Search for the QCD critical endpoint in high-statistics lattice simulations

Workshop at ECT*

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Introduction

The data : $\chi_2, \chi_4, \chi_6, \chi_8, \chi_{10}$

[Adam et al. 2507.13254]
Previous talk by S. Borsanyi

- Volume : $16^3 \times 8$
- ≈ 2 million configs. per T at $\mu = 0$
- Jackknife with $N_J = 48$
- 2+1 flavours with 4 HEX smearing
- Simulated at physical quark mass
- B-Spline with χ^2 fit

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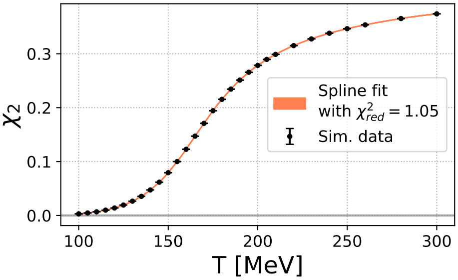

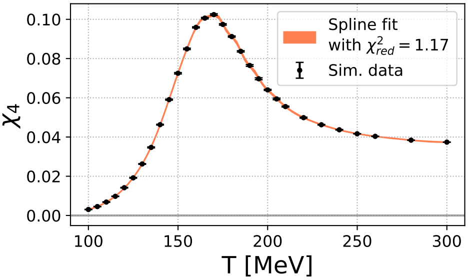

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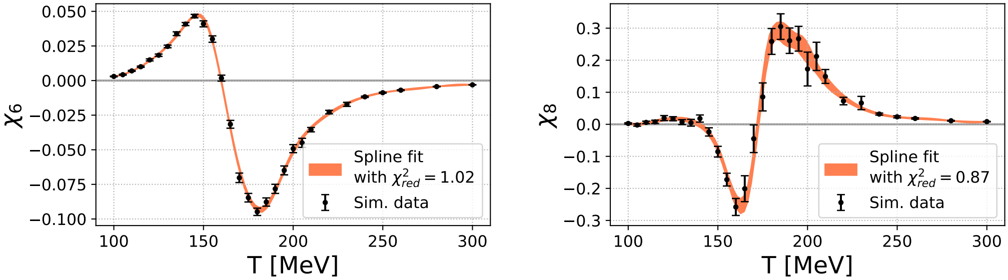

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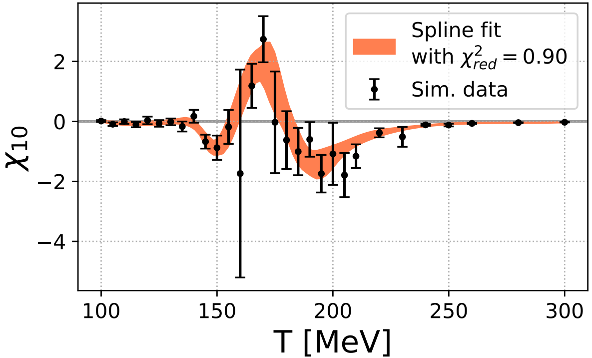
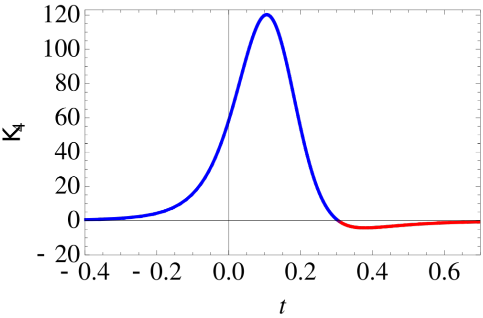


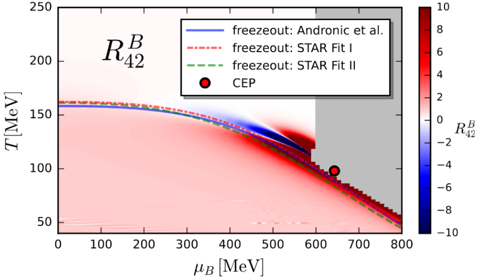
Search for CEP via $\chi's$

1) Search via Non-Gaussian fluctuations M. A. Stephanov [0809.3450]

[Stephanov 1104.1627]



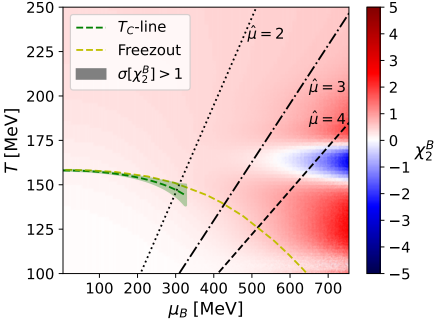
(DSE: [Lu et al. 2504.05099])
FRG: [Fu et al. 2308.15508]



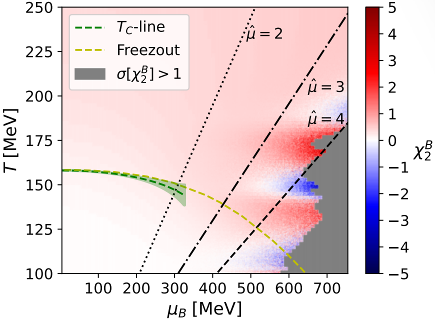
$$\kappa_4 = \frac{6T}{V}\left[2(\lambda_3\xi)^2 - \lambda_4\right]\xi^8$$ correlation length: $\xi \longrightarrow \infty$ at CP

Extrapolate χ_2 using Taylor

$$\chi_2^B(T,\mu_B) = \left(\frac{\partial^2(p/T^4)}{\partial(\mu_B/T)^2}\right)_{\mu_B} = \chi_2 + \chi_4\frac{\hat{\mu}_B^2}{2!} + \chi_6\frac{\hat{\mu}_B^4}{4!} + \dots$$



χ_2^B using up to χ_8



χ_2^B using up to χ_{10}

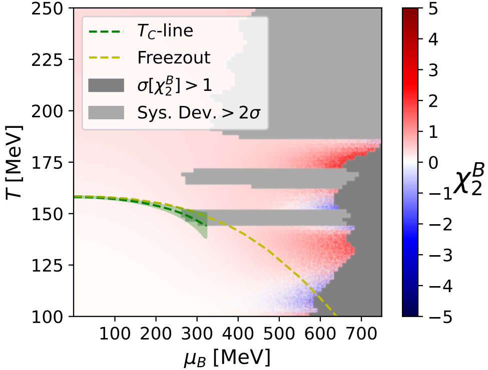
T_C-line : [Borsanyi et al. 2002.02821]   Freezout : [Andronic et al. 1710.09425]

