Locating the critical point using lattice QCD[1]

D. A. Clarke, F. Di Renzo, P. Dimopoulos, J. Goswami, C. Schmidt, S. Singh, K. Zambello

University of Utah

RHIC-BES Seminar, 11 June 2024

[1] B.-P. collaboration, arXiv:2405.10196, (May 2024).

The lattice approach

Lattice QCD expectation values given by

$$\begin{aligned}\langle O\rangle &\sim \int \mathrm{d}\bar\psi\,\mathrm{d}\psi\, e^{\bar\psi D\psi} \quad \mathrm{d}U\, e^{-S(U)}\, O(U)\\ &= \int \det D \qquad \mathrm{d}U\, e^{-S(U)}\, O(U)\\ &\approx \frac{1}{N_{\text{conf}}}\sum_n O_n\end{aligned}$$

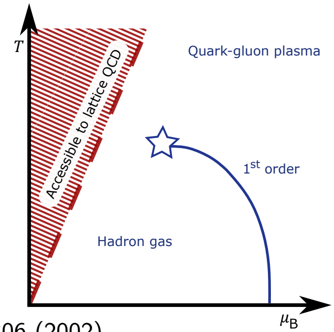
- Draw configuration U_n according to $\mathrm{d}P \sim \mathrm{d}U \det D\, e^{-S}$
- Create time series of measurements O_n of O
- $\det D \in \mathbb{R}$ when $\mu = 0$
- If $\mu \neq 0$, it is in general complex (sign problem)

The infamous problem

Trick: μ_B pure imaginary avoids sign problem; can analytically continue to $\mu_B \in \mathbb{R}$[2,3].

Trick: Expand pressure P/T^4 in μ_B/T[4,5]. (Up to 8^{th} order.)

The latter is too pricey! Popularity of resummation schemes[6,7,8,9].



[2] P. de Forcrand and O. Philipsen, Nuclear Physics B, 642.1-2, 290–306 (2002).
[3] M. D'Elia and M.-P. Lombardo, Phys. Rev. D, 67.1, 014505 (2003).
[4] C. R. Allton et al., Phys. Rev. D, 66.7, 074507 (2002).
[5] R. V. Gavai and S. Gupta, Phys. Rev. D, 68.3, 034506 (2003).
[6] S. Borsányi et al., Phys. Rev. Lett. 126.23, 232001 (2021).
[7] D. Bollweg et al., Phys. Rev. D, 105.7, 074511 (2022).
[8] S. Mitra, P. Hegde, and C. Schmidt, Phys. Rev. D, 106.3, 034504 (2022).
[9] S. Mondal, S. Mukherjee, and P. Hegde, Phys. Rev. Lett. 128.2, 022001 (2022).

Lee-Yang edges

Taylor where $P \sim T \log \mathcal{Z}_{\rm QCD}$ is analytic.

Lee-Yang theorem[10]: Zeroes of the partition function that approach the real axis as $V \to \infty$ correspond to phase transitions.

Intuition: Indications of non-analyticities in P

- may hint at phase transitions
- or singularities in $\mathbb{C}$
- constrain validity of Taylor series

Ising: Generically have branch cuts on imaginary axis. (Pinch real axis at T_c.)

Lee-Yang edge (LYE): The singularities closest to real axis.

LYE is the nearest singularity to the origin, position fixed at[11],

$$z_c = |z_c| e^{\pm i\pi/2\beta\delta}, \qquad z \equiv t h^{-1/\beta\delta}$$

with $t \sim |T - T_c|$, h magnetization, critical exponents β, δ.

[10] C. N. Yang and T. D. Lee, Phys. Rev. 87.3, 404–409 (1952).
[11] M. E. Fisher, Phys. Rev. Lett. 40.25, 1610–1613 (1978).

Extracting singularities

Singularities $\Rightarrow$ **rational functions**,

$$R_n^m(x) \equiv \frac{\sum_{i=0}^{m} a_i x^i}{1+\sum_{j=1}^{n} b_j x^j}.$$

Singularities captured/mimicked by poles.

Let f have formal Taylor series

$$f(x) = \sum_{k=0}^{\infty} c_k x^k.$$

Padé approximant of order $[m,n]$: R_n^m with coefficients to equal the Taylor series up to order $m+n$.

Say we know Taylor series up to some order s. The Multi-point Padé is the R_n^m satisfying

$$\left.\frac{\mathrm{d}^l R_n^m}{\mathrm{d}x^l}\right|_{x_i} = \left.\frac{\mathrm{d}^l f}{\mathrm{d}x^l}\right|_{x_i}$$

for N points x_i, $0 \le l < s-1$.

