quanties (χ_1^B, χ_2^B), also singular!

- Model the approach to the critical point:

$$\text{Im}(\mu_{LY})^{1/\beta\delta} = A(T - T_c)$$

  Systematics # 2: repeat the procedure for equivalent functional forms:

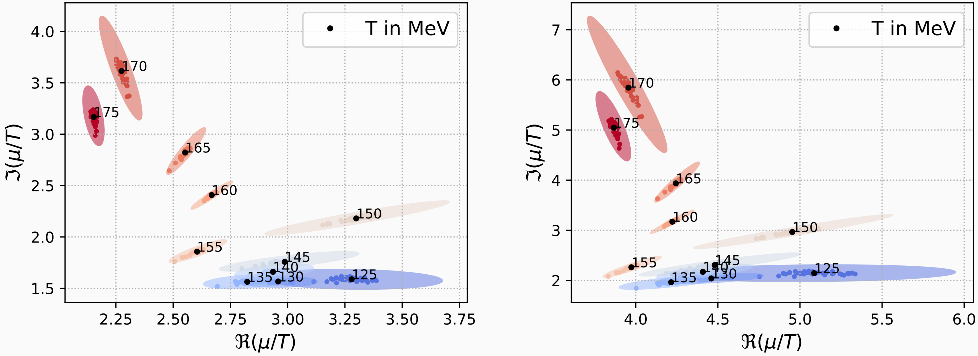
$$\text{Im}(\mu_{LY}/T)^{1/\beta\delta} \qquad \text{Im}(\mu_{LY}^2)^{1/\beta\delta} \qquad \text{Im}((\mu_{LY}/T)^2)^{1/\beta\delta}$$

- **Systematics # 3**: vary the fit range in T

Note: we do not fit, but fix a_n, b_n directly from the χ_n^B

LYE estimates

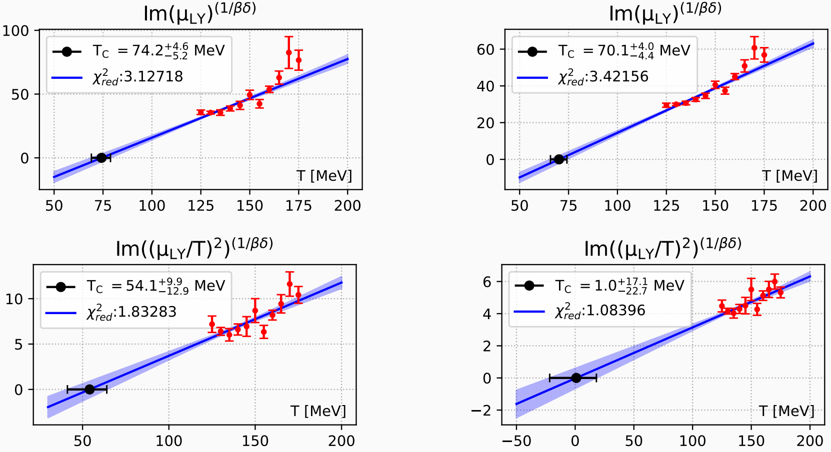
Estimates for the LYE singularities from χ_2 (left) and p (right)



The spreads reflect the statistical errors only

Systematics

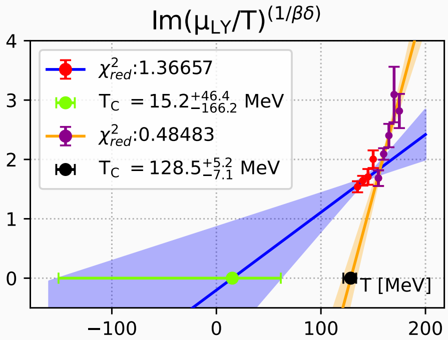
Estimates for T_c from χ_2 (left) and p (right)

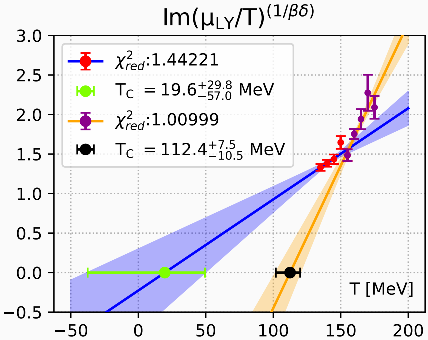


We can notice quite some variability changing the observable and the ansatz

Systematics

Dependence on fit range for T_c estimate from χ_2 (left) and p (right)