Extrapolate χ_2 incl. systematic error

Sys. Dev.: Deviation of the extrapolation between the usage of χ_8 or χ_{10} above 2σ

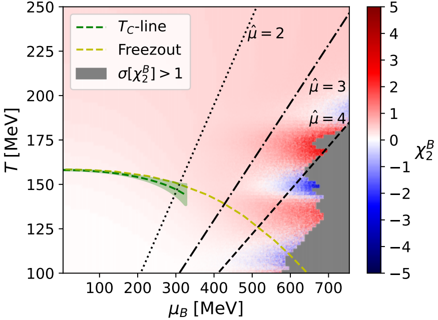
$$\Delta = \text{Taylor}_{\chi_8}[\chi_2^B] - \text{Taylor}_{\chi_{10}}[\chi_2^B]$$

$$\frac{\Delta}{\text{std dev}(\Delta)} > 2$$

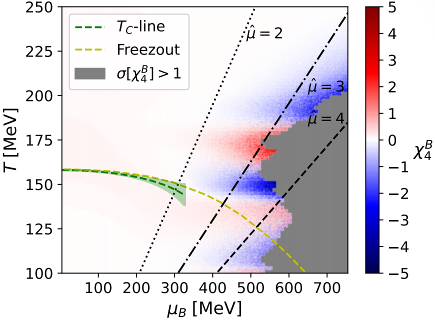


Extrapolate χ_2 & χ_4 using Taylor

$$\chi_4^B(T,\mu_B) = \left(\frac{\partial^4(p/T^4)}{\partial(\mu_B/T)^4}\right)_{\mu_B} = \chi_4 + \chi_6\frac{\hat{\mu}_B^2}{2!} + \chi_8\frac{\hat{\mu}_B^4}{4!} + \dots$$



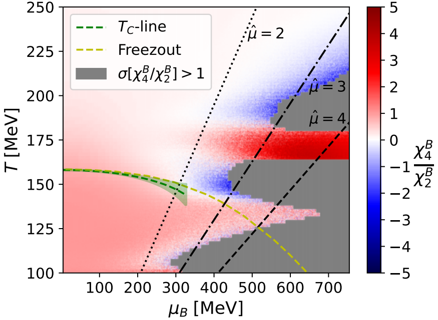
χ_2^B using up to χ_{10}



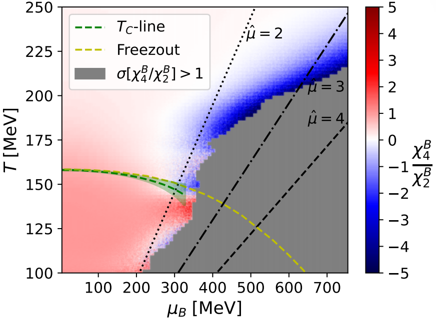
χ_4^B using up to χ_{10}

Ratio of Taylor vs Taylor of Ratio

$$\frac{\chi_4}{\chi_2} = \frac{\text{Taylor}[\chi_4^B](T,\mu_B)}{\text{Taylor}[\chi_2^B](T,\mu_B)} \quad \text{or} \quad \frac{\chi_4}{\chi_2} = \text{Taylor}\left[\frac{\chi_4^B}{\chi_2^B}\right](T,\mu_B)$$



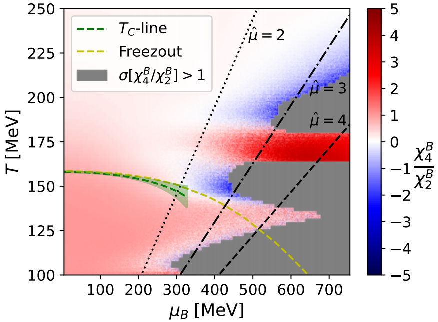
Ratio of Taylor

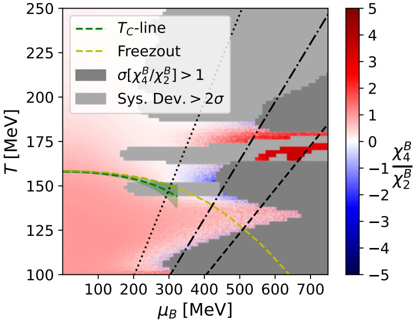


Taylor of Ratio

Extrapolate χ_4/χ_2 using Ratio of Taylor

$$\frac{\chi_4^B(T,\mu_B)}{\chi_2^B(T,\mu_B)} \approx \frac{\chi_4 + \chi_6\frac{\hat{\mu}_B^2}{2} + \chi_8\frac{\hat{\mu}_B^4}{4!} + \chi_{10}\frac{\hat{\mu}_B^6}{6!}}{\chi_2 + \chi_4\frac{\hat{\mu}_B^2}{2} + \chi_6\frac{\hat{\mu}_B^4}{4!} + \chi_8\frac{\hat{\mu}_B^6}{6!} + \chi_{10}\frac{\hat{\mu}_B^8}{8!}},$$





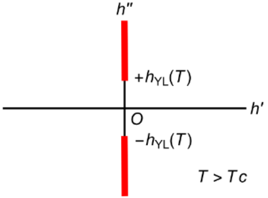
using up to χ_{10}

Lee-Yang Zeros & Padé

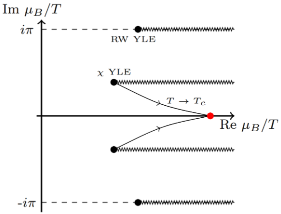
Lee-Yang theory

GC partition function: $Z_{\rm GC}^{N} = \sum_{N_i} Z(N_i, V, T)\, z^{N_i}$,

Path of complex roots in finite system is indicative of the phase transition :
If they pinch the real axis $\Longrightarrow$ second order phase transition



Ising model [Wei 1611.08074]



QCD [Skokov 2411.02663]

