Towards lattice QCD at *not so small* chemical potentials

based on [2102.06625] [2102.06660] [2108.09213]

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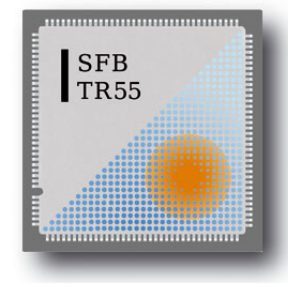
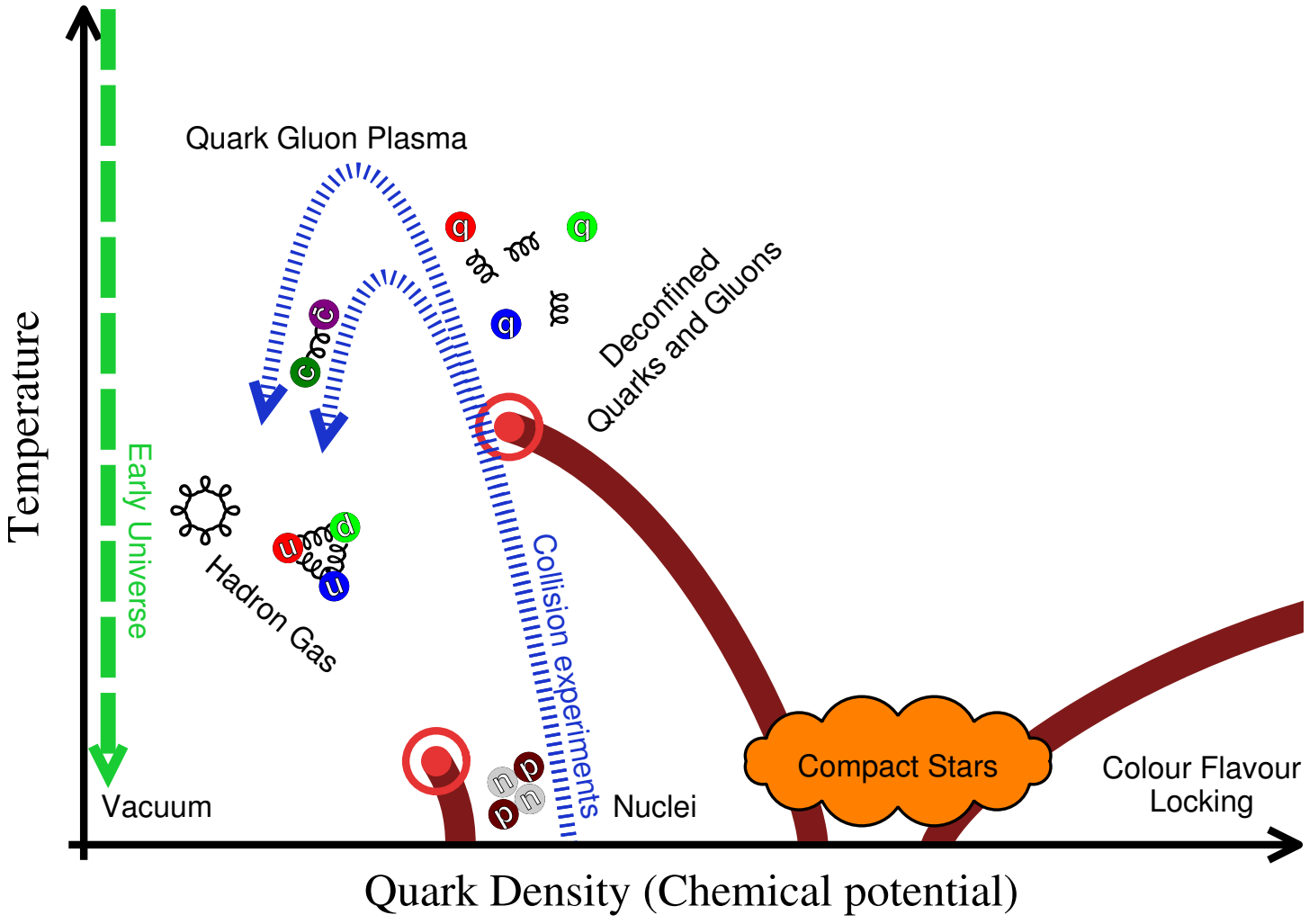
RHIC BES Seminar



The QCD phase diagram



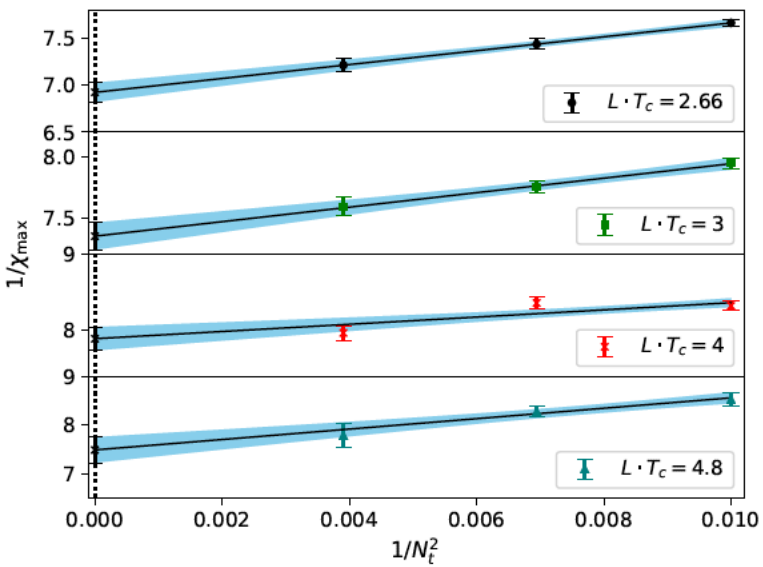
Lattice QCD still sees a crossover at $\mu_B = 0$

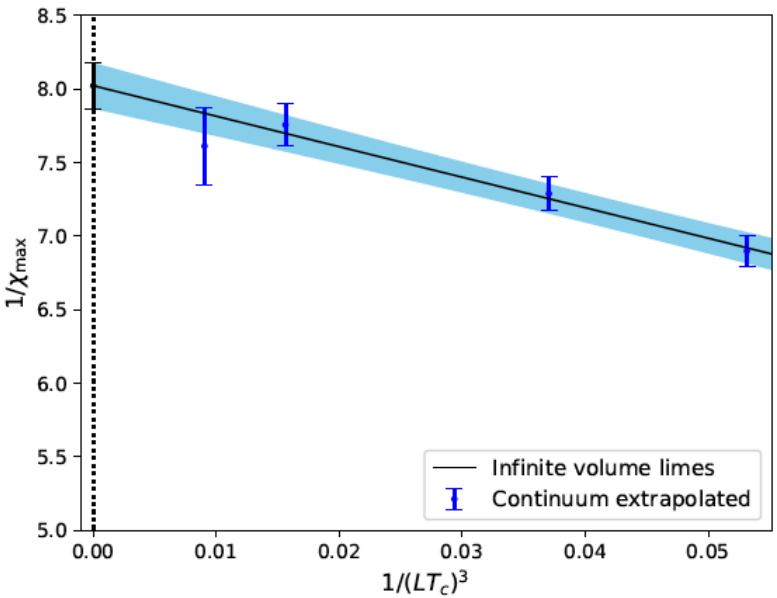
If it was a real transition:

the inverse chiral susceptibility $1/\chi \to 0$ with Volume$\to \infty$

Left) Continuum limit with every volume

Right) Thermodynamic limit of continuum ($1/\chi(V)$) results: **finite**





Byproduct: $T_c(\mu_B = 0) = 158.0 \pm 0.6$ MeV

width of the transition $\Delta T = 15\ MeV$.

[First result: Fodor et al Nature 443 (2006) 675-678]

[Update: Ruben Kara's diploma thesis, QM'19 Wuhan]

Outline

Why is finite μ_B difficult for lattice?

Lattice QCD is a tool to integrate the Euclidean path integral.

$$Z = \int DAD\bar{\psi}D\psi e^{-\int \frac{1}{4}F_{\mu\nu}F_{\mu\nu} - \int \bar{\psi}(m+\gamma_\mu D_\mu)\psi}$$

We get rid of the Grassmann variables by integrating the ferminos analytically:

$$Z = \int DA \det M(A) e^{-\int \frac{1}{4}F_{\mu\nu}F_{\mu\nu}}$$

where M is the fermion matrix. We can simulate this if det M is

real and positive

because then we can associate a probility weight with every gauge configuration.
This determinant is real and positive if

- chemical potential = zero
- nonzero isospin chemical potential $(\mu_u = -\mu_d)$
- nonzero imaginary baryon chemical potential $(\mathrm{Re}\ \mu_B = 0)$

Otherwise we face a **complex action problem** *and importance sampling fails.*

How to avoid the complex action problem?

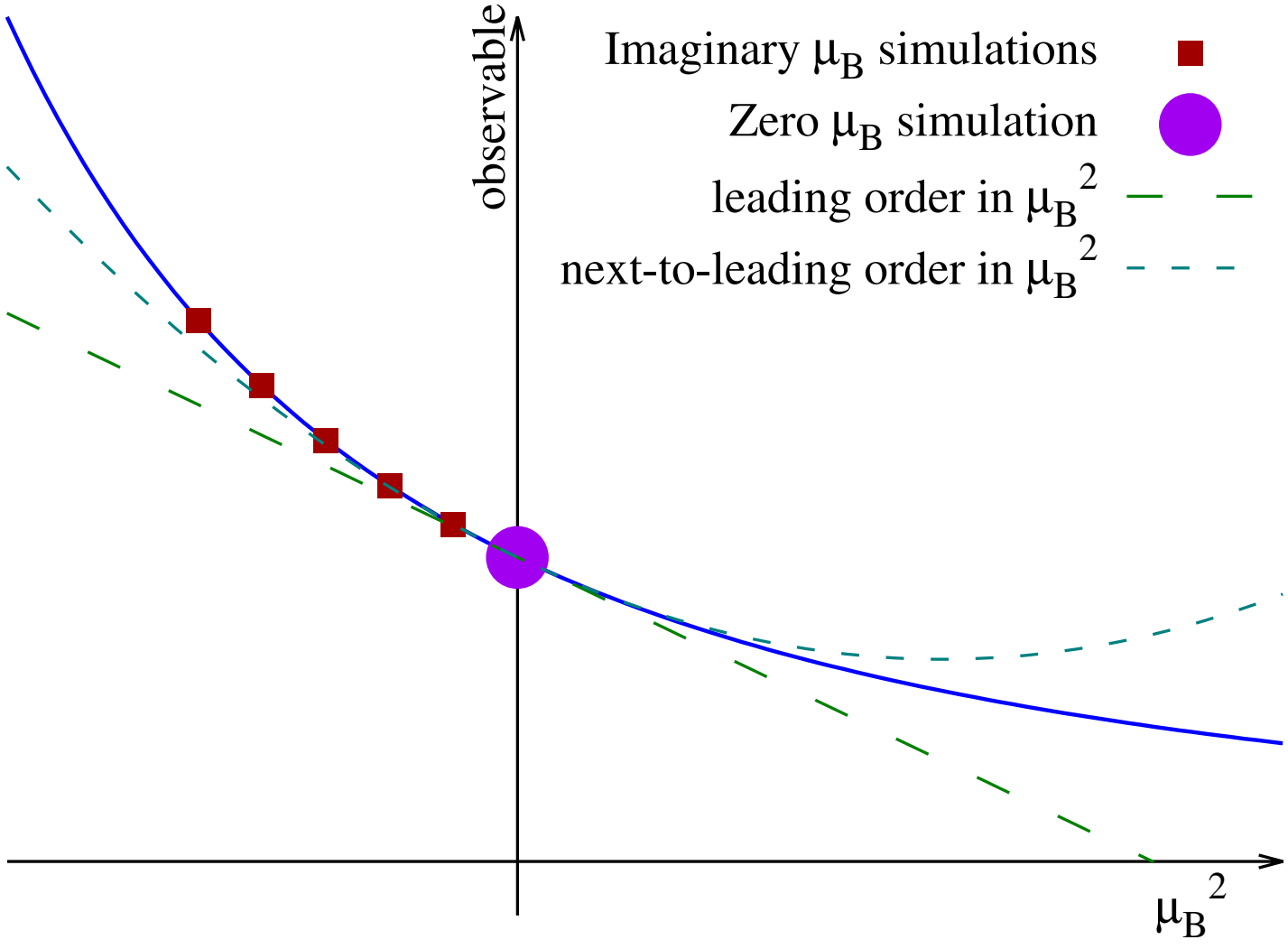
- zero chemical potential
  At $\mu_B = 0$ one can simulate and calculate derivatives, like

$$\left.\frac{\partial^n \langle \text{Observable} \rangle}{(\partial \mu_B)^n}\right|_{\mu_B=0}$$

  This is the **Taylor method** since one simulates the expanson coefficients of the power series in μ_B.
  Higher derivatives are **not cheap**.

