Lattice QCD and Equation of State

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- **Lattice QCD Basics:** Why Lattice QCD, different lattice actions, continuum limit, scale setting.

- **Equation of State at $\mu = 0$:** Properties of strong interaction matter at the QCD crossover, approach to the perturbative limit at high T, effective description through Hadron Resonance Gas at low T.

- **Cumulants of conserved charge fluctuations:** The Equation of State at $\mu_B > 0$, probing the hadronic mass spectrum, melting of mesons, critical behaviour and the search for the QCD critical point

- **The QCD Phase diagram:** The chiral phase transition, The Roberge-Weiss Transition, Lee Yang edge singularities.

Textbooks:

- Christof Gattringer, Christian B. Lang, “Quantum Chromodynamics on the Lattice, An Introductory Presentation”, Springer-Verlag Berlin, 2010.
- István Monty and Gernot Münster, “Quantum Fields on a Lattice”, Cambridge University Press 1994.
- Jan Smit, “Introduction to Quantum Fields on a Lattice”, Cambridge University Press 2002.
- Heinz J Rothe “Lattice Gauge Theories: An Introduction”, World Scientific Publishing Company; 4th edition (14 Mar. 2012).
- Thomas Degrand, Carlton Detar “Lattice Methods for Quantum Chromodynamics”, World Scientific Publishing Company; Illustrated edition (27 Sept. 2006).
- Michael Creutz “Quarks Gluons and Lattices”, Cambridge University Press 1985.

Review articles:

- Heng-Tong Ding, Frithjof Karsch, Swagato Mukherjee, “*Thermodynamics of strong-interaction matter from Lattice QCD*”, Int.J.Mod.Phys.E **24** (2015) 10, 1530007 • e-Print: 1504.05274 [hep-lat].

- Owe Philipsen, “*Lattice Constraints on the QCD Chiral Phase Transition at Finite Temperature and Baryon Density*”, Symmetry **13** (2021) 11, 2079 • e-Print: 2111.03590 [hep-lat].

- CS, Sayantan Sharma, “*The Phase Structure of QCD*”, *J.Phys.G* 44 (2017) 10, 104002 • e-Print: 1701.04707 [hep-lat].

Lattice QCD Basics

- A (non-abelian) gauge theory of quarks, gluons, and their interactions, gauge group is SU(N_c) with $N_c = 3$.

- The Lagrange density is given by

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F^{\mu\nu}_a + i\bar{\psi}\gamma^\mu D_\mu \psi$$

Field strength tensor
$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^b_\mu A^c_\nu$

Covariant Derivative
$D_\mu = \partial_\mu - i g T_a A^a_\mu$

Gauge field A^a_μ

Spinors: $\psi \equiv \psi^{f,c,\alpha}$ (Quarks)
$\bar{\psi} \equiv \gamma_0 \psi^\dagger$ (Anti-Quarks)

$f = u, d, s, \ldots$ (flavor-indices)
$c = 1,2,3$ (color-indices)
$\alpha = 0,1,2,3$ (Dirac-indices)

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- The Lagrange density is given by

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F_a^{\mu\nu} + i\bar{\psi}\gamma^\mu D_\mu \psi$$

  - No dimensionfull parameter, the bare coupling is defined as $\bar{\alpha}_s = \dfrac{g^2}{4\pi}$

  - A scale μ is developed via “dimensional transmutation” [Coleman, Gross, PRL **31**, 851 (1973)]

- In perturbation theory the UV divergencies need to be subtracted (regularisation), which is done at the (arbitrary) scale μ.
  - Observables should not depend on μ.
  - Idea: make $\bar{\alpha}_s$ scale dependent (running coupling).

- The purpose of making $\bar{\alpha}_s$ scale-dependent is to transfer to $\bar{\alpha}_s$ all terms involving μ in the perturbative series of any dimensionless observable R.

$$
\begin{aligned}
0 &= \mu^2 \frac{\mathrm{d}}{\mathrm{d}\mu^2} R(Q^2/\mu^2, \bar{\alpha}_s(\mu)) \\
&= \left[\mu^2 \frac{\partial}{\partial \mu^2} + \mu^2 \frac{\partial \bar{\alpha}_s}{\partial \mu^2} \frac{\partial}{\partial \bar{\alpha}_s}\right] R(Q^2/\mu^2, \bar{\alpha}_s(\mu))
\end{aligned}
$$

$\beta(\bar{\alpha}_s)$

Beta-function

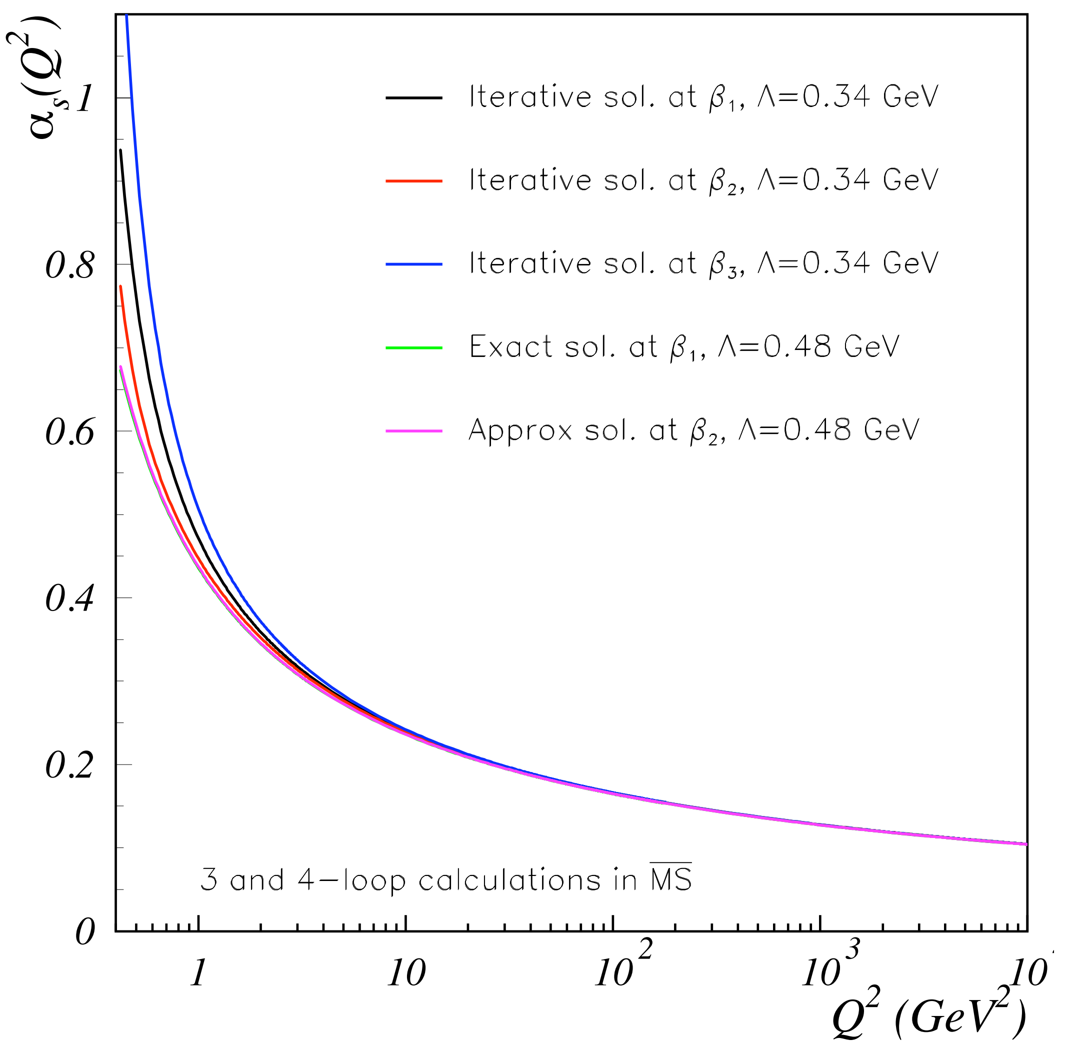
Callan-Symanzik relation

[Callan, PRD **2**, 1541 (1970);
Symanzik, Commun. Math. Phys. **18,** 227 (1970);
Commun. Math. Phys. **23**, 49 (1971)]

- Callan-Symanzyk relation can be solved in perturbation theory, the exact 1-loop solution is

$$\alpha_s(Q^2) = \frac{4\pi}{\beta_0 \ln(Q^2/\Lambda^2)}$$

  - Feature of the perturbative solutions: appearance of (unphysical) Landau Pole at $Q = \Lambda$, signals breakdown of pQCD.
  - Scale parameter Λ is scheme dependent.
  - Scale $\Lambda_{\bar{MS}} \approx 340$ MeV is often associated with the confinement scale or hadronic mass sale.
  - pQCD could work for $Q \gg \Lambda$ (at high T the situation is more complex).



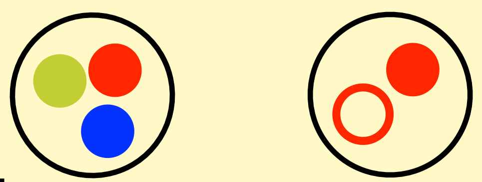
[Deur, Brodsky, de Teramond, Prog. Part. Nucl. Phys.90 (2016) 1-74]

QCD exhibits important non-perturbative phenomena, some examples:

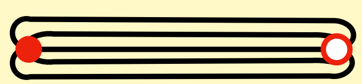
- **Long distance properties:** we have $r \sim Q^{-1}$

  - Confinement

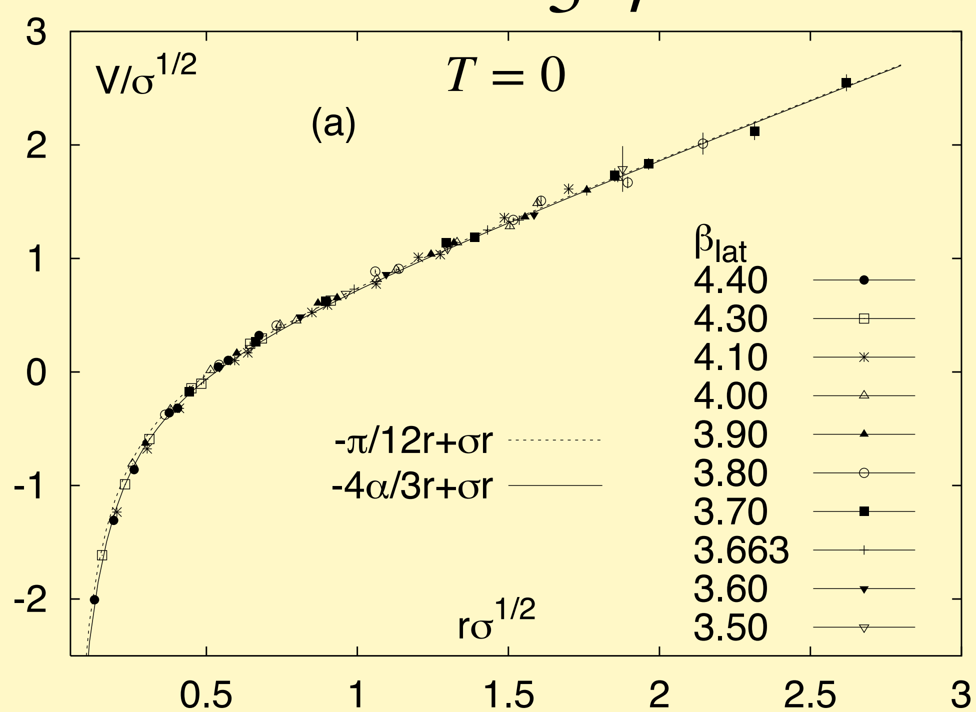
Ground state: hadrons



Flux tube



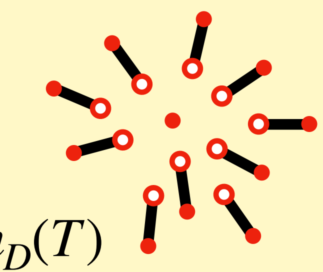
Potential: $V(r) = -\frac{4}{3}\frac{\alpha_s}{r} + \sigma r$



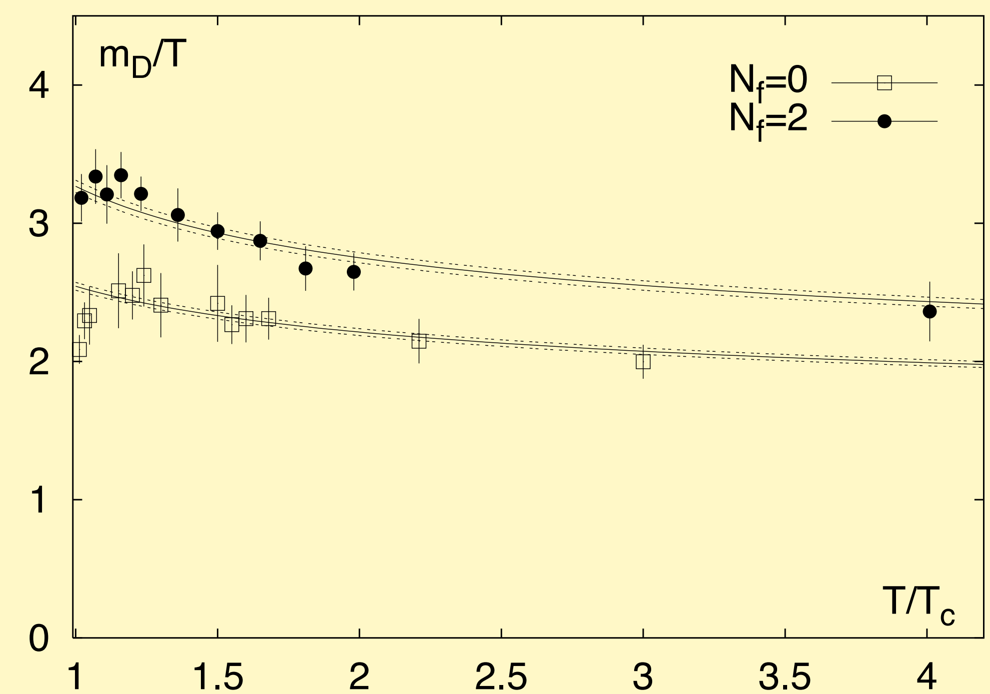
[Kaczmarek, Zantow, PRD **71** (2005) 114510]

  - Screening

At hight T, vacuum polarisation modifies the short distance part of the potential



$$-\frac{4\alpha_s}{3r} \rightarrow \frac{4\alpha_s(T)}{3r} e^{-r m_D(T)}$$



[Kaczmarek, Zantow, PRD **71** (2005) 114510]

QCD exhibits important non-perturbative phenomena, some examples:

- **Chiral symmetry breaking:** in the chiral limit the QCD Lagrangian is invariant under separate unitary rotations of left- and right handed quarks

$$\psi_L \to e^{i\theta_L^a T^a}\psi_L \quad \text{and} \quad \psi_R \to e^{i\theta_R^a T^a}\psi_R \quad \text{with} \quad \psi_{R,L} = \frac{1 \pm \gamma^5}{2}\psi$$

The symmetry $U_L(N_f) \times U_R(N_f)$ decomposes into

$$\underbrace{SU_L(N_f) \times SU_R(N_f)} \times U_V(1) \times U_A(1)$$

spontaneously broken to $SU_V(N_f)$ at low T

$U_V(1)$: Baryon number conservation

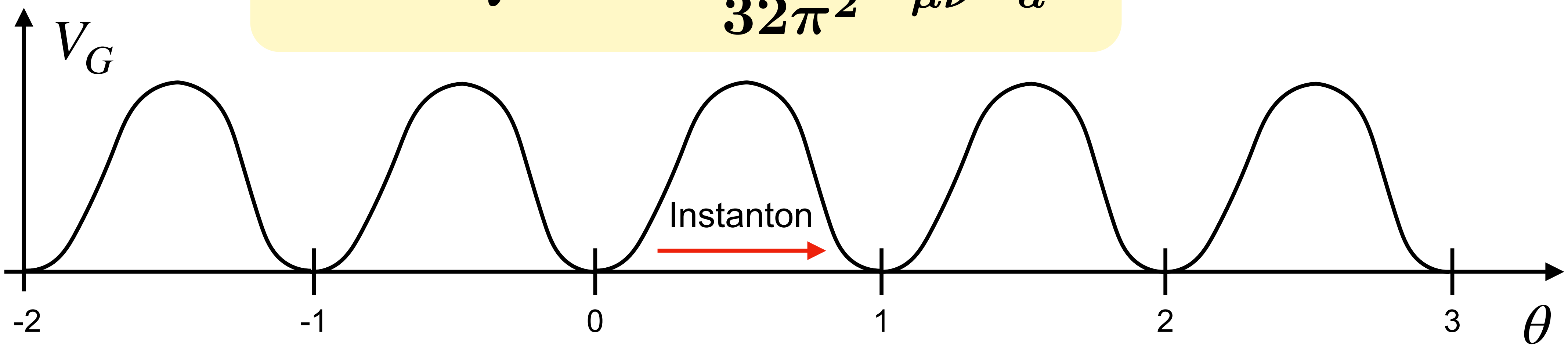
$U_A(1)$: Axial anomaly, broken by quantum effects

- mass term introduces explicit symmetry breaking
- remaining approximate symmetry explains observed patterns in the mass spectrum of hadrons (Goldstone bosons, chiral partners)
- Weak coupling expansion is an expansion around the wrong vacuum
- Chiral perturbation theory is an effective description

QCD exhibits important non-perturbative phenomena, some examples:

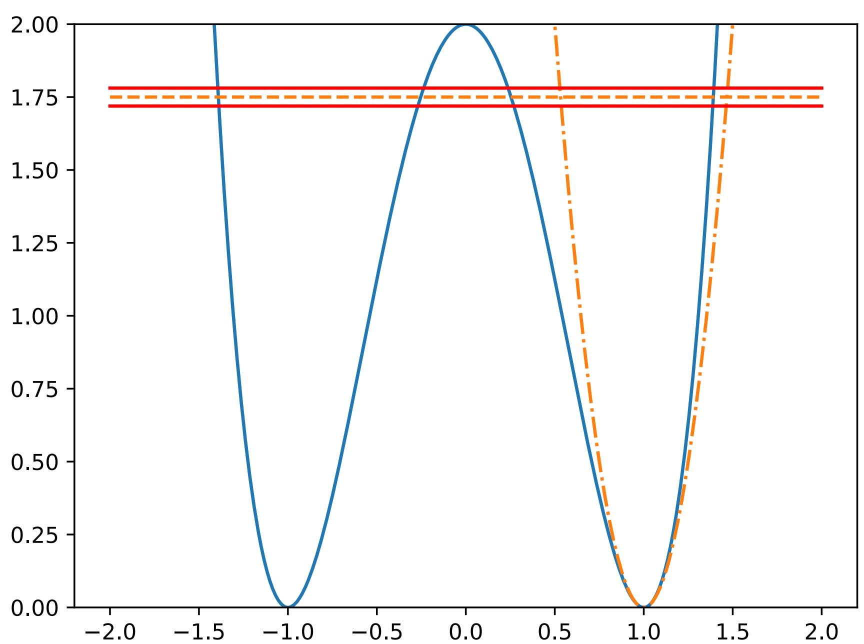
- **Topology:** Gauge fields can have non-trivial topology, i.e. non-trivial winding number, different vacua with different topology are separated by a potential barrier

$$\mathcal{L} = \mathcal{L}_{QCD} - \theta \frac{n_f g^2}{32\pi^2} F^a_{\mu\nu} \tilde{F}^{\mu\nu}_a$$



Toy model in QM

$V(x) = \lambda(x^2 - 1)^2$



- In QCD Instantons induce the chiral anomaly
- Perturbation theory completely misses the level splitting due to Instanton solutions

$$\Delta E = \sqrt{\frac{6S_0}{\pi}} \omega e^{-S_0}, \quad S_0 = \frac{\omega^3}{12\lambda}$$

Lattice QCD if formulated as a numerical calculation of the path integral

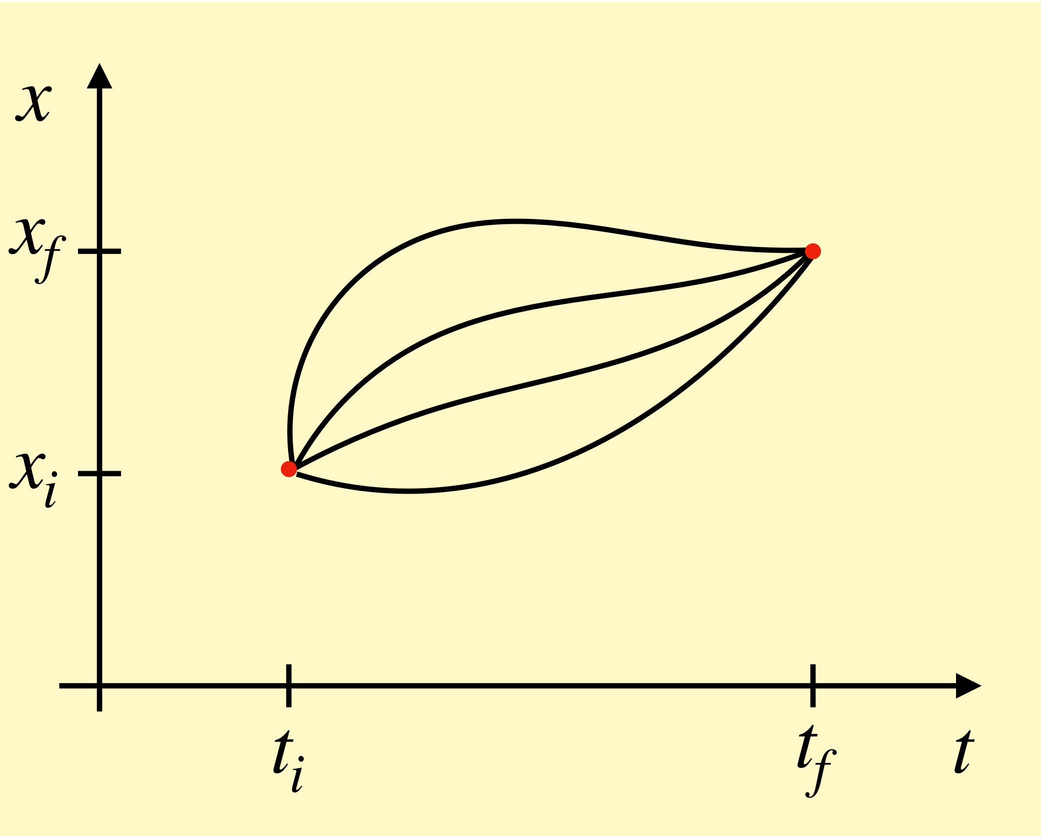
- It focusses in the action, rather than the Hamiltonian (Time is put on equal footing with space, relativistic symmetries become manifest.
- Operators are eliminated and QFT is mapped to a ***classical statistical system***.
- It allows for a more efficient organisation of perturbation theory.
- It goes back to Feynman (1948).

Transition amplitudes in QM as weighted sum over all paths connecting $x_i(t_i)$ and $x_f(t_f)$

$$< f \,|\, e^{-\frac{i}{\hbar}(t_f - t_i)\hat{H}} \,|\, i > = \int_{q(t_i)=x_i}^{q(t_f)=x_f} \mathscr{D}q(t)\; e^{\frac{i}{\hbar}S[q]}$$

$$S[q] = \int_{t_i}^{t_f} dt\; \mathscr{L}(q, \dot{q})$$

Classical action



Example: Path Integral in QM

- Start with discretising the time evolution

$$\hat{H} = K(\hat{p}) + V(\hat{q})$$

$$G(y,t'';x,t') = < y | e^{-\frac{i}{\hbar}(t''-t')\hat{H}} | x > = \lim_{n\to\infty} < y | \underbrace{e^{-\frac{i}{\hbar}\delta t\,\hat{H}} \cdots e^{-\frac{i}{\hbar}\delta t\,\hat{H}}}_{\text{n-times: } \delta t = (t''-t')/n} | x >$$

- For small δt we can use Baker-Campbell-Hausdorff $e^{K+V} \approx e^K e^V (1 + \mathcal{O}(\delta t^2))$

- Insert compete sets of position eigenstates every were

$$G(y,t'';x,t') = \lim_{n\to\infty} \int dz_1 \cdots dz_{n-1} < y | e^{-\frac{i}{\hbar}\delta t K} e^{-\frac{i}{\hbar}\delta t V} | z_1 > < z_1 | \cdots$$

$$\cdots | z_{n-1} > < z_{n-1} | e^{-\frac{i}{\hbar}\delta t K} e^{-\frac{i}{\hbar}\delta t V} | x >$$

$$= \lim_{n\to\infty} \int dz_1 \cdots dz_{n-1} < y | e^{-\frac{i}{\hbar}\delta t K} | z_1 > e^{-\frac{i}{\hbar}\delta t V(z_1)} < z_1 | \cdots$$

$$\cdots < z_{n-1} | e^{-\frac{i}{\hbar}\delta t K} | x > e^{-\frac{i}{\hbar}\delta t V(x)}$$

Example: Path Integral in QM

- Now insert complete sets of momentum eigenstates

$$G(y,t'';x,t') = \lim_{n\to\infty} \int dz_1 \cdots dz_{n-1} dp_1 \cdots dp_{n-1} < y \,|\, e^{-\frac{i}{\hbar}\delta t K} \,|\, p_1 > < p_1 \,|\, z_1 > e^{-\frac{i}{\hbar}\delta t V(z_2)}$$
$$\cdots < z_{n-1} \,|\, e^{-\frac{i}{\hbar}\delta t K} \,|\, p_{n-1} > < p_{n-1} \,|\, x > e^{-\frac{i}{\hbar}\delta t V(x)}$$

$$= \lim_{n\to\infty} \int dz_1 \cdots dz_{n-1} dp_1 \cdots dp_{n-1} < y \,|\, p_1 > e^{-\frac{i}{\hbar}\delta t K(p_1)} < p_1 \,|\, z_1 > e^{-\frac{i}{\hbar}\delta t V(z_2)}$$
$$\cdots < z_{n-1} \,|\, p_{n-1} > e^{-\frac{i}{\hbar}\delta t K(p_{n-1})} < p_{n-1} \,|\, x > e^{-\frac{i}{\hbar}\delta t V(x)}$$

- Integrate over the momentum, using the overlap $< z \,|\, p > = e^{ipz}/\sqrt{2\pi\hbar}$ and choosing $K(p) = p^2/2m$ we obtain

$$G(y,t'';x,t') = \lim_{n\to\infty} \left(\frac{m}{2\pi\hbar i \delta t}\right)^{\frac{n-1}{2}} \int dz_1 \cdots dz_{n-1} \; e^{\frac{i}{\hbar}S_n}$$

Diverging Faktor!
Still finite for finite n

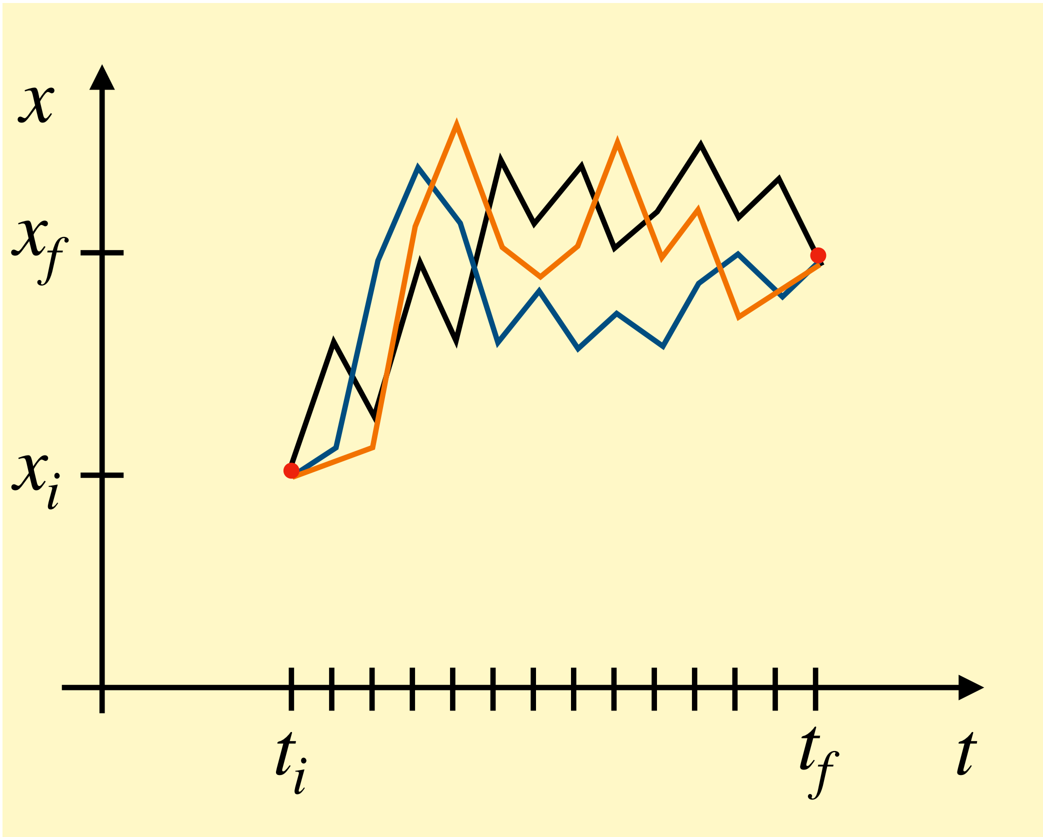
Example: Path Integral in QM

… with $S_n = \sum_{k=1}^{n} \frac{m}{2\delta t}(z_k - z_{k-1})^2 - \delta t V(z_k)$ $\qquad z_0 = x, \quad z_{n+1} = y$

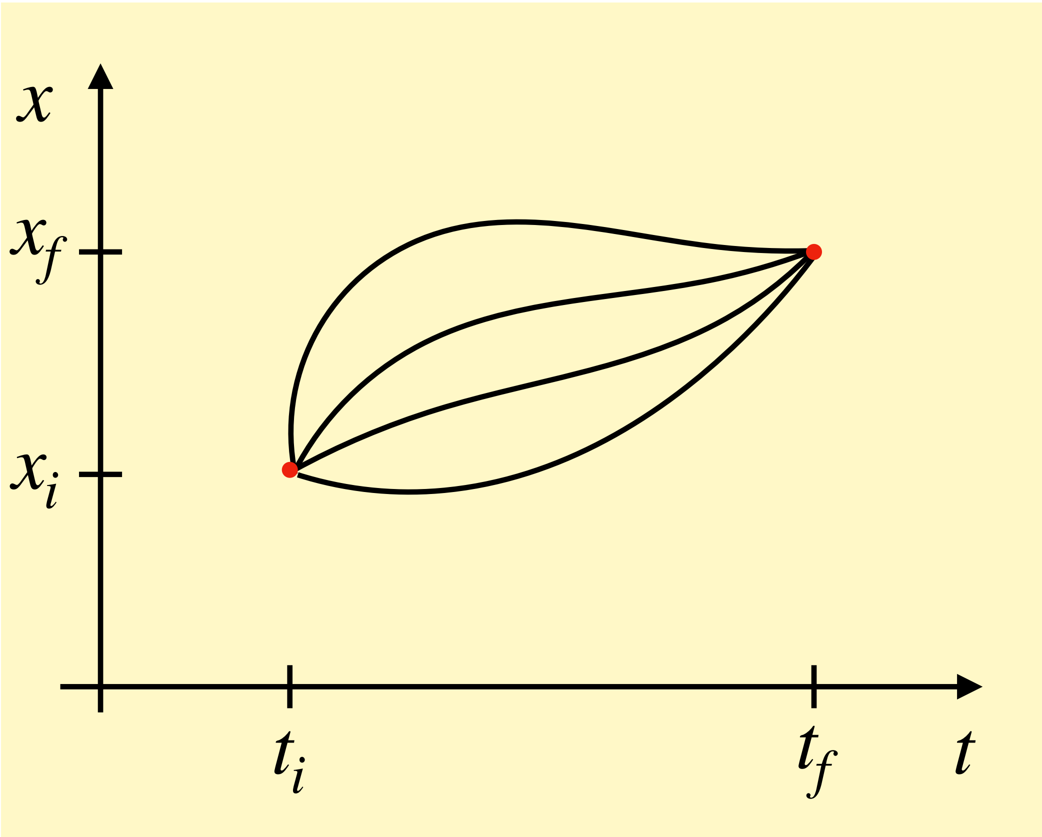
$$= \delta t \sum_{k=1}^{n} \frac{m}{2}\left(\frac{z_k - z_{k-1}}{\delta t}\right)^2 - V(z_k)$$

and $\lim_{n\to\infty} S_n = \int_{t'}^{t''} \mathrm{d}t \left\{ \frac{m}{2}\dot{z}^2(t) - V(z(t)) \right\} = \int_{t'}^{t''} \mathrm{d}t\, \mathscr{L}(z(t), \dot{z}(t))$ *q.e.d.*

Discretized Path Integral



Kontinuum



Special case: periodic paths. Consider $y = z(t_f) = z(t_i) = x$

and define $\tilde{Z}(t) = \int \mathrm{d}x\, G(x, t; x, 0) = \int \mathrm{d}x \; < x | e^{-\frac{i}{\hbar} t \hat{H}} | x >$

- Insert energy eigenstates

$$\tilde{Z}(t) = \int \mathrm{d}x \sum_n \; < x | e^{-\frac{i}{\hbar} t \hat{H}} | E_n > < E_n | x >$$

$$= \sum_n \int \mathrm{d}x \; < x | E_n > < E_n | x > e^{-\frac{i}{\hbar} t E_n}$$

$$= \sum_n \int \mathrm{d}x \, |\psi_n(x)|^2 e^{-\frac{i}{\hbar} t E_n} = \sum_n e^{-\frac{i}{\hbar} t E_n} = \mathrm{Tr}\; e^{-\frac{i}{\hbar} t H}$$

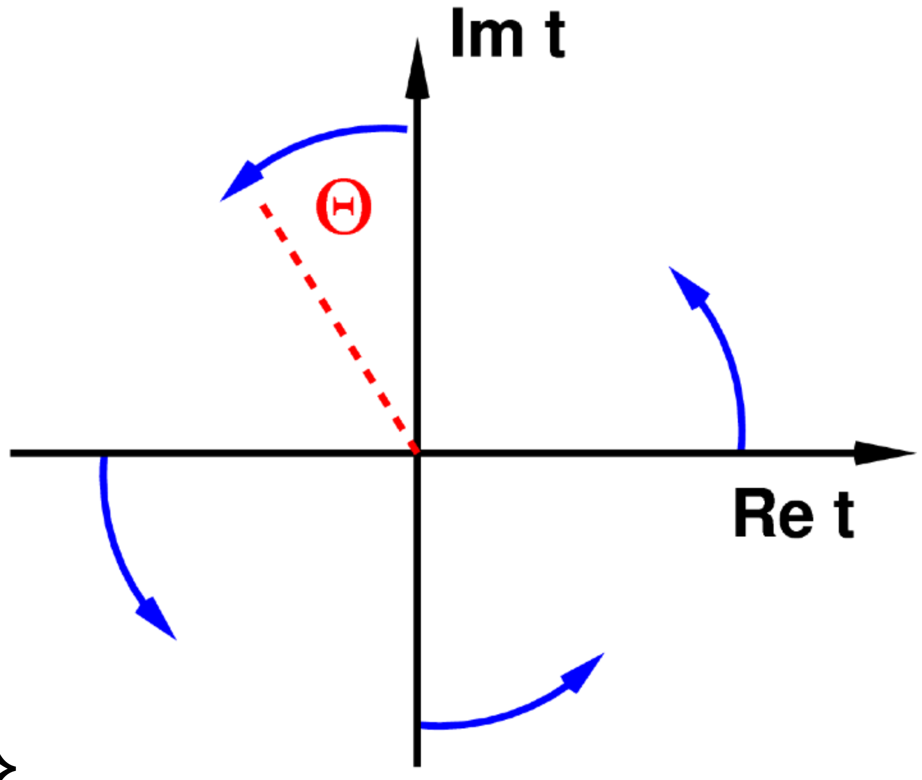
- Relation to the partition function in statistical mechanics

$$Z(T) = \int \mathrm{Tr} e^{-\beta H} = \sum_n e^{-\beta E_n}, \quad \beta \equiv \frac{1}{T}$$

$\tilde{Z}(t) = Z(T)$ with $t = -i\hbar/T$

Perform analytic continuation from real to imaginary time

Complex time: $t = |t| e^{-i\theta}$



$$S(z) = \int_0^t \mathrm{d}t \left\{ \frac{m}{2} \left(\frac{\mathrm{d}z(t)}{\mathrm{d}t} \right)^2 - V(z(t)) \right\}$$

$$\Rightarrow S_\theta(z) = \int_0^{|t|} \mathrm{d}|t|\, e^{-i\theta} \left\{ \frac{m}{2} e^{2i\theta} \left(\frac{\mathrm{d}z(t)}{\mathrm{d}|t|} \right)^2 - V(z(t)) \right\}$$

$$= \int_0^{|t|} \mathrm{d}|t|\, e^{i\theta} \left\{ \frac{m}{2} \left(\frac{\mathrm{d}z(t)}{\mathrm{d}|t|} \right)^2 - e^{-2i\theta} V(z(t)) \right\}$$

- Euclidian formulation, rotate to imaginary time $\theta = \pi/2$

$$S_{\pi/2}(z) = i \int_0^{|t|} \mathrm{d}|t| \left\{ \frac{m}{2} \left(\frac{\mathrm{d}z(t)}{\mathrm{d}|t|} \right)^2 + V(z(t)) \right\} \equiv i S_E(z)$$

Euclidean action

- Euclidian formulation, rotate to imaginary time $\theta = \pi/2$

$$S_{\pi/2}(z) = i \int_0^{|t|} \mathrm{d}|t| \left\{ \frac{m}{2} \left(\frac{\mathrm{d}z(t)}{\mathrm{d}|t|} \right)^2 + V(z(t)) \right\} \equiv iS_E(z)$$

Euclidean action

$$\tilde{Z}(-i\tau) \equiv Z_E(\tau) = \mathrm{Tr} e^{-\tau H/\hbar} \quad \text{with} \quad t = -i\tau \ \text{(imaginary time)}$$

- No oscillatory terms, convergence properties of integrals under control
- Probability interpretation: $e^{-S_E(z)} \geq 0, \quad e^{-\tau E_n} \geq 0$

- Euclidian path integral (now wet set $\hbar \equiv 1$)

$$Z_E(\tau) = \int \mathrm{d}x \int_{z(0)=x}^{z(\tau)=x} \mathscr{D}z(\tau)\, e^{-S_E[z(\tau)]} = \mathrm{Tr} e^{-\tau H} = \sum_n e^{-\tau E_n} = e^{-\tau E_0} \left(1 + \sum_{n>0} e^{-\tau(E_n - E_n)} \right)$$

Ground state: $E_0 = \lim_{\tau \to \infty} \frac{1}{\tau} \ln Z_E(\tau)$

- The Euclidean path integral over all paths with period τ is the partition function of a system at temperature $T = 1/\tau$

- The probability density

$$P_E = \frac{1}{Z_E(\tau)} e^{-S_E(\tau)}$$

- Observable

$$< \mathcal{O} >_\tau = \frac{1}{Z_E(\tau)} \int_\tau \mathcal{D}q(\tau)\ \mathcal{O}[q(\tau)]\ e^{-S_E[q(\tau)]}$$
$$= \frac{\text{Tr}\ \hat{\mathcal{O}}\ e^{-\tau \hat{H}}}{\text{Tr} e^{-\tau \hat{H}}}$$

- n-point functions

$$< \mathcal{O}(\tau_1)\mathcal{O}(\tau_2)\cdots\mathcal{O}(\tau_n) >_\tau = \frac{1}{Z_E(\tau)} \int_\tau \mathcal{D}q(\tau)\ \mathcal{O}(\tau_1)\mathcal{O}(\tau_2)\cdots\mathcal{O}(\tau_n)\ e^{-S_E[q(\tau)]}$$
$$= \frac{\text{Tr}\ T[\hat{\mathcal{O}}(\tau_1)\hat{\mathcal{O}}(\tau_2)\cdots\hat{\mathcal{O}}(\tau_n)]\ e^{-\tau \hat{H}}}{\text{Tr} e^{-\tau \hat{H}}}$$

thermal

$$< \mathcal{O}(\tau_1)\mathcal{O}(\tau_2)\cdots\mathcal{O}(\tau_n) > = \lim_{\tau \to \infty} < \mathcal{O}(\tau_1)\mathcal{O}(\tau_2)\cdots\mathcal{O}(\tau_n) >_\tau$$
$$= < 0 | T[\hat{\mathcal{O}}(\tau_1)\hat{\mathcal{O}}(\tau_2)\cdots\hat{\mathcal{O}}(\tau_n)] | 0 >$$

vav

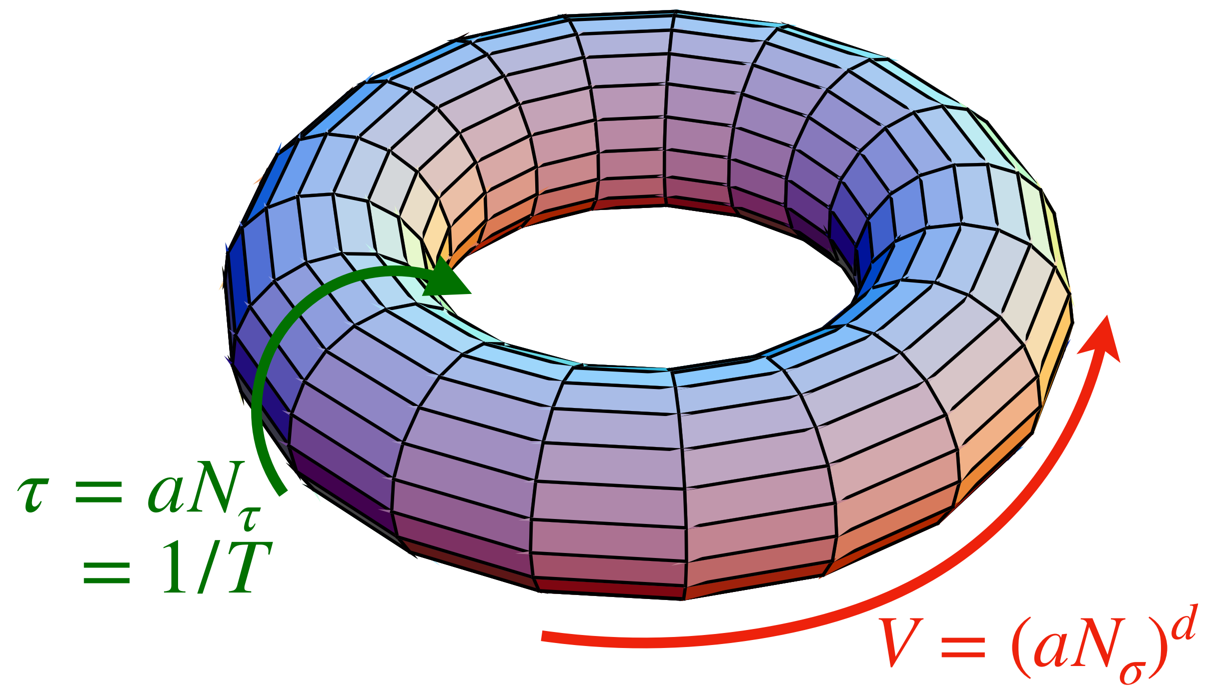
Time-ordering

- all n-point functions can be mapped to a classical statistical system
- this can be generalised to many d.o.f, i.e. to a (bosonic) QFT

- A suitable discretisation for the Euclidian action has to be chosen.
- The path integral is regularised by introducing a space-time grid with lattice constant a.

$$\int \mathscr{D}\phi \rightarrow \int \prod_{n}^{N_\tau \times N_\sigma^d} \mathrm{d}\phi_n \, .$$

- The topology often resembles a torus.
  - Periodic boundary condition in space are used to reduce finite size effects.



