Staggered fermions and the QCD phase diagram

[2108.09213,2208.05398,2308.06105]

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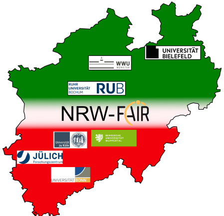
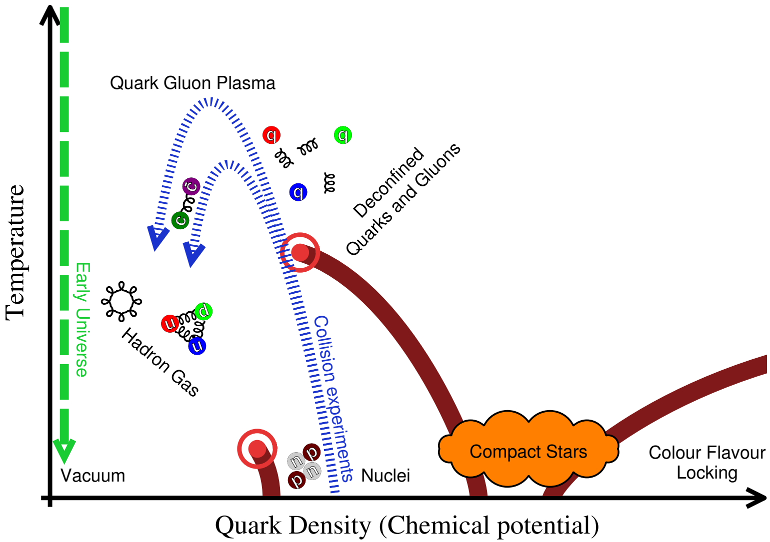
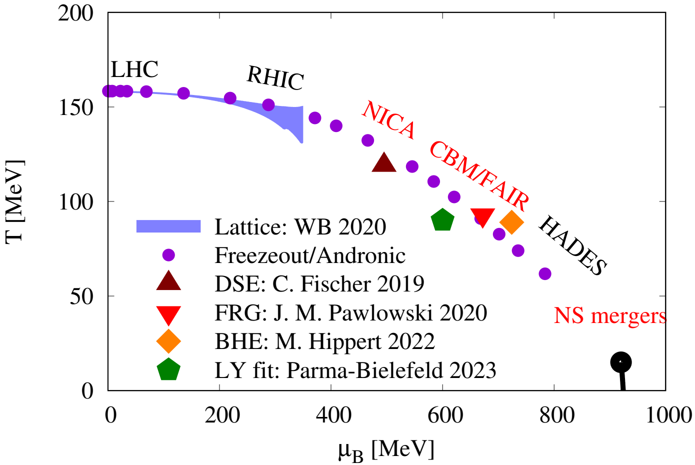
Regensburg, Sep 18, 2023
QCD on and off the lattice (and a few other topics)



The QCD phase diagram (2007)





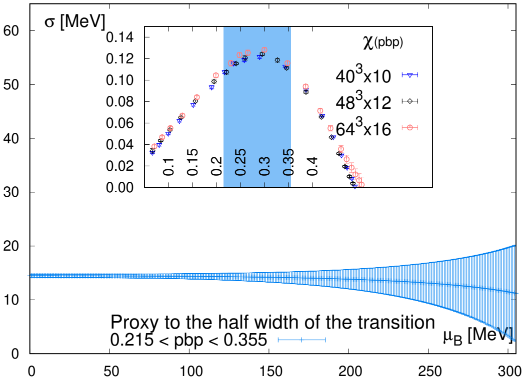
Low μ_B: $T_{\mathrm{freeze-out}} \approx T_c(\mu_B)$ [Braun-Munzinger, Stachel, Wetterich, nucl-th/0311005]
High μ_B: $T_{\mathrm{freeze-out}} < T_c(\mu_B)$ [Floerchinger, Wetterich 1202.1671]

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.



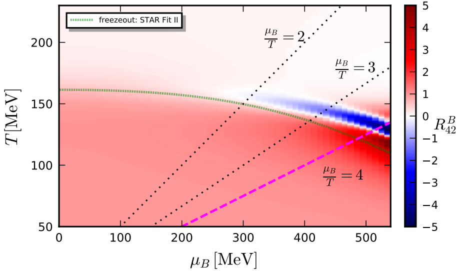
Stephanov [0809.3450,1104.1627] : Non-monotonic high order fluctuations near a critical end point.

