The QCD phase diagram and Lee-Yang zeros

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[PRD 109 (2024) 11, 114516, arXiv: <u>2403.09390</u>] [PRD 105 (2022) 7, 074511, arXiv: 2202.09184]





Bielefeld Parma Collaboration:

David Clarke, Petros Dimopoulos, Francesco Di Renzo, Jishnu Goswami, Guido Nicotra, CS, Simran Singh, Kevin Zambello [arXiv: 2405.10196] [PRD 105 (2022) 3, 034513, arXiv: 2110.15933]

ECT,* Trient, September 9-13, 2024

- * Track Lee-Yang edge singularity in the complex $\frac{\mu_B}{T}$ -plane, as function of T
- * We can think of three distinct critical points/ scaling regions: Roberge Weiss transition, chiral transition, QCD critical point

* Solve $t/h^{1/\beta\delta} \equiv z_{YL}$ for different scaling fields and non-universal constants.





 \rightarrow different temperature intervals are sensitive to different scaling of the Lee-Yang edge singularity

* Universal scaling of Lee-Yang zeros and Lee-Yang edge Singularity

- ➡ Finite size vs infinite size scaling
- * First Lee-Yang zero via Padé and multi-point Padé
 - Scaling evidence from Roberge-Weiss transition (and 2d-Ising model)
 - ➡ First Estimates of the QCD critical end-point
- * Estimate via Fourier coefficients

Universal scaling of the zeros of the partition function



Finite size scaling function of the partition function $Q(tL^{1/\nu}, h^2L^{2\beta\delta/\nu}) = 0$ [tzykson et al. NPB 220 (1983) 415]

* Finite size scaling: scaling of the zeros is well understood, universal angels $\varphi, \psi = \pi/(2\beta\delta)$ indicate the universality class.

* Infinite size scaling: Lee-Yang condense to a branch cut in the infinite size limit. The edge singularity has a universal position in terms of $z = t/h^{1/\beta\delta}$



Lee-Yang edge singularities in the complex μ_B/T -plane

Scaling variable: $z = t/h^{1/\beta\delta}$ Use universal constant $z_{LY} = |z_c| e^{i\frac{\pi}{2\beta\delta}}$ Solve for $\mu_{LY}(T)$

Roberge-Weiss transition:

$$t = t_0 \left(\frac{T_{RW} - T}{T_{RW}} \right)$$
 and $h = h_0 \left(\frac{\hat{\mu}_B - i\pi}{i\pi} \right)$

Chiral transition:

$$t = t_0 \left[\frac{T - T_c}{T_c} + \kappa_2^B \left(\frac{\mu_B}{T} \right)^2 \right] \text{ and } h = h_0 \frac{m_l}{m_s^{\text{phys}}}$$

QCD critical point:

$$t = \alpha_t (T - T_{cep}) + \beta_t (\mu_B - \mu_{cep}) \text{ and}$$
$$h = \alpha_h (T - T_{cep}) + \beta_h (\mu_B - \mu_{cep})$$

 \rightarrow different temperature intervals exhibits different scaling of the Lee-Yang edge singularity



Simulation Strategie: first Lee-Yang zero in a finite volume

*Calculate derivatives of the pressure $\frac{p}{T^4} = \frac{\ln Z}{VT^3}$

 $(T, \mu_B = 0)$: Taylor expansion in μ_B^2

 $(T, \mu_B^2 < 0)$: Taylor expansion in μ_B



⇒ perform a Padé resummation to obtain the complex singularity that limit the radius of convergence



[De Frorcrand, Philipsen (2002); D'Elia, Lombardo (2003)]

- ⇒ obtain a rational approximation of the data (e.g. by the multi-point Padé) to obtain the closest singularity
- ⇒ alternatively, analyse the (asymptotic) behaviour of the Fourier coefficients



