Fourier coefficients of the net baryon number density

Christian Schmidt

UNIVERSITÄT BIELEFELD
Faculty of Physics

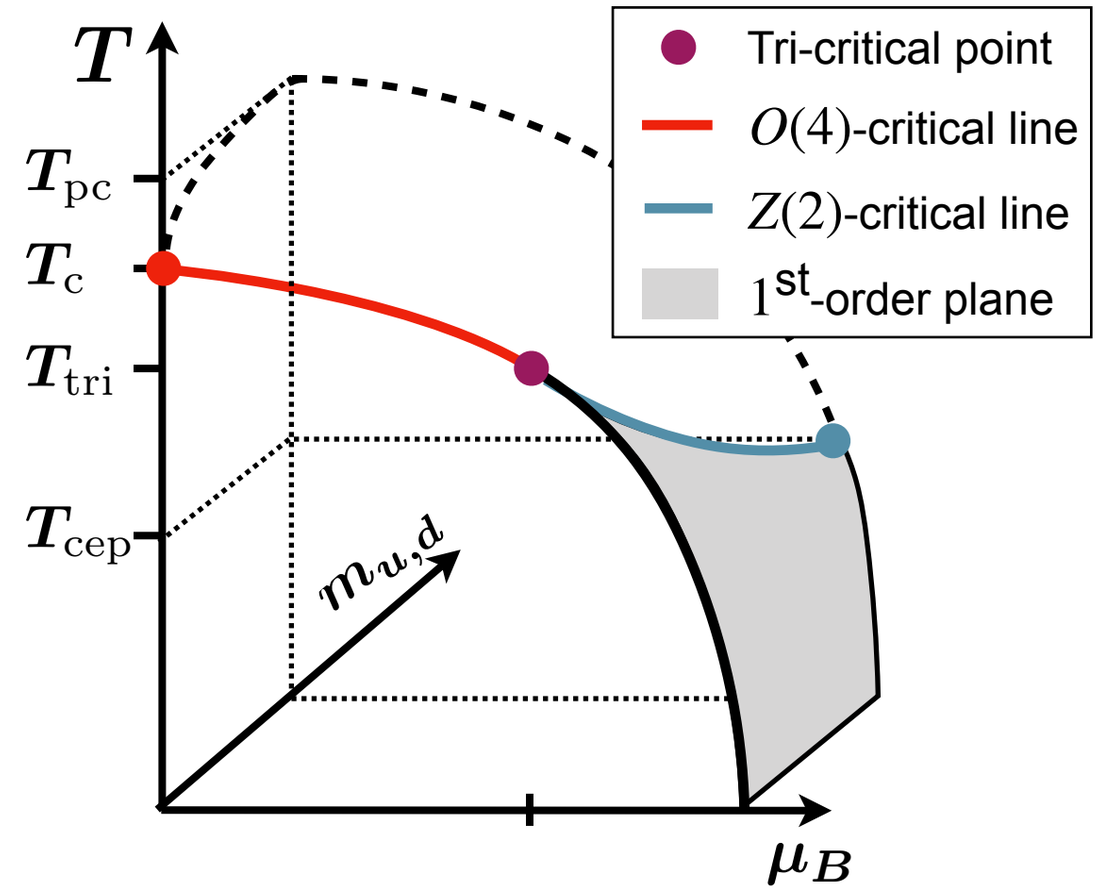
CRC-TR 211

August 8-13, Bonn, Germany

Bielefeld Parma Collaboration:
David Clarke, Petros Dimopoulos, Francesco Di Renzo, Jishnu Goswami, Guido Nicotra, CS, Simran Singh, Kevin Zambello

We want to investigate the analytic structure of the partition function ($\ln Z$)

- Locating singularities in the complex μ_B/T -plane might help to find the elusive QCD critical point
- We have theoretical guidance by the Lee-Yang theorem, which predicts branch-cuts in the scaling function of the order parameter, located at universal positions.



We use lattice QCD data of the baryon number density ($\partial_\mu \ln Z$) at imaginary chemical potential

- Asymptotic behaviour of Fourier coefficient encodes information on the branching point singularity of the scaling function.

Are we sensitive enough to see that?

- The first Fourier coefficient is related to the interaction in the excluded volume HRG model. Modeling the Fourier coefficients might help to improve analytic continuation to real chemical potential.

[Vovchenko et al., PLB 775, 71 (2017); Vovchenko et al., PRD 97, 114030 (2018); Almási et al. PRD 100 (2019) 1, 016016]

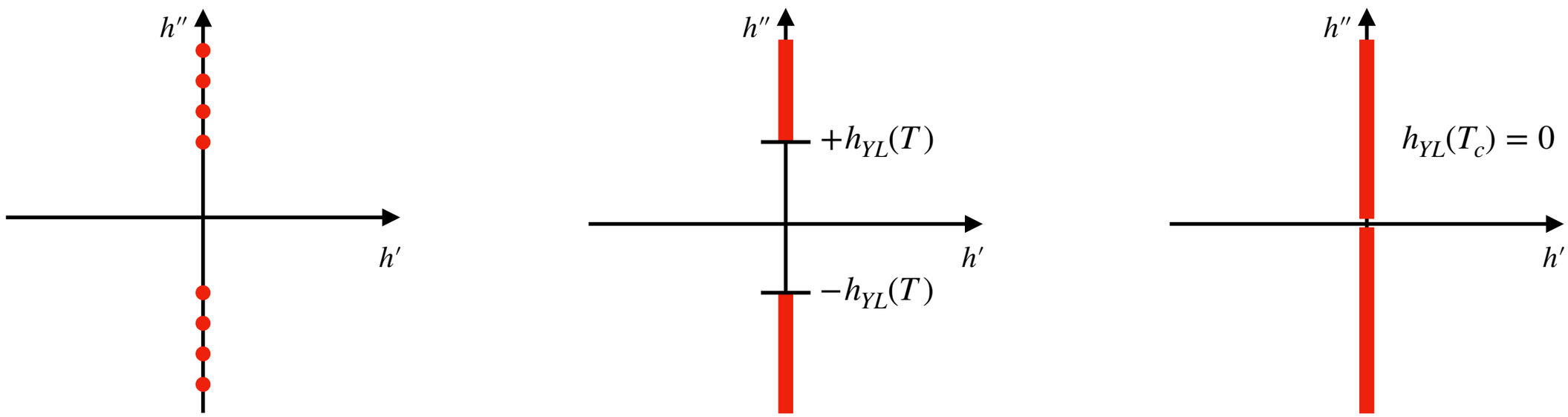
Plan

- **Lee-Yang edge singularities related to Roberge-Weiss, chiral, and QCD critical points**
  - Scaling variables
  - Universal behaviour
- **Our approach to Fourier Coefficients**
  - The lattice setup
  - Definition of the Fourier coefficients
  - Interpolation of the Lattice data
- **Preliminary Results and Conclusions**