- Can trade lower Taylor order for more x_i.
- Translates to simulations at multiple $i\mu_B$ using low-order cumulants.

Strategy and setup

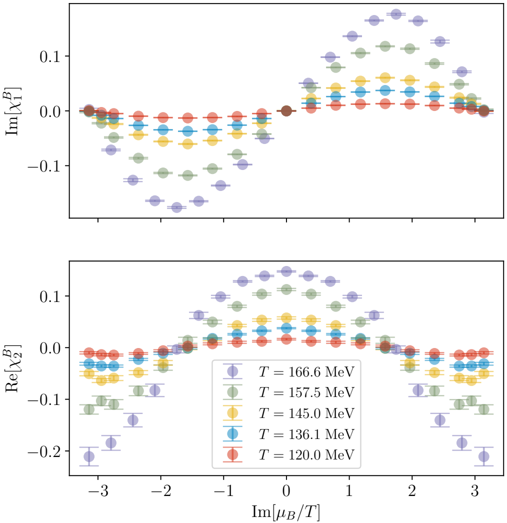
Roughly follow this procedure:

1. What transition are you interested in? (CEP)
2. How should the singularities scale? ($z_c = |z_c| e^{\pm i\pi/2\beta\delta}$)
3. Lattice calculations at multiple, pure imaginary μ_B
4. Estimate singularities with multi-point Padé
5. Analytically continue results to $\mu_B \in \mathbb{R}$

Set up:

- $N_f = 2 + 1$ sea quarks, physical masses $m_s/m_l = 27$
- $\mu_u = \mu_d = \mu_s \equiv \mu$ which gives $\mu_B = 3\mu$ and $\mu_S = 0$
- Imaginary μ_B only at one lattice spacing $N_\tau = 6$

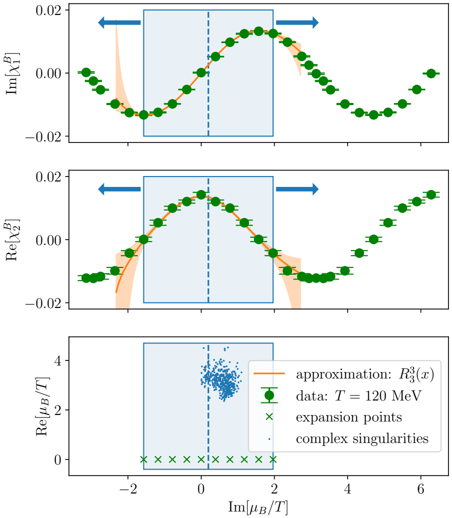
Lattice observables



Cumulants $\chi_n^B \sim \partial^n_{\hat{\mu}_B} \log \mathcal{Z}_{\rm QCD}$

- $\log \mathcal{Z}_{\rm QCD}$ even in $\hat{\mu}_B = i\theta$ and 2π-periodic
- Simulate on 10 $\hat{\mu}_B \in [0, i\pi]$
- Other points by periodicity and parity

Constructing rational approximations



- Singularities have some interval dependence
- Hence try many intervals per T
- R_3^3 simulataneous fit to χ_1^B and χ_2^B
- Try 55 intervals, collect poles as singularities

Toward the CEP

CEP in 3-d, $\mathbb{Z}_2$ universality class, so $\beta\delta \approx 1.5$. Mapping to Ising not yet known. Ansatz:

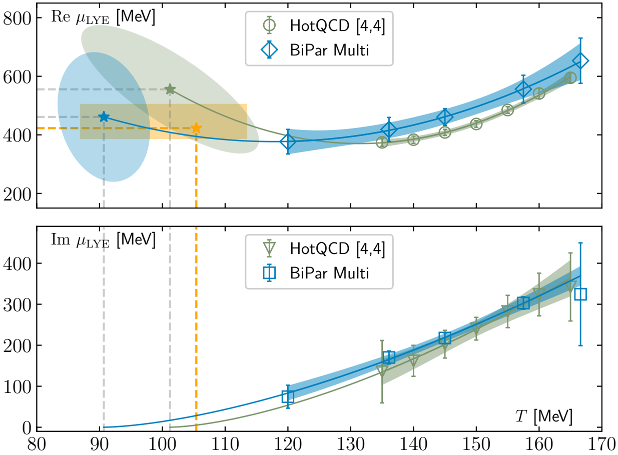
$$t = \alpha_t \Delta T + \beta_t \Delta\mu_B$$
$$h = \alpha_h \Delta T + \beta_h \Delta\mu_B,$$

where $\Delta T \equiv T - T^{\mathrm{CEP}}$ and $\Delta\mu_B \equiv \mu_B - \mu_B^{\mathrm{CEP}}$; leads to singularity scaling[12]

$$\mu_{\mathrm{LY}} = \mu_B^{\mathrm{CEP}} + c_1 \Delta T + i c_2 |z_c|^{-\beta\delta} \Delta T^{\beta\delta} + c_3 \Delta T^2 + \mathcal{O}\left(\Delta T^3\right).$$