- The number of integration variables is very high $\sim 10^6$. A numerical integration is only possible since the Boltzmann factor e^{-S_E} is very localised.
  - Importance sampling is essential!

$$< \mathcal{O} >_\tau = \frac{1}{N} \sum_{k=1}^{N} \mathcal{O}(\phi^{(k)})$$

Sum over all generated field configurations.

- Markov Chain Monte Carlo is used to approach the correct equilibrium distribution.
  - For scalar and gauge theories several local update algorithms are known (Metropolis, heat-bath, micro-canonical, over relaxation, …).

- For fermions we can also find a path integral representation.
  - Important difference: Fermions require anti-periodic boundary conditions!
  - Example: the 1-particle Hamiltonian, derivation analog to the bosonic case

$$\hat{H}_1 = \omega \hat{a}^\dagger \hat{a} \quad \longleftrightarrow \quad \hat{H}_1 = \omega \frac{\partial}{\partial z} z = \omega - \omega z \frac{\partial}{\partial z}$$

$$\mathrm{Tr}_F e^{-\beta \hat{H}_1} = \int \mathrm{d}\eta \int \mathrm{d}\bar{\eta} \int_{\psi(0)=\eta}^{\psi(t)=-\eta} \int_{\bar{\psi}(0)=\bar{\eta}}^{\bar{\psi}(t)=-\bar{\eta}} \mathscr{D}\psi \mathscr{D}\bar{\psi}\, e^{-S} = 1 + e^{-\beta\omega}$$

$$\text{with } S = -\int_0^\beta \mathrm{d}\tau\ \bar{\psi}(\tau)(\partial_\tau + \omega)\psi(\tau)$$

- Integrating out the Grassmann fields
  - Action is bilinear in ψ, perform (Gauss) integration

d.o.f	bosonic	fermionic
1	$\int \mathrm{d}x\ e^{-\frac{1}{2}ax^2} = \sqrt{2\pi} a^{-1}$	$\int \mathrm{d}z \mathrm{d}\bar{z}\ e^{-\bar{z}az} = \int \mathrm{d}z\mathrm{d}\bar{z}\ (1 - \bar{z}az) = a$
$n \times n$	$\int \prod_{i=1}^{n} \mathrm{d}x_i\ e^{-\frac{1}{2}x_i a_{ij} x_j} = (2\pi)^{n/2} (\det A)^{-1}$	$\int \prod_{i=1}^{n} \mathrm{d}z_i \mathrm{d}\bar{z}_i\ e^{-\bar{z}_i a_{i,j} z_j} = \det A$

- The fermion matrix

$$S = -\int_0^\beta \mathrm{d}\tau \, \bar{\psi}(\tau)\underbrace{(\partial_\tau + \omega)}\psi(\tau) \approx -\delta\tau \sum_i \bar{\psi}_i Q_{i,j} \psi_j$$

Obvious discretization

$$Q = \begin{pmatrix} \omega & \frac{1}{2\delta\tau} & & & \frac{1}{2\delta\tau} \\ -\frac{1}{2\delta\tau} & \omega & \ddots & & \\ & \ddots & \ddots & & \\ & & -\frac{1}{2\delta\tau} & \omega & \frac{1}{2\delta\tau} \\ -\frac{1}{2\delta\tau} & & & -\frac{1}{2\delta\tau} & \omega \end{pmatrix}$$

We can absorb the diagonal entries in the fields

$$\psi_i \to \psi_i/\sqrt{\omega} \quad \bar{\psi}_i \to \bar{\psi}_i/\sqrt{\omega}$$

$$Z(\tau) = \propto \det[1 + \kappa D]$$

- Hoppingparameter expansion

$$Z(\tau) = \propto \det[1 + \kappa D] = e^{\ln\det[1+\kappa D]} = e^{Tr\ln[1+\kappa D]} = e^{-\sum_{l=0}^{\infty} \frac{\kappa^l}{l} Tr\, D^l}$$

  - Expansion of the effective action
  - Good for heavy fermions $\kappa \sim 1/m$

Pseudo Fermions

- We can write the determinant as

$$Z(\tau) = \det Q = \mathcal{N} \int \prod_{i=1}^{n} \mathrm{d}\bar{\chi}_i \mathrm{d}\chi_i \, e^{\bar{\chi}_i Q^{-1}_{i,j} \chi_j} \text{ with bosonic fields } \bar{\chi}_i, \chi_i$$

  - Requires the inversion of the fermion matrix for the MCMC → expensive.
  - Inversion can be done by iterative methods (Q is sparse).
  - If we can further write $Q = M^\dagger M$, a heat bath algorithm can be used for the update of the pseudo fermion fields.

… more problems later!

SU(3) Gauge Fields

$$\mathscr{L}_G = -\frac{1}{4} F^a_{\mu\nu} F^{\mu\nu}_a \quad \text{(Minkowski)}$$

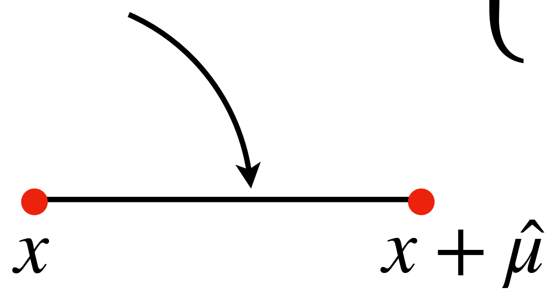
- Perform the Wick rotation

$$x_0 \to -ix_4, \quad A_0 \to +iA_4, \quad \partial_0 \to +i\partial_4$$

$$S_G(T,V) = + \int^{1/T} \mathrm{d}x_4 \int^{V} \mathrm{d}^3x \, \frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu} \quad \text{(Euclidian)}$$

- Introduce **link variables**, associated with the parallel transporter along the links between lattice points. [Wilson, PRD **10** (1974) 2445]

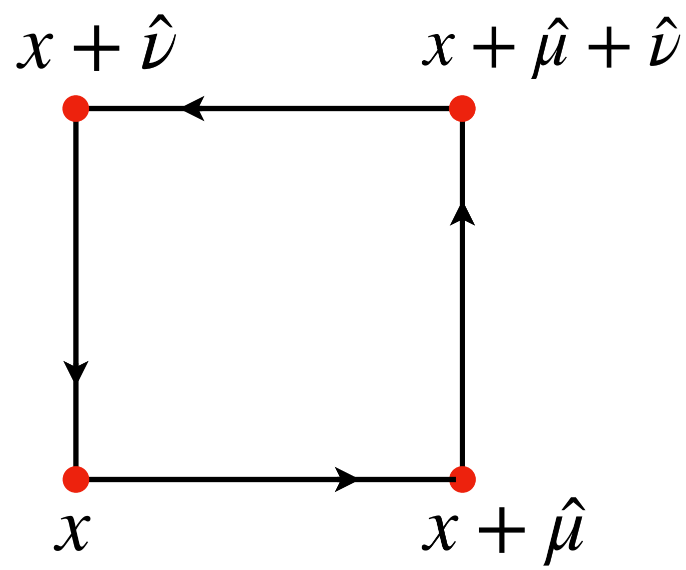
$$U_\mu(x) = P \exp\left\{ ig \int_x^{x+\hat{\mu}} \mathrm{d}x_\mu \, A^a_\mu T^a \right\} \in SU(3)$$



$$\lim_{a\to 0} U_\mu(x) = 1 + igaA^a_\mu T^a - \frac{g^2a^2}{2}(A^a_\mu T^a)^2 + \cdots$$

- No need to store gauge fields $A_\mu = A^a_\mu T^a$, which live in the algebra $\mathfrak{su}(3)$, explicitly.

- Need discretisation of the field strength tensor, consider the Plaquette $W^{(1,1)}_{\mu\nu}$



$$W^{(1,1)}_{\mu\nu}(x) = U_\mu(x)U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x)$$

$$= \underbrace{e^{iagA_\mu(x)}e^{iagA_\nu(x+\hat{\mu})}}\, e^{-iagA_\mu(x+\hat{\nu})}e^{-iagA_\nu(x)}$$

use Backer-Campbell-Hausdorff repeatedly

$$e^{iag(A_\mu(x)+A_\nu(x+\hat{\mu}))-a^2g^2[A_\mu(x),A_\nu(x+\hat{\mu})]}$$

$$\Rightarrow \frac{1}{N_c}\text{ReTr}W^{(1,1)} = 1 - a^4\frac{g^2}{2}\text{Tr}F_{\mu\nu}F_{\mu\nu} + \mathcal{O}(a^6)$$

$$\beta S_G = \beta\sum_x \sum_{1\leq\mu<\nu\leq 4}\left(1 - \frac{1}{N_c}\text{ReTr}W^{(1,1)}_{\mu\nu}\right) + \mathcal{O}(a^2)$$ **(Wilson action)**

$$\beta \equiv \frac{6}{g^2}$$ gauge coupling, not to be confused with the inverse temperature!

- Check local gauge invariance. Link variables transform under gauge transformations $G(x) = e^{i\Lambda(x)} \in SU(3)$ as $U_\mu(x) \to G(x)U_\mu(x)G^{-1}(x+\hat{\mu})$

$$\Rightarrow \mathrm{Tr}W_{\mu\nu}^{(1,1)} \to \mathrm{Tr}\left[G(x)U_\mu(x)\underbrace{G^{-1}(x+\hat{\mu})G(x+\hat{\mu})}_{1}\,U_\nu(x+\hat{\mu})G^{-1}(x+\hat{\mu}+\hat{\nu})\cdots G^{-1}(x)\right]$$

cyclic permutation

- Need to specify the integration measure

$$Z = \int \prod_{n,\mu} \mathrm{d}U\mu(n)\; e^{-\beta S_G(U)}$$

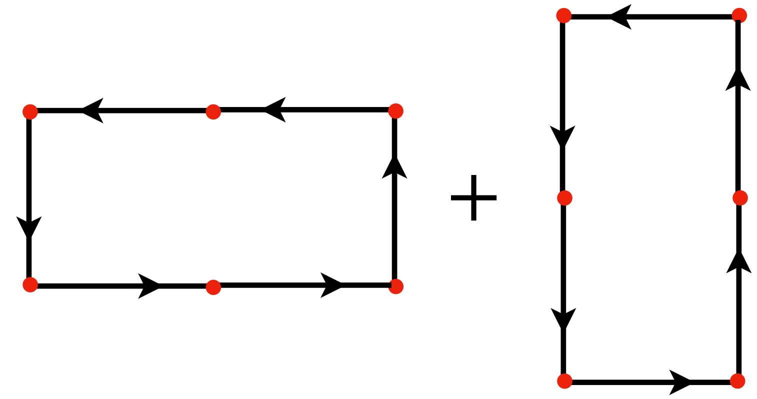
(pure gauge partition function)

Use group invariant Haar measure

- Action and measure are gauge invariant!

- We can reduce the cut-off effects of the gauge action by adding further (irrelevant) operators, we define

$$W^{(2,1)}_{\mu\nu}(x) =$$



$$\beta S_G = \beta \sum_n \sum_{1\le\mu<\nu\le4} c_{1,1}\left(1 - \frac{1}{3}\text{ReTr}W^{(1,1)}_{\mu\nu}\right) + c_{2,1}\left(1 - \frac{1}{6}\text{ReTr}W^{(2,1)}_{\mu\nu}\right)$$

$$+\mathcal{O}(g^2a^2) + \mathcal{O}(a^4)$$

with $c_{1,1} = \frac{5}{3}$, $c_{2,1} = \frac{1}{6}$ and $\beta = \frac{10}{g^2}$

- Symanzik (tree-level) $\mathcal{O}(a^2)$-improved
  [Symanzik, Nucl. Phys. B226, 187 (1983); Nucl. Phys. B226, 205 (1983)] [Weisz, Nucl. Phys. B212, 1 (1983); Weisz and R. Wohlert, Nucl. Phys.B236, 397 (1984); Nucl. Phys. B247, 544 (1984)] [Lüscher and P. Weisz, Comm. Math. Phys. 97, 59 (1985)]

- In principle, we can further improve the action at order g^2a^2 or even non-perturbatively
  [Iwasaki, Nucl. Phys. B258, 141 (1985)]

- The Euclidian action

$$S_F = \int \mathrm{d}^4x\ \bar{\psi}(\gamma_\mu D_\mu(A_\mu) + m)\psi$$

ψ : 4-spinor $\qquad D_\mu(A_\mu)$: covariant derivative

$\bar{\psi} = \gamma_4 \psi^\dagger \qquad D_\mu(A_\mu) = \partial_\mu + igA_\mu$

γ-matrices: $\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu\nu}$

- Discretization

Free case: $\left(\partial_\mu f\right)(x) \rightarrow \left(\mathring{\partial}_\mu f\right)(x) = \dfrac{1}{2a}\left(f(x+\hat{\mu}) - f(x-\hat{\mu})\right)$

Interacting case: $\left(D_\mu f\right)(x) \rightarrow \left(\mathring{D}_\mu f\right)(x) = \dfrac{1}{2a}\left(U_\mu(x)f(x+\hat{\mu}) - U_\mu^\dagger(x-\hat{\mu})f(x-\hat{\mu})\right)$

Problem: corresponding momentum modes $\mathring{\partial}_\mu \longleftrightarrow \mathring{p}_n = \sin(ap_n)$ with $p_n = \dfrac{2\pi n}{N_\sigma}$

(anti-periodic boundary condition require $p_n = \dfrac{(2+1)\pi n}{N_\tau}$ for $\mu = 4$)

Number of lattice points

- Propagator in momentum space

Continuum

$$(\gamma_\mu \partial_\mu)^{-1} = \frac{-i\sum_\mu \gamma_\mu p_\mu}{p^2}$$

one pole at
$p = (0,0,0,0)$

Lattice

$$(\gamma_\mu \mathring{\partial}_\mu)^{-1} = \frac{-i\sum_\mu \gamma_\mu p_\mu}{\sum_\mu \sin^2(p_\mu)}$$

15 additional poles at
$p = (\pi/a,0,0,0), (0,\pi/a,0,0),$
$\cdots, (\pi/a, \pi/a, \pi/a, \pi/a)$

- Pros: $\mathring{\partial}_\mu$ has chiral symmetry and γ_5-hermiticity (eigenvalues come in complex conjugated pairs)
- Cons: $\mathring{\partial}_\mu$ has doubles in the spectrum

How to get rid of the doublers?

- Nielsen-Ninomiya Theorem

There is no Dirac operator D on the lattice, fulfilling simultaneously the properties

(1) Locality: $D(x-y) \leq e^{-\gamma(x-y)}$

(2) Correct continuum limit: $\lim_{a\to 0} \tilde{D}(p) = \sum_\mu \gamma_\mu p_\mu$

(3) No doublers: $\tilde{D}(p)$ *is invertible if* $p > 0$

(4) Chiral Symmetry: $\{\gamma_5, D\} = 0$

[Nielsen-Ninomiya Nucl. Phys B **185**, 20; Nucl. Phys. B **193**, 173]
[Friedan, Commun. Math. Phys. **85**, 481]

- Chiral symmetry on the lattice is difficult!

- Decouple doublers in the continuum limit

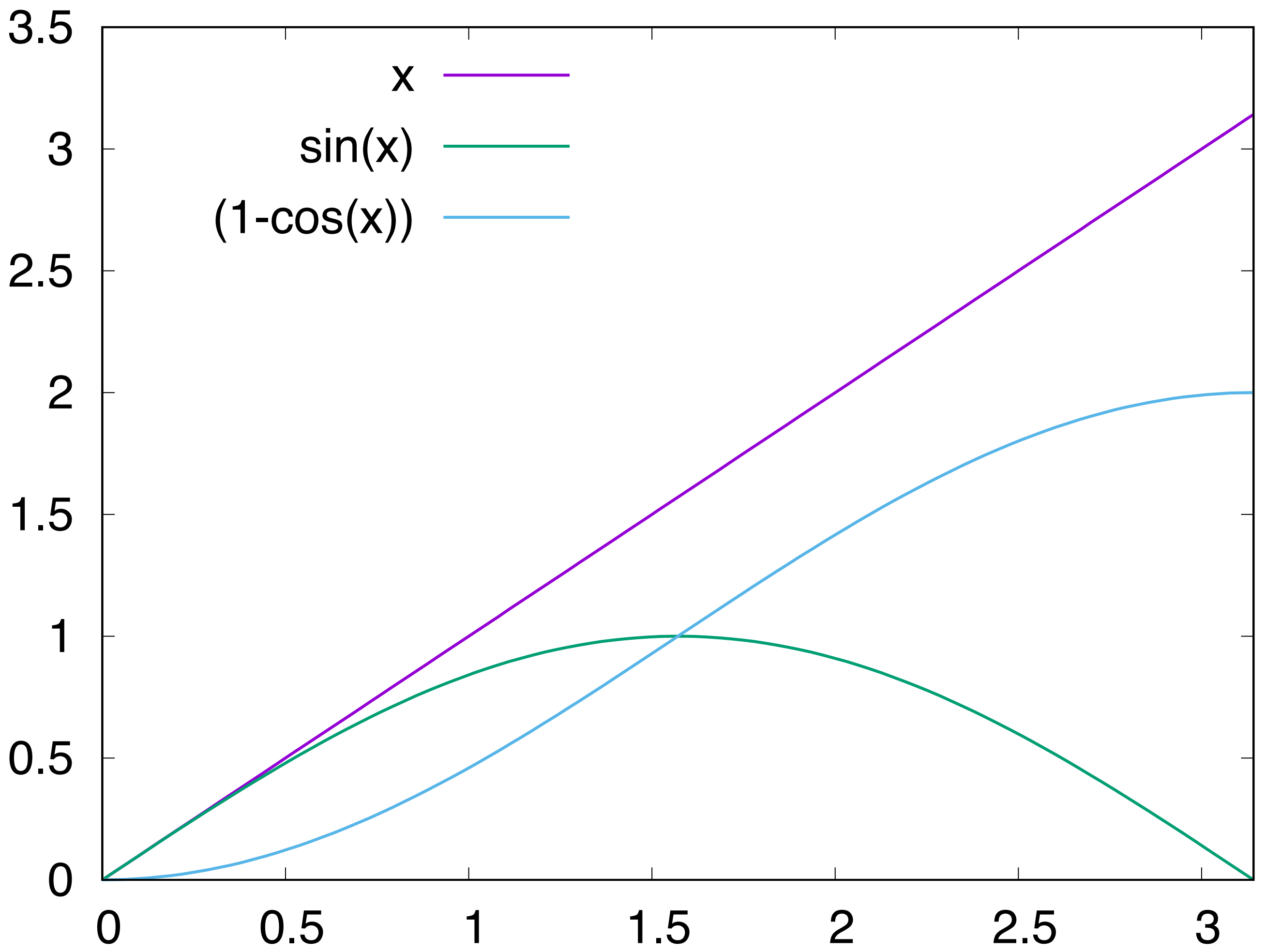
$$\left(\partial_\mu f\right)(x) \to \left(\mathring{\partial}_\mu f + r\hat{\Delta} f\right)(x)$$

$$\left(\hat{\Delta} f\right)(x) = a\frac{1}{2a^2}\left(2f(x) - f(x+\hat{\mu}) - f(x-\hat{\mu})\right) \quad \to \quad \frac{1}{a}(1-\cos(ap_\mu))$$

- Dose not change the continuum limit
- Lifts doublers at $p = \pi/a$
- Wilson parameter usually chooses as $r = 1$, i.e. we obtain with gauge files

$$D\!\!\!\!/_\mu^W = -\frac{1}{2a}\Big[(1-\gamma_\mu)U_\mu(x)\delta_{x,y-\hat{\mu}} + (1+\gamma_\mu)U_\mu^\dagger(x-\hat{\mu})\delta_{x,y+\hat{\mu}}\Big] + \frac{4}{a}\delta_{x,y}$$

[Wilson 1975]



$\Rightarrow$ breaks chiral symmetric, $\{D\!\!\!\!/_\mu^W, \gamma_5\} \neq 0$

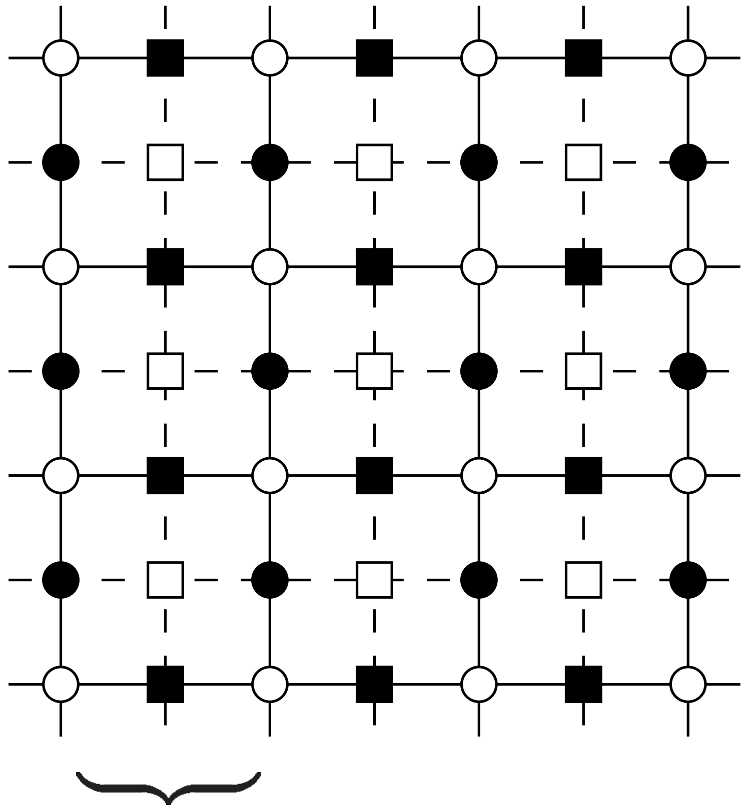
- Distribute spinor degrees of freedom over the lattice, effectively double the lattice spacing

  Hyper cube with $2^d = 2^4 = 16$ sites

  fits 4×4 components

  Dirac (spin) flavor (taste)

  $\Rightarrow$ KS-spinor describes 4 degenerate Dirac-spinors in the continuum limit



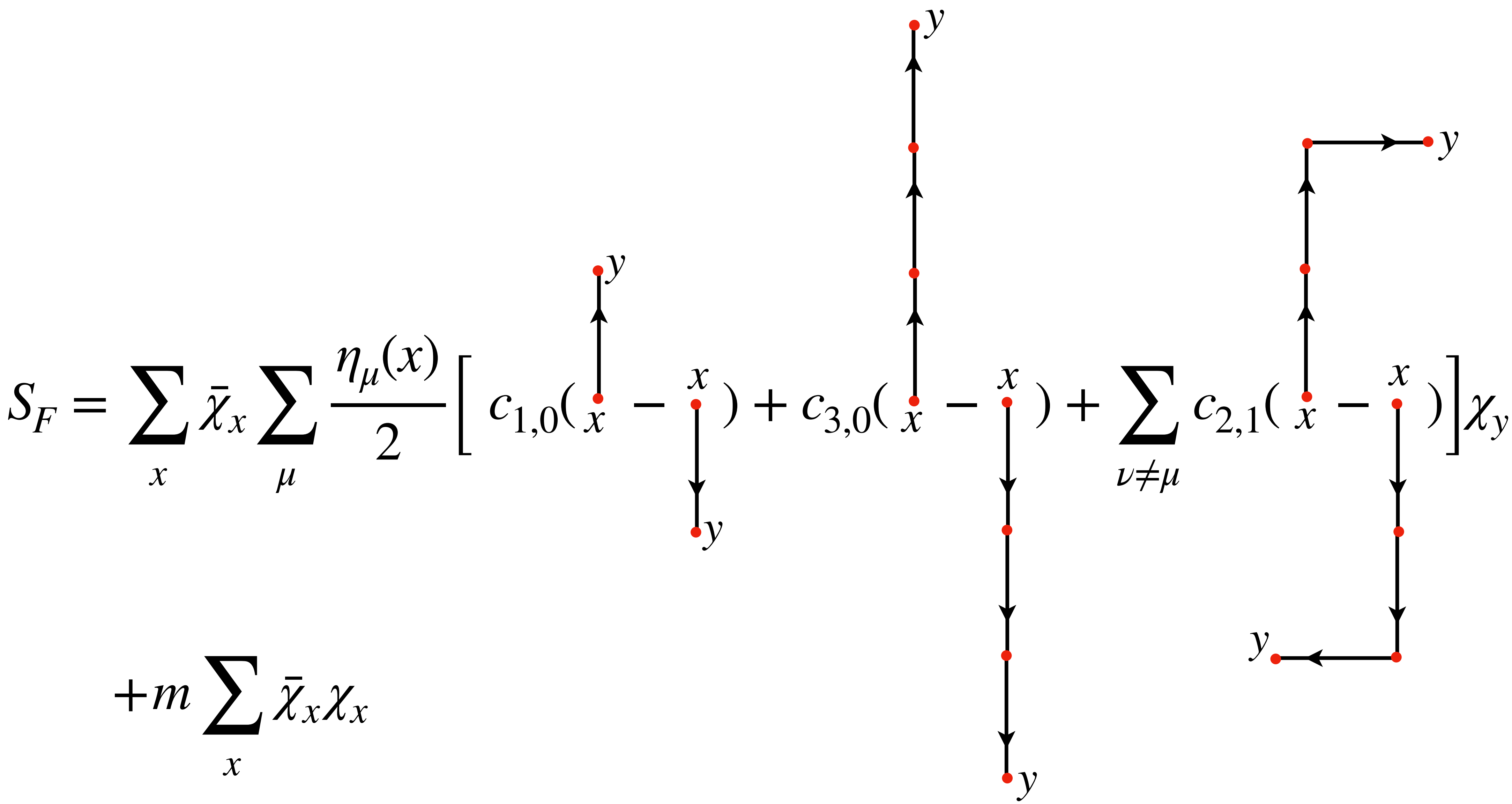
$$D\!\!\!/_\mu^{KS} = \frac{\eta_\mu(x)}{2a}\left[U_\mu(x)\delta_{x,y-\hat{\mu}} - U_\mu^\dagger(x-\hat{\mu})\delta_{x,y+\hat{\mu}}\right]$$

[Kogut-Susskind PRD **11** (1975) 396]

with staggered phases $\eta_\mu(x) = (-1)^{x_1+x_2+\cdots x_{\mu-1}}$

- Pros: computationally relatively cheap, KS-spinor has just 3 color components, reduces number of doublers to 4, remains subgroup of the chiral symmetry
- Cons: correlation function are alternating, doublers are not completely removed, chiral symmetry is not completely preserved

- Similarly to the gauge action we can improve the fermion action, the standard Willson and Kogut-Susskind actions receive corrections at $\mathcal{O}(a^2)$.
- We can add straight and bended 3-link terms to the KS action



Naik-action: $c_{1,0} = 9/16, \quad c_{3,0} = -1/48, \quad c_{2,1} = 0$

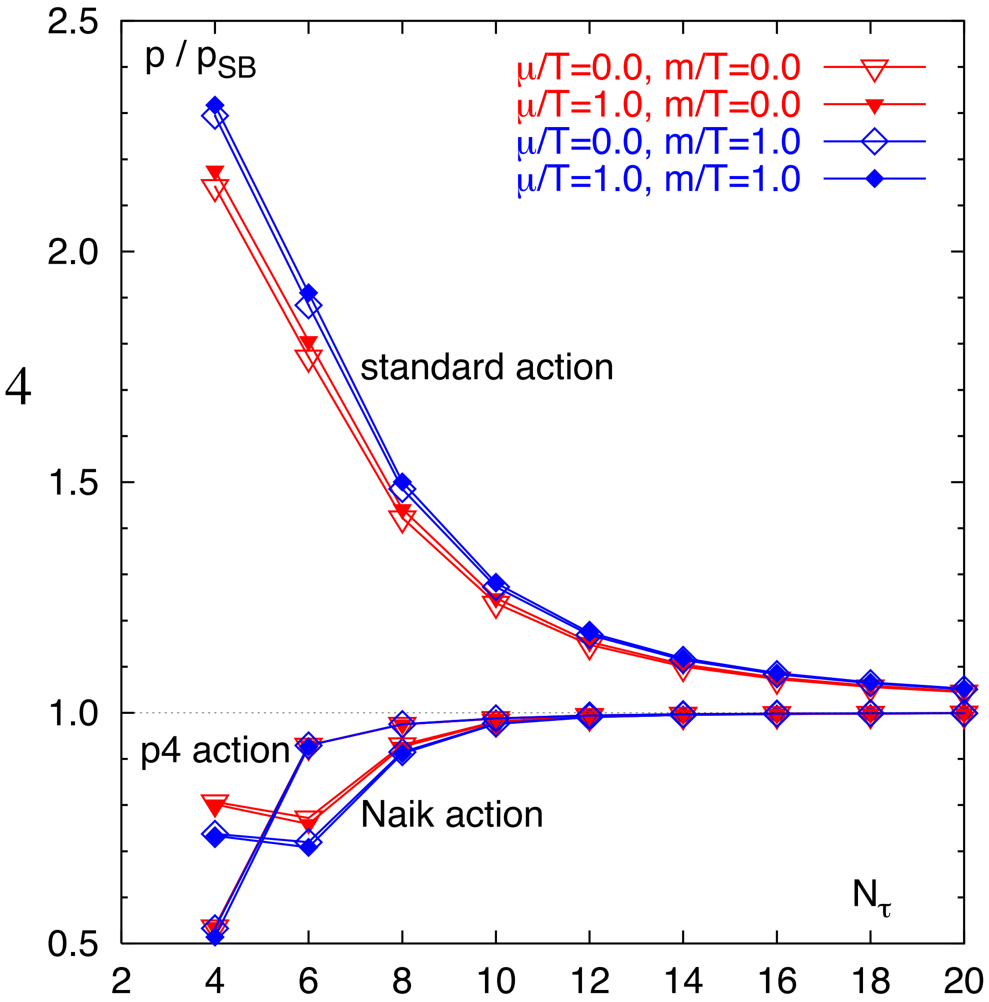
p4-action: $c_{1,0} = 3/8, \quad c_{3,0} = 0, \quad c_{2,1} = 1/48$

[Heller, Karsch, Strum PRD **60** (1999) 114502]

- The improvement at tree-level affects the approach to the free gas limit

$$p_{SB} \equiv \frac{p}{T^4}\bigg|_{\infty} = \frac{7 n_f \pi^2}{60} + \frac{n_f}{2}\left(\frac{\mu_q}{T^2}\right)^2 + \frac{n_f}{4\pi^2}\left(\frac{\mu_q}{T^4}\right)^4$$

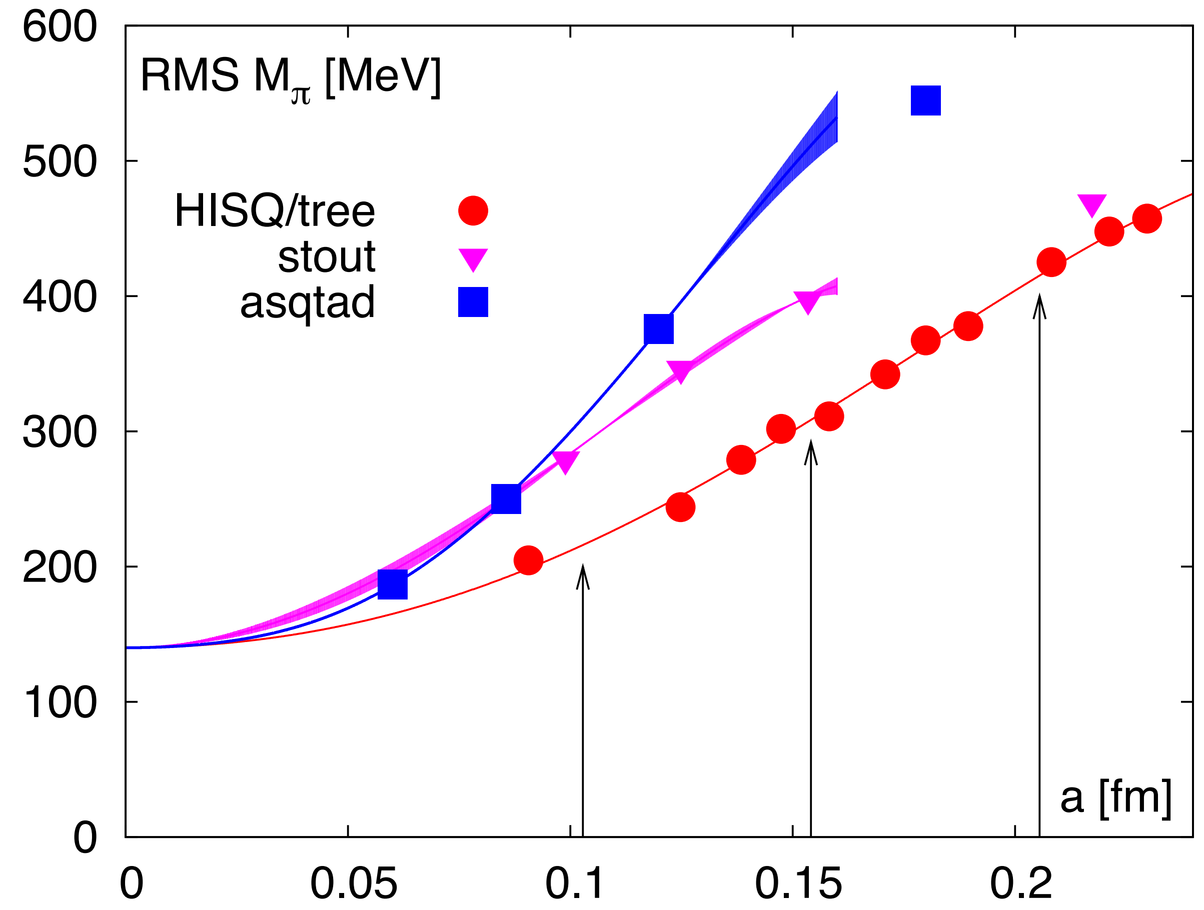
Ideal quark gas



$$\frac{\frac{p}{T^4}}{\left(\frac{p}{T^4}\right)_{\rm SB}} = 1 + \begin{cases} \frac{248}{147}\left(\frac{\pi}{N_\tau}\right)^2 + \frac{635}{147}\left(\frac{\pi}{N_\tau}\right)^4 + \frac{13351}{8316}\left(\frac{\pi}{N_\tau}\right)^6 & \text{std. Wilson} \\ \frac{248}{147}\left(\frac{\pi}{N_\tau}\right)^2 + \frac{635}{147}\left(\frac{\pi}{N_\tau}\right)^4 + \frac{3796}{189}\left(\frac{\pi}{N_\tau}\right)^6 & \text{std. staggered} \\ \qquad\qquad - \frac{1143}{980}\left(\frac{\pi}{N_\tau}\right)^4 - \frac{365}{77}\left(\frac{\pi}{N_\tau}\right)^6 & \text{Naik} \\ \qquad\qquad - \frac{1143}{980}\left(\frac{\pi}{N_\tau}\right)^4 + \frac{73}{2079}\left(\frac{\pi}{N_\tau}\right)^6 & \text{p4} \end{cases}$$

[Hegde, Karsch, Laermann, Shcheredin, Eur. Phys. J. C 55 (2008) 423]

- Staggered quarks consists out of four "tastes", which become degenerate in the continuum limit $\longrightarrow$ trivial factor in bulk thermodynamics.
- At finite lattice spacing a, rough gauge fields induce interactions between "tastes". Gluons at high momentum can scatter quarks from one corner of the Brillouine zone to another.
- Due to additional tastes, we have additional pions on the lattice. Taste-interactions disturb the pion spectrum. A measure for this effect is the pion root-mean-square mass.

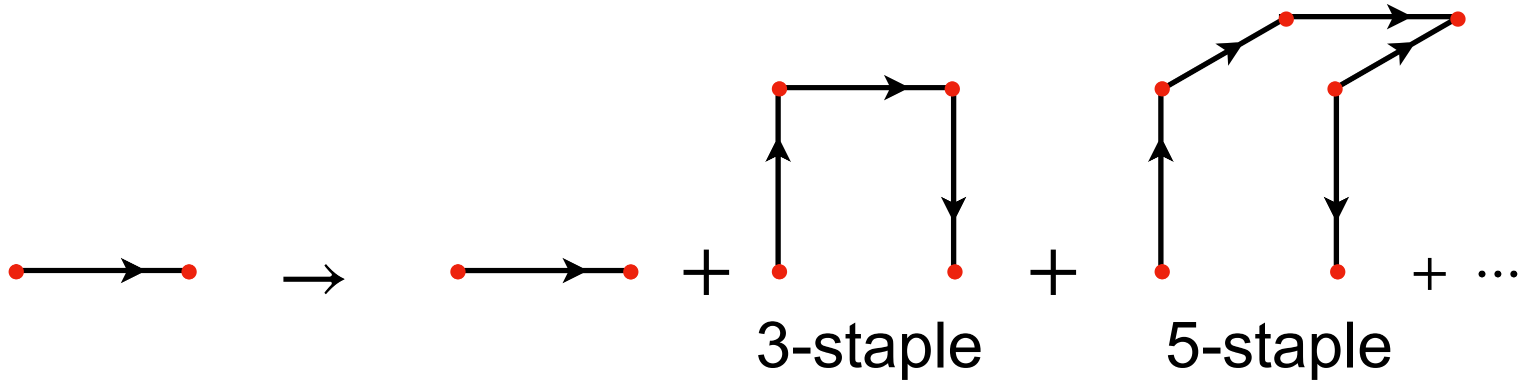


[Bazavov et al (HotQCD) *PRD* **85** (2012) 054503]

$$m_{RMS} = \sqrt{m^2_{\gamma_5} + m^2_{\gamma_0\gamma_5} + m^2_{\gamma_i\gamma_5} + m^2_{\gamma_0} + m^2_{\gamma_i} + m^2_{\gamma_0\gamma_i} + m^2_{\gamma_i\gamma_j} + m^2_1}$$

Smearing techniques:

- Smear the one link-term by staples up to length 7 (fat7 smearing)



[Orginos et al (MILC), *PRD* **60** (1999) 054503]

- Exponentiated 3-staple smearing (stout-smearing)

[Morningstar Peardon PR*D* **69** (2004) 05450]

Overview of some frequently used staggered actions:

Name	tree-level	1-loop	smearing
HISQ/tree	Naik (3-link)	none	2-times fat7
2-stout	none	none	2-times stout
aqtad	Naik (3-link)	tadpole	none

- All parameters of the action are dimensionless β, N_σ, N_τ, $\hat{m}_l = am_l$, $\hat{m}_s = am_s$ (quark masses are given in units of the lattice spacing)

- All observables Γ are measured in units of the lattice spacing: $\hat{\Gamma} = a^{d_\Gamma}\Gamma$

- The lattice cut-off is our renormalisation scale, and all observables should be come independent of a, i.e. $a\frac{\mathrm{d}}{\mathrm{d}a}\Gamma = 0$

- Since $\Gamma = \Gamma(a, g)$ the Callan-Symanzik equation reads now

$$\left(a\frac{\partial}{\partial a} - \beta(a)\frac{\partial}{\partial g}\right)\Gamma = 0 \quad \text{with} \quad \beta(g) = -a\frac{\partial g}{\partial a}$$

$$\text{Solution: } \frac{a}{a_0} = \exp\left\{\int_g^{g_0} \frac{1}{\beta(a)}\right\}$$

- Lattice spacing $a \to 0$ requires $\beta(g) \to 0$ (fix-point)
- The coupling controls the lattice spacing
- β-function has perturbative expansion for small g (large $6/g^2$)

- In the non-perturbative regime we require input information from experiment to set the scale. Typically one hadron mass, decay constant or a parameter of the heavy quark potential.