Here : fourth cumulant $\langle B^4 \rangle_c$, normalized to the second cumulant $\langle B^2 \rangle_c$

FRG-Lattice assisted LEFT

Pawlowski et al. [2101.06035]

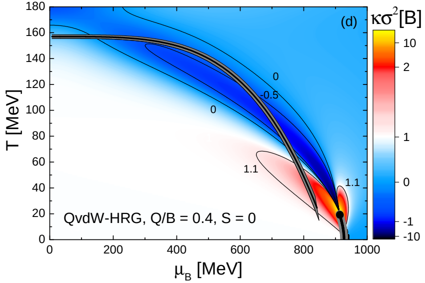
CEP = (93 MeV, 672 MeV)



QVdW gas

Vovchenko et al [1906.01954]

Liquid-Gas CEP = (19.7 MeV, 922 MeV)



- Taylor coefficients of the pressure

$$\frac{p(\mu_B)}{T^4} = \frac{p(0)}{T^4} + \frac{1}{2!}\frac{\mu_B^2}{T^2}\chi_2^B(T) + \frac{1}{4!}\frac{\mu_B^4}{T^4}\chi_4^B(T) + \frac{1}{6!}\frac{\mu_B^6}{T^6}\chi_6^B(T) + \dots$$

- These Taylor coefficients are equal to the Grand Canonical fluctuations

$$\langle B^2 \rangle - \langle B \rangle^2 = \frac{1}{VT}\frac{\partial^2 \log Z(V,T,\mu_B,\mu_Q,\mu_S)}{\partial {\mu_B}^2} = \chi_2^B$$

- Higher fluctuations are the Taylor coefficients of lower fluctuations

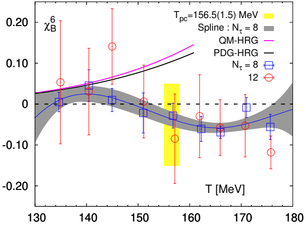
$$\chi_2^B(\mu_B) = \chi_2^B(\mu_B = 0) + \frac{1}{2!}\frac{\mu_B^2}{T^2}\chi_4^B(\mu_B = 0) + \frac{1}{4!}\frac{\mu_B^4}{T^4}\chi_6^B(\mu_B = 0) + \dots$$

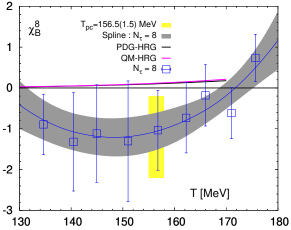
- Taylor coefficients can be used to reveal analytic structure of the thermodynamic potential
  - Repulsive interactions beyond ideal HRG
  - Searching the critical end point
- Hints for chiral O(4) universality

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*



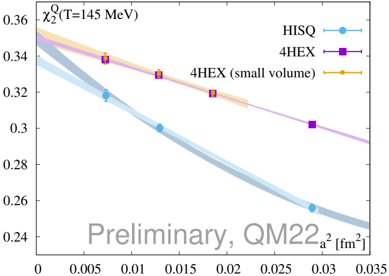


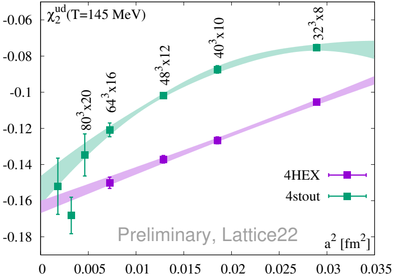
$N_\tau = 8$		$N_\tau = 12$	
T[MeV]	#conf.	T[MeV]	#conf.
134.64	1,275,380	134.94	256,392
140.45	1,598,555	140.44	368,491
144.95	1,559,003	144.97	344,010
151.00	1,286,603	151.10	308,680
156.78	1,602,684	157.13	299,029
162.25	1,437,436	161.94	214,671
165.98	1,186,523	165.91	156,111
171.02	373,644	170.77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

[Lattice results: HotQCD 2001.08530]

New in Wuppertal: 4HEX staggered action with strongly reduced taste breaking.