The Roberge-Weiss temperature



* The approach of the LY edge to the RW critical point: By solving $z = t/h^{1/\beta\delta} \equiv z_c$ we find

$$\hat{\mu}_{LY}^R = a(N_{ au}) \left(rac{T_{RW}(N_{ au}) - T}{T_{RW}(N_{ au})}
ight)^{eta \delta}$$

with
$$\hat{\mu}_{LY}^R = ext{Re}[\mu_B/T]$$

We assume $T_{RW} = T_{RW}^{(0)} + T_{RW}^{(2)}/N_{ au}^2$
 $a = a^{(0)} + a^{(2)}/N_{ au}^2$

* Obtain continuum result

$$T_{RW}^{(0)} = 211.1 \pm 3.1 \text{ MeV}$$

 \Rightarrow in good agreement with previous results from the Pisa group

[Bonati et al., PRD 93 (2016) 074504]

Fischer and Lee-Yang zeroes in the 2d Ising model

- * The multi-point method works well in the Ising model when applied to the magnetisation or the specific heat.
- * A finite size scaling analysis reproduces the transition temperature β_c and the critical exponents ν and $\beta\delta$



[Singh et al, PRD 109 (2024) 7, 07450, arXiv: 2312.03178]

The Padé resummation

- Detecting phase transitions via Padé and post-Padé approximants has a long history in statistical and high energy physics
- They are often used in combination with perturbation theory
- *QCD is nonperturbative in the vicinity of the phase
- * The numerical calculation of the pressure series in μ_B is difficult



HotQCD, PRD 108 (2023) 1, 014510, arXiv: 2212.09043]

- Construct [4,4]-Padé from 8th order Taylor Expansion
- Calculate complex roots of the denominator
- Find apparent
 approach to the real
 axis with decreasing
 temperature
- Can also be combined with conformal maps [Basar, 2312.06952]

$$P[4,4] = \frac{P_2\hat{\mu}_B^2 + (P_4 + (P_2^2 P_8)/P_4^2)\hat{\mu}_B^4}{1 + ((P_2 P_8)/P_4^2)\hat{\mu}_B^2 - (P_8/P_4)\hat{\mu}_B^4}$$



[PRD 105 (2022) 7, 074511, arXiv: 2202.09184]

Lattice Setup ($N_{\tau} = 6$)

Code:



Simulation Parameters:

- * Use (2+1)-flavor of *Highly Improved Staggered Quarks* (HISQ) with physical masses $(m_l/m_s = 1/27)$.
- ***** Lattice size: $36^3 \times 6$
- Use Line of Constant Physics (LCP) and scale setting from HotQCD
- * Introduce non-zero imaginary chemical potential $\hat{\mu}_u = \hat{\mu}_d = \hat{\mu}_s = i\theta$, which corresponds to $\mu_B = 3\mu_u$ and $\mu_S = 0$

Statistics:

N_{μ}	$N_{ m conf}/N_{\mu}$
10	1800
10	4780
10	5300
10	6840
10	24000
	$ \begin{array}{r} N_{\mu} \\ 10 \\ 10 \\ $

Machines:

- #Juwels-Booster @ JSC
- * Marconi100 @ CINECA
- * Leonardo @ CINECA

Lattice Data



Observables:

* Derivatives of $\ln Z$, w.r.t $\hat{\mu}_B = \mu_B/T$

$$\chi^B_n(T) = rac{V}{T^3} \left(rac{\partial}{\partial \hat{\mu}_B}
ight)^n \ln Z(T, \hat{\mu}_B)$$

- * $\ln Z$ is even in $\hat{\mu}_B = i\theta$ and periodic, with periodicity 2π
- * Choose 10 equidistant $\hat{\mu}_B$ -points in $[0, i\pi]$, all further points are obtained by periodicity and parity
- * Odd (even) derivatives are imaginary (real) at $\hat{\mu}_B = i\theta$

Sliding Window Analysis



Procedure:

- * Perform simultaneous fits to χ_1^B and χ_2^B for each temperature
- *Use [3,3]-Padé
- * Varry length of the fit interval in $[\pi, 2\pi]$ and the center of the interval in $[-\pi/2, +\pi/2]$
- * bootstrap over the data by assuming independent and normal distributed errors
- Calculate roots of the denominator and keep only roots in the first quadrant
- Collect all the results for Lee-Yang scaling fits. We have 55 different intervals per temperature.