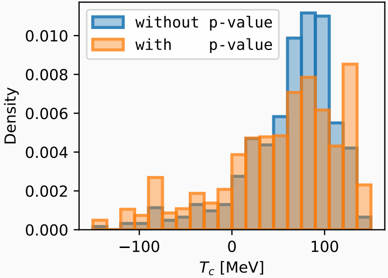


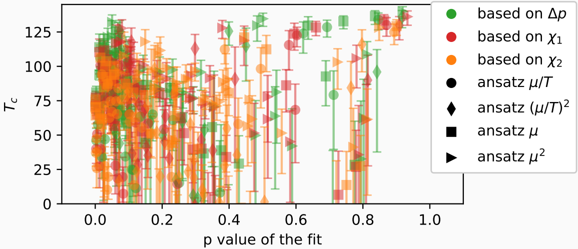


Very large dependence on the fitted range, but *a priori* we can't know where the scaling ansatz is valid!

Systematics: wrap up

Putting together the $3 \times 4 \times 36 = 432$ analyses:





When considering the systematic errors, it is extremely hard to make any predictions on the location of the CP.

Results that do not include systematic uncertainties should be taken with extreme care

Summary

The mapping of the phase diagram of QCD continues!

- Looking at chiral and deconfinement-related observables we determined the dependence of the transition temperature on the volume and the chemical potential
- Much smaller volume effects for deconfinement than for chiral symmetry restoration, but similar μ_B dependence
- Results in a small volume $LT = 2$ with a new, improved action, with large statistics to search for the critical point
- Thorough analysis of LYE singularities with *systematic errors*. The conclusion is no conclusion

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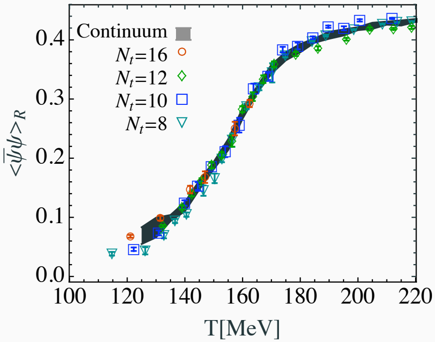
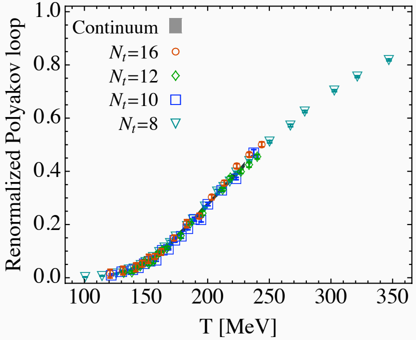
GRAZIE!

BACKUP

Confinement and chiral symmetry breaking

At low temperature and density, quarks and gluons are **confined** inside hadrons. The approximate **chiral symmetry** of QCD is **spontaneously broken**





At large temperature and/or density, a **deconfined medium** is formed, with quasi-free quarks and gluons, with **effectively restored chiral symmetry**

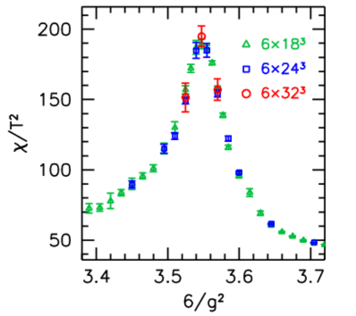
Borsányi *et al.*, JHEP 1009:073 (2010)

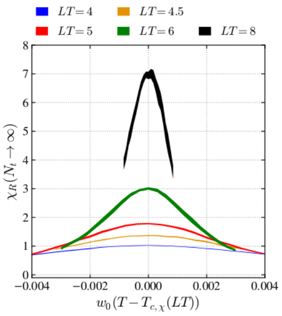
The QCD transition: crossover vs. first order

On the lattice we study the volume scaling of certain quantities to determine the order of the transition

Left: physical masses

Right: infinite masses (pure gauge)



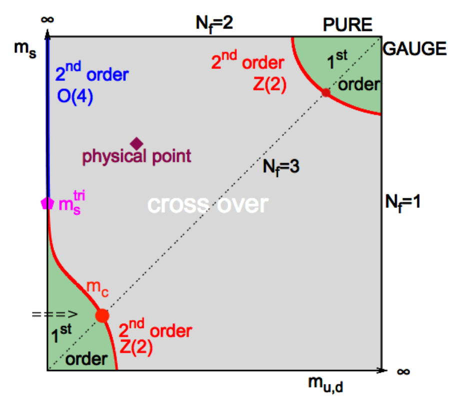


- For a crossover (left), **the peak height is independent of the volume**
- For a first order transition, **it scales linearly with the volume**