Continuum extrapolation $T = 145$ MeV



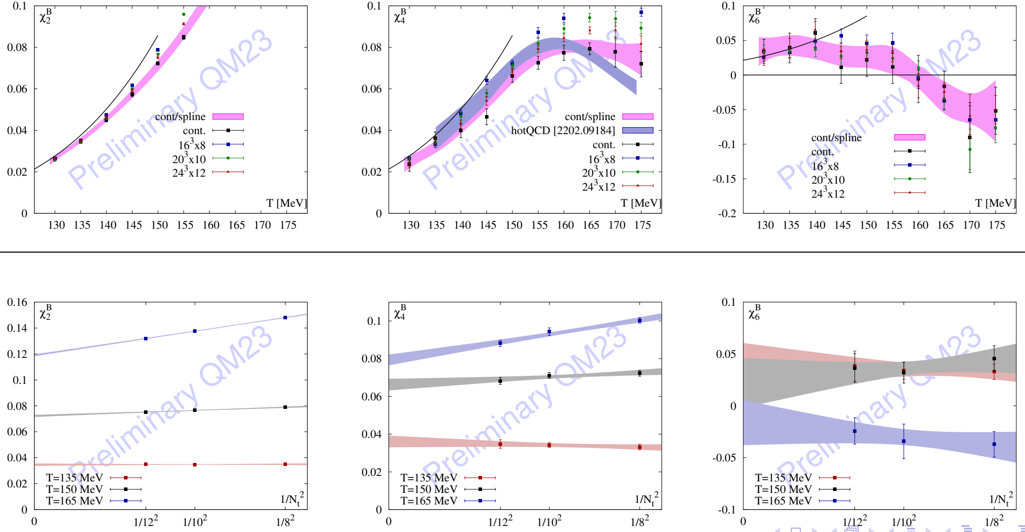


Wuppertal-Budapest (2013–2023) 4stout results: [Wuppertal-Budapest [1507.04627]]
BNL-Bielefeld (2011–. . .) HISQ results: [HotQCD [2107.10011]]
Wuppertal-Budapest (2022–. . .) 4HEX results: [Wuppertal-Budapest **QM2022**]

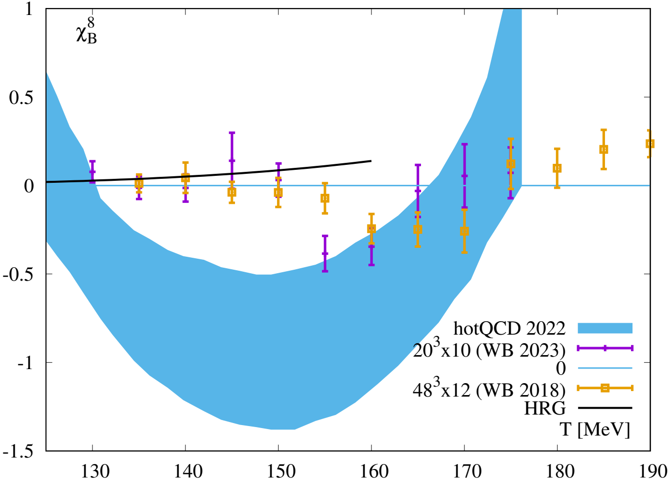
Results are at a lattice size of $LT = 4$. The label "small volume" is $LT = 3$ in the plot, we will use $LT = 2$ for high order fluctuations.

