# Finite density QCD thermodynamics from lattice simulations

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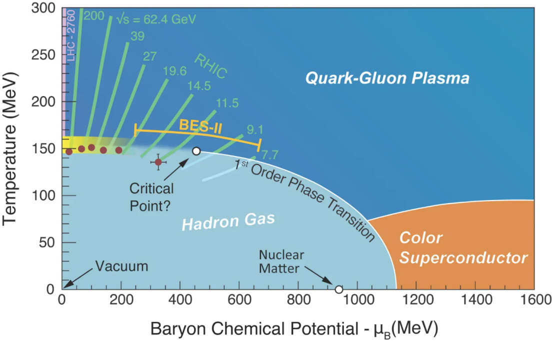
October 4, 2025, Cortona, Italy

**TNPI2025 - XX Conference on Theoretical Nuclear Physics in Italy**

# The thermodynamics of QCD

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

- **Early Universe-like** conditions at $\mu_B = 0$ (matter-anti-matter symmetry), large $T$
- **Hadron gas** at low $T$ & $\mu$
- **Quark gluon plasma** (QGP) at high $T \,||\, \mu$
- **Crossover** at zero density at $T \simeq 160\,\mathrm{MeV}$
- **Ordinary nuclear matter** at $T \simeq 0$ and $\mu_B \simeq 922\,\mathrm{MeV}$ + liquid-gas transition
- **Critical point?** Exotic phases?




**Main exploration tools:** simulations of QCD on the lattice and heavy-ion collisions (LHC, RHIC, SPS, AGS, FAIR†, JPARC†)

† in the future

# Theory: lattice QCD

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

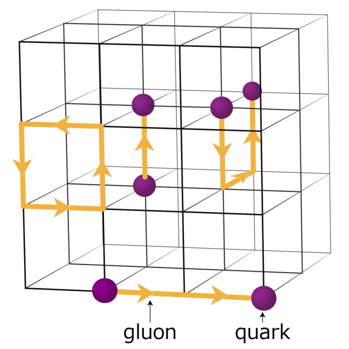
$$\mathcal{Z}[A,\bar{\psi},\psi] = \int \mathcal{D}A_\mu(x)\,\mathcal{D}\bar{\psi}(x)\,\mathcal{D}\psi(x)\,e^{-\int d^4x\,\mathcal{L}_E[A,\bar{\psi},\psi]}$$

by defining the theory on a discretized 3+1d lattice with $N_s^3 \times N_\tau$ sites.

- Quark fields $\bar{\psi}, \psi$ are defined on lattice sites, gauge fields $A_\mu$ are the lattice links $U_\mu = \exp[iaA_\mu] \in \mathrm{SU}(3)$.
- 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 and fermion actions.



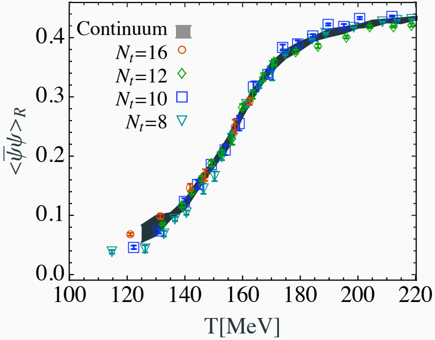

Ideally, take the continuum ($N_\tau \to \infty$) and infinite volume ($N_s/N_\tau \to \infty$) limits

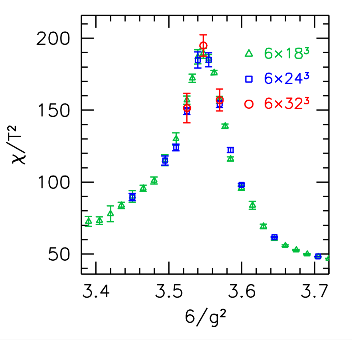
# QCD transition: chiral symmetry breaking

**Chiral symmetry**: exact for $m_q \to 0$. **Chiral condensate** $\langle\bar{\psi}\psi\rangle$ (order parameter) and **chiral susceptibility**:

$$\langle\bar{\psi}\psi\rangle = \frac{T}{V}\frac{\partial \log \mathcal{Z}}{\partial m} \qquad\qquad \chi = \frac{T}{V}\frac{\partial^2 \log \mathcal{Z}}{\partial m^2}$$

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




Borsanyi *et al.*, JHEP 1009:073 (2010); Aoki *et al.*, Nature 443, 675–678 (2006)

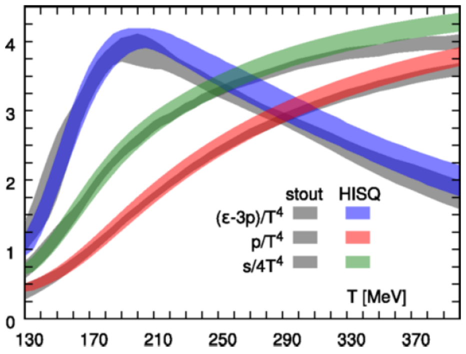
No volume scaling in susceptibility → **QCD transition is a crossover**

# The equation of state of QCD

- Crucial input for modeling QCD matter, e.g. hydro simulations of heavy-ion collisions
- 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 $\mathcal{Z}$