- nonzero imaginary baryon chemical potential $(\text{Re}\ \mu_B = 0)$
  Charge conjugation symmetry: C-even observables: $f(\mu_B^2)$
  Imaginary μ_B: $\mu_B^2 < 0$
  Real μ_B: $\mu_B^2 > 0$
  Analytical continuation from $\mu_B^2 \leq 0$ to $\mu_B^2 > 0$.
  Many expansion schemes can be defined (ambiguous).

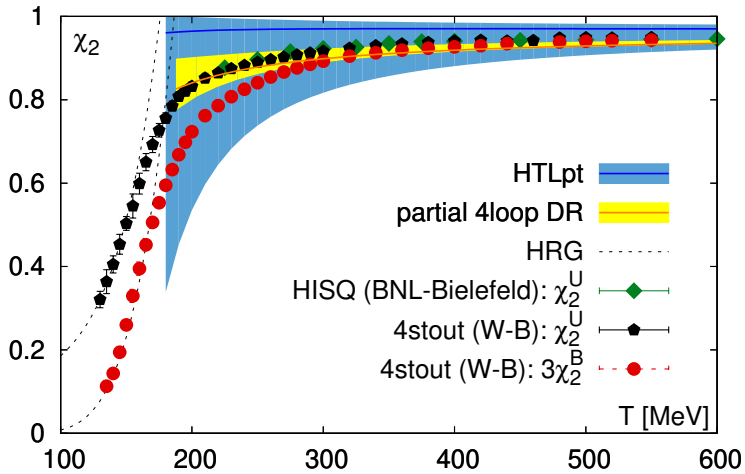
Extrapolation approaches to $\mu_B^2 > 0$

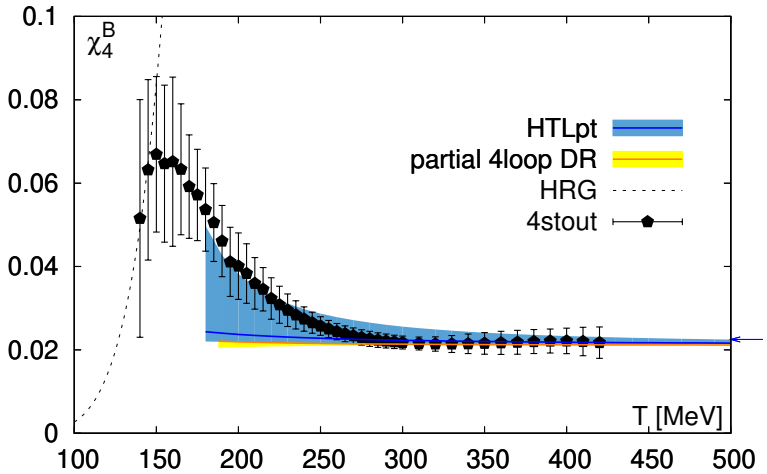


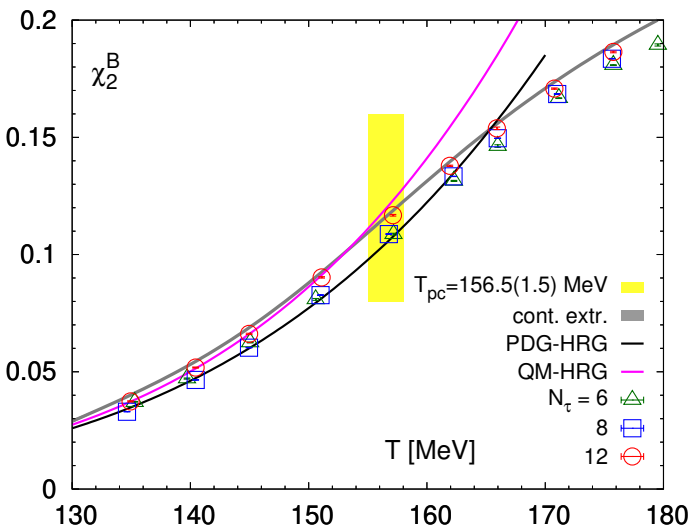
Imaginary μ_B: numerical derivatives with some *lever arm*.
Taylor from $\mu_B = 0$: exact derivatives based on the tails of a distribution.

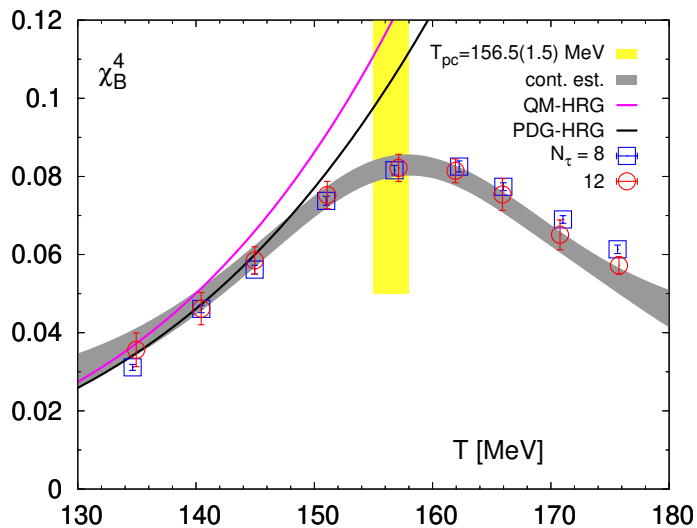
Baryon fluctuations: lattice connects HRG and HTL

$$\frac{\langle \delta B^2 \rangle}{V} = \chi_2^B = T^{-2} dp/d\mu_B^2$$









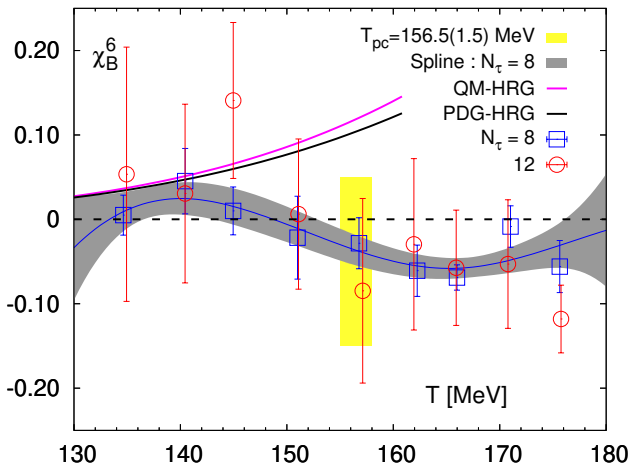
[HTL results: Haque et al 1309.3968,1402.6907]

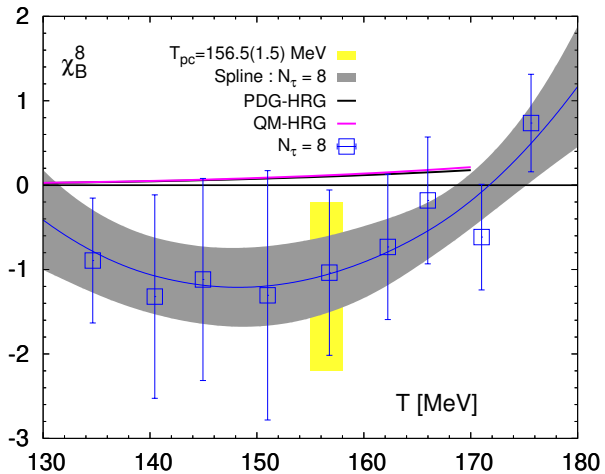
[Lattice results: (top) BW 1507.04627 (see also 1805.04445), (bottom) HotQCD 2001.08530]

Taylor method

$$\frac{p}{T^4} = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n p/T^4}{(\partial \mu_B)^n} = \sum_{n=0}^{\infty} \frac{1}{n!} \chi_B^n$$

Sixth and eight order baryon fluctuations = $\mathcal{O}(\mu_B^6)$ and $\mathcal{O}(\mu_B^8)$ coefficients

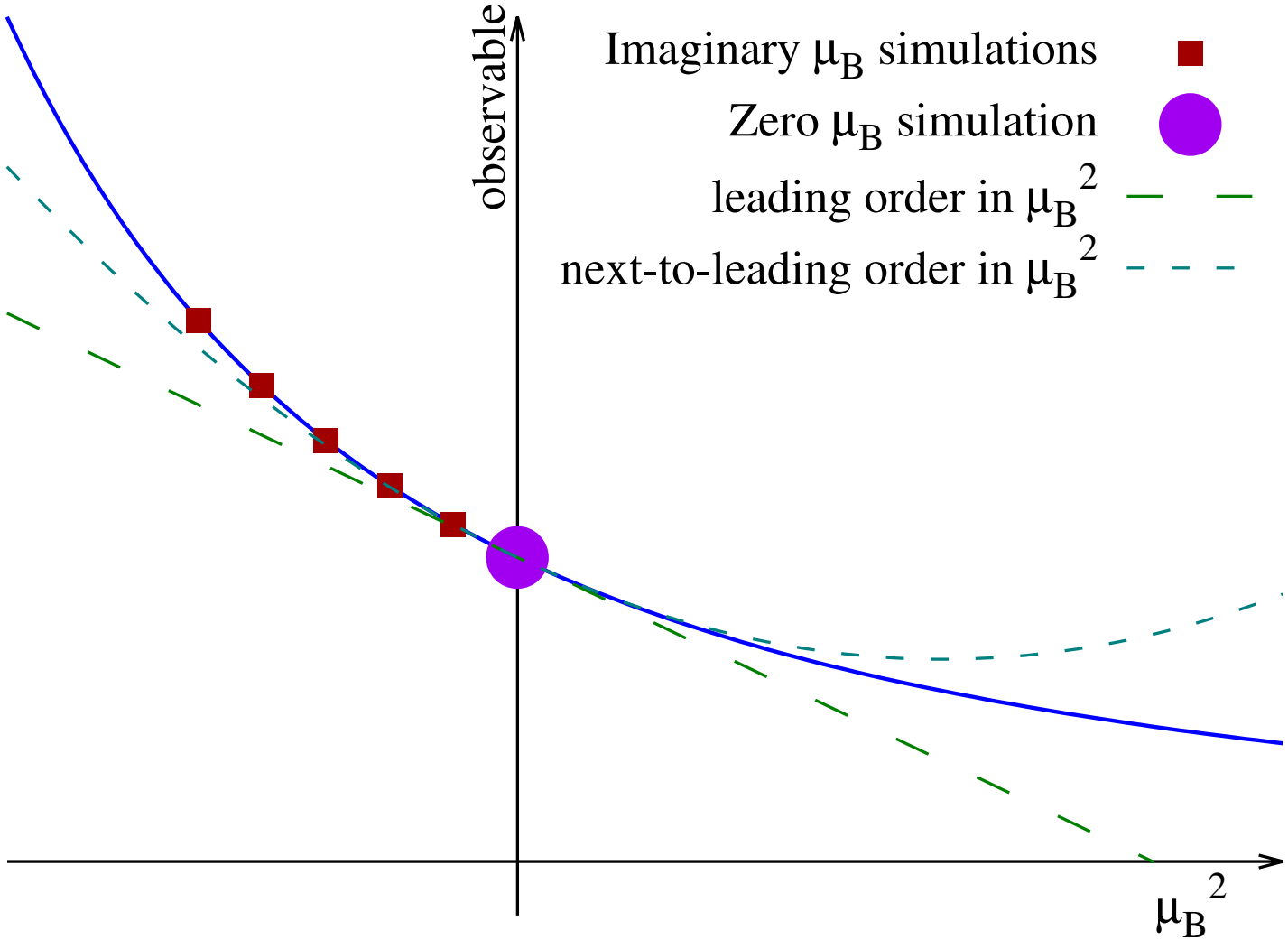




N_τ = 8		N_τ = 12	
T[MeV]	#conf.	T[MeV]	#conf.
134.64	1,275,380	134.94	256,392
140.45	1,598,555	140.44	368,491
144.95	1,559,003	144.97	344,010
151.00	1,286,603	151.10	308,680
156.78	1,602,684	157.13	299,029
162.25	1,437,436	161.94	214,671
165.98	1,186,523	165.91	156,111
171.02	373,644	170.77	144,633
175.64	294,311	175.77	131,248