Consider a generic Ising or O(N) model:

* One finds zeros of the partition function only at imaginary values of the symmetry breaking field [Lee, Yang 1952]
* In the thermodynamic limit the zeros become dense on the line $h' = 0$

$Z(V, T, h) \equiv 0, \quad h = h' + ih''$



V finite, $T > T_c$ $\qquad$ $V \to \infty, T > T_c$ $\qquad$ $V \to \infty, T \to T_c$

→ a brach cut is observed in the free energy density and order parameter

* The position of the branch cut singularity is universal. In terms of the scaling variable $z = t/h^{1/\beta\delta}$, we have $z_{LY} = |z_c| e^{i\frac{\pi}{2\beta\delta}}$, where $t = T/T_c - 1$. [Connelly et al. PRL 125 (2020) 19]

Solve for $z_{LY} = |z_c| e^{i\frac{\pi}{2\beta\delta}}$

with different scaling fields and non-universal parameters

Roberge-Weiss transition:

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

Chiral transition:

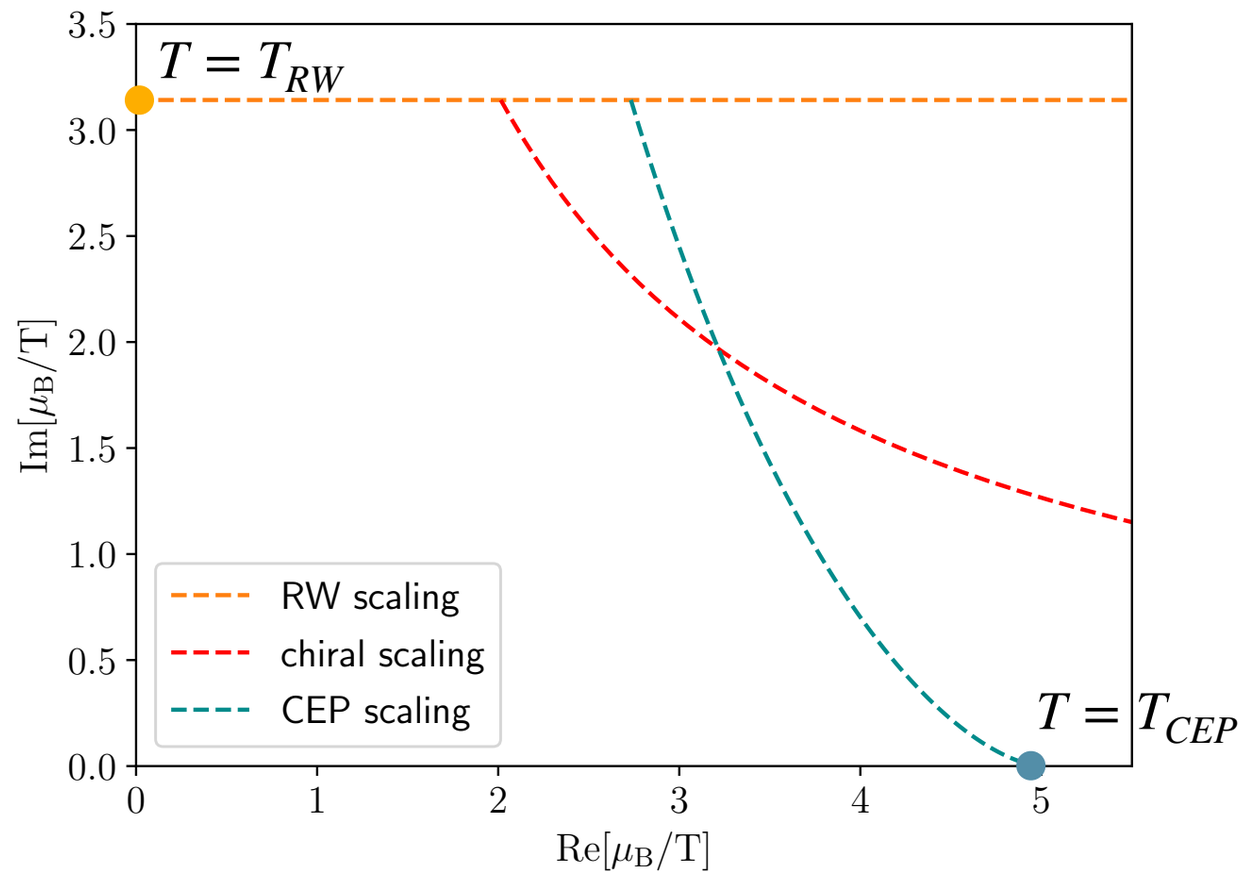
$$t = t_0 \left[\frac{T - T_c}{T_c} + \kappa_2^B \left(\frac{\mu_B}{T} \right)^2 \right] \quad \text{and} \quad h = h_0 \frac{m_l}{m_s^{\text{phys}}}$$