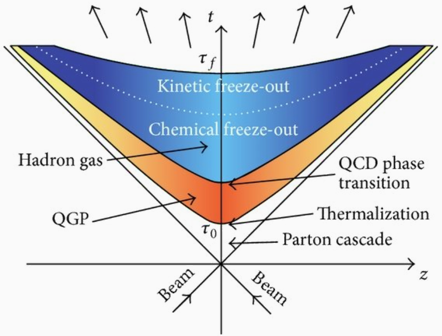
* **Pressure**: $p = -k_B T \frac{\partial \ln \mathcal{Z}}{\partial V}$
* **Entropy density**: $s = \left(\frac{\partial p}{\partial T}\right)_{\mu_i}$
* **Charge densities**: $n_i = \left(\frac{\partial p}{\partial \mu_i}\right)_{T,\mu_{j\neq i}}$
* **Energy density**: $\epsilon = Ts - p + \sum_i \mu_i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

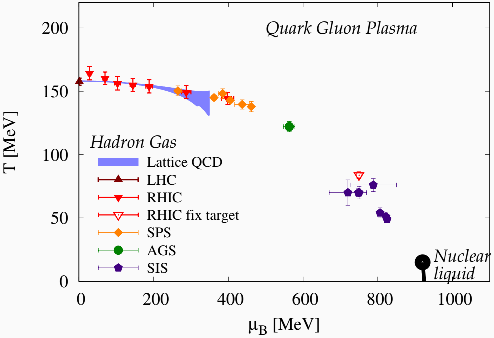



Borsányi *et al.*, PLB 370 (2014) 99, Bazavov *et al.*, PRD 90 (2014) 094503

# Experiment: heavy ion collisions

Heavy nuclei colliding at different energy create media with different baryon density




Measuring the number of final-state hadrons we have an "experimental" sketch of the phase diagram → **chemical freeze-out**

⇒ First-principle theoretical methods don't yet reach as far: **what's beyond?**

# Finite density QCD: the sign/complex action problem

Euclidean path integrals are calculated with MC methods using importance sampling and the Boltzmann weights $\det M[U]\, e^{-S_G[U]}$

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

When a chemical potential is introduced, a problem appears:

$$[\det M(\mu)]^* = \det M(-\mu^*)$$

in general the determinant is complex and cannot serve as a statistical weight.

However, that is **not the case if**:

- there is particle-antiparticle-symmetry ($\mu = 0$):
- the chemical potential is *purely imaginary* ($\mu^2 < 0$)

$$[\det M(\mu)]^* = \det M(-\mu^*) = \det M(\mu) \in \mathbb{R}$$

# The sign/complex action problem

Because finite-$\mu_B$ physics is of great interest, alternatives have been widely explored:

- **Taylor expansion** around $\mu_B = 0$
  One calculates derivatives of the QCD pressure at $\mu_B = 0$, then construct the expansion:

$$\frac{p(T,\mu_B)}{T^4} = \sum_n c_{2n}(T)\left(\frac{\mu_B}{T}\right)^{2n} , \qquad c_n(T) = \frac{1}{n!}\left.\frac{\partial^n (p/T^4)}{\partial \mu_B^n}\right|_{\mu_B=0} = \frac{1}{n!}\chi_n(T)$$

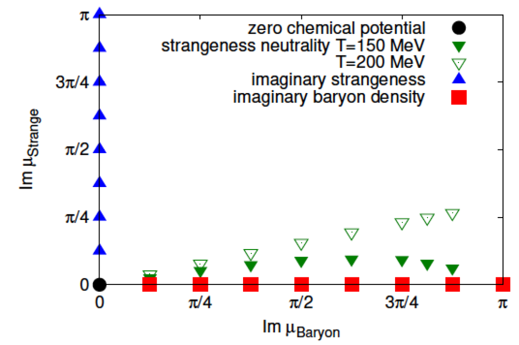
- **Reweighting**
  Because the Boltzmann weight contains $\det M(\mu_B)$, which is complex, move it to the observable:

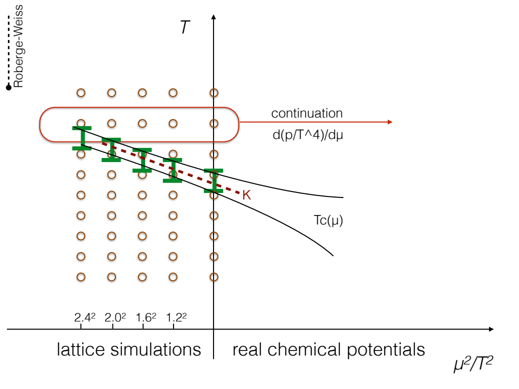
$$\det M(\mu_B) = \frac{\det M(\mu_B)}{\det M(\mu_B = 0)} \det M(\mu_B = 0)$$

- **Imaginary chemical potential**
  Simulate at imaginary $\mu_B$, then (somehow) analytically continue to real $\mu_B$

# Simulations at imaginary chemical potential

Since the QCD transition is analytic, we can analytically continue from $\mu_B^2 < 0$ to $\mu_B^2 > 0$



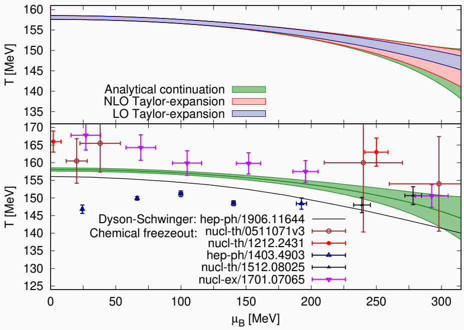



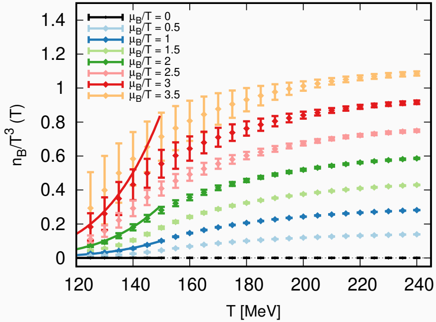

To mimic experiment, one can impose **strangeness neutrality**, i.e. fix the chemical potentials $\mu_B, \mu_Q, \mu_S$ associated to $B, Q, S$ such that:

$$\langle n_S \rangle = 0 \qquad \langle n_Q \rangle = 0.4 \langle n_B \rangle$$

# Finite density QCD from imaginary $\mu_B$ simulations

Among the quantities we can reliably extrapolate to real $\mu_B$ are the **transition line** $T_c(\mu_B)$ and the **equation of state**