Aoki *et al.* Nature 443 (2006), Borsányi, PP *et al.*, PRD 105 (2022)

The QCD transition: Columbia plot

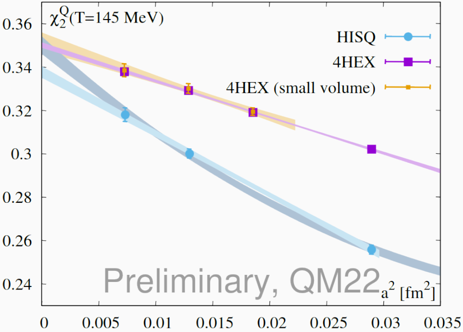
As a function of the light (u,d) and strange quark masses, the order of the transition changes

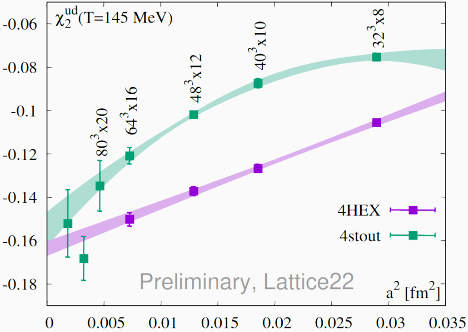


- At the physical point $m_s/m_{ud} \simeq 27$, the transition is a smooth crossover!
- In the heavy-quark limit (pure gauge), the transition is first order

Continuum extrapolation with 4HEX action

Smaller taste breaking $\longrightarrow$ smaller discretization effects $\longrightarrow$ cleaner continuum limit

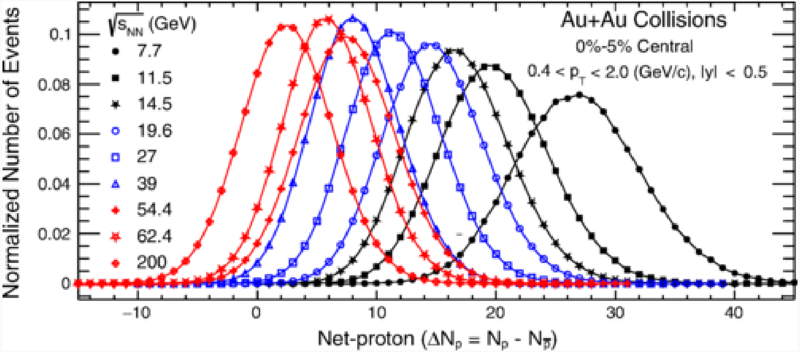




Bellwied+ '15; Bollweg+ '21; Borsanyi, PP+ 'QM '22

Heavy-ion collisions: event-by-event fluctuations

- Conserved charges in QCD are all quark numbers
  $\longrightarrow$ B (baryon number), Q (electric charge), S (strangeness)
- Weak effects are not considered (time's too short)
- Charm is ignored (might not thermalize)
- Conserved charges are conserved only on average in experiment