To detect LYZ use ansatz allowing for singularity $\Longrightarrow$ Padé

Taylor and Padé for $f(x) = 1/\cosh(x)$

$$T_l(x) = \sum_{i=0}^{l} c_i x^i \qquad \text{Pade}[m,n] : \frac{P_m(x)}{1+Q_n(x)} = \frac{\sum_{i=0}^{m} a_i x^i}{1+\sum_{i=1}^{n} b_i x^i}$$

Taylor of f up to $l = 6$: $\frac{1}{\cosh(x)} \approx 1 - \frac{x^2}{2} + \frac{5x^4}{25} - \frac{61x^6}{720}$

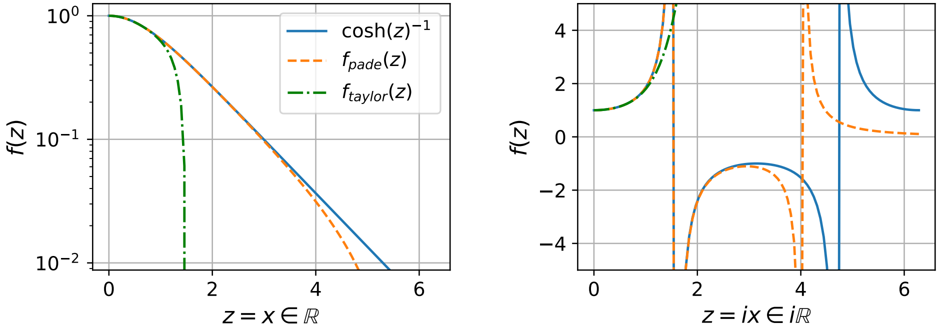
Convert by solving $P_m(x) - T_l(x)Q_n(x) = T_l(x)$ order by order ($l \overset{!}{=} m+n+1$)

$$\left.\frac{\partial}{\partial x}\right|_{x=0} P_m(x) - T_l(x)Q_n(x) = \left.\frac{\partial}{\partial x}\right|_{x=0} T_l(x) = c_i i! \implies M(\vec{c})\begin{pmatrix}\vec{a}\\ \vec{b}\end{pmatrix} = \vec{c}$$

[2,4]-Padé: $\frac{1}{\cosh(x)} \approx \frac{1-\frac{1}{30}x^2}{1+\frac{7}{15}x^2+\frac{1}{40}x^4}$

Plot of Taylor and Padé for $f(x) = 1/\cosh(x)$

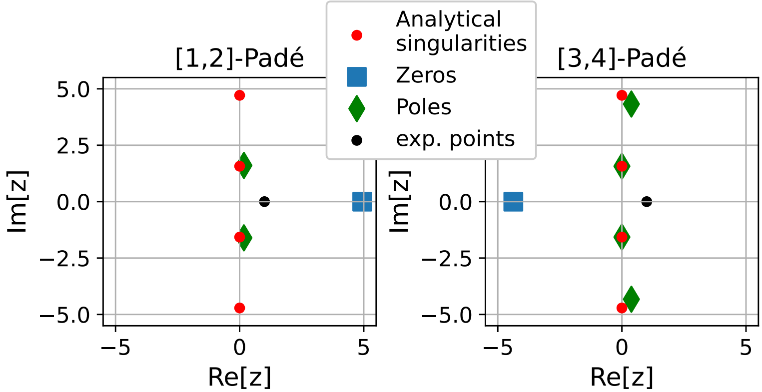
$$T_l(x) = \sum_{i=0}^{l} c_i x^i \qquad \text{Pade}[m,n] : \frac{P_m(x)}{1+Q_n(x)} = \frac{\sum_{i=0}^{m} a_i x^i}{1+\sum_{i=1}^{n} b_i x^i}$$



Extract Poles from Padé

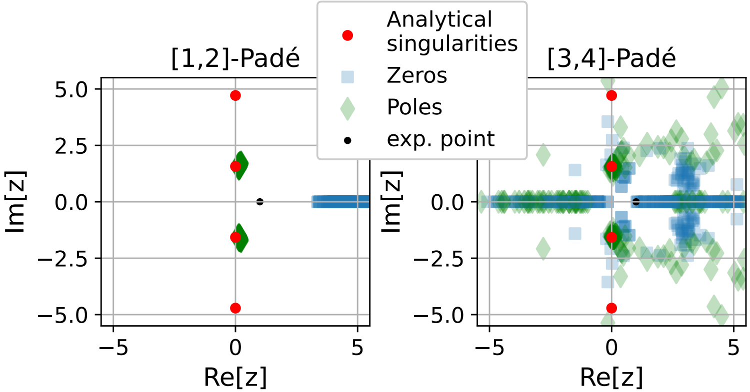
$$T_l(x) = \sum_{i=0}^{l} c_i x^i \qquad \text{Pade}[m,n] : \frac{P_m(x)}{1+Q_n(x)} = \frac{\sum_{i=0}^{m} a_i x^i}{1+\sum_{i=1}^{n} b_i x^i}$$

solving the equation $1 + Q_n(x) \overset{!}{=} 0$ gives the Poles ($z_0 = 1 + 0i$)



Padé with Noise

Emulating error on the derivatives:
Drawing $N = 100$ samples of from Gaussian distribution with $\mu = \partial_z^n f(x)$ and 3% relative error.



Padé for QCD

$$T_l(x) = \sum_{i=0}^{l} c_i x^i \qquad \text{Pade}[m,n] : \frac{P_m(x)}{1+Q_n(x)} = \frac{\sum_{i=0}^{m} a_i x^i}{1+\sum_{i=1}^{n} b_i x^i}$$

What expansion variable? Motivation by symmetries!