4HEX continuum extrapolations of $\chi_B^n(T)$

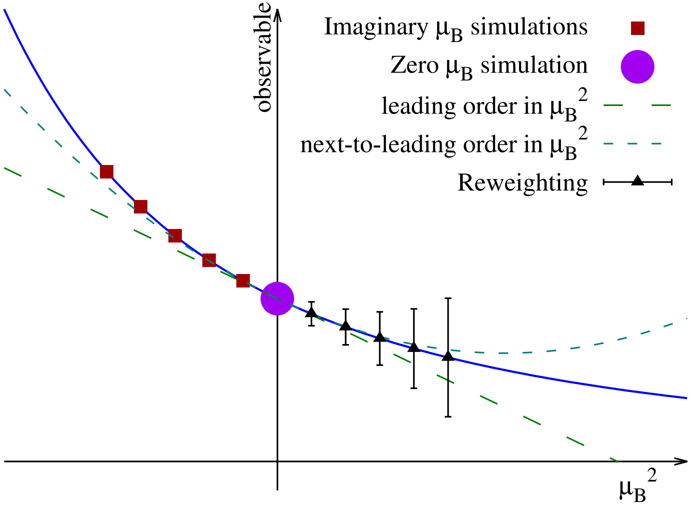
Baryon Taylor coefficients



Focusing on $\chi_8^B(T)$



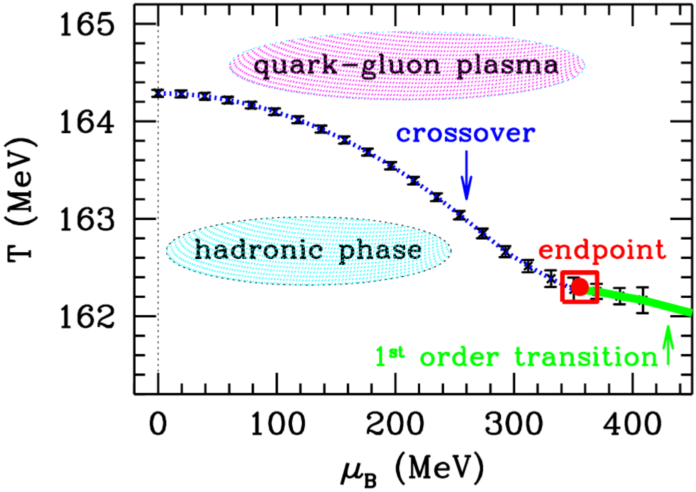
Extrapolation approaches to $\mu_B^2 > 0$



Imaginary μ_B: numerical derivatives with some *lever arm*.

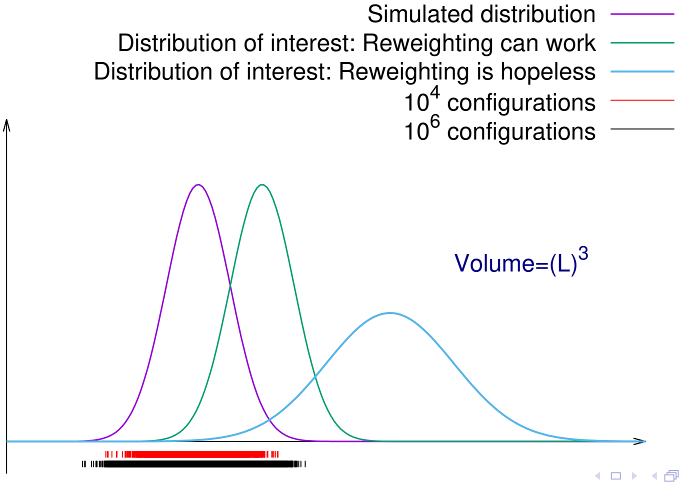
Taylor from $\mu_B = 0$: exact derivatives based on the tails of a distribution.

Can we use lattice QCD to perform simulations at finite μ_B directly?

