From extrapolation to direct simulations at finite chemical potential

based on [2002.02821] [2102.06625] [2102.06660] [2108.09213]

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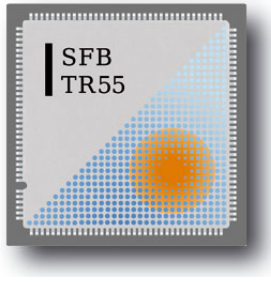
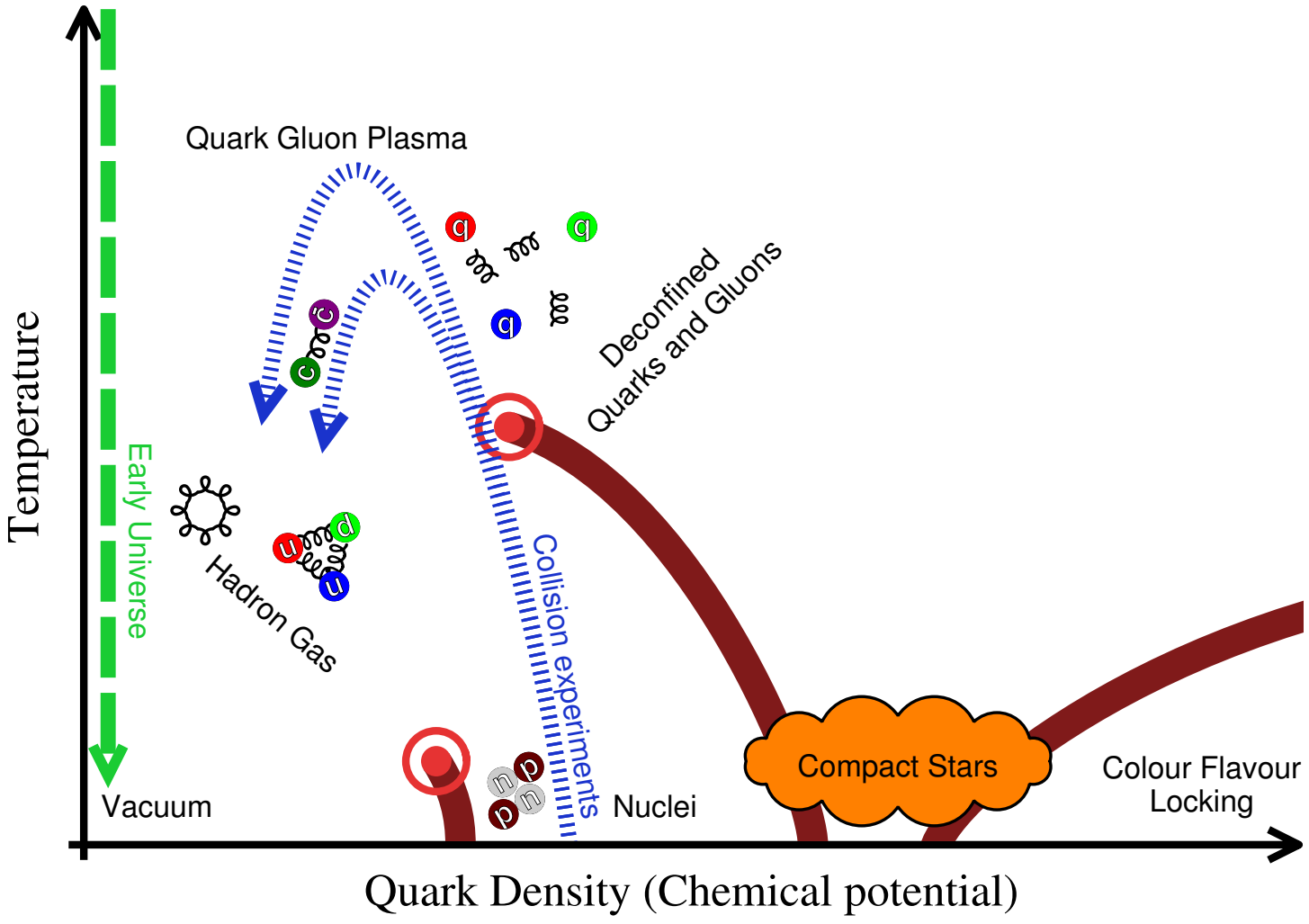
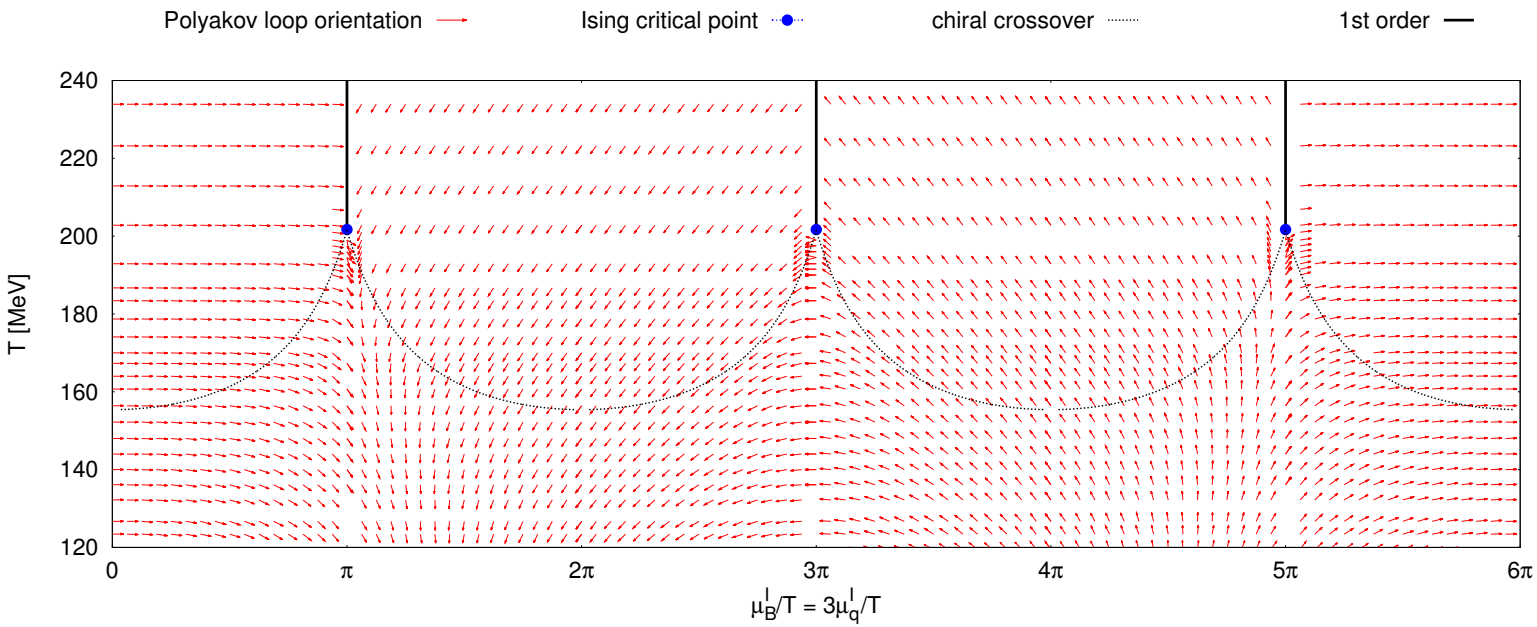
29 October, 2021 YTIP
QCD phase diagram and lattice QCD



The QCD phase diagram

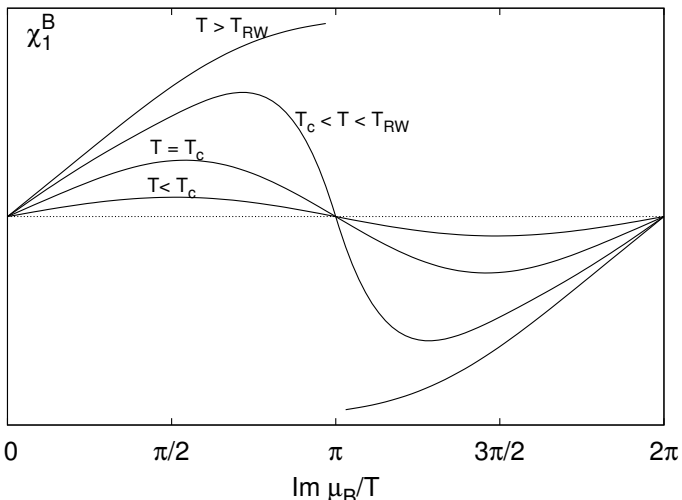


Phase diagram at imaginary baryo-chemical potential:



[Fodor &Katz hep-lat/0104001] [de Forcrand & Philipsen hep-lat/0205016] [D'Elia & Lombardo hep-lat/0209146]

[D'Elia et al 0705.3814] [Philipsen 0708.1293, 1402.0838] [Cea et al hep-lat/0612018,0905.1292,1202.5700]



At low T only B states contribute:

$$\chi_1^B \sim \sin(\mu_B/T)$$

At high T fractional charges are required to make a first order transition at $\mu_B = \pi T$:

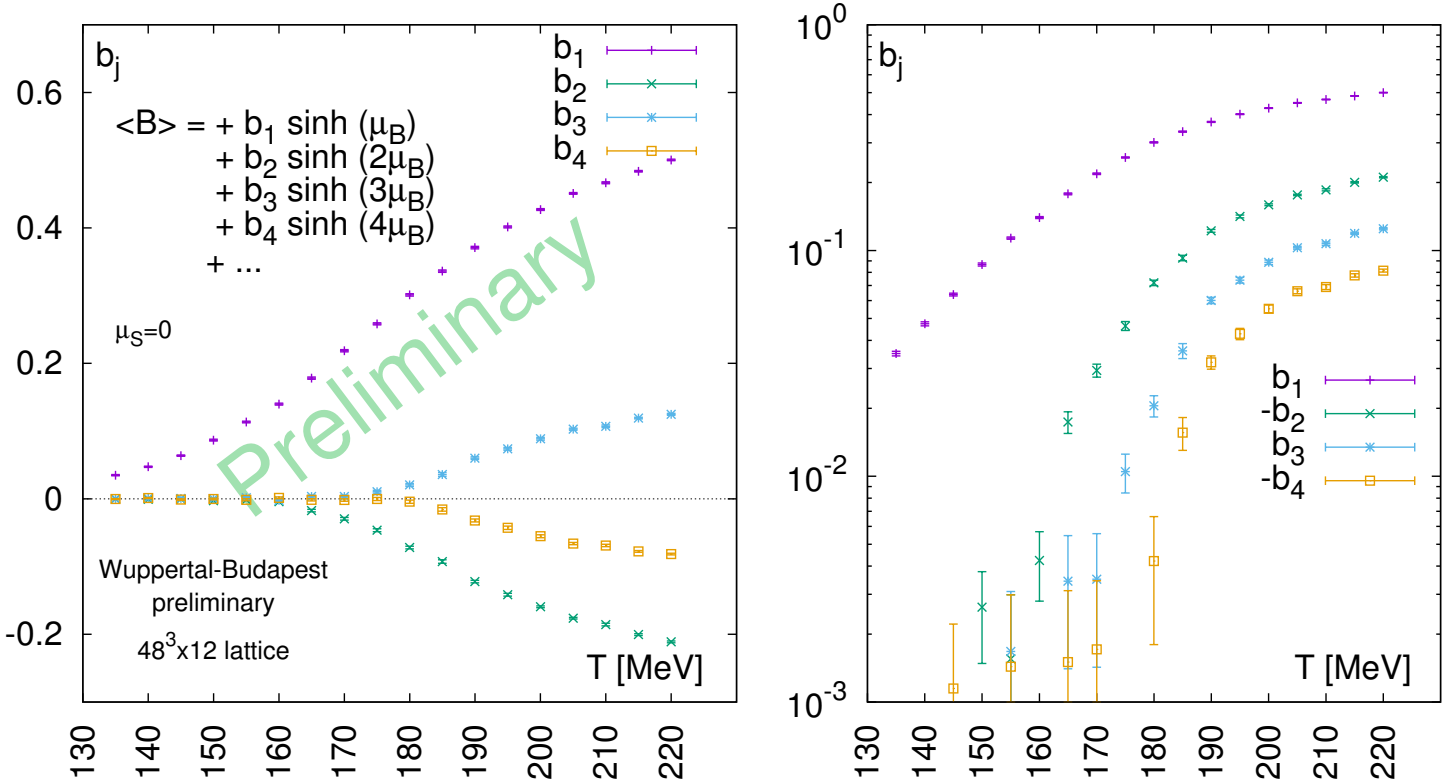
$$\chi_1^B \sim \sin(\mu_B/T/3)$$

A Fourier analysis of the imaginary density

HRG prediction *(Boltzmann approximation)*:

$$\langle B \rangle \sim VT^3 \chi_2^B(T) \sinh(\mu_B/T)$$

Using imaginary μ_B we represent $\langle B \rangle = i \sum_{j=1} b_j \sin(j \cdot \mathrm{Im}\mu_B/T)$

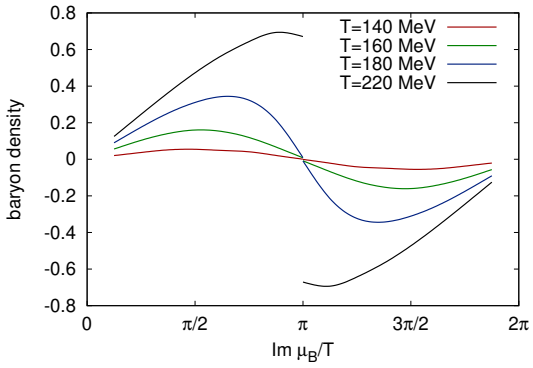


The negative $\sinh(2\mu_B/t)$ *contribution signals a repulsive interaction.*

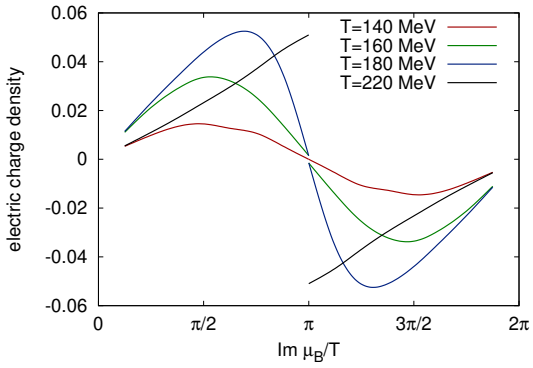
Modelling of $b_3, b_4 \ldots$ basedon b_1 and b_2 [Vovchenko et al: 1708.02852, 1711.01261]