- We also need the bare quark masses as function of the coupling (if we want to keep the renormalised masses constant during the simulation)

  - Requires tuning of the bare quark masses at T=0

Equation of state at $\mu = 0$

- We use HISQ fermions with two degenerate light quarks and one strange quark

Partition function

$$Z(T,V) = \int \mathcal{D}U \mathcal{D}\bar{\chi} \mathcal{D}\chi \, e^{-S_E} \text{ with } S_E = \beta S_G(U) - S_F(\bar{\chi}, \chi, U)$$

$$S_F = \bar{\chi}_l M_l^{-2/4} \chi_l + \bar{\chi}_s M_s^{-1/4} \chi_s$$

Bulk thermodynamics

$$\frac{p}{T^4} = \frac{1}{VT^3} \ln Z$$

$$\frac{\epsilon}{T^4} = \frac{1}{VT^4} \frac{\mathrm{d}}{\mathrm{d}T^{-1}} \ln Z$$

- All thermodynamic potentials are obtained from $\ln Z$
- We can not calculate the pressure directly, we are using the **integral method**

[see e.g. Cheng et. al *PRD* **77** (2008) 014511]

- The basic quantity is the **trace anomaly** (also called interaction measure)

$$\frac{\epsilon - 3p}{T^4} = T \frac{\mathrm{d}}{\mathrm{d}T} \frac{p}{T^4}$$

$$\Rightarrow \frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = \int_{T_0}^{T} \mathrm{d}T \, \frac{1}{T} \left(\frac{\epsilon - 3p}{T^4} \right)$$

Integration constant

$$\frac{\epsilon - 3p}{T^4} = T\frac{\mathrm{d}}{\mathrm{d}T}\frac{p}{T^4}$$

$$T = \frac{1}{aN_\tau}$$

The temperature is usually dialled by a, keeping N_τ fixed

We need to express this differential operator in terms of lattice parameter

$$T\frac{\mathrm{d}}{\mathrm{d}T} = T\frac{\mathrm{d}(1/T)}{\mathrm{d}T}\frac{\mathrm{d}}{\mathrm{d}(1/T)} = -T^{-1}\frac{\mathrm{d}}{\mathrm{d}(1/T)} = -aN_\tau\frac{\mathrm{d}}{\mathrm{d}(aN_\tau)} = -a\frac{\mathrm{d}}{\mathrm{d}a}$$

- The lattice spacing is controlled by the coupling β. Also the bare quark masses depend on a (LCP).

$$-a\frac{\mathrm{d}}{\mathrm{d}a} = -a\frac{\mathrm{d}\beta}{\mathrm{d}a}\frac{\partial}{\partial\beta} - a\underbrace{\frac{\mathrm{d}m_s}{\mathrm{d}a}\frac{\partial}{\partial m_s}} = -a\frac{\mathrm{d}\beta}{\mathrm{d}a}\left(\frac{\partial}{\partial\beta} + a\frac{\mathrm{d}m_s}{\mathrm{d}\beta}\frac{\partial}{\partial m_s}\right)$$

R_β R_m (Lattice β-functions)

note that we fix $m_l = m_s/27$ (physical point), i.e. we need here just one quark mass parameter

- Now we can construct our lattice observables

$$\frac{\Theta_{\mu\mu}}{T^4} = \frac{\epsilon - 3p}{T^4} = T \frac{\mathrm{d}}{\mathrm{d}T} \frac{p}{T^4}$$

Trace of the energy momentum tensor

$T = 0$ obtained by $N_0 \geq N_\sigma$

$$= R_\beta \left(\frac{\partial}{\partial \beta} + R_m \frac{\partial}{\partial m_s} \right) N_\tau^4 \left[\frac{1}{N_\sigma^3 N_\tau} \ln Z(\tau) - \frac{1}{N_\sigma^3 N_0} \ln Z(0) \right]$$

Renormalisation by subtracting the zero temperature result

$$= N_\tau^4 R_\beta \left[\left\langle s_G \right\rangle_0 - \left\langle s_G \right\rangle_\tau \right]$$ (*gluonic contribution*)

$$+ N_\tau^4 R_\beta R_m \left[\frac{2}{27} \left(\langle \bar{\psi}\psi \rangle_{l,\tau} - \langle \bar{\psi}\psi \rangle_{l,0} \right) + \left(\langle \bar{\psi}\psi \rangle_{s,\tau} - \langle \bar{\psi}\psi \rangle_{s,0} \right) \right]$$

(*fermionic contribution*)

$$\frac{\Theta_{\mu\mu}}{T^4} = N_\tau^4 R_\beta \left[\langle s_G \rangle_0 - \langle s_G \rangle_\tau \right]$$

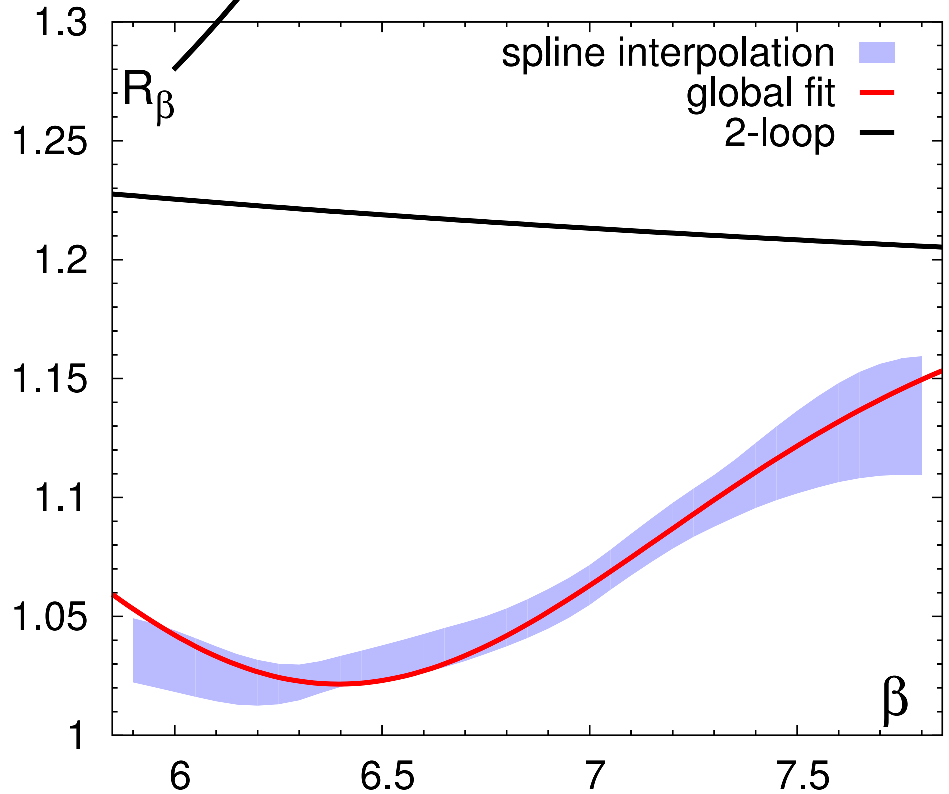
(*gluonic contribution*)

$$+ N_\tau^4 R_\beta R_m \left[\frac{2}{27} \left(\langle \bar{\psi}\psi \rangle_{l,\tau} - \langle \bar{\psi}\psi \rangle_{l,0} \right) + \left(\langle \bar{\psi}\psi \rangle_{s,\tau} - \langle \bar{\psi}\psi \rangle_{s,0} \right) \right]$$

(*fermionic contribution*)

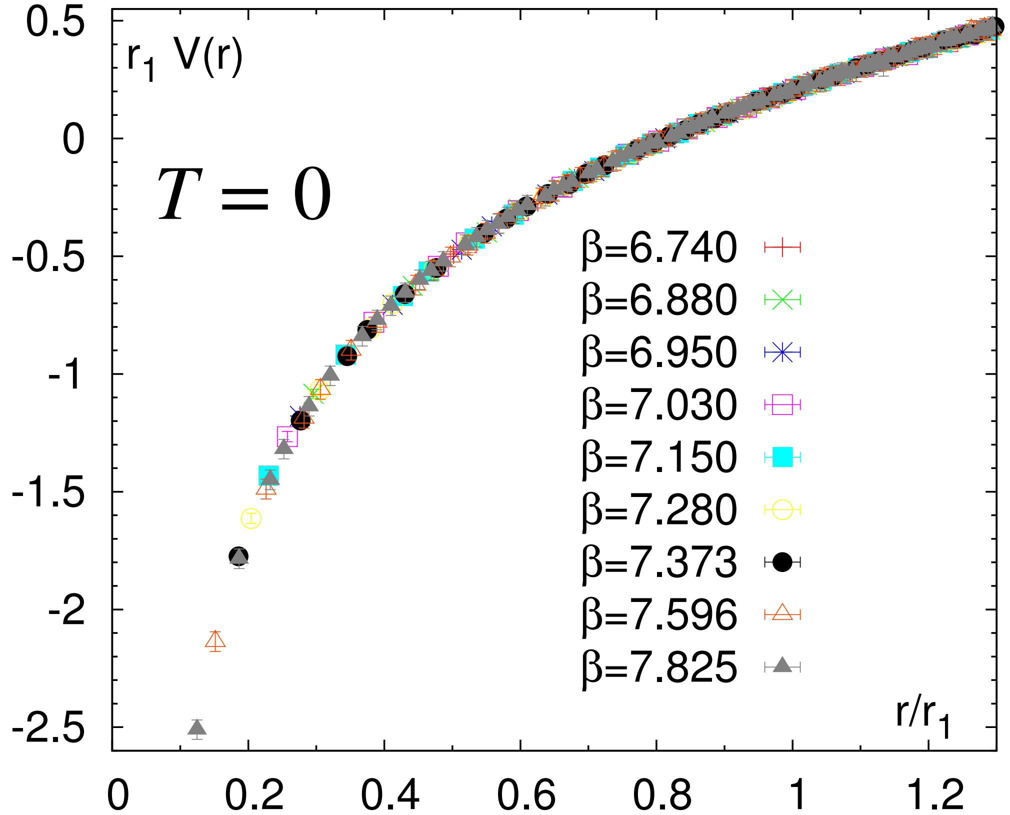
$$\left\langle \frac{1}{4} \mathrm{Tr} \left[M_l^{-1} \right] \right\rangle \qquad \left\langle \frac{1}{4} \mathrm{Tr} \left[M_s^{-1} \right] \right\rangle$$

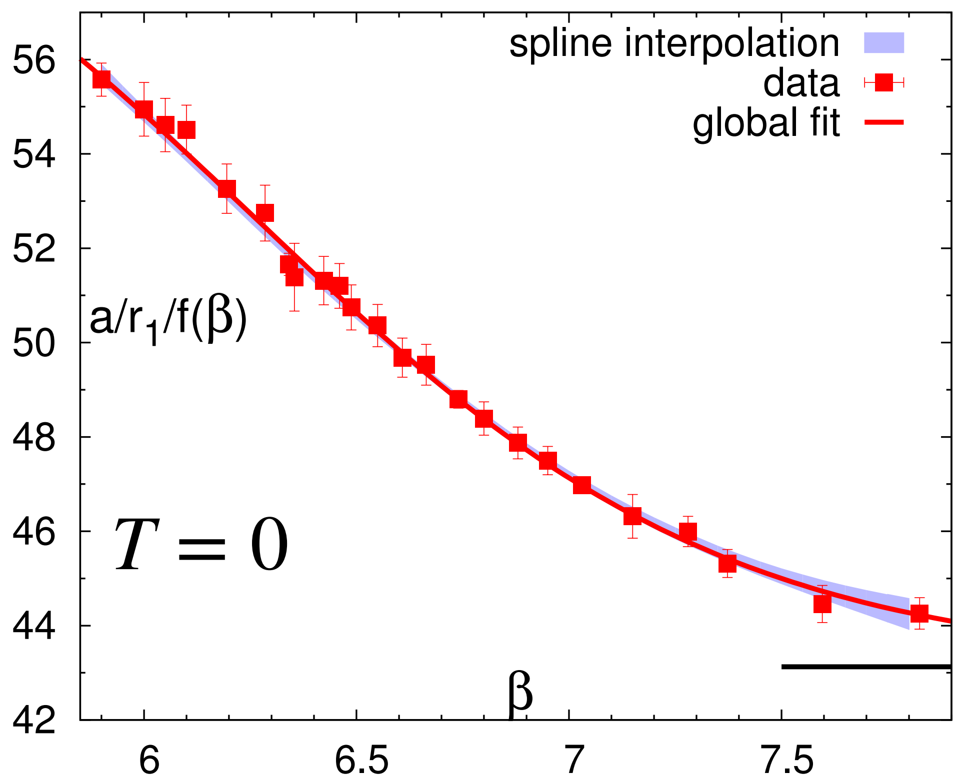
We use stochastic estimators to calculate the traces



[Bazavov et al. (HotQCD), PRD **90** (2014) 094503]

- For the 2014 HotQCD EoS we extracted R_β from the static quark potential





[Bazavov et al. (HotQCD), PRD **90** (2014) 094503]

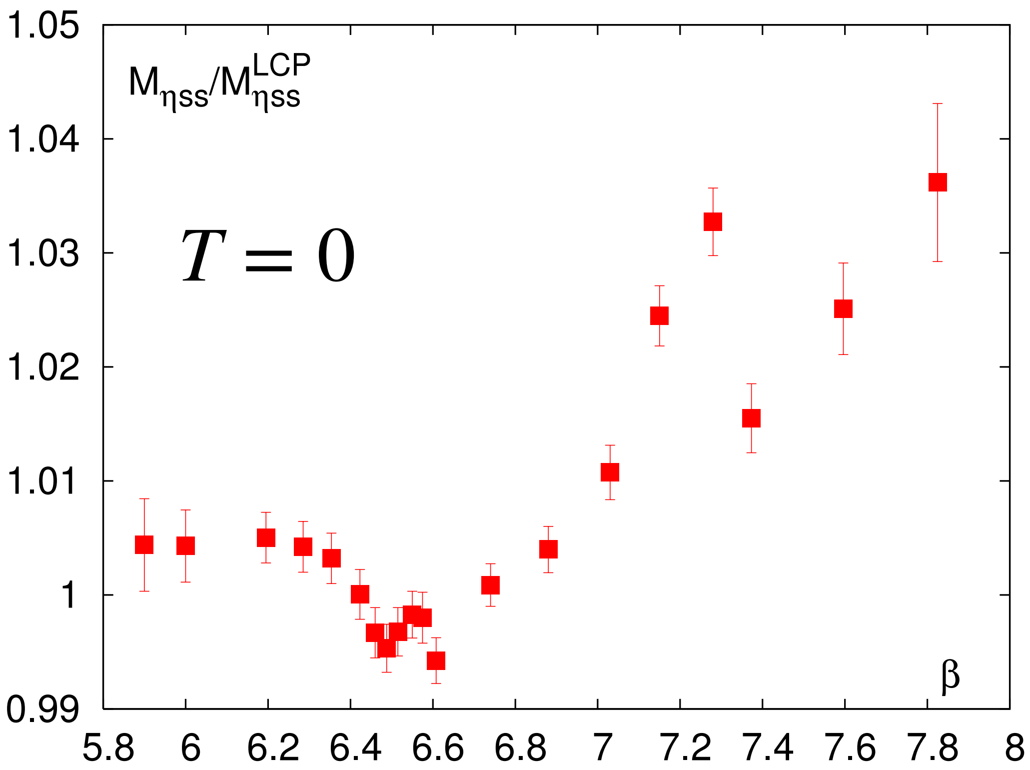
- The static quark potential shows almost no cut-off effects
- The scale r_1 is defined as

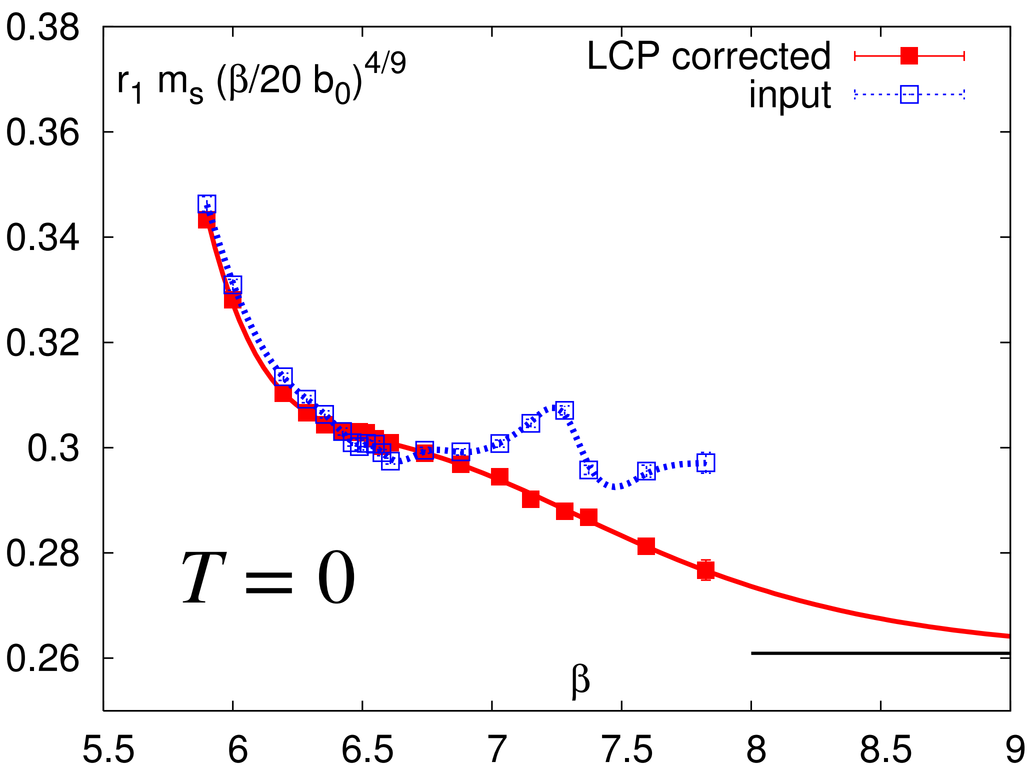
$$\left[r^2 \frac{\mathrm{d}}{\mathrm{d}r} V(r) \right]_{r=r_1} = 1$$

- The r_1-scale is indirectly determined by the spectrum of the $(\bar{c}c)$ and $(\bar{b}b)$ states. In physical units we have $r_1 = 0.3106$ fm
- We can write R_β as

$$R_\beta = -a\frac{\mathrm{d}\beta}{\mathrm{d}a} = \frac{r_1}{a}\left(\frac{\mathrm{d}(r_1/a)}{\mathrm{d}\beta}\right)^{-1}$$

- We extract R_β through fits/splines to $\dfrac{r_1 f(\beta)}{a}$, with $f(\beta)$ being the 2-loop perturbative β-function





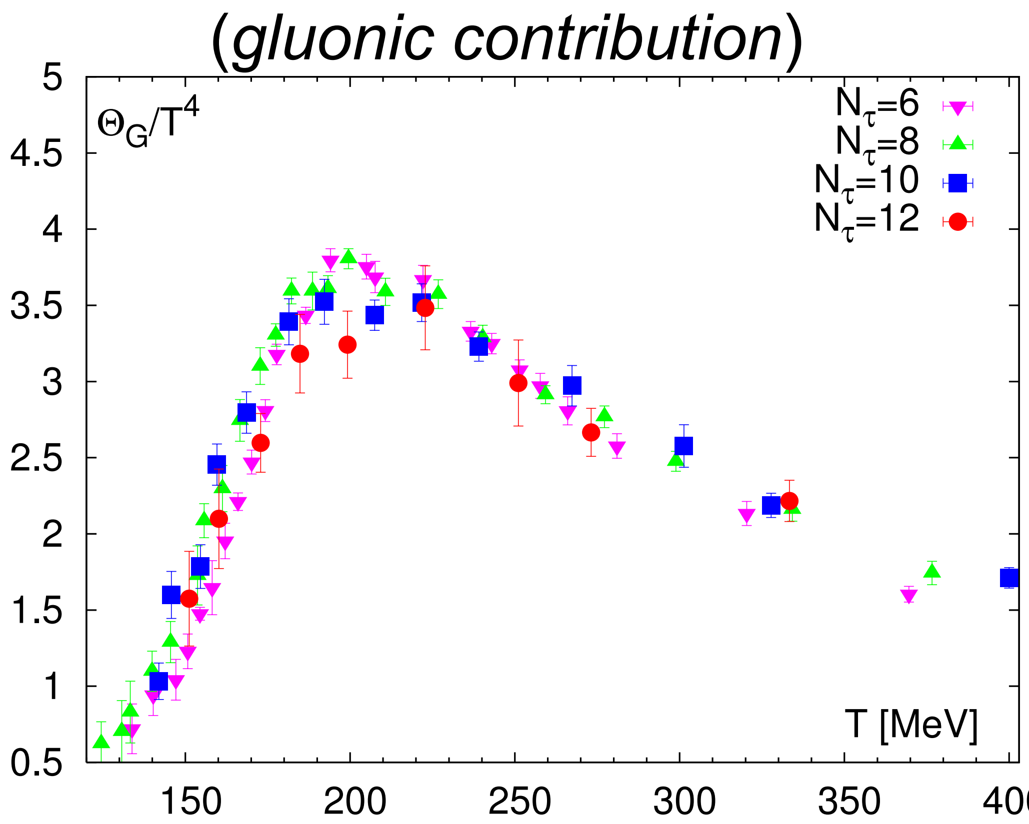
[Bazavov et al. (HotQCD), PRD **90** (2014) 094503]

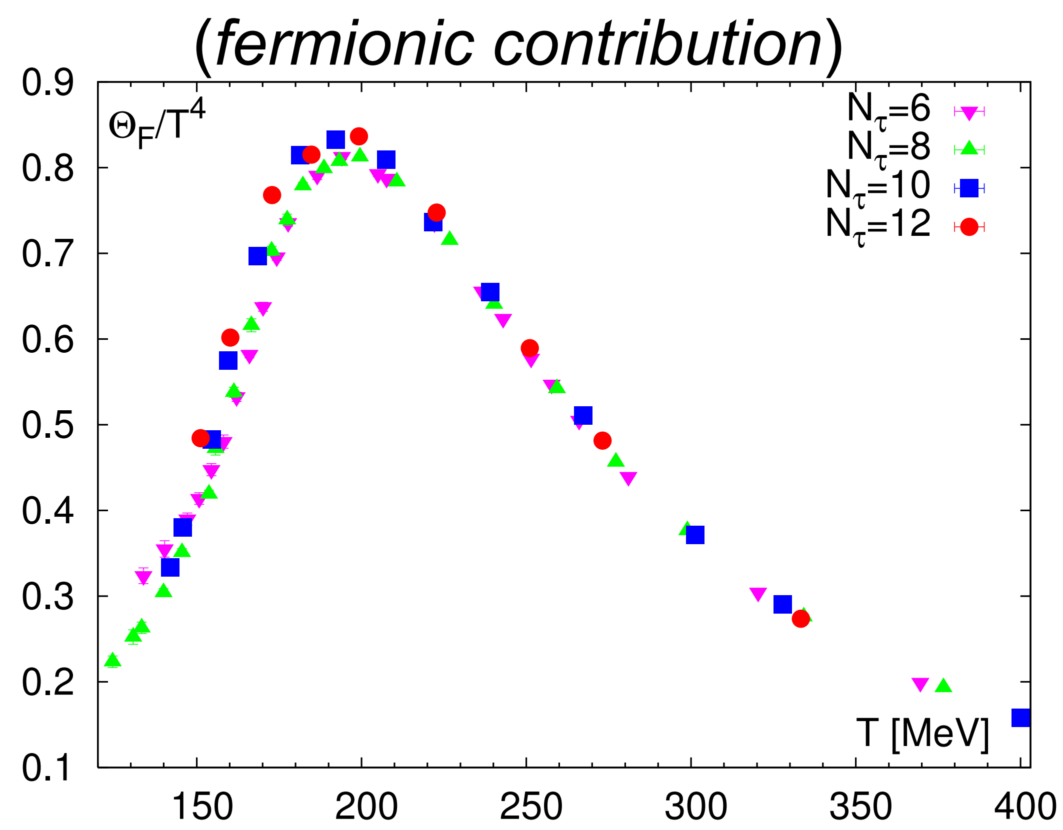
- We tune bare quark masses to keep the (un-mixed) $\eta_{\bar{s}s}$ meson constant
- Chiral perturbation theory predicts

$$m_{\eta_{\bar{s}s}} = \sqrt{2m_K^2 + m_\pi^2} = 686 \text{ MeV},$$

and a linear dependence of $m_{\eta_{\bar{s}s}}$ on m_s.

- We correct mistuned quark masses by LO chiral perturbation theory
- We calculate R_m by a fit to $r_1 m_s$
- We check the LCP also by calculating vector mesons $(\rho, K^\star, \phi)$ and pseudo scalar decay constants $(f_\pi, f_K, f_{\eta_{\bar{s}s}})$

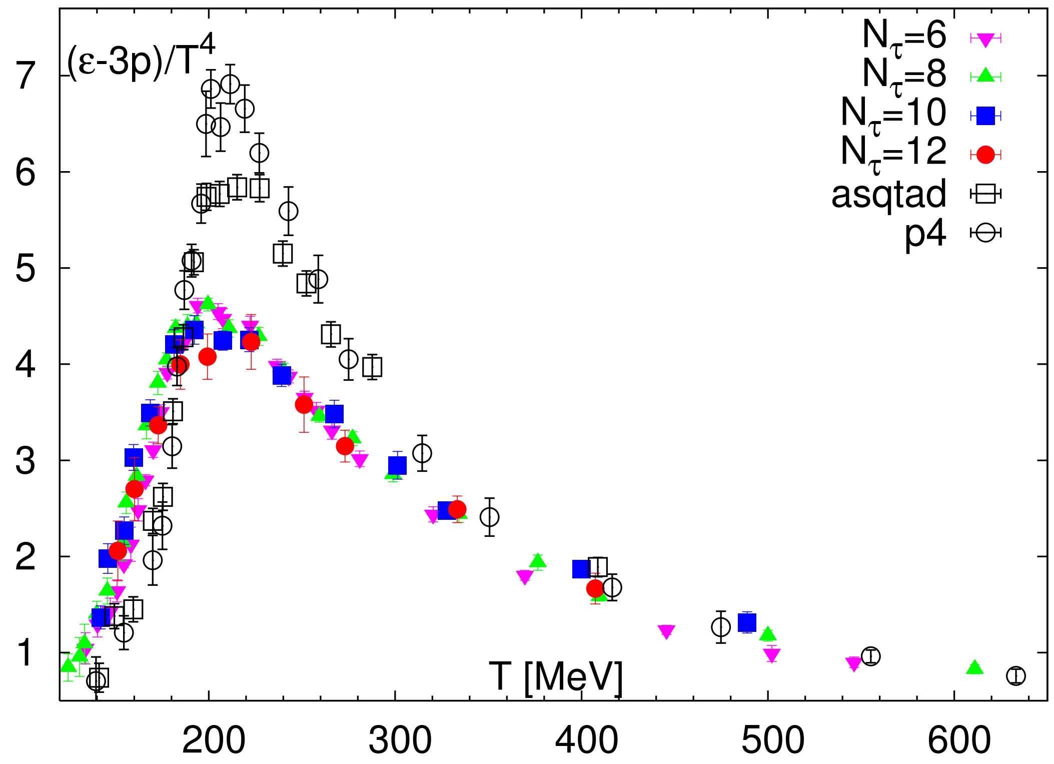




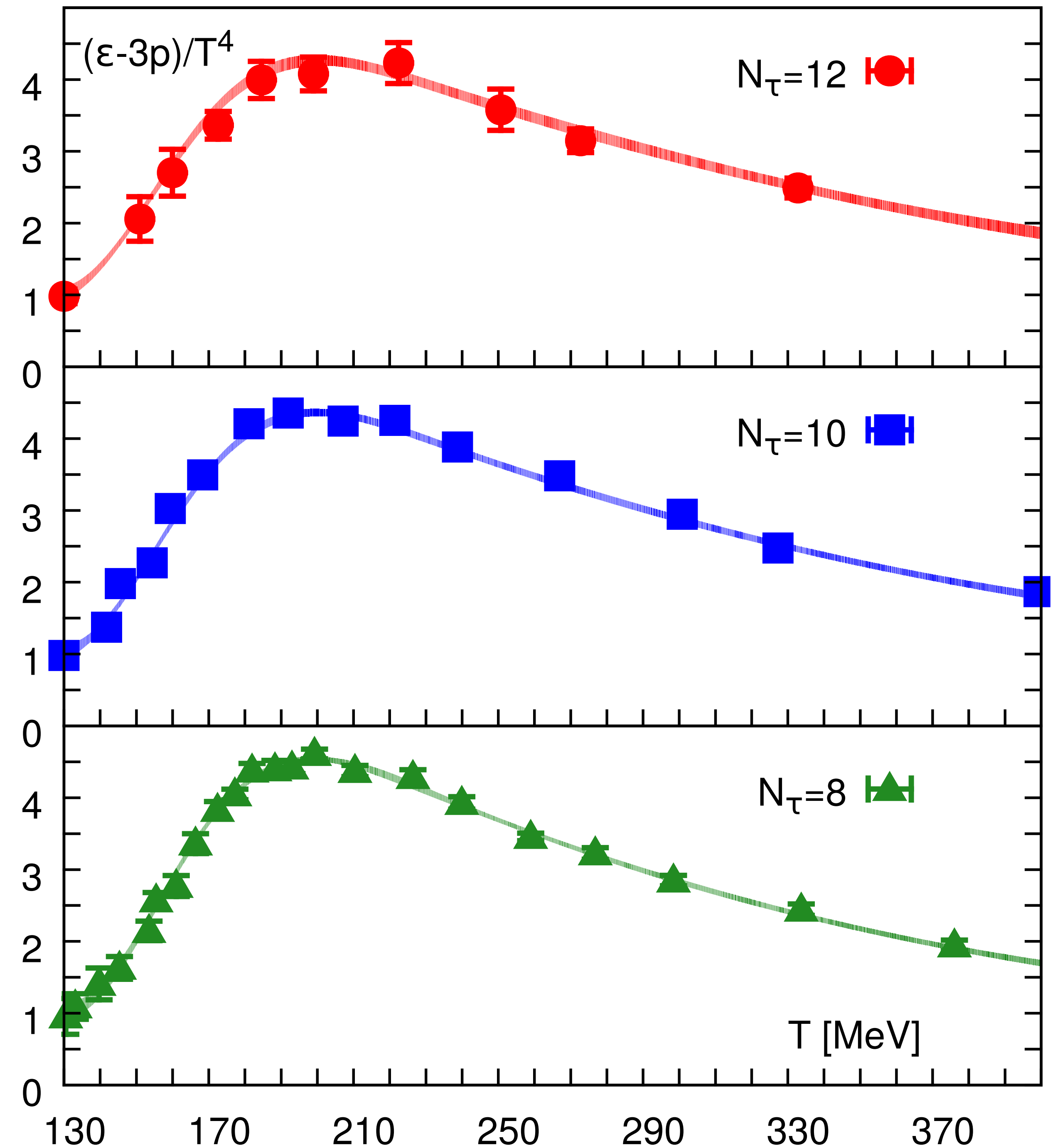
[Bazavov et al. (HotQCD), PRD **90** (2014) 094503]

- Simulations at $N_\tau = 6{,}8{,}10{,}12$, which corresponds to $a = 0.16,\ 0.12,\ 0.1,\ 0.08$ fm at $T = 200$ MeV.
- Used $\mathcal{O}(10^4)$ gauge field configurations per temperature value.
- Simulations are parallelized and are performed on leadership HPC-systems.
- Code for GPU-accelerated Clusters is available on GitHub https://github.com/LatticeQCD/SIMULATeQCD

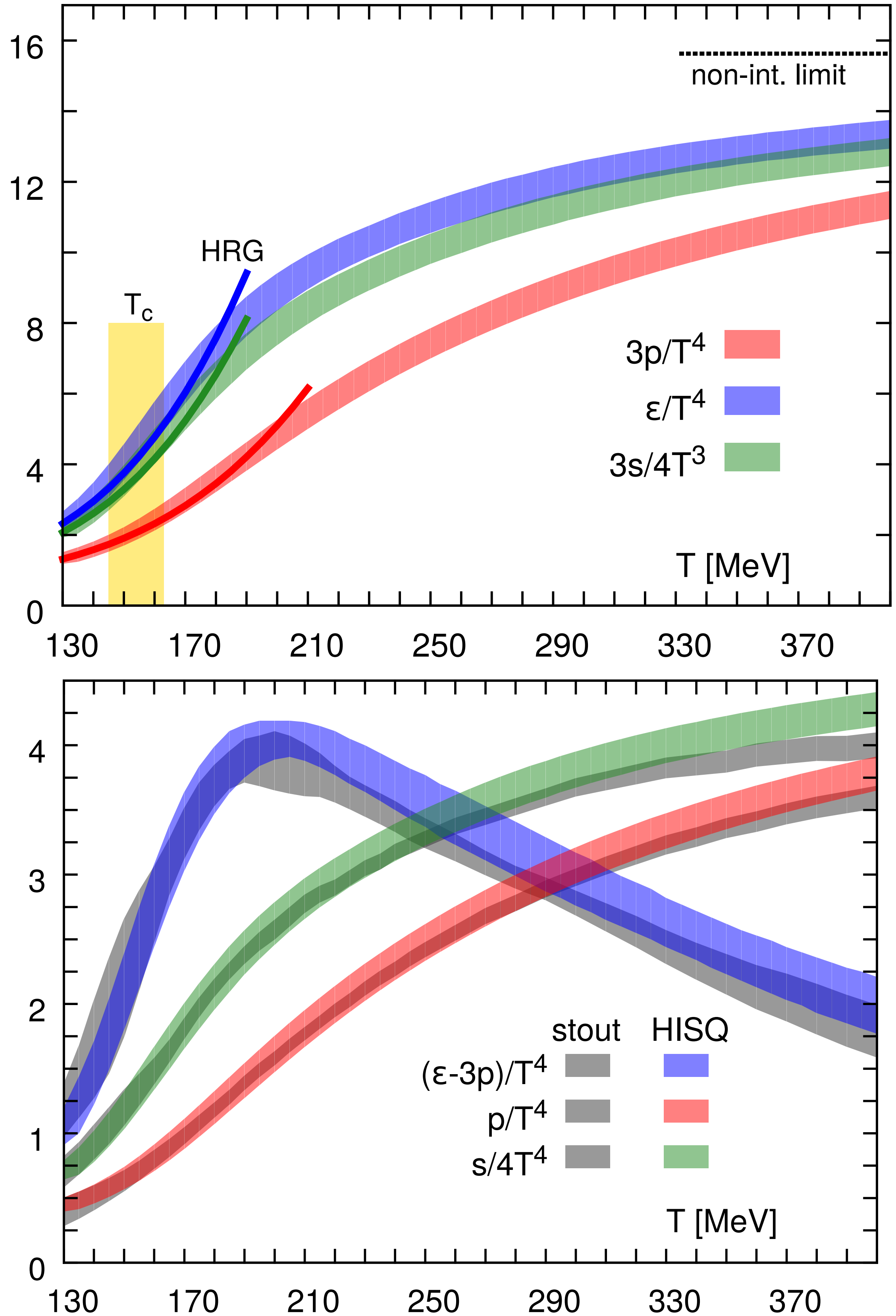
The continuum extrapolation



- Cut-off effects are much reduced compared to un-smeared actions
- Continuum extrapolations are done by N_τ-dependent spline fits with variable number and positions of knots
- For staggered fermions the cut-off effects are expected to be $(aT)^2 \sim (1/N_\tau)^2$



[Bazavov et al. (HotQCD), PRD **90** (2014) 094503]

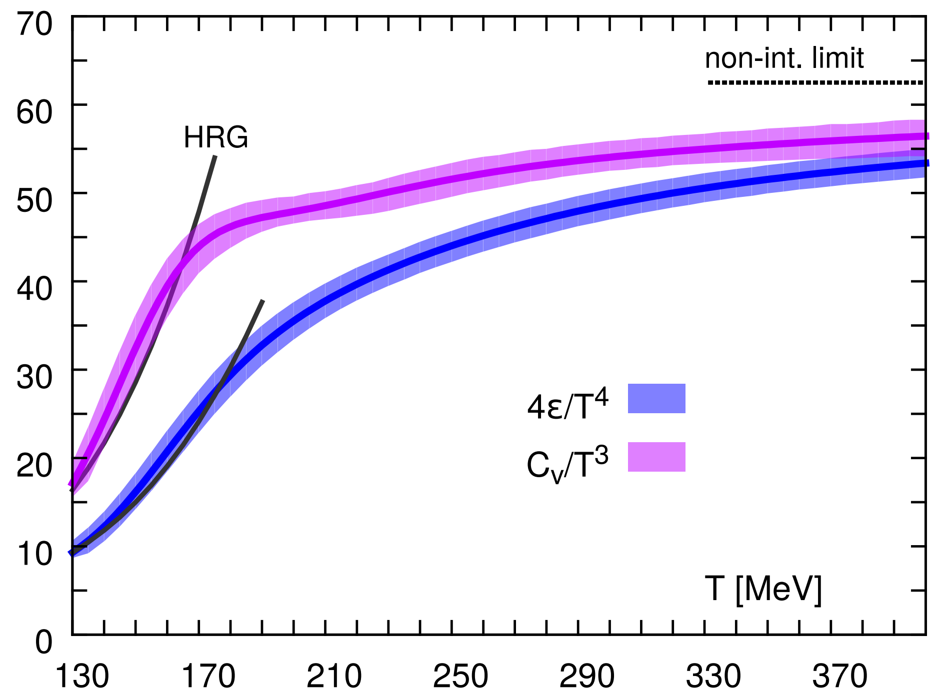


[Bazavov et al. (HotQCD), PRD **90** (2014) 094503]

Calculation of the pressure:

- Perform numerical integration of bootstrap samples of $\Theta_{\mu\mu}(T)$ between 130 and 400 MeV
- For the integration constant we choose $p_0/T_0^4 = 0.4391$ from HRG with a normal-distributed error of 10%
- From $(\epsilon - 3p)/T^4$ and p/T^4 we can get energy density ϵ/T^4 and entropy $s = (\epsilon + p)/T$
- We provide a parametrization of the EoS
- Results agree with the calculation of the Budapest-Wuppertal collaboration using the stout-action

[S. Borsanyi, et al. (BW) Phys.Lett. B370, 99 (2014), 1309.5258]

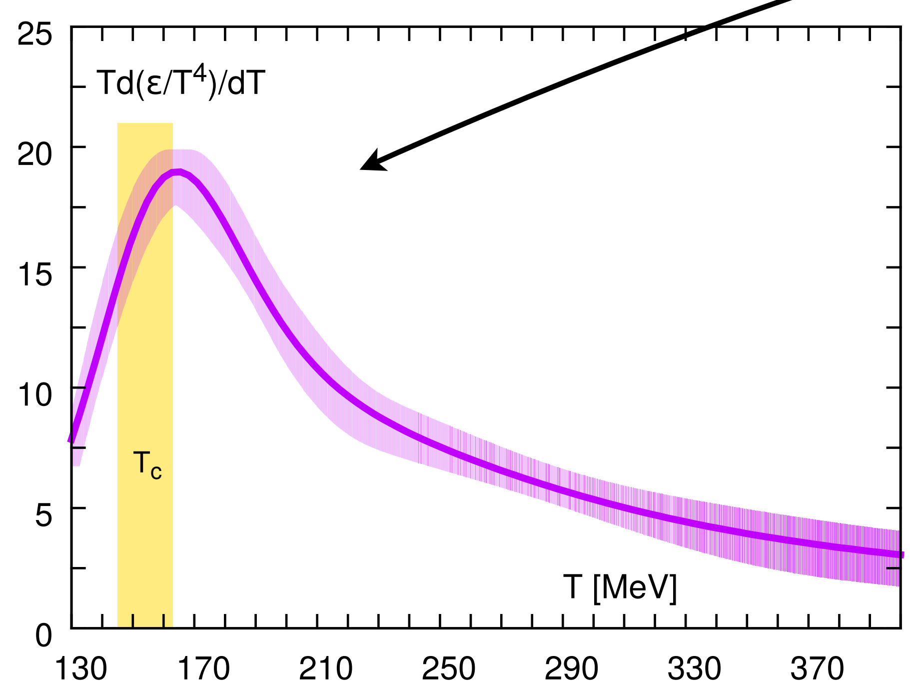


- Energy density should develop an infinite slope in the chiral limit $m_l \to 0$
- Specific heat should develop a cusp

$$C_V = \frac{\partial \epsilon}{\partial T}\bigg|_V = \left(4\frac{\epsilon}{T^4} + T\frac{\partial(\epsilon/T^4)}{\partial T}\bigg|_V\right)T^3$$

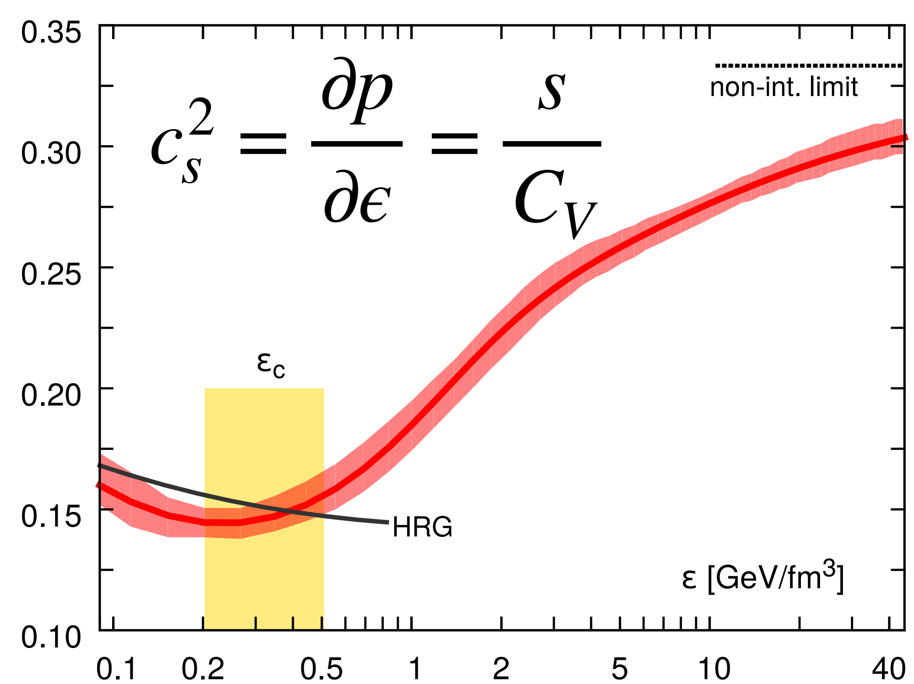
$$\underset{m_l \to 0}{\sim} \quad c_0 + \frac{A_\pm}{\alpha}\left|\frac{T-T_c}{T_c}\right|^\alpha + \mathcal{O}(T-T_c)$$

$$\alpha \approx -0.21$$



Dominating singular part of the specific heat

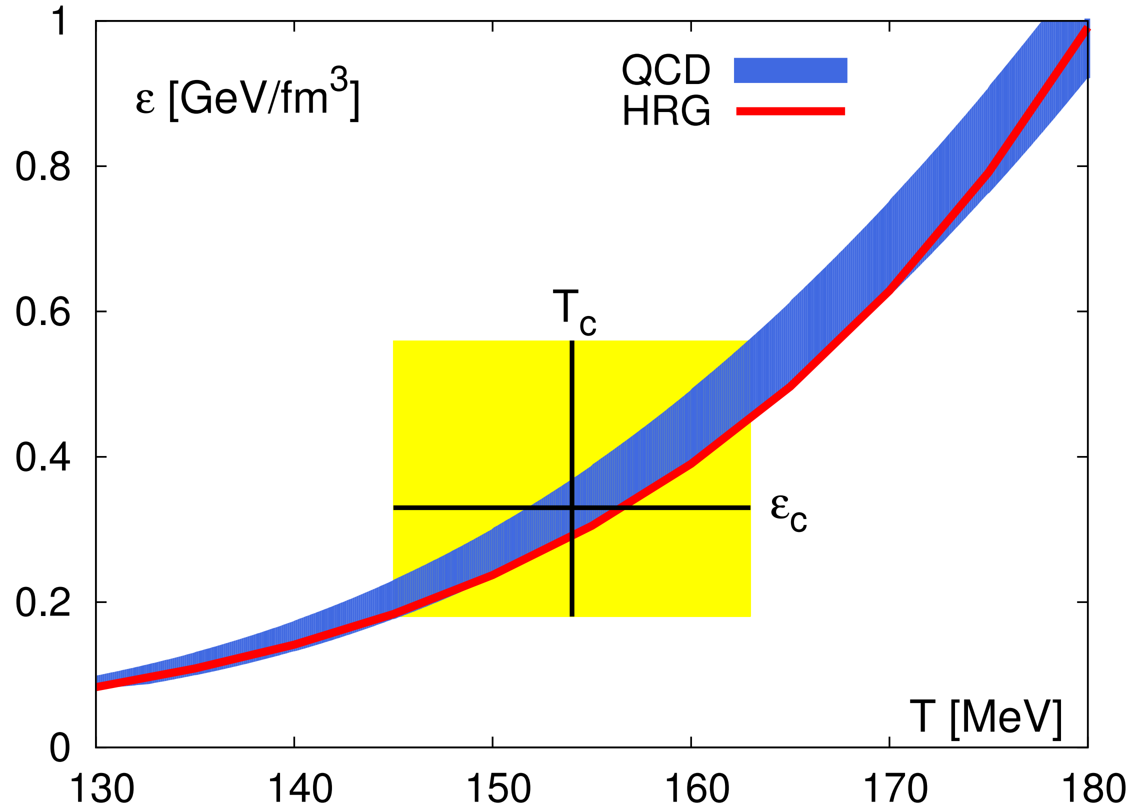
- The speed of sound



- Find softest point at

$$\left(c_s^2\right)_{\text{min}} \approx \frac{1}{2}\left(c_s^2\right)_{\text{free}}$$

[Bazavov et al. (HotQCD), PRD **90** (2014) 094503]



[Ding, Karsch, Mukherjee, Int.J.Mod.Phys.E **24** (2015) 10, 1530007]

- Temperature and energy density at the crossover

$$T_{pc} = (156 \pm 1.5)\text{ MeV}$$

$$\epsilon_{pc} = \left(0.35 \pm 0.08\right)\text{ GeV/fm}^3$$

- Referenz values

$$\epsilon_{\text{(nucl. mat.)}} \simeq 0.15\text{ GeV/fm}^3$$

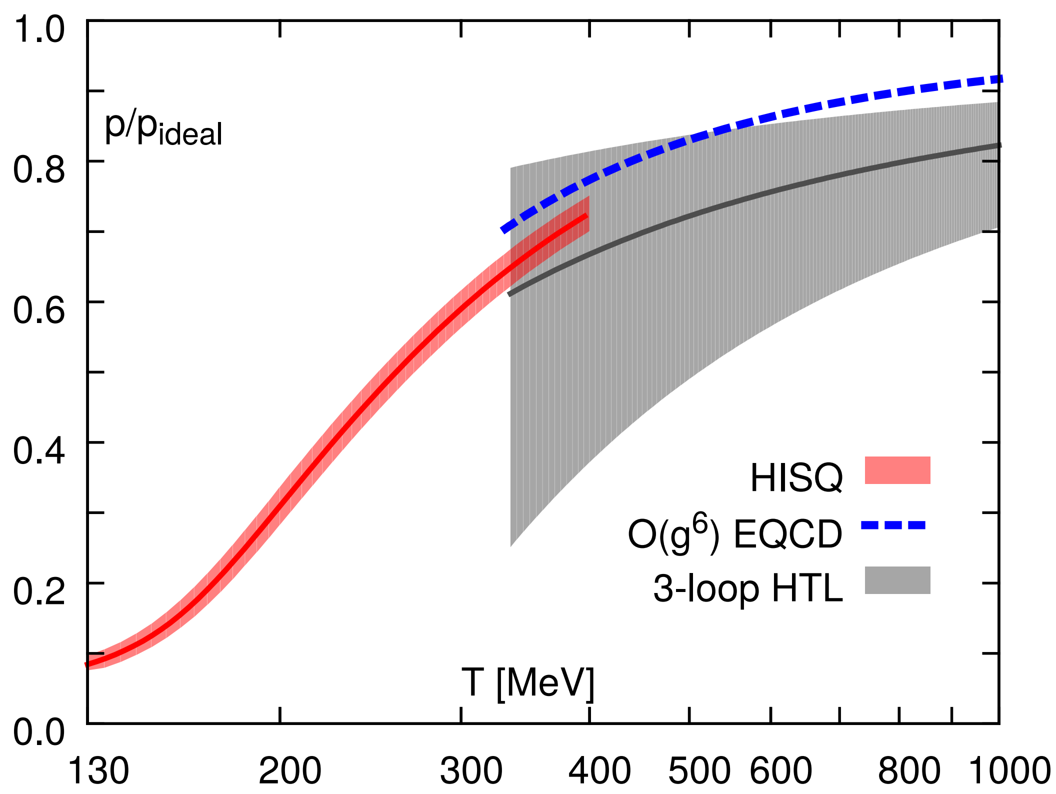
$$\epsilon_{\text{(nucleon)}} \simeq 0.45\text{ GeV/fm}^3$$

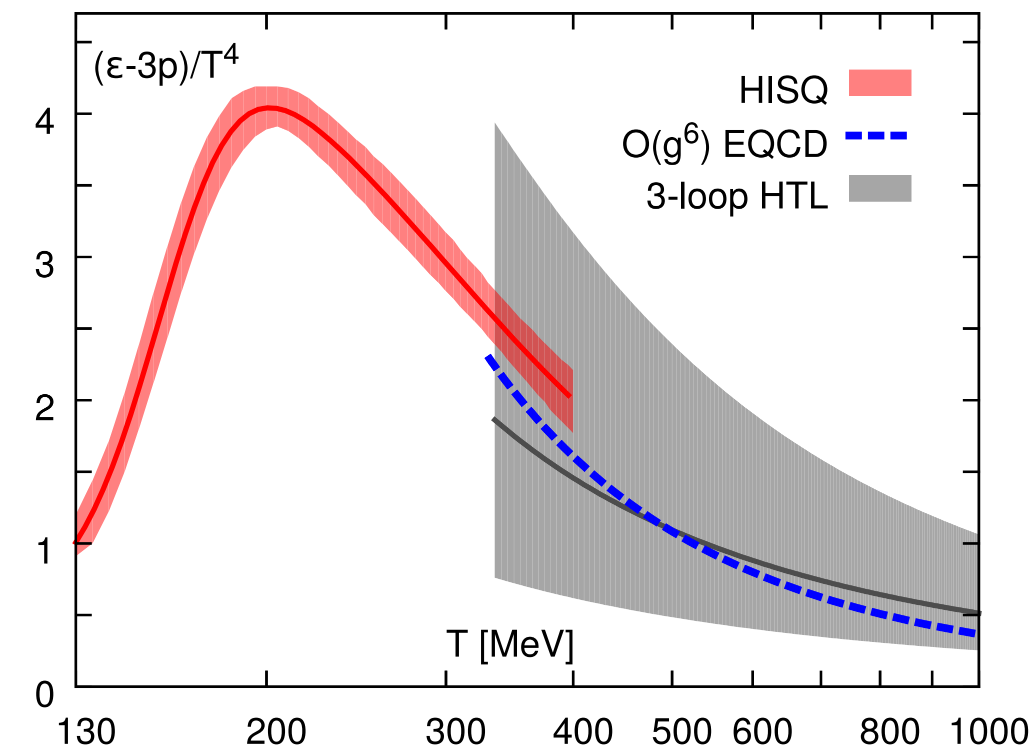
- Dense packing of spheres (DPS)

$$\epsilon_{\text{(DPS)}} \simeq 0.74 \times \epsilon_{\text{(nucleon)}}$$

$$\simeq 0.33\text{ GeV/fm}^3$$

- Overlapping nucleons = QGP??