Scaling in the vicinity of the QCD critical point

Mixing of scaling fields:

* Scaling fields are unknown, a frequently used ansatz is given by a linear mixing of T, μ_B

$$\begin{split} t &= A_t \Delta T + B_t \Delta \mu_B, \\ h &= A_h \Delta T + B_h \Delta \mu_B, \end{split}$$
 with $\Delta T &= T - T^{\rm CEP}$ and $\Delta \mu_B = \mu_B - \mu_B^{\rm CEP}$





Fit Ansatz:

* For a constant $z = z_c$ we obtain $\operatorname{Re}[\mu_{\text{LYE}}] = \mu_B^{\text{CEP}} + c_1 \Delta T + c_2 \Delta T^2 + O(\Delta T^3)$ $\operatorname{Im}[\mu_{\text{LYE}}] = c_3 \Delta T^{\beta \delta},$

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

* The fit parameter c_1 gives the (inverse) slope of the 1st order line at the critical point: $c_1 = -A_h/B_h$

Fit results

* Perform one fit for $N_{\tau} = 8$ and $\mathcal{O}(10^5)$ fits for $N_{\tau} = 6$



- * Ellipses show 1 σ confidence region, using the Pearson correlation coefficient ${
 m Im}[$
- * $N_{\tau} = 6$ singularities show here are chosen on the basis of the χ^2 of the scaling fit ("best fit")



- $\operatorname{Re}[\mu_{\mathrm{LYE}}] = \mu_B^{\mathrm{CEP}} + c_1 \Delta T + c_2 \Delta T^2$ $\operatorname{Im}[\mu_{\mathrm{LYE}}] = c_3 \Delta T^{\beta \delta},$
- * Orange box shows the AIC weighted result for $N_{\tau} = 6$, based on $\mathcal{O}(10^5)$ scaling fits

Statistical analysis of fits



* Histogram over the $T^{\rm CEP}$ and $\mu_B^{\rm CEP}$ from the $\mathcal{O}(10^5)$ fits

* Error bars are based on the inner 68-percentile

Observe interesting structure

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Dashed line

continuum

indicates the

extrapolated

crossover line

Statistical analysis of fits



* For $N_{\tau} = 8$: similar results by [Basar, arXiv: 2312.06952]

Crossover line and cutoff effects

 Continuum estimate might suffer from large systematic effects (Padé vs multi-point Padé)

* $\kappa_2 = \bar{\kappa}_2 = -0.015(1)$ [HotQCD, <u>2403.09390</u>]

* Many results seem to favour a small $\bar{\kappa}_4 \approx - \ 0.0002(1)$



Parametrizations of the crossover line: * 1.)
$$T_{\rm pc}(\mu_B) = T_{\rm pc}(0) \left[1 + \kappa_2^B \left(\frac{\mu_B}{T} \right)^2 + \kappa_4^B \left(\frac{\mu_B}{T} \right)^4 \right]$$
*** 2.)** $T_{\rm pc}(\mu_B) = T_{\rm pc}(0) \left[1 + \bar{\kappa}_2^B \left(\frac{\mu_B}{T_{\rm pc}(0)} \right)^2 + \bar{\kappa}_4^B \left(\frac{\mu_B}{T_{\rm pc}(0)} \right)^4 \right]$

→ <u>Talk by A. Adam@Lattice24</u>: single point Padé approximation of the pressure based on χ_2^B , χ_4^B , χ_6^B , χ_8^B (LT=2)