[Lattice results: HotQCD 2001.08530]

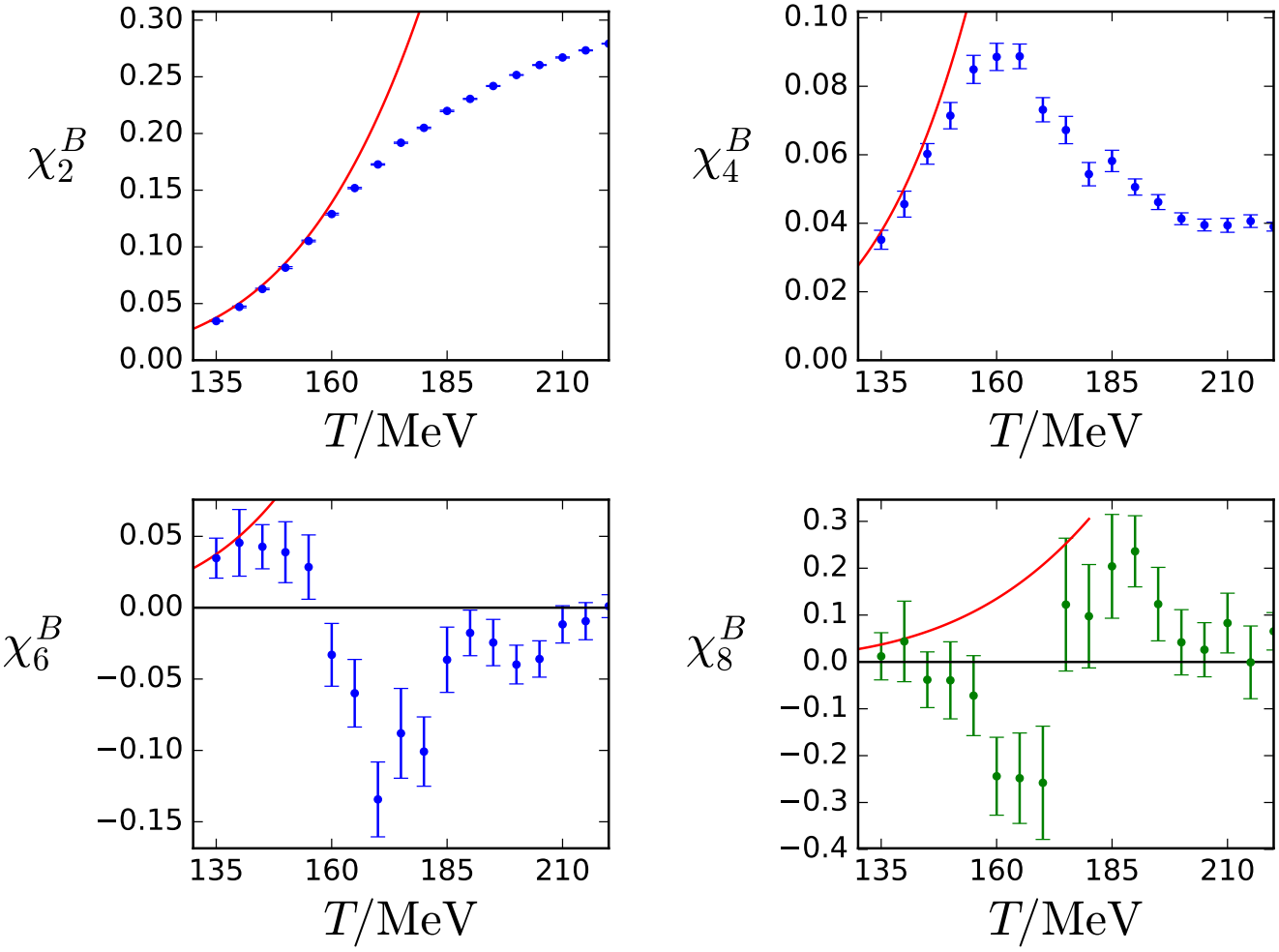
Extrapolation approaches to $\mu_B^2 > 0$



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]

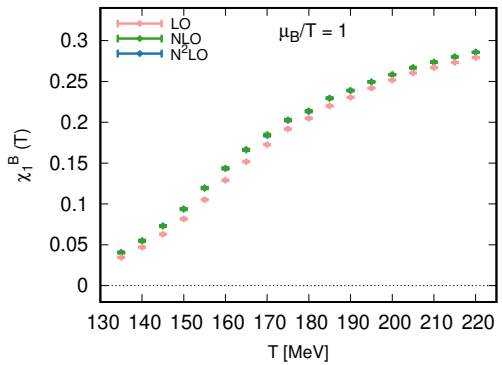


This structure is already known from chiral effecive models. [Friman et al 1103.3511]

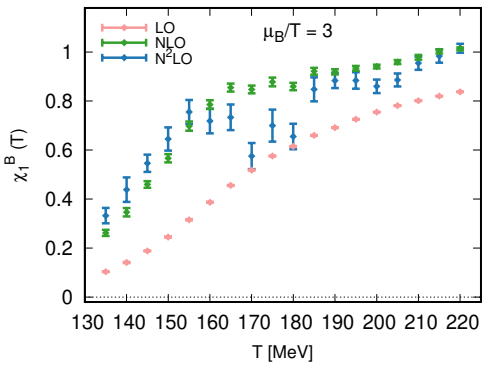
There is a rather simple model that quantitatively describes the χ coefficients

Baryon density at finite μ_B - Taylor expansion

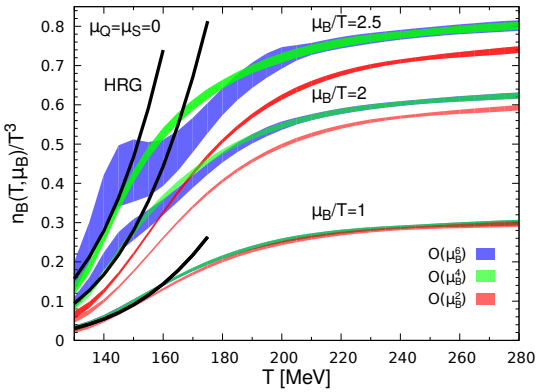
- Thermodynamic quantities at large chemical potential become problematic
- Higher orders do not help with the convergence of the series



[Wuppertal Budapest 1805.04445]



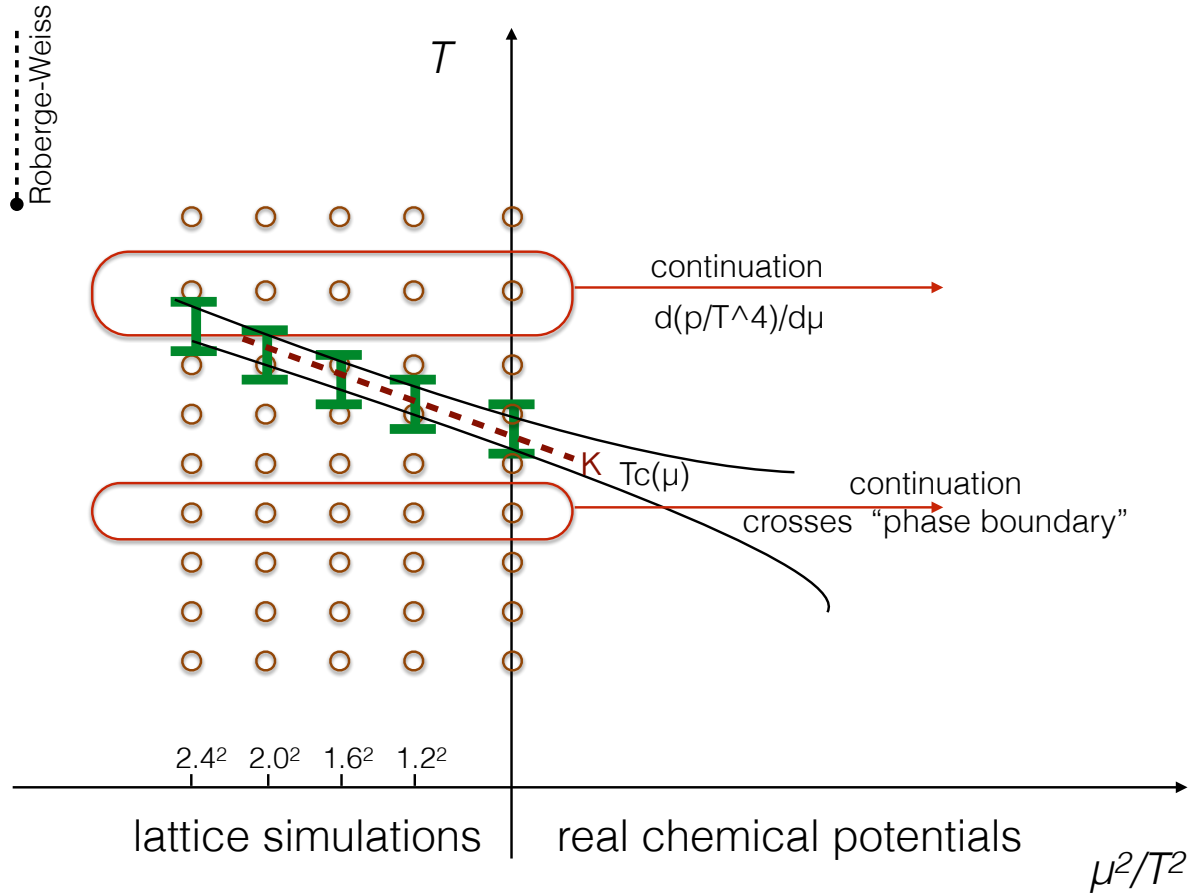
[Wuppertal Budapest 1805.04445]



[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 $Tc(\mu_B)$

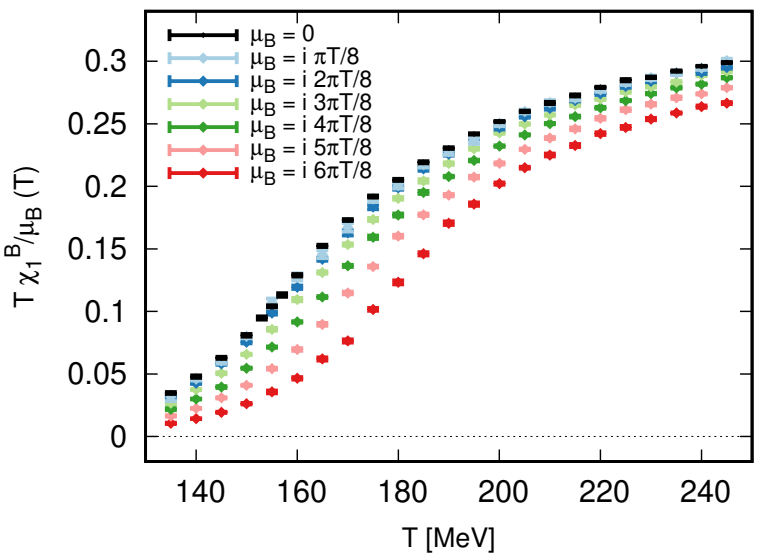
Further observations from imaginary μ_B

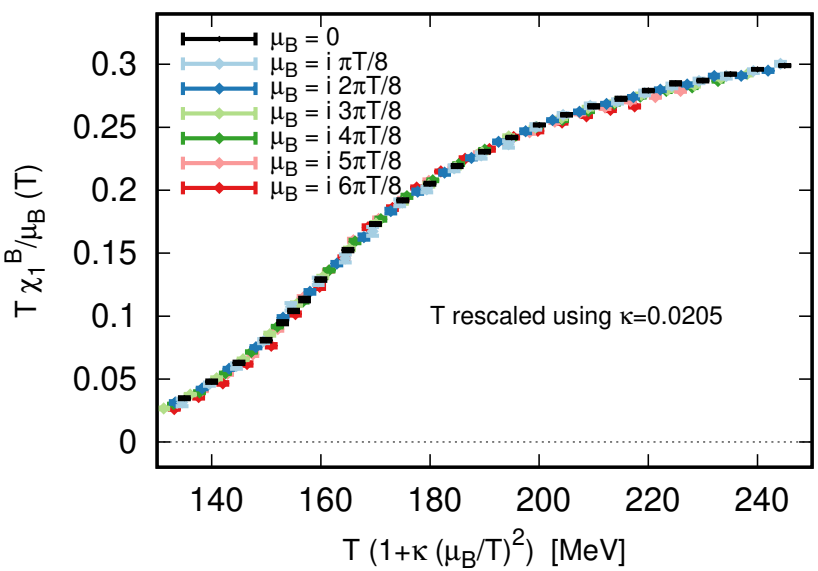
Baryon density: $\chi_1^B(T, \hat{\mu}_B)$