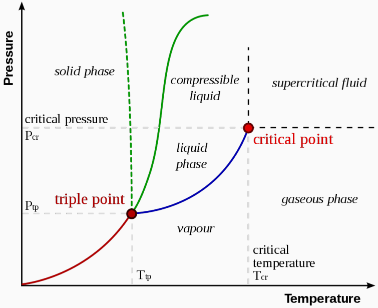




Borsányi, PP, *at el.*, PRL 125 (2020) 052001; Borsányi, PP, *at el.*, PRL 126 (2021) 232001

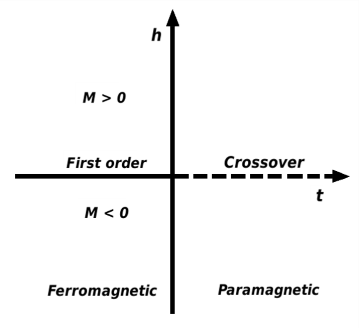
# How about critical behavior?

“a critical point is the end point of a phase equilibrium curve. [...] At the critical point, defined by a critical temperature $T_c$ and a critical pressure $p_c$, phase boundaries vanish. [...]”

**Water**




**Ising model**

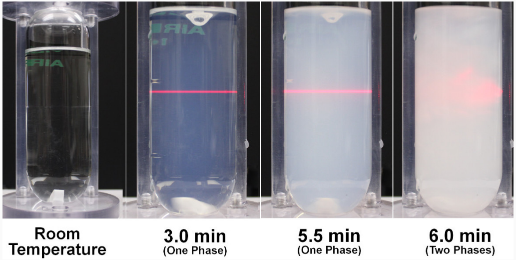



- The correlation length $\xi$ diverges: $\xi \to \infty$ for $T \to T_c$, $p \to p_c$ (i.e. $\mu \to \mu_c$, $\rho \to \rho_c$)
- Some quantities show power-law divergences governed by **critical exponents** $\alpha, \beta, \gamma, \delta, \ldots$
- Very different phenomena share the same critical exponents $\to$ **universality class**

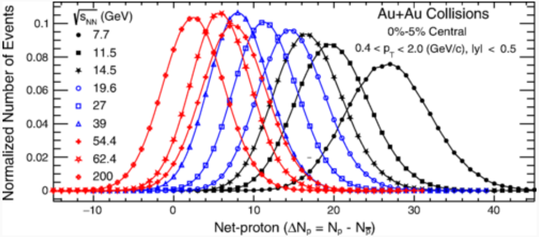
# The critical point of QCD

In general, in order to observe criticality one can tune the system to the critical point

This is possible e.g. for water and watery mixtures




Williamson *et al.*, J. Chem. Educ. 2021, 98, 7, 2364-2369




STAR Collaboration, PRL 112 (2014) 032302

**In QCD we can't!** In heavy-ion collisions, we can observe final state hadrons

Search for large event-by-event fluctuations:

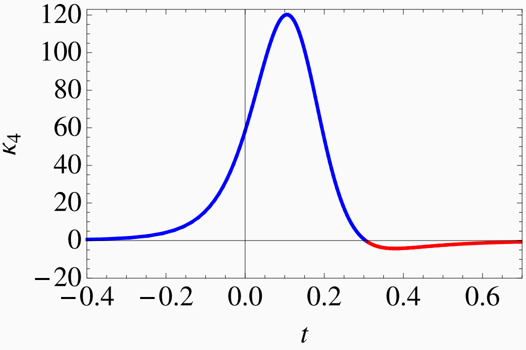
$$\kappa_2 \sim \xi^2 \qquad \kappa_3 \sim \xi^{9/2} \qquad \kappa_4 \sim \xi^7$$

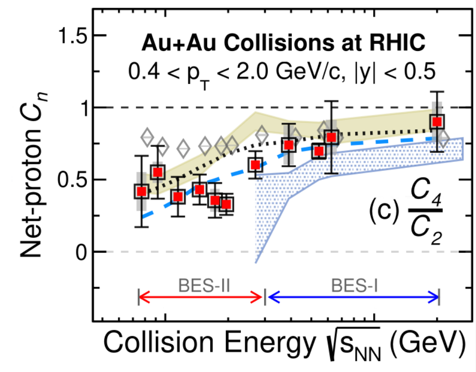
Stephanov, PRL 102 (2009) 032301

# Signals of critical behavior

**We do know:** the critical point of QCD has same universality class as 3D Ising model
Pisarski, Wilczek, PRD 29 (1984) 338

We expect **non-monotonic dependence** of net-proton kurtosis vs collision energy (left)
Stephanov, PRL 107 (2011) 052301