Response to an imaginary chemical potential

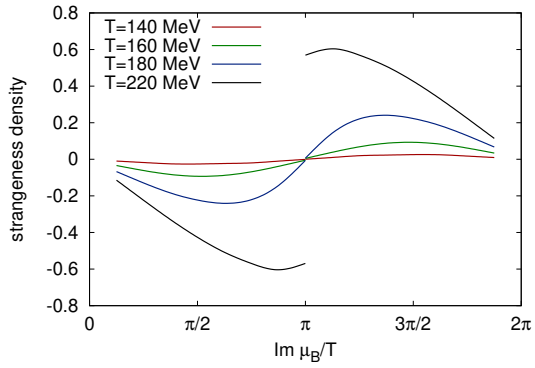
$\langle B \rangle$ vs. μ_B



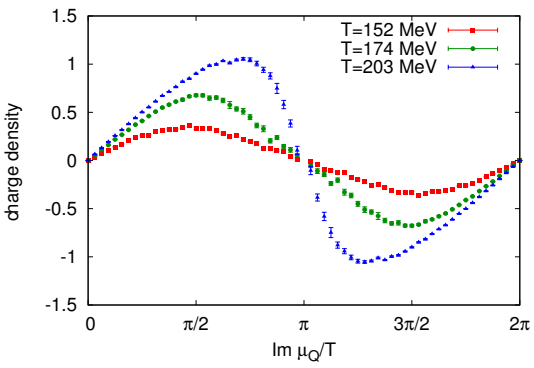
$\langle Q \rangle$ vs. μ_B



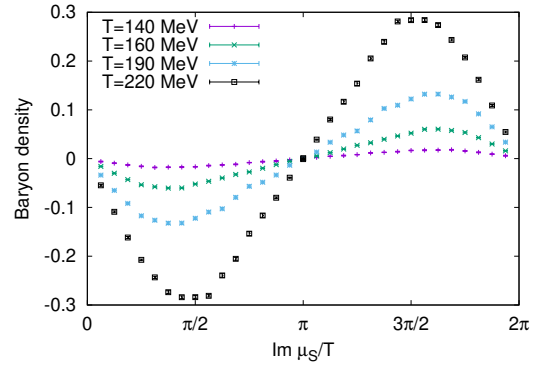
$\langle S \rangle$ vs. μ_B



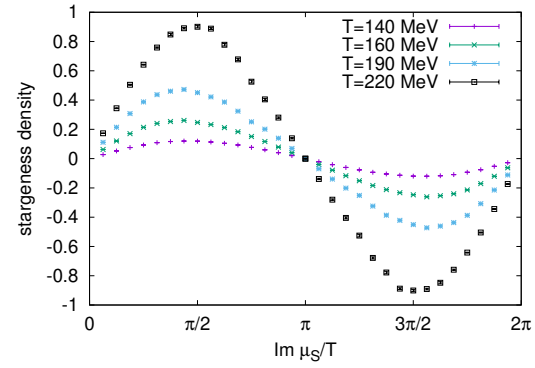
$\langle Q \rangle$ vs. μ_Q



$\langle B \rangle$ vs. μ_S



$\langle S \rangle$ vs. μ_S

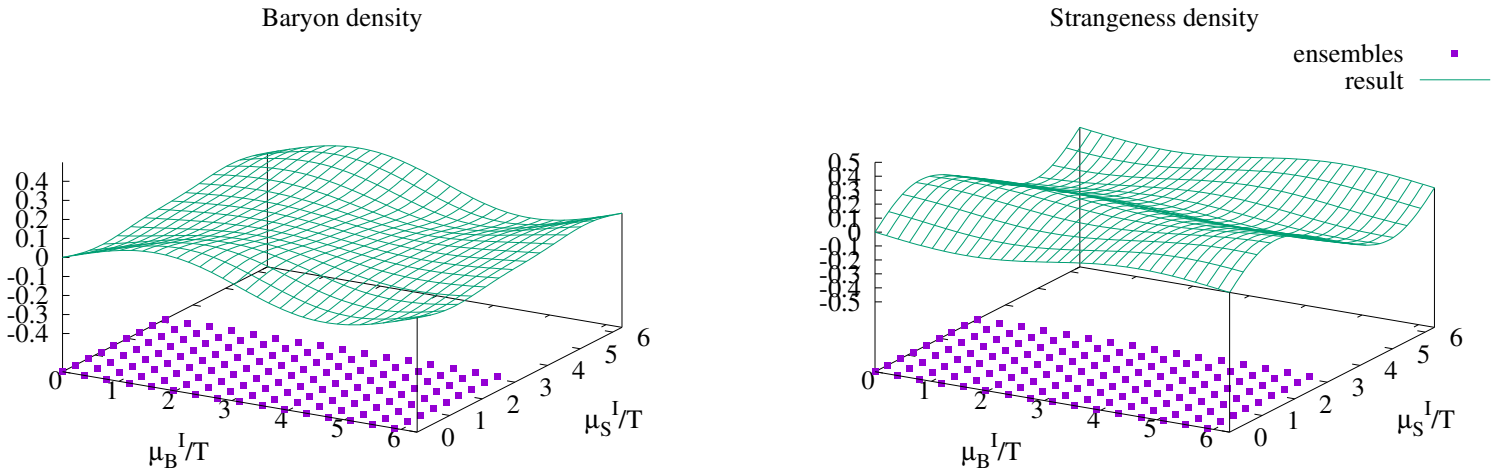


Data: Wuppertal-Budapest

Two-dimensional mapping of μ_B, μ_S

144 ensembles for each temperature and lattice spacing.

Example at $T = 155$ MeV:



A surface is fitted on the baryon and strangeness densities, as well as on their susceptibilities.

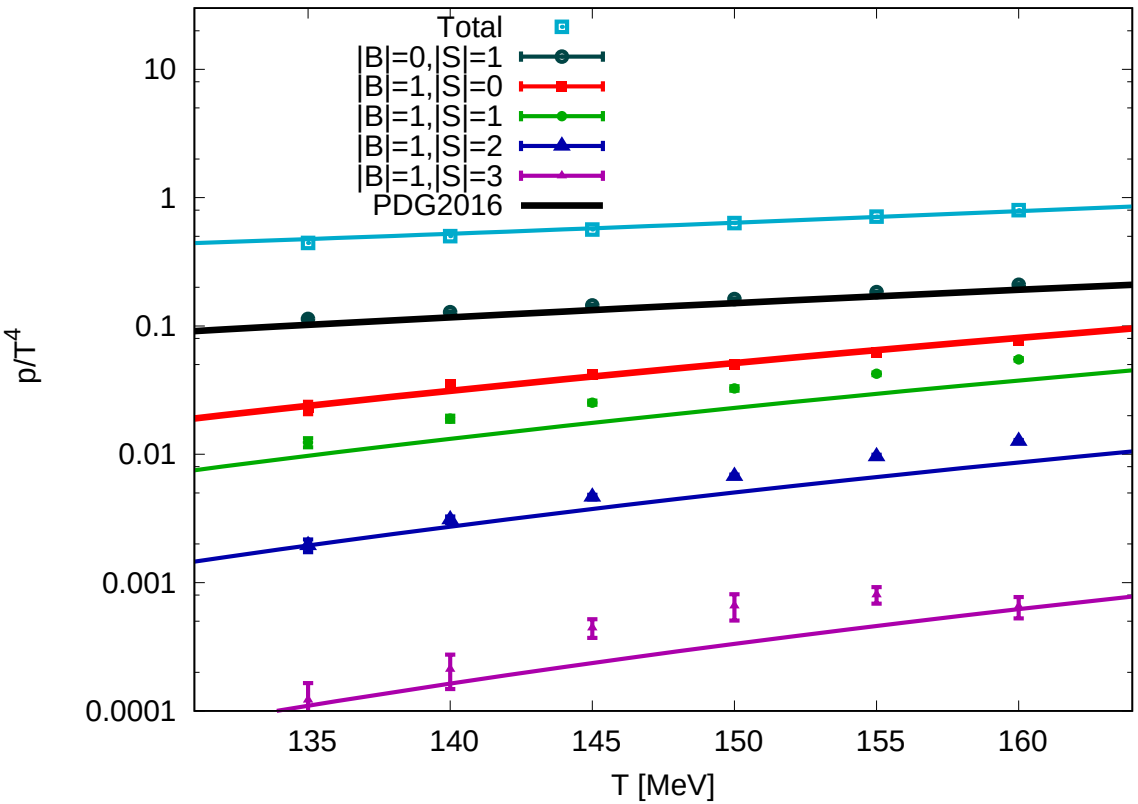
$$P(T, \hat{\mu}_B^I, \hat{\mu}_S^I) = \sum_{j,k} P_{jk}^{BS}(T) \cos(j\hat{\mu}_B^I - k\hat{\mu}_S^I) \ .$$

$$\begin{aligned} -S &= -1, 0, 1, 2, 3 \\ B &= 0, 1, 2, 3 \end{aligned}$$

Sector decomposition of the QCD free energy

$$P(T,\hat{\mu}_B^l,\hat{\mu}_S^l) = \sum_{j,k} P_{jk}^{BS}(T)\cos(j\hat{\mu}_B^l - k\hat{\mu}_S^l)\ .$$

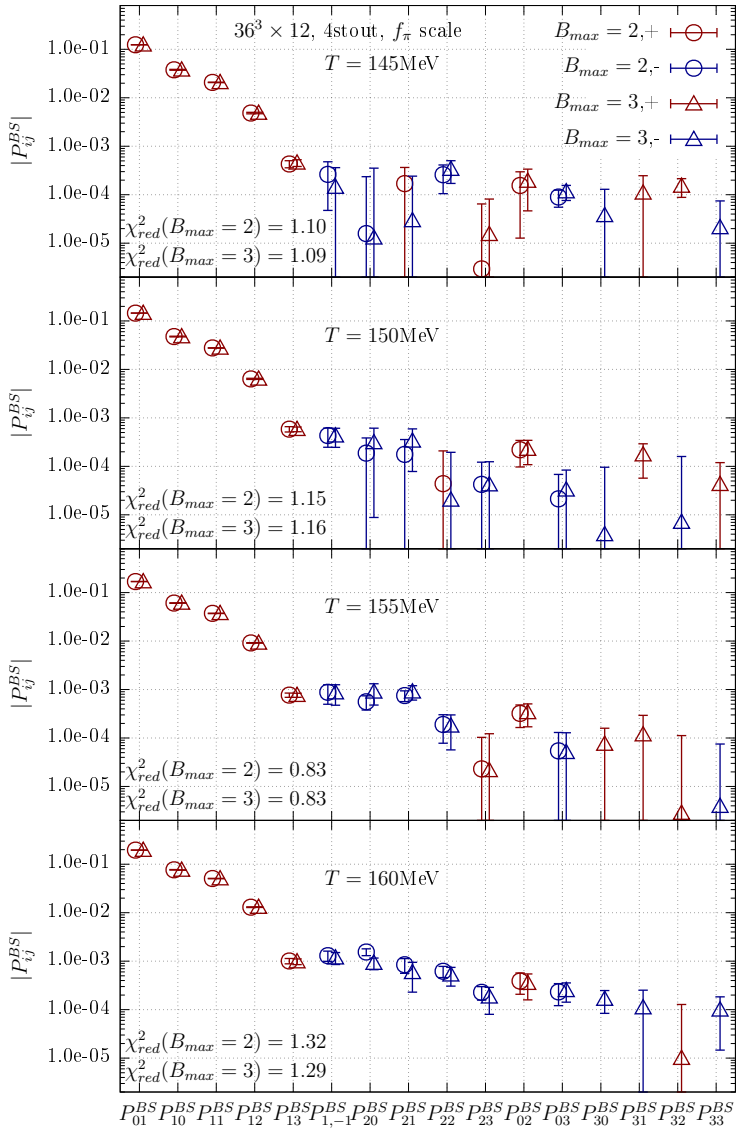
Sectors that contribute to the ideal HRG:

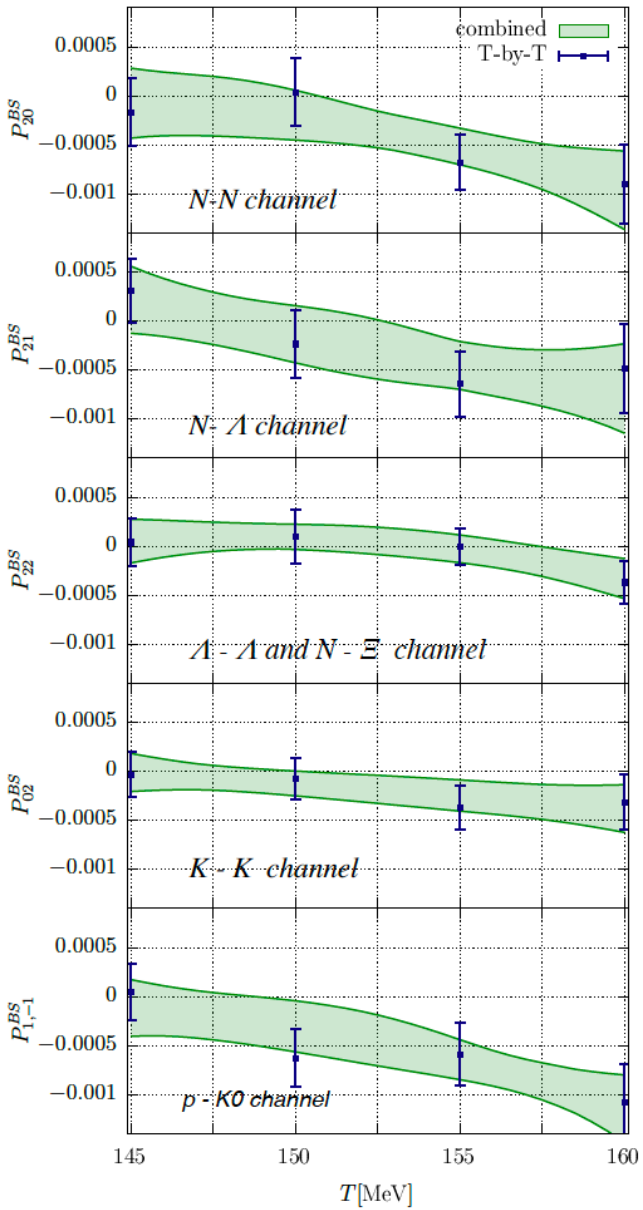


[Wuppertal-Budapest 1702.01113]