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

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

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

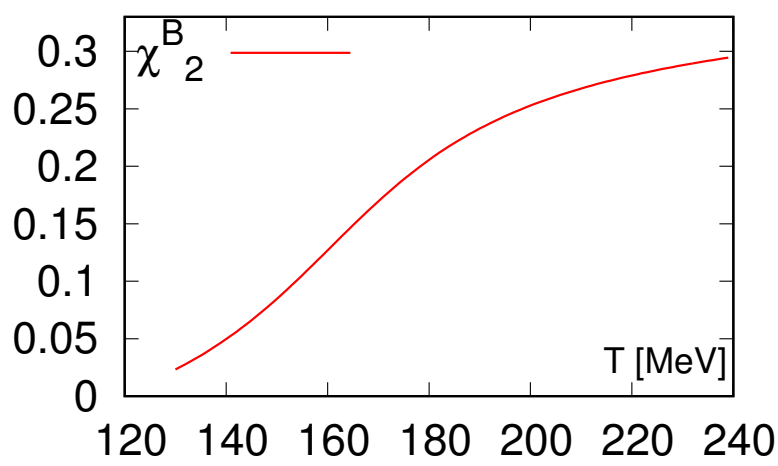


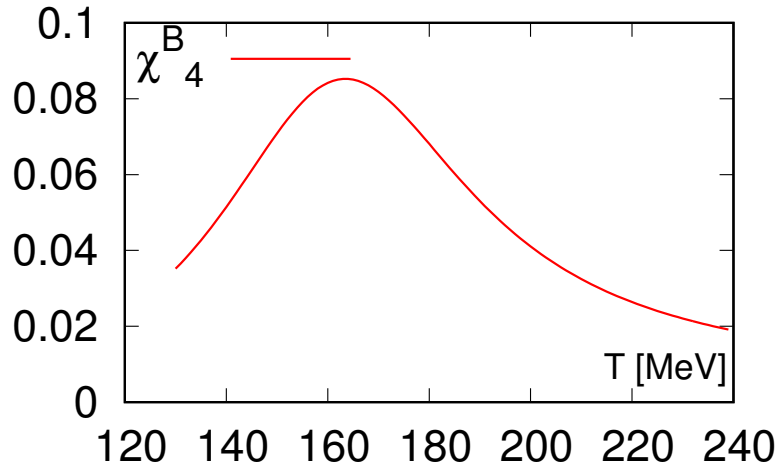


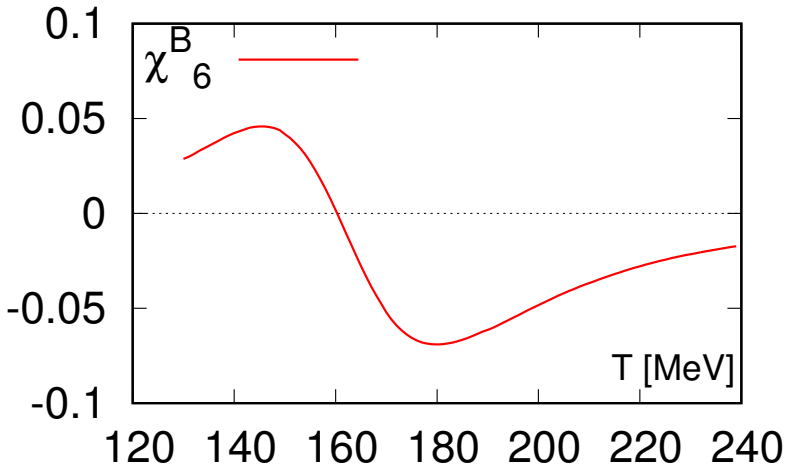
[Wuppertal Budapest 2102.06660]

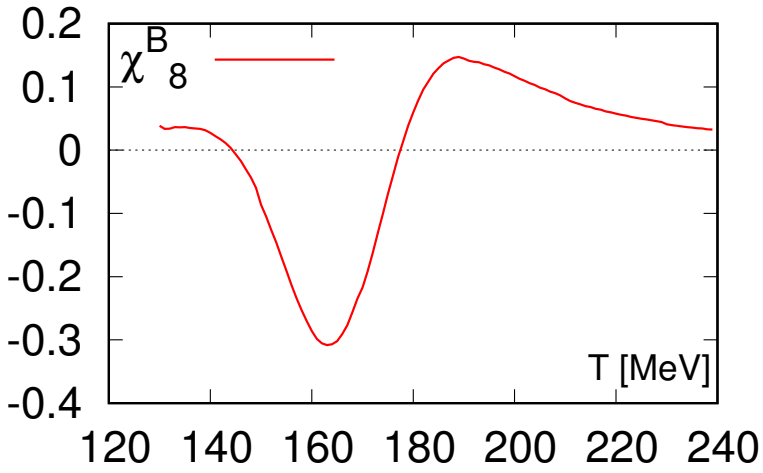
Higher order χ_B in the simple model

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



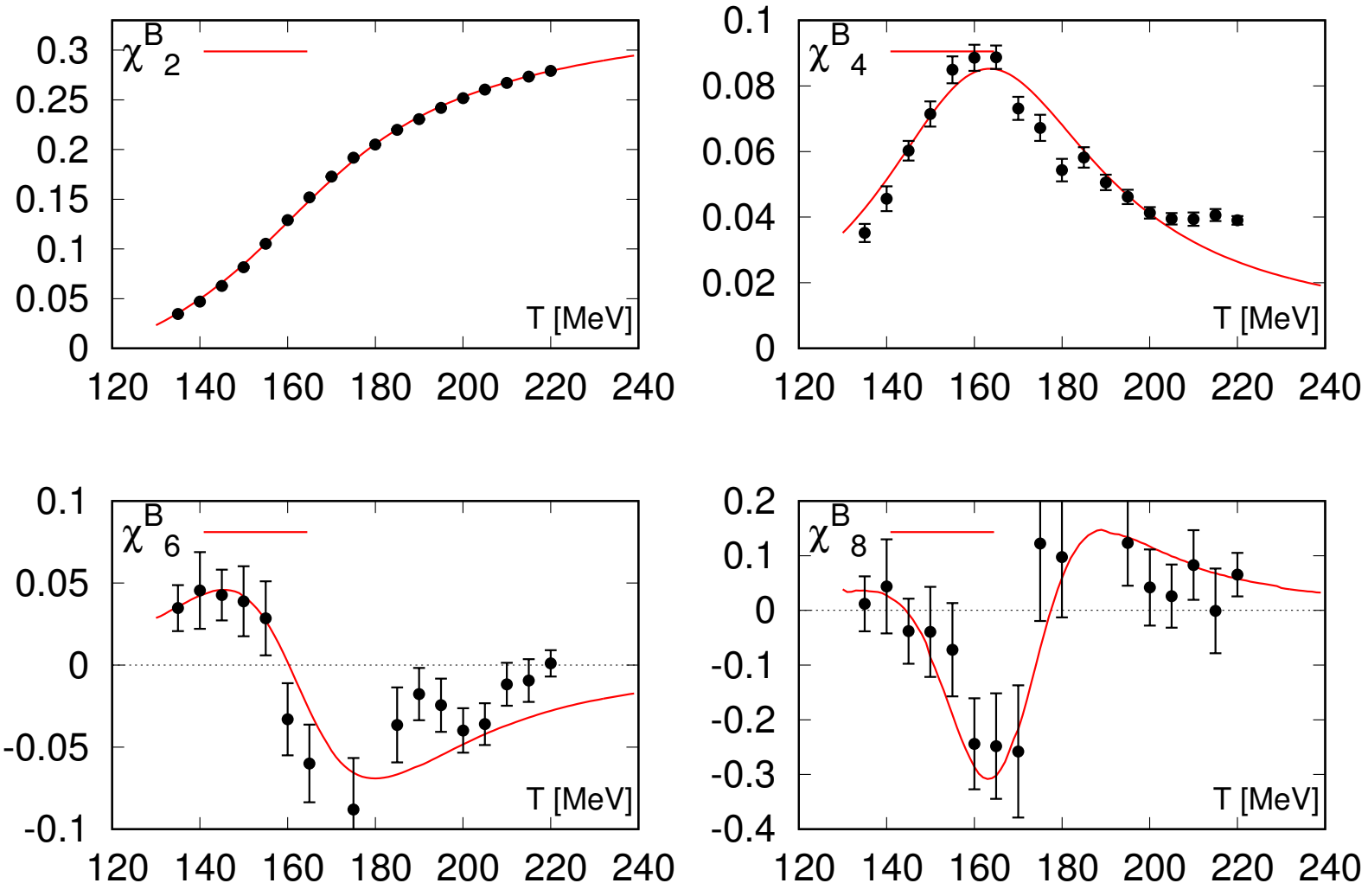






Higher order χ_B in the simple model

Comparing the simple model with our lattice result:



Simple model describes lattice result surprisingly well.

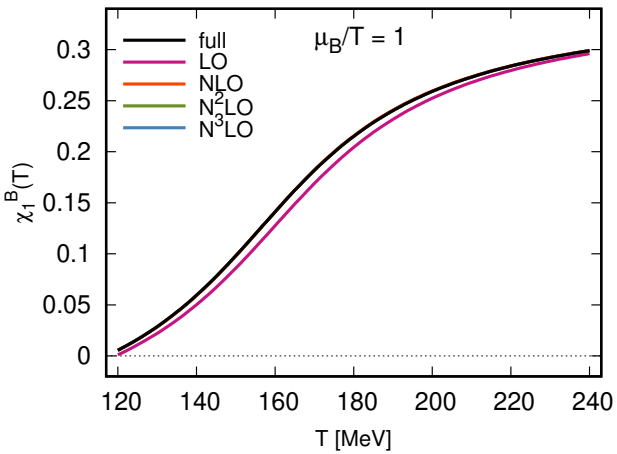
Result is consistent with the no-critical-end-point scenario.