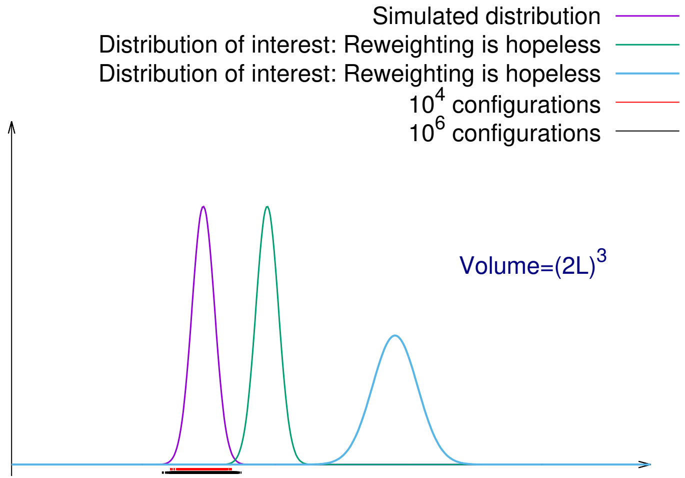


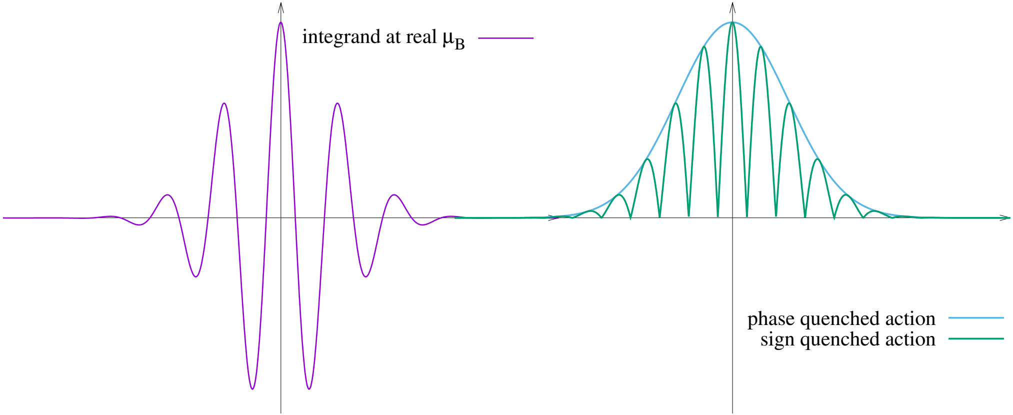
Using physical quark masses, 2 + 1 flavors, $N_t = 4$ [Fodor&Katz hep-lat/0402006]

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



Reweighting: Costs explode with volume.





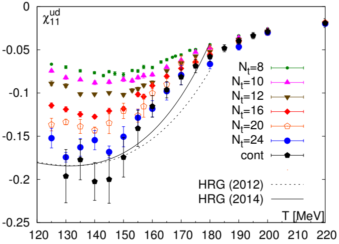
Sign problem: Large cancellations between positive and negative contributions of $\mathrm{Re}\left[\det M[U]\right]$.

Overlap problem: Problem solved.

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)]

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

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



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

Idea: *sign quenched simulations:* $\mathrm{Re}\, e^{i\theta} = \underbrace{\pm}_{\text{reweighting}} \underbrace{|\cos(\theta)|}_{\text{simulation}}$

[Budapest 2004.10800]

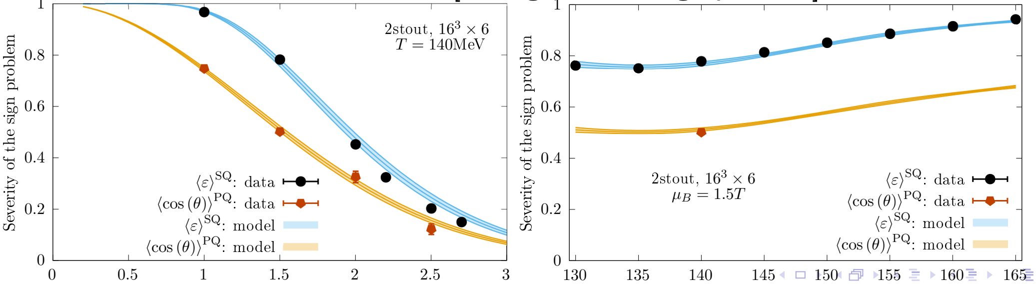
For a concrete case:

– 2-stout-staggered action,

– physical quarks with 2+1 flavors,

– $16^3 \times 6$ lattice.

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

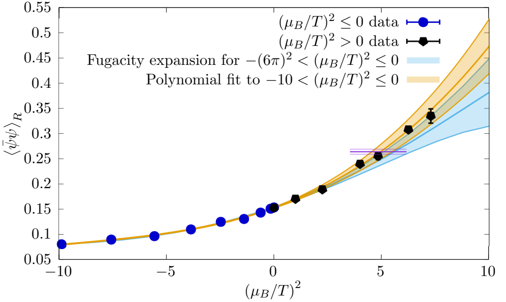


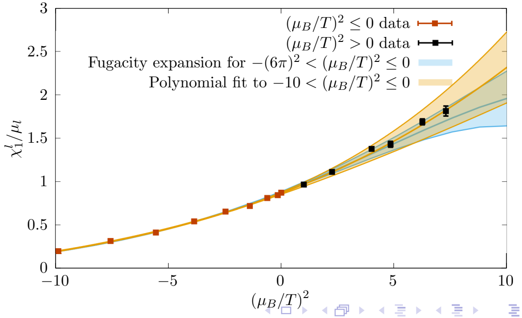
How far can we go in the chemical potential?