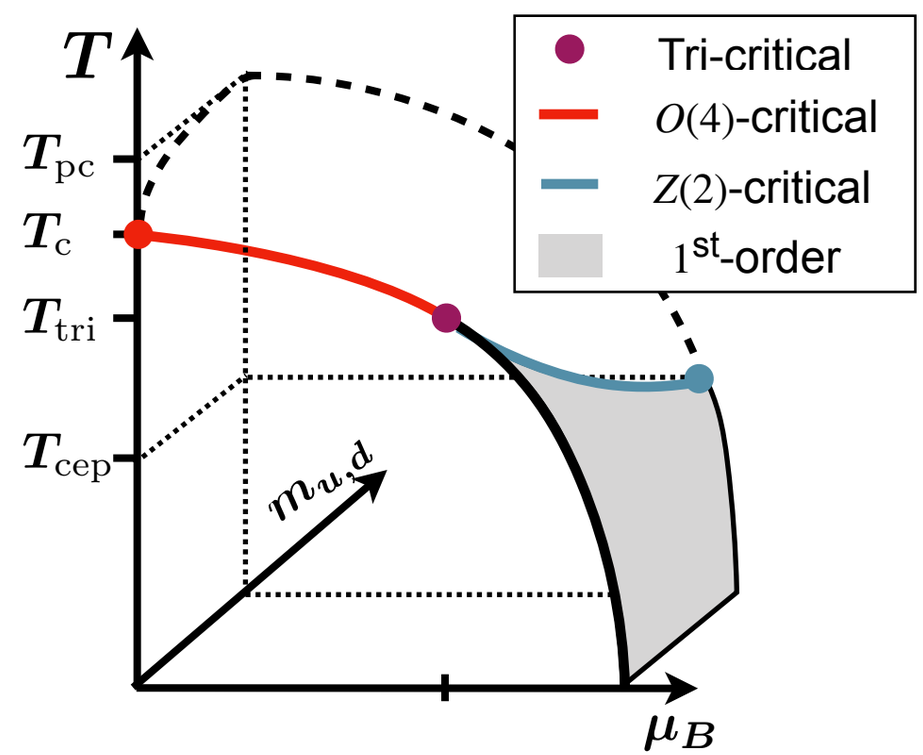
QCD critical point:

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

$$h = \alpha_h (T - T_{cep}) + \beta_h (\mu_B - \mu_{cep})$$

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

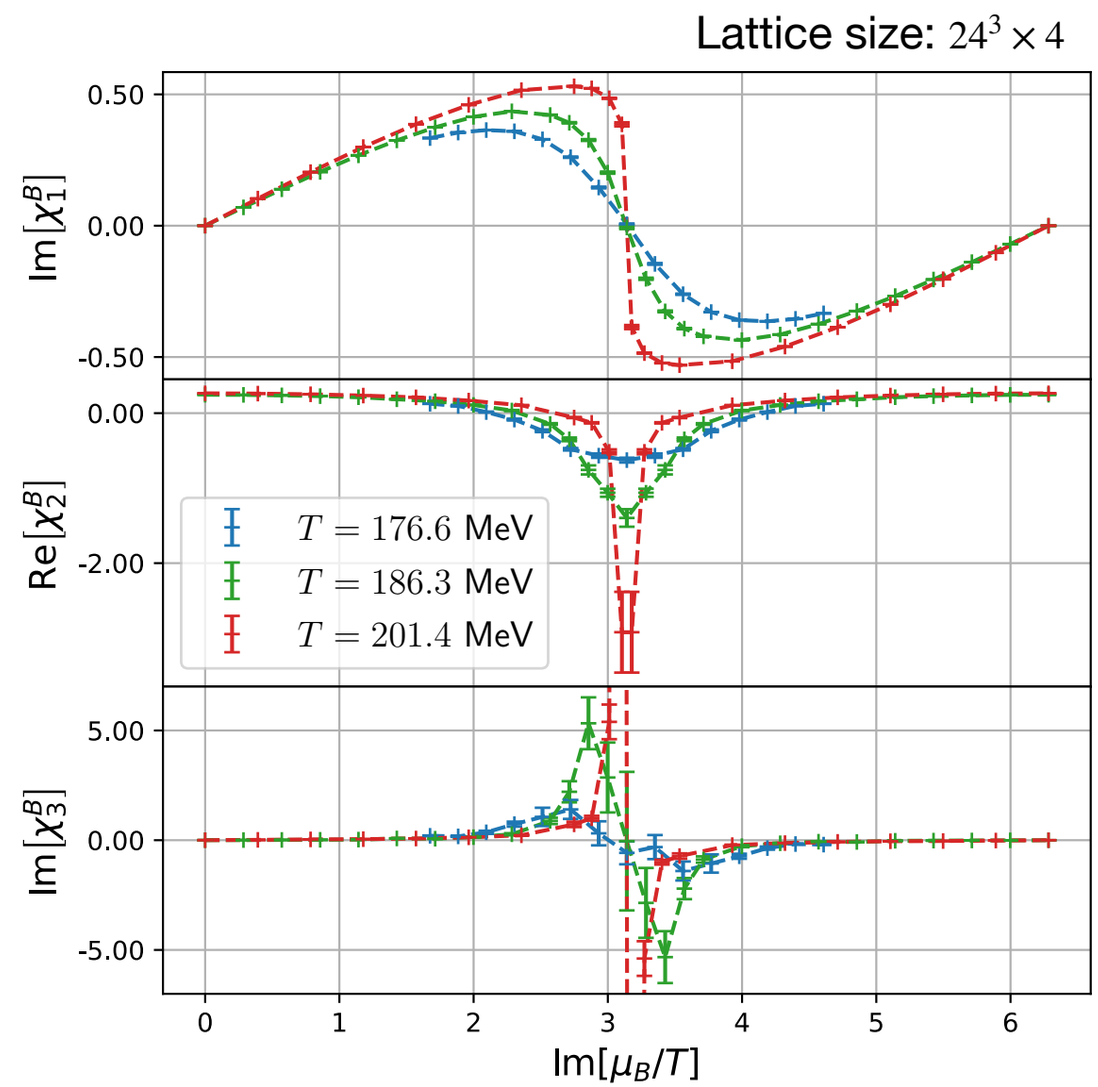




Lattice Data

- We use (2+1)-flavor of highly improved staggered quarks (HISQ)
- Simulations at $\mu_B > 0$ are not possible due to the infamous sign problem
- Instead we perform calculations at imaginary chemical potential $\mu_B = i\mu_B^I$
  [De Frorcrand, Philipsen (2002); D'Elia, Lombardo (2003)]
- The temperature scale and line of constant physics is taken from previous HotQCD calculations
  [see e.g., Bollweg et al. PRD 104 (2021)]
- We measure cumulants of net baryon number in the interval $i\mu_B^I/T \in [0,\pi]$
  [Allton et al. PRD 66 (2002)]
- The cumulants χ_n^B are odd and imaginary for n odd and even and and real for n even