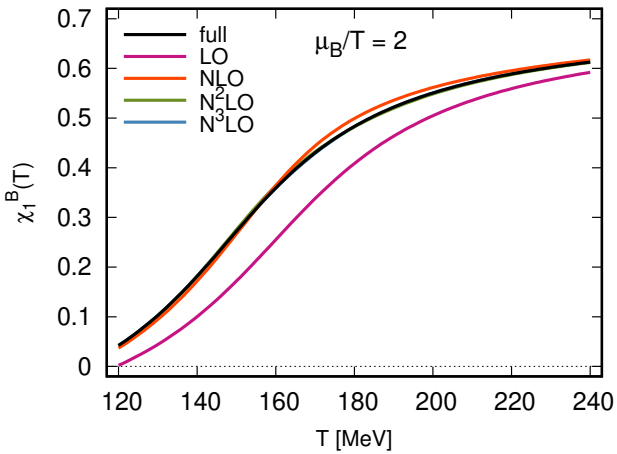
Taylor expanding a (shifting) sigmoid

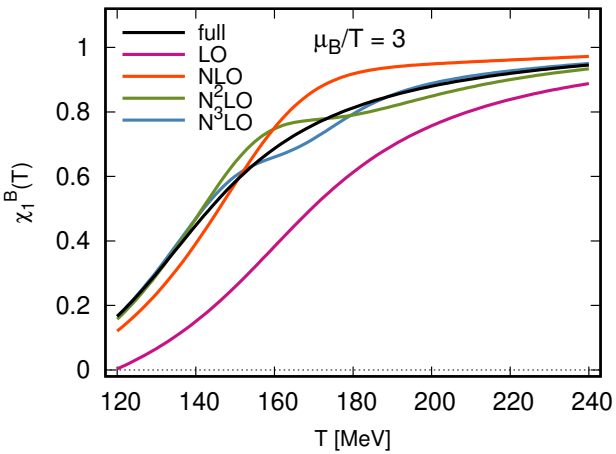
Assume we have a sigmoid function $f(T)$ which shifts with $\hat{\mu}$, with a simple T-independent shifting parameter κ. How does Taylor cope with it?

$$f(T,\hat{\mu}) = f(T',0)\ , \qquad T' = T(1+\kappa\hat{\mu}^2)\ ,$$

We fitted $f(T,0) = a + b\arctan(c(T-d))$ to $\chi_2^B(T,0)$ data for a 48×12 lattice







[Wuppertal Budapest 2102.06660]

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

- $\chi(T)$: 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:

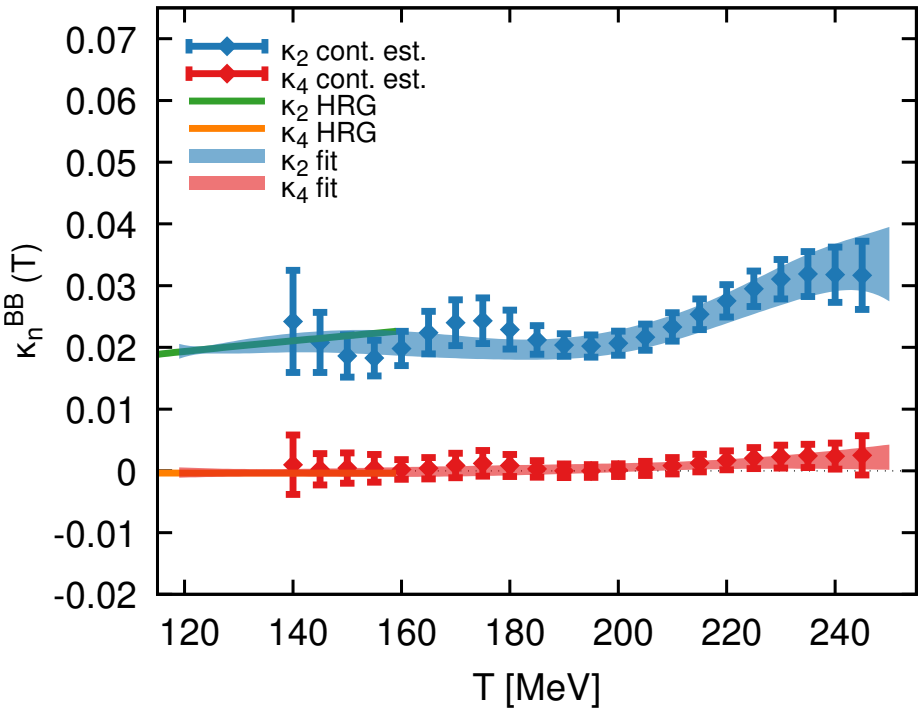
$$\kappa_2(T) = \frac{1}{6T}\frac{\chi_4^B(T)}{\chi_2^{B\prime}(T)}$$

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

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)



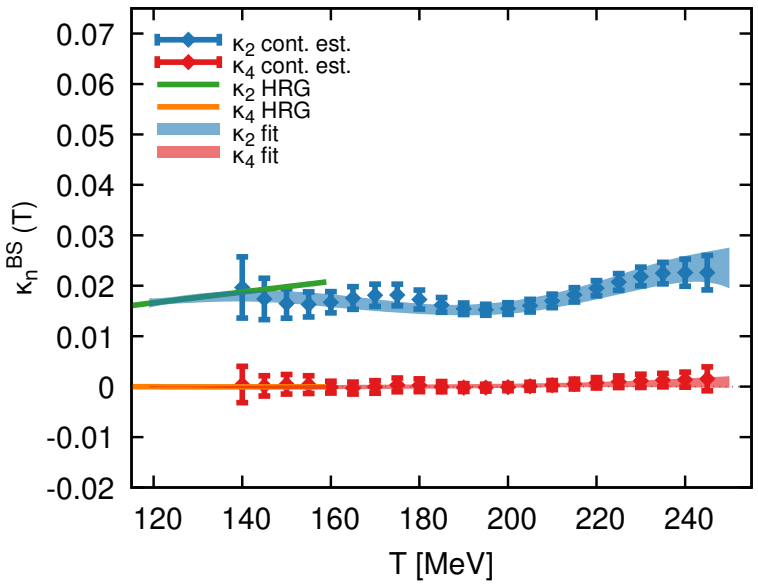
NOTE: polynomial fits take into account both statistical and systematic correlations.

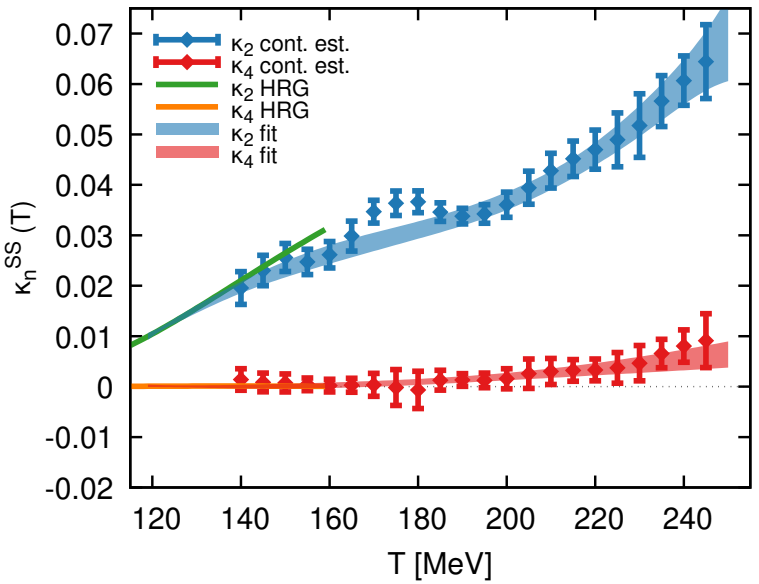
[Wuppertal Budapest 2102.06660]

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

A similar picture appears for strangeness density and susceptibility:

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





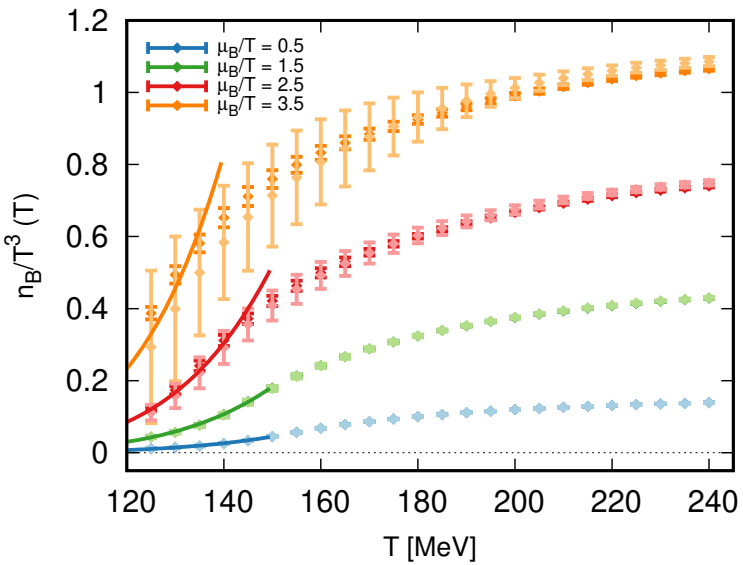
NOTE: polynomial fits take into account both statistical and systematic correlations.

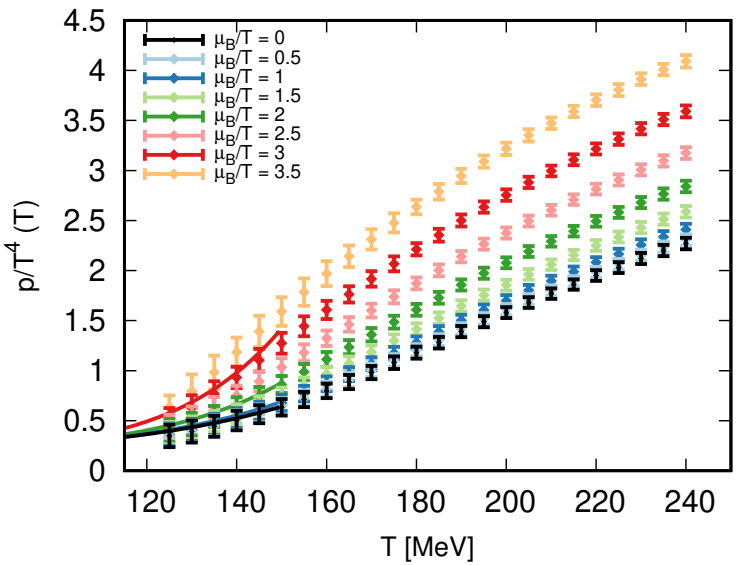
[Wuppertal Budapest 2102.06660]

Thermodynamics at finite (real) μ_B

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





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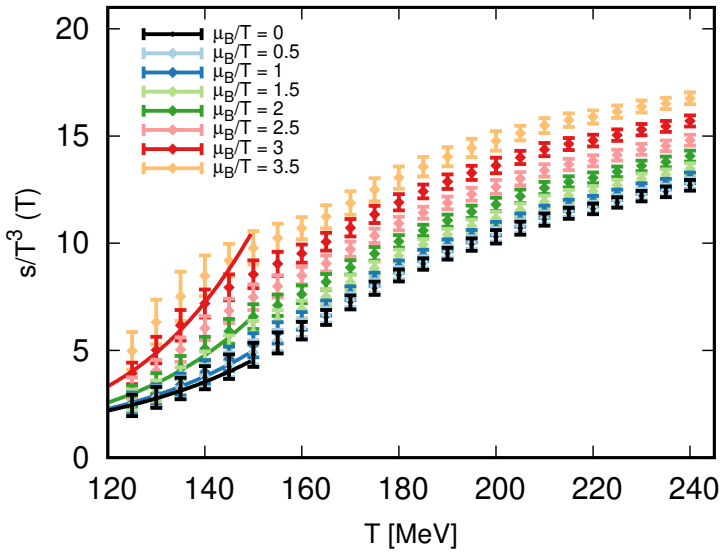
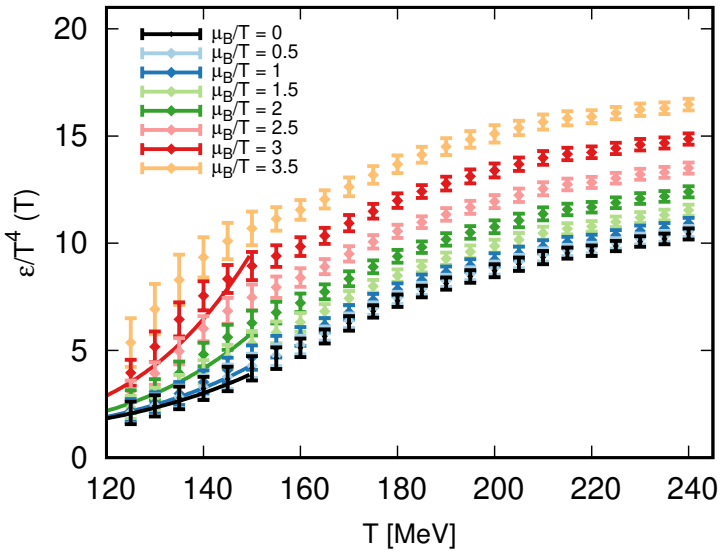
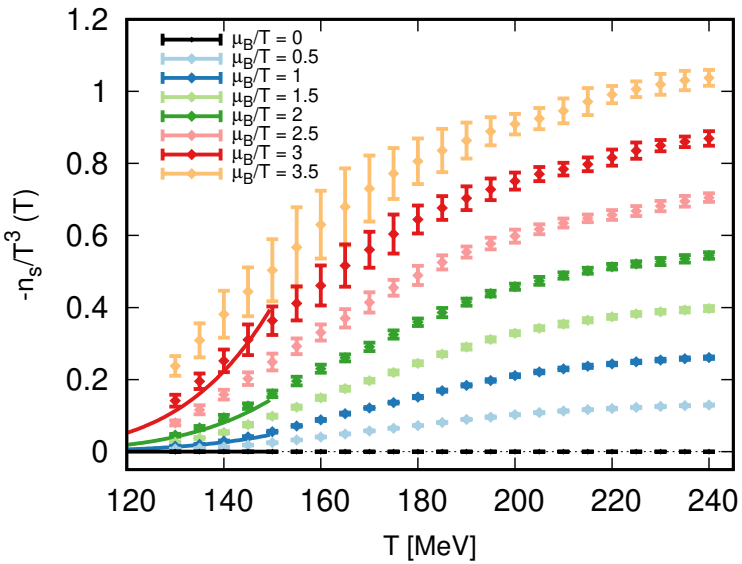
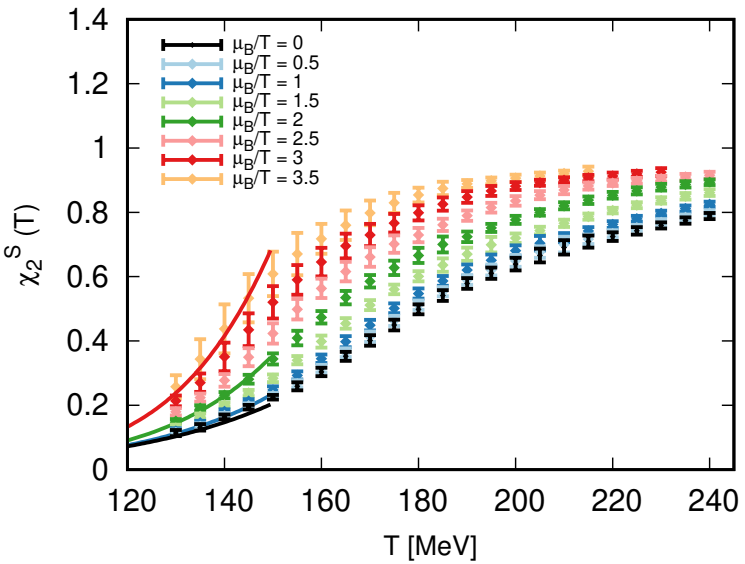
Thermodynamics at finite (real) μ_B