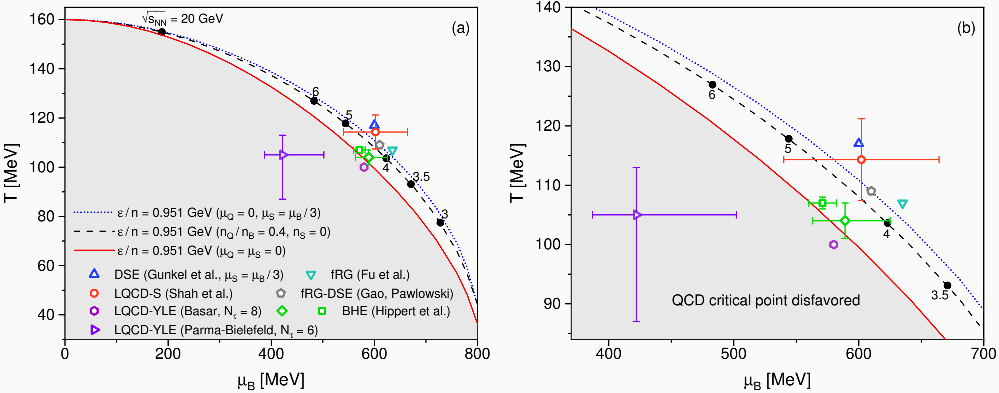




STAR Collaboration, PRL 135 (2025) 142301

Recent **data show only hints**, it's not clear if and where there is non-monotonicity

# The QCD critical point

From the theory side, many different models predicting a critical point




Vovchenko, PRC 111 (2025) 054903

→ and recent estimates seem to “converge”

# Large density QCD from the lattice

## I. Large lattices in the continuum limit

Exclusion region for the critical point from lattice simulations!

**Borsànyi, PP *et al.*, 2502.10267**

## II. Extreme statistics on a $16^3 \times 8$ lattice

Yang-Lee edge singularities

**Adam, PP *et al.*, 2507.13254**

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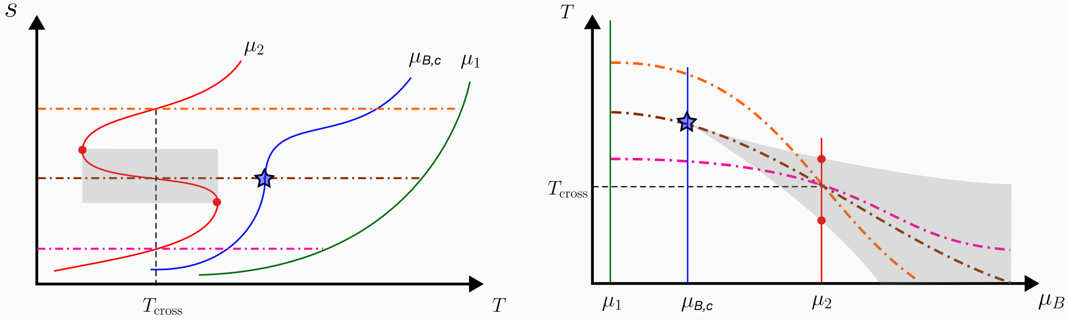
# Critical point location from entropy contours

Recently proposed to look at contours of constant entropy, and search for where they meet
**Shah *et al.*, 2410.16206**

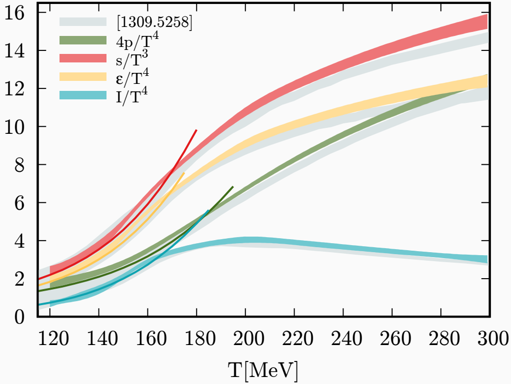



Through Taylor expansion, predicted a critical point at $T \sim 100$ MeV, $\mu_B \sim 600$ MeV

# Critical point location from entropy contours

**Full quantitative analysis** with same method, but:

- analytical continuation from imaginary $\mu_B$
- new equation of state at $\mu_B = 0$ with 2x better precision

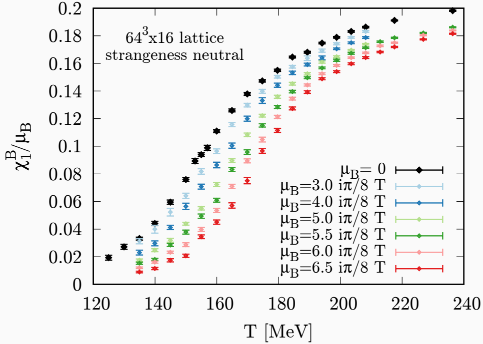


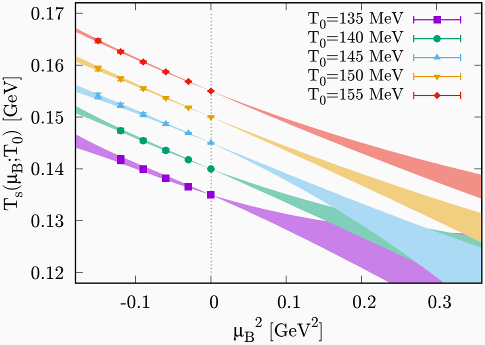

and **different goal**: try to exclude the CP somewhere in the phase diagram

# Our entropy contours

We generalized the approach and employed new data. Starting from baryon density at imaginary $\mu_B$, obtain the entropy entropy at imaginary $\mu_B$ (**total** 16x systematics here)

$$s(T,\mu_B) = s(T,\mu_B=0) + \int_0^{\mu_B} d\mu_B' \frac{\partial n_B(T,\mu_B')}{\partial T}$$