- Interesting to check results with the Budapest-Wuppertal data
- Preliminary results for single Point Padé analysis on 16³ × 8 lattices, multi-Point is work in progress
- Preliminary result on the transition temperature based on extrapolations 432 on different approximations and fit ranges
- T^{CEP} around 90 MeV, in agreement with
 [BiePar, <u>2405.10196</u>]
- Results are very sensitiv to noise

Histogram of the T^{CEP} results



One example of the extrapolations



Talk by T. Wada@Lattice24: Finite size scaling of Lee-Yang zeros in 3d Pots model and heavy-quark QCD

- Construct ratios of the LYZ locations
- Scaling is in accordance with a ratio of scaling function: nonuniversal pre-factors cancel, intersection point of different volumes is universal.
- Ratios show reduced corrections to scaling and regular parts
- T^{CEP} is shifted to higher
 values, results from
 extrapolation of first LYZ can
 serve as a lower bound









Method:

- Interpolate Im χ_1^B , take also it's derivative Re χ_2^B and eventually higher derivatives up to order *s* into account \rightarrow Hermite-interpolation (spline)
- Piecewise integration can be done analytically

$$b_{k} = \frac{2}{\pi} \sum_{i=0}^{N-1} \int_{\theta_{B}^{(i)}}^{\theta_{B}^{(i+1)}} \mathrm{d}\theta_{B} \ p(\theta_{B}) \sin(k\theta_{B}) \quad \text{with} \quad 0 = \theta_{B}^{(0)} < \theta_{B}^{(1)} < \dots < \theta_{B}^{(N)} = \pi$$

 \rightarrow variant of a Filon-type quadrature: error decreases as $\mathcal{O}(k^{-s-2})$ (for exact data)

• Statistical error is estimated by bootstrapping over the error of Im χ_1^B and Re χ_2^B .

• We can deform the integration contour to integrate along the cuts



Assume that we can express the density along the cuts as

$$n_B(\hat{\mu}) = \underbrace{A(\hat{\mu} - \hat{\mu}^{\mathbf{br}})^{\sigma}}_{\text{Leading order}} (1 + B(\hat{\mu} - \hat{\mu}^{\mathbf{br}})^{\theta_c} + \ldots) + \underbrace{\sum_{n=0}^{\infty} a_n (\hat{\mu} - \hat{\mu}^{\mathbf{br}})^n}_{\text{analytic part}}$$

analytic part

• The final result for one cut is

$$b_k = \frac{e^{-\mu^{\operatorname{br}}k}}{i\pi} A \frac{\Gamma(1+\sigma)}{k^{1+\sigma}} \left(1 - e^{i2\pi\sigma} + \frac{B}{k^{\theta_c}} \left[1 - e^{i2\pi(\sigma+\theta_c)} \right] \frac{\Gamma(1+\sigma+\theta_c)}{\Gamma(1+\sigma)} + \dots \right)$$

Absorbing k-independent factors into A and B we get

$$b_k = ilde{A} rac{e^{-\hat{\mu}^{\mathrm{br}}k}}{k^{1+\sigma}} \left(1 + rac{ ilde{B}}{k^{ heta_c}} + \ldots
ight)$$
 Note that the cancels composited on the concels composited on the concentration of the concentration of the cancel of the concentration of the concentratic definition of the concentration of the concentrat

regular part oletely

• The final result for both cuts is (dropping NLO)

$$b_{k} = |\tilde{A}_{\text{YLE}}| \frac{e^{-\hat{\mu}_{r}^{\text{YLE}}k}}{k^{1+\sigma}} \cos(\hat{\mu}_{i}^{\text{YLE}}k + \phi_{a}^{\text{YLE}}) + |\hat{A}_{\text{RW}}|(-1)^{k} \frac{e^{-\hat{\mu}_{r}^{\text{RW}}k}}{k^{1+\sigma}}$$

$$\hat{\mu}_{i}^{RW} = \pi$$

Test of the analytic form in the quark-meson model

- The analytic form fits the Fourier coefficients from the quark-meson model well. Details of the Model can be found here [Skokov et al., PRD 82 (2010) 034029]
- In Mean-Field and LAP approximation fits to the Fourier coefficients reproduce the correct location of the LY edge up to (5 – 7)%.