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

  Direct = reweigting from sign quenched





Simulation in two steps:

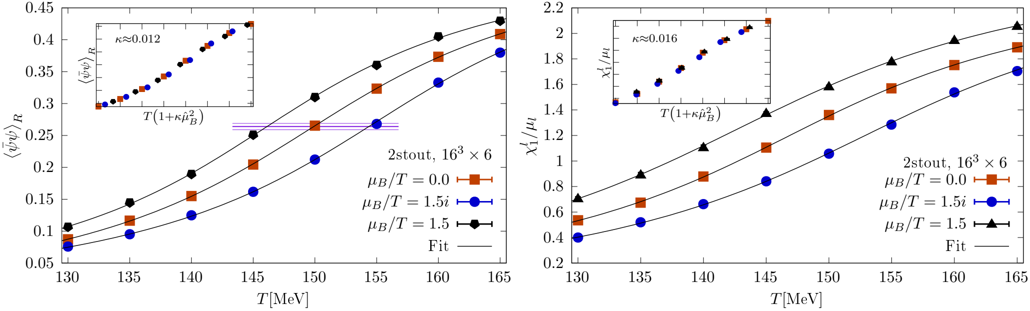
1. Simulate the real (sign quenched) action
2. Reweight each configuartion with the correct sign

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

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

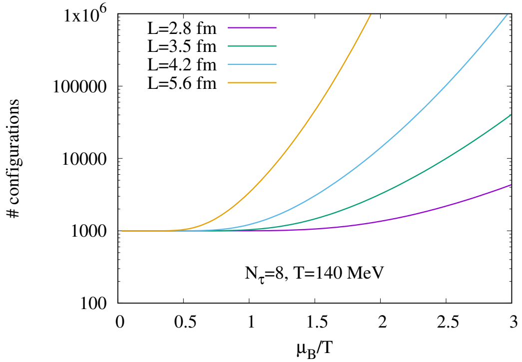
Drawback: the simulation algorithm is more expensive *(subject to research)*

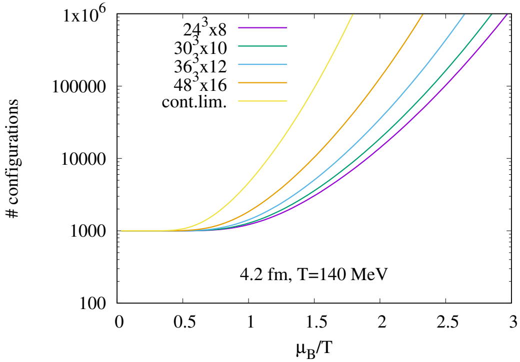
The chiral condensate (left) and the real quark density(right).



The plots show the matching imaginary μ_B results for comparison.

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:

What do we learn from "direct" simulations?

- Simulations are limited to small volumes.

  $\rightarrow$ *Explore phase diagram in a small volume*

  (1st step in a finite size scaling)

- Extrapolations are available on larger volumes, too.

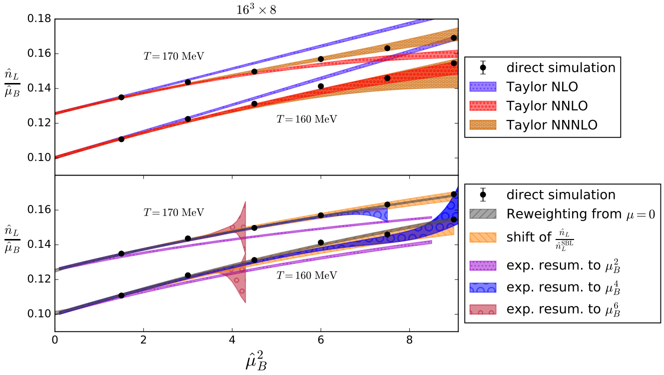
  Extrapolations are susceptible to a bias with respect to scheme

Strategy:

- Perform extrapolations in small volumes
- Perform "direct" simulations
- Check which scheme works

Comparison at fixed $T > T_c$

Let's look at the light quark density as a function of μ_B.

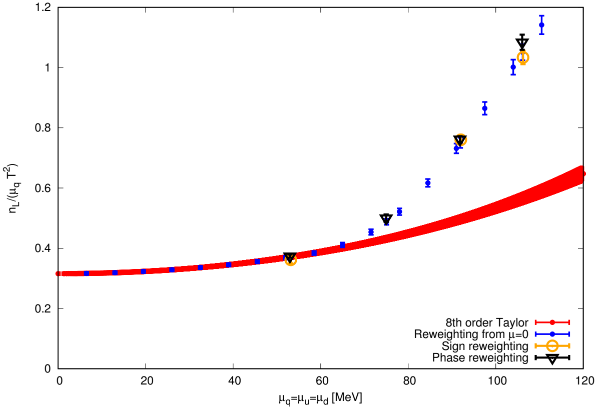


[Wuppertal-Budapest 2102.06660]

1. Direct points use sign qunched [Wuppertal-Budapest 2208.05398] *(smallest error bars!)*
2. Shift method uses the *alternative scheme* adapted to this setup [Wuppertal-Budapest 2102.06660] *(good agreement with "direct" at next-to-leading order)*
3. Taylor method is complemented with $\mu_B \neq 0$ points *(good agreement with "direct" at next-to-next-to-leading order)*

Full result vs. Taylor at $T < T_c$

Staggered simulations with three different reweighting schemes.