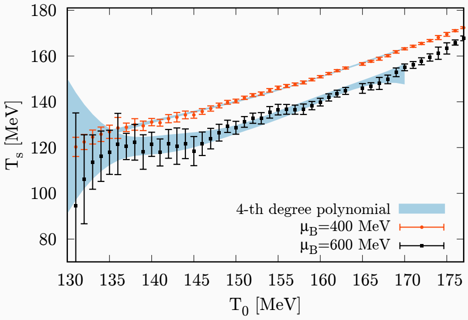

The points (right) are where the entropy has the same exact value (color-by-color)

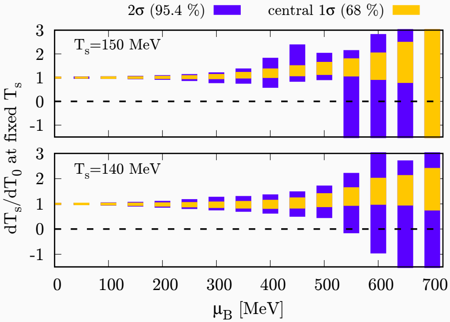
# Our entropy contours

Now we extrapolate $T_s(\mu_B, T_0)$, i.e. the temperature at which the entropy has the value it has at $T_0, \mu_B = 0$. We use two functional forms:

$$T_s(\mu_B^2, T_0) = \frac{T_0 + a\mu_B^2}{1 + b\mu_B^2} \qquad\qquad T_s(\mu_B^2, T_0) = T_0 + a\mu_B^2 + b\mu_B^4$$

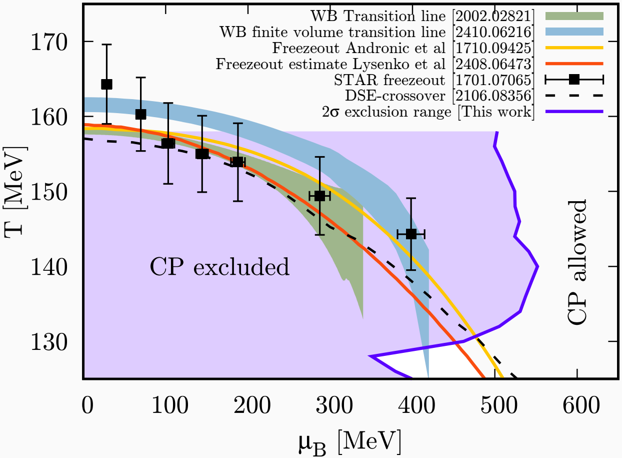
**If there is a critical point**, $T_s$ is non-monotonic above $\mu_B > \mu_{BC}$, so we look for the smallest values of the derivative at $1\sigma$ and $2\sigma$ levels (**total** 48x systematics per $\mu_B$ value)



# The exclusion region

This gives us indication of where the derivative is compatible with 0 at the $1\sigma$ and $2\sigma$ levels, temperature by temperature $\rightarrow$ $2\sigma$ **exclusion region**




This is the first rigorous exclusion range from lattice QCD.

## Large lattices in the continuum limit

Exclusion region for the critical point from lattice simulations!

**Borsànyi, PP *et al.*, 2502.10267**

## II. Extreme statistics on a $16^3 \times 8$ lattice

Yang-Lee edge singularities

**Adam, PP *et al.*, 2507.13254**

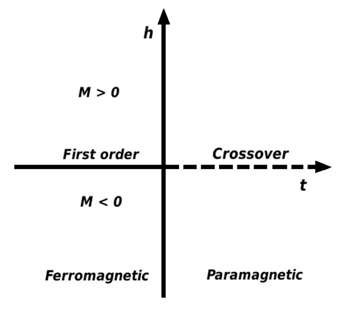
# Critical point and universality

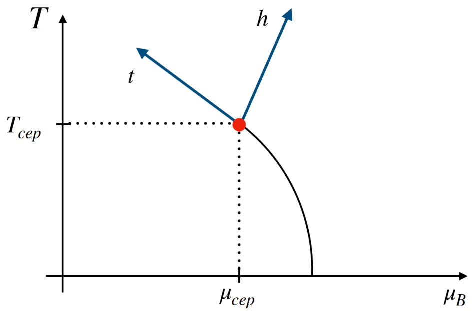
In the Ising model, scaling fields are the reduced temperature $t = \frac{T - T_c}{T_c}$ and the magnetic field $h$. Universality implies they can be mapped onto QCD coordinates as:

$$t = A_t \Delta T + B_t \Delta \mu_B$$

$$h = A_h \Delta T + B_h \Delta \mu_B$$

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

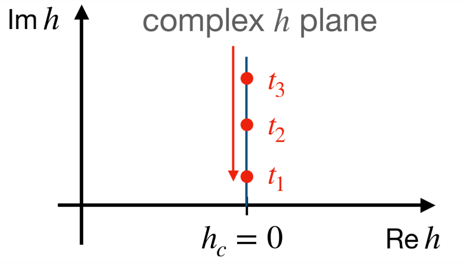



C. Schmidt, Lattice 24

# Critical point: Yang-Lee 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 ($\mu_B$) axis
- Zeroes of $\mathcal{Z}$ are singularities of the free energy $f \sim \log \mathcal{Z}$, and they accumulate at the so-called Yang-Lee edge (YLE) singularities




C. Schmidt, Lattice 24

- In the vicinity of a critical point, the **scaling variable** $z = t/h^{\beta\delta}$ is the only "coordinate", and the YLE are universally located at:

$$z_c = |z_c| \exp\left(\frac{i\pi}{2\beta\delta}\right)$$

- In QCD this translates to expected scaling forms for the real and imaginary parts:

$$\mathrm{Re}\Delta\mu_B = \mu_{BC} + c_1\Delta T \ (+c_2\Delta T^2) \qquad \text{and} \qquad \mathrm{Im}\Delta\mu_B = c_3\Delta T^{\beta\delta}$$