- * Universal scaling is a very powerful tool if the scaling fields and the universality class are known.
- * Pseudo-critical lines correspond (asymptotically) to a constant real $z = t/h^{1/\beta\delta}$, the Lee-Yang edge to a universal complex z_c
- New Strategy: Determine the QCD critical point by the temperature scaling of the Lee-Yang edge singularity
- * Technically this requires Pade or multi-point Pade analysis of $\ln Z$ derivatives. The later eliminates the need for the calculation of high order expansion coefficients but introduces some interval dependence.
- * Find encouraging results for $N_{\tau} = 6$: $(T^{\text{CEP}}, \mu_B^{\text{CEP}}) = (105^{+8}_{-18}, 422^{+80}_{-35})$ MeV .
- * No continuum result yet

* Current estimates of the cutoff effects increase $\mu_B^{
m CEP}$ towards $\mu_B^{
m CEP} pprox 650$ MeV

Back Up Slides



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Chiral scaling fields and operators



* chiral condensates couple to the temperaturelike scaling field

Magnetic equation of state

$$M=h^{1/\delta}\left(f_G(z)-f_\chi(z)
ight)$$

* $f_G(x)$ and $f_{\chi}(z)$ are universal function of a single scaling variable $z = t/h^{1/\beta\delta}$

<u>Order parameter</u>

$$M_l = rac{\displaystyle \int \mathop{\mathrm{Remove\ multiplicative\ UV\ divergences}}}{\displaystyle \int _{K_{K_{L}}^4} rac{\displaystyle T}{\displaystyle \int \frac{\partial \ln Z}{\partial m_l}} }{\displaystyle \int _{\partial m_l}^4 = rac{\displaystyle \partial }{\displaystyle \partial m_u} + rac{\displaystyle \partial }{\displaystyle \partial m_d}}$$

$$\frac{Magnetic \ susceptibility}{\chi_l = m_s \frac{\partial}{\partial m_l} M_l}$$

"Improved" order parameter

$$M = M_l - H\chi_l$$

[PRD 109 (2024) 11, 114516, arXiv: <u>2403.09390</u>]

Curvature coefficients

*****Remember:

$$t=rac{1}{t_0}\left(\Delta T+\kappa_2^l\hat{\mu}_l^2+\kappa_2^s\hat{\mu}_s^2+2\kappa_{11}^{ls}\hat{\mu}_l\hat{\mu}_s
ight)$$

Ratio of mixed susceptibilities are related to the curvature coefficients

$$\kappa_2^l = rac{1}{2T_c} \left(rac{\partial^2 M_l / \partial \hat{\mu}_l^2}{\partial M_l / \partial T}
ight) \Big|_{(T=T_c, ec{\mu}=0)}$$

$$\kappa_{11}^{ls} = \frac{1}{2T_c} \left(\frac{\partial^2 M_l / \partial \hat{\mu}_l \hat{\mu}_s}{\partial M_l / \partial T} \right) \Big|_{(T=T_c, \vec{\mu}=0)}$$

results may be transformed to the hadronic basis



[PRD 109 (2024) 11, 114516, arXiv: 2403.09390]

$$egin{aligned} &\kappa_2^{B,\hat{\mu}_S=0}\equiv\kappa_2^B=0.015(1)\ &\kappa_2^{B,n_S=0}=0.893(35)\kappa_2^B\ &\kappa_2^{B,\hat{\mu}_s=0}=0.968(23)\kappa_2^{n_S=0} \end{aligned}$$