- In principle perturbation theory should work for $T \gg \Lambda_{QCD}$
- The perturbative regime breaks down at $\mathcal{O}(g^6)$ (Linde Problem)
- At $g \ll 1$ there is a clear separation of scales $m_{\text{mag}} \sim g^2 T \ll m_{\text{elec}} \sim gT \ll m_{\text{hard}} \sim \pi T$
- After integrating out the scale πT we arrive at eQCD
- Another resummation scheme is the Hard Thermal Loop (HTL) resummation
- We obtain reasonable agreement with both schemes at $T \simeq 400$ MeV

Cumulants of Conserved Charge Fluctuations

$$\frac{p}{T^4} = \frac{\ln Z}{T^3 V} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi_{ijk,0}^{BQS} \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$

Gavai, Gupta (2001)
Bielefeld-Swansea (2002)

Cumulants of conserved charge fluctuations, can also be measured as event-by-event fluctuations in heavy ion collisions

$$\chi_{ijk,0}^{BQS} = \frac{\partial^i}{\partial(\mu_B/T)} \frac{\partial^j}{\partial(\mu_Q/T)} \frac{\partial^k}{\partial(\mu_S/T)} \frac{\ln Z}{T^3 V}$$

- Compare with HRG model calculation
- Compare with measurements at RHIC and LHC
- Investigate critical behaviour

- The chemical potential is introduced as the fourth component of a vector potential

$$U_4(x) \rightarrow U_\mu(x) e^{a\mu}$$

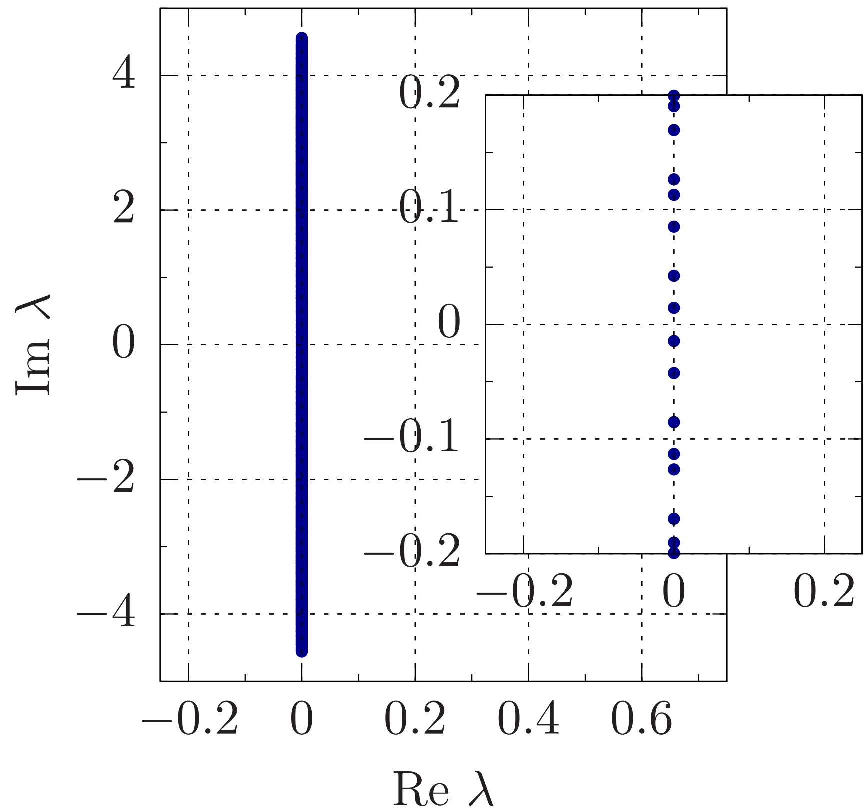
$$U_4^\dagger(x) \rightarrow U_4^\dagger(x) e^{-a\mu}$$

[Hasenfratz, Karsch, Phys.Lett.B 125 (1983) 308]

- Determinant becomes complex for $\mu > 0$. $\longrightarrow$ MCMC does not work anymore!

$$\mu = 0$$

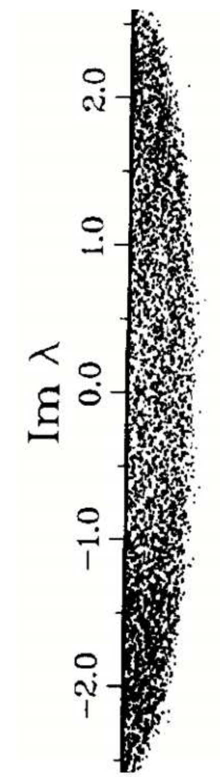
$$\gamma_5 D \gamma_5 = D^\dagger$$



[Jäger, de Forcrand, *PoS* LATTICE2018 (2018) 178]

$$\mu > 0$$

$$\gamma_5 D(\mu) \gamma_5 = D^\dagger(\mu^*)$$



[Barbour et. al, *Nucl.Phys.B* 275 (1986) 296]

The (2+1)-flavor partition function depends on the quark chemical potentials

$$Z(T,V,\hat{\mu}_u,\hat{\mu}_d,\hat{\mu}_s) = \int \mathscr{D}U \, e^{Tr \ln M_u(\hat{\mu}_u)} \, e^{Tr \ln M_d(\hat{\mu}_d)} \, e^{Tr \ln M_s(\hat{\mu}_s)} \, e^{-\beta S_G}$$

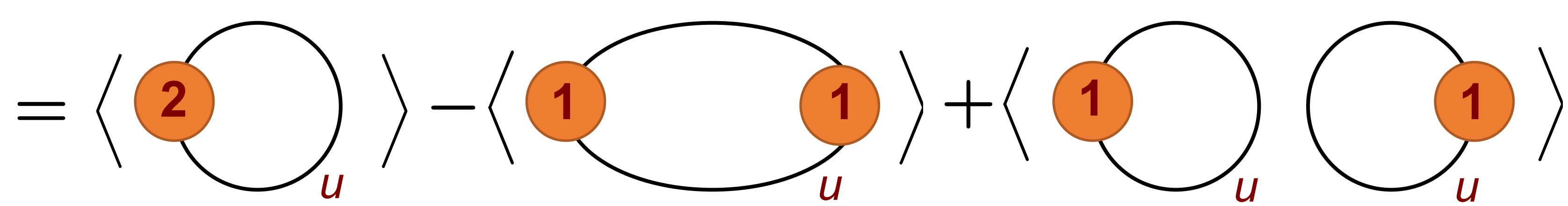
Aim: express the pressure (thermodynamic potential) as Taylor series in μ

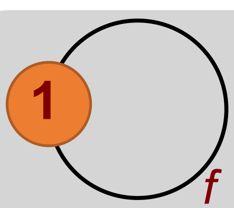
$$\frac{p(\vec{\mu},T)}{T^4} = \frac{\ln Z(\vec{\mu},T)}{T^3 V} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi_{ijk}^{uds}(T) \left(\frac{\mu_u}{T}\right)^i \left(\frac{\mu_d}{T}\right)^j \left(\frac{\mu_s}{T}\right)^k$$

Interpretation:

$$\chi_{200}^{uds} = \frac{\partial^2}{\partial(\mu_u/T)^2}\left(\frac{\ln Z}{T^3 V}\right) = \left\langle D_2^u \right\rangle + \left\langle \left(D_1^u\right)^2 \right\rangle$$

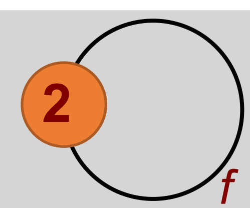
$$= \left\langle \mathrm{Tr}\left[M_u^{-1} M_u^{(2)}\right] \right\rangle - \left\langle \mathrm{Tr}\left[M_u^{-1} M_u^{(1)} M_u^{-1} M_u^{(1)}\right] \right\rangle + \left\langle \mathrm{Tr}\left[M_u^{-1} M_u^{(1)}\right] \mathrm{Tr}\left[M_u^{-1} M_u^{(1)}\right] \right\rangle$$





$$= \left[M_f^{-1} M_f^{(1)}\right]_{xx}$$

≙ local f-quark density



$$= \left[M_f^{-1} M_f^{(2)}\right]_{xx}$$

≙ un-physical contact term

Random noise method:

- Choose a number of random vectors $\eta^{(k)}$ with
- The trace of a matrix A is approximated as

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k}^{N} \eta_i^{(k)} \cdot \eta_j^{(k)} = \delta_{ij}$$

$$\mathrm{Tr}\, A \approx \frac{1}{N} \sum_{k}^{N} \eta^{(k)\dagger} A\, \eta^{(k)}$$

$$\mathrm{std}\, [\mathrm{Tr}\, A] \sim \frac{1}{\sqrt{N}}$$

⇒ $A := M^{-1}$: matrix inversion can be reduced to a linear problem $Mx = \eta$.

Unbiased estimators:

- Need unbiased estimators for powers of traces: $(\mathrm{Tr}\ A)^m$

$$(\mathrm{Tr}\, A)^m \approx \frac{1}{N} \sum_{k_1 \neq k_2, \cdots \neq k_m} \left(\eta^{(k_1)\dagger} A\, \eta^{(k_1)}\right) \cdot \left(\eta^{(k_2)\dagger} A\, \eta^{(k_2)}\right) \cdots \left(\eta^{(k_m)\dagger} A\, \eta^{(k_m)}\right)$$

⇒ we need at least m random vectors, more might be necessary to improve precision

(signal to noise ratio can be quite low)

⇒ we have developed an efficient recursive method to calculate unbiased estimators

[Mitra, Hegde, CS, arXiv:2205.08517 [hep-lat]]

Hadronic fluctuations:

- Convert quark number fluctuations χ_{ijk}^{uds} to fluctuation of hadronic charges χ_{ijk}^{BQS}, e.g., we have

$$\chi_{200}^{BQS} = \frac{\partial}{\partial \hat{\mu}_B} \frac{\ln Z}{VT^3} = \frac{1}{9}\left(\frac{\partial}{\partial \hat{\mu}_u} + \frac{\partial}{\partial \hat{\mu}_d} + \frac{\partial}{\partial \hat{\mu}_s}\right)^2 \frac{\ln Z}{VT^3} = \chi_{200}^{uds} + \chi_{020}^{uds} + \chi_{002}^{uds} + \chi_{110}^{uds} + \chi_{101}^{uds} + \chi_{011}^{uds}$$

Constraints:

- We can also reorganize the expansion in μ_B, μ_Q, μ_S to incorporate up to two constraints, e.g.

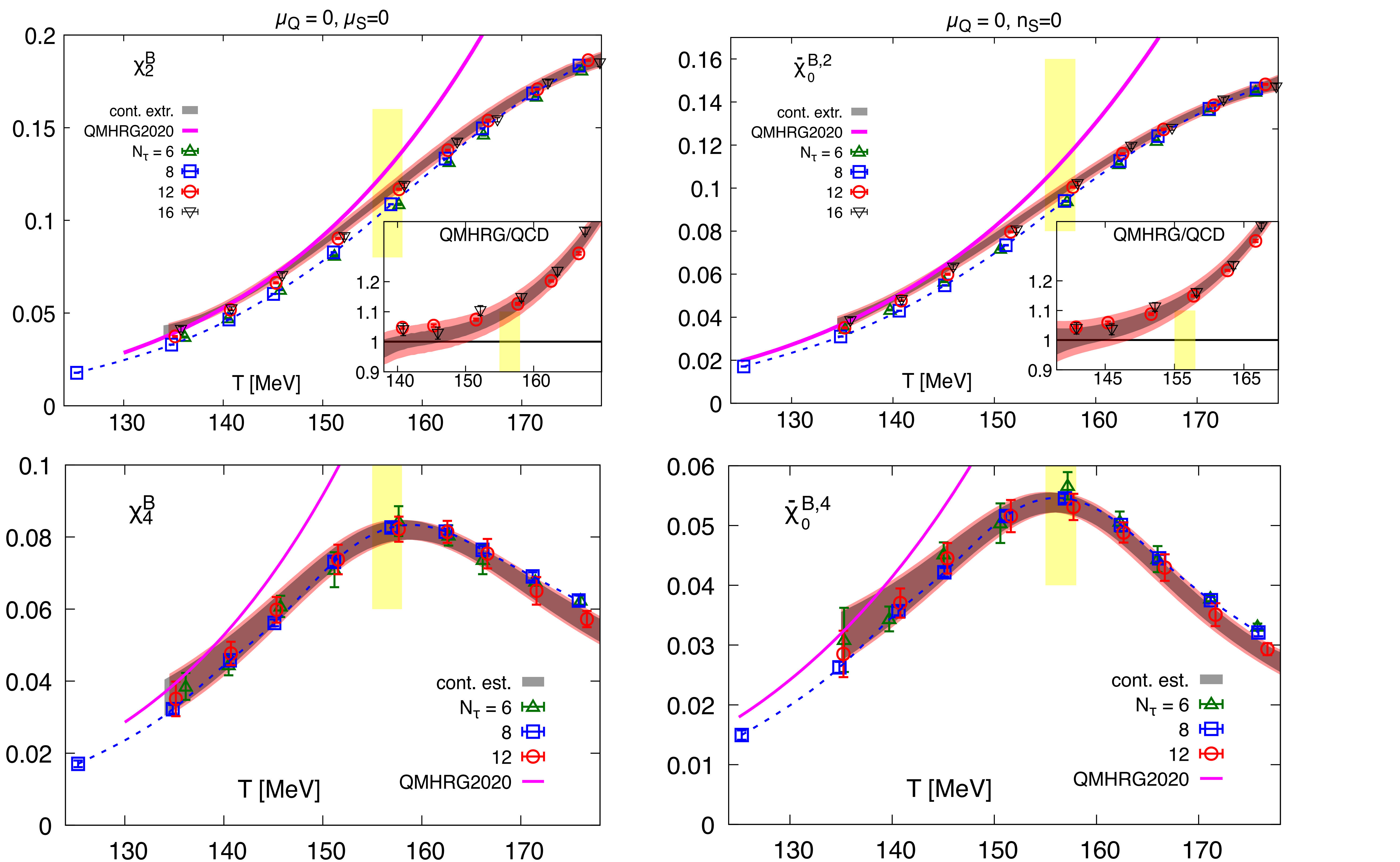
$$\frac{p}{T^4}\left[T, \hat{\mu}_B, \hat{\mu}_Q, \hat{\mu}_S\right] = \frac{p}{T^4}\left[T, \hat{\mu}_B, \hat{\mu}_Q(\hat{\mu}_B), \hat{\mu}_S(\hat{\mu}_B)\right] \equiv \sum_k \frac{1}{(2k)!} \tilde{\chi}_{2k}^{B} \hat{\mu}_B^{2k}$$ with

new expansion coefficients

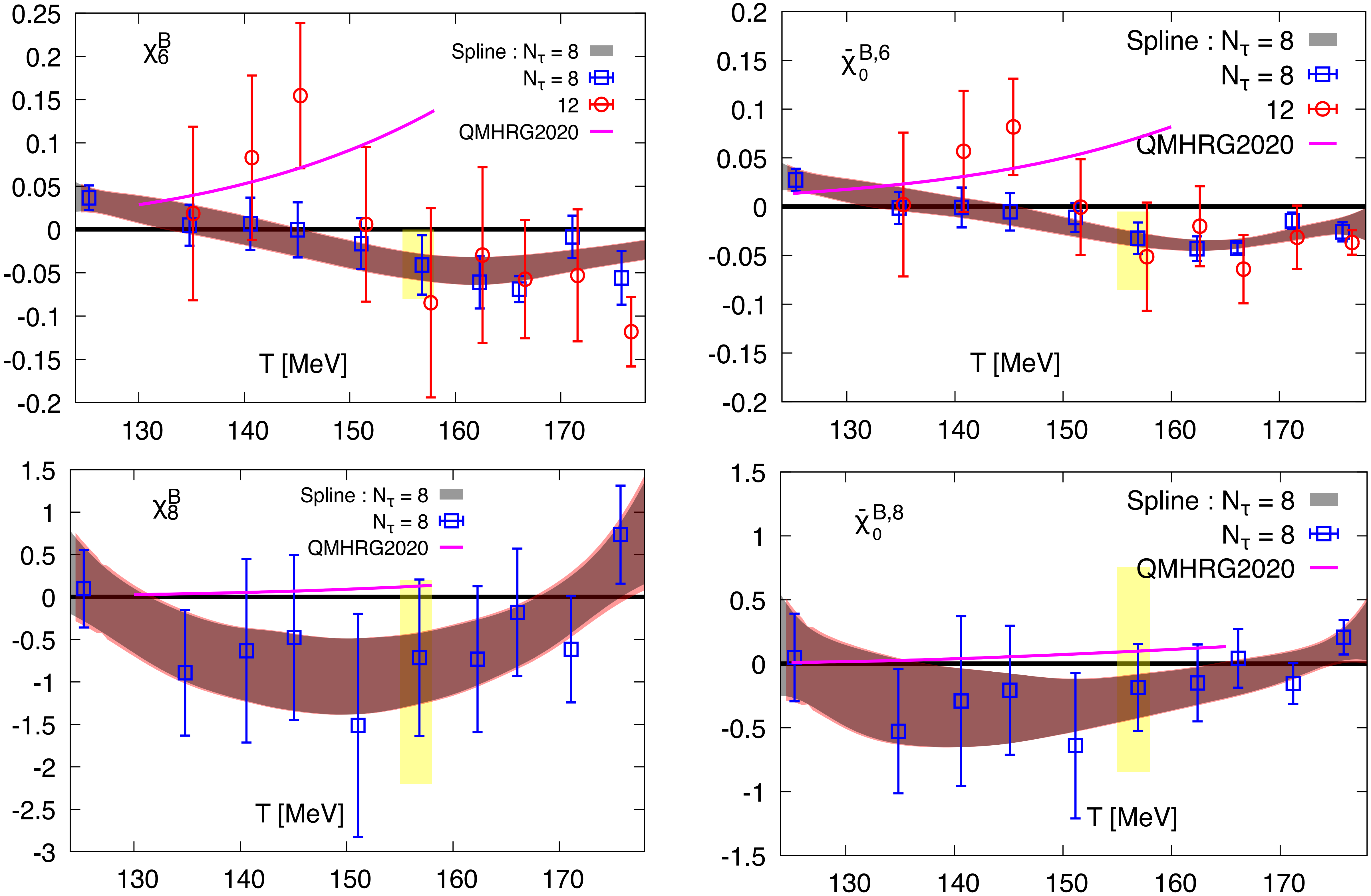
$$\hat{\mu}_Q(\hat{\mu}_B) = q_1 \hat{\mu}_B + q_3 \hat{\mu}_B^3 + \cdots$$
$$\hat{\mu}_S(\hat{\mu}_B) = s_1 \hat{\mu}_B + s_3 \hat{\mu}_B^3 + \cdots$$

Where q_i, s_i are determined such that $n_Q/n_B = 0.4$ and $n_S = 0$ (order by order)

Baryon number cumulants

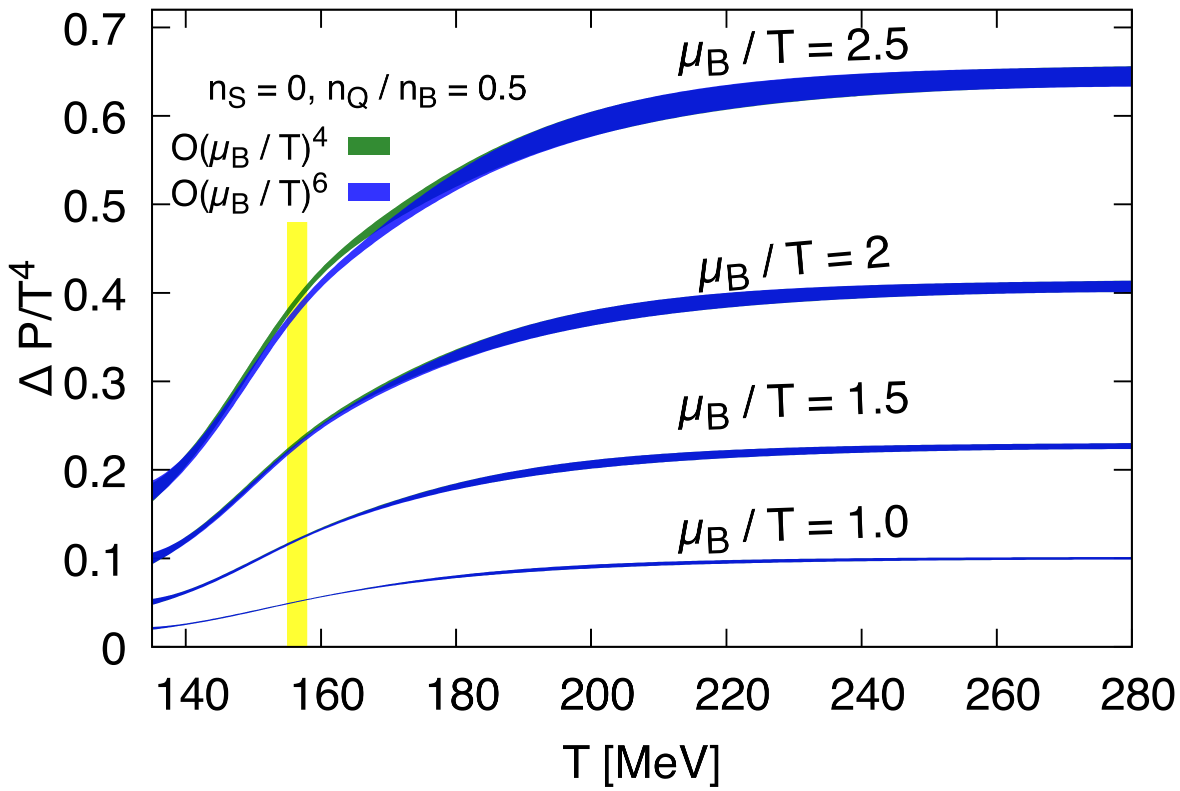


Baryon number cumulants



- Corrections to the pressure due to finite μ_B

$$\Delta\hat{p} \equiv \frac{p(T,\mu_B)}{T^4} - \frac{p(T,0)}{T^4} = \sum_{k=1}^{\infty} P_{2k}(T)\hat{\mu}_B^{2k}$$



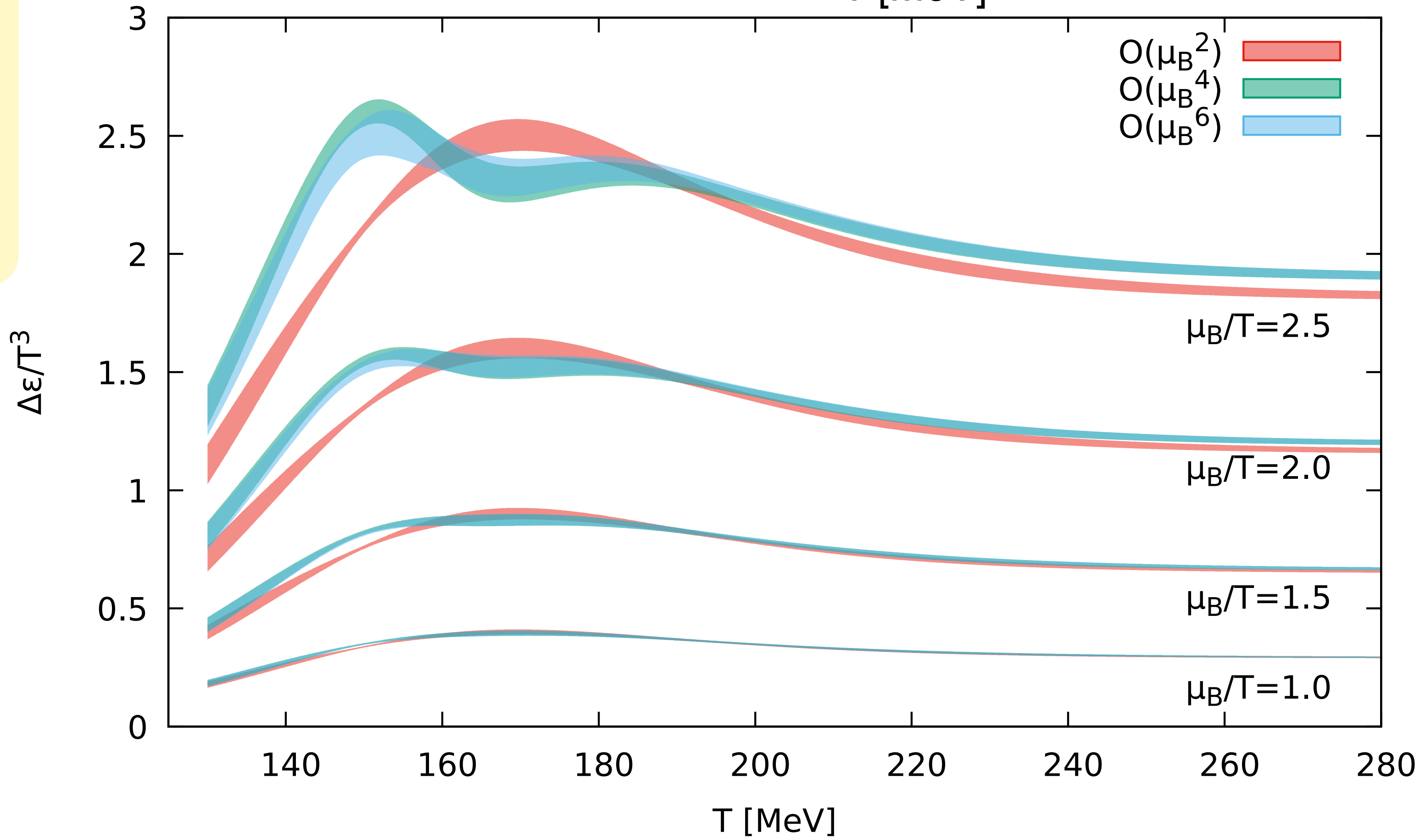
- From $\Delta\hat{p}$ we can compute $\Delta\hat{\epsilon}$:

energy density at finite μ_B

$$\hat{\epsilon} = \frac{1}{VT^3} T \frac{\partial \ln Z(T,V,\hat{\mu}_B,\hat{\mu}_Q,\hat{\mu}_S)}{\partial T} = 3\hat{p} + T\frac{\partial \hat{p}}{\partial T}$$

$$\Delta\hat{\epsilon} \equiv \frac{\epsilon(T,\mu_B)}{T^4} - \frac{\epsilon(T,0)}{T^4} = \sum_{k=1}^{\infty} \epsilon_{2k}(T)\hat{\mu}_B^{2k} ,$$

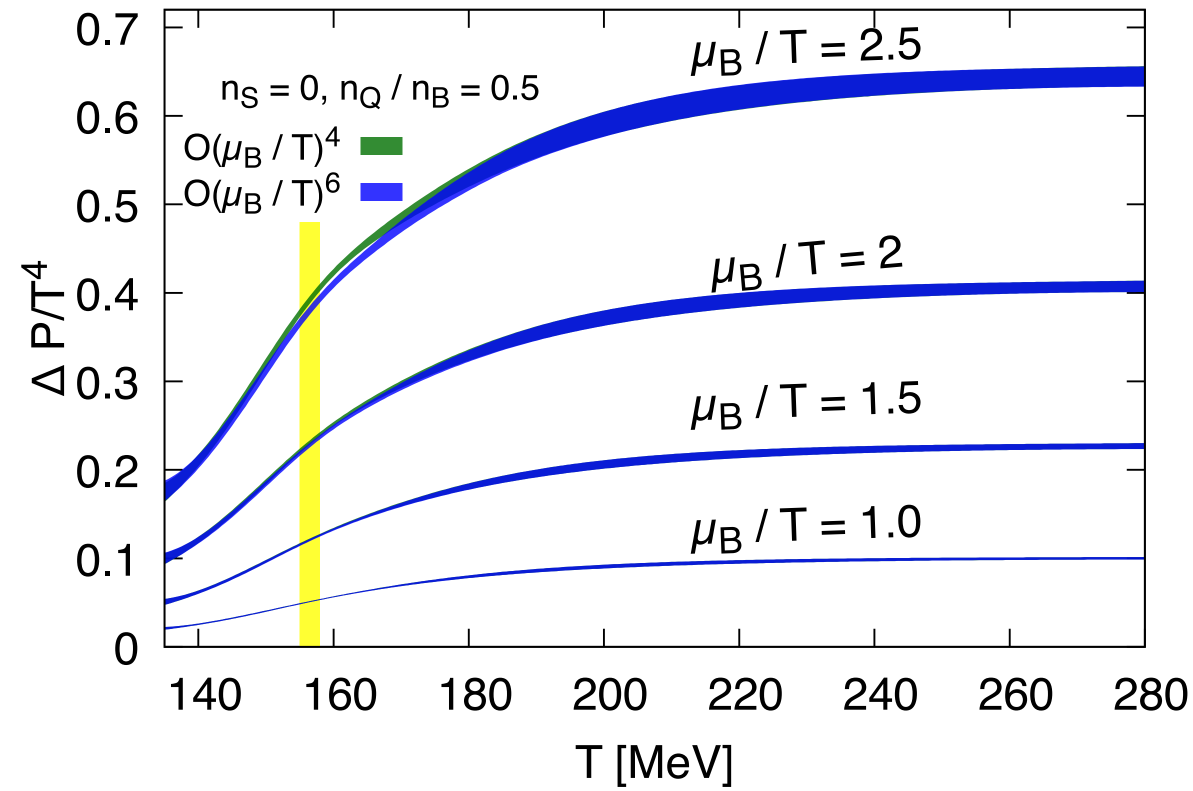
[A. Bazavov et al., HotQCD, PRD 95 (2017) 054504]



[D. Bollweg, QM2022; HotQCD in preparation]

- Corrections to the pressure due to finite μ_B

$$\Delta\hat{p} \equiv \frac{p(T,\mu_B)}{T^4} - \frac{p(T,0)}{T^4} = \sum_{k=1}^{\infty} P_{2k}(T)\hat{\mu}_B^{2k}$$



- From $\Delta\hat{p}$ and $\Delta\hat{\epsilon}$ we can compute $\Delta\hat{s}$:

  entropy density at finite μ_B

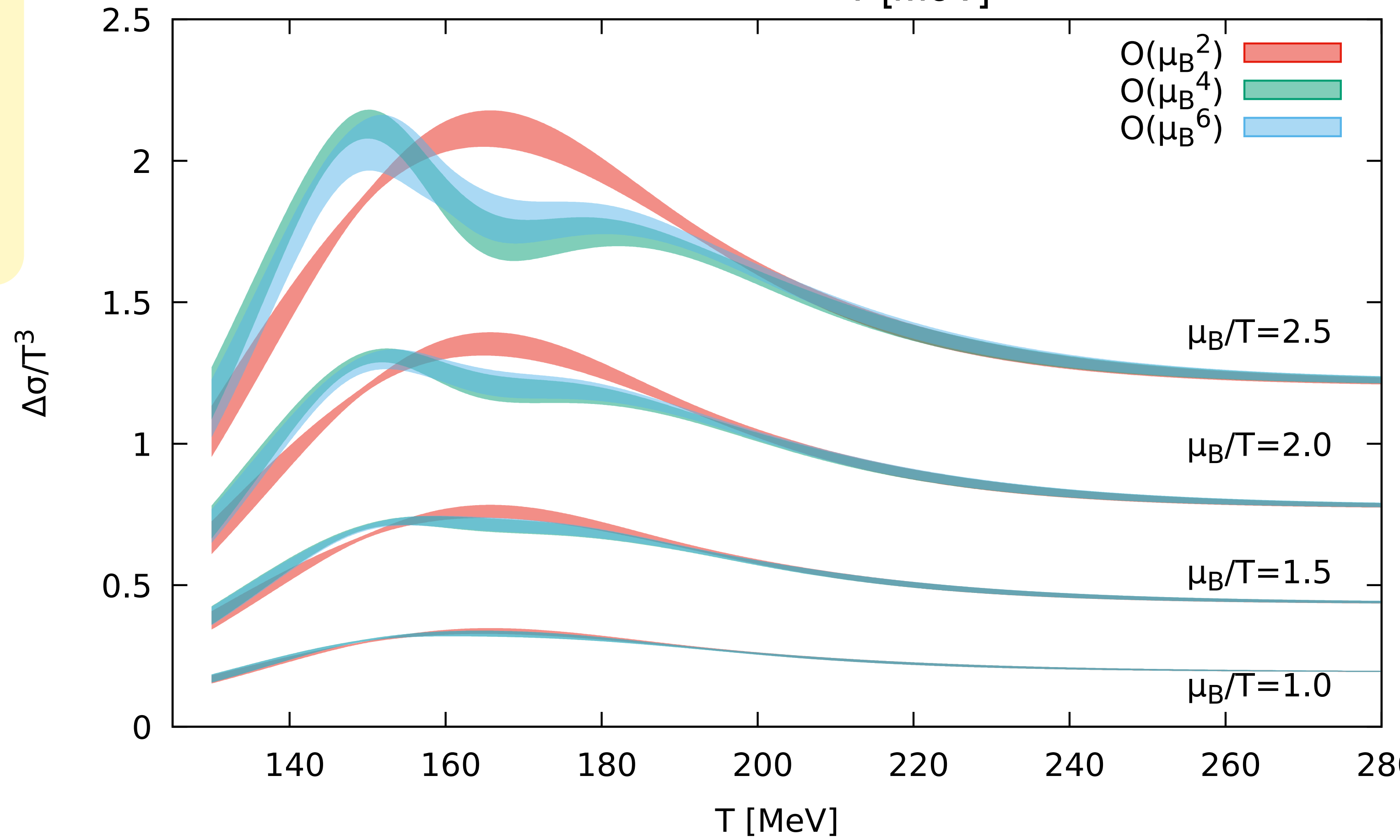
$$\hat{s} = \hat{\epsilon} + \hat{p} - \hat{\mu}_B\hat{n}_B - \hat{\mu}_Q\hat{n}_Q - \hat{\mu}_S\hat{n}_S$$

$$= \hat{\epsilon} + \hat{p} + \mu_B\frac{\partial\hat{p}}{\hat{\mu}_B} + \mu_Q\frac{\partial\hat{p}}{\hat{\mu}_Q} + \mu_S\frac{\partial\hat{p}}{\hat{\mu}_S}$$

$$\Delta\hat{s} \equiv \frac{s(T,\mu_B)}{T^3} - \frac{s(T,0)}{T^3}$$

$$= \sum_{k=1}^{\infty} \sigma_{2k}(T)\hat{\mu}_B^{2k}$$

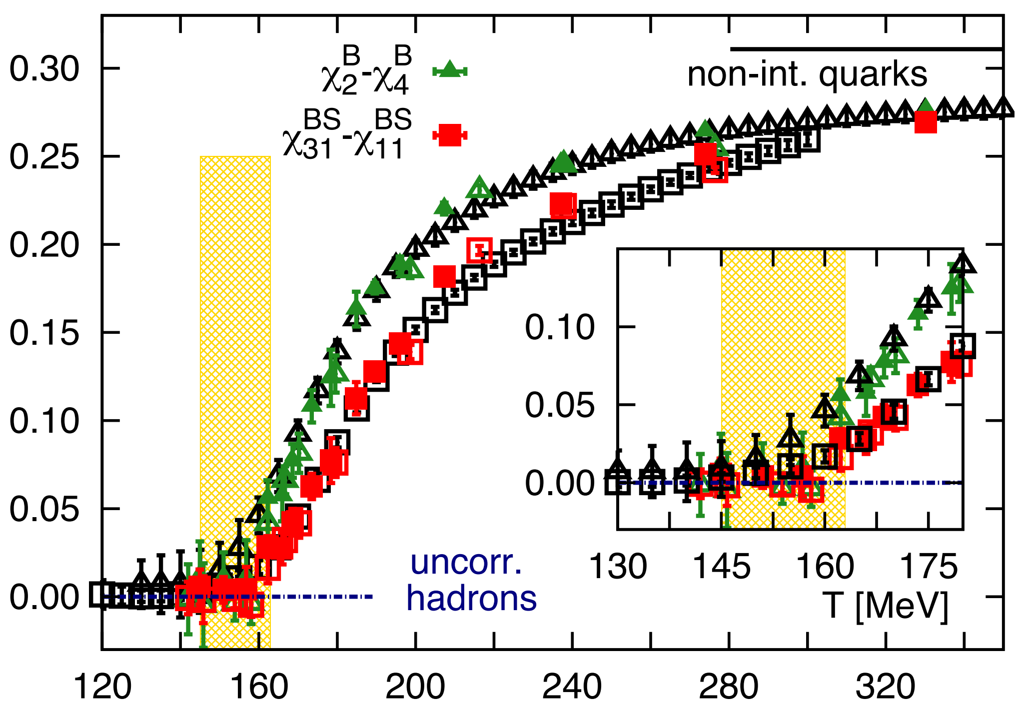
[A. Bazavov et al., HotQCD, PRD 95 (2017) 054504]



[D. Bollweg, QM2022; HotQCD in preparation]

- **cumulants are sensitive to effective charges:** compare cumulants from non-perturbative (lattice) QCD calculations to other scenarios such as an uncorrelated gas of hadrons (HRG) or perturbative QCD

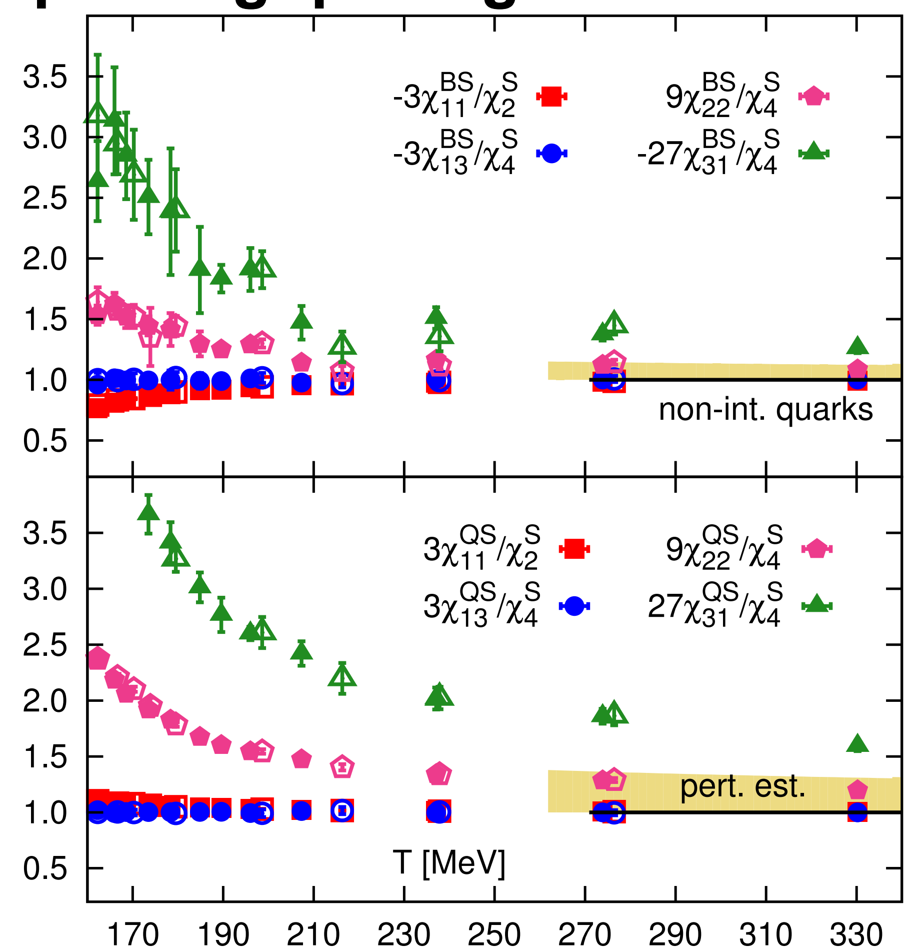
probing HRG DoFs:



Bazavov et al., PRL 111 (2013)
Bellwied et al., PRL 111 (2013)

$\Rightarrow$ relevant degrees of freedom are hadronic and uncorrelated for $T \lesssim T_c$

probing quark gas DoFs:



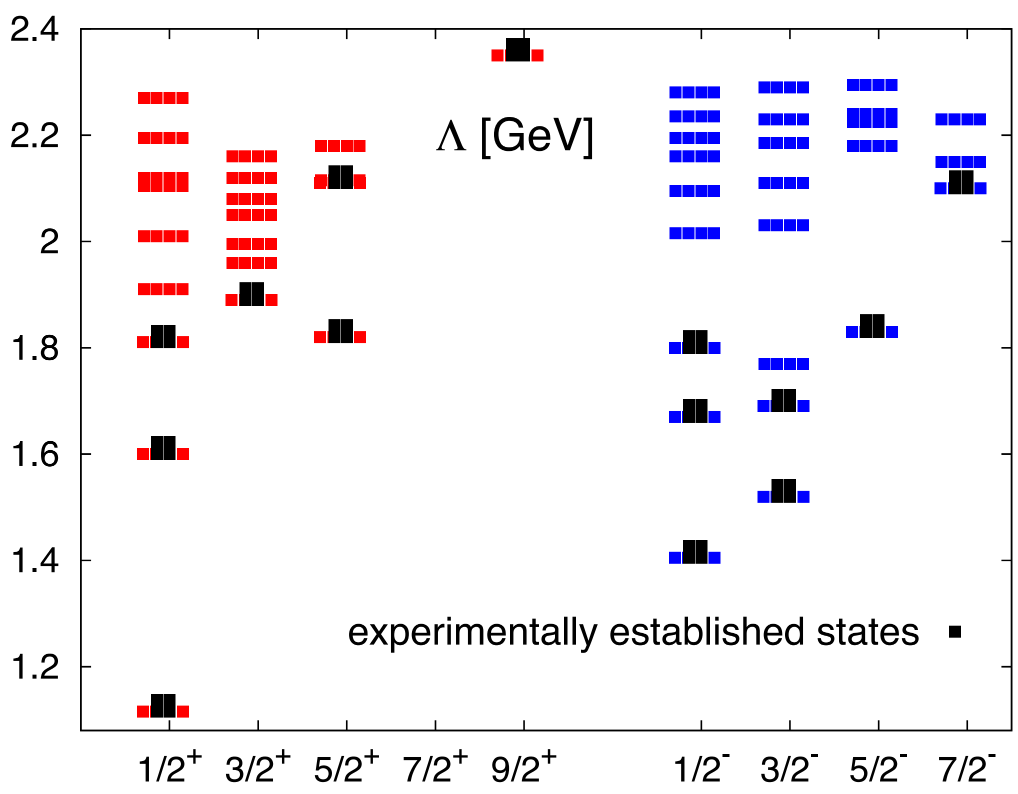
$\Rightarrow$ relevant degrees of freedom are that of a weakly interact. quark gas for $T \gtrsim 2T_c$

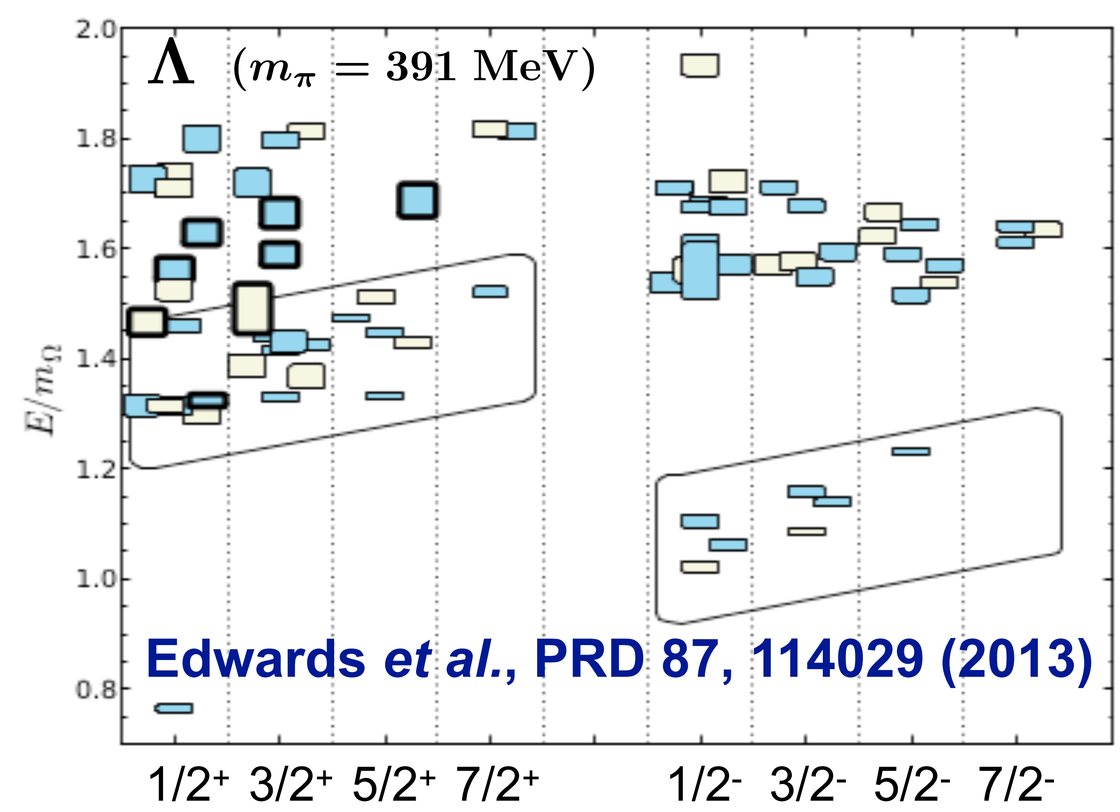
Are there missing strange states in the PDG?