Sectors describing interactions

Continuum estimate from $N_\tau = 8, 10$ and 12 [Wuppertal-Budapest: 2102.06625]





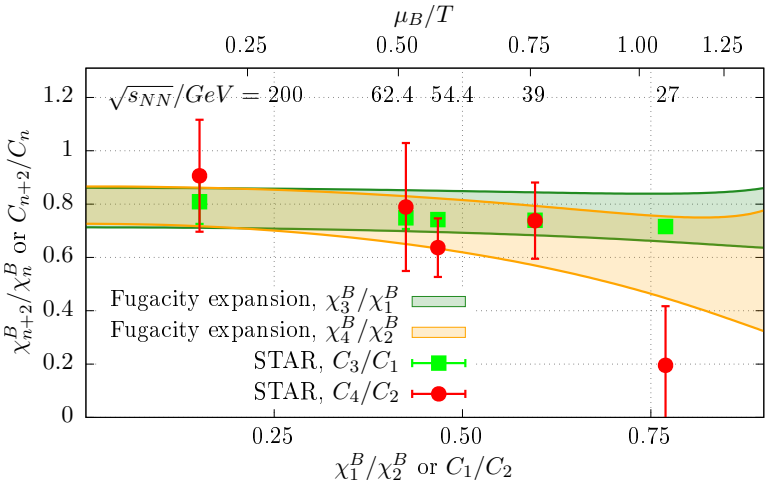
Hadronic phase: Fourier (virial/fugacity) expansion

Our scheme converges in the transition regime the fastest.
Deep in the confined phase an other scheme may be more useful:

$$\frac{p}{T^4} = \cdots + f_{-2}(T)e^{-2\hat{\mu}_B} + f_{-1}(T)e^{-\hat{\mu}_B} + f_0 + f_1(T)e^{\hat{\mu}_B} + f_2(T)e^{2\hat{\mu}_B} + \ldots$$

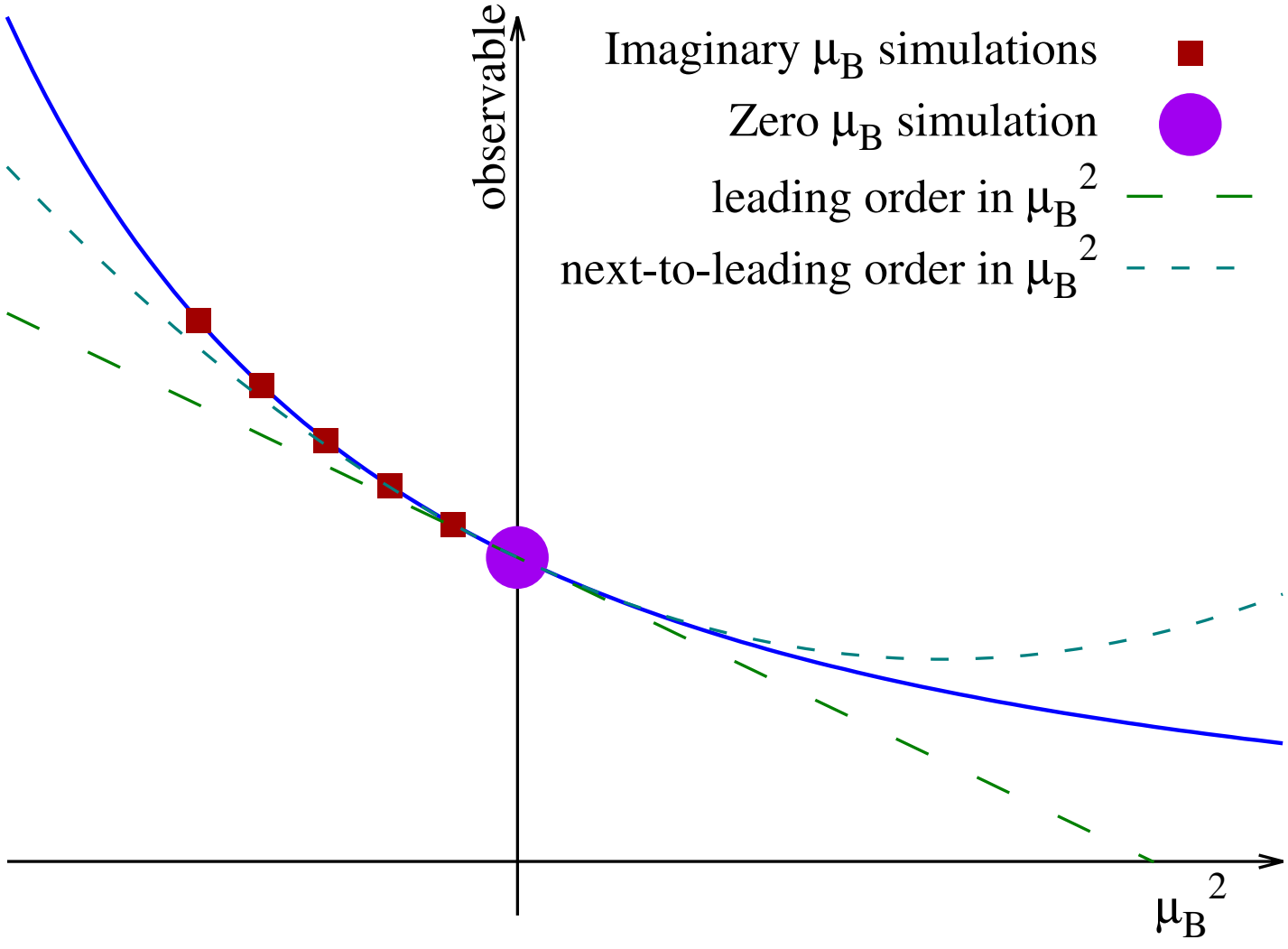
Leading order: HRG / Next-to-leading order: scattering states

We extended this to a $e^{B\hat{\mu}_B - S\hat{\mu}_S}$ expansion scheme and find at NLO:



[Wuppertal-Budapest 2102.06660]

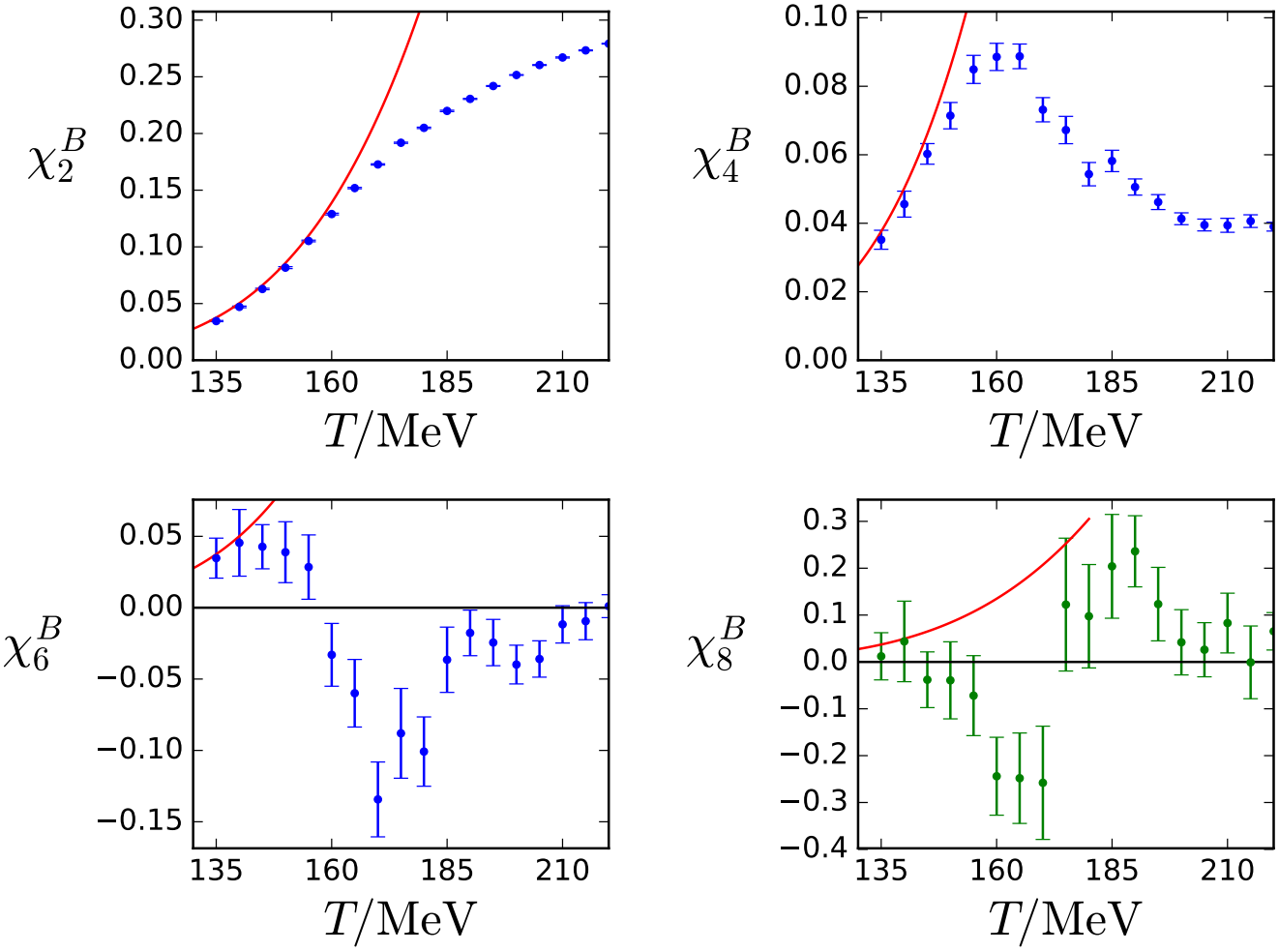
Extrapolation approaches to $\mu_B^2 > 0$



Imaginary μ_B: numerical derivatives with some *lever arm*.
Taylor from $\mu_B = 0$: exact derivatives based on the tails of a distribution.

Higher order χ_B from imaginary μ_B

"Numerical derivatives" from $\mu_B^2 \leq 0$ simulations: [WB 1805.04445]

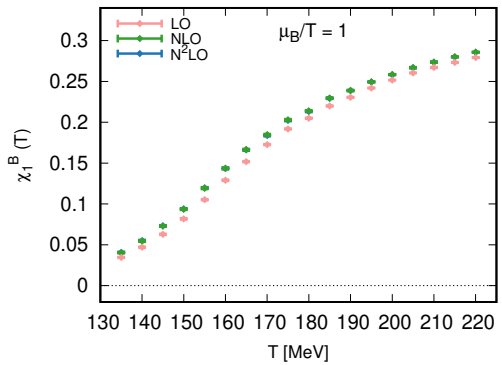


This structure is already known from chiral effecive models. [Friman et al 1103.3511]

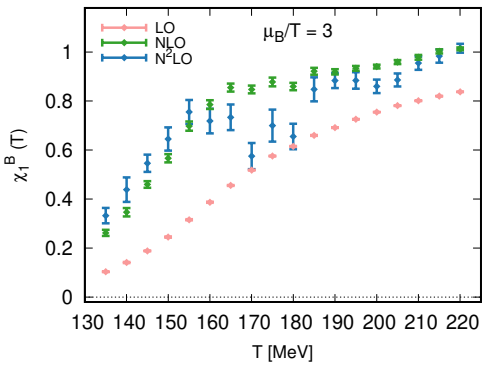
There is a rather simple model that quantitatively describes the χ coefficients

Baryon density at finite μ_B - Taylor expansion

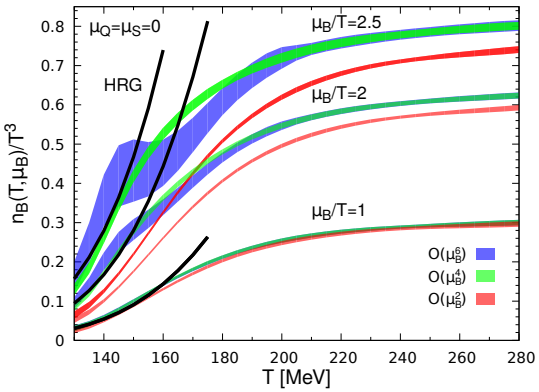
- Thermodynamic quantities at large chemical potential become problematic
- Higher orders do not help with the convergence of the series



[Wuppertal Budapest 1805.04445]