[Wuppertal Budapest 2102.06660]

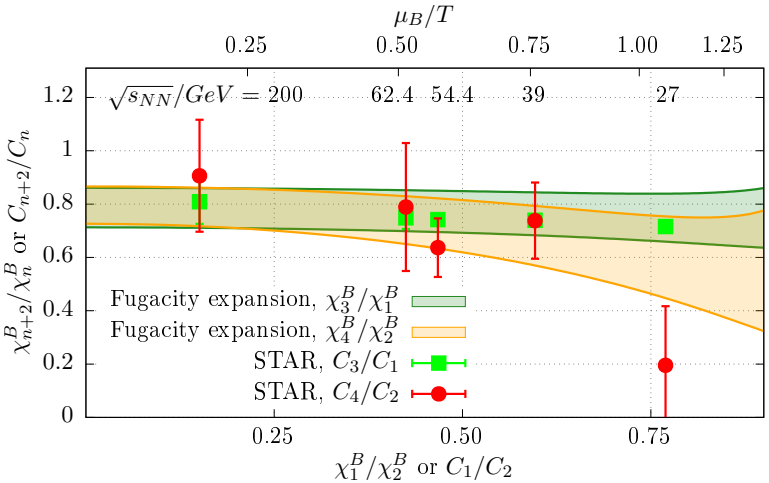
Hadronic phase: Fourier (virial/fugacity) expansion

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]

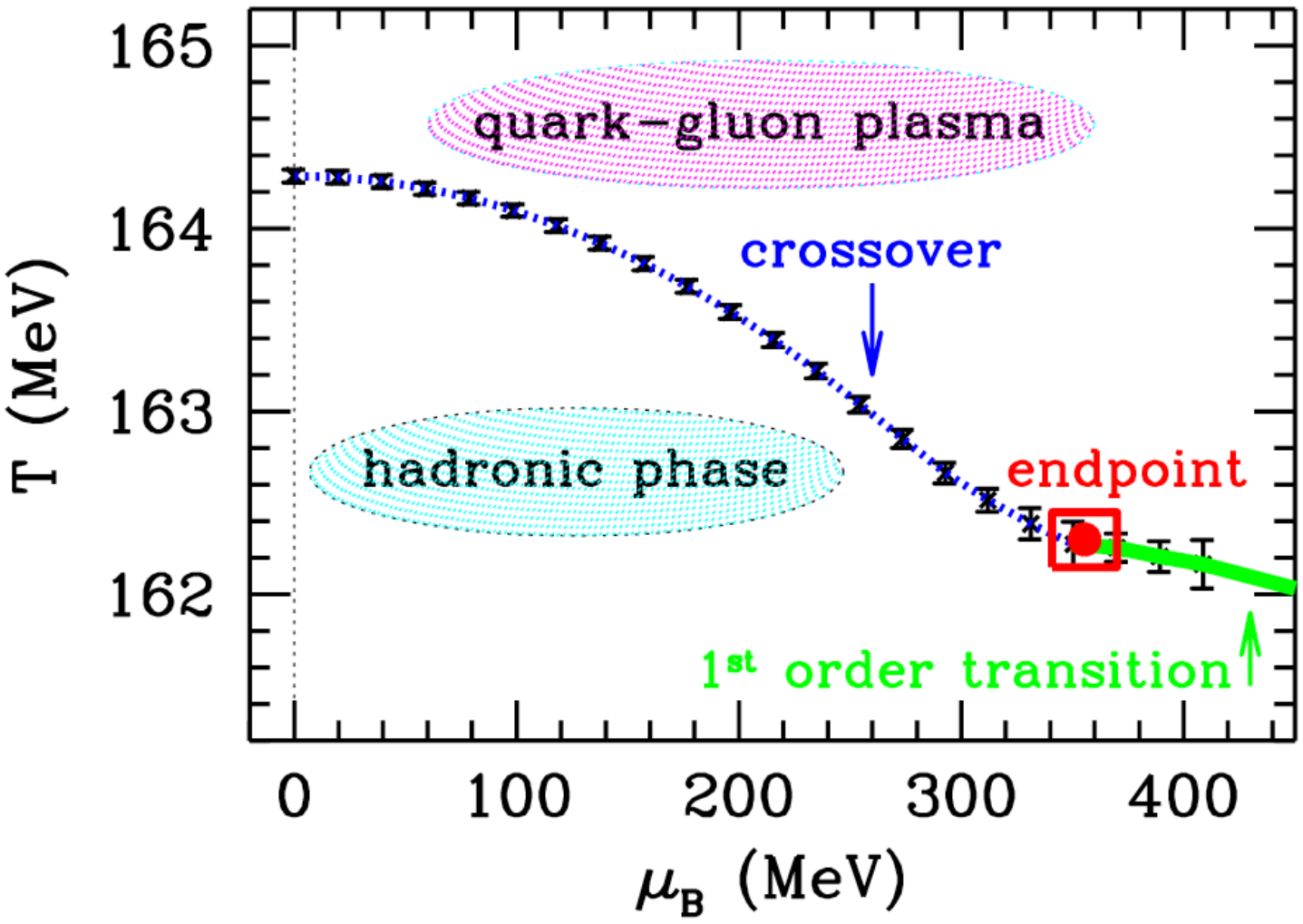
Extrapolation schemes: summary

We discussed three extrapolation schemes:

- **Taylor method:**
  - Power series in μ_B at fixed T:
  - robust, well motivated at high T,
  - convergence problems around the transition
- **Fugacity expansion:**
  - Fourier series in imaginary $\mu_B \longrightarrow \sum_B sinh(B\mu_B)$ series,
  - explodes at high μ_B
  - motivated in the confined phase
- **Extrapolation in temperature:** *(not in the observable)*
  - extrapolations to larger μ_B
  - well motivated by the nature of the crossover transition *(quasi-constant width and strength)*
  - does not try to extrapolate through a transition

All these schemes are just reorderings of the μ_B expansion.
All these schemes assume an analytic cross-over.