- Charge conjugation symmetry $Z(T,-\theta) = Z(T,\theta)$ ($\mu_B = i\theta T$)
  $\implies$ even function in $i\mu_B$
- Roberge Weiss symmetry $Z(T,\theta) = Z(T,\theta+2\pi)$
  $\implies$ periodic function in $i\mu_B$

Simplest function for both symmetries: $\cos(i\mu_B) = \cosh(\mu_B)$ Other collaborations used for example:

- HotQCD collaboration μ_B^2 : [Bollweg et al. 2202.09184]
- Parma Bielefeld μ_B : [Clarke et al. 2405.10196]

Models

The resulting models incorporating the respective symmetries:

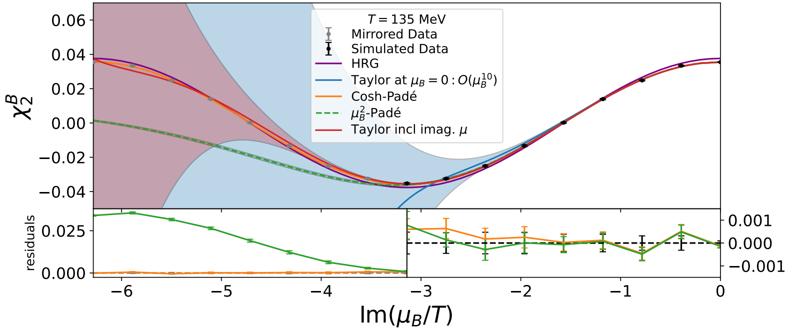
$$\text{Cosh-Padé for } \Delta\hat{p} : \frac{a \cdot (\mathbf{cosh}(\hat{\mu}) - 1)}{1 + c(\cosh(\hat{\mu}) - 1) + d(\cosh(\hat{\mu}) - 1)^2}$$

$$\text{Cosh-Padé for } \chi_1 : \frac{a \cdot \mathbf{sinh}(\hat{\mu})}{1 + c(\cosh(\hat{\mu}) - 1) + d(\cosh(\hat{\mu}) - 1)^2}$$

$$\text{Cosh-Padé for } \chi_2 : \frac{(a + b \cdot (\mathbf{cosh}(\hat{\mu}) - 1))}{1 + c(\cosh(\hat{\mu}) - 1) + d(\cosh(\hat{\mu}) - 1)^2}$$

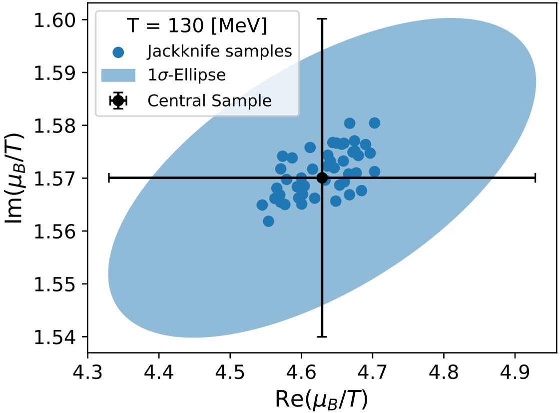
Exemplary fit results for χ_2 at $T = 135$ MeV

- Simulated Data: Performed at $\hat{\mu}_B = i\pi(j/8)$ with ~ 100k per j and T
- Taylor:
  - Using data at $\hat{\mu}_B = 0$
  - χ^2-Fit to full data ($\hat{\mu}_B = 0 \quad \& \quad \hat{\mu}_B = i\pi(j/8)$)
- Padé via χ^2-Fit to full data: Cosh-Padé & μ_B^2-Pade



Example LYZ/Pole extraction

$$\left(1 + c(\cosh(\hat{\mu}) - 1) + d(\cosh(\hat{\mu}) - 1)^2\right) \stackrel{!}{=} 0$$



LYZ Analysis

Analysis Overview:

- $\overbrace{\chi_2, \chi_4, \chi_6, \chi_8, \chi_{10}}^{\text{each} \sim 2\text{M cfgs per T}}$ at $\mu^2 = 0$ & $\overbrace{\chi_1, \chi_2, \chi_3, \chi_4}^{\text{each} \sim 100\text{k cfgs per T}}$ at $\mu^2 < 0$
  $\Longrightarrow$ Cosh-Padé via χ^2 minimization

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$$f(\hat{\mu}) = \frac{a(\cosh(\hat{\mu}) - 1)}{1 + c(\cosh(\hat{\mu}) - 1) + d(\cosh(\hat{\mu}) - 1)^2}$$

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- Repeat for each jackknife sample and independently for each temperature.

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- Repeat for each jackknife sample and independently for each temperature.
- Extrapolate T_c, via eg. $\text{Im}[f(\mu_B^{\text{LYZ}}, T)] = \kappa\,(\Delta T)^{\beta\delta}$

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$$f(\hat{\mu}) = \frac{a(\cosh(\hat{\mu}) - 1)}{1 + c(\cosh(\hat{\mu}) - 1) + d(\cosh(\hat{\mu}) - 1)^2}$$

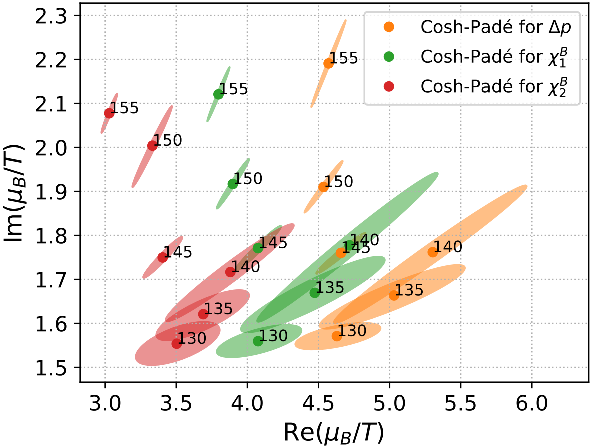
- Poles:

$$(1 + c(\cosh(\hat{\mu}) - 1) + d(\cosh(\hat{\mu}) - 1)^2) \stackrel{!}{=} 0$$

- Repeat for each jackknife sample and independently for each temperature.
- Extrapolate T_c, via eg. $\mathrm{Im}[f(\mu_B^{\text{LYZ}}, T)] = \kappa\,(\Delta T)^{\beta\delta}$
- Estimation of systematic effects
  - Use Δp or χ_1 or χ_2
  - Vary fit range in temperature
  - Use different scaling observables: μ, μ^2, μ^3, μ^4

Varying the scheme used

Numbers next to data points indicate temperature

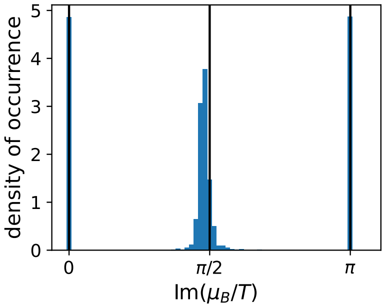


Non Critical Baseline: nHRG

Use HRG to create noncritical input data:

$$\hat{p} = \frac{p_B}{T^4} = \sum_{i \in baryons} \frac{g_i}{\pi^2} \left(\frac{m_i}{T}\right)^2 K_2\left(\frac{m_i}{T}\right) \mathbf{cosh}\left(\frac{\mu_B}{T}\right).$$

with gaussian noise determined by the relative error on the lattice data.
Imaginary part of LYZ $\mathrm{Im}(\mu_{LYZ}/T)$ over all temperatures:

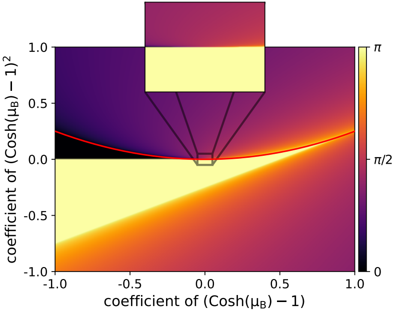


nHRG behavior explained

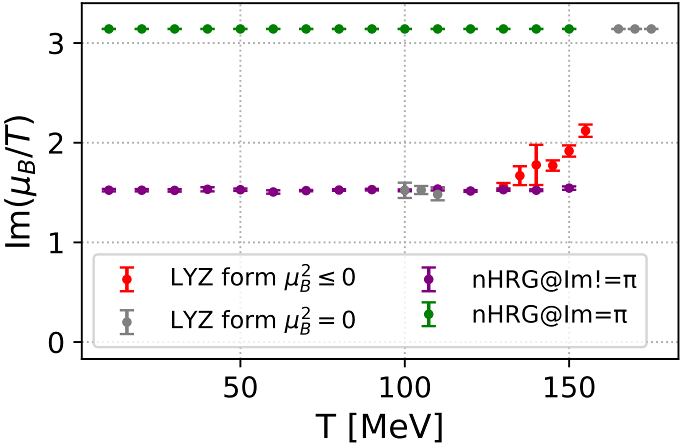
$$(1 + q_1(\cosh(\hat{\mu}) - 1) + q_2(\cosh(\hat{\mu}) - 1)^2) \stackrel{!}{=} 0$$

$$1 + q_1 x + q_2 x^2 \stackrel{!}{=} 0 \implies x_{1/2} = \frac{-q_1 \pm \sqrt{q_1^2 - 4q_2}}{2}$$

Imaginary part of the LYZ based on q_1 and q_2:



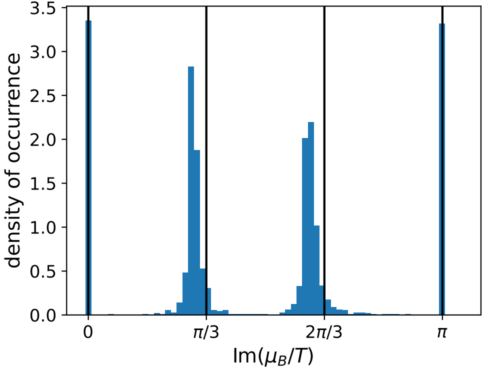
nHRG & Lattice



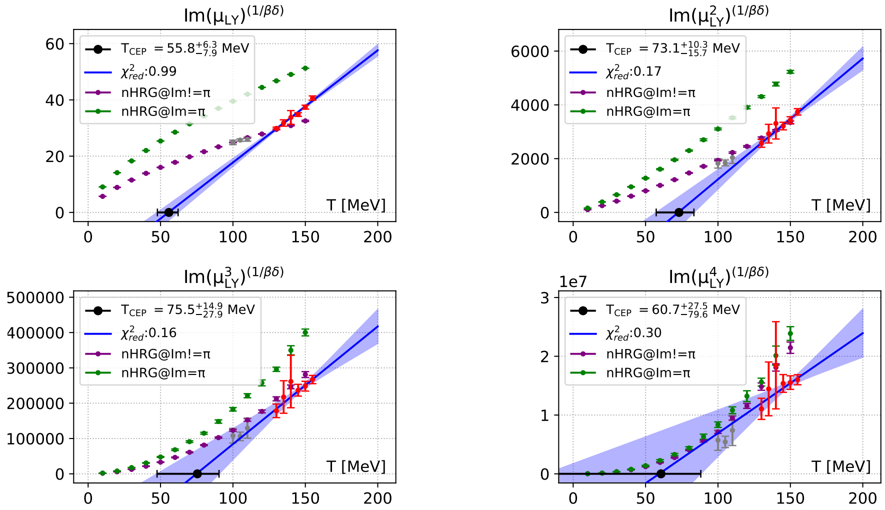
3rd order nHRG

Can the non critical baseline be improved?: Yes!

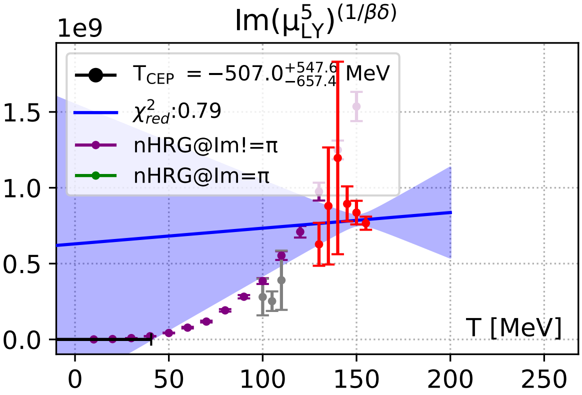
$$(1 + c(\cosh(\hat{\mu}) - 1) + d(\cosh(\hat{\mu}) - 1)^2) + e(\cosh(\hat{\mu}) - 1)^3) \stackrel{!}{=} 0$$



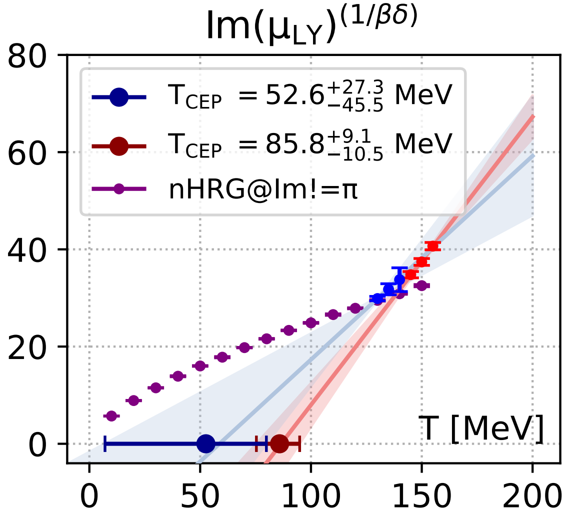
Varying the scaling observable for χ_1: $\kappa\Delta T = \mathrm{Im}(x)^{1/\beta\delta}$



Why not go further?