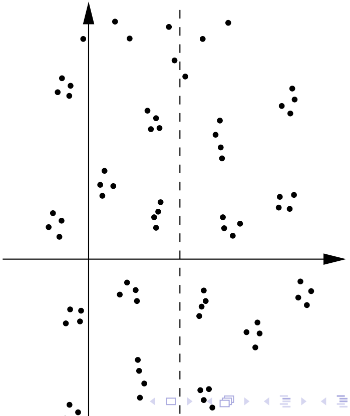


[Wuppertal-Budapest 2308.06105]

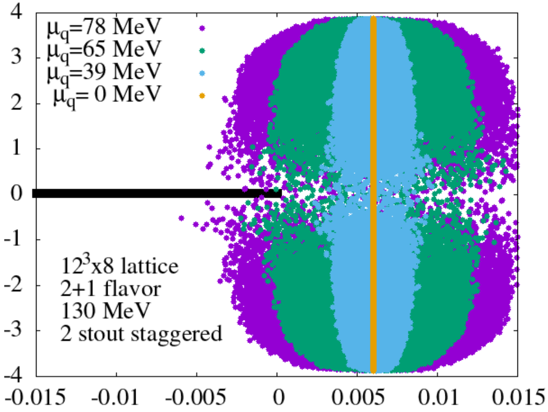
Golterman, Shamir, Svetitsky: [hep-lat/0602026]

$$(\det M)^{1/4} = \left[\prod_i \lambda_i\right]^{1/4} = \prod_{i,i+4,\ldots} [\lambda_i \lambda_{i+1} \lambda_{i+2} \lambda_{i+3}]^{1/4} \neq \prod_i \lambda_i^{1/4}$$

1. Staggered fermions describe four flavors
2. At finite μ this brings in a complex rooting
3. At $\mu_q > m_\pi/2$ quartets spread the full complex plane, leaving the square root ambigous
4. On fine lattices eigenvalues are structured as quartets of size $\mathcal{O}(a)$
5. Quartets could be separated by the branch cut of the root even with fine lattices

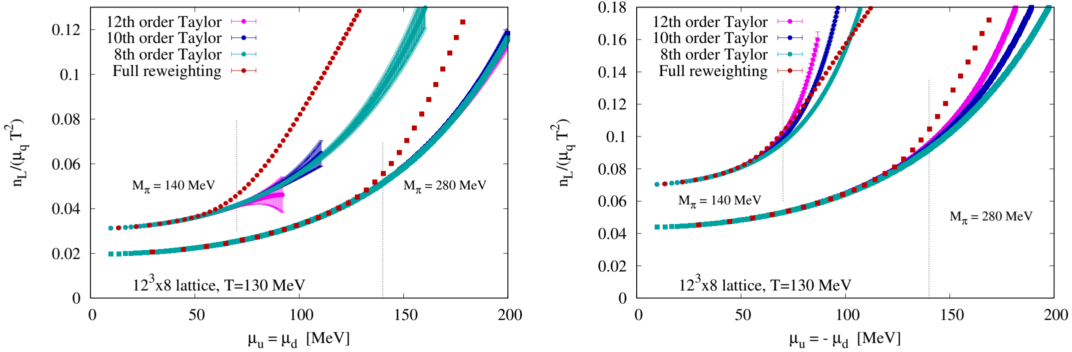


At $\mu_B = 0$ we have $\lambda = m + ix$, with $x \in \mathbb{R}$.



The eigenvalues reach the cut at $\mu_q = m_\pi/2$.

Let's vary the pion mass.