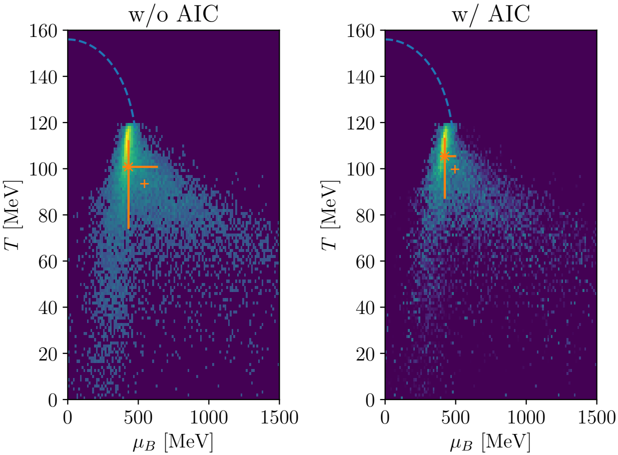
[12] M. A. Stephanov, Phys. Rev. D, 73.9, 094508 (2006).

Toward the CEP: Single-point and multi-point



- Simultaneous fit to real and imaginary
- One $N_\tau = 8$ fit to HotQCD
- Representative $N_\tau = 6$ MPP fit
- Yellow: AIC-weighted result (bootstrap MPP over multiple singularity sets)

Toward the CEP: Multi-point histogram



Distribution of μ_B^{CEP}, T^{CEP} from bootstrap:

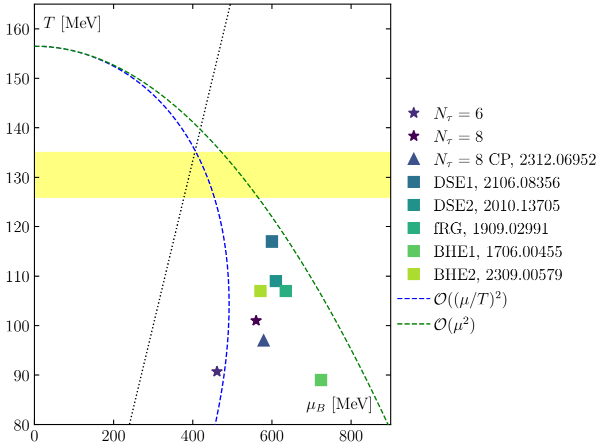
- Hotter means more results in that pixel
- Bars give 68% confidence, centered at median
- Cross gives arithmetic mean
- Dashed line gives crossover

Toward the CEP: Evaluation

$$T_{\text{pc}}(\mu_B) \approx T_{\text{pc}}(0)\left(1+\kappa_2^B\left(\frac{\mu_B}{T}\right)^2\right)$$

$$T_{\text{pc}}(\mu_B) \approx T_{\text{pc}}(0)\left(1+\kappa_2^B\left(\frac{\mu_B}{T_{\text{pc}}(0)}\right)^2\right)$$

- $T^{\text{CEP}} < T_{\text{c}}$
- Outside $\mu/T \gtrsim 3$
- NOT extrapolated

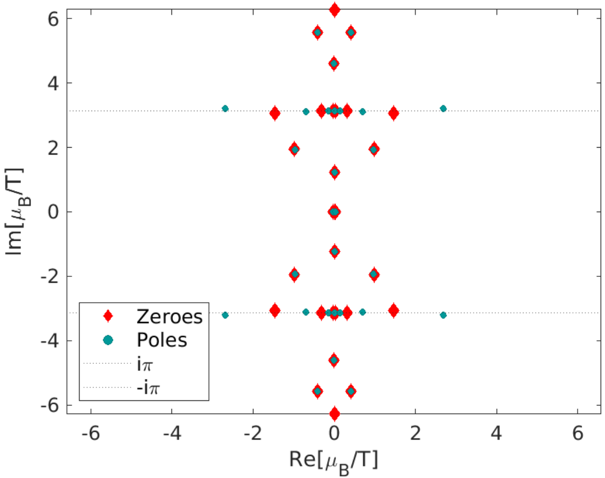


Summary and Outlook

- Use Padé and MPP to find singularities in $\log \mathcal{Z}_{\text{QCD}}$
- Follow the LYE according to scaling expectation
- Encouraging MPP results for $N_\tau = 6$ at $(T^{\text{CEP}}, \mu_B^{\text{CEP}}) = (105^{+8}_{-18}, 422^{+80}_{-35})$ MeV
- Working on lower T
- Working on finer lattices

Thanks for your attention.