# Critical point: Yang-Lee edge singularities

So, the idea is:

- somehow **determine the complex locations** of the YLE
- **use the expected scaling** to find where $\mathrm{Im}\Delta\mu_B = 0$, i.e. where the critical point is

**Our setup:**

- Single $16^3 \times 8$ lattice, **huge statistics** ($\mathcal{O}(10^6)$ at each $T = 110 - 300$ MeV)
- $N_f = 2 + 1$ flavours of **physical quark masses**
- Our recent 4HEX **action has small discretization effects** (i.e., $N_\tau = 8$ is not that small)

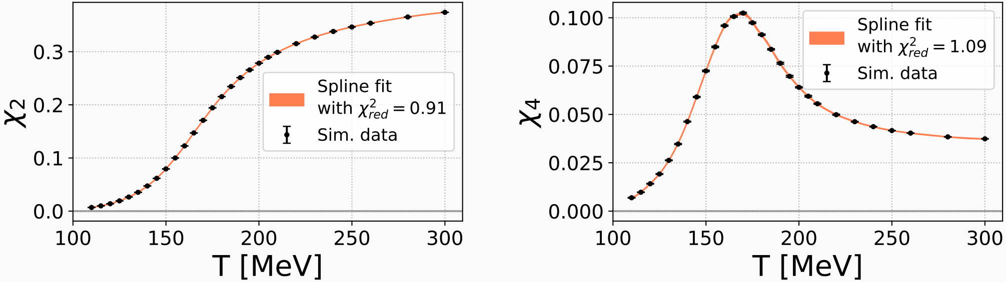
**Important caveats:** (due to prohibitive cost)

- <u>No continuum limit</u>, as only $N_\tau = 8$ lattices were used
- <u>No infinite volume limit</u>, nor a finite volume scaling analysis
- Truncated Taylor series will affect the location of the YLE singularities
- The extrapolation to $T_{\mathrm{CEP}}$ covers a large portion of the phase diagram

# Input: fluctuation observables

The fluctuations are the expansion coefficients of the pressure:

$$\chi_n^B(T) = \left.\frac{\partial^n (p/T^4)}{\partial(\mu_B/T)^n}\right|_{\mu_B=0}$$




The extreme statistics is reflected in tiny errors, unprecedented precision

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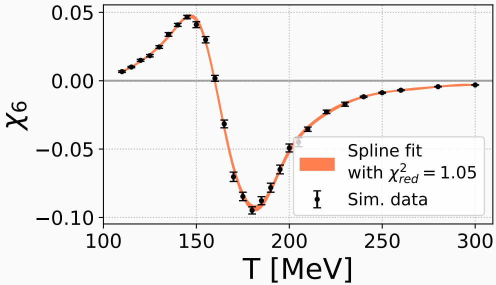


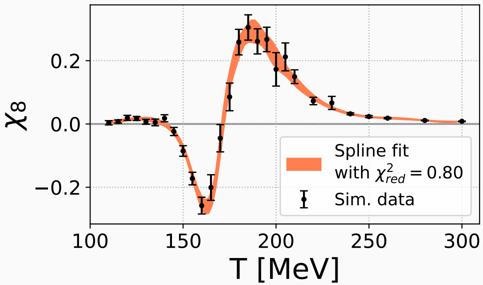


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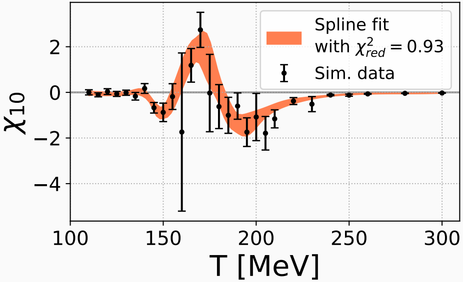



The extreme statistics is reflected in tiny errors, unprecedented precision

# Systematics

We model the pressure with a functional form allowing for singularities, retaining the known symmetries (charge conjugation $\mu_B \leftrightarrow -\mu_B$ and Roberge-Weiss periodicity)

- For each $T$, we use a 2/2 Padé in $\cosh(\mu_B) - 1$, fitted to our $\chi_n^B$ coefficients:

$$F(\mu_B) = \frac{a(\cosh(\mu_B) - 1)}{1 + c(\cosh(\mu_B) - 1) + d(\cosh(\mu_B) - 1)^2}$$

  **Systematics # 1**: repeat the procedure for related quanties ($\chi_1^B$, $\chi_2^B$), also singular!

- Universality fixes the approach to the critical point:

$$(\mathrm{Im}\mu_{LY})^{1/\beta\delta} = c_3(T - T_c)$$

  **Systematics # 2**: but other asymptotically equivalent ansätze are allowed:

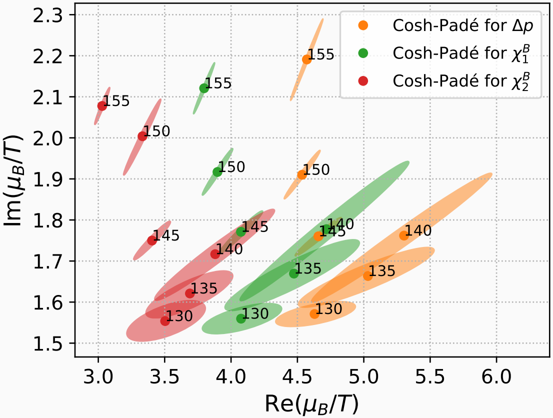
$$(\mathrm{Im}\mu_{LY}^2)^{1/\beta\delta} \sim (\mathrm{Im}\mu_{LY}^3)^{1/\beta\delta} \sim (\mathrm{Im}\mu_{LY}^4)^{1/\beta\delta}$$