- Obvious in the charm sector
- How large could be the effect of missing states in the strange sector?

⇒ construct **QM-HRG**, including additional states predicted by Quark-Model

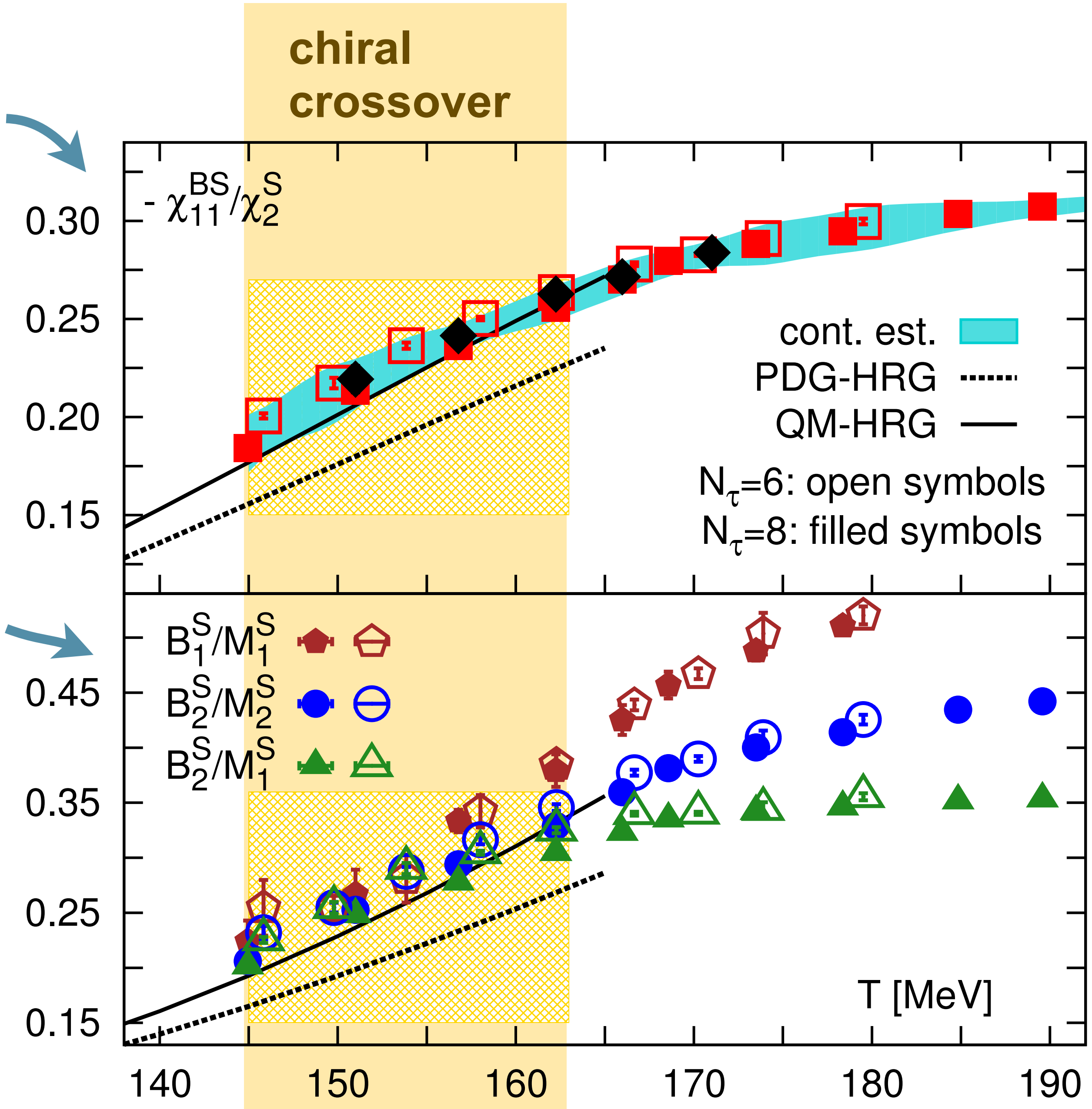
- **Use mesonic states from:** **S. Capstick and N. Isgur, PRD 34, 2809 (1986)**.
- **Use baryonic states from:** **D. Ebert *et al.*, PRD 79, 114029 (2009)**





- Similar to the spectrum of strange baryons on the lattice

- **BS-correlation χ_{11}^{BS}**
  at low T: weighted sum of partial pressure of strange baryons
- Different **linear combinations** of
  $$\chi_2^S, \chi_4^S, \chi_{11}^{BS}, \chi_{31}^{BS}, \chi_{22}^{BS}, \chi_{13}^{BS}$$
  are used to project onto partial pressure of strange baryons (B_i^S) and mesons (M_i^S) in the hadronic phase, e.g.
  $$B_1^S = -\frac{1}{6}(11\chi_{11}^{BS} + 6\chi_{22}^{BS} + \chi_{13}^{BS})$$
  $$B_2^S = \frac{1}{12}(\chi_4^S - \chi_2^S) - \frac{1}{3}(4\chi_{11}^{BS} - \chi_{13}^{BS})$$

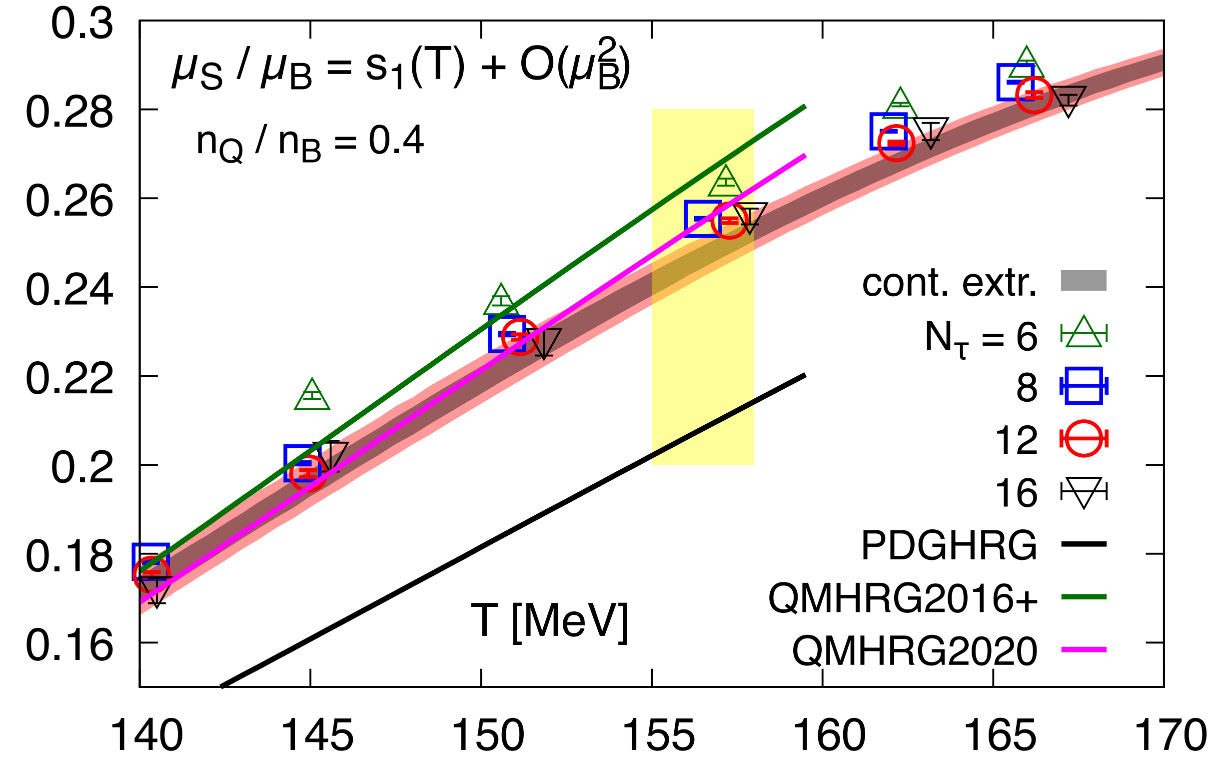


⇒ **QM-PDG provides more accurate description of lattice data**

⇒ Re-confirmation of our previous findings [**PRL 111,082301**]: onset of melting of open strange hadrons consistent with chiral crossover

$$\frac{\mu_S}{\mu_B} \equiv s_1(T) = -\frac{\chi_{11}^{BS}}{\chi_2^S} - \frac{\chi_{11}^{QS}}{\chi_2^S} q_1 + \mathcal{O}(\mu_B^2)$$

- Very sensitive to the strange spectrum
- Clear evidence for missing strangeness in the PDG list



[A. Bazavov et al., HotQCD, *PRD* 104 (2021), 074512]

HRG:

$$\frac{p^{HRG}}{T^4} = \frac{1}{VT^3} \sum_{i \in \, mesons} \ln \mathcal{Z}^M_{m_i}(T, V, \mu_S) + \frac{1}{VT^3} \sum_{i \in \, baryons} \ln \mathcal{Z}^B_{m_i}(T, V, \mu_B, \mu_S)$$

with

$$\ln \mathcal{Z}^{M/B}_{m_i} = \frac{VT^3}{\pi^2} d_i \left(\frac{m_i}{T}\right)^2 \sum_{k=1}^{\infty} \frac{(\pm 1)^{k+1}}{k^2} K_2(k m_i/T) \cosh\left(k(B_i \hat{\mu}_B + S_i \hat{\mu}_S)\right)$$

here we have set $\mu_Q \equiv 0$

- From the pressure expansion we readily obtain the expansions for the nth-order cumulants:

$$\chi_n^B(T,\mu_B) = \sum_{k=0}^{k_{\max}} \tilde{\chi}_n^{B,k}(T)\hat{\mu}_B^k, \quad \text{with} \quad \hat{\mu}_B = \mu_B/T$$

- Define ratios to eliminate the leading order volume dependence

$$R_{nm}^B = \frac{\chi_n^B(T,\mu_B)}{\chi_m^B(T,mu_B)} = \frac{\sum_{k=0}^{k_{\max}} \tilde{\chi}_n^{B,k}(T)\hat{\mu}_B^k}{\sum_{l=0}^{l_{\max}} \tilde{\chi}_m^{B,l}(T)\hat{\mu}_B^l}$$

- In terms of the shape parameters of the distribution we find

$$R_{12} = M/\sigma^2$$

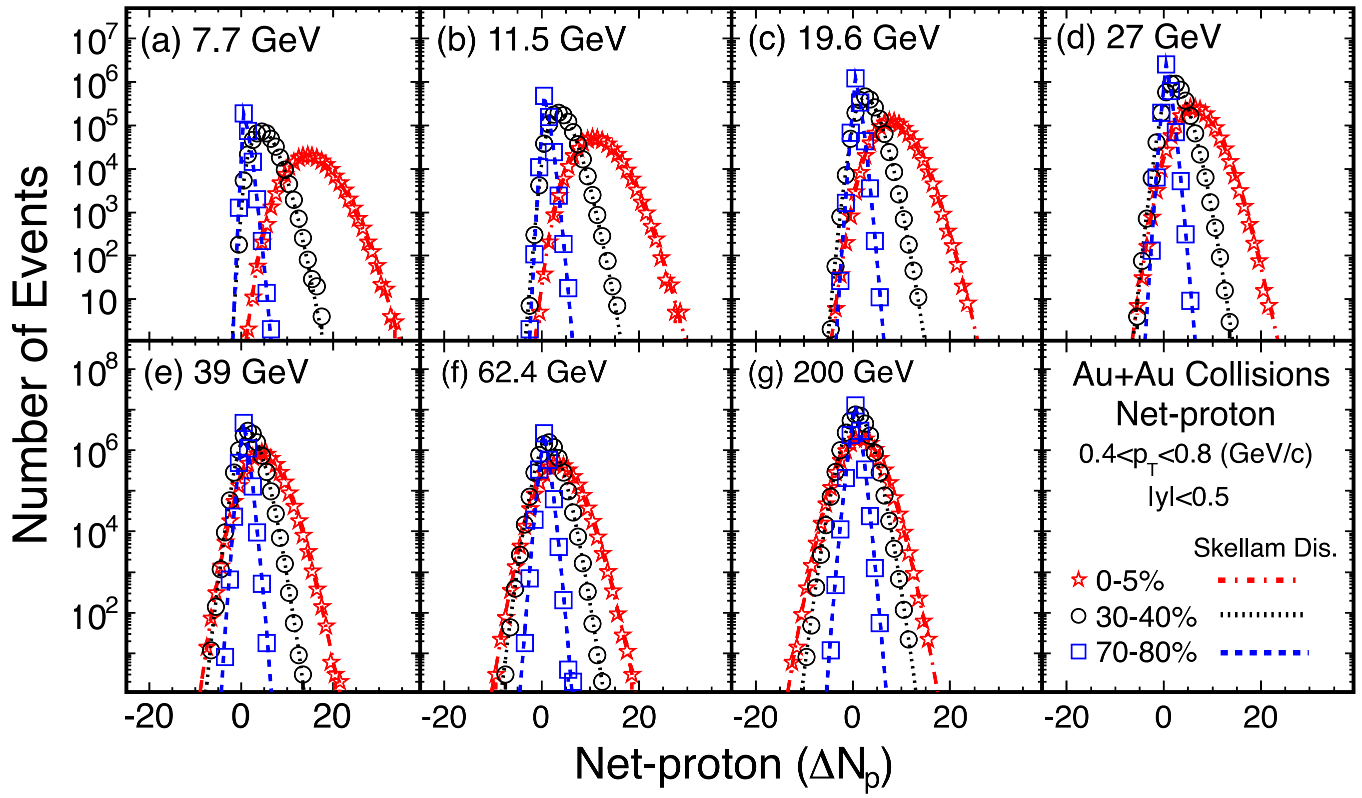
$$R_{31} = S\sigma^3/M$$

$$R_{32} = S\sigma$$

$$R_{42} = \kappa\sigma^2$$

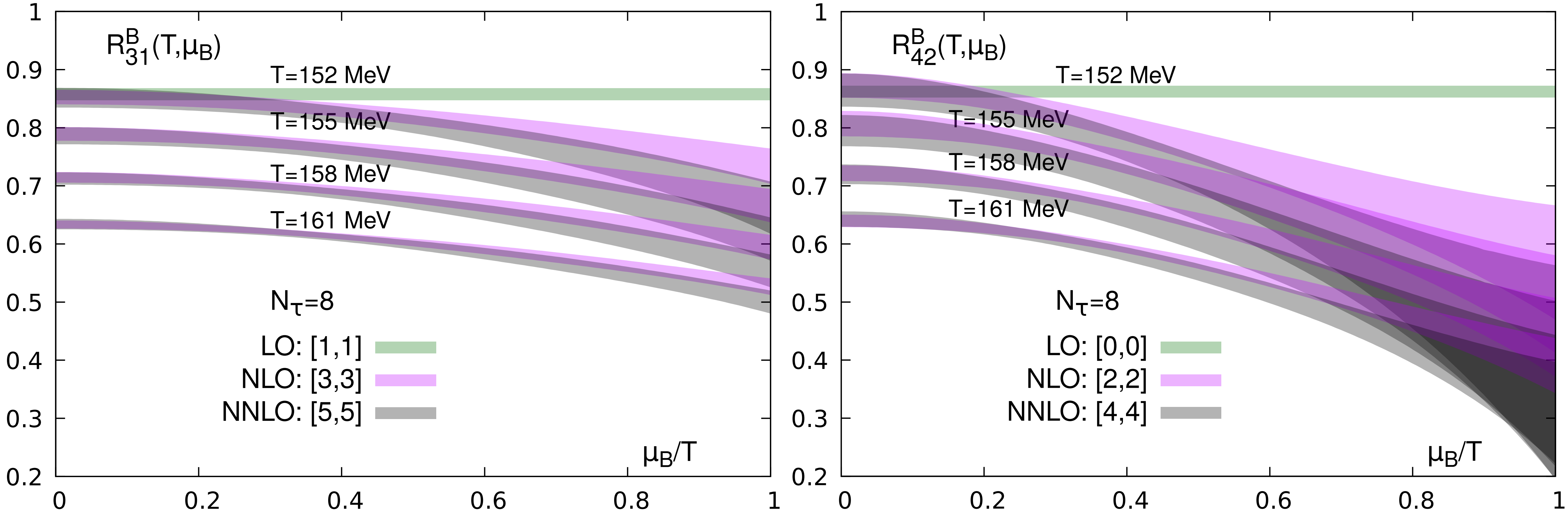
[Karsch, Redlich, Phys.Lett. B695 (2011) 136]

[Friman, Karsch, Redlich, Skokov, Eur.Phys.J.C (2011) 1694]



[STAR, PRL 112 (2014) 032302]

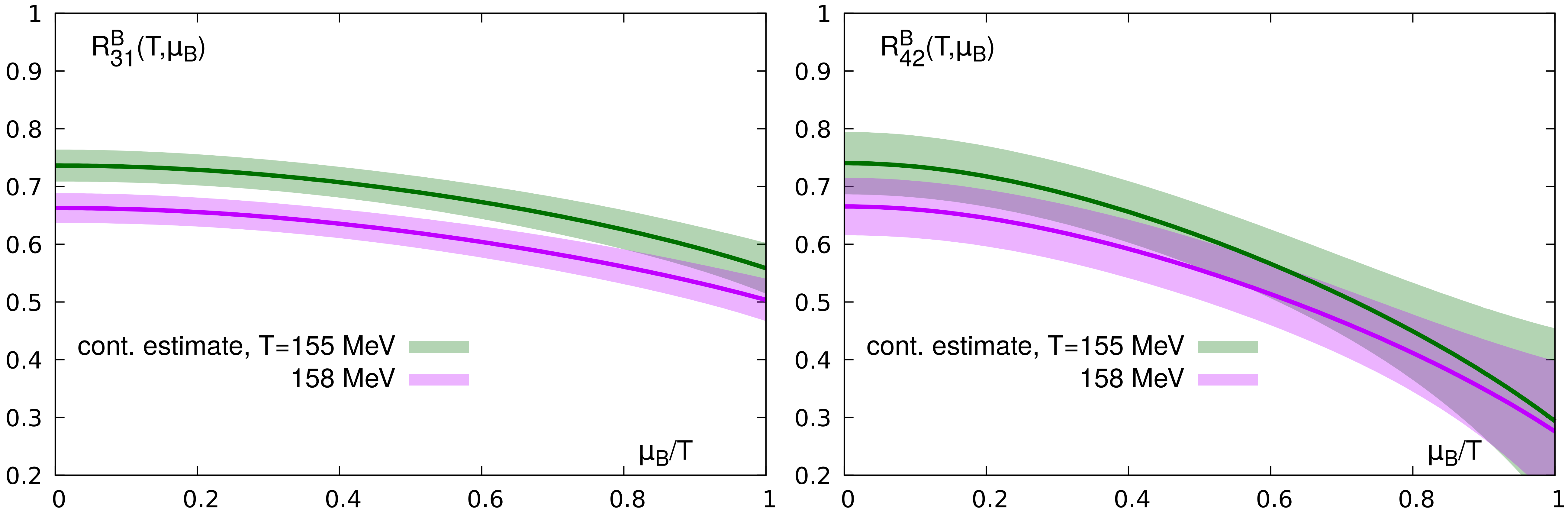
- Skewness and kurtosis ratios R^B_{31} and R^B_{42} on ($N_\tau = 8$)-lattices



- Convergence gets worth with increasing order of the cumulant and with decreasing temperature.
- NLO and NNLO corrections are negative.

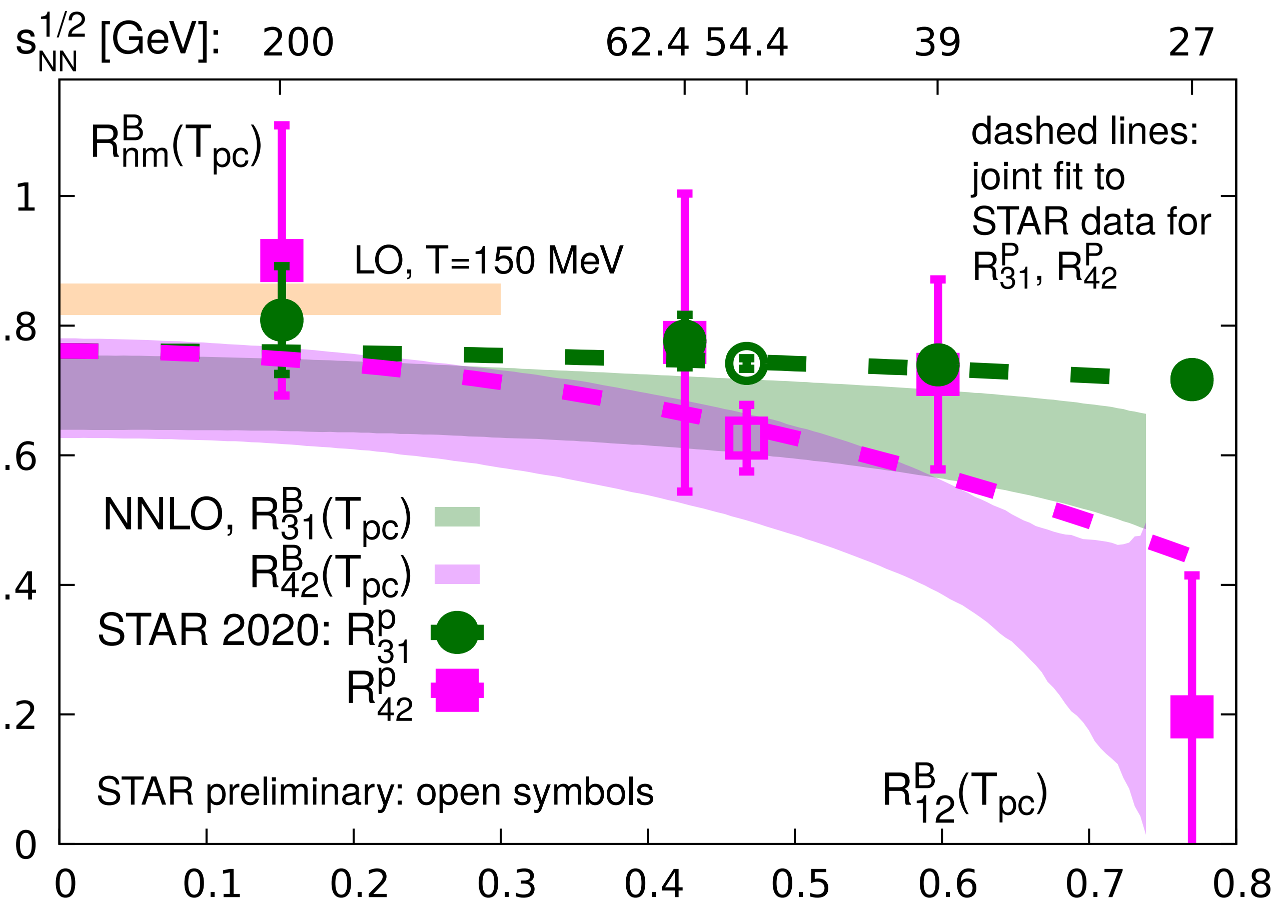
[Bazavov et al., HotQCD, *PRD* 101 (2020) 074502]

- Continuum estimates of R_{31}^B and R_{42}^B as function of μ_B/T for various temperatures.



- Ratios drop with increasing μ_B/T and with increasing temperature.

[Bazavov et al., HotQCD, *PRD* 101 (2020) 074502]



[Bazavov et al., HotQCD, *PRD* 101 (2020) 074502]

- Continuum estimates of $\boldsymbol{R^B_{31}}$ and $\boldsymbol{R^B_{42}}$ as function of $\boldsymbol{R^B_{12}}$ on the crossover line.
- Star data at $\sqrt{s_{NN}} = \mathbf{54.4}$ GeV favours a freeze-out temperature slightly below the crossover.
- The estimate of the freeze-out temperature $T_{\mathrm{f}} = \mathbf{165}$ MeV for $\sqrt{s_{NN}} = \mathbf{200}$ GeV (from a statistical model analysis) is not consistent with a determination of T_{f} from the skewness and kurtosis data by STAR.

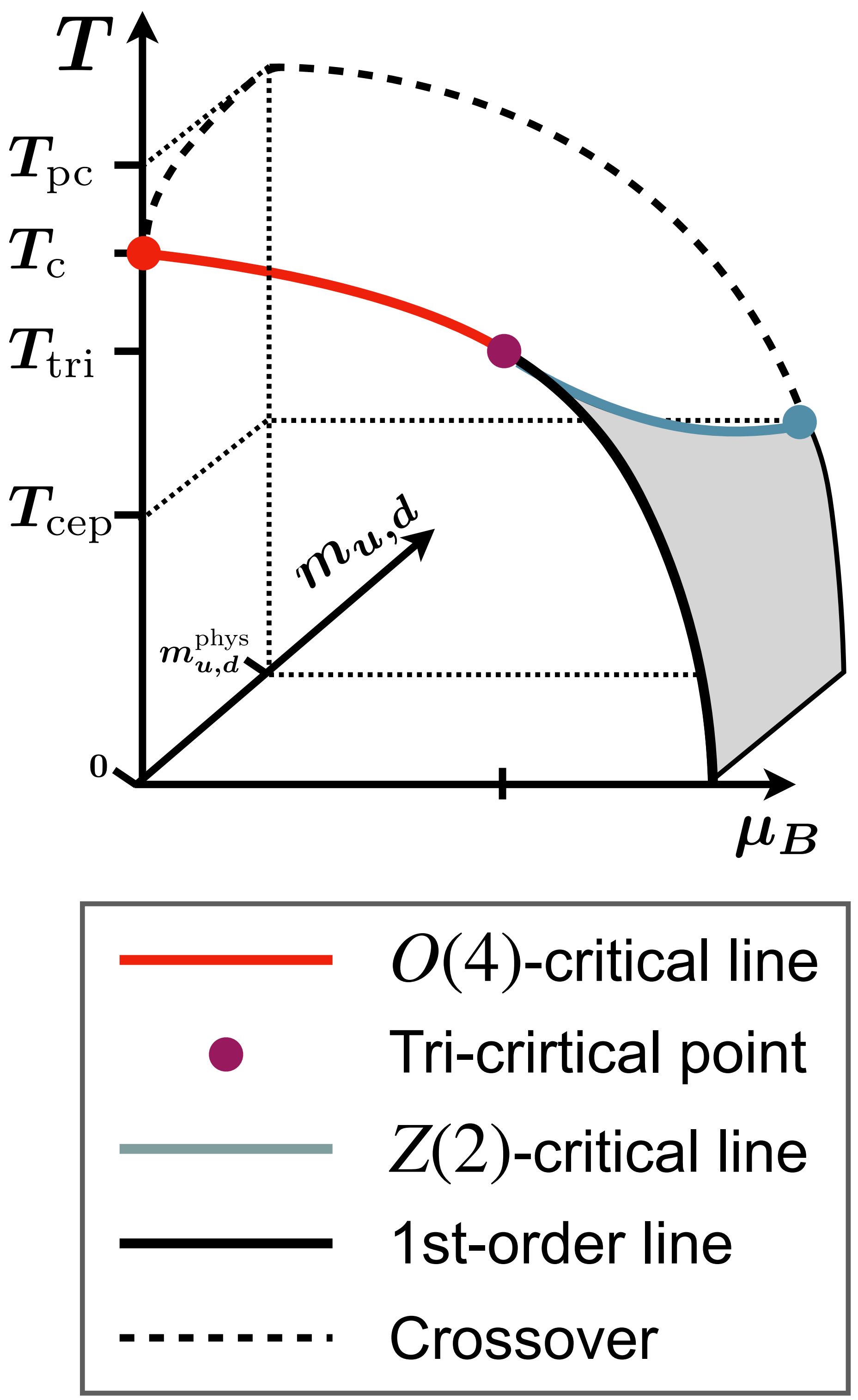
In principle baryon number fluctuation and proton number fluctuations are not the same thing!

[Asakawa, Kitazawa, Phys.Rev.C 86 (2012) 024904]

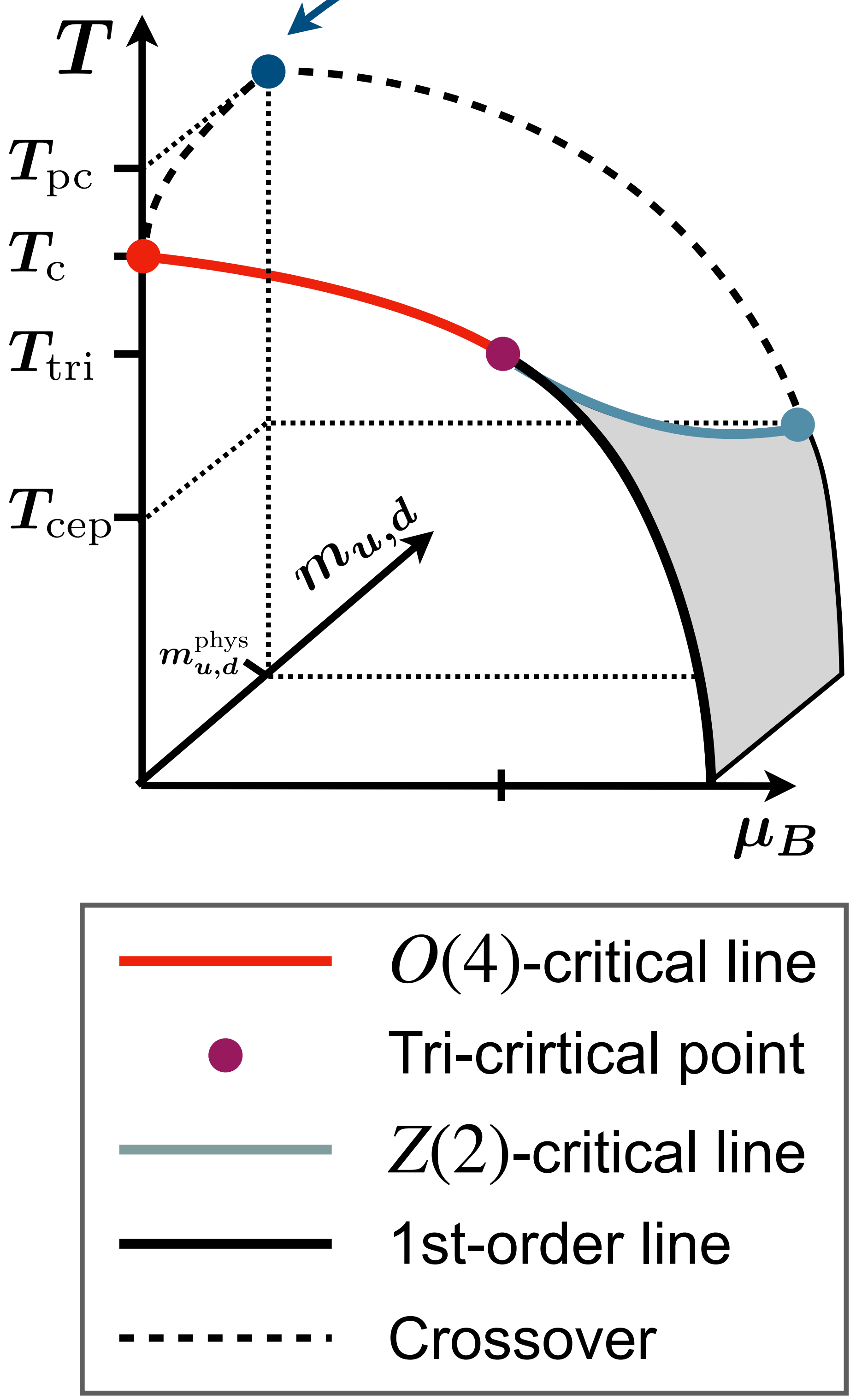
[Bazdak, Koch, Skokov, *Phys.Rev.C* 87 (2013) 014901]

[Vovchenko et al., Phys.Lett. B 811 (2020) 135868]

The QCD phase diagram

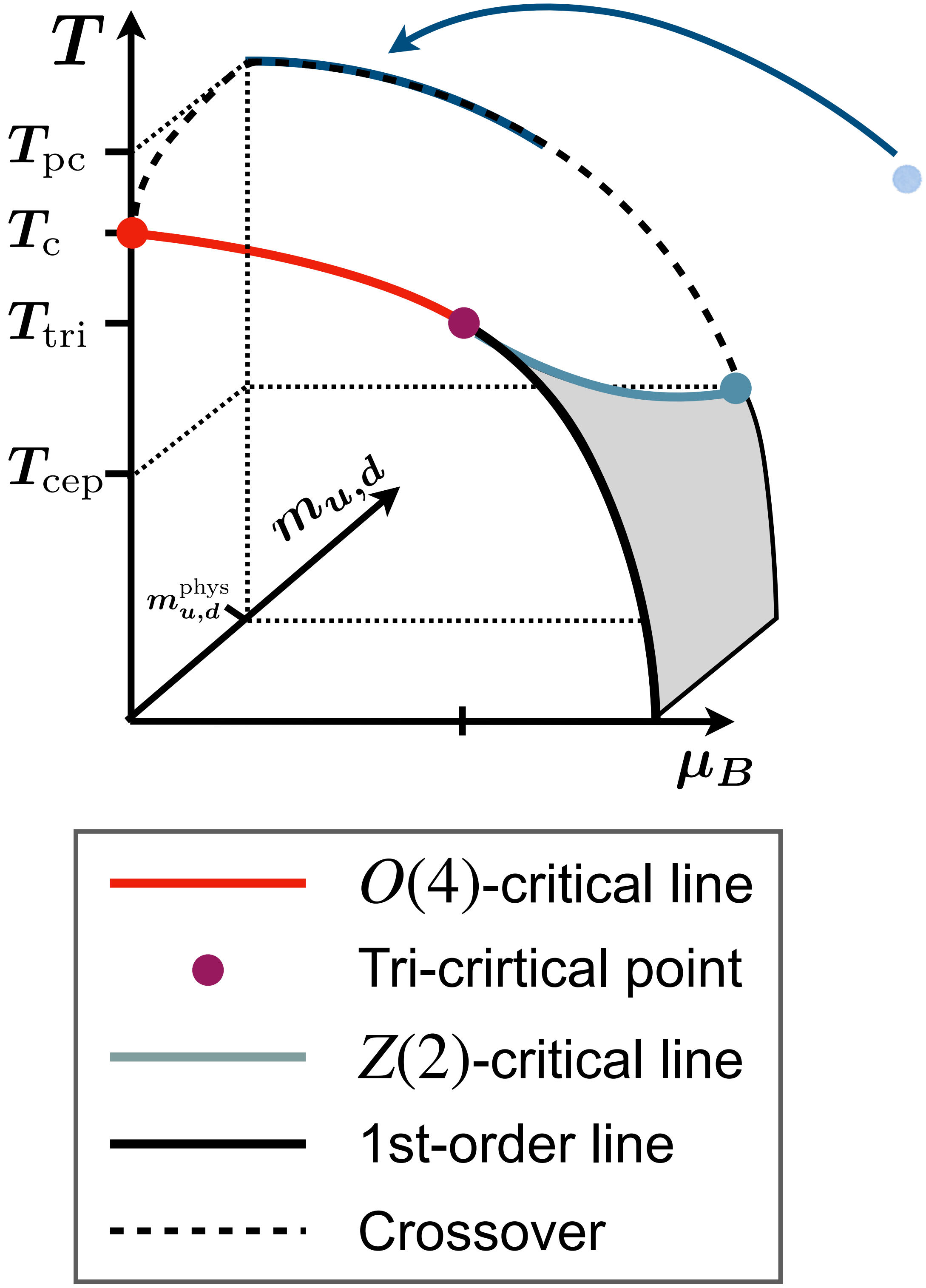


T
$T_{\rm pc}$
$T_{\rm c}$
$T_{\rm tri}$
$T_{\rm cep}$
$m_{u,d}$
$m_{u,d}^{\rm phys}$
0
μ_B
$O(4)$-critical line
Tri-crirtical point
$Z(2)$-critical line
1st-order line
Crossover



- Precise determination of the QCD transition temperature $T_{\rm pc} = \mathbf{156.5 \pm 1.5}$ MeV

HotQCD: PLB 795 (2019) 15



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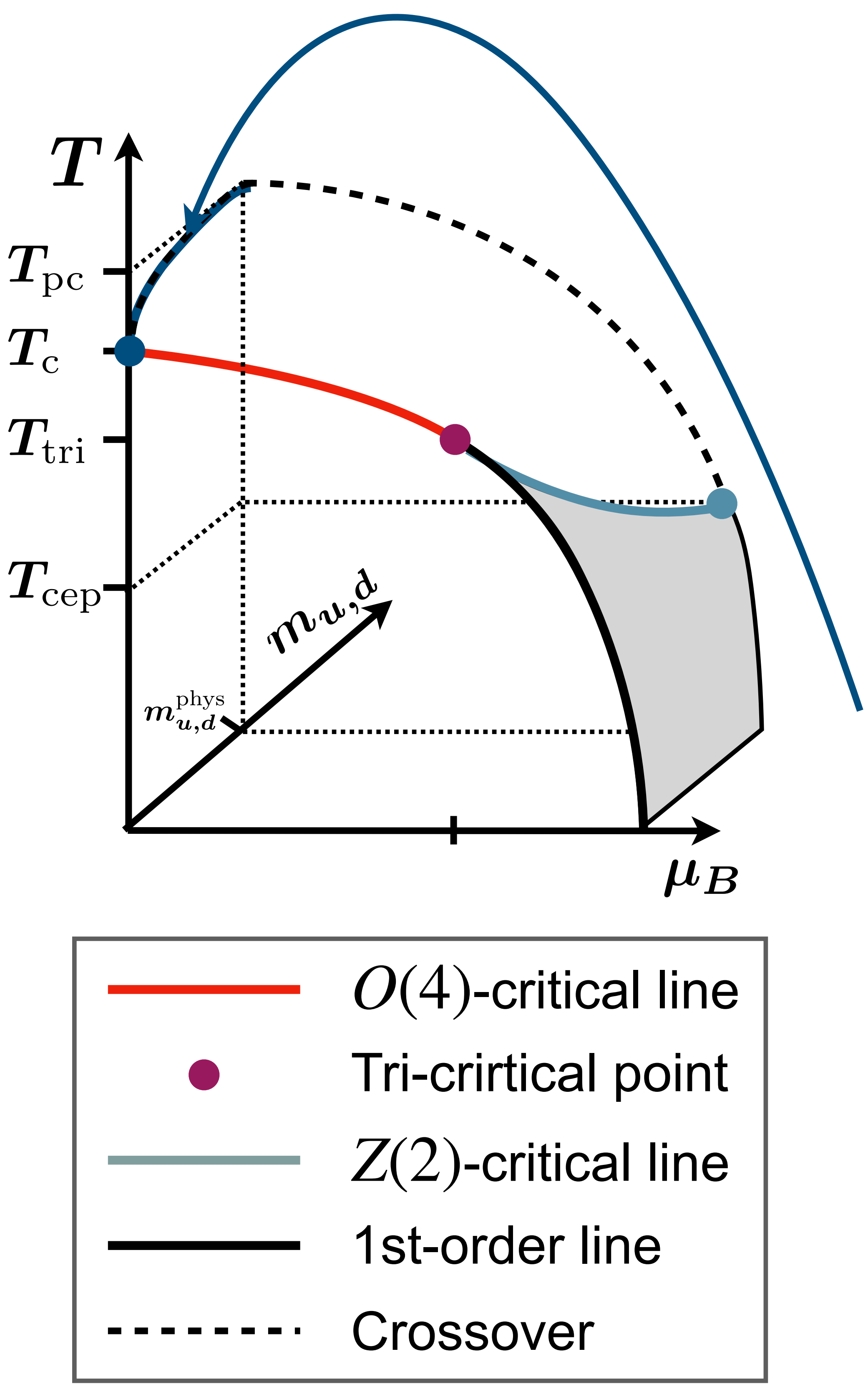
HotQCD: PLB 795 (2019) 15