Temperature-like derivatives of the order parameter

$$\chi_{t(T)}^{M_{\ell}} = -T_{c} \frac{\partial M_{\ell}}{\partial T} ,$$

$$\chi_{t(f,f)}^{M_{\ell}} = -\frac{\partial^{2} M_{\ell}}{\partial \hat{\mu}_{f}^{2}} ,$$

$$\chi_{t(\ell,s)}^{M_{\ell}} = -\frac{\partial^{2} M_{\ell}}{\partial \hat{\mu}_{\ell} \partial \hat{\mu}_{s}} ,$$

Peak-position of susceptibilities determine a pseudo critical line (constant z_{y})



Perform joined fit to peak positions of mixed susceptibilities, including corrections to scaling \rightarrow results for T_c , z_0 are in good agreement with EoS fits.

Standard Padé:

* Starting point is a power series L

$$f(x) = \sum_{i=0}^{L} c_i x^i + \mathcal{O}(x^{L+1}).$$

- * A Padé approximation is constructed such that the expansion of the Padé is identical to the Taylor series about x = 0
- * We denote the [m/n]-Padé as

$$R_n^m(x) = \frac{P_m(x)}{\tilde{Q}_n(x)} = \frac{P_m(x)}{1 + Q_n(x)} = \frac{\sum_{i=0}^{m} a_i x^i}{1 + \sum_{j=1}^{n} b_j x^j}$$

т

* One possibility to solve for the coefficients a_i, b_j , is by solving the tower of equations

$$P_m(0) - f(0)Q_n(0) = f(0)$$
$$P'_m(0) - f'(0)Q_n(0) - f(0)Q'_n(0) = f'(0)$$
$$\vdots$$

→ Linear system of size m + n + 1, need m + n derivatives of f(x)

Multipoint Padé:

- * We have power series at several points x_k
- * We demand that at all points x_k the expansion of the Padé is identical to the Taylor series about $x = x_k$
- * One possibility (method I) to solve for the coefficients a_i, b_j , is by solving the tower of equations

$$P_{m}(x_{0}) - f(x_{0})Q_{n}(x_{0}) = f(x_{0})$$

$$P'_{m}(x_{0}) - f'(x_{0})Q_{n}(x_{0}) - f(x_{0})Q'_{n}(x_{0}) = f'(x_{0})$$

$$\vdots$$

$$P_{m}(x_{1}) - f(x_{1})Q_{n}(x_{1}) = f(x_{1})$$

$$P'_{m}(x_{1}) - f'(x_{1})Q_{n}(x_{1}) - f(x_{1})Q'_{n}(x_{1}) = f'(x_{1})$$

$$\vdots$$

→ again a linear system of size m + n + 1, need much less derivatives, we have $m + n + 1 = \sum_{k} (L_k + 1)$

[Dimpopoulos et al. Phys.Rev.D 105 (2022) 3, 034513]

A parametrisation of of the scaling function

$$M=m_0R^eta heta\ t=R(1- heta^2)\ h=h_0R^{eta\delta}h(heta)^{-1/eta\delta}\ z(heta)=rac{1- heta^2}{ heta_0^2-1} heta_0^{1/eta}\left(rac{h(heta)}{h(1)}
ight)^{-1/eta\delta}$$

$$> h(heta) = heta \left(1 + h_3 heta^2 + h_5 heta^4 + h_7 heta^6 + \cdots
ight)$$

- The coefficients h_3 , h_5 can be determined perturbatively and non-perturabively

[Guida, Zinn-Justin, NPB 489 (1997)] [Karsch et al. PRD 108 (2023) 014505]



- the coefficient h_7 is not known precisely (zero within current precision)
- $h_7 \neq 0$ introduces an additional pair of singularities (imaginary if $h_7 > 0$, real if $h_7 < 0$)
- h_7 can be used to tune the phase of the LY edge singularity

[Karsch, CS, Singh, arXiv:2311.13530]