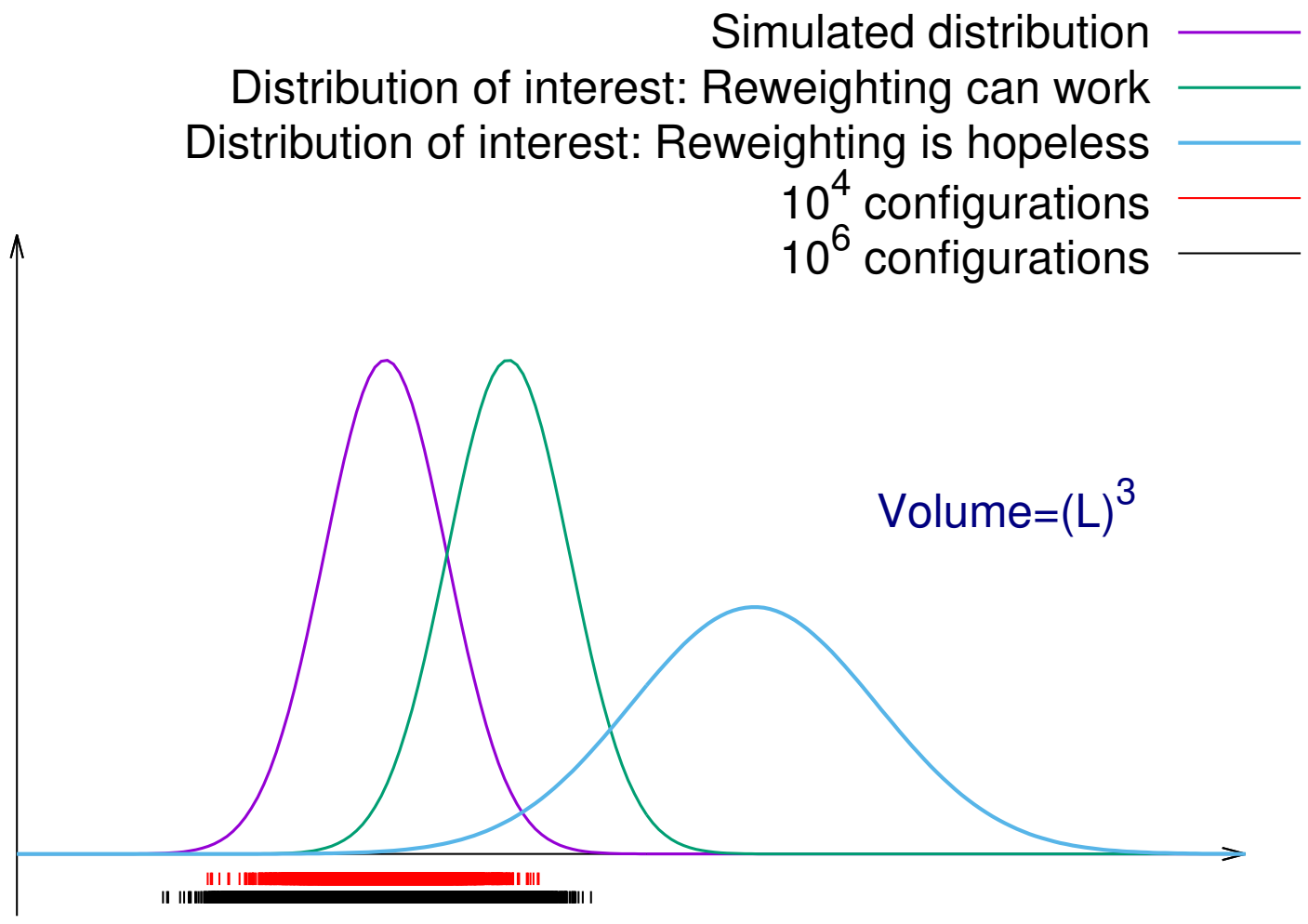
Reweighting to real μ_B



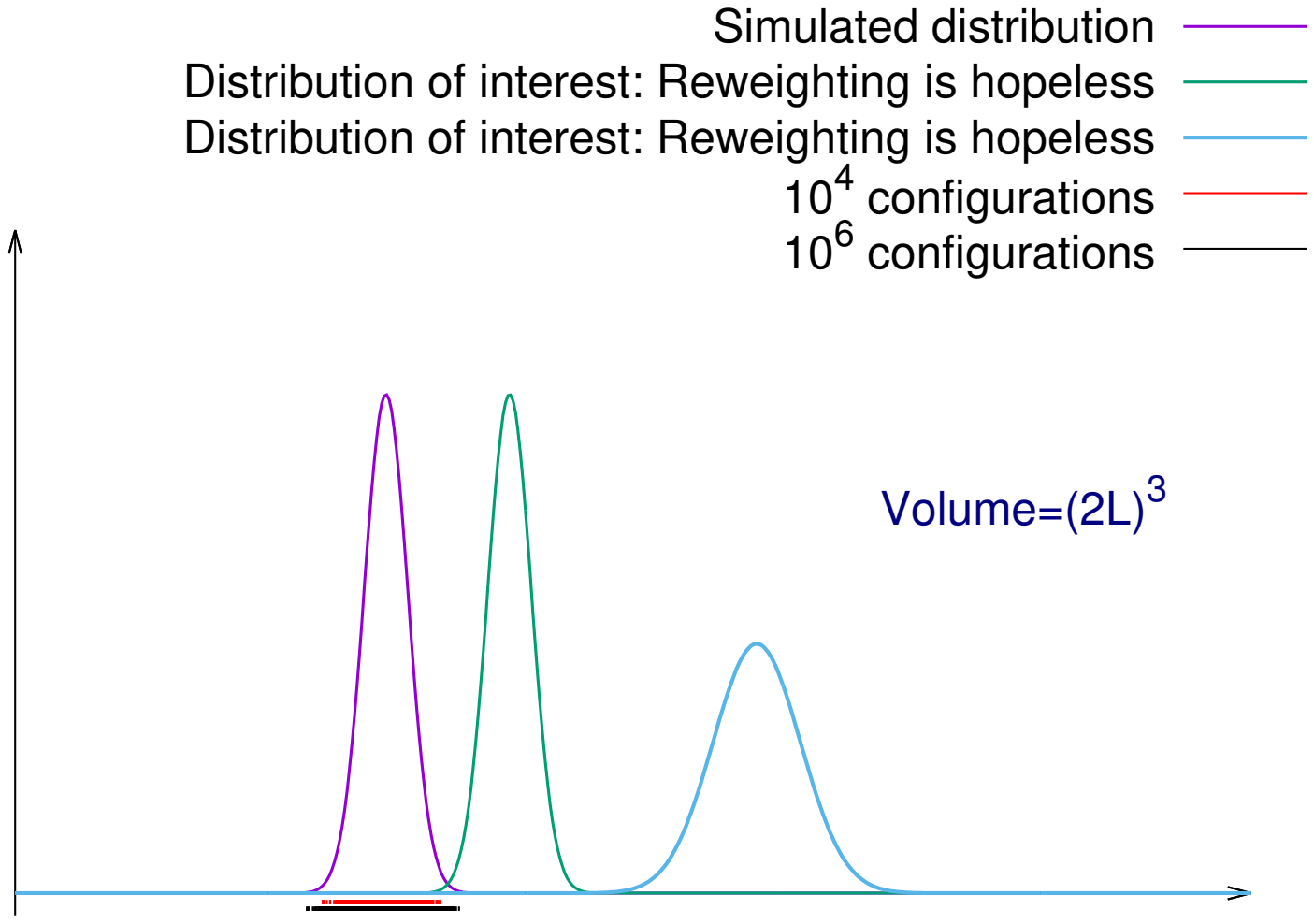
Using physical quark masses, $2+1$ *flavors,* $N_t = 4$ [Fodor&Katz hep-lat/0402006]

The overlap problem

Reweighting: Simulalate with parameters A and try to transform the distribution as if you simulated with parameters B.



Reweighting: Costs explode with volume.



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)*

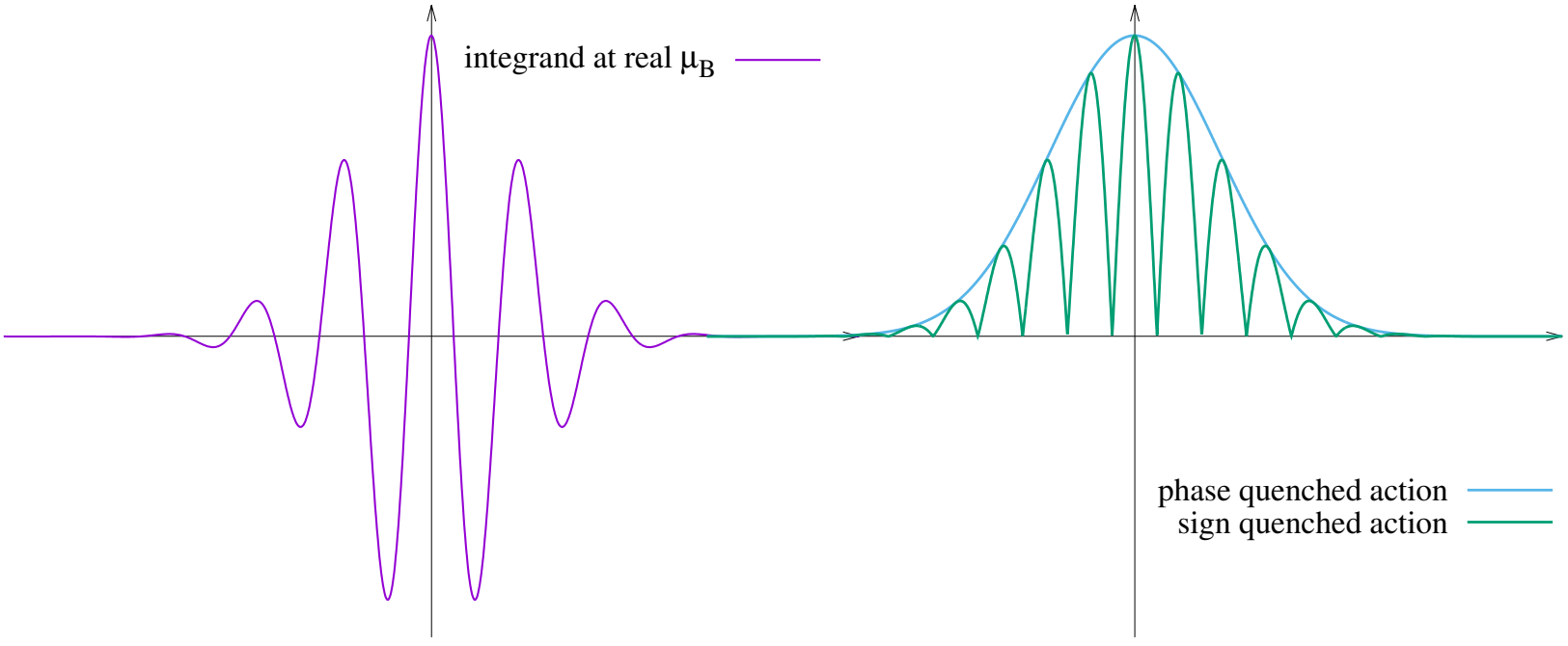
$$\int DU \,\big|\det M[U]\big|\, e^{-S_g(U)}$$

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]

The sign problem



Sign problem: Large cancellations between positive and negative contributions of $\mathrm{Re}\big[\det M[U]\big]$.

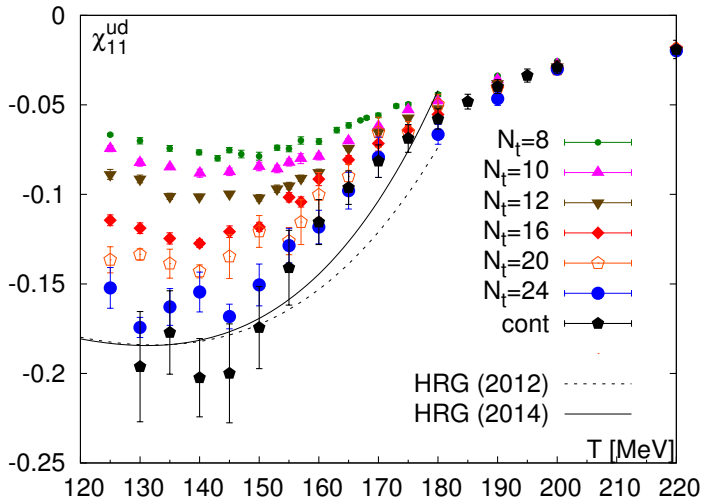
Overlap problem: Problem solved.

How strong is the sign problem?

The complex phase of the fermion determinant is linked to a physical observable, the light quark density.

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

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



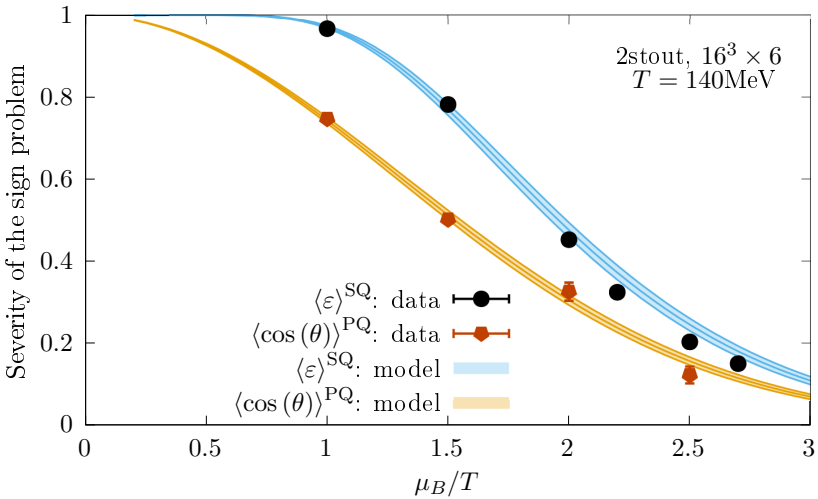
The sign problem is weak for coarse lattices and at high temperatures.