→ see also talks by K. Zambello and F. Di Renzo



[Dimopoulos et al., *PRD* 105 (2022)]

$$\chi_n^B(T,V,\mu_B) = \left(\frac{\partial}{\partial\hat{\mu}_B}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$

$$= \left(\frac{1}{3}\frac{\partial}{\partial\hat{\mu}_l} + \frac{1}{3}\frac{\partial}{\partial\hat{\mu}_s}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$

Definition:

$\mu_B/T = i\theta_B, \text{ with } \theta_B \in \mathbb{R}$

$$b_k(T) = \frac{1}{\pi}\int_0^{2\pi} \mathrm{d}\theta_B \, \mathrm{Im}\,\chi_1^B(T, i\theta_B)\,\sin(k\theta_B)$$

highly oscillatory for large k

Data only defined on a discrete set of points

Method 1:

- Interpolate $\mathrm{Im}\,\chi_1^B$, take also it's derivative $\mathrm{Re}\,\chi_2^B$ and eventually higher derivatives up to order s into account → Hermite-interpolation (spline)
- Piecewise integration can be done analytically

$$b_k = \frac{2}{\pi}\sum_{i=0}^{N-1}\int_{\theta_B^{(i)}}^{\theta_B^{(i+1)}} \mathrm{d}\theta_B \; p(\theta_B)\sin(k\theta_B) \quad \text{with} \quad 0 = \theta_B^{(0)} < \theta_B^{(1)} < \cdots < \theta_B^{(N)} = \pi$$

  → 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 $\mathrm{Im}\,\chi_1^B$ and $\mathrm{Re}\,\chi_2^B$.

Definition:

$$\mu_B/T = i\theta_B, \text{ with } \theta_B \in \mathbb{R}$$

$$b_k(T) = \frac{1}{\pi}\int_0^{2\pi} \mathrm{d}\theta_B \, \mathrm{Im}\,\chi_1^B(T, i\theta_B)\,\sin(k\theta_B)$$

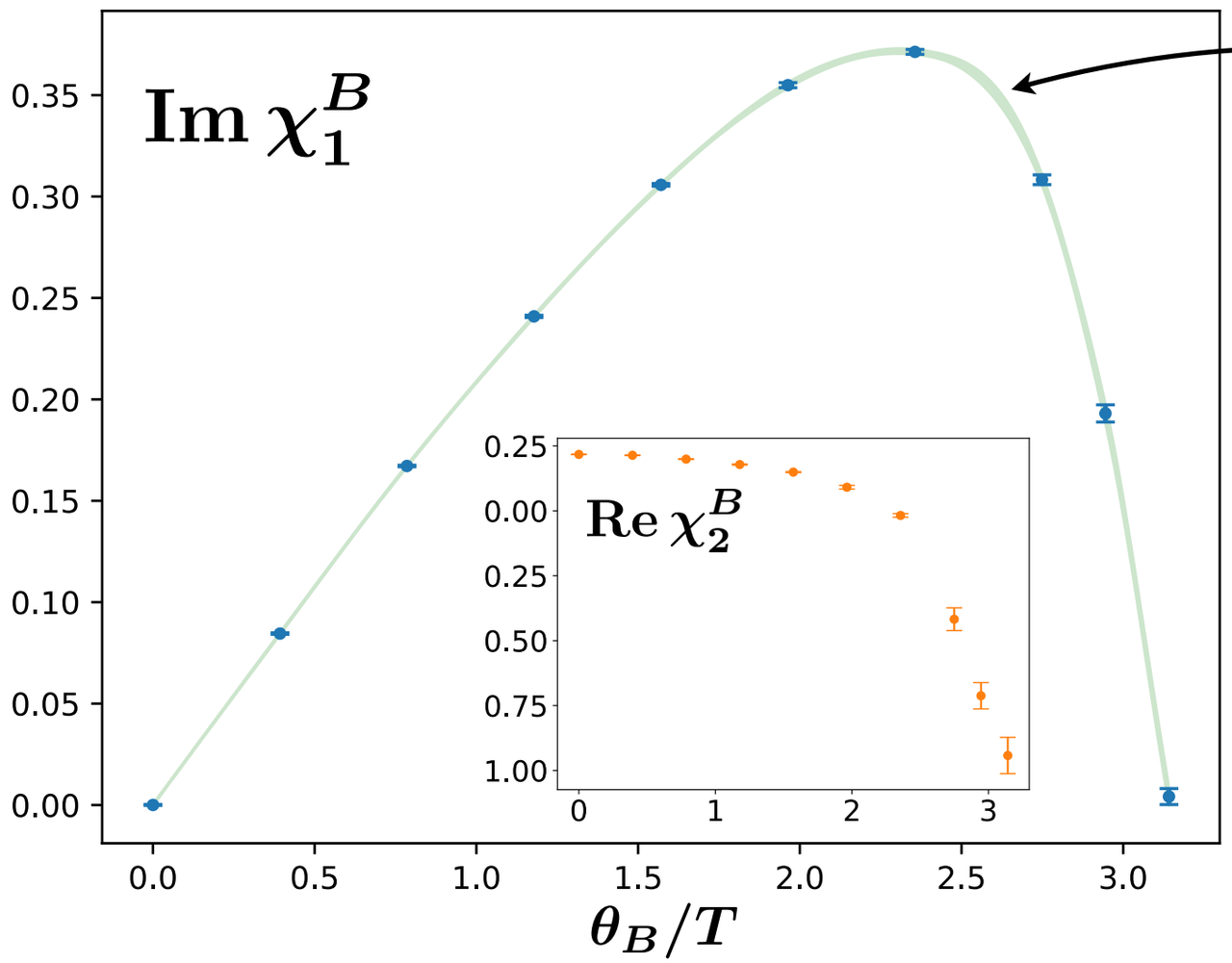
highly oscillatory for large k

Data only defined on a discrete set of points

Method 2:

- Determine a (global) rational approximation of $\mathrm{Im}\,\chi_1^B$, e.g. by multi-point Padé (see talk by Kevin Zambello) or by fitting a specific Ansatz-function
- Integrate analytically or numerically by Gaussian quadrature or perform a Fast Fourier Transformation (FFT)
- Estimate systematic error by comparing to Method 1

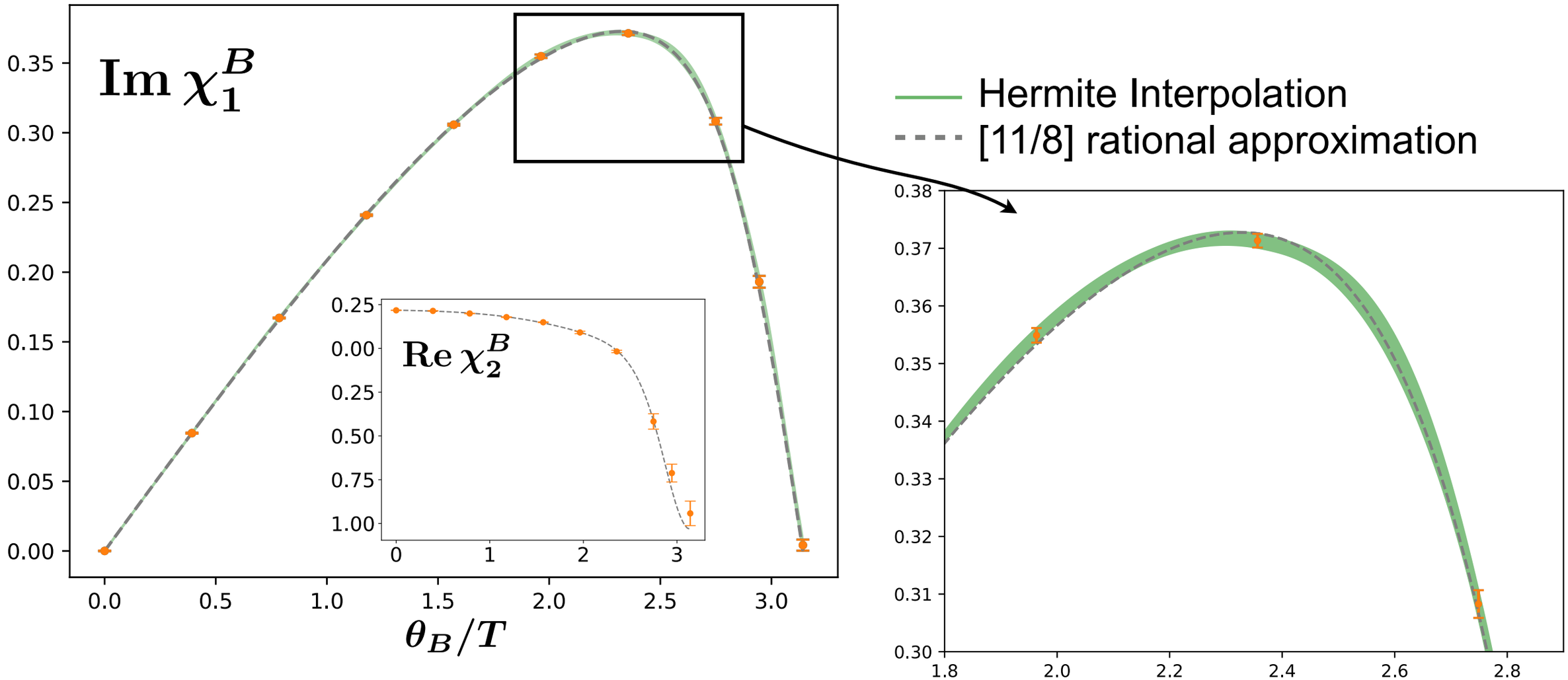
Interpolation at $T = 190$ MeV



Error band of the Hermite-Interpolation (piecewise cubic, taking $\mathrm{Im}\,\chi_1^B$ and $\mathrm{Re}\,\chi_2^B$ into account)

- Note asymmetry of the data, w.r.t a sin function: data can be described by $\mathcal{O}(10)$ Fourier-coefficients

Interpolation at $T = 190$ MeV, $36^3 \times 6$



- Note asymmetry of the data, w.r.t a sin function: need $\mathcal{O}(10)$ Fourier-coefficients to describe the data

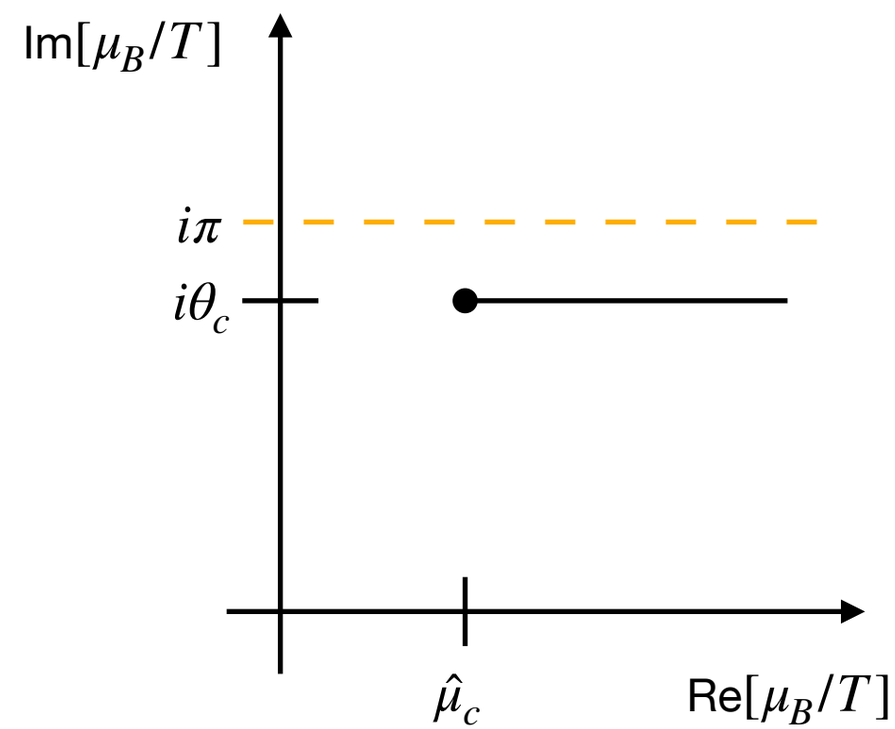
- Both interpolations agree within error.