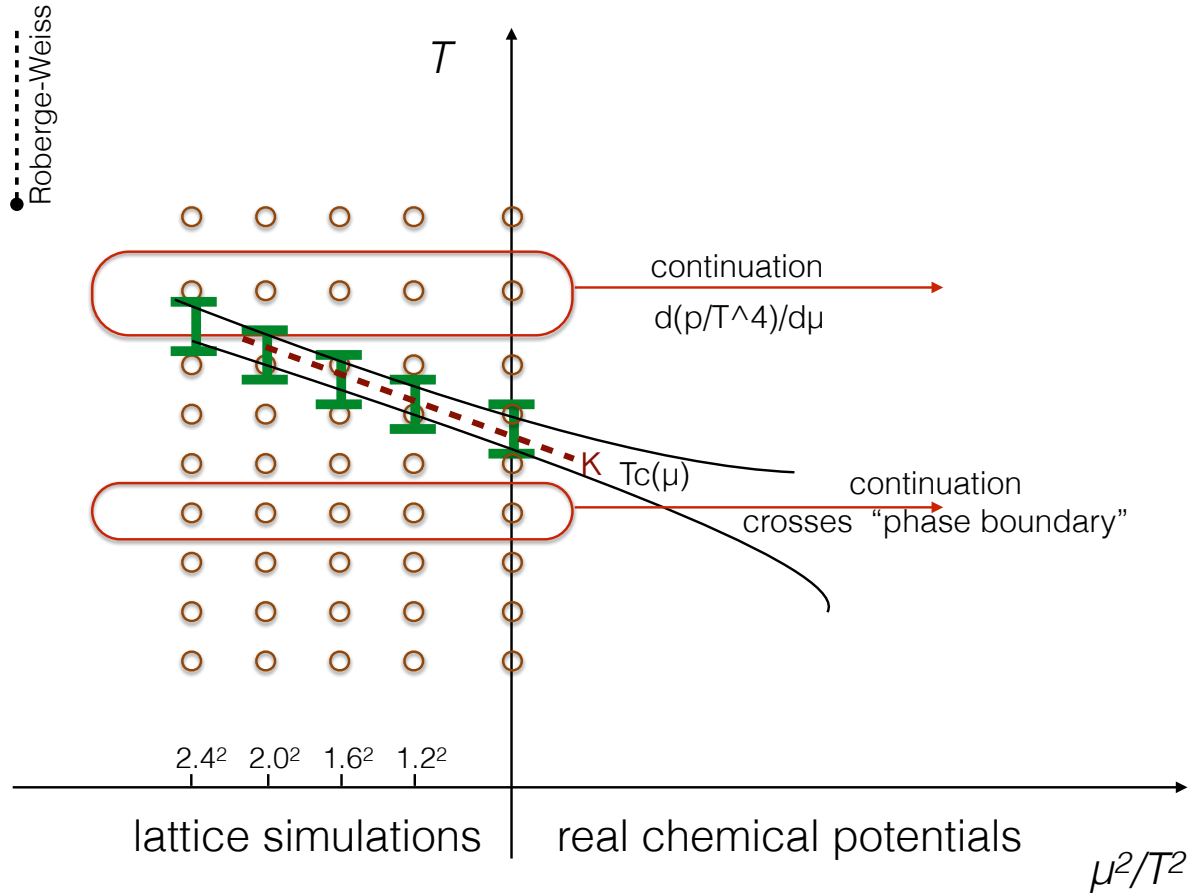
[Wuppertal Budapest 1805.04445]



[HotQCD 1701.04325]

- Inherent problem with Taylor expansion: carried out at $T = \text{const.}$ This doesn't cope well with $\hat{\mu}_B-$dependent transition temperature
- Can we find an alternative expansion to improve finite-$\hat{\mu}_B$ behavior?

Extrapolation in the presence of a transition line



Problematic extrapolation:

- the transition line is crossed
- the Taylor coefficients are dominated by a nearby transition line

In such cases the covergence of the Taylor series is slow.

An unproblematic case: extrapolation of the $Tc(\mu_B)$

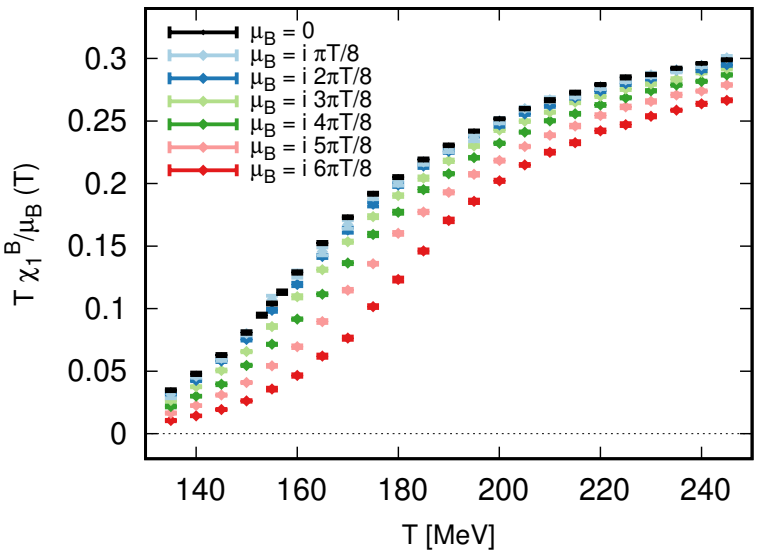
Further observations from imaginary μ_B

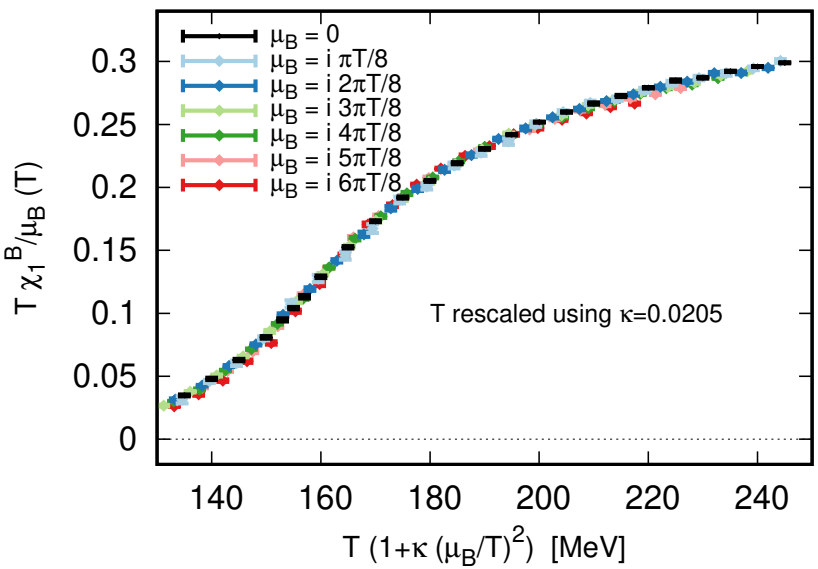
Baryon density: $\chi_1^B(T, \hat{\mu}_B)$

From simulations at imaginary μ_B we *observe* that $\chi_1^B(T, \hat{\mu}_B)$ is to good approximation:

$$\chi_1^B(T, \hat{\mu}_B) = \mu_B \, \chi_2^B\left(T\left(1 + \kappa \hat{\mu}_B^2\right), 0\right)$$

$$\chi_1^B(T, \hat{\mu}_B) = \hat{\mu}_B \chi_2^B(T, 0) + \frac{\hat{\mu}_B^3}{6} \chi_4^B(T, 0) + \ldots$$

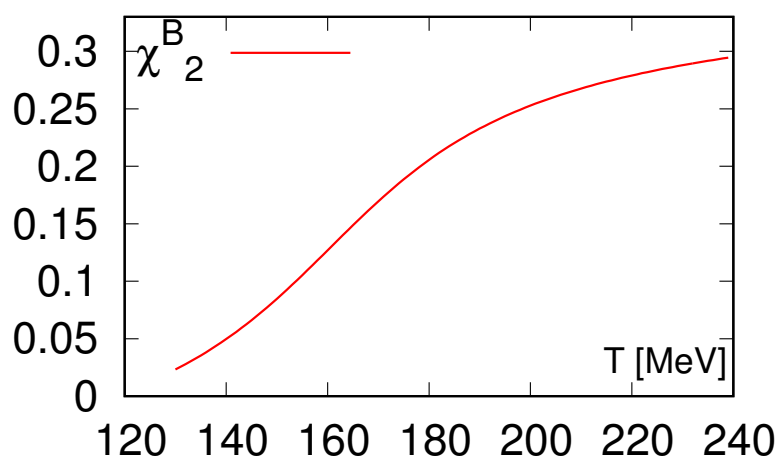


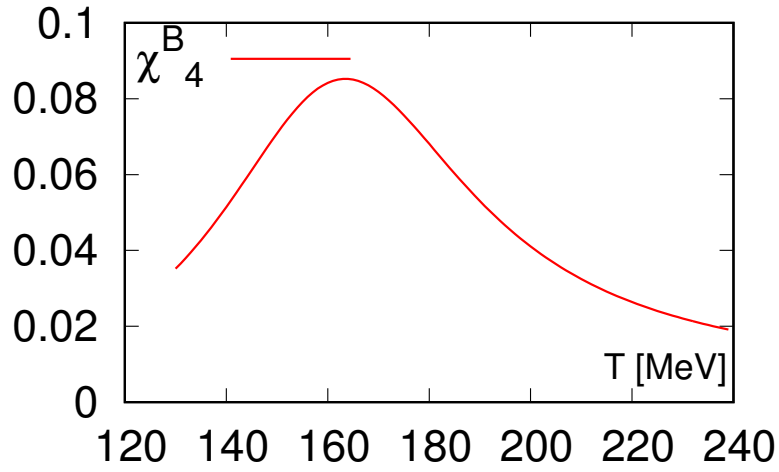


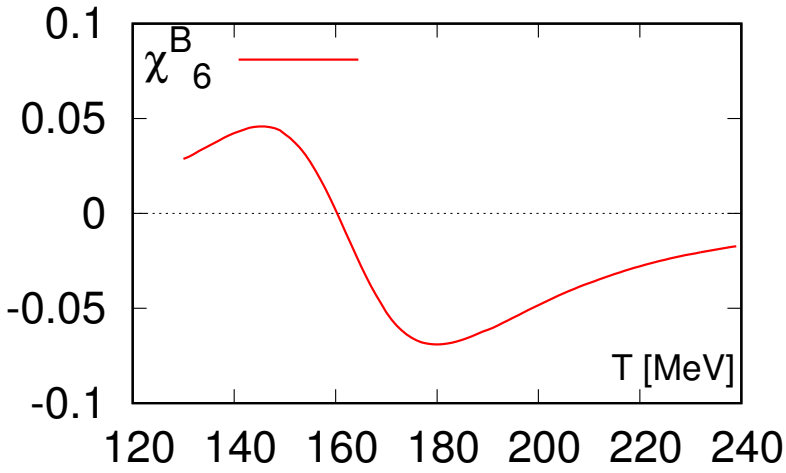
[Wuppertal Budapest 2102.06660]

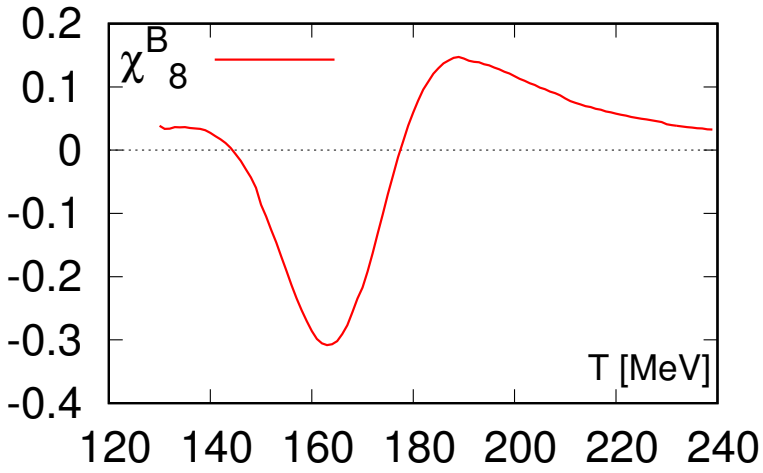
Higher order χ_B in the simple model

Input: $\chi_2^B(T, \mu = 0)$ from Wuppertal-Budapest, and $\kappa = 0.02$ [see 1508.07599]:



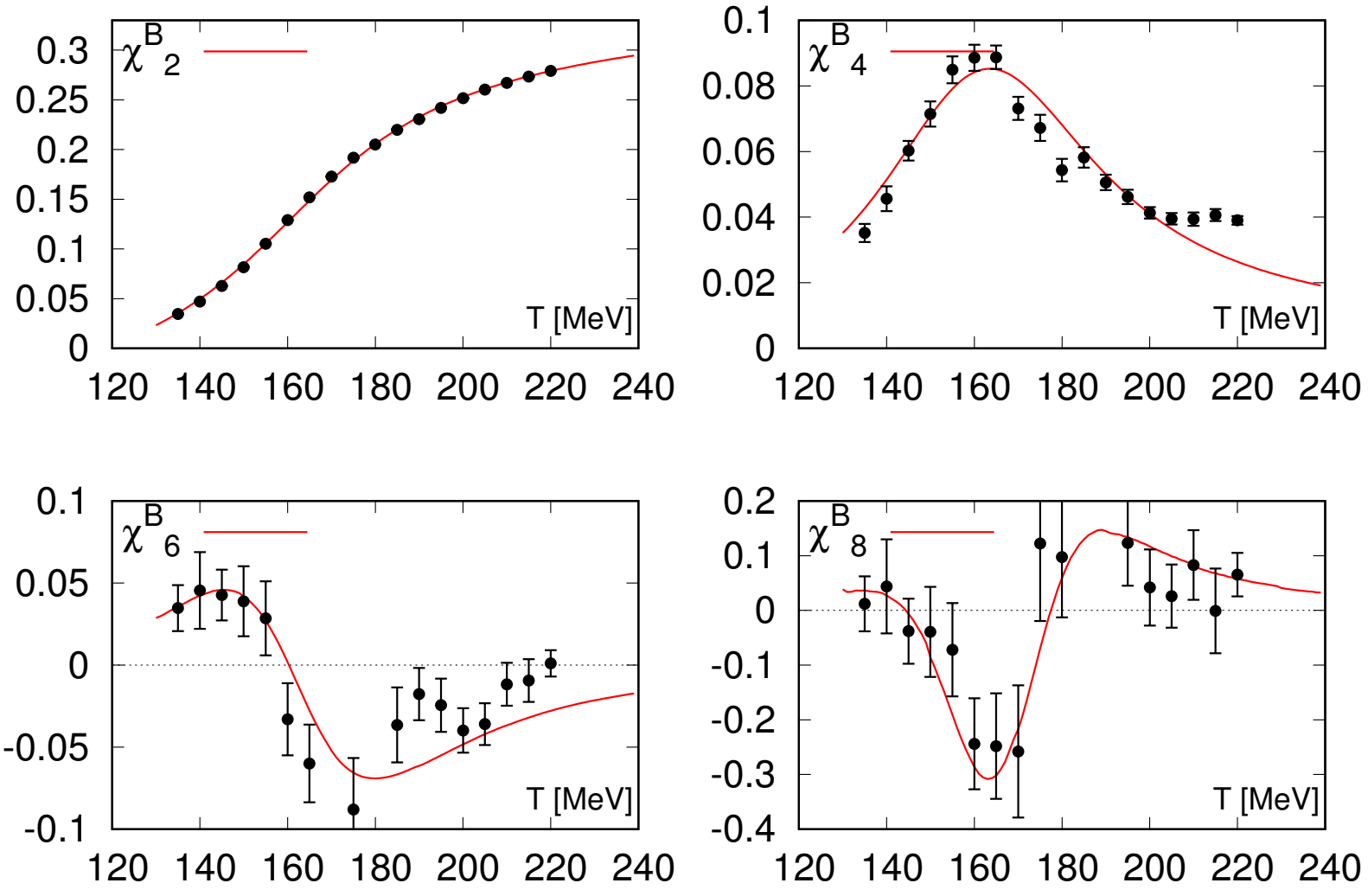






Higher order χ_B in the simple model

Comparing the simple model with our lattice result:



Simple model describes lattice result surprisingly well.