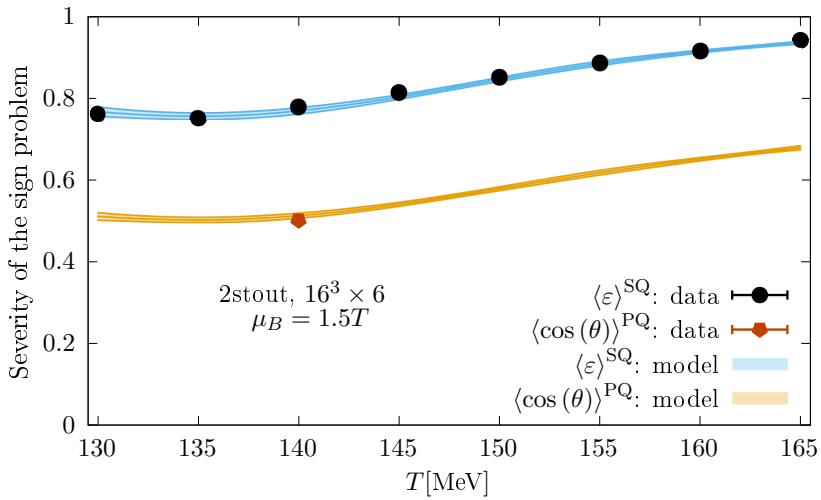
[Wuppertal-Budapest 1507.04627]

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]

Direct simulations at $\mu_B > 0$

Simulation in two steps:

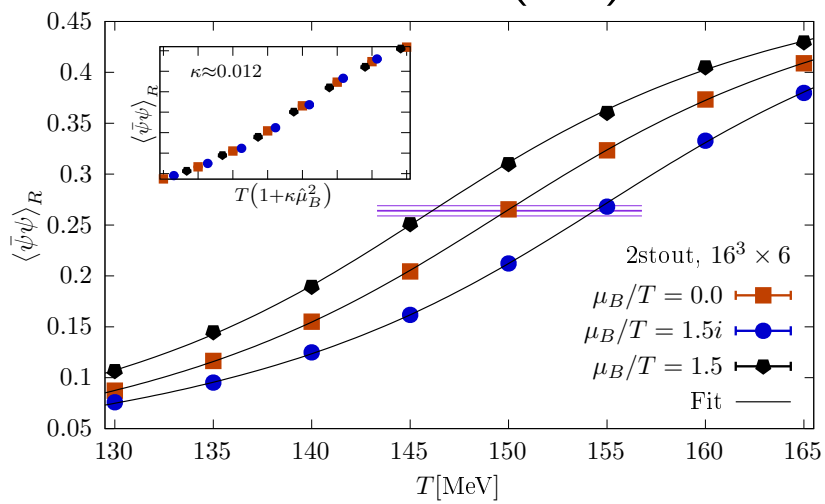
1. Simulate the real (sign quenched) action
2. Reweight each configuartion with the correct sign

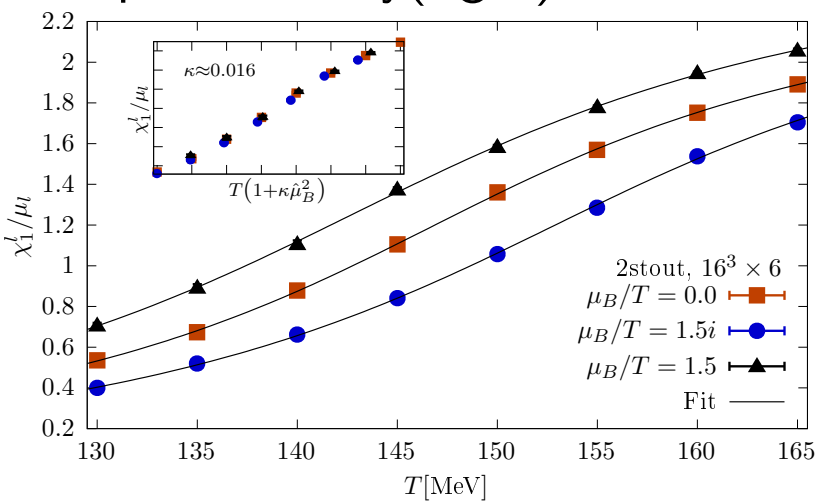
Feasible as long as the sign problem is not too severe.

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 !

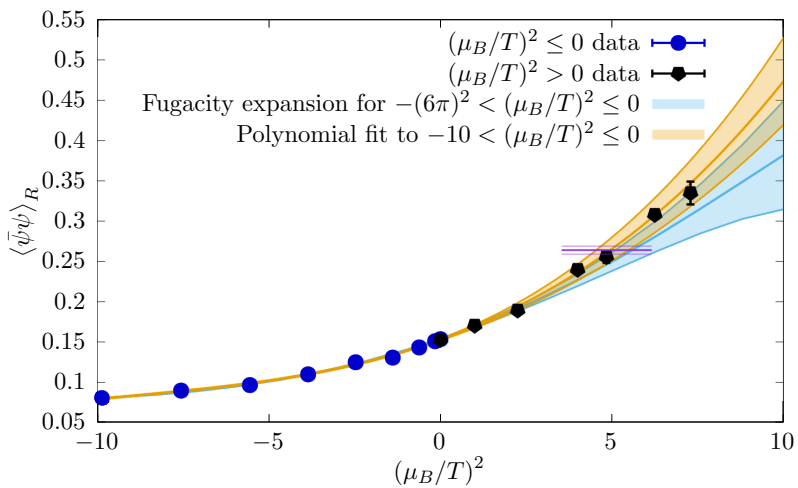
[Wuppertal-Budapest 2108.09213]

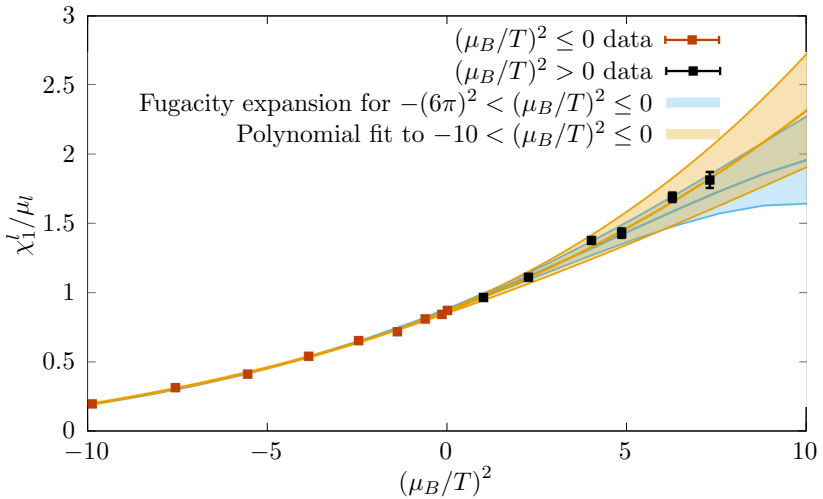
Direct simulations at $\mu_B > 0$

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

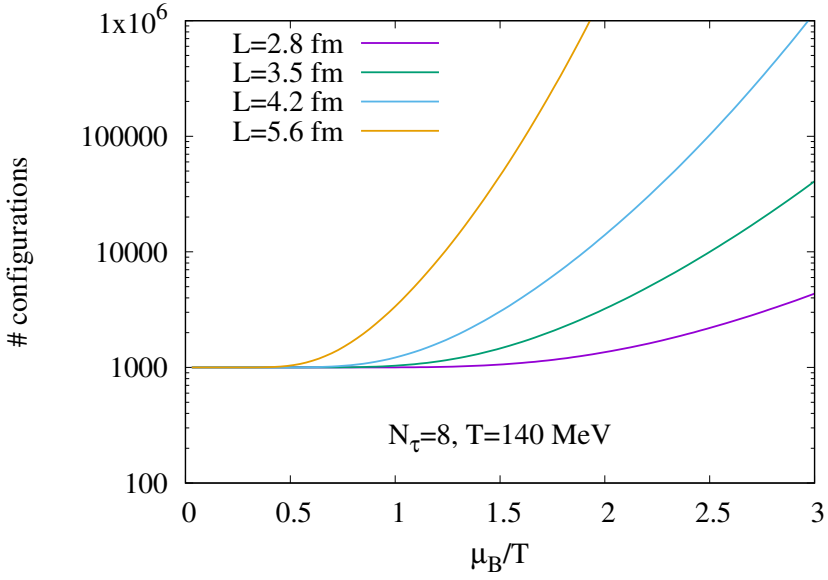


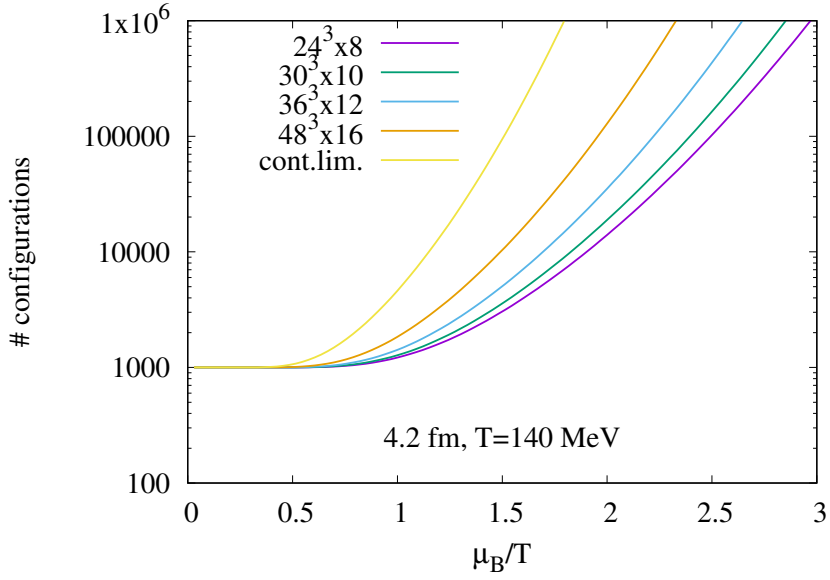


The direct result has the smallest errors.

[Wuppertal-Budapest 2108.09213]

What are the limits of the direct simulations

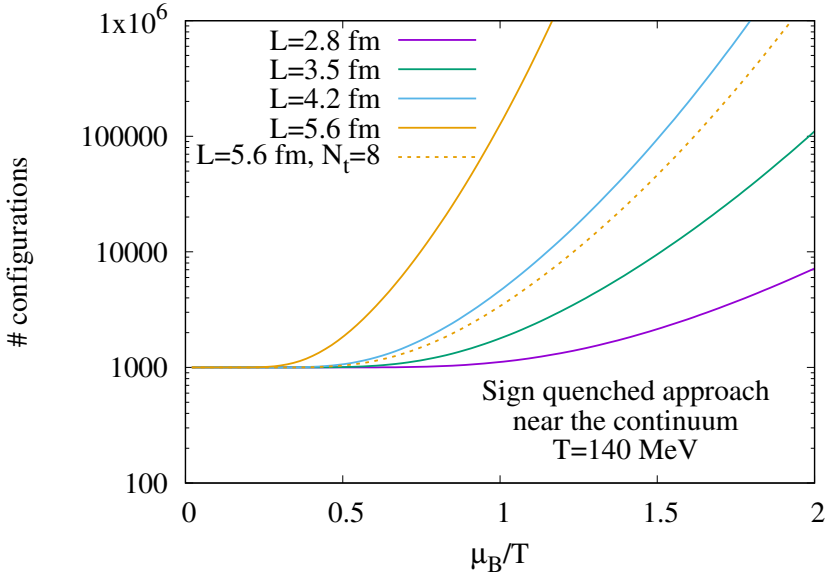


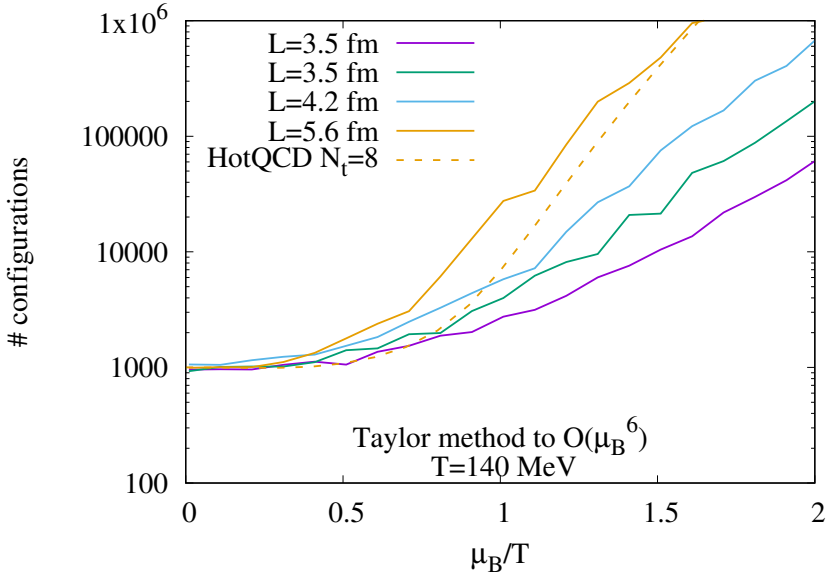


- The most important limiting factor is **volume** and μ_B.
  (The same is true for the $\mu_B = 0$ Taylor method.)
- This is bad news for the CEP search
  (finite volume scaling is very difficult)
- Below $\mu_B/T < 1$ the sign problem is weak.
- Deeper temperature and μ_B scans are feasible:
  Is the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

Statistics: direct simulation vs Taylor

We compare the number of independent configurations for fine lattices:





Let's admit:

– the direct (sign quenched) approach has more costs per config

– the direct approach must simulate at each $\mu_B > 0$,

while Taylor uses $\mu_B = 0$ only

- Sign Quenched and Taylor statistics are in the same ball park
- both face an exponential problem that deteriorates with volume
- Taylor is an extrapolation scheme, Sign Quenched is a direct result.

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!