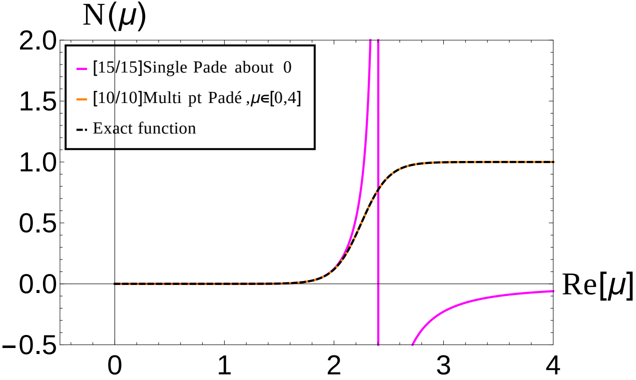
Extracting a LYE[13]



[13] P. Dimopoulos et al., Phys. Rev. D, 105.3, 034513 (2022).

Test: 1-d Thirring model[14,15]

Number density $N(\mu)$ can be worked out exactly.

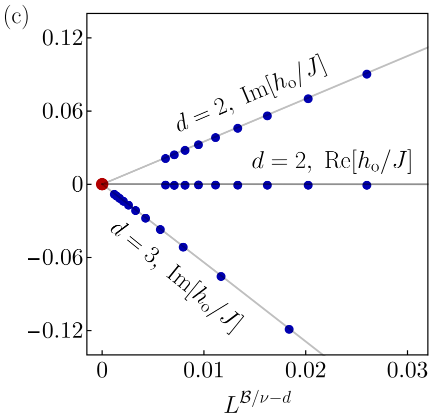


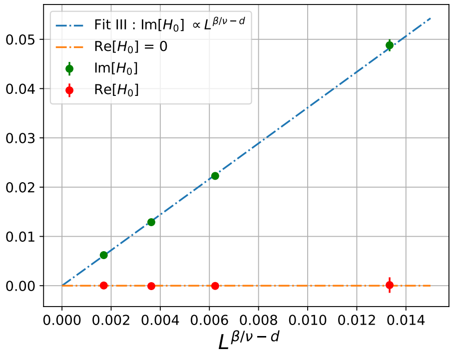
Multi-point captures the exact $N(\mu)$ well, outperforms single point.

[14] P. Dimopoulos et al., Phys. Rev. D, 105.3, 034513 (2022).

[15] F. Di Renzo, S. Singh, and K. Zambello, Phys. Rev. D, 103.3, 034513 (2021).

Test: 2-d Ising model[16,17]





Reproduces correct scaling and critical exponents extremely well.

[16] A. Deger and C. Flindt, Phys. Rev. Research, 1.2, 023004 (2019).
[17] S. Singh, M. Cipressi, and F. Di Renzo, Phys. Rev. D, 109.7, 074505 (2024).

$\mathcal{Z}_{\text{QCD}}$ at $\hat{\mu}_f = i\hat{\mu}_I$ has $\mathbb{Z}_3$ periodicity

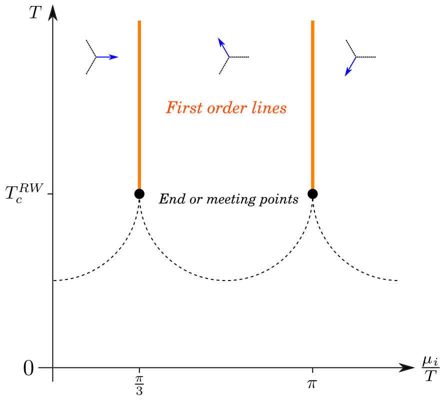
$$\hat{\mu}_I \to \hat{\mu}_I + 2\pi n/3$$

with $\hat{\mu} \equiv \mu/T$. First order lines separate phases distinguished by Polyakov loop

$$P \sim \sum_{\vec{x}} \text{tr} \prod_{\tau} U_4(\vec{x}, \tau).$$

Endpoint in 3-d, $\mathbb{Z}_2$ universality class. Critical exponents[18]:

$$\beta = 0.3264, \qquad \delta = 4.7898$$



[18] S. El-Showk et al., J Stat Phys, 157.4-5, 869–914 (2014).
[19] F. Cuteri et al., Phys. Rev. D, 106.1, 014510 (2022).