* A branch cut at $\hat{\mu}_c + i\theta_c$ will give rise to an

  - exponential damping $b_k \sim \exp\{-k\,\hat{\mu}_c\}$
  - oscillation $b_k \sim \sin(k\,\theta_c)$
  - in addition there is an algebraic decay $b_k \sim k^{-2}$

→ in principle we can determine μ_{LY} from b_k

[Almási et al. PRD 100 (2019) 1, 016016]



Roberge-Weiss transition:

$$T = T_{RW}$$

$$b_k \sim \frac{-1^{k+1}}{k^{1+1/\delta}}$$

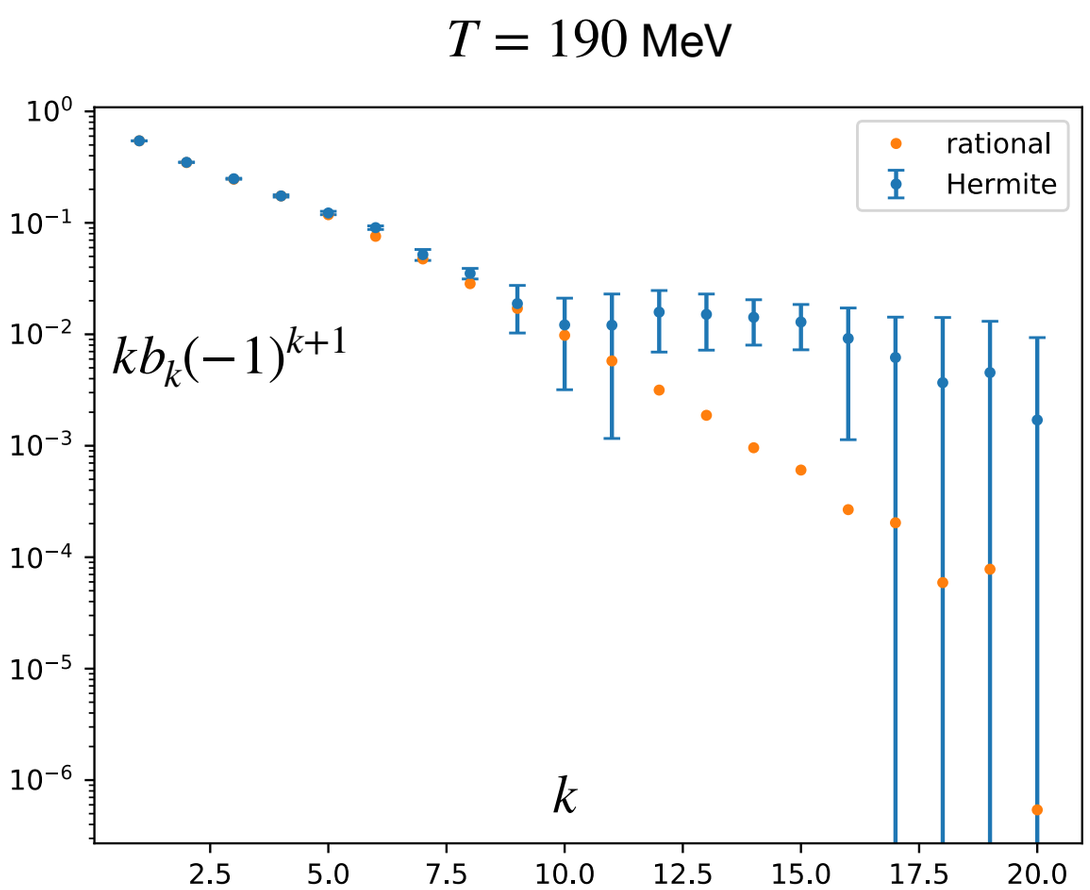
Chiral transition:

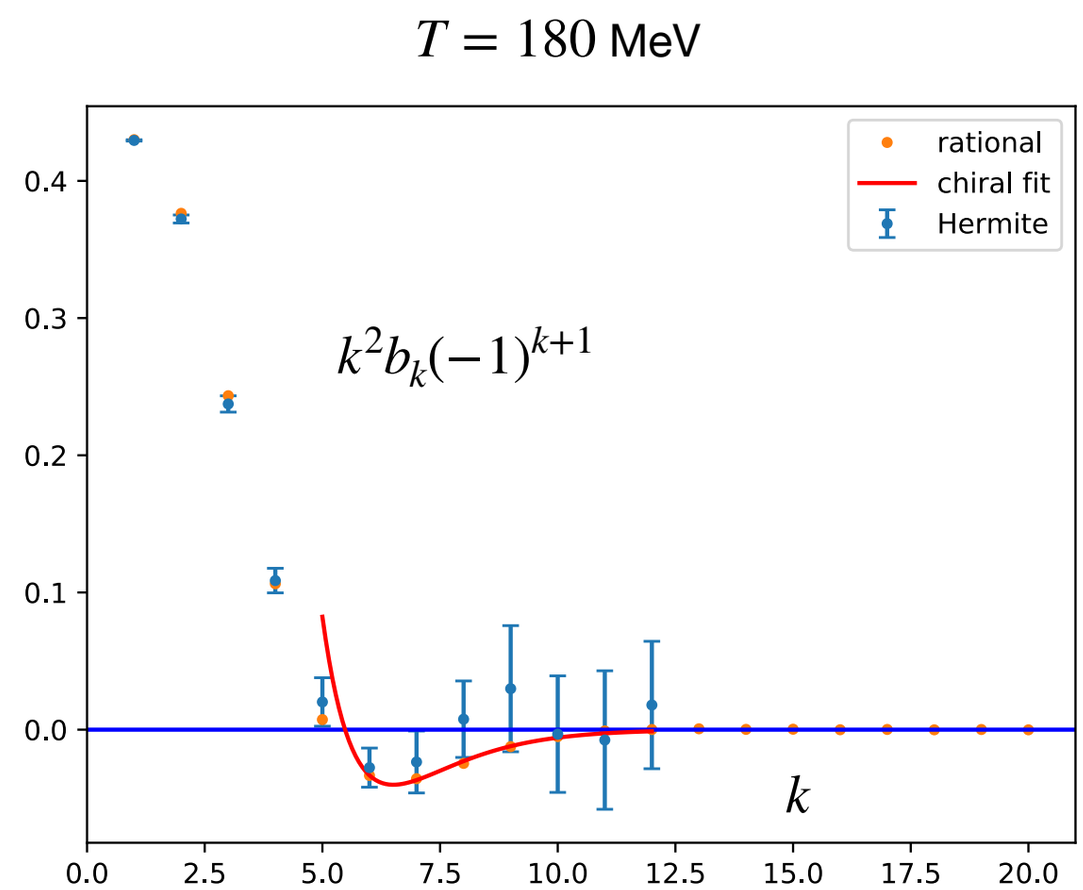
$$T < T_{RW}$$

$$b_k \sim \frac{e^{-k\hat{\mu}_c}(\sin(k\theta_c - \alpha\pi/2) + R_\pm \sin(k\theta_c + \alpha\pi/2))}{k^{2-\alpha}}$$

[Almási et al., *Phys.Lett.B* 793 (2019) 19-25]