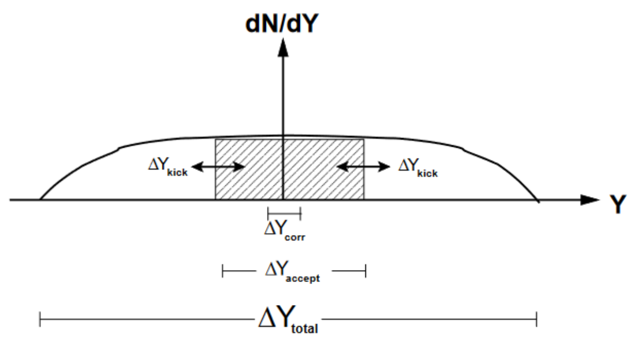


STAR Collaboration: PRL 112 (2014) 032302

Fluctuations of conserved charges

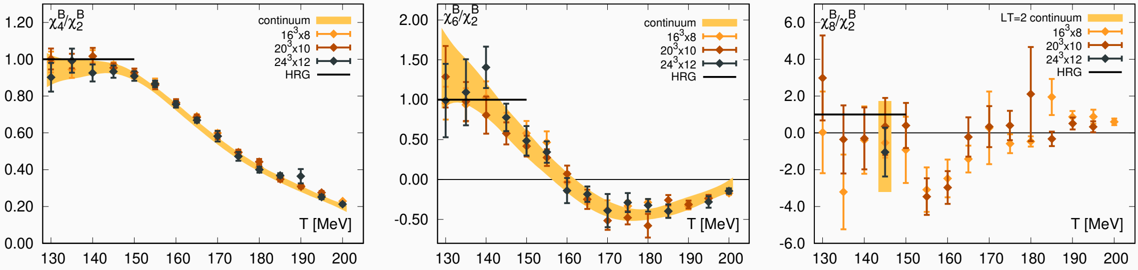
How can CONSERVED CHARGES fluctuate?

- If we could measure ALL particles in a collision, they would not
- If we look at a small enough subsystem, fluctuations occur and become meaningful



High-order baryon fluctuations

Continuum extrapolation of baryon fluctuation ratios B_4/B_2, B_6/B_2, B_8/B_2 (only at $T = 145\,\mathrm{MeV}$)



Small discretization effects, the continuum limit is very clean

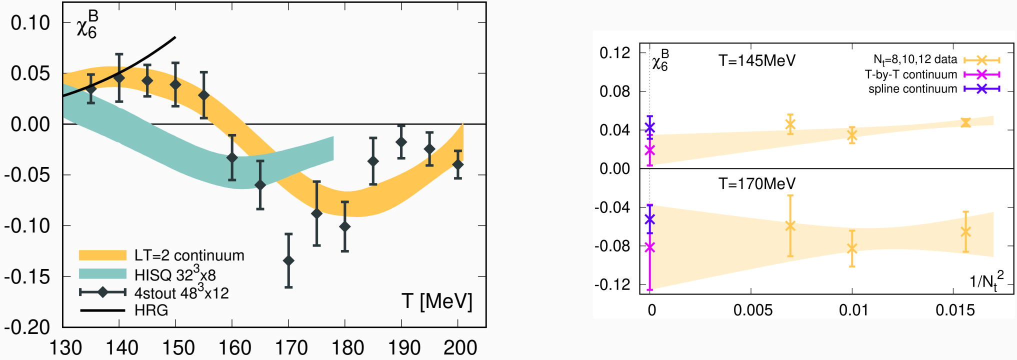
These are the first ever continuum $\mathcal{O}(\mu_B^6)$ and $\mathcal{O}(\mu_B^8)$ results

Borsanyi, PP+ '23

High-order baryon fluctuations: comparisons

Continuum extrapolated χ_6^B with same ansatz, compared to non-continuum results:

- small finite volume effects (especially at low T)
- **not** small cutoff effects in existing $N_\tau = 8$ data (sign is opposite, slope is opposite)

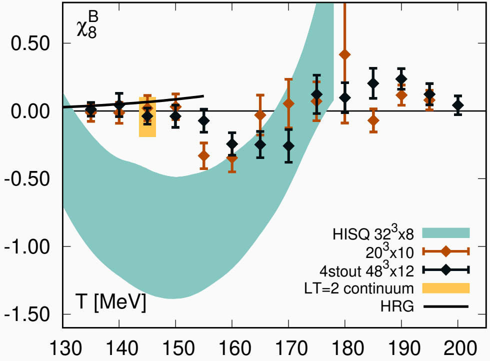


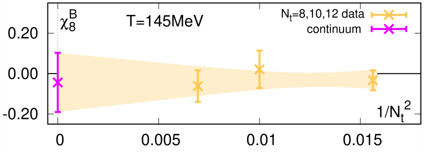
4stout: Borsanyi+ '18; HISQ: Bollweg+ '22; 4HEX (new): Borsanyi, PP+ '23

High-order baryon fluctuations: comparisons

Continuum extrapolated χ_8^B at $T = 145\,\text{MeV}$ only, compared to non-continuum results:

- again, small finite volume effects (especially at low T)
- cutoff effects way out of control in existing $N_\tau = 8$