Result is consistent with the no-critical-end-point scenario.

Expansion scheme: formal definition

Our naive obsrevation (almost correct):

$$\chi_1^B(T,\hat{\mu}_B) = \hat{\mu}_B \chi_2^B\left(T\cdot(1+\kappa_2\hat{\mu}_B^2),0\right)$$

Let's generalize this to endorse any sigmoid $\chi_1^B(T,\hat{\mu}_B)$ result:

$$\chi_1^B(T,\hat{\mu}_B) = \hat{\mu}_B \cdot \chi_2^B\left[T\cdot(1+\kappa_2(T)\cdot\hat{\mu}_B^2+\kappa_4(T)\cdot\hat{\mu}_B^4+\dots)\right]$$

The complete finite denesity equation of state is then contained in

- $\chi_2^B(T)$: baryon number susceptibility (known precisely)
- $\kappa_2(T),\kappa_4(T)$ a series of slowly varying functions

These functions are directly related to the Taylor coefficients:

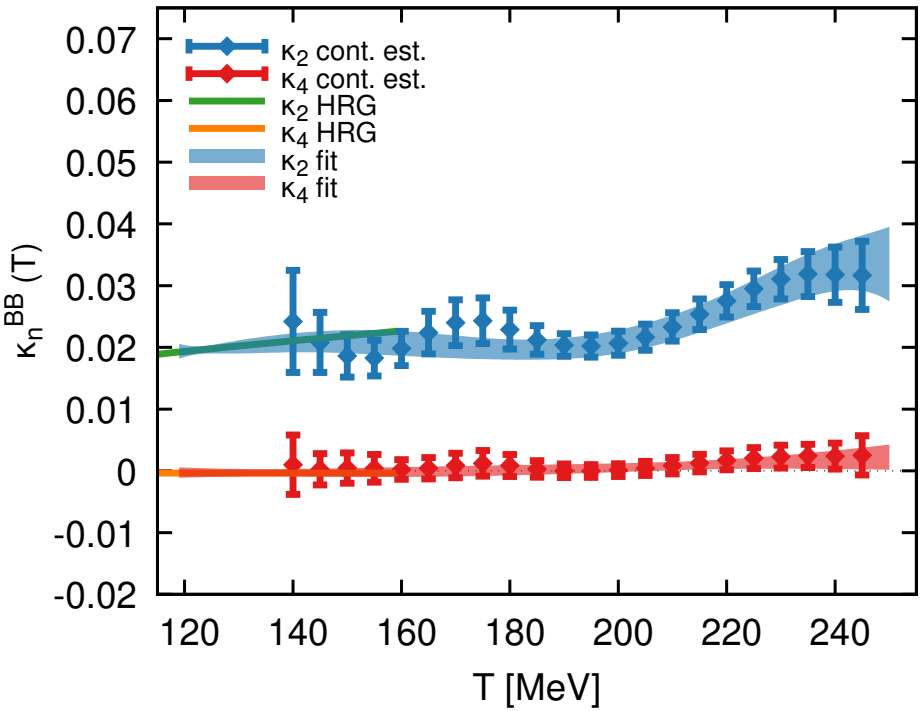
$$\kappa_2(T) = \frac{1}{6T}\frac{\chi_4^B(T)}{\chi_2^{B\prime}(T)}$$

$$\kappa_4(T) = \frac{1}{360\chi_2^{B\prime}(T)^3}\left(3\chi_2^{B\prime}(T)^2\chi_6^B(T) - 5\chi_2^{B\prime\prime}(T)\chi_4^B(T)^2\right)$$

The results for $\kappa_2(T)$, $\kappa_4(T)$

Our initial guess was not far-off:

- Fairly constant $\kappa_2(T)$ over a large T-range
- Clear separation in magnitude between $\kappa_2(T)$ and $\kappa_4(T)$ hints at better convergence
- Agreement with the HRG model results at low temperatures
- Polynomial fits of $\kappa_2(T)$ and $\kappa_4(T)$ before use in thermodynamics (good fit qualities)



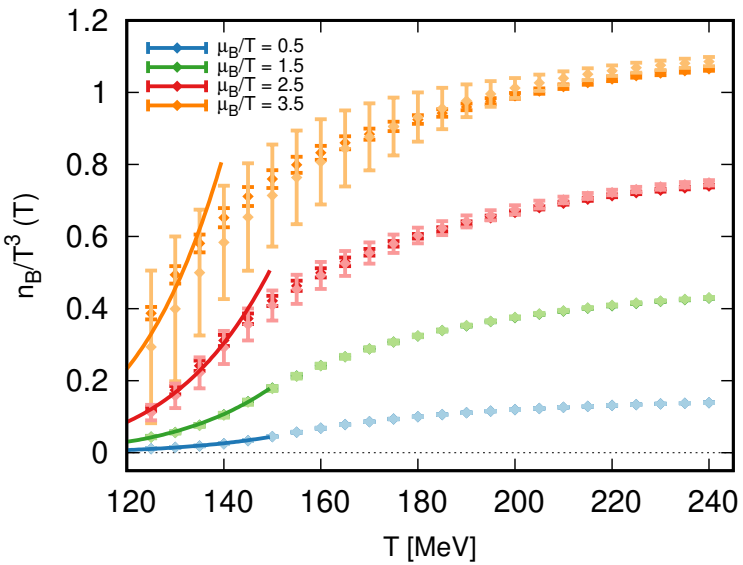
NOTE: polynomial fits take into account both statistical and systematic correlations.

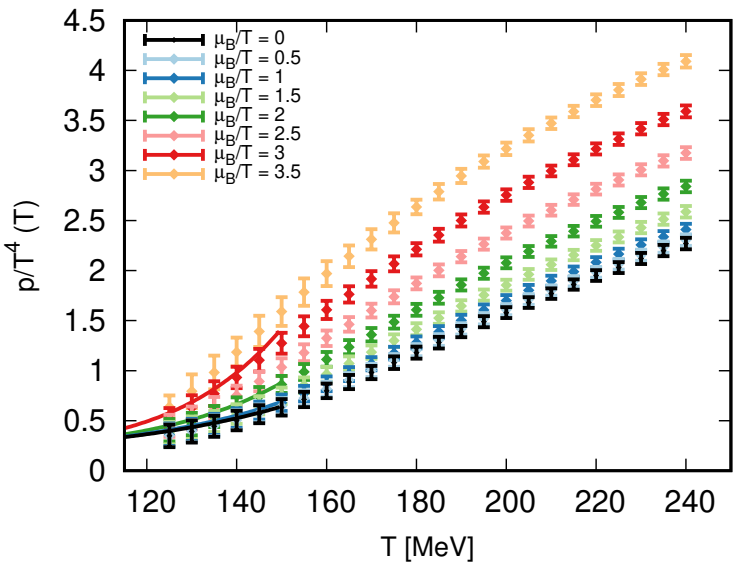
[Wuppertal Budapest 2102.06660]

Thermodynamics at finite (real) μ_B

baryon density and pressure

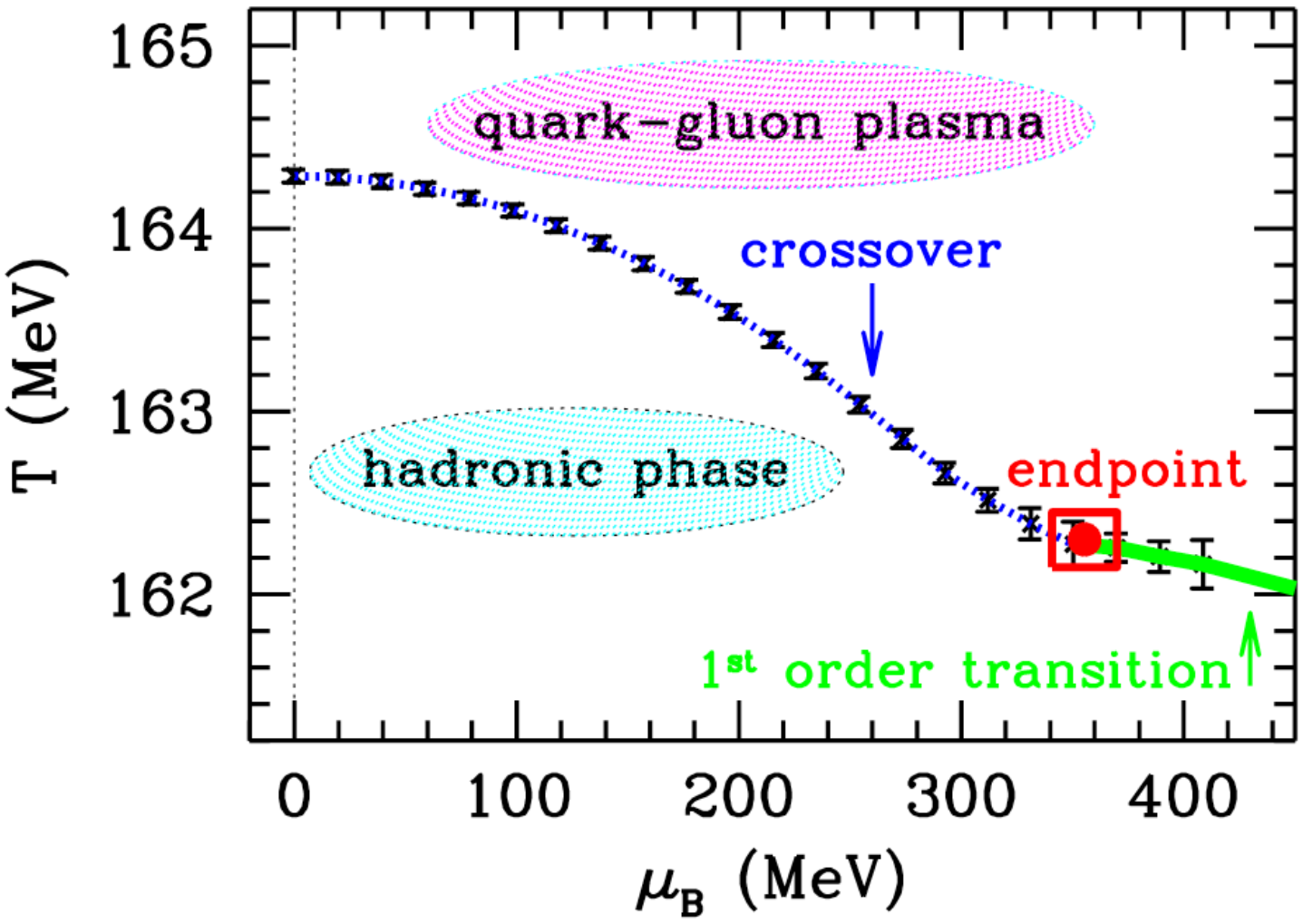
- We reconstruct thermodynamic quantities up to $\hat{\mu}_B \simeq 3.5$ with uncertainties well under control
- Agreement with HRG model calculations at small temperatures
- No pathological (non-monotonic) behavior is present





[Wuppertal Budapest 2102.06660]

Reweighting to real μ_B



Using physical quark masses, $2+1$ *flavors,* $N_t = 4$ [Fodor&Katz hep-lat/0402006]

The sign problem

The complex action problem can be simplified to a sign problem

$$Z = \int DU \det M[U]\, e^{-S_g(U)}$$

Since both the gauge part $e^{-S_g(U)}$ and the result Z are real:

$$Z = \int DU \,\mathrm{Re}\big[\det M[U]\big]\, e^{-S_g(U)}$$

Two main options to make the probability weight positive:
Phase quenched: *(more popular)*

$$\int DU \,\big|\det M[U]\big|\, e^{-S_g(U)}$$

Sign quenched: *(difficult to simulate, weakest sign problem)*

$$\int DU \,\big|\mathrm{Re}\big[\det M[U]\big]\big|\, e^{-S_g(U)}$$

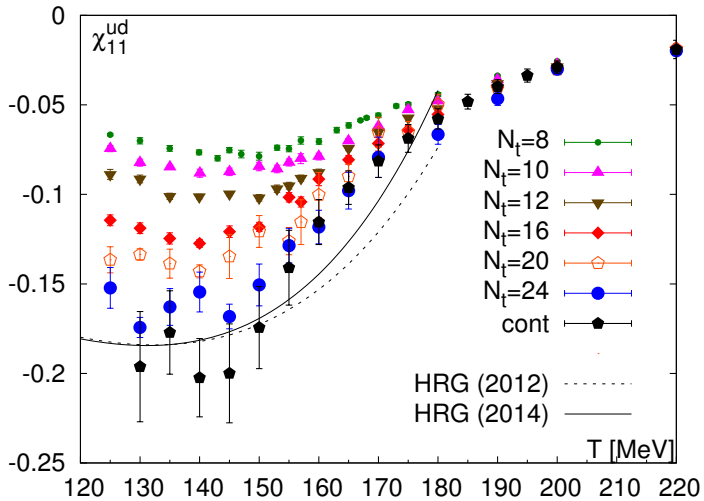
[Giordano et al 2004.10800]

How strong is the sign problem?