Preliminary results





systematic errors under control for $k \lesssim 10$

→ no oscillation

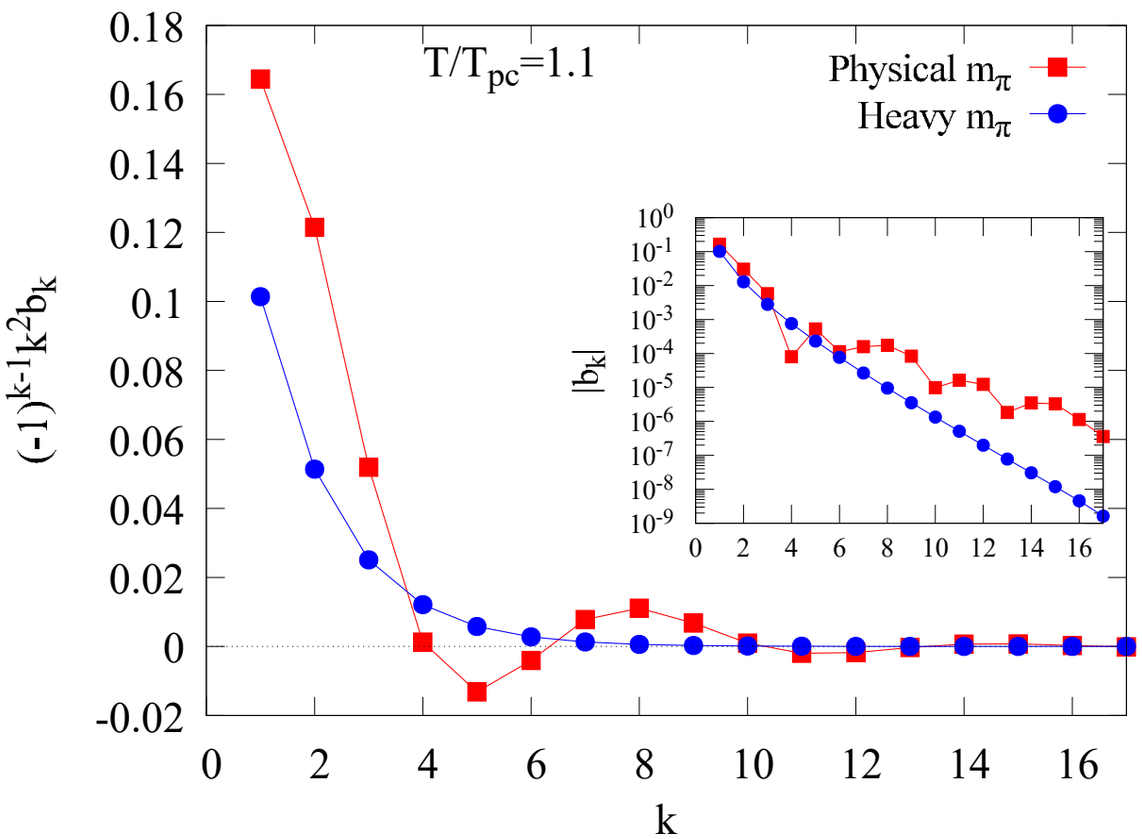
→ damed oscillations

Sensitivity to the chiral transition,

chiral fits yield reasonable Lee-Yang edge singularity

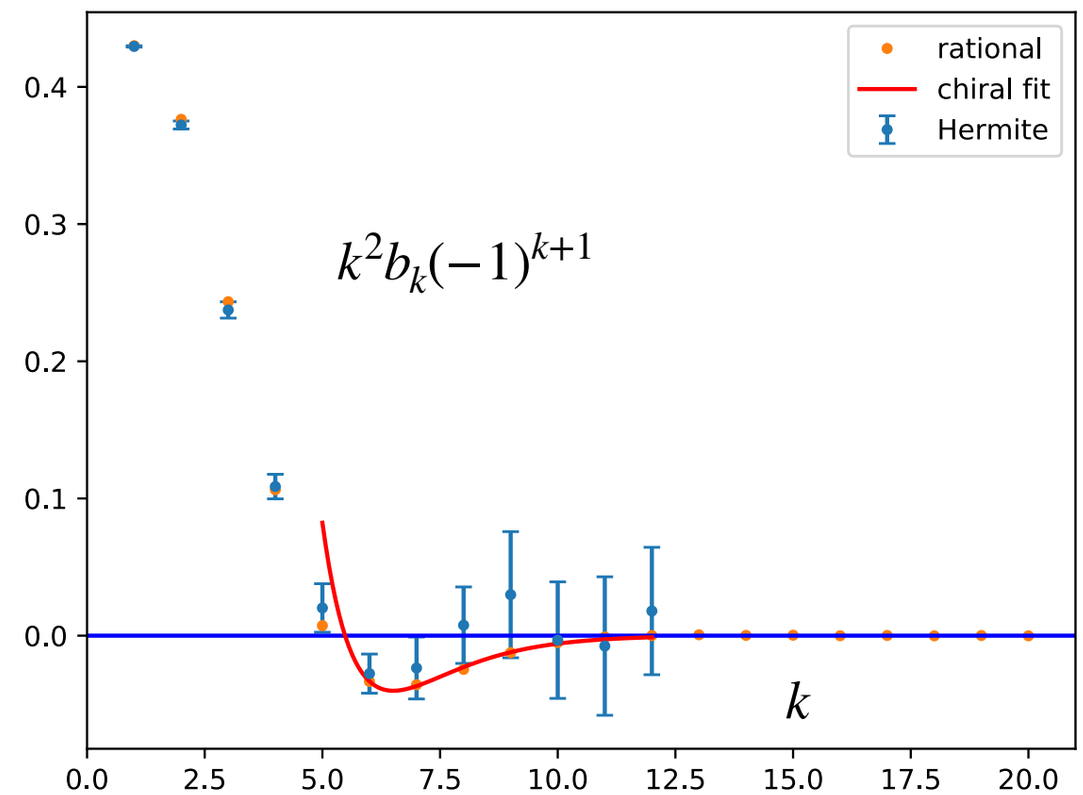
$\hat{\mu}_{LY} = 0.97(6) + 3.123(3)\, i$

PQM model



[Almási et al. PRD 100 (2019) 1, 016016]

$T = 180$ MeV



→ damed oscillations

Sensitivity to the chiral transition,

chiral fits yield reasonable Lee-Yang edge singularity

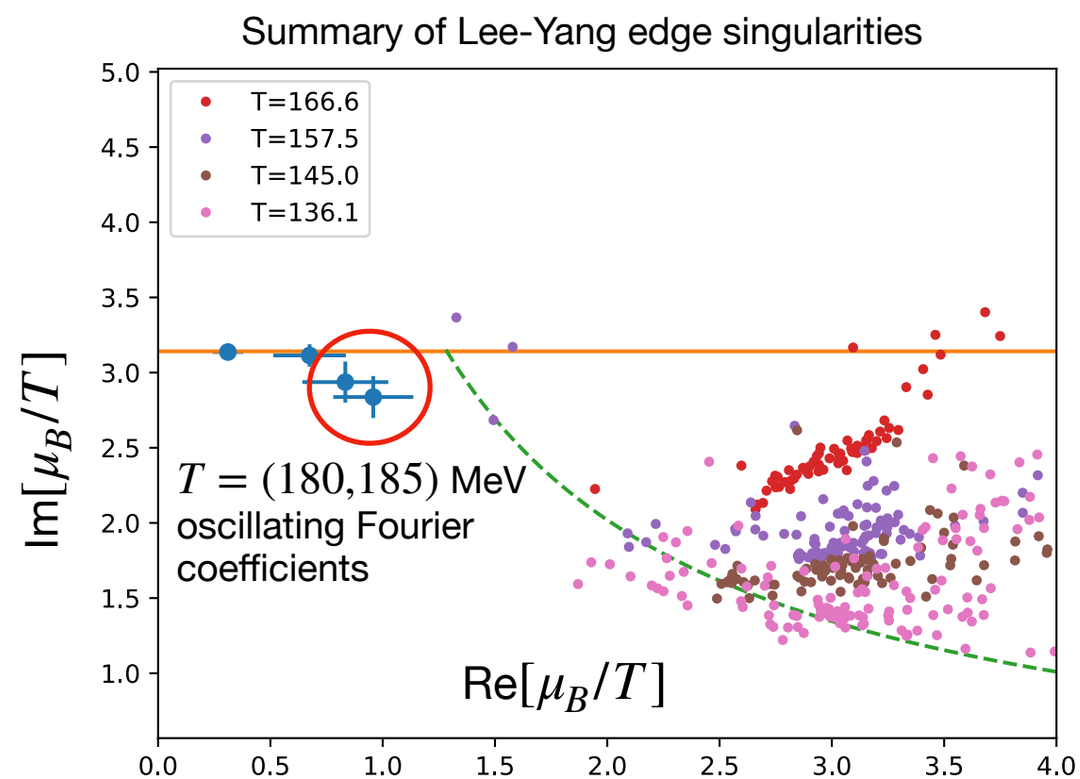
$\hat{\mu}_{LY} = 0.97(6) + 3.123(3)\, i$

Summary and Conclusions

- At different temperature intervals we expect to see different scaling behaviour of the Lee-Yang edge singularly (Roberge-Weiss, chiral, QCD critical point)
- The Fourier coefficients of the baryon number density start to oscillate for $T \lesssim 180$ MeV

  →sensitivity to the chiral phase transition
- The exponential decay is a problem for $\hat{\mu}_c > 1$

  →exponentially small coefficients



Outlook:

- perform more systematic fits to Fourier coefficients
- investigate phenomenological motivated models
- performing smaller than physical mass calculations

  →the real part of the branch cut singularity will be reduced!