- The range where the ansätze hold is not known a priori (non universal)

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

# Systematics #1, different observables (x3)

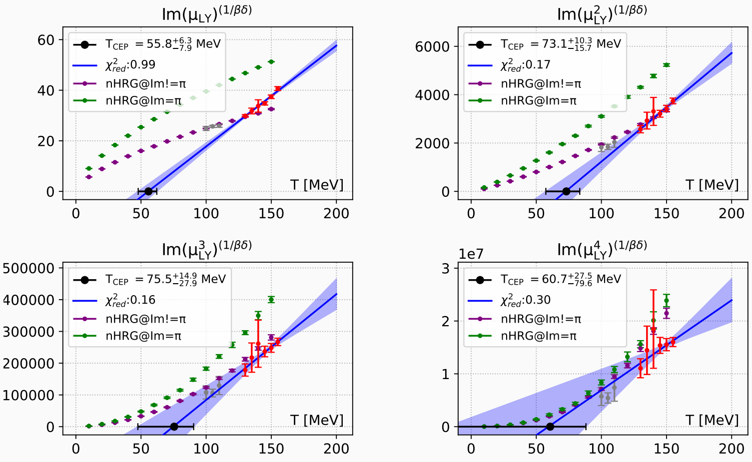
Estimates for the LYE singularities from $p$ $(\chi_0)$, $\chi_1$ and $\chi_2$




**NOTE:** here the spreads reflect the statistical errors only

# Systematics #2, different ansätze for $T$ dependence (x4)

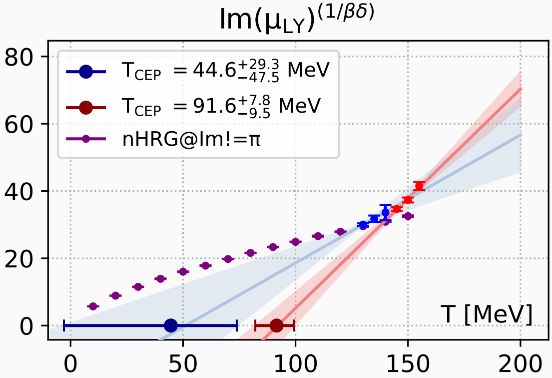
Different ansätze all give good fits




but different results!

# Systematics #3, fit range (x6)

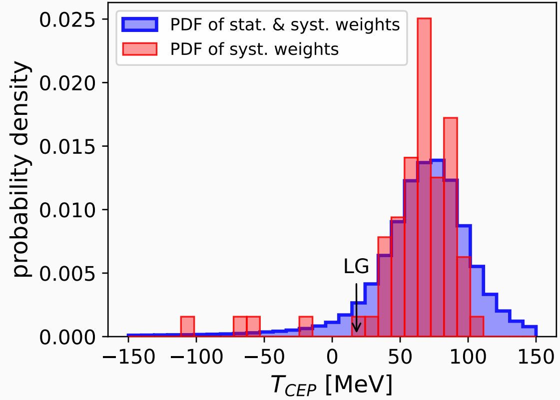
Since we can't know *a priori* where the scaling ansatz is valid, fits with different $T$ ranges must be treated equally




The dependence on the fit range is substantial.

# Systematics: wrap up

Putting together the $3 \times 4 \times 6 = 72$ analyses:




We find an 84% probability that the critical point is at $T < 103$ MeV or does not exist.

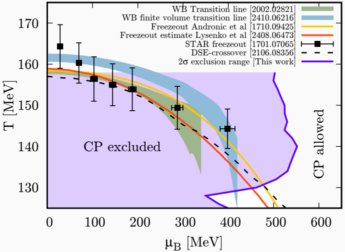
# Summary

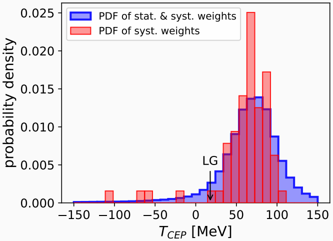
Is there a critical point in the QCD phase diagram? Can lattice say something?

**YES!** (it can say something)

i. **Critical point exclusion range**: first ever, admittedly not very stringent yet, but the method is systematically improvable

ii. **Yang-Lee edge singularities** offer an intriguing chance, but the numerics suggest to be very cautious



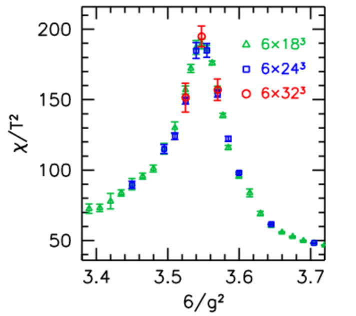



# BACKUP

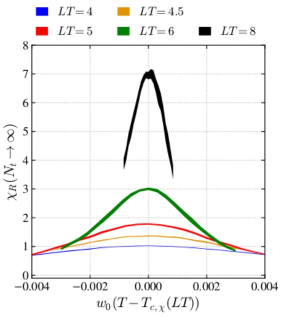
# The QCD transition: crossover vs. first order

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)