The complex phase of the fermion determinant is linked to a physical observable, the light quark density. [(See formula 5.2 of Allton et al hep-lat/0501030)]

$$\theta = \frac{1}{4} N_f \mathrm{Im} \left[\mu \underbrace{\frac{\partial \ln \det M}{\partial \mu}}_{\text{light quark density}} + \ldots \right]$$

$$\langle \theta^2 \rangle = -\frac{1}{9} \mu_B^2 L^3 T N_f^2 \chi_{11}^{ud} \qquad \text{with} \quad \chi_{11}^{ud} \sim \partial^2 \log Z / \partial \mu_u \partial \mu_d \,.$$



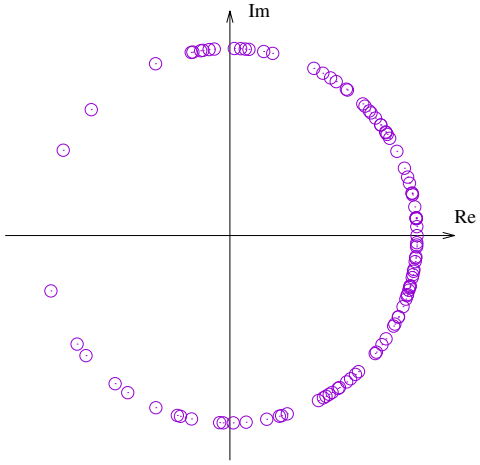
The sign problem is weak for coarse lattices and at high temperatures.

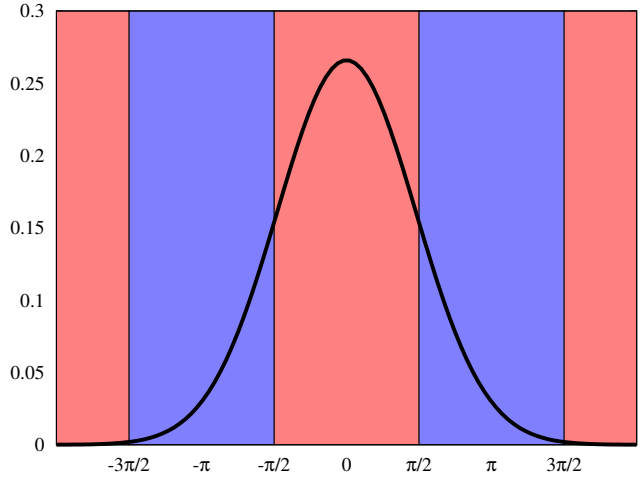
[Wuppertal-Budapest 1507.04627]

How to calculate the severity of the sign problem

Simplification: The distribution of the phase of the determinant shall be *Gaussian*.

$$\rho(\theta) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\theta^2}{2\sigma^2(\mu)}}$$





Phase Quenched: $\langle \cos\theta \rangle = e^{-\sigma^2(\mu)/2}$

Sign Quenched: $\langle \epsilon \rangle = \frac{\langle \cos\theta \rangle}{\langle |\cos\theta| \rangle} \approx 1 - \frac{4}{\pi} \left(\frac{2\sigma^2(\mu)}{\pi} \right)^{\frac{3}{2}} e^{-\frac{\pi^2}{8\sigma^2(\mu)}}$

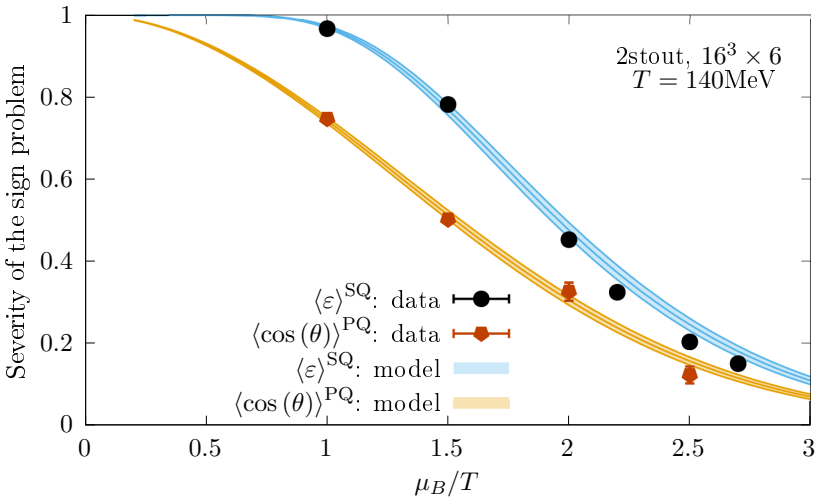
Small μ: $\sigma^2(\mu) = -\frac{4}{9}\chi_{11}^{ud}(T)(LT)^3\hat{\mu}_B^2$

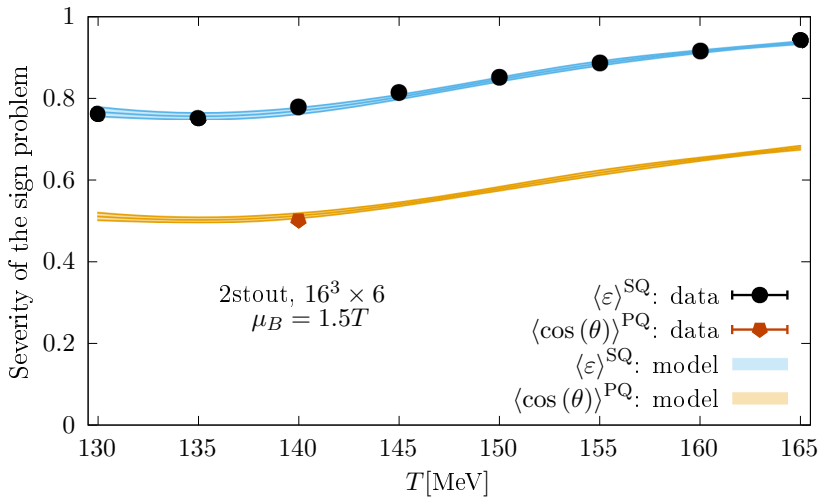
Large μ advantage of the sign quenched approach:
factor $(\pi/2)^2 \approx 2.5$ in the statistics.

Sign problem in the practice

For a concrete case:
– 2-stout-staggered action,
– physical quarks with 2+1 flavors,
– $16^3 \times 6$ lattice.

$$\textbf{Statistics required} \sim \frac{1}{[\textbf{Strength of the sign problem}]^2}$$





The data points are actual simulations!

[Wuppertal-Budapest 2108.09213]

Staggered fermions at finite chemical potential

The staggered rooting is ill-defined at $\mu_B > 0$.

$$Z(T,\mu) = \int \mathcal{D}U \, [\det M \int \mathcal{D}U \, \mathrm{Re}\{[\det M(U, m_{ud}, \mu)]^{\frac{1}{2}}\} [\det M(U, m_s, 0)]^{\frac{1}{4}} e^{-S_g[U]} \, .$$

We can calculate the determinant up to a sign: $\pm\sqrt{\det M}$

To reinsert the missing sign is the whole point of the reweighting.

Let Λ_i be the eigenvalues of the reduced matrix;

$$\begin{aligned} \det M(\mu) &= e^{3V\hat{\mu}} \prod_{i=1}^{6V} \left[\Lambda_i - e^{-\hat{\mu}}\right] = \det M(0) \prod_{i=1}^{6V} \left[\frac{\Lambda_i e^{\hat{\mu}/2} - e^{-\hat{\mu}/2}}{\Lambda_i - 1}\right] \\ \sqrt[\mathbb{C}]{\det M(\mu)} &= \sqrt{\det M(0)} \prod_{i=1}^{6V} \sqrt[\mathbb{C}]{\frac{\Lambda_i e^{\hat{\mu}/2} - e^{-\hat{\mu}/2}}{\Lambda_i - 1}} \end{aligned}$$

This way $\sqrt[\mathbb{C}]{\det M(\mu^2)}$ is analytically connected to the real function $\sqrt{\det M(-\mu^2)}$.

Direct simulations at $\mu_B > 0$

Simulation in two steps:

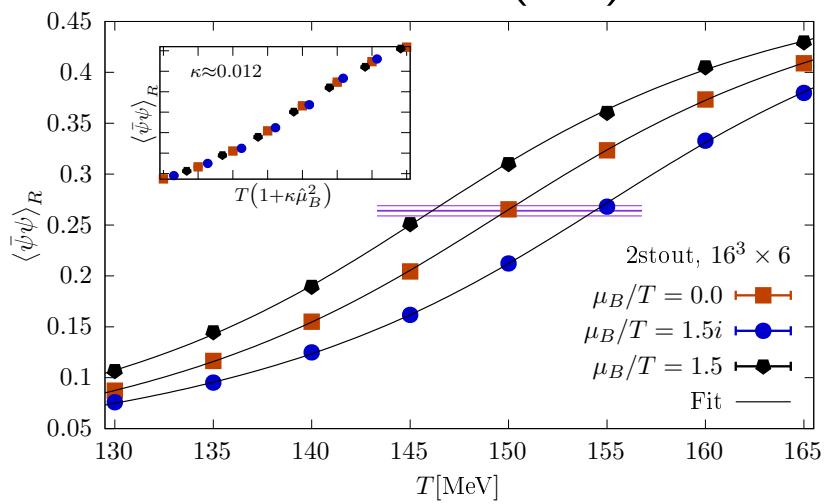
1. Simulate the real (sign quenched) action
2. Reweight each configuartion with the correct sign

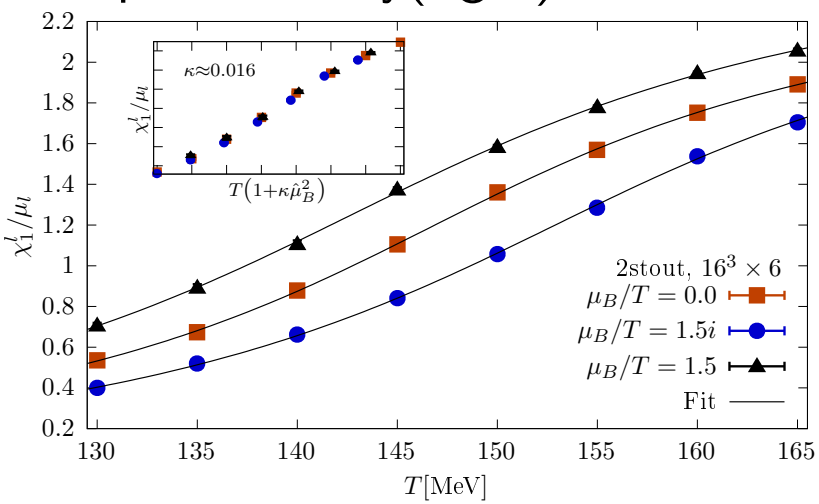
Feasible as long as the sign problem is not too severe.

The earlier, tighter constraint of the overlap problem was removed.

Drawback: the simulation algorithm is more expensive *(subject to research)*

The chiral condensate (left) and the real quark density(right).





The plots show the matching imaginary μ_B results for comparison.

Inset plots: the scaling with temperature survives to real μ_B !

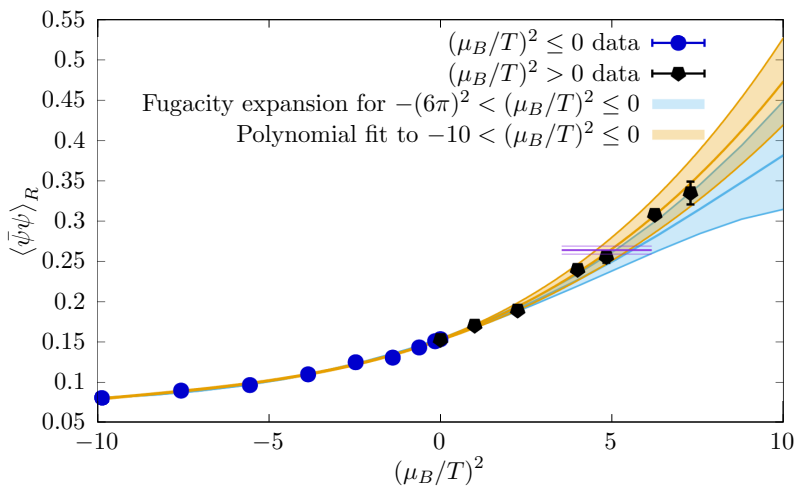
[Wuppertal-Budapest 2108.09213]

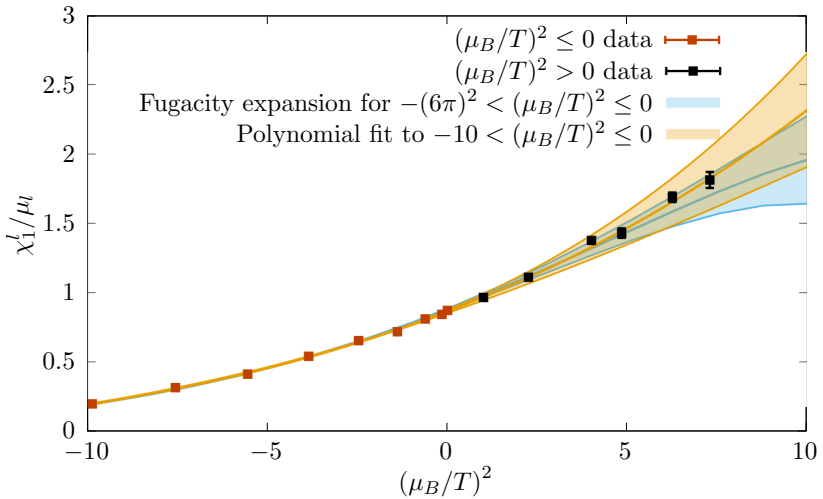
Direct simulations at $\mu_B > 0$

How far can we go in the chemical potential?