Varying the fit range for χ_1



Combination for Lattice Data

Based on $3[\Delta p, \chi_1, \chi_2] \times 4\left[\mu, \mu^2, \mu^3, \mu^4\right] \times 6$ Temp. ranges $= \ 72$ Fits

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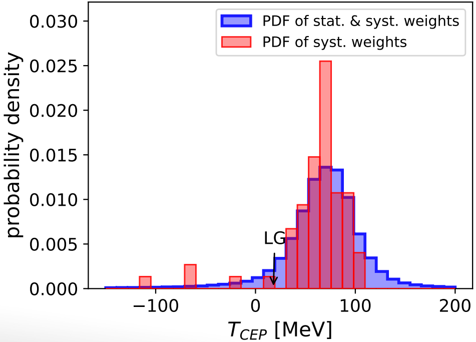

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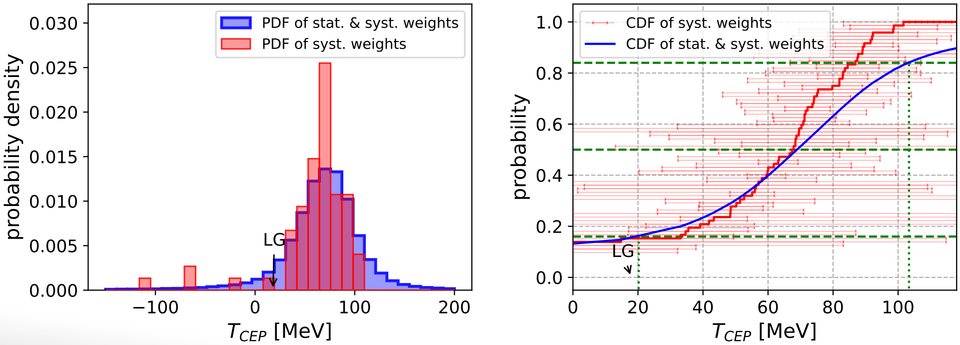
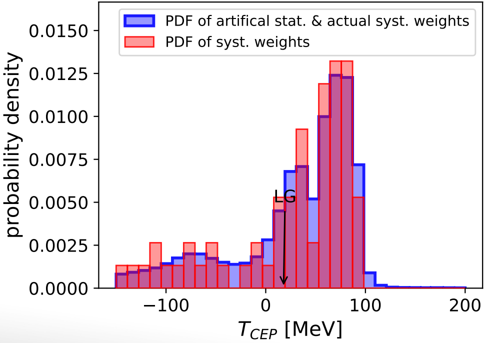
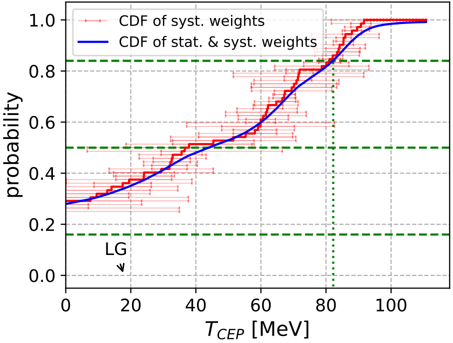


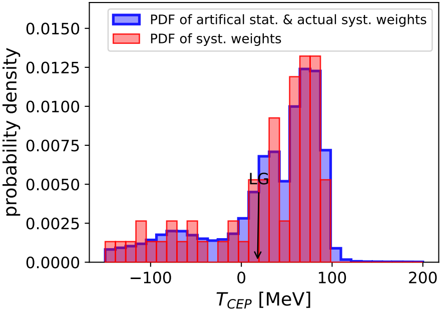
Combination for nHRG

Based on the same $3[\Delta p, \chi_1, \chi_2] \times 4\left[\mu, \mu^2, \mu^3, \mu^4\right] \times 6$ Temp. ranges $=\ 72$ Fits

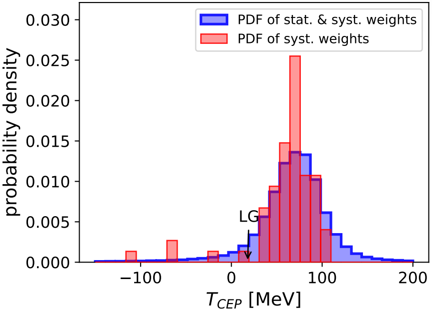




Conclusion from LYZ



Non critical Baseline

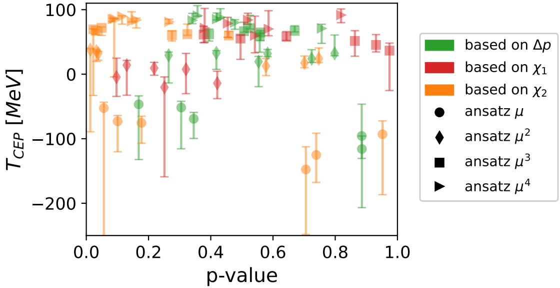


Lattice result

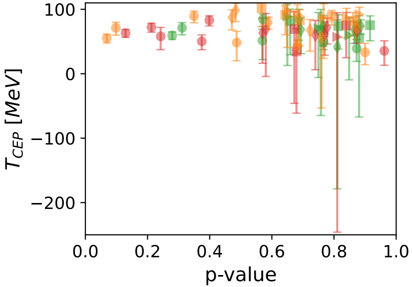
Lattice CDF result:
84% probability the CP either lies below $T = 103\,\mathrm{MeV}$ or does not exist