- The chiral crossover line with respect to μ_B

$$T_{\rm pc}(\mu_B) = T_{\rm pc}^0 \left(1 - \kappa_2^{B,f}\left(\frac{\mu_B}{T_{\rm pc}^0}\right)^2 - \kappa_4^{B,f}\left(\frac{\mu_B}{T_{\rm pc}^0}\right)^4\right)$$

$$\kappa_2^{B,f} = 0.012(4), \quad \kappa_4^{B,f} = 0.00(4)$$

HotQCD: PLB 795 (2019) 15



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HotQCD: PLB 795 (2019) 15

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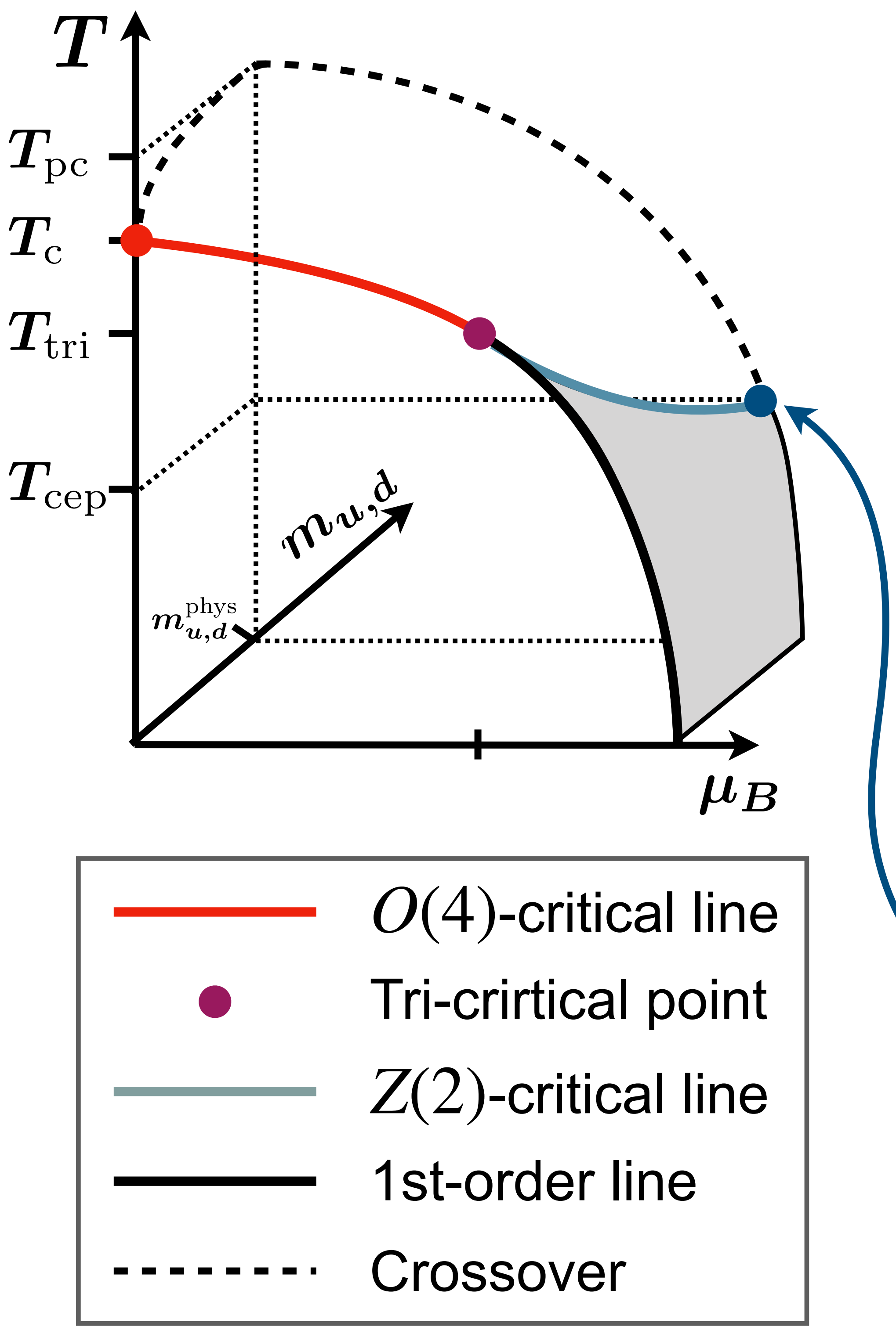
HotQCD: PLB 795 (2019) 15

- The chiral phase transition temperature and pseudo-critical line $T_{\rm c} = 132^{+3}_{-6}$ MeV

HotQCD: PRL 123 (2019) 062002



- Precise determination of the QCD transition temperature $T_{\rm pc} = 156.5 \pm 1.5$ MeV

HotQCD: PLB 795 (2019) 15

- The chiral crossover line with respect to μ_B

$$T_{\rm pc}(\mu_B) = T^0_{\rm pc}\left(1 - \kappa_2^{B,f}\left(\frac{\mu_B}{T^0_{\rm pc}}\right)^2 - \kappa_4^{B,f}\left(\frac{\mu_B}{T^0_{\rm pc}}\right)^4\right)$$

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HotQCD: PLB 795 (2019) 15

- The chiral phase transition temperature and pseudo-critical line $T_{\rm c} = 132^{+3}_{-6}$ MeV

HotQCD: PRL 123 (2019) 062002

- Expected bounds on the QCD critical end-point

$$T_{\rm cep} < T_{\rm c} = 132^{+3}_{-6}\ \text{MeV}$$
$$\mu_B^{\rm cep} \gtrsim 3\ T_c$$

- Universal critical behaviour guides our thinking on the QCD phase diagram. Often considered in the vicinity of the chiral critical point.

$$\frac{p}{T^4} = \frac{1}{VT^3}\ln Z(V,T,\vec{\mu}) = -h^{(2-\alpha)/\beta\delta} f_f(z) - f_r(V,T,\vec{\mu})$$

Universal scaling function, depending on $z = t/h^{1/\beta\delta}$

Effective model O(4)/O(2)/Z(2):

- 3 relevant scaling fields

t reduced temperature

h reduced symmetry breaking field

L^{-1} inverse system size

map QCD to the effective model

controlled by non-universal parameter:

t_0, h_0, l_0
T_c, H_c, κ_2^B

(2+1)-flavor QCD:

$$t = t_0\left[\left(\frac{T-T_c}{T_c}\right) + \kappa_2^B\left(\frac{\mu_B}{T}\right)^2\right]$$

$$h = h_0(H - H_c), \quad H = \frac{m_l}{m_s}$$

$$l = l_0 L^{-1}$$

- Universal critical behaviour guides our thinking on the QCD phase diagram. Often considered in the vicinity of the chiral critical point.

$$\frac{p}{T^4} = \frac{1}{VT^3} \ln Z(V,T,\vec{\mu}) = -h^{(2-\alpha)/\beta\delta} f_f(z) - f_r(V,T,\vec{\mu})$$

Universal scaling function

- We can calculate derivatives of $\ln Z$. Singular behaviour is characteristic to the universality class. E.g. here: O(4)

O(4)-critical exponents:

$\alpha = -0.21$

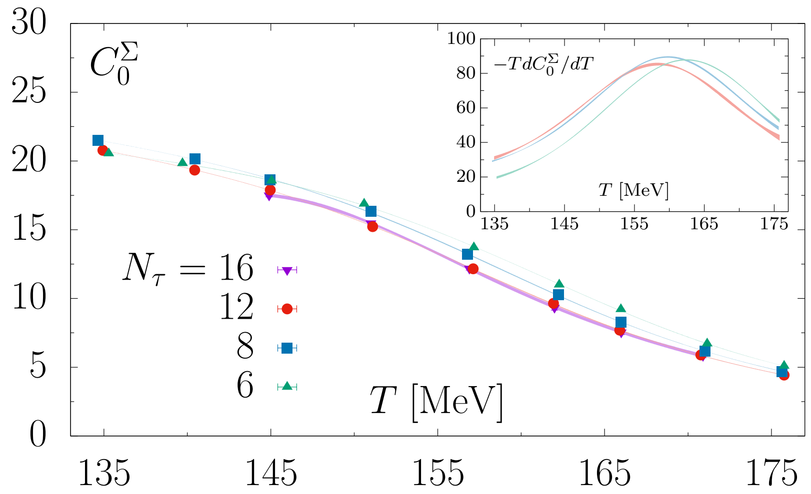
$\beta = -0.38$

$\delta = 4.82$

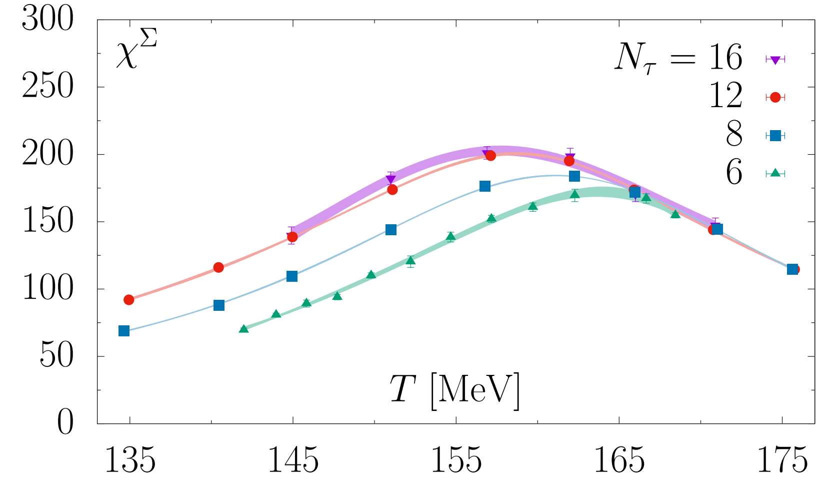
	Magnetic	**Mixed**	**Thermal**
	$\frac{\partial^2 \ln Z}{\partial h^2}$	$\frac{\partial^2 \ln Z}{\partial h\, \partial t}$	$\frac{\partial^2 \ln Z}{\partial t^2}$
	$\sim \left(\frac{m_l}{m_s}\right)^{1/\delta-1}$	$\sim \left(\frac{m_l}{m_s}\right)^{(\beta-1)/\beta\delta}$	$\sim \left(\frac{m_l}{m_s}\right)^{-\alpha/\beta\delta}$
	$\sim \left(\frac{m_l}{m_s}\right)^{-0.79}$	$\sim \left(\frac{m_l}{m_s}\right)^{-0.34}$	$\sim \left(\frac{m_l}{m_s}\right)^{+0.11}$
Divergence:	**strong**	**moderate**	**none**

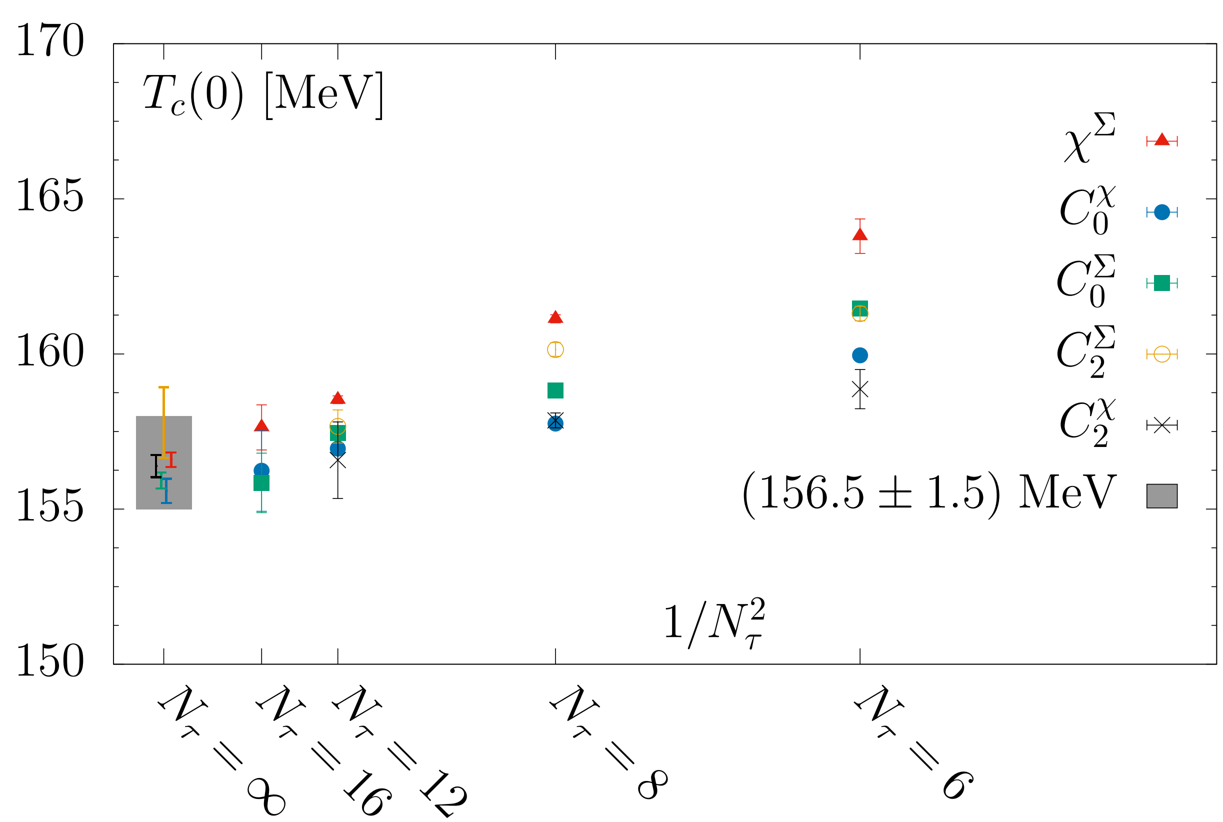
The pseudo critical temperature

$$M \sim \frac{\partial f}{\partial H}$$



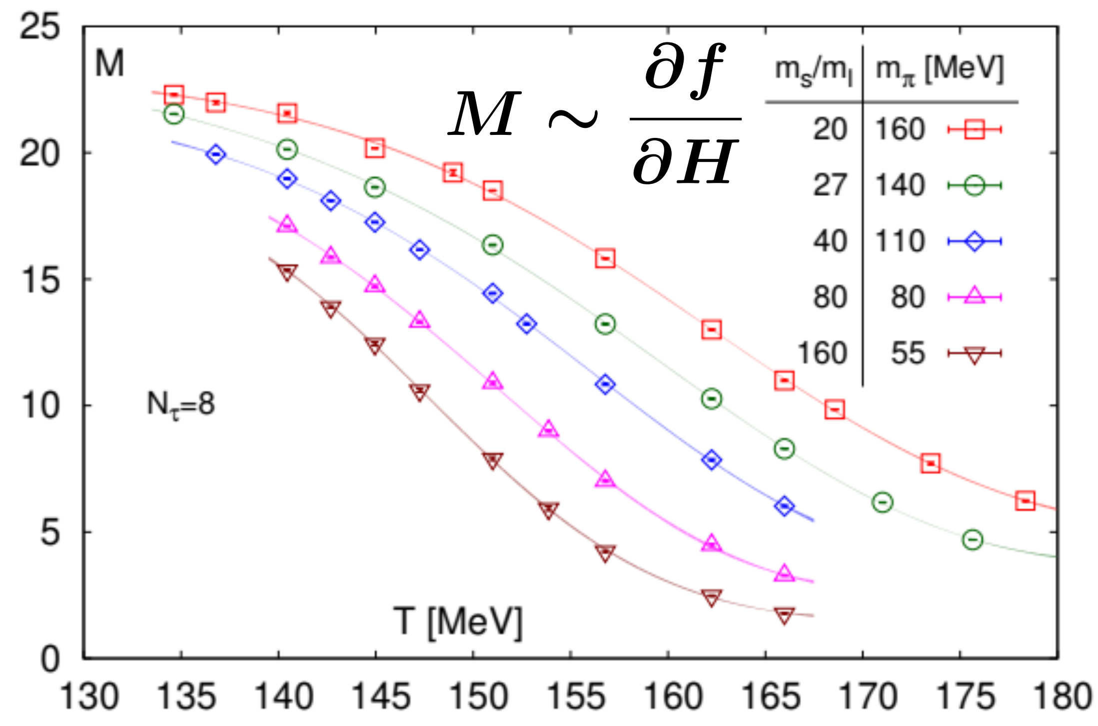
$$\chi_M \sim \frac{\partial^2 f}{\partial H^2}$$





- Transition is a crossover, various definitions of T_{pc} do not need to agree
- Study 5 different definitions and perform continuum limit
- Find good agreement in the continuum limit: $T_{pc} = 156.5\ (1.5)$ MeV

A. Bazavov et al [HotQCD], Phys. Lett. B795, 15 (2019), arXiv:1812.08235



Magnetic susceptibility

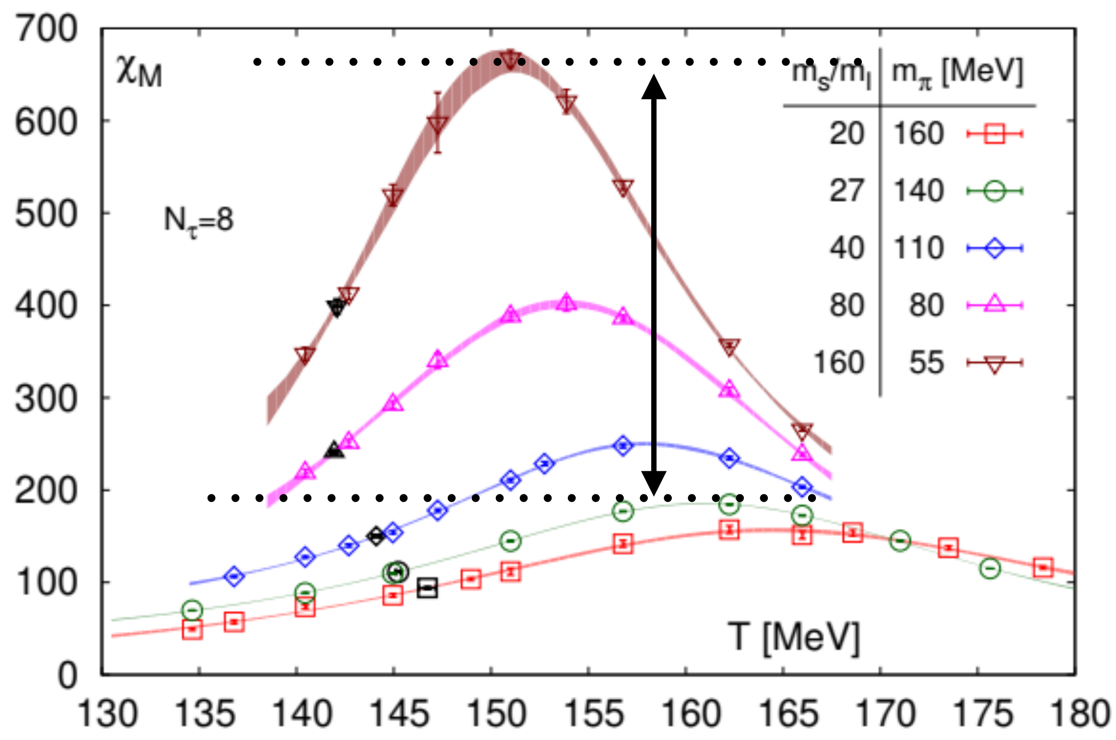
$$\sim \left(\frac{m_l}{m_s}\right)^{-0.79}$$

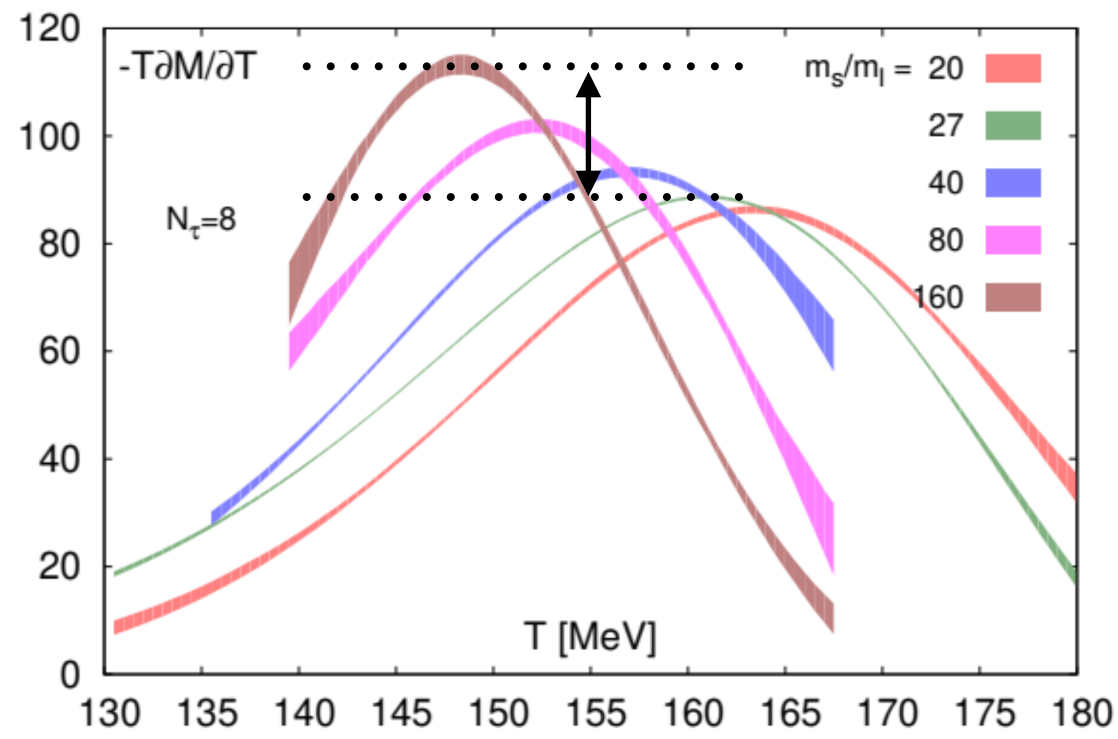
Mixed susceptibility

$$\sim \left(\frac{m_l}{m_s}\right)^{-0.34}$$

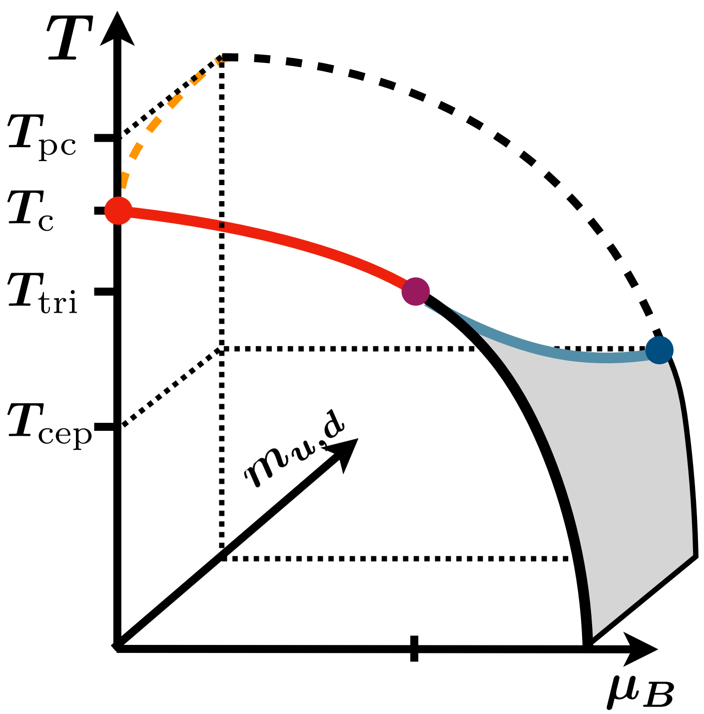
$$(160/27)^{0.79} \approx 4$$

$$(160/27)^{0.34} \approx 1.8$$

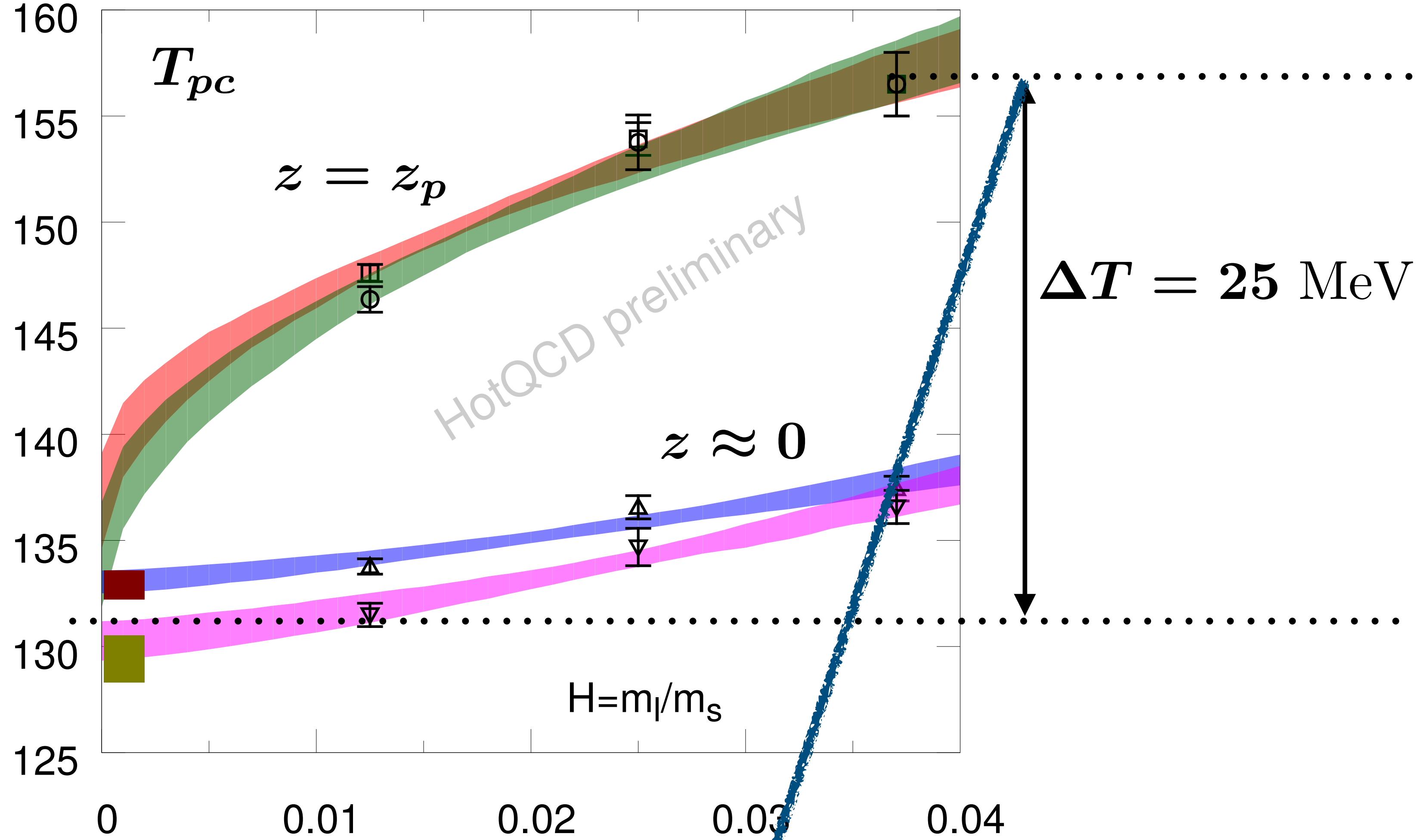




H.T. Ding et al. (HotQCD), PRL 123 (2019) 15, arXiv:1903.04801



A. Lahiri et al, arXiv:2010:1559



Chiral extrapolations:

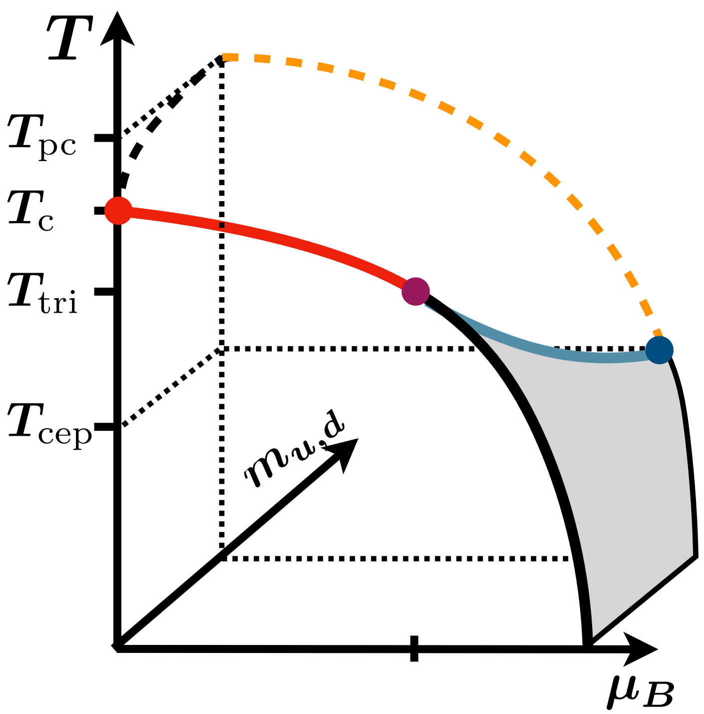
$T_c^0 = 132^{+3}_{-6}$ MeV

H.T. Ding et al. (HotQCD), PRL 123 (2019) 15, arXiv:1903.04801

Physical masses:

$T_{pc} 156.5\ (1.5)$ MeV

A. Bazavov et al [HotQCD], Phys. Lett. B795, 15 (2019), arXiv:1812.08235



- Consider a μ_B-dependent shift of the peak of the susceptiblities. Defining conditions are thus

$$\left.\frac{\partial^2 M(T,\mu_B)}{\partial T^2}\right|_{\mu_B} = 0 \quad \text{or} \quad \left.\frac{\partial \chi_M(T,\mu_B)}{\partial T}\right|_{\mu_B} = 0$$

- The condition lead to equations for κ_2, κ_4

$$T_{\rm pc}(\mu_B) = T_{\rm pc}^0\left(1 - \kappa_2^{B,f}\left(\frac{\mu_B}{T_{\rm pc}^0}\right)^2 - \kappa_4^{B,f}\left(\frac{\mu_B}{T_{\rm pc}^0}\right)^4\right)$$

$$\kappa_2^{B,f} = 0.012(4), \quad \kappa_4^{B,f} = 0.00(4)$$

A. Bazavov et al [HotQCD], Phys. Lett. B795, 15 (2019), arXiv:1812.08235

- Universal scaling relates derivatives of M

$$t = t_0\left[\left(\frac{T-T_c}{T_c}\right) + \kappa_2^B\left(\frac{\mu_B}{T}\right)^2\right] \Longleftrightarrow \frac{\partial^2}{\partial(\mu_B/T)^2} \simeq \frac{\partial}{\partial T}$$

$$\kappa_2 \sim \frac{T^2\partial^2 M/\partial\mu_B}{2T\partial M/\partial T}$$

Kaczmarek et al, PRD 83 (2011) 014504

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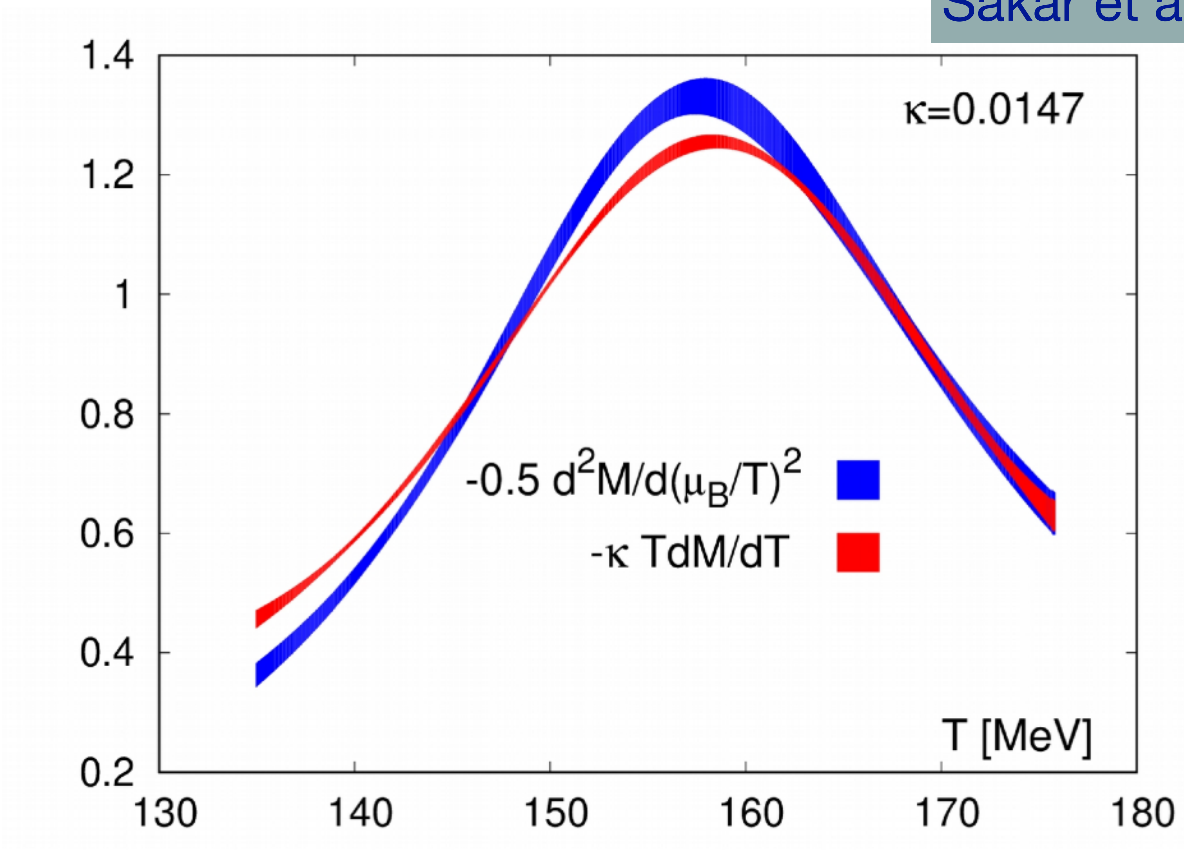
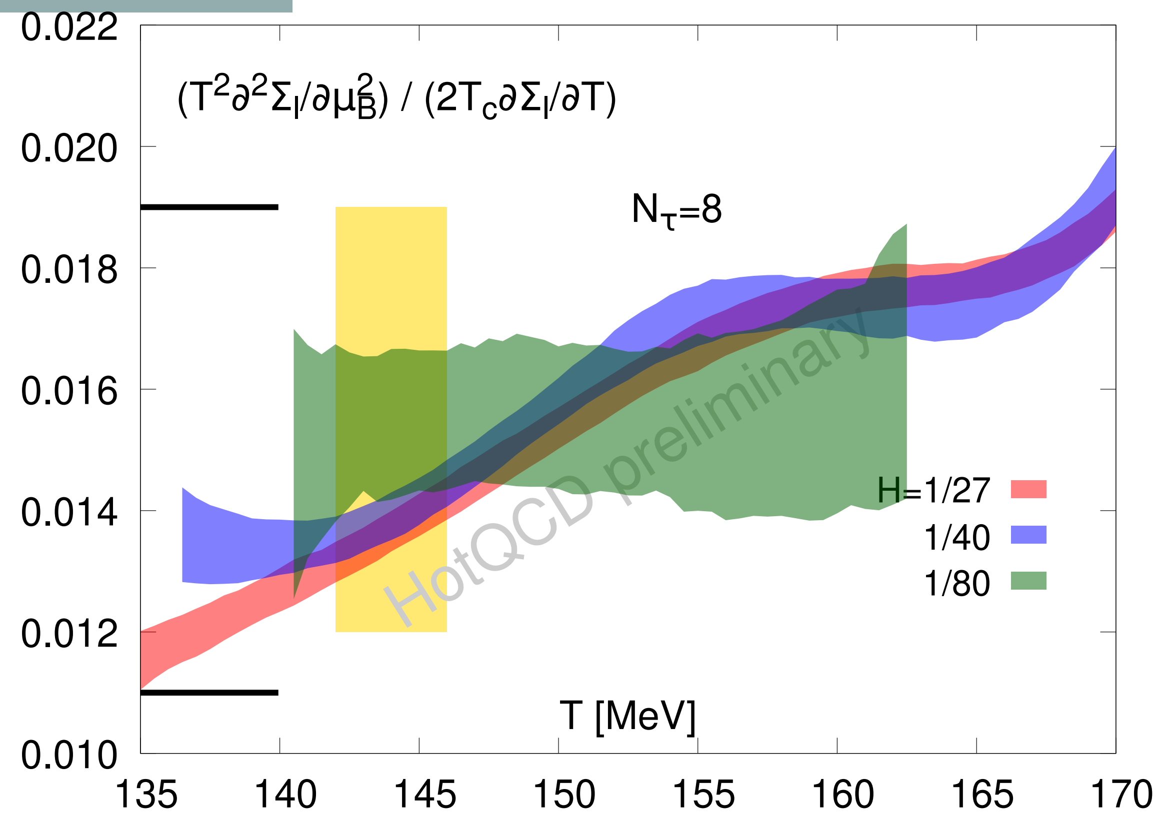
Kaczmarek et al, PRD 83 (2011) 014504

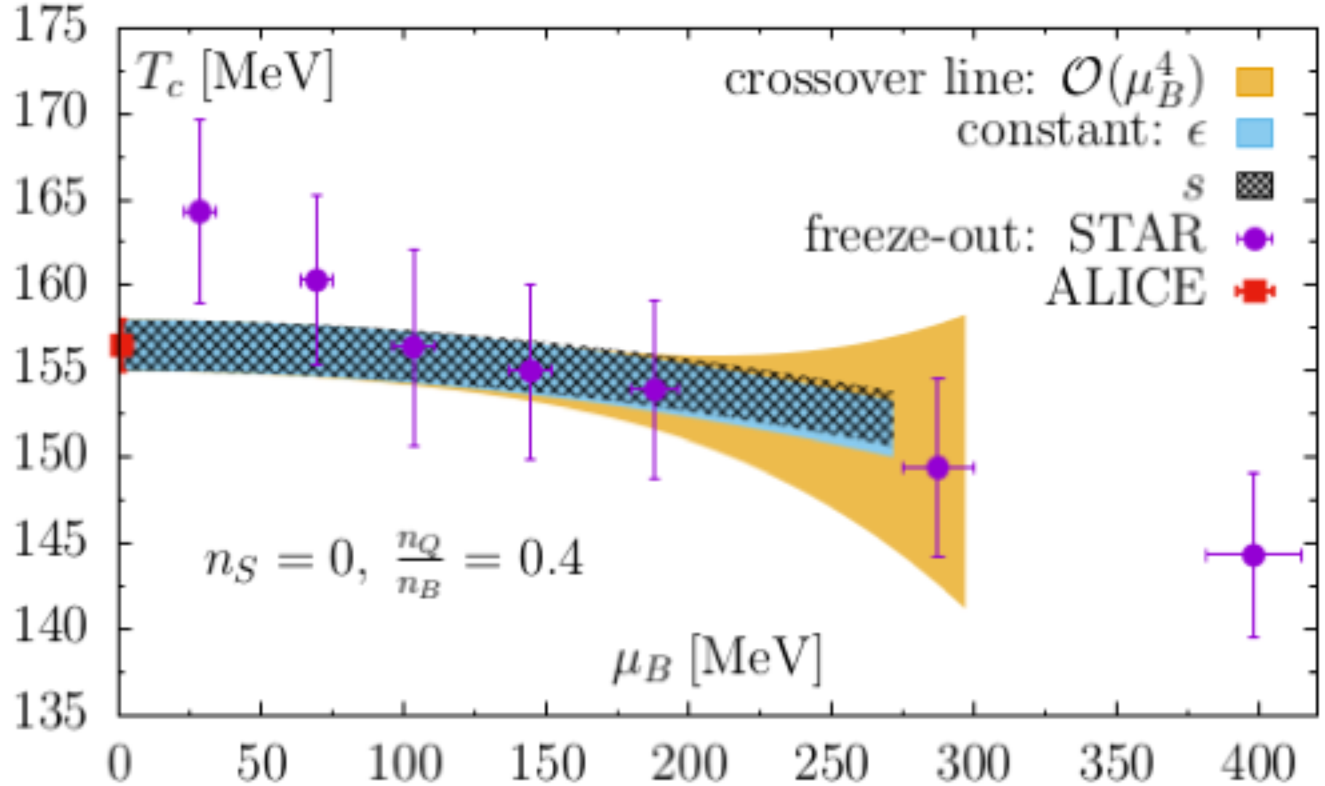
Sakar et al, Lattice 2021





- Curvature of the pseudo critical line depends only mildly on H

$$T_{\rm pc}(\mu_B) = T^0_{\rm pc}\left(1 - \kappa_2^{B,f}\left(\frac{\mu_B}{T^0_{\rm pc}}\right)^2 - \kappa_4^{B,f}\left(\frac{\mu_B}{T^0_{\rm pc}}\right)^4\right)$$



STAR: arXiv:1701.07065

A. Andronic et al., Nature 561 (2018) 321

T_{pc} 156.5 (1.5) MeV
$\kappa_2 = 0.012(4)$
$\kappa_4 = 0.00(4)$

A. Bazavov et al [HotQCD], Phys. Lett. B795, 15 (2019), arXiv:1812.08235

T_{pc} 158.0 (0.6) MeV
$\kappa_2 = 0.0153(18)$
$\kappa_4 = 0.00032(67)$

S. Borsanyi et al, arXiv: 2002.02821

* We can estimate the radius of convergence $r_c = \lim_{n\to\infty} r_{c,n}$ by ratios of expansion coefficients

Simple ratio estimator: $r_{c,n} = \sqrt{|A_n|}$ $\quad A_n = \dfrac{c_n}{c_{n+2}}$, n even

Mercer-Roberts estimator: $r_{c,n}^{MR} = |A_n^{MR}|^{1/4}$ $\quad A_n^{MR} = \dfrac{c_{n+2}\,c_{n-2} - c_n^2}{c_{n+4}\,c_n - c_{n+2}^2}$, n even

* The Estimators A_n and A_n^{MR} are related to the poles of the [n,2] and [n,4] Padé, respectively.