We compare in these plots for 140 MeV

- Taylor expansion from imaginary μ_B
- Fugacity expansion from imaginary μ_B
- Direct finite density simulations at $0 < \mu_B \leq 380$ MeV

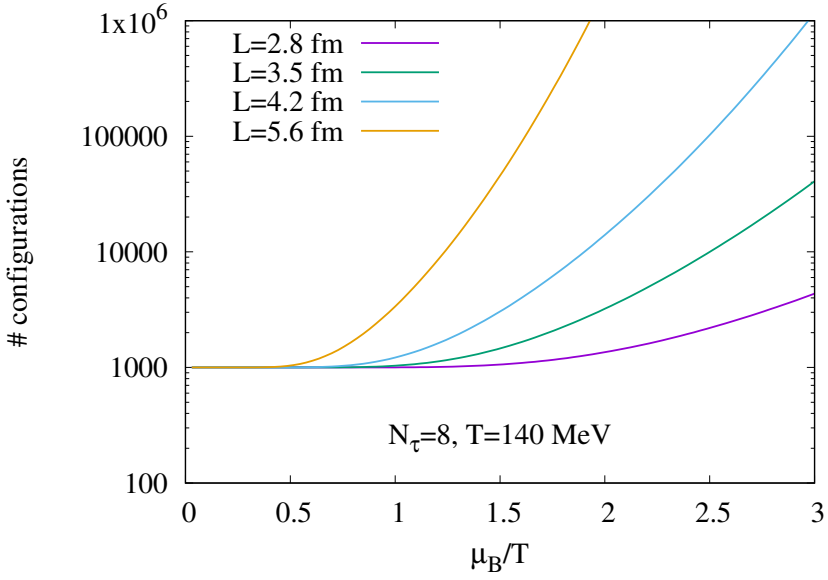


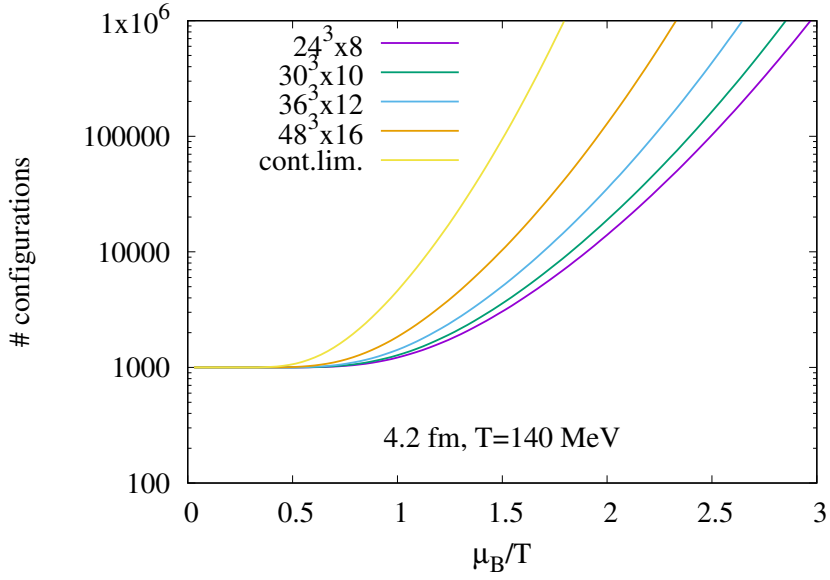


The direct result has the smallest errors.

[Wuppertal-Budapest 2108.09213]

What are the limits of the direct simulations





- The most important limiting factor is **volume** and μ_B.
  (The same is true for the $\mu_B = 0$ Taylor method.)
- This is bad news for the CEP search
  (finite volume scaling is very difficult)
- Below $\mu_B/T < 1$ the sign problem is weak.
- Deeper temperature and μ_B scans are feasible:
  Is the transition getting any stronger?
  How long are EoS extrapolation schemes valid?
- The continuum extrapolation brings no further conceptual problems.

Conclusions

Indirect methods:

1. **Taylor expansion:** perfect for high T
2. **Fugacity expansion:** perfect for confinement
3. **New expansion scheme in temperature:** perfect for the transition

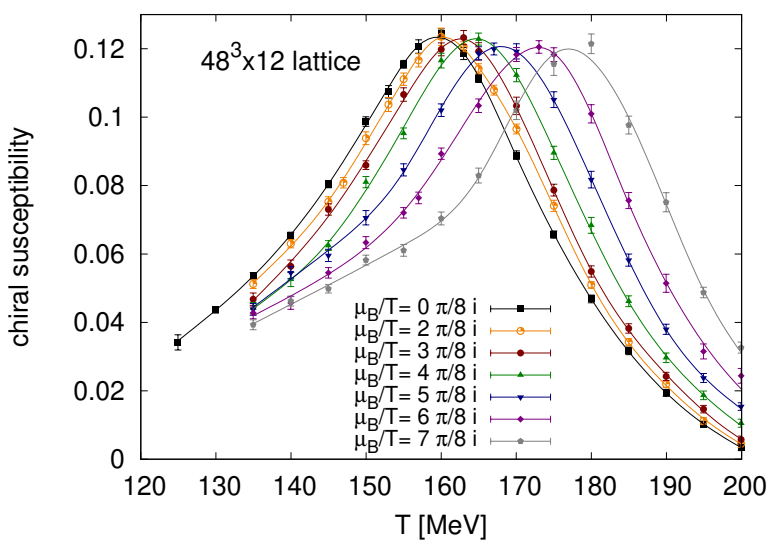
Direct simulations (sign quenched + reweighting):

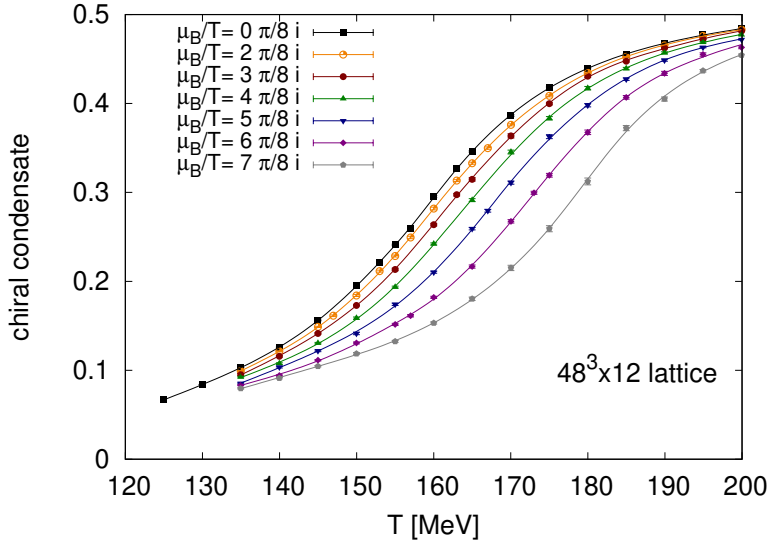
1. Expensive, but increasingly feasible
2. Can be simulated today (in modest volumes)
3. EoS can be mapped
4. Active research: cutting the costs with algorithmic tricks
5. First results shown here.

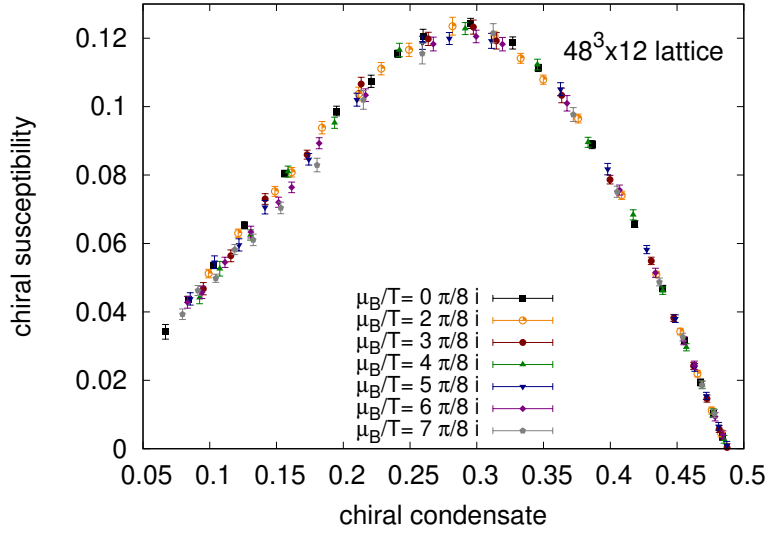
THANK YOU!

backup

An observation: Chiral susceptibility

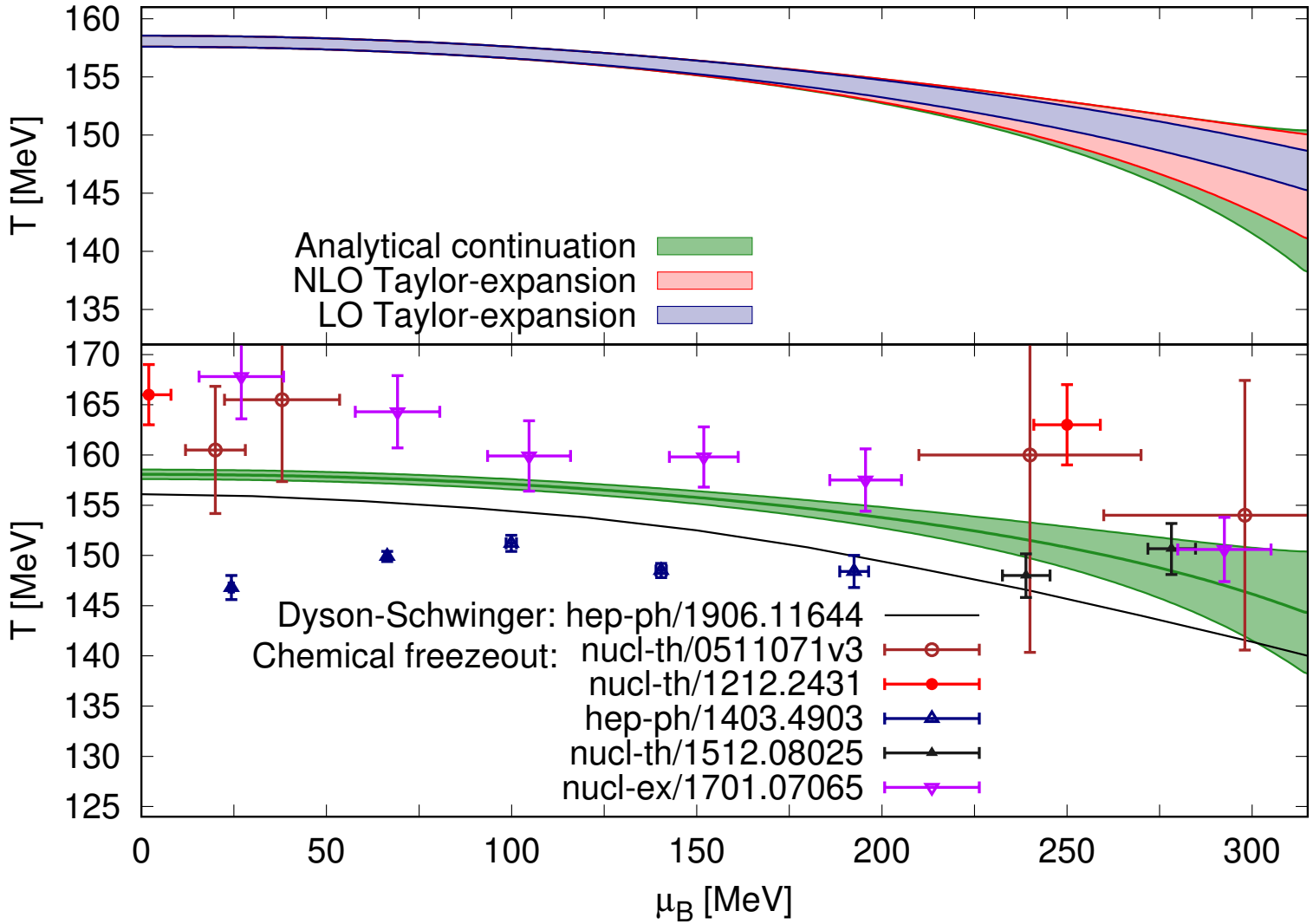






The strength of the transition is μ_B independent [WB 2002.02821]

The transition line



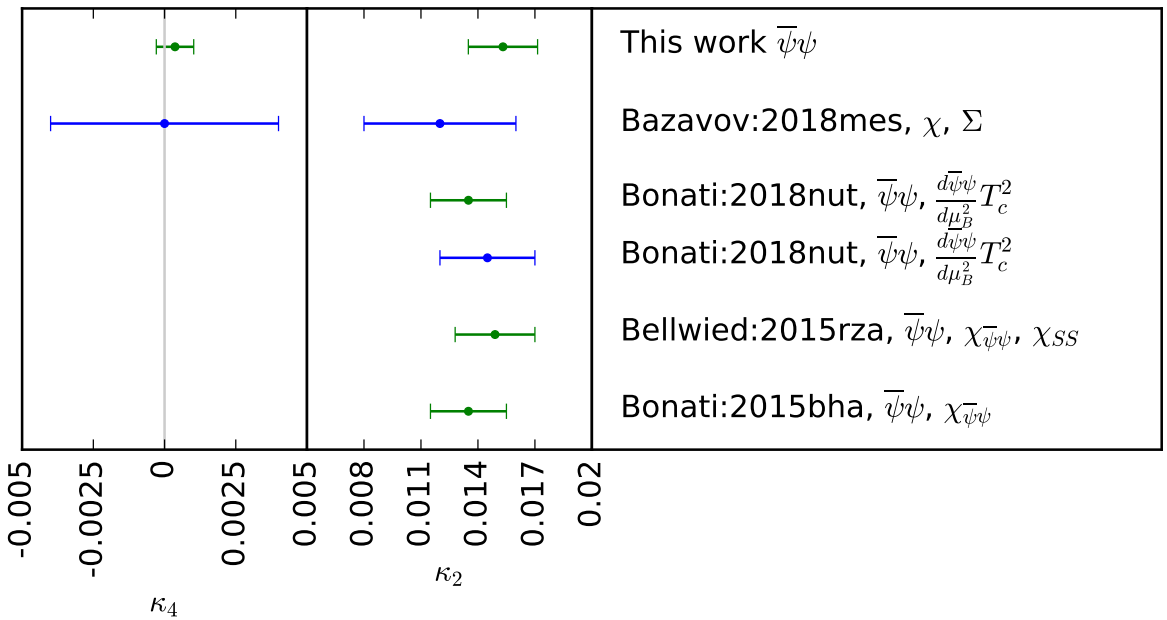
Result for the transition line

Continuum extrapolation using lattices $40^3 \times 10$, $48^3 \times 12$ and $64^3 \times 16$.

[Wuppertal Budapest 2002.02821 (PRL (2020) 125, 052001]

$$\frac{T_c(\mu_B)}{T_c(\mu_B = 0)} = 1 - \kappa_2 \left(\frac{\mu_B}{T_c(\mu_B)} \right)^2 - \kappa_4 \left(\frac{\mu_B}{T_c(\mu_B)} \right)^4 \ldots$$

$$\kappa_2 = \mathbf{0.0153(18)} \text{ and } \kappa_4 = \mathbf{0.00032(67)}$$

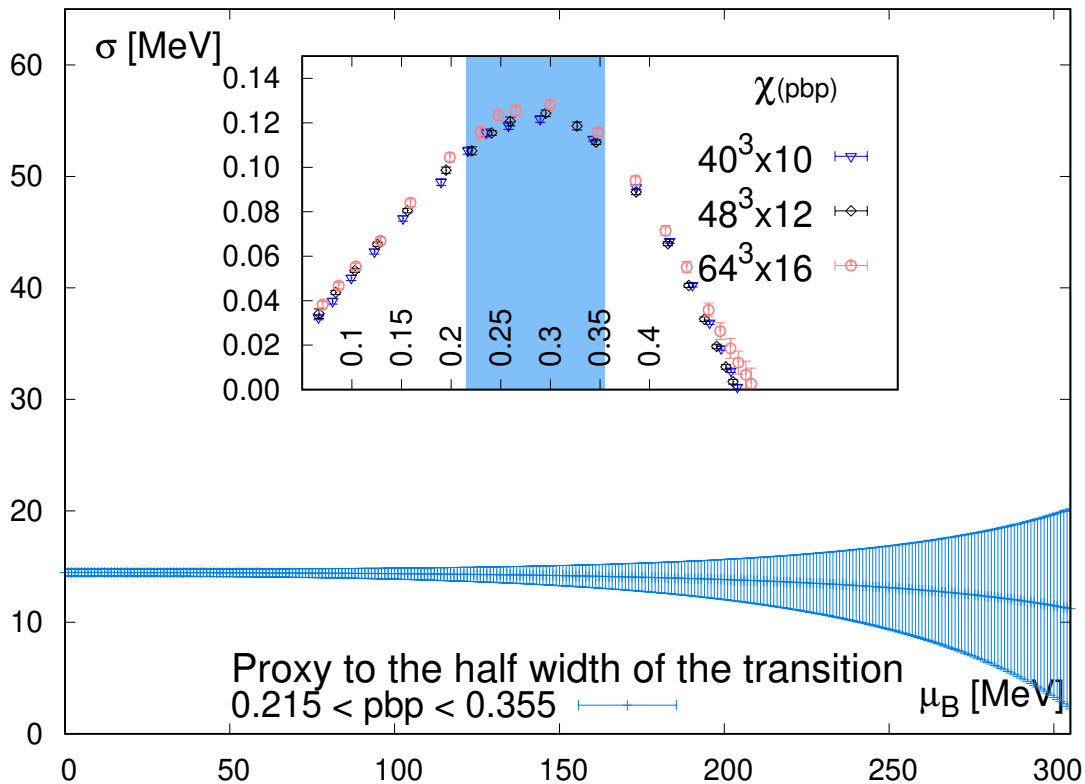


The width of the transition extrapolated

To accurately obtain the width we use a proxy: $\sigma(\mu_B)$

$$\langle\bar{\psi}\psi\rangle(T_c \pm \sigma/2) = \langle\bar{\psi}\psi\rangle_c \pm \Delta\langle\bar{\psi}\psi\rangle/2$$

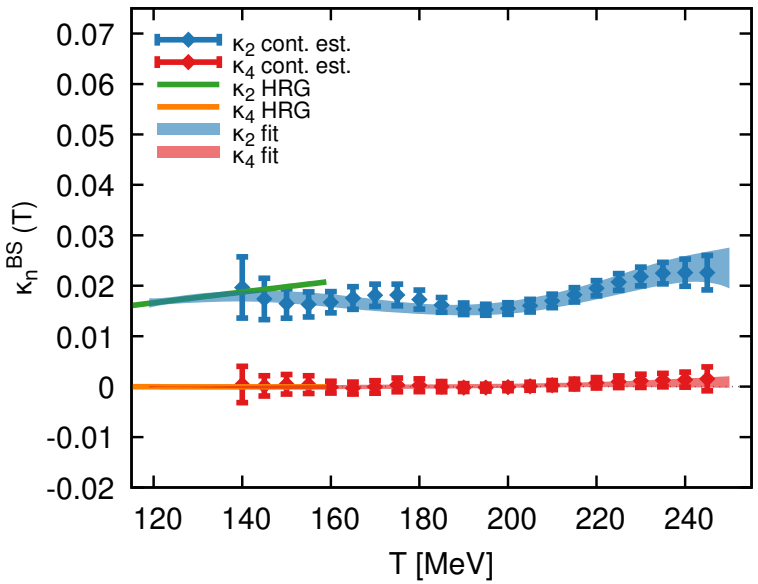
The width is basically independent of $\mathrm{Im}\hat{\mu}_B$ in our data.
We extrapolate using a cubic polynomial.

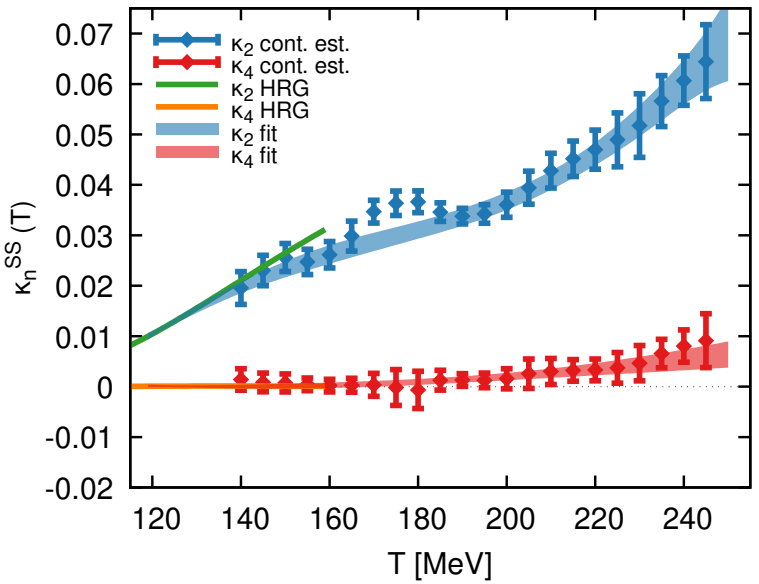


The results for $\kappa_2(T)$, $\kappa_4(T)$

A similar picture appears for strangeness density and susceptibility:

$$\chi_1^S(T,\hat{\mu}_B) = \mu_B \cdot \chi_{11}^{BS}\left[T \cdot (1 + \kappa_2^{BS}(T) \cdot \hat{\mu}_B^2 + \kappa_4^{BS}(T) \cdot \hat{\mu}_B^4 + \ldots)\right]$$
$$\chi_2^S(T,\hat{\mu}_B) = \chi_2^S\left[T \cdot (1 + \kappa_2^{SS}(T) \cdot \hat{\mu}_B^2 + \kappa_4^{SS}(T) \cdot \hat{\mu}_B^4 + \ldots)\right]$$

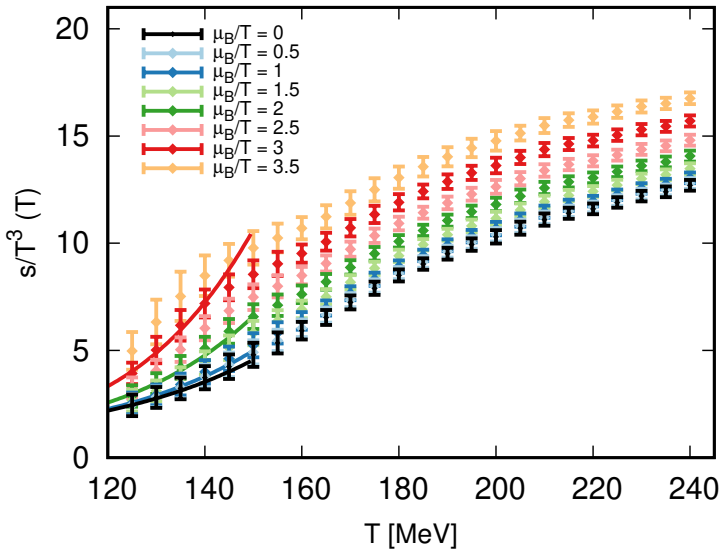


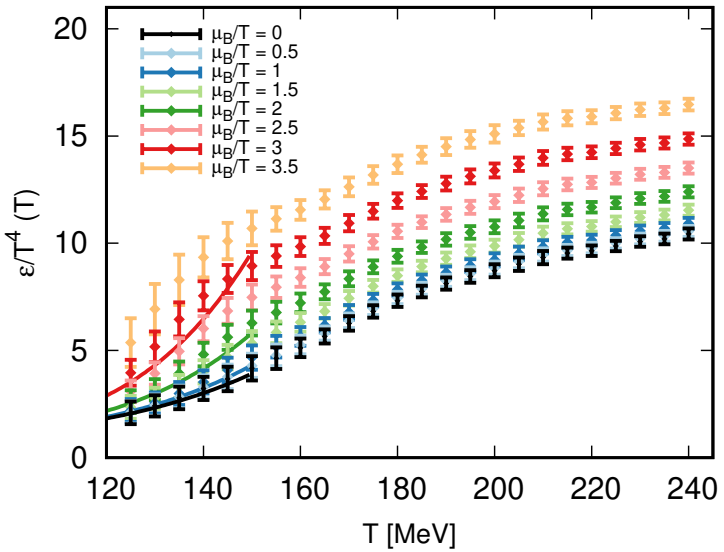


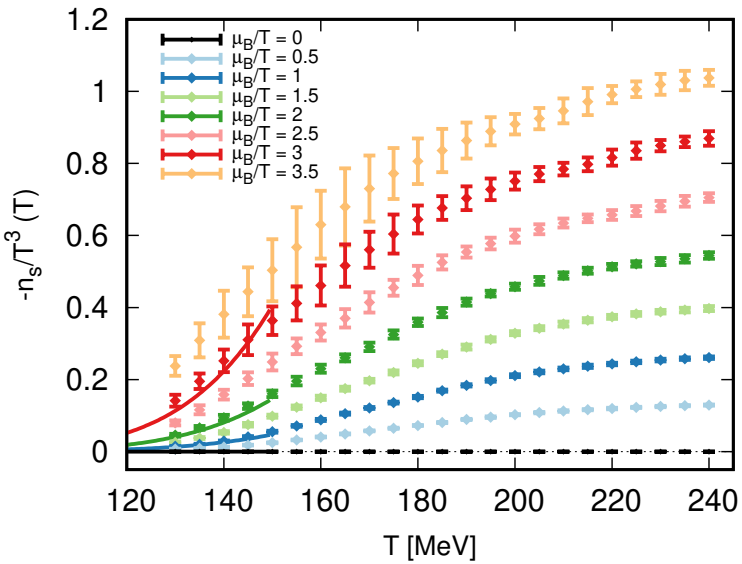
NOTE: polynomial fits take into account both statistical and systematic correlations.

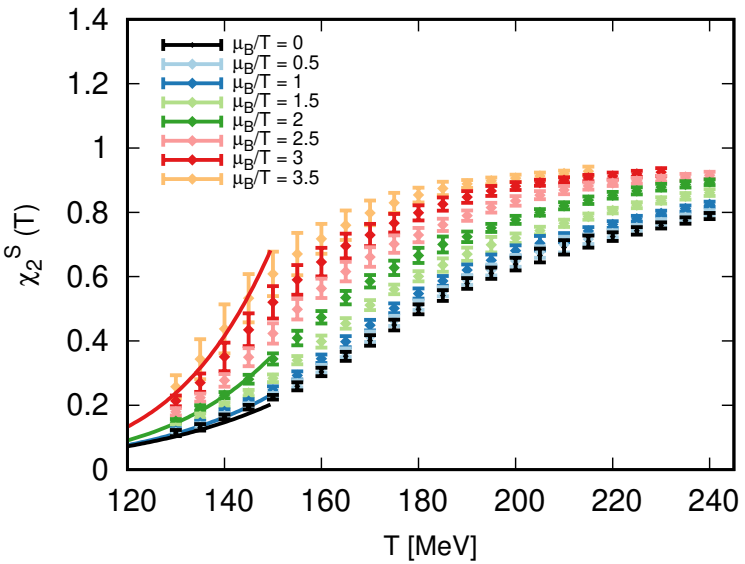
[Wuppertal Budapest 2102.06660]

Thermodynamics at finite (real) μ_B









[Wuppertal Budapest 2102.06660]