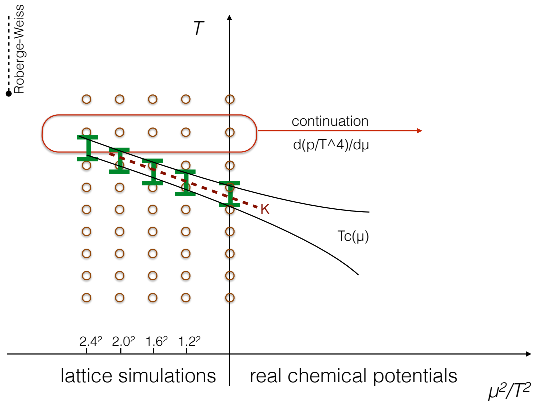


4stout: Borsanyi+ '18; HISQ: Bollweg+ '22; 4HEX (new): Borsanyi, PP+ '23

Simulations at imaginary chemical potential

- While for real chemical potential ($\mu^2 > 0$) $\det M(U)$ is complex, for **imaginary** chemical potential ($\mu^2 < 0$) $\det M(U)$ is real
- We perform simulations at imaginary chemical potentials:

$$\hat{\mu}_B = i\frac{j\pi}{8} \quad j = 0, 1, 2, \ldots$$



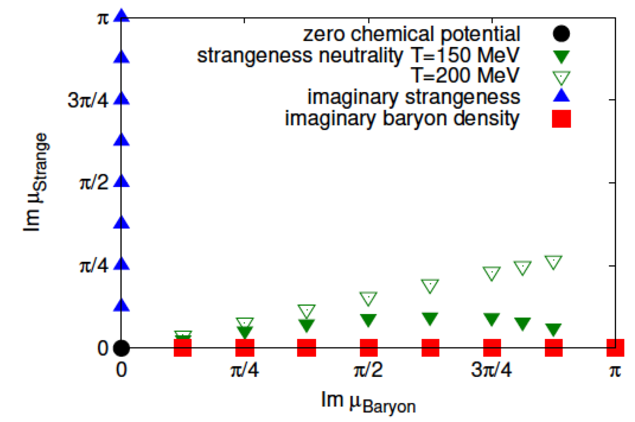
We then analytically continue to $\mu^2 > 0$ by means of suitable extrapolation schemes

Simulations at imaginary chemical potential

Strangeness neutrality (or not)

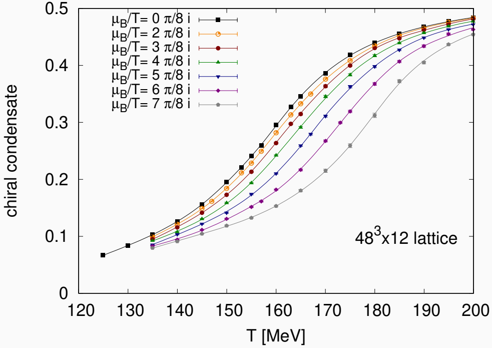
Set the chemical potentials for heavy-ion collisions scenario, or simpler setup:

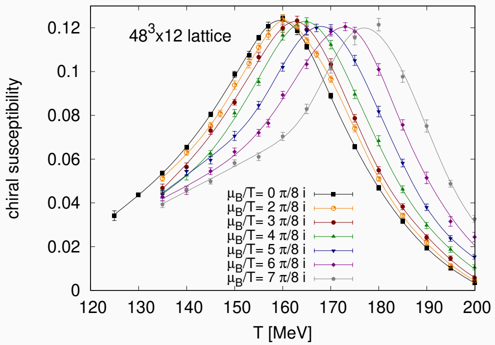
$$\langle n_S \rangle = 0 \qquad \langle n_Q \rangle = 0.4 \langle n_B \rangle \qquad \text{or} \qquad \mu_Q = \mu_S = 0$$



Chiral observables at imaginary μ_B

Chiral condensate and chiral susceptibility at imaginary chemical potential





- From here, we could determine the inflection point of $\langle\bar{\psi}\psi\rangle(T)$ and the peak of $\chi(T)$ (this was done in e.g., [Bellwied:2015rza])
- However, we are after great precision, and the complicated shapes of these curves are an obstacle

Lattice QCD at finite μ_B - Taylor coefficients

cane

cane

- Fluctuations of baryon number are the Taylor expansion coefficients of the pressure

$$\chi_{ijk}^{BQS}(T) = \left.\frac{\partial^{i+j+k} p/T^4}{\partial\hat{\mu}_B^i \partial\hat{\mu}_Q^j \partial\hat{\mu}_S^k}\right|_{\vec{\mu}=0}$$

- Signal extraction is increasingly difficult with higher orders, especially in the transition region

- Higher order coefficients present a more complicated structure