Backup

Systematic origin



Non critical Baseline



Lattice result

Roberge Weiss

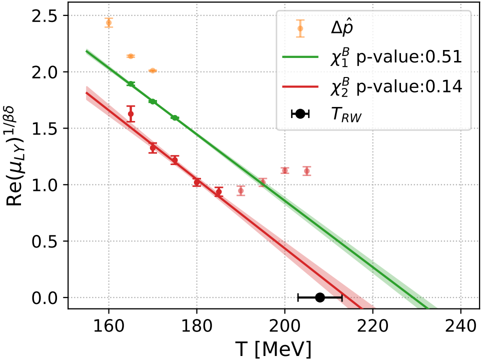


Figure 1: RW scaling

Backup Statistical Methods

Jackknife

Jackknife samples/Replicas

$$\bar{\theta}_{(i)} = \frac{1}{N_J - 1} \sum_{j \neq i} \theta_j, \qquad i = 1, \ldots, N_j. \tag{1}$$

The variance of a observable with $\bar{\theta}_{\text{jack}} = \frac{1}{n} \sum_{i=1}^{n} \bar{\theta}_{(i)}$:

$$\widehat{\text{var}}(\bar{\theta})_{\text{jack}} = \frac{N_J - 1}{N_J} \sum_{i=1}^{N_J} (\bar{\theta}_{(i)} - \bar{\theta}_{\text{jack}})^2 \tag{2}$$

The general covariance for multiple observables $\vec{\theta}$:

$$C_{lm} = \frac{N_J - 1}{N_J} \sum_{i=1}^{N_J} (\bar{\theta}_{l,(i)} - \bar{\theta}_{l,\text{jack}})(\bar{\theta}_{m,(i)} - \bar{\theta}_{m,\text{jack}}) \tag{3}$$

Least-squares spline approximation

General spline as linear combination of B-splines:

$$S_{n,\mathbf{t}}(x) = \sum_i \beta_i B_{i,n}(x). \tag{4}$$

Least-squares objective function:

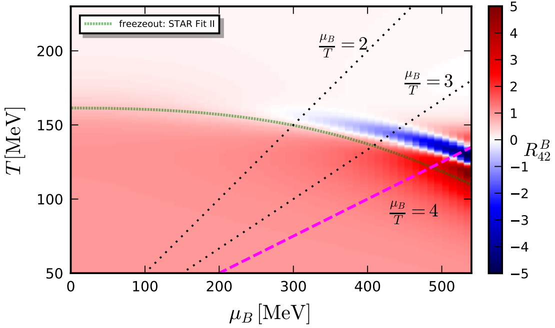
$$U = \sum_j \left\{ W \left[y_j - \sum_i \beta_i B_{i,k,\mathbf{t}}(x_j) \right] \right\}^2 . \tag{5}$$

Exact solution since $S_{n,\mathbf{t}}(x)$ is linear in $\vec{\beta}$:

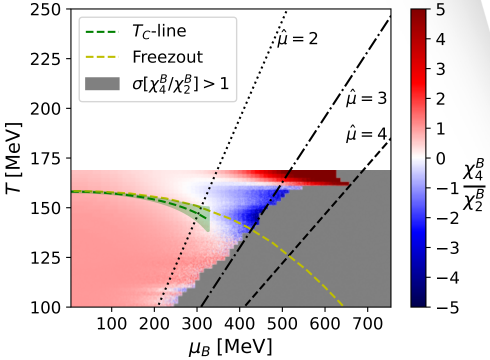
$$\begin{aligned} \hat{\beta} &= (B^T \cdot W \cdot B)^{-1} B^T \cdot W \cdot \vec{y} \\ M^\beta &= \left(B^T \cdot W \cdot B\right)^{-1} . \end{aligned} \tag{6}$$

T [MeV]	β	m_l	m_s	# configurations at $\mu_B = i\pi(j/8)$								
	$16^3 \times 8$ lattice			$j=0$	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$	$j=7$	$j=8$
100	0.4846	0.00490631	0.1355610	915010	-	-	-	-	-	-	-	-
105	0.5050	0.00458740	0.1267500	894220	-	-	-	-	-	-	-	-
110	0.5236	0.00432111	0.1193920	760795	-	-	-	-	-	-	-	-
115	0.5406	0.00409845	0.1132400	1054502	-	-	-	-	-	-	-	-
120	0.5560	0.00390982	0.1080280	1082567	-	-	-	-	-	-	-	-
125	0.5700	0.00374705	0.1035310	1726868	-	-	-	-	-	-	-	-
130	0.5829	0.00360381	0.0995733	2132329	-	96440	-	96082	-	95775	-	95625
135	0.5947	0.00347548	0.0960274	1453169	110859	105287	104348	120205	103744	103749	103196	103084
140	0.6056	0.00335869	0.0928007	4010320	99904	105232	104911	359058	103501	99483	102589	113865
145	0.6158	0.00325107	0.0898270	2579944	106703	106386	105027	121944	103958	103239	102471	115049
150	0.6252	0.00315088	0.0870590	1688860	114258	114018	112067	117290	109804	97932	96239	109087
155	0.6341	0.00305689	0.0844619	1623503	109132	108649	107158	125765	104061	102762	101464	115855
160	0.6425	0.00296817	0.0820105	2229437	112026	111086	108615	128345	104466	95570	101203	108589
165	0.6504	0.00288403	0.0796857	1768242	103692	101652	89855	121047	95726	92934	86765	105389
170	0.6579	0.00280394	0.0774727	1204210	-							
175	0.6651	0.00272748	0.0753604	1602383	-							
180	0.6719	0.00265434	0.0733394	1357330	-							
185	0.6785	0.00258424	0.0714026	855048	-							
190	0.6848	0.00251696	0.0695436	318710	-							
195	0.6909	0.00245231	0.0677573	362672	-							
200	0.6968	0.00239013	0.0660393	324768	-							
205	0.7025	0.00233028	0.0643856	159500	-							
210	0.7080	0.00227263	0.0627928	260084	-							
220	0.7188	0.00216352	0.0597782	249068	-							
230	0.7290	0.00206205	0.0569745	257480	-							
240	0.7389	0.00196759	0.0543644	270856	-							
250	0.7485	0.00187961	0.0519336	430495	-							
260	0.7580	0.00179768	0.0496700	281616	-							
280	0.7765	0.00165052	0.0456040	289961	-							
300	0.7946	0.00152351	0.0420946	297512	-							