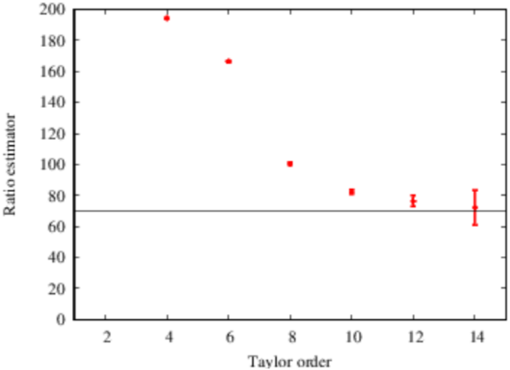


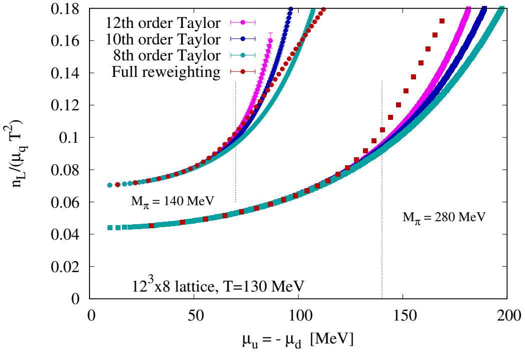
Left: Baryon chemical potential; Right: Isospin chemical potential (phase quenched)

[Wuppertal-Budapest 2308.06105]

Phase Quenched = Isospin chemical potential: 2nd order transition

[Son&Stephanov hep-ph/0005225, Brand&Endrődi 1712.08190]

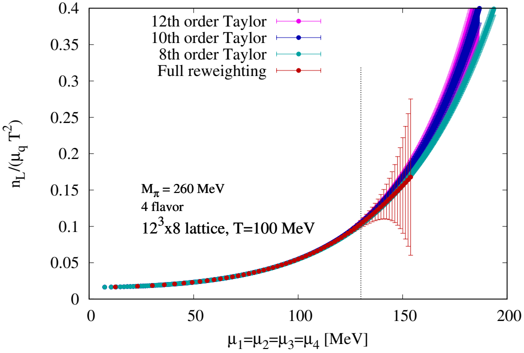


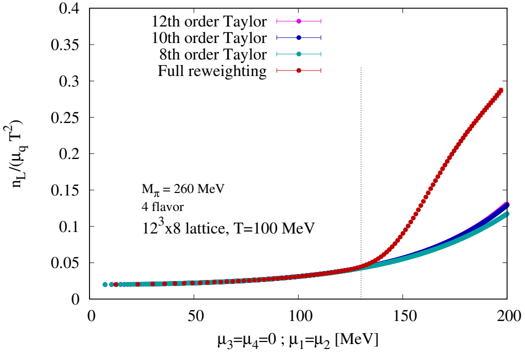


The radius of convergence estimators clearly display this for the phase quenched case, but not for the case of the baryo-chemical potential.

[Attila Pásztor, Preliminary]

Let's try the 4 flavor theory



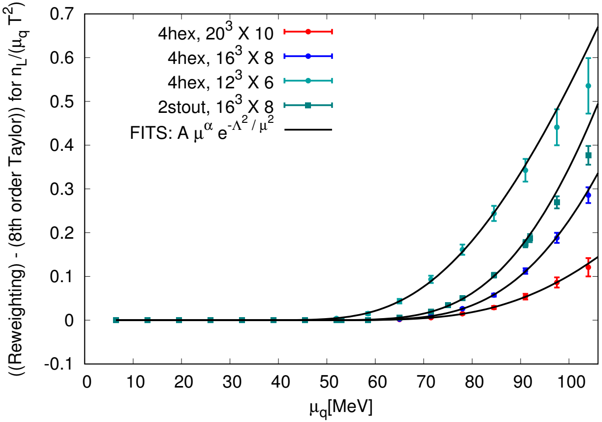


Left: No rooting ; Right: chemical potential introduced to 2 flavors (rooting)

[Wuppertal-Budapest 2308.06105]

This is a cut-off effect

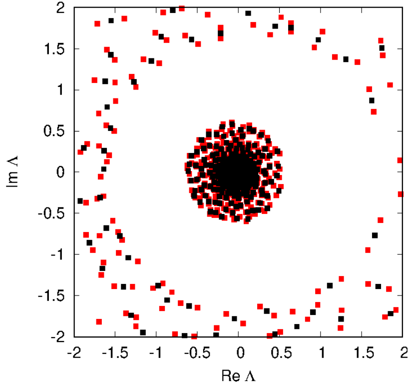
Reweighted result - Taylor