* For the analysis of the Padé, we take advantage of the positivity of $\chi_2^B\,(\bar{\chi}_2^B)$ and $\chi_4^B\,(\bar{\chi}_4^B)$ and rescale the pressure series by a factor P_4/P_2^2 and redefine the expansion parameter to $\bar{x} = \sqrt{P_4/P_2}\;\hat{\mu}_B \equiv \sqrt{\bar{\chi}_4^B/(12\bar{\chi}_2^B)}\;\hat{\mu}_B$.

$$\frac{(\Delta P(T,\mu_B)/T^4)P_4}{P_2^2} = \sum_{k=1}^{\infty} c_{2k,2}\bar{x}^{2k} = \bar{x}^2 + \bar{x}^4 + c_{6,2}\bar{x}^6 + c_{8,2}\bar{x}^8 + \ldots$$

with $c_{6,2} = \dfrac{P_6 P_2}{P_4^2} = \dfrac{2}{5}\,\dfrac{\bar{\chi}_6^B\bar{\chi}_2^B}{(\bar{\chi}_4^B)^2}$ and $c_{8,2} = \dfrac{P_8 P_2^2}{P_4^3} = \dfrac{3}{35}\,\dfrac{\bar{\chi}_8^B(\bar{\chi}_2^B)^2}{(\bar{\chi}_4^B)^3}$

→The singular structure of the 8th order expansion depends only on two coefficients

* In term of the expansion parameter $\bar{x}$, the Padé is given as

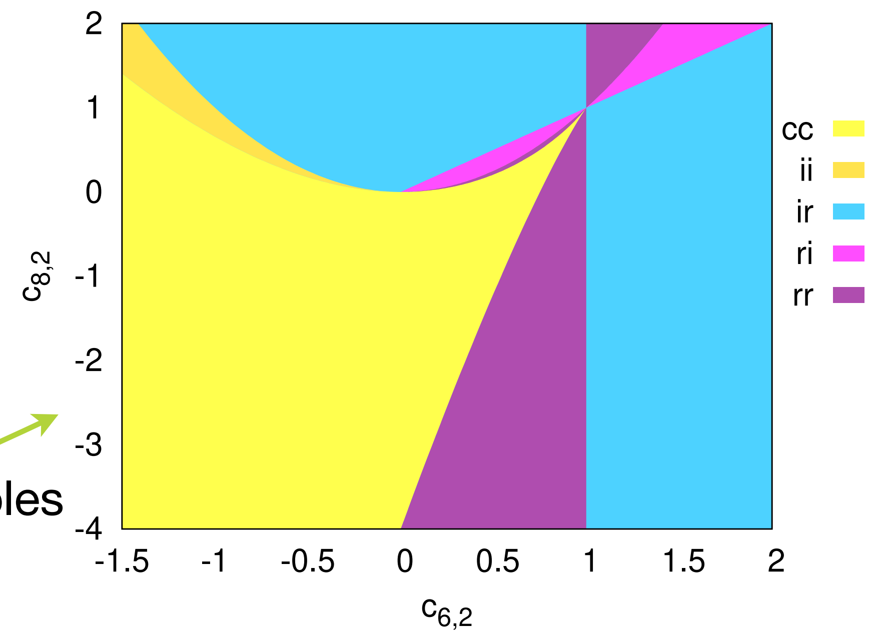
$$P[2,2] = \frac{\bar{x}^2}{1-\bar{x}^2}$$

Poles on the real axis at

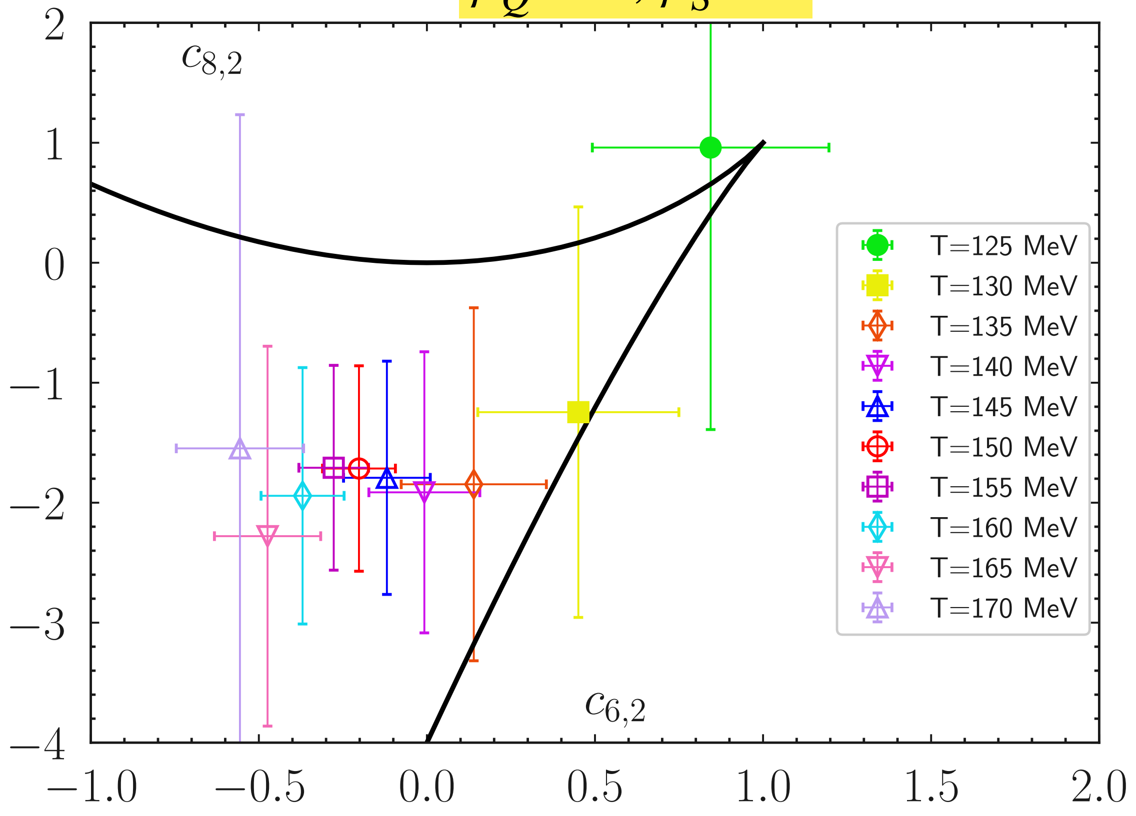
$$\bar{x}^2 = 1 \quad \Leftrightarrow \quad \hat{\mu}_{B,c} = \sqrt{12\bar{\chi}_2^B/\bar{\chi}_4^B}$$

$$P[4,4] = \frac{(1-c_{6,2})\bar{x}^2 + \left(1-2c_{6,2}+c_{8,2}\right)\bar{x}^4}{(1-c_{6,2}) + (c_{8,2}-c_{6,2})\bar{x}^2 + (c_{6,2}^2 - c_{8,2})\bar{x}^4}$$

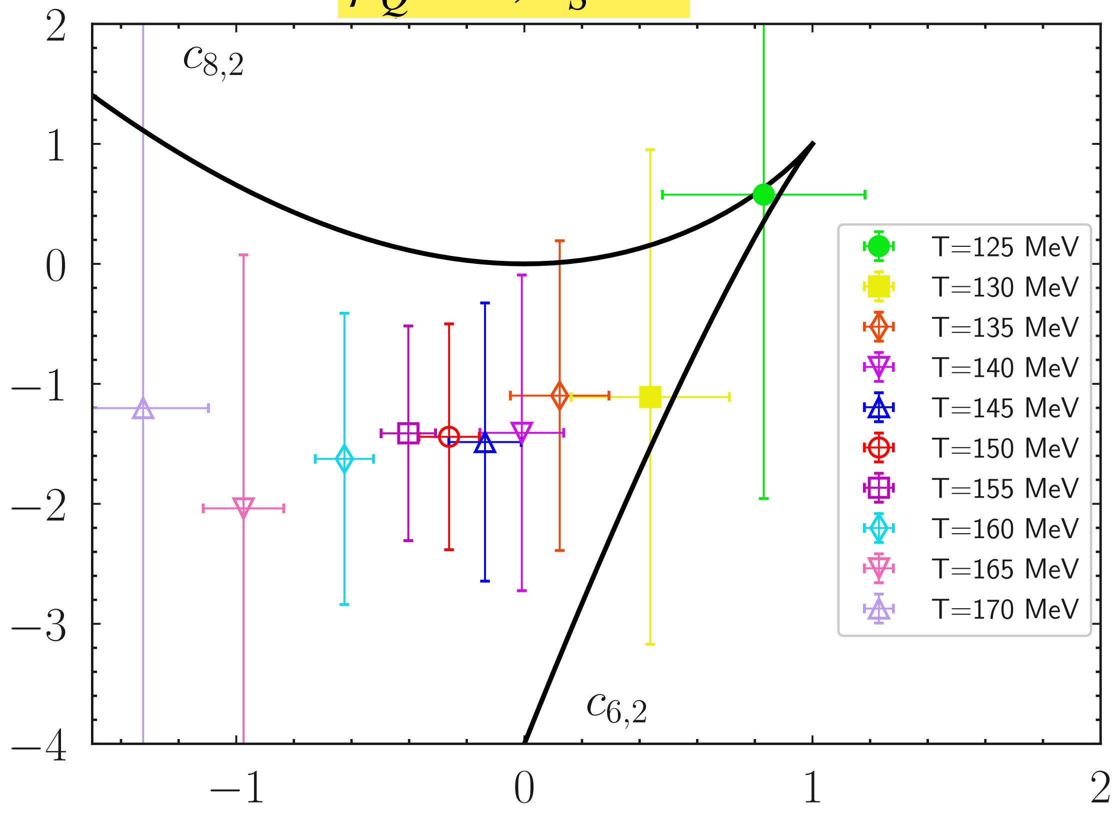
4 poles (two pairs)



$\mu_Q = 0, \mu_S = 0$

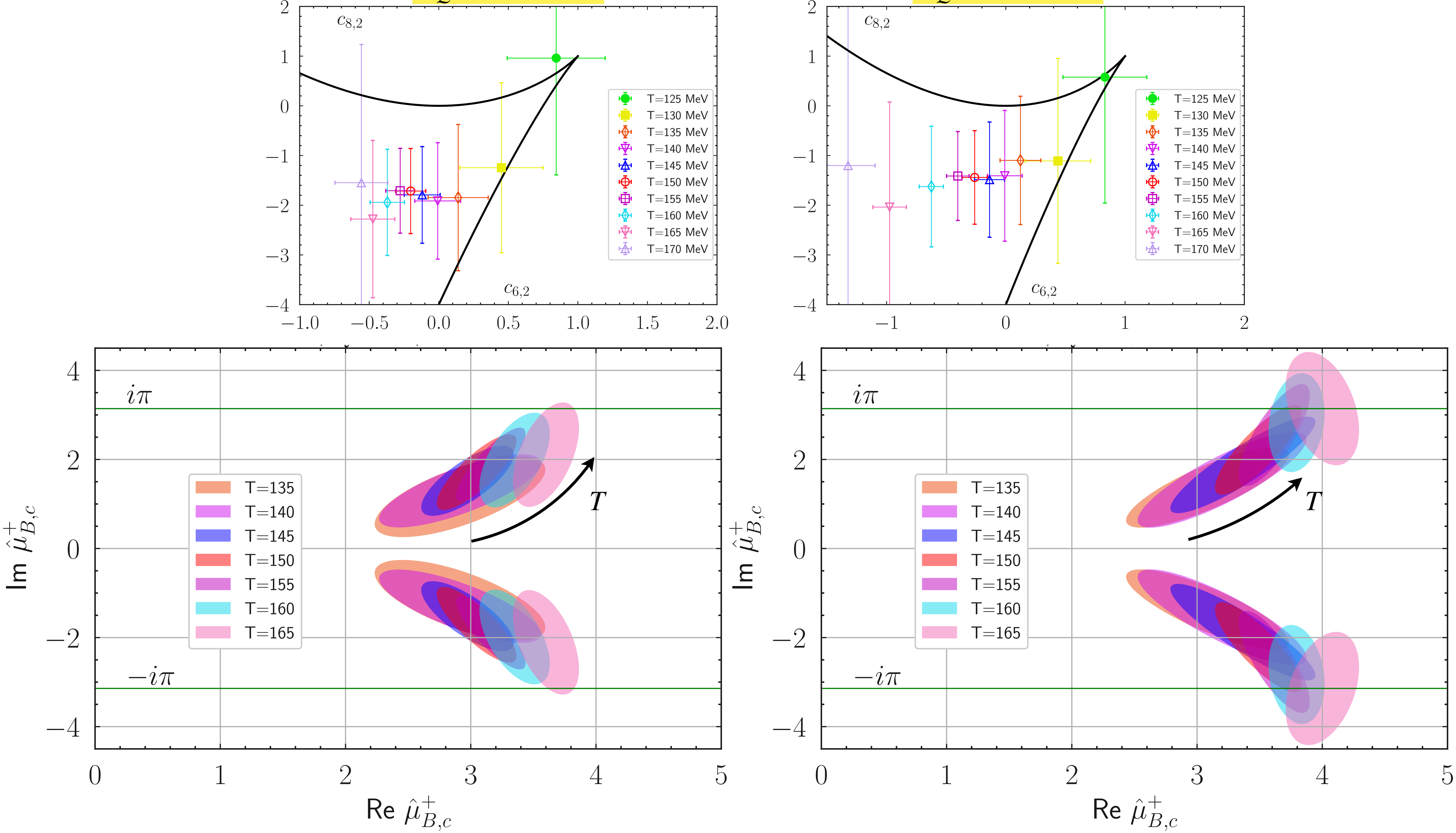


$\mu_Q = 0, n_S = 0$



→ For $T > 135$ MeV we find only complex poles

$\mu_Q = 0, \mu_S = 0$ $\mu_Q = 0, n_S = 0$



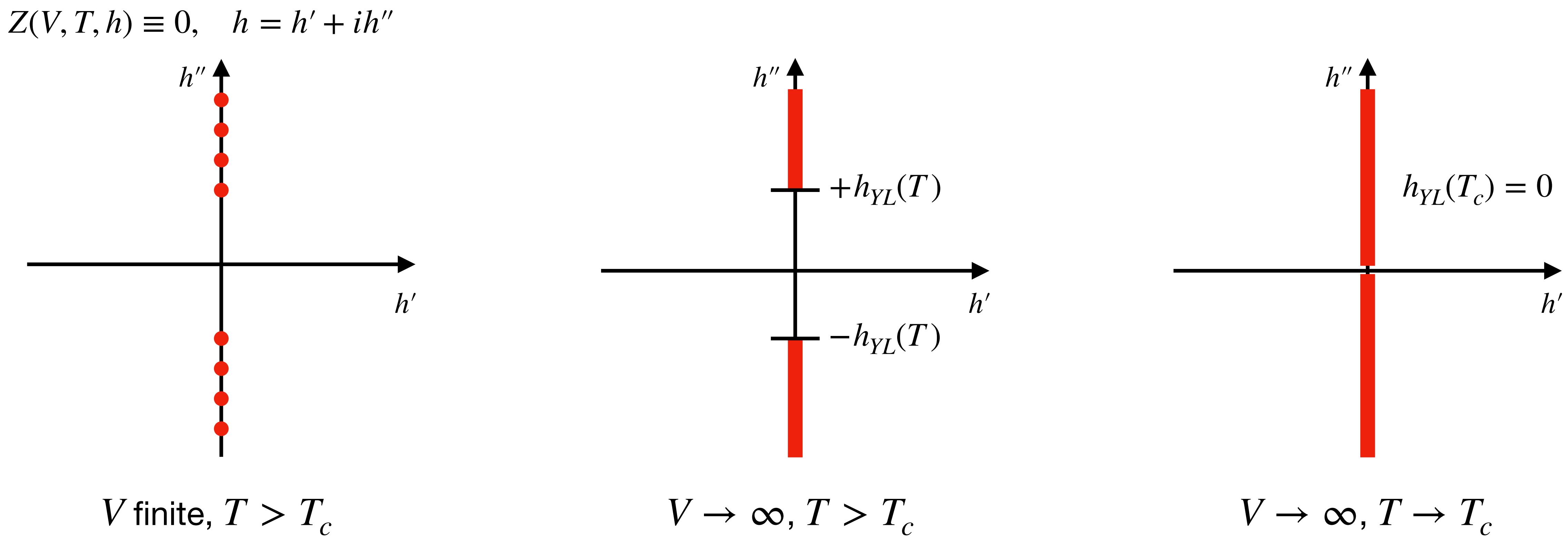
→ Poles approach the real axis with decreasing temperature

→Temperature dependence is currently not in consistence with expected universal scaling

What is a Lee-Yang edge singularity?

Consider a generic ferromagnetic 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 $h' = 0$



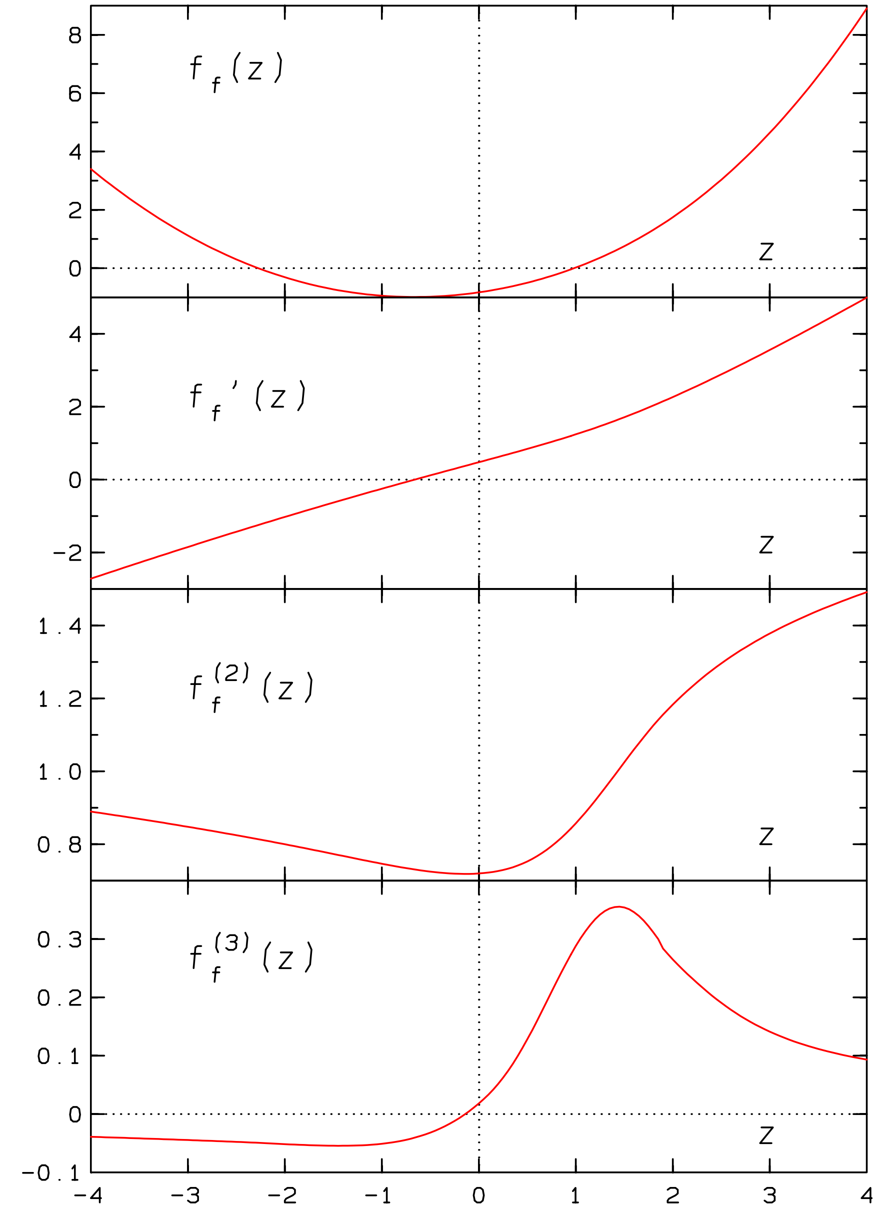
- The density of Lee-Yang zeros $g(T, h'')$ behaves as $g(T, h'') \sim |h'' - h_{YL}(T)|^{\sigma_{LY}}$ for $h'' \to h_{LY}(T)$ from above [Kortman, Griffiths 1971; Fischer 1978].
- Fischer connected the edge-singularity with a phase transition in an φ^3-theory with imaginary coupling [Fischer 1978]
- 5-Loop calculation of this theory yields $\sigma_{LY} \sim 0.075$ (d=3) [Borinsky et al., Phys. Rev. D 103, 116024 (2021)]

What are the universal properties of Lee-Yang edge singularities?

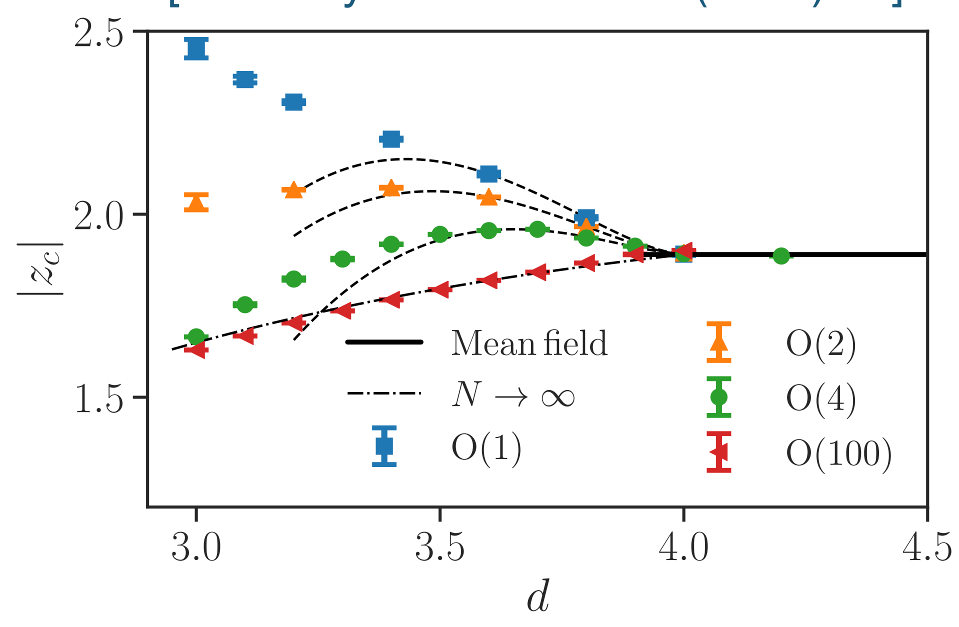
* Scaling relies on the assumption that the singular part of the free energy is a generalised homogeneous function $f(t,h) = b^{-d} f(b^{y_t} t, b^{y_h} h)$ with $t = T - T_c$. We can get rid of one argument by introducing a scaling variable, e.g., $z = t/h^{1/\beta\delta}$ which yields $f = h^{\frac{2-\alpha}{\beta\delta}} f_f(z)$.

* In terms of the scaling variable z, the position of the the Lee-Yang edge singularity is universal. We find $z_{LY} = |z_c| e^{i\frac{\pi}{2\beta\delta}}$. The modulus has been calculated recently by means of functional renormalization group methods

[Engels, Karsch, PRD 85 (2012) 094506]



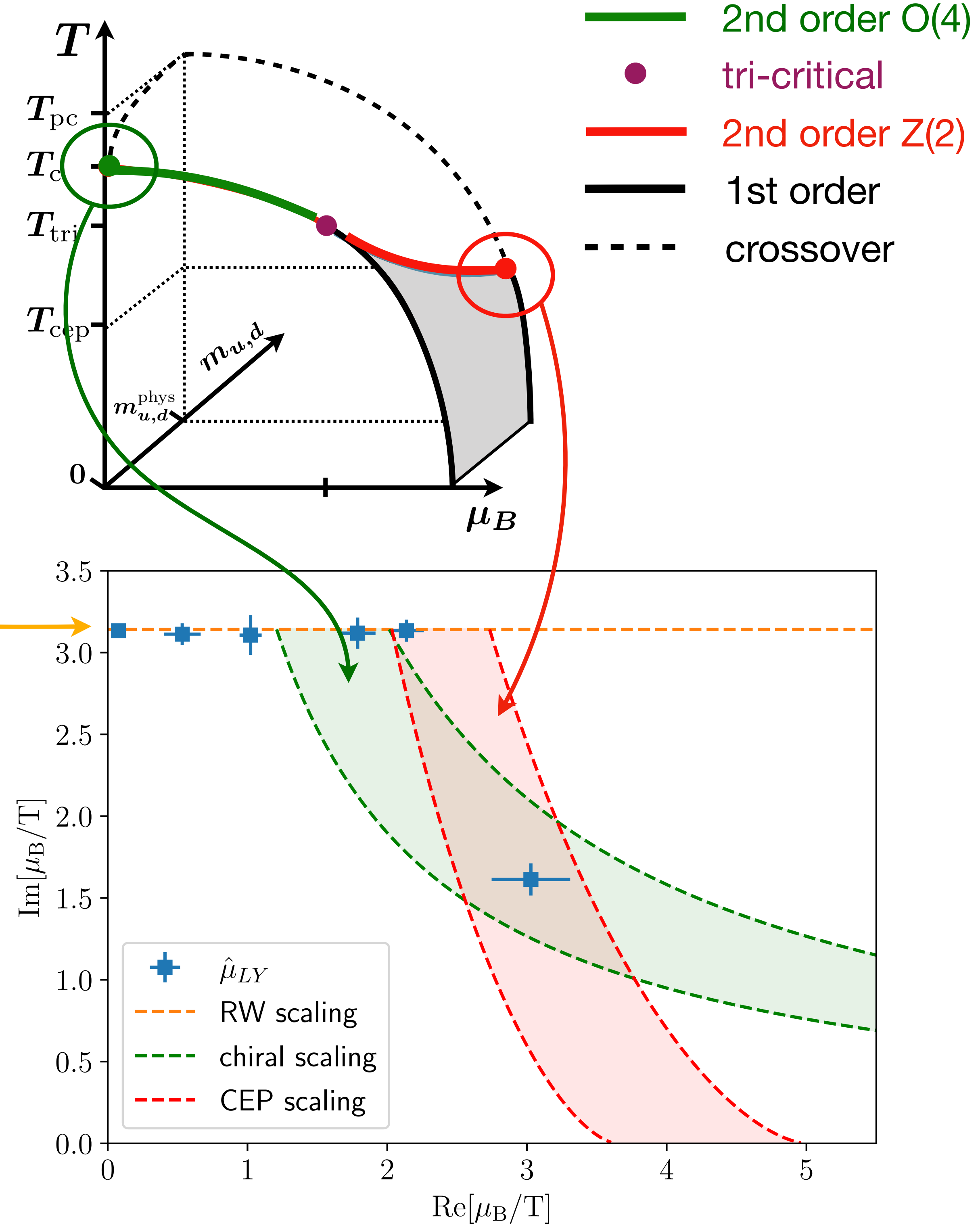
[Connelly et al. PRL 125 (2020) 19]

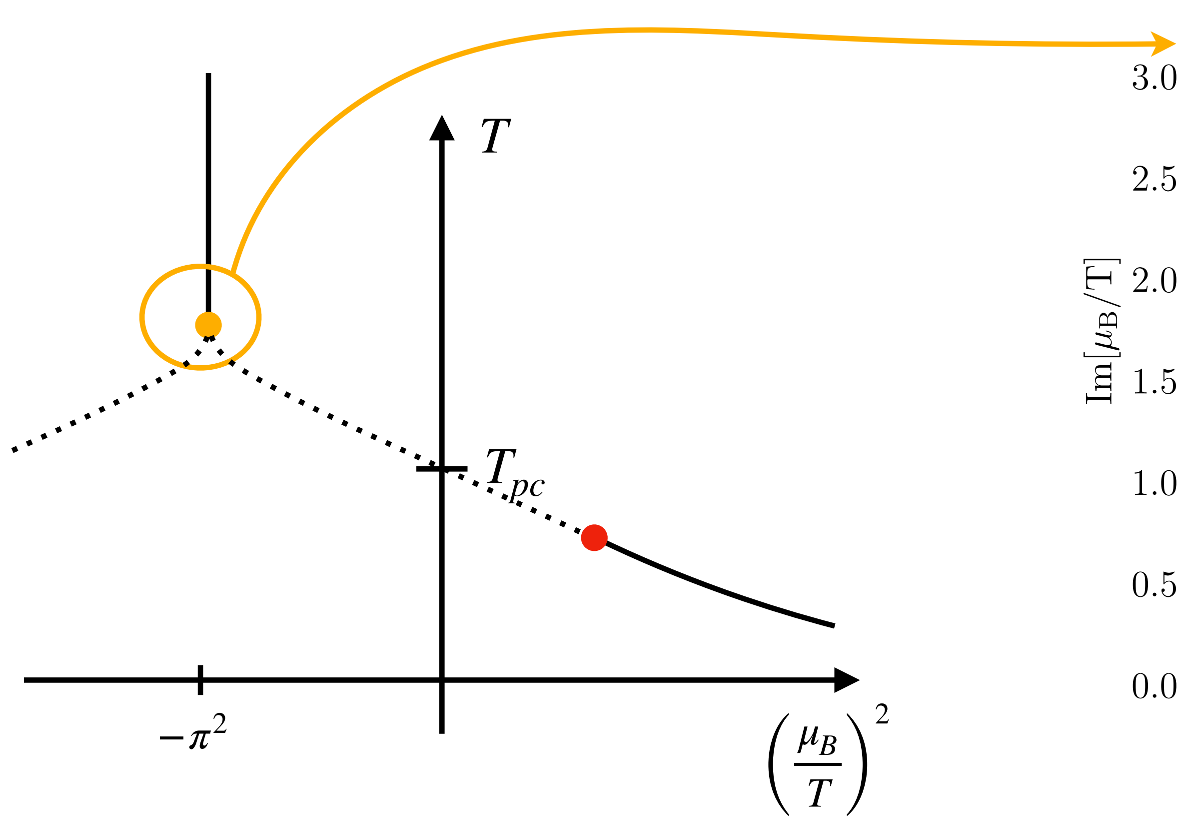


* Eos: $M = h^{1/\delta} f_G(z)$;
The universal scaling function $f_G(z)$ exhibits a branch cut starting at $z = z_{LY}$

Where can we apply our knowledge of Lee-Yang edge singularities in QCD?

* The ultimate goal is the location of the QCD critical point
* We can think of three distinct critical points/ scaling regions: Roberge Weiss transition, chiral transition, QCD critical point



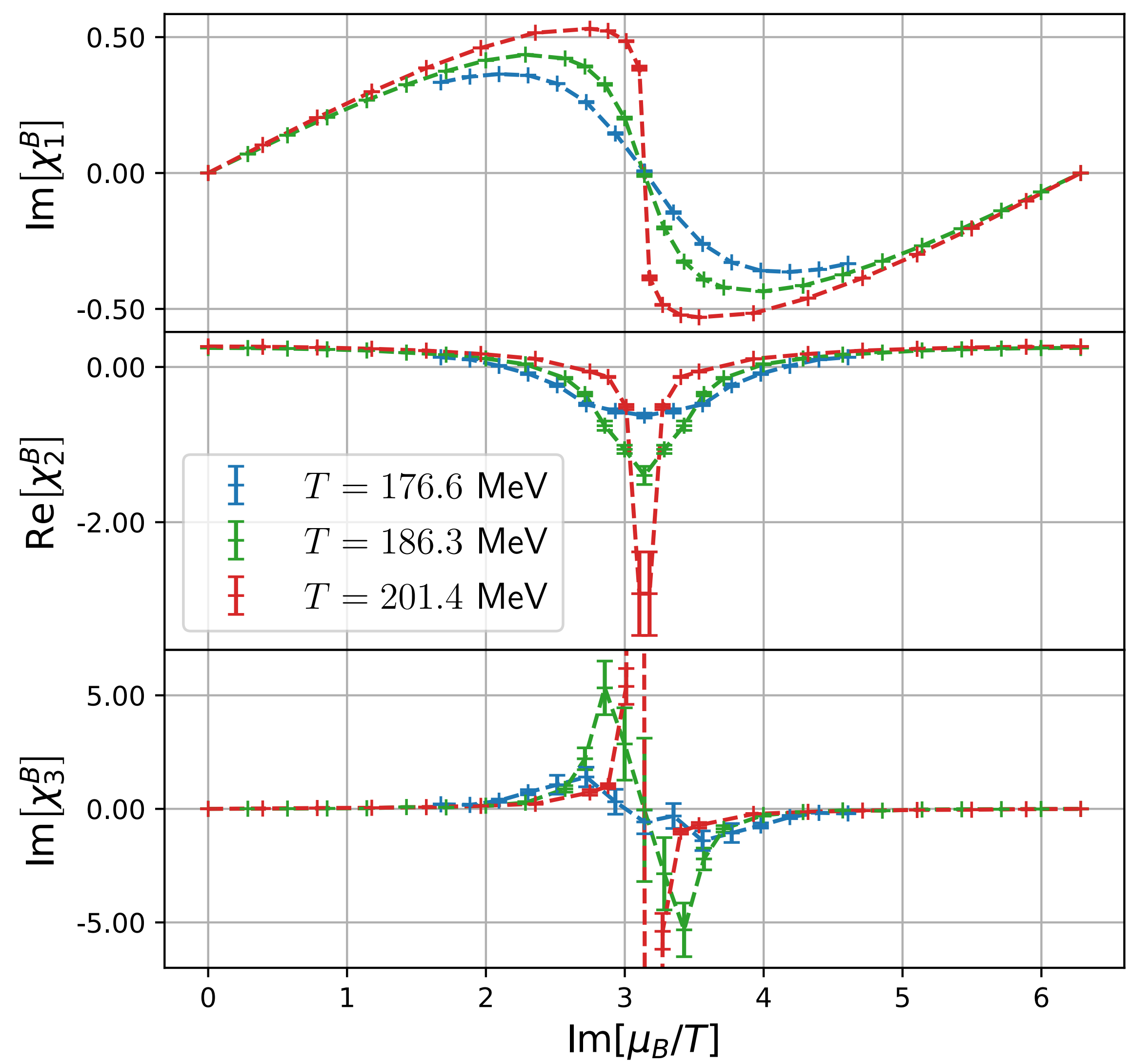


[Dimpoulos et al. (Bielefeld-Parma) PRD 105 (2022) 034513]

Input data from Lattice QCD:

- 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

Lattice size: $24^3 \times 4$



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

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

Standard Padé:

* Starting point is a power series

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

* 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

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

* 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 $m + n + 1 = \sum_k (L_k + 1)$

- Here we use $f = \chi_1^B$ and $x = \mu_B$
- Solving the linear system in the μ_B/T plane with two different *Ansatz* functions
- The most general form (*Ansatz* **NS**)

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

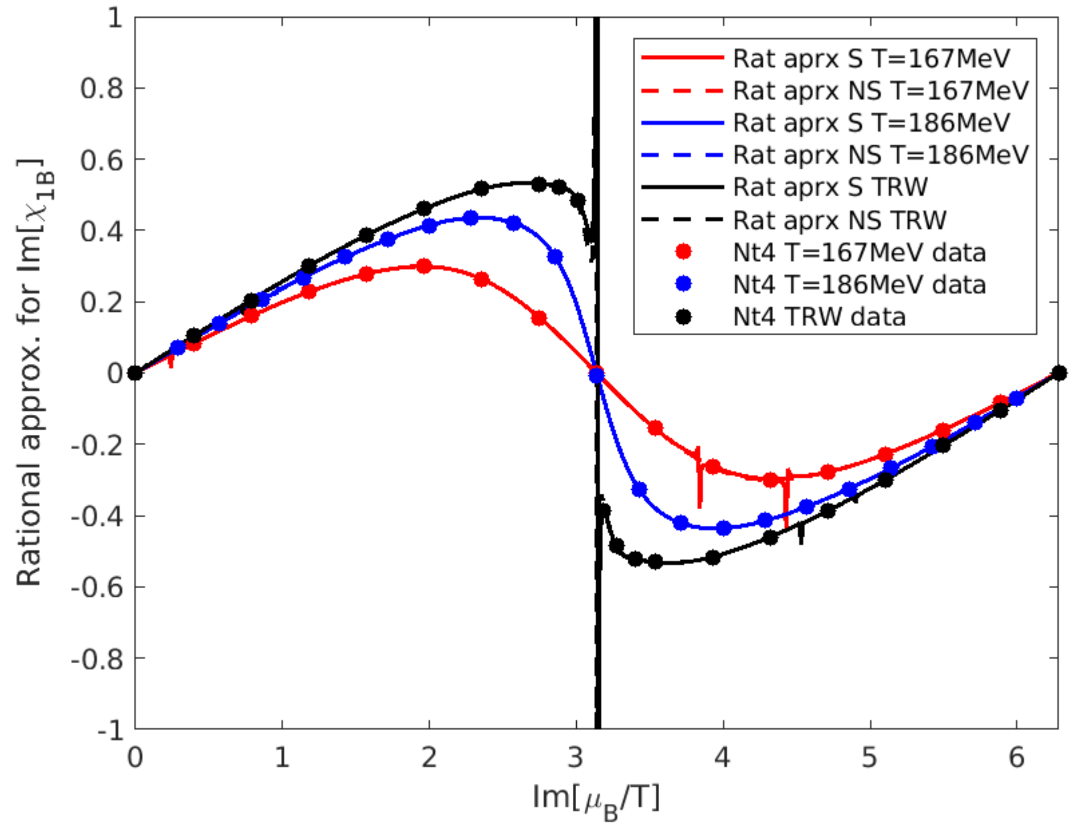
- Taking into account the expected parity of the net baryon number density (*Ansatz* **S**)

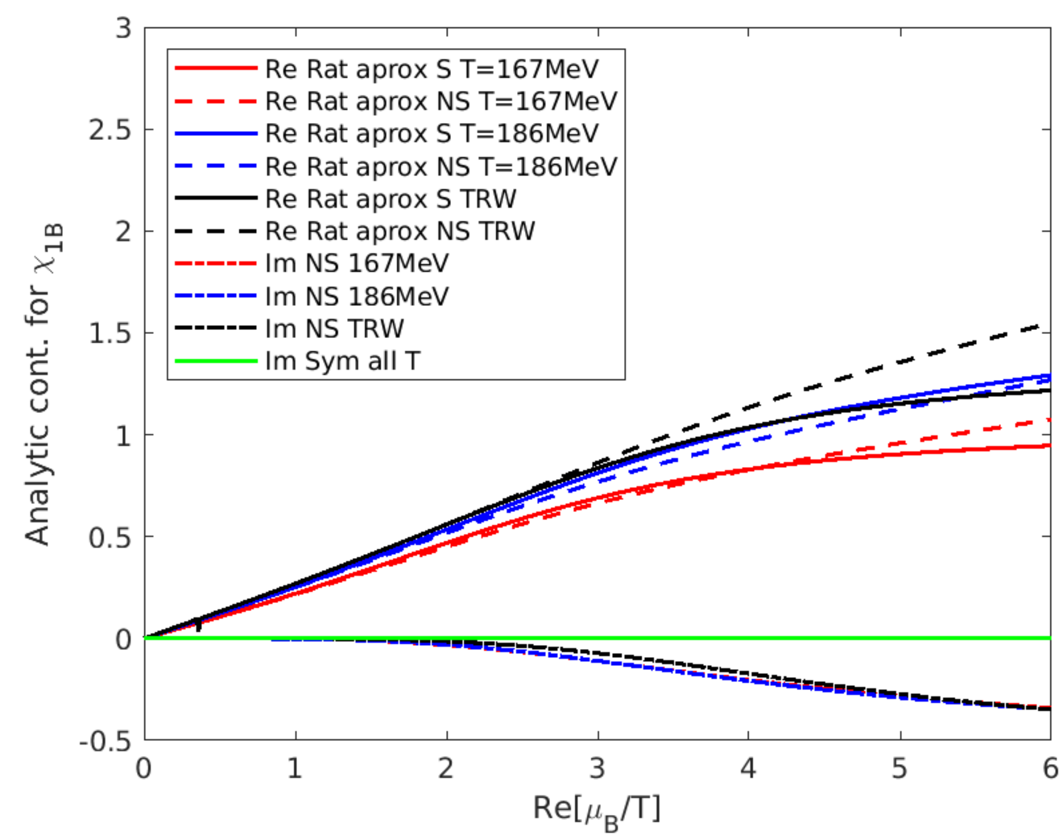
$$R_n^m(x) = \frac{\sum_{i=0}^{m'} a_{2i+1}\, x^{2i+1}}{1 + \sum_{j=1}^{n/2} b_{2j}\, x^{2j}} \qquad \text{with}$$

$$m = 2m' + 1;\ \ a_i, b_i \in \mathbb{R};\ \ a_1 = \chi_2^B(T, V, 0)$$

This ensures the correct parity for all χ_n^B, and a real valued analytic continuation.