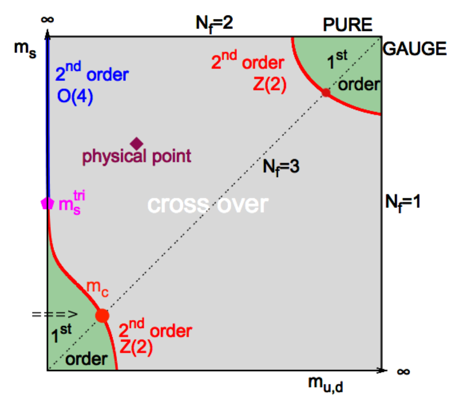



- For a crossover (left), **the peak height is independent of the volume**
- For a first order transition, **it scales linearly with the volume**

**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

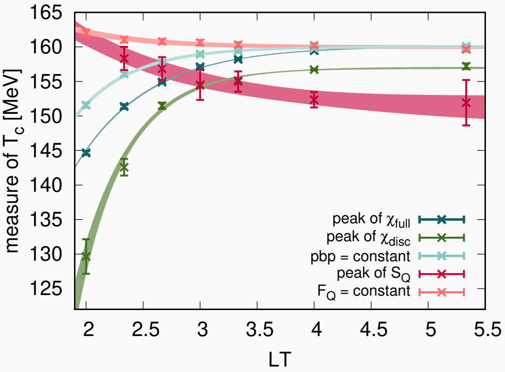



- At the physical point $m_s/m_{ud} \simeq 27$, the transition is a smooth crossover!
- In the heavy-quark limit (pure gauge), the transition is first order

# 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 $\sim 10$ MeV for $LT > 2.5$
- Clear ordering $T_c^{\chi} < T_c^{S_Q}$ appears above $LT = 3$

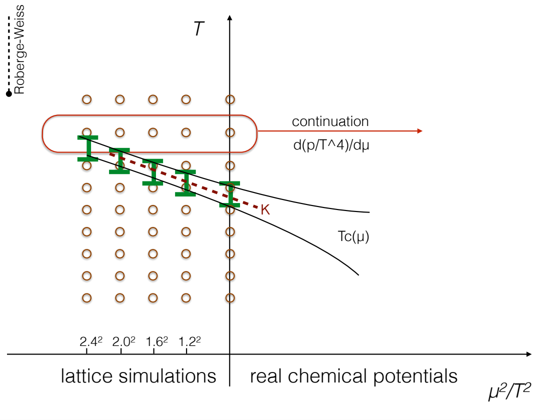



This suggests that studies of $T_c$ can be performed on lattice with smaller volumes based on deconfinement-related observables

# 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:

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



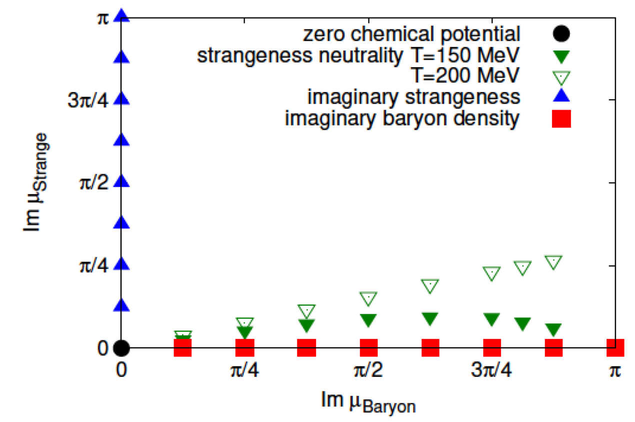

We then analytically continue to $\mu^2 > 0$ by means of suitable extrapolation schemes

# Simulations at imaginary chemical potential

**Strangeness neutrality** (or not)

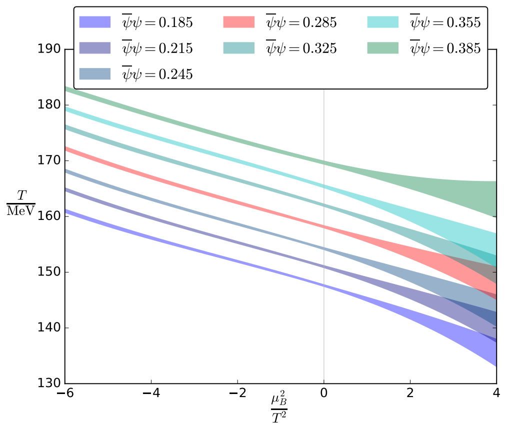
Set the chemical potentials for heavy-ion collisions scenario, or simpler setup:

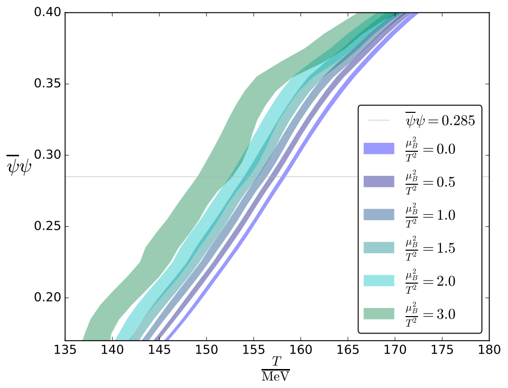
$$\langle n_S \rangle = 0 \qquad \langle n_Q \rangle = 0.4 \langle n_B \rangle \qquad \text{or} \qquad \mu_Q = \mu_S = 0$$



# The width of the transition at finite chemical potential

We can extrapolate our results for $\langle\bar{\psi}\psi\rangle$ along contours of constant $\langle\bar{\psi}\psi\rangle$ (left) or constant $\mu_B/T$ (right)




The extrapolated $\langle\bar{\psi}\psi\rangle$ at finite $\mu_B$ is quite precise for $\mu_B < 3T$