Test: The Roberge-Weiss transition[20,21]

Lattice setup:

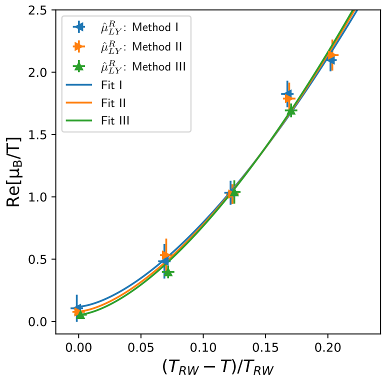
- 2+1 dynamical HISQ quarks
- m_s/m_l fixed to physical value
- $N_\tau = 4$, 6 with $N_s/N_\tau = 6$

$$h \sim \hat{\mu}_B - i\pi \qquad t \sim T - T_{\rm RW}$$

$$z = th^{-1/\beta\delta} \qquad z_c = |z_c| e^{\pm i\pi/2\beta\delta}$$

$$\Rightarrow \ \mathrm{Re}\,\hat{\mu}_{\mathsf{LY}} = \pm\pi \left(\frac{z_0}{|z_c|}\right)^{\beta\delta}$$

Taking $|z_c| = 2.43$ yields $9.1 \lesssim z_0 \lesssim 9.4$.

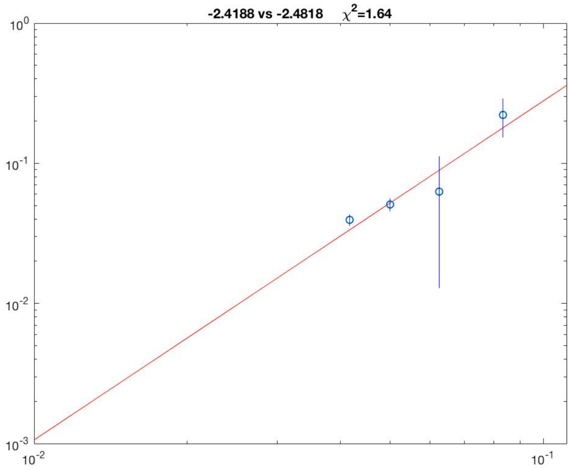


Taking $T_{\rm RW}^{N_\tau=4} = 201.4$ MeV yields $\beta\delta \approx 1.5635$, compare 1.563495(15).

Prelim: $T_{\rm RW} = 211.1(3.1)$ MeV, compare 208(5) MeV.

[20] C. Bonati et al., Phys. Rev. D, 93.7, 074504 (2016).
[21] G. Johnson et al., Phys. Rev. D, 107.11, 116013 (2023).

Test: Roberge-Weiss FSS



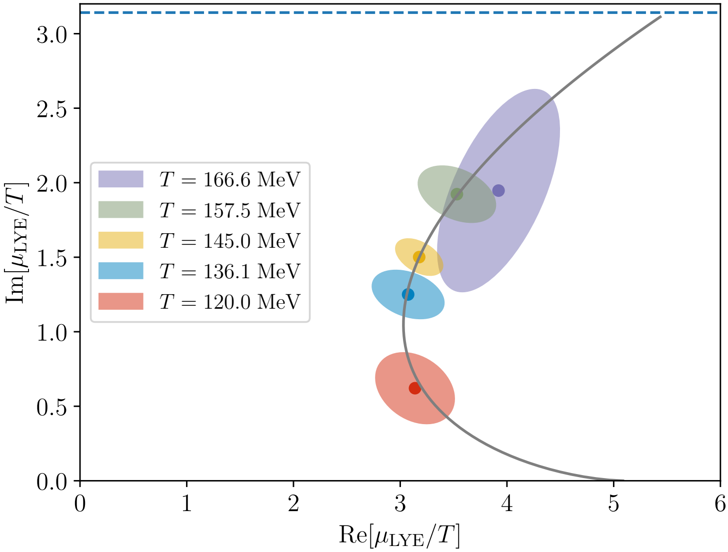
FSS scaling of $\mathrm{Re}\,\hat{\mu}_{\mathsf{LY}}$ near RW transition reasonably captured.

More simulation details

- Generate HISQ using RHMC of `SIMULATeQCD`
- Set scale with f_K

β	T [MeV]	N_μ	N_{conf}/N_μ
6.170	166.6	10	1800
6.120	157.5	10	4780
6.038	145.0	10	5300
5.980	136.1	10	6840
5.850	120.0	10	24000

Simulataneous fit



CEP distribution