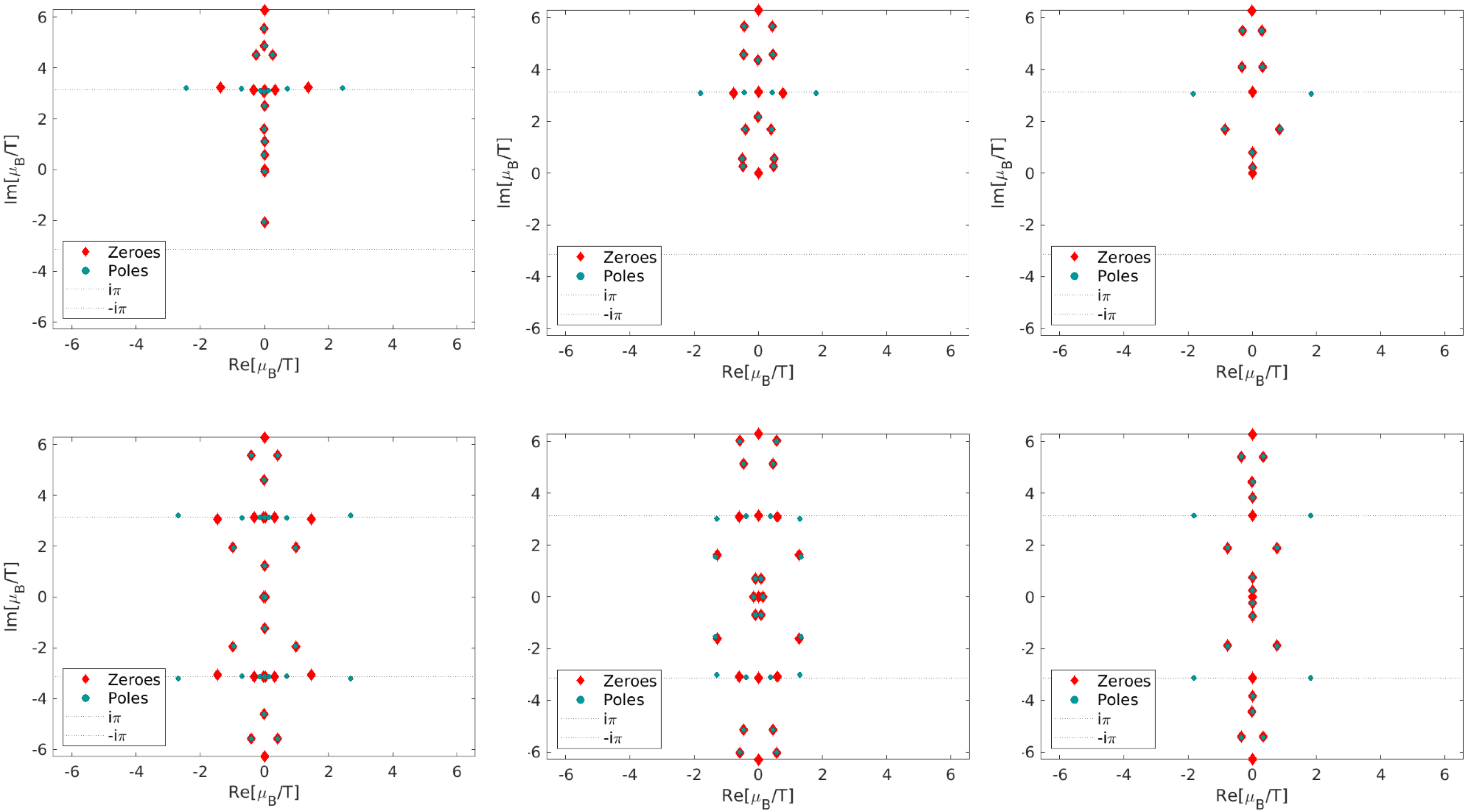
→ find agreement in analytic continuation of both *for* $\mu_B/T \lesssim 2.5$





[Dimpoulos et al. (Bielefeld-Parma) PRD 105 (2022) 034513]

$T = 201\,MeV = T_{RW}$ | $T = 186\,MeV$ | $T = 167\,MeV$



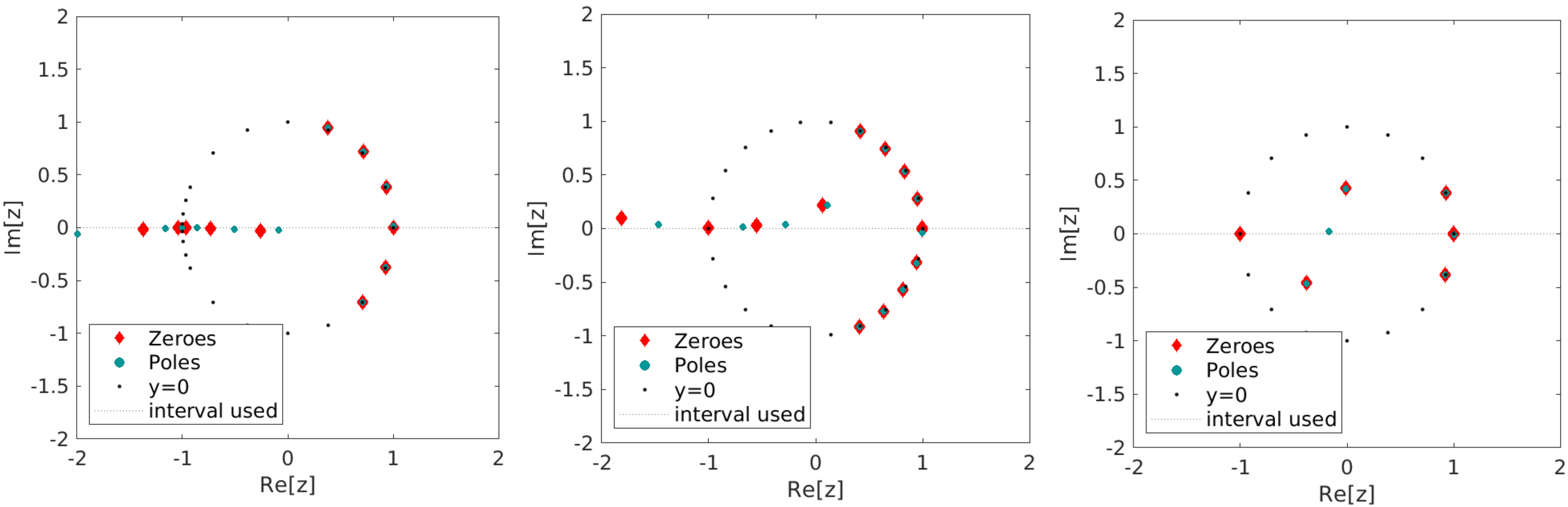
(NS)

(S)

→ find almost perfect cancelation of many zeros and poles

→ find signature for branch cut along $\mu_B/T = \mu_B^R \pm i\pi$ at $T = \{201,186\}$ MeV

[Dimpoulos et al. (Bielefeld-Parma) PRD 105 (2022) 034513]



- We can solve the linear system in the fugacity plane

  → find signature for branch cut along $z = -z^R$ at $T = \{201{,}186\}$ MeV

- First steps toward using more complicated conformal mappings [Skokov, Morita, Friman PRD 83 (2011); Basar Dunne 2112.14269]
- It has been argued that certain conformal mappings improve analytic continuation and sensitivity to the QCD critical point

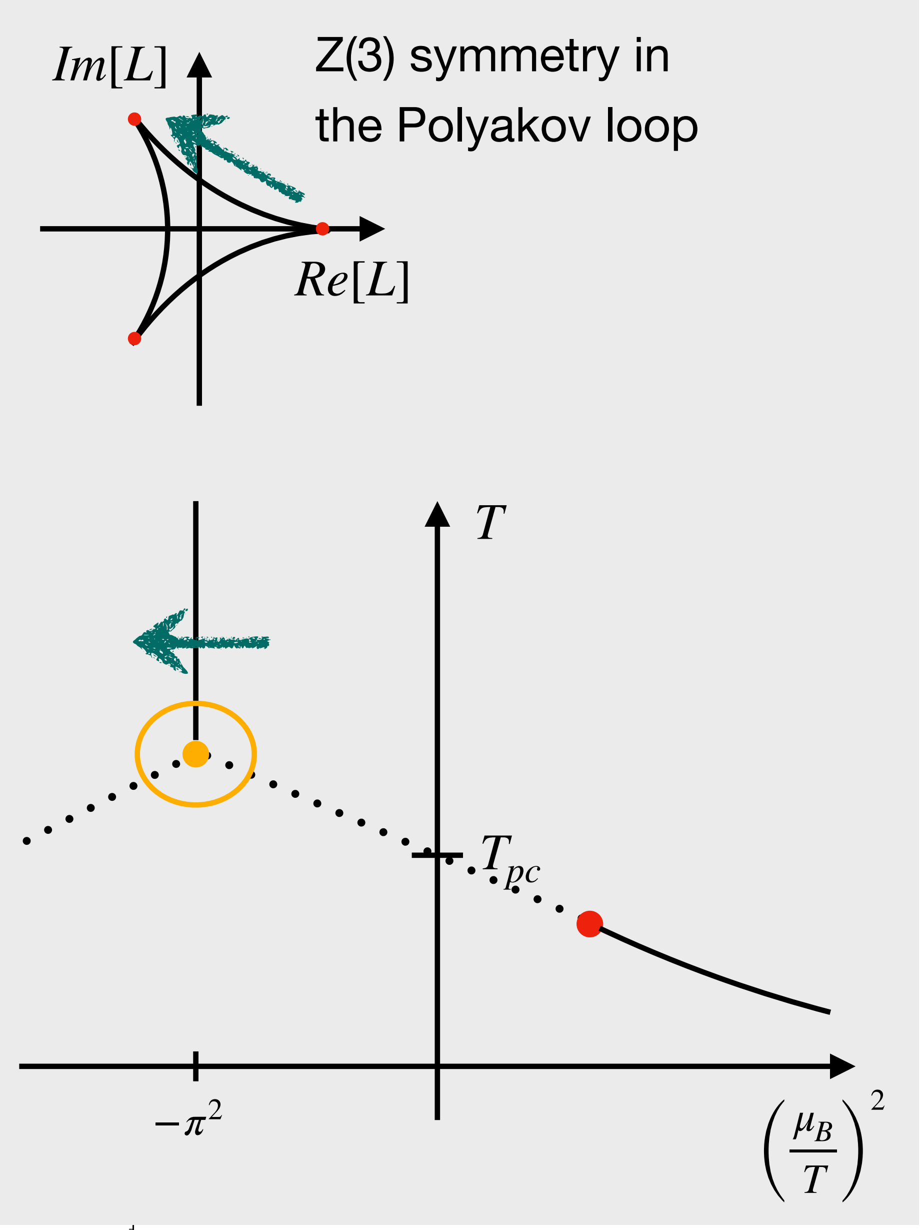
[Dimpoulos et al. (Bielefeld-Parma) PRD 105 (2022) 034513]

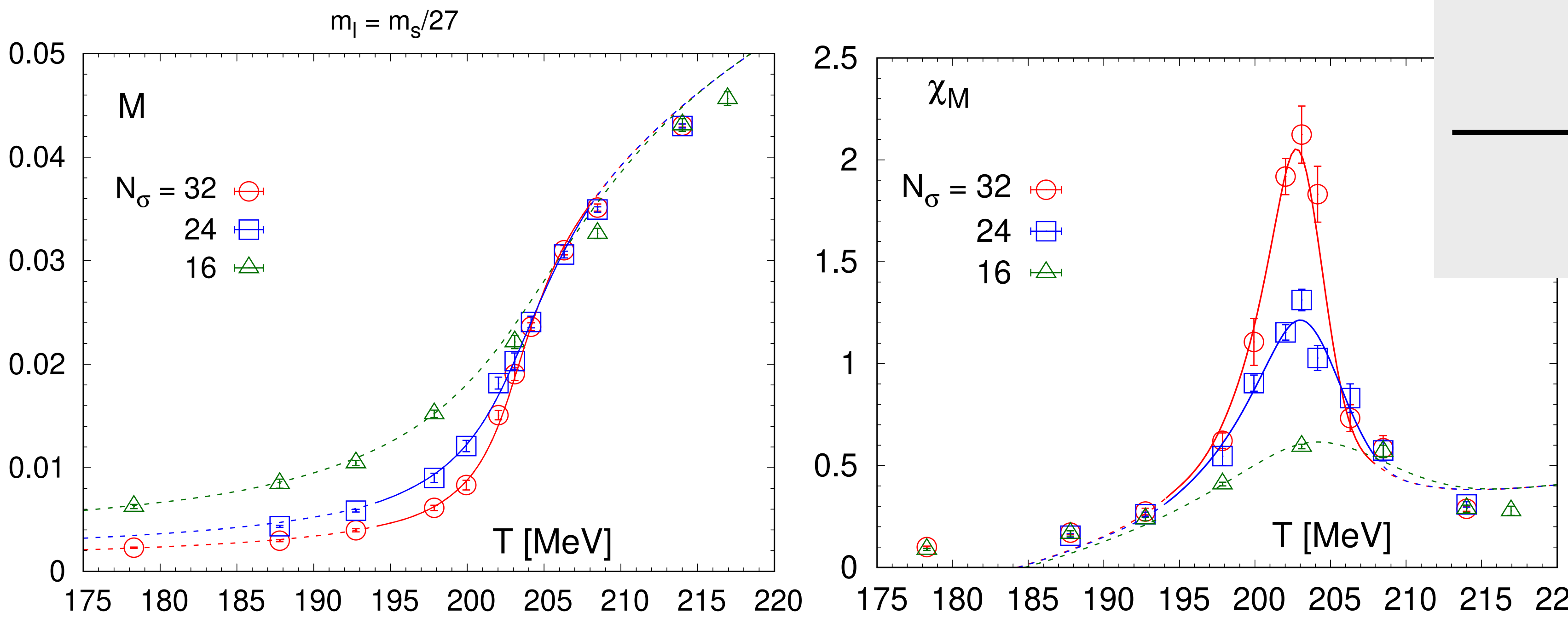
Can we interpret the closest singularity as Lee-Yang edge singularity?

- At physical quark masses the Roberge-Weiss critical point is the Z(2) symmetric end point of a line of first order transitions.
- Need to map QCD parameter to the scaling fields t, h. For the Roberge-Weiss Transition we make the following Ansatz

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

- For our lattice setup [(2+1)-flavor of HISQ, $N_\tau = 4$] we know the position of the critical point $(T_{RW}, \mu_{B_{RW}} = (201\ \text{MeV}, i\pi))$





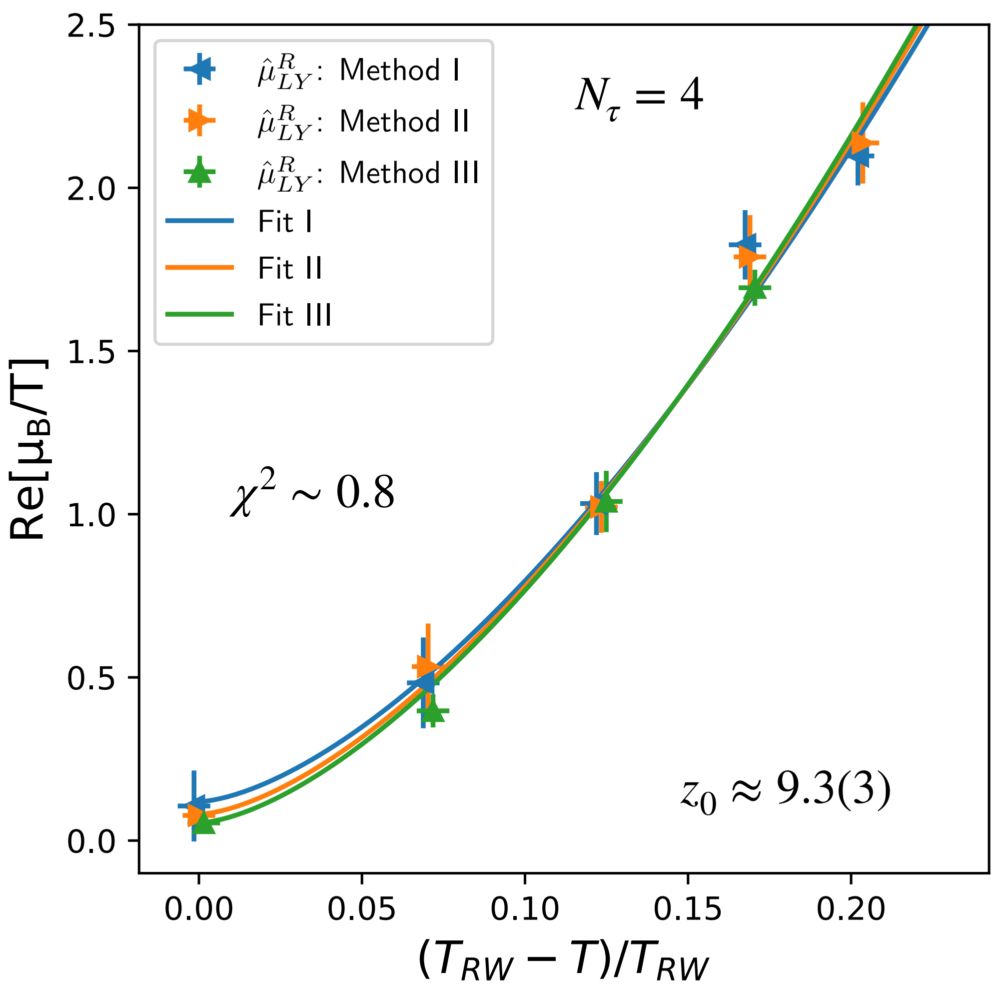
[J. Goswami, Lattice 2021]
[Bielefeld-Frankfurt, arXiv:2205.12707]

Can we interpret the closest singularity as Lee-Yang edge singularity?

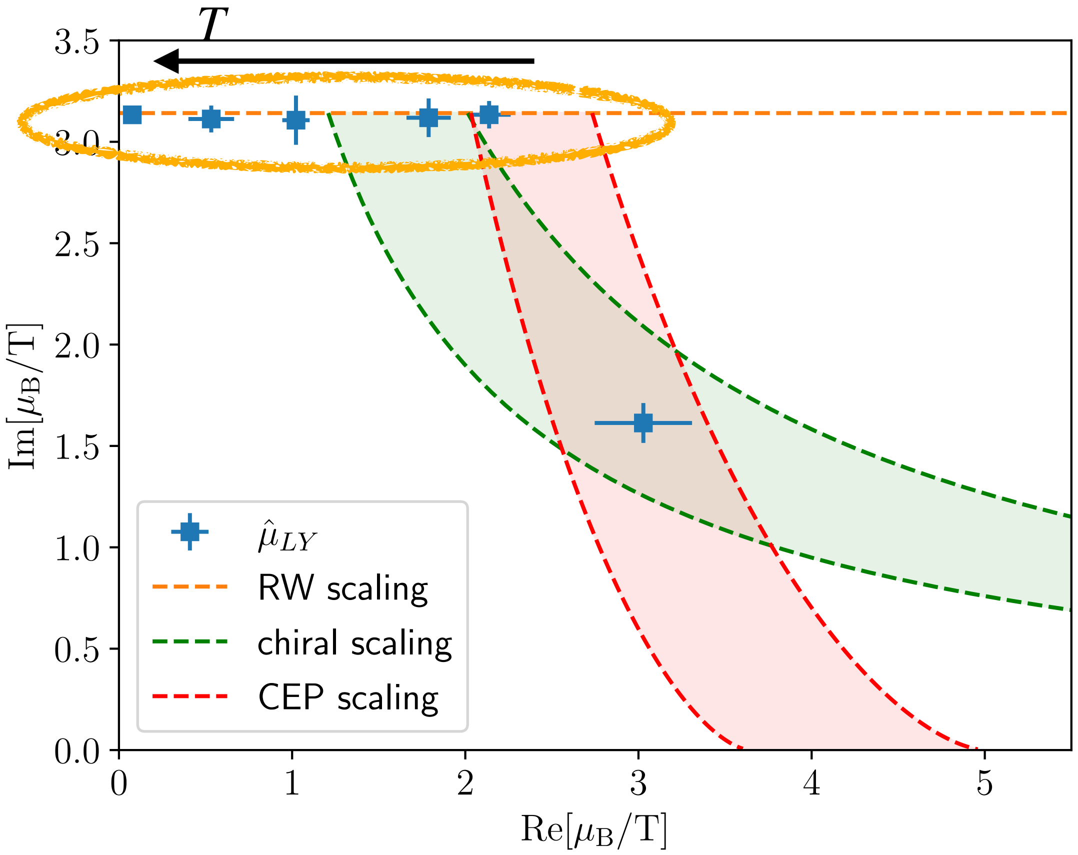
- We can look at the temperature dependence of our singularities. By solving $z = t/h^{1/\beta\delta} \equiv z_c$ we find

$$\hat{\mu}^R_{LY} = \pm \pi \left(\frac{z_0}{|z_c|}\right)^{\beta\delta} \left(\frac{T_{RW} - T}{T_{RW}}\right)^{\beta\delta} \text{ and } \hat{\mu}^I_{LY} = \pm \pi$$

with $z_0 = t_0/h_0^{1/\beta\delta}$ and $\hat{\mu} = \mu/T$.



→find good agreement with RW-scaling



Method I: solving the linear system in the $\hat{\mu}_B$ plane

Method II: minimize a generalised $\tilde{\chi}^2$, (combined fit to all data)

$$\tilde{\chi}^2 = \sum_{j,k} \frac{\left| \frac{\partial^j R^m_n}{\partial \hat{\mu}^j_B}(\hat{\mu}_{B,k}) - \chi^B_{j+1}(\mu_{B,k}) \right|^2}{\left| \Delta\chi^B_{j+1}(\hat{\mu}_{B,k}) \right|^2}$$

Method III: solving the linear system in the z plane, and mapping the result back to $\hat{\mu}_B$

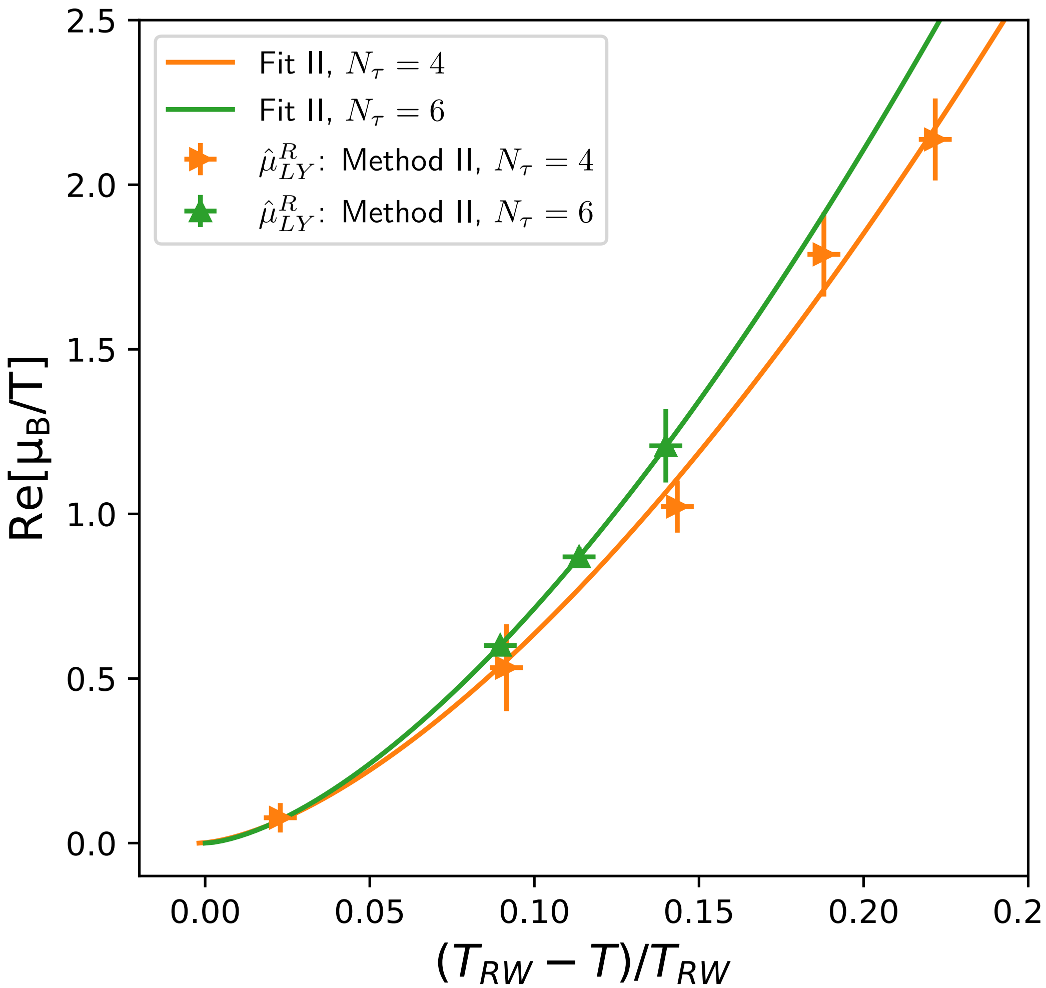
[Dimpoulos et al. (Bielefeld-Parma) PRD 105 (2022) 034513]

Can we interpret the closest singularity as Lee-Yang edge singularity?

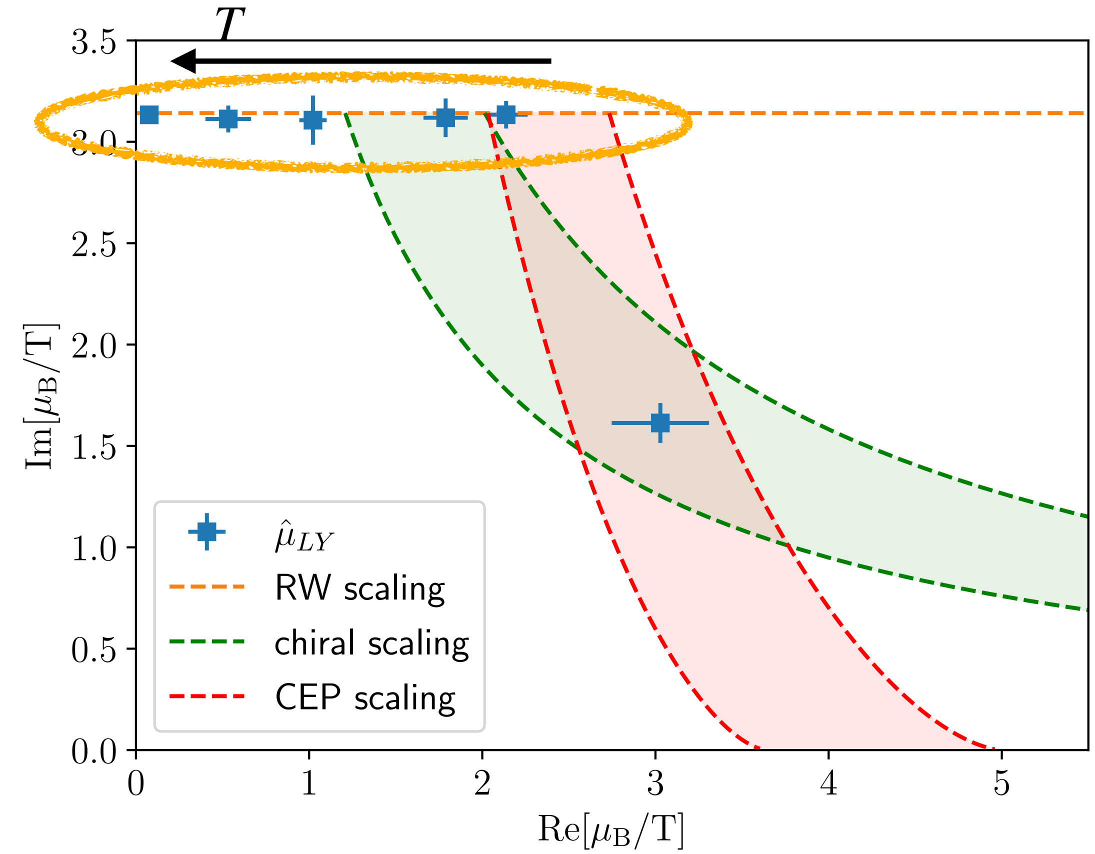
* We can look at the temperature dependence of our singularities. By solving $z = t/h^{1/\beta\delta} \equiv z_c$ we find

$$\hat{\mu}_{LY}^{R} = \pm \pi \left(\frac{z_0}{|z_c|}\right)^{\beta\delta} \left(\frac{T_{RW}-T}{T_{RW}}\right)^{\beta\delta} \quad \text{and} \quad \hat{\mu}_{LY}^{I} = \pm \pi$$

with $z_0 = t_0/h_0^{1/\beta\delta}$ and $\hat{\mu} = \mu/T$.



→find good agreement with RW-scaling



Method I: solving the linear system in the $\hat{\mu}_B$ plane

Method II: minimize a generalised $\tilde{\chi}^2$, (combined fit to all data)

$$\tilde{\chi}^2 = \sum_{j,k} \frac{\left|\frac{\partial^j R_n^m}{\partial \hat{\mu}_B^j}(\hat{\mu}_{B,k}) - \chi_{j+1}^B(\mu_{B,k})\right|^2}{\left|\Delta\chi_{j+1}^B(\hat{\mu}_{B,k})\right|^2}$$

Method III: solving the linear system in the z plane, and mapping the result back to $\hat{\mu}_B$

[Dimpoulos et al. (Bielefeld-Parma) PRD 105 (2022) 034513]

* The chiral transition is very well studied by the HotQCD collaboration. Important nonuniversal constants are known.

* Ansatz for the scaling fields is give by

$$t = t_0 \left[\frac{T - T_c}{T_c} + \kappa_2^B \left(\frac{\mu_B}{T} \right)^2 \right]$$

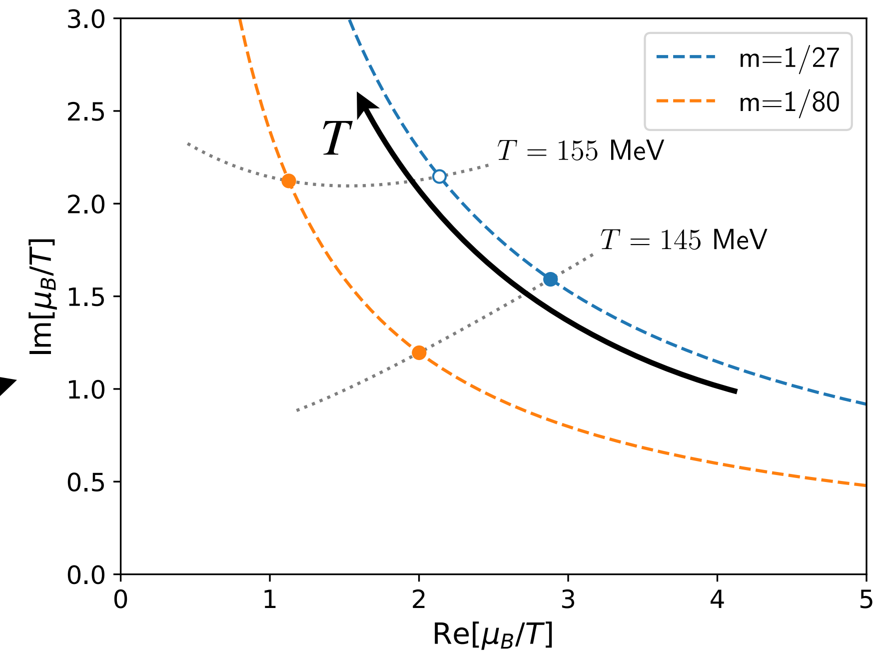
$$h = h_0 \frac{m_l}{m_s^{\text{phys}}}$$

* We solve again for $\hat{\mu}_{LY}$ by setting $z = z_c$ and obtain

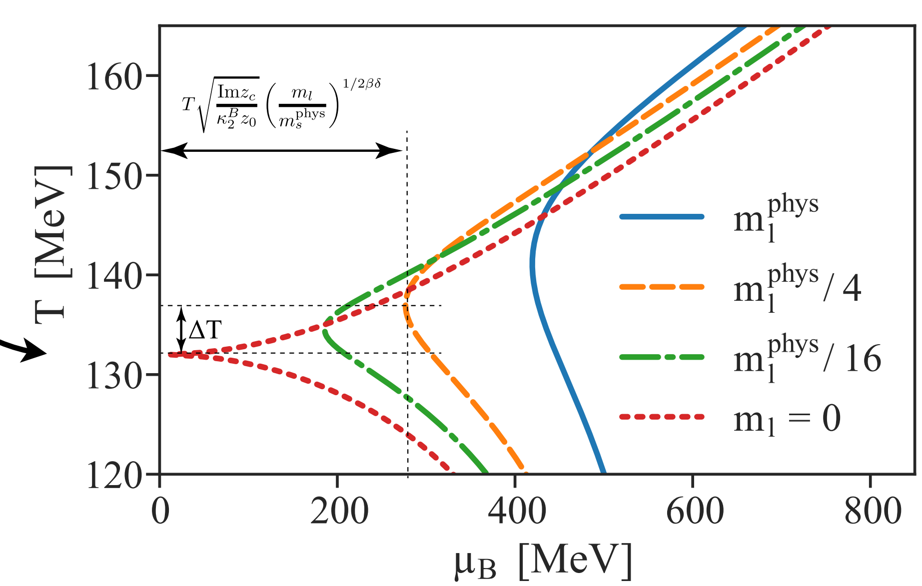
$$\hat{\mu}_{LY} = \left[\frac{1}{\kappa_2^B} \left(\frac{z_c}{z_0} \left(\frac{m_l}{m_s^{\text{phys}}} \right)^{1/\beta\delta} - \frac{T - T_c}{T_c} \right) \right]^{1/2}$$

Required input: T_c, κ_2^B, z_0, z_c

Position of the LYE

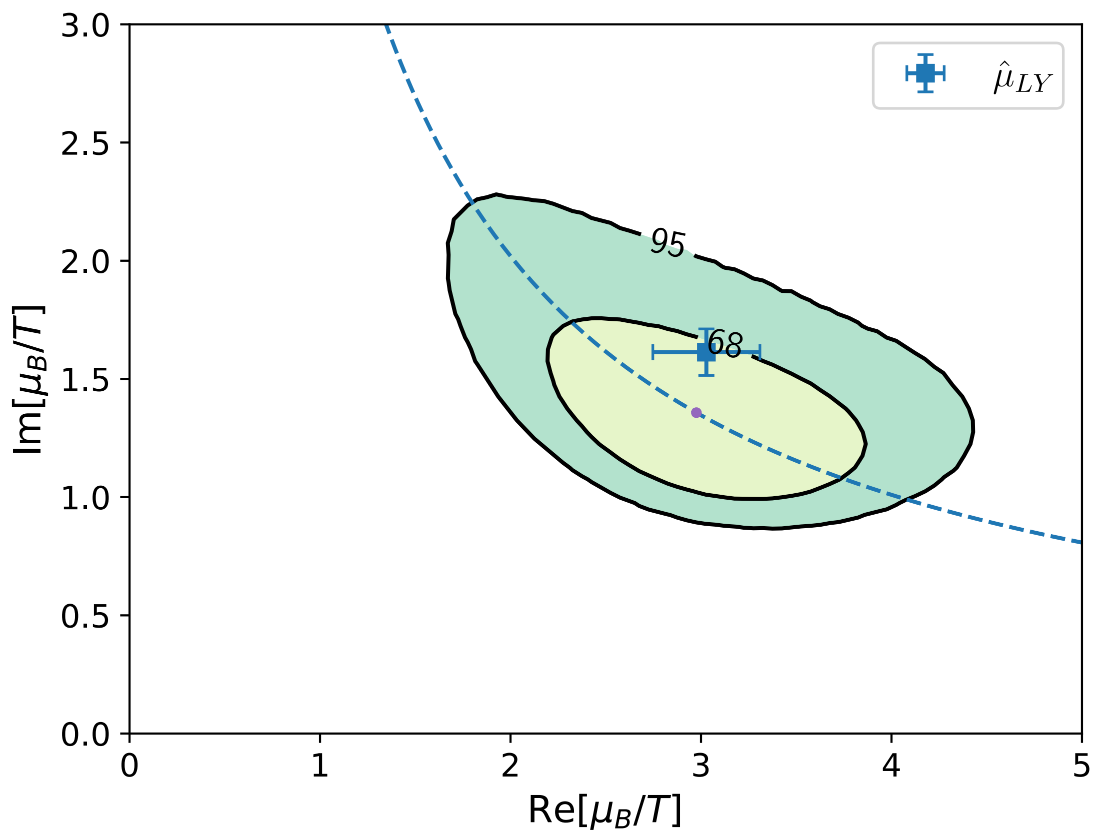


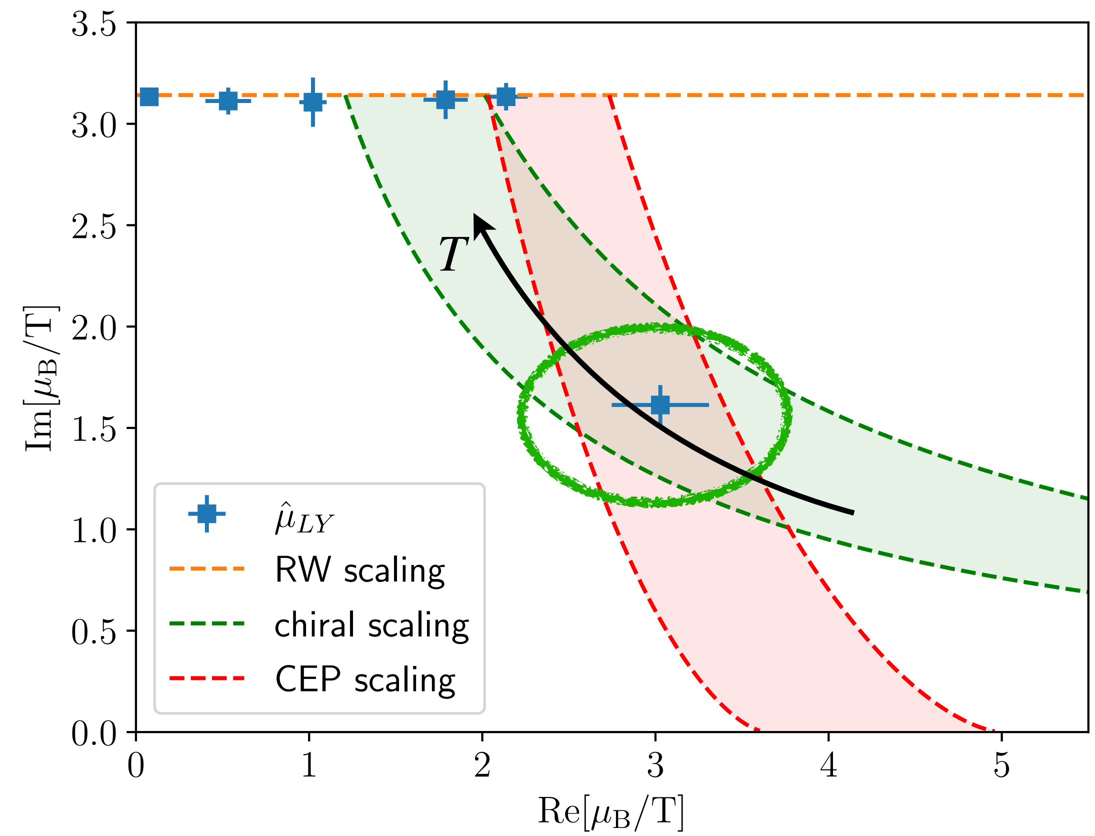
The radius of convergence



[Mukherjee, Skokov, PRD 103 (2021) 071501]

* Comparison of the prediction with the actually found singularity of the multipoint Padé





* 68% and 95% confidence regions of the prediction are generated with the following $N_\tau = 6$ specific values for the nonuniversal constants

$$
\left.\begin{aligned}
T_c &= (147 \pm 6)\ \text{MeV}\,, \\
z_0 &= 2.35 \pm 0.2\,, \\
\kappa_2^B &= 0.012 \pm 0.002\,,
\end{aligned}\right\}
$$

[HotQCD], Gaussian error distribution assumed

$|z_c| = 2.032$ (O(2)) value [Connelly et al. PRL 125 (2020) 19]

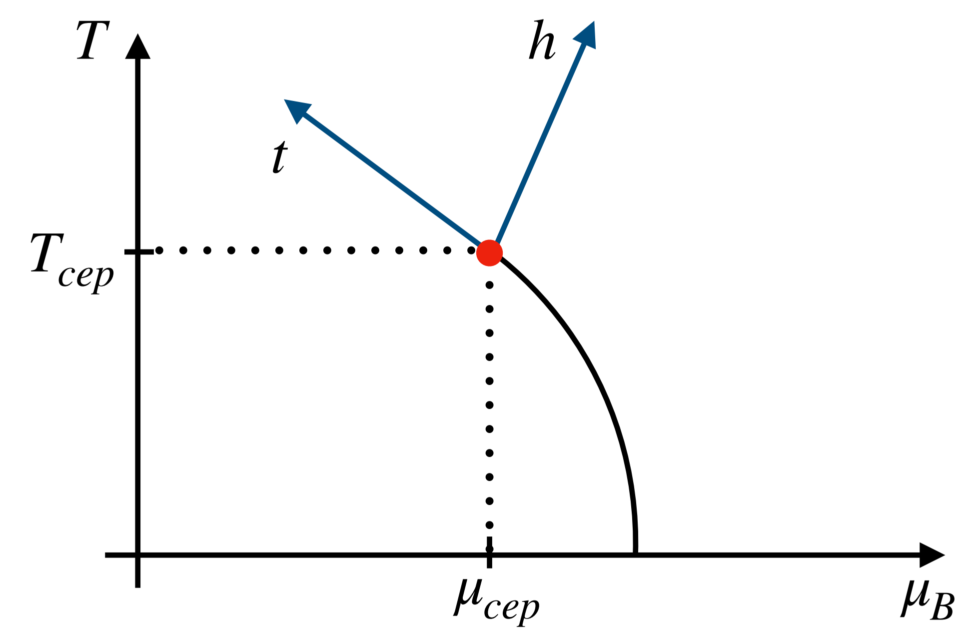
→find good agreement. Coincidence? Need more data.

[Dimpoulos et al. (Bielefeld-Parma) PRD 105 (2022) 034513]

* Scaling fields are unknown, a frequently used *ansatz* is given by a linear mapping

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

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



* For the Lee-Yang edge singularity we obtain

$$\mu_{LY} = \mu_{cep} - c_1(T - T_{cep}) + ic_2|z_c|^{-\beta\delta}(T - T_{cep})^{\beta\delta},$$

Real part: linear in T

Imaginary part: power law

The coefficient only depends on the slope of the crossover line

$$c_1 = \beta_T/\beta_\mu$$

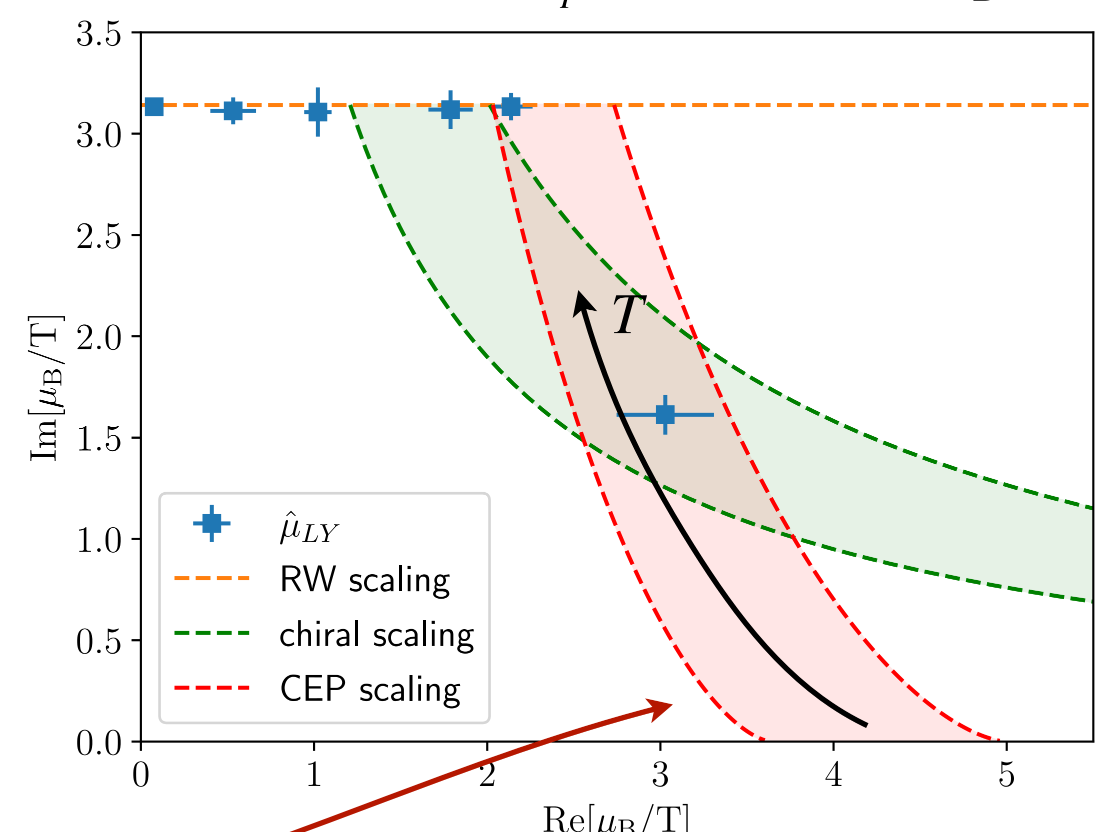
* To visualise the scaling we use some ad-hoc values

$\mu_{cep} = 500 - 630$ MeV

$T_{cep} = T_{pc}(1 - \kappa_2^B \hat{\mu}_B^2)$

$\kappa_2^B = 0.012$ $\quad c_1 = 0.024$

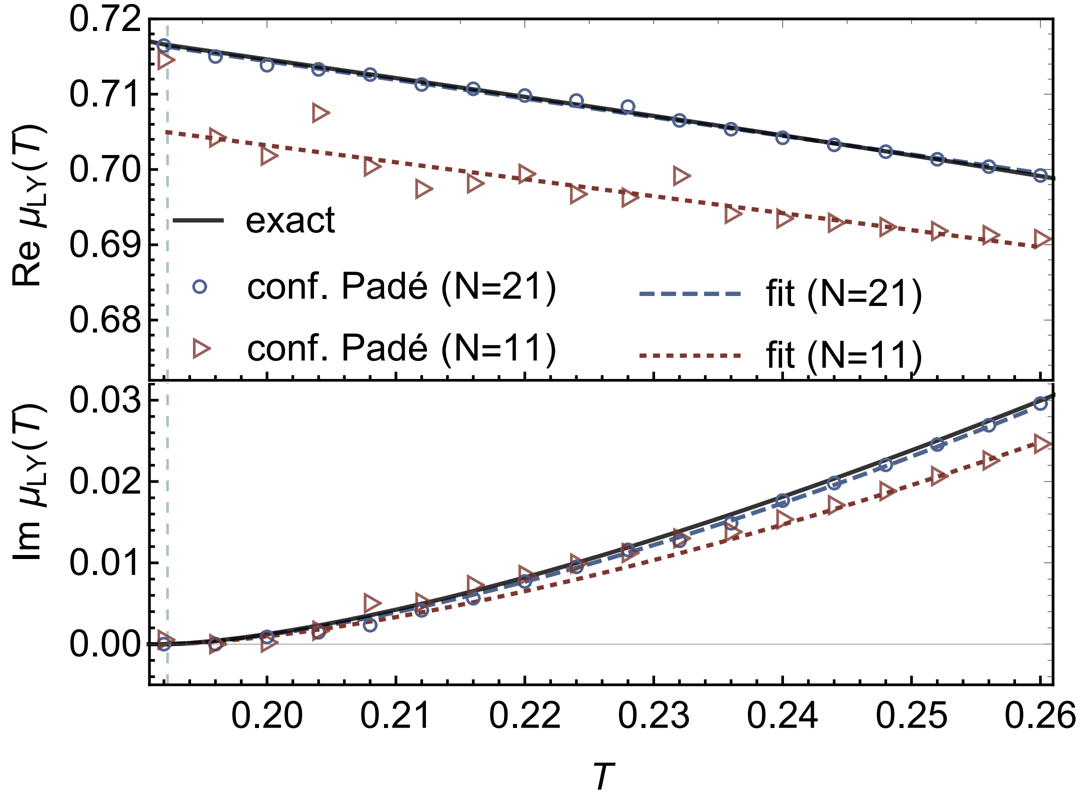
$T_{pc} = 156.5$ MeV $\quad c_2 = 0.5$



- In the Gross-Neveu model, it has been demonstrated that a scaling analysis of the Lee-Yang edge singularities can be used to determine the critical point

- However, 8th order is not sufficient to extract the correct results.

→ Need more precise data from lattice QCD



[Basar, PRL 127 (2021) 171603]