Comparing χ_4/χ_2 with cosh-Padé



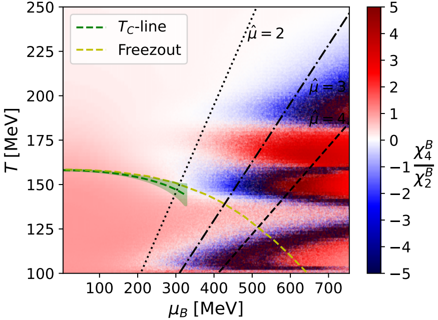
FRG: Fu et al. [2101.06035]



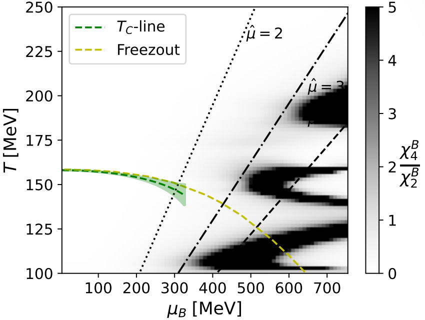
Cosh-Padé using up to χ_{10}

Separate value and error on χ_4/χ_2

Ratio based on Taylor extrapolation using up to χ_{10}



sampled value



error

Example for the susceptibility

$$(a_1 + a_2\mu^2) = (\chi_2 + \chi_4\mu^2 + \chi_6\mu^4 + \chi_8\mu^6)(1 + b_1\mu^2 + b_2\mu^4)$$

$$\left.\frac{\mathrm{d}^0}{\mathrm{d}\mu^0}\right|_{\mu=0} : \quad a_1 = \chi_2$$

$$\left.\frac{\mathrm{d}^2}{\mathrm{d}\mu^2}\right|_{\mu=0} : \quad 2a_2 = 2b_1\chi_2 + 2\chi_4$$

$$\left.\frac{\mathrm{d}^4}{\mathrm{d}\mu^4}\right|_{\mu=0} : \quad 0 = 24(b_2\chi_2 + b_1\chi_4 + \chi_6) \iff \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & \chi_2 & 0 \\ 0 & 0 & \chi_4 & \chi_2 \\ 0 & 0 & \chi_6 & \chi_4 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} \chi_2 \\ \chi_4 \\ \chi_6 \\ \chi_8 \end{pmatrix}$$

$$\left.\frac{\mathrm{d}^6}{\mathrm{d}\mu^6}\right|_{\mu=0} : \quad 0 = 720(b_2\chi_4 + b_1\chi_6 + \chi_8)$$

Computation on the lattice

$$Z(T,\mu) = \int \mathcal{D}U \ \det \mathbf{M}(U,\mu)\, e^{-S_g(U)}$$

$$\log\det M_j^{1/4}(U,m_j,\hat\mu_j) = \log\det M_j^{1/4}(U,m_j,0) + A_j\hat\mu_j + \frac{1}{2!}B_j\hat\mu_j^2 + \frac{1}{3!}C_j\hat\mu_j^3 + \dots$$

With ABCD:

$$\partial_j\langle X\rangle = \langle XA_j\rangle - \langle X\rangle\langle A_j\rangle + \langle\partial_j X\rangle.$$

$$\partial_i \log Z = \frac{1}{Z}\int \mathcal{D}U\, \partial_i e^{-S_{\text{eff}}} = \langle A_i\rangle, \quad \partial_i\partial_j \log Z = \partial_i\langle A_j\rangle \overset{\mu_i=0}{=} \langle A_iA_j\rangle + \delta_{ij}\langle B_i\rangle.$$

Reduced matrix formalism:

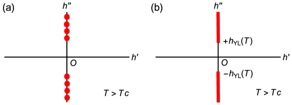
$$\frac{\det M(\hat\mu,m,U)}{\det M(0,m,U)} = e^{-3N_s^3\hat\mu}\prod_{i=1}^{6N_s^3}\frac{\xi_i[m,U]-e^{\hat\mu}}{\xi_i[m,U]-1} \implies \begin{array}{ll} A = \frac{i}{4}\mathrm{Im}\sum_i \frac{1}{(1-\xi_i)} & B = \frac{1}{4}\mathrm{Re}\sum_i \frac{-\xi_i}{(1-\xi_i)^2}, \\ C = \frac{i}{4}\mathrm{Im}\sum_i \frac{\xi_i(1+\xi_i)}{(1-\xi_i)^3}, & D = \frac{1}{4}\mathrm{Re}\sum_i \frac{-\xi_i(\xi_i^2+4\xi_i+1)}{(1-\xi_i)^4} \end{array}$$

LYZ in 3D Ising

$$\sum_{(\sigma)=\pm 1} \exp \underbrace{\left\{ \beta \sum_{\langle ij \rangle} (\sigma_i \sigma_j - 1) + h \sum_i (\sigma_i - 1) \right\}}_{\text{Hamiltonian}} = Z_L = \sum_{m=0}^{M} \sum_{n=0}^{N} C_{m,n} \, y^m t^n .$$

Studied by Lee and Yang & Fisher leading to the Circle Theorem: and the scaling relation to CP:

$$h r^{-1/\beta\delta} = x = \pm i x_{\rm LY} = \pm i (z_c)^{-\beta\delta}$$



[Wei 1611.08074]

Scaling for QCD

Map Ising onto QCD:

$\Delta T \equiv T - T_{\mathrm{CEP}}, \Delta\mu \equiv \mu - \mu_{\mathrm{CEP}}$

$$r = A_r\,\Delta T + B_r\,\Delta\mu,$$
$$h = A_h\,\Delta T + B_h\,\Delta\mu,$$

$$h = \pm i z_c^{-\beta\delta}\, r^{\beta\delta} \implies (A_h\,\Delta T + B_h\,\Delta\mu) = \pm i z_c^{-\beta\delta}\,(A_r\,\Delta T + B_r\,\Delta\mu)^{\beta\delta}. \quad (7)$$

Up to leading order:

$$\mathrm{Im}(\mu_{LY}) = c_1\,(\Delta T)^{\beta\delta}, \quad (8)$$
$$\mathrm{Re}(\mu_{LY}) = \mu_{\mathrm{CEP}} + c_2\,\Delta T, \quad (9)$$

c_1, c_2 : non-universal constants.

CEP via Lee-Yang zeros

- Use theory of Lee-Yang zeros (LYZ) and Lee-Yang edge singularity [Lee,Yang'59]
- assume the chiral CEP in QCD is in the same universality class as the 3D Ising model
- Use the scaling relation form 3D Ising by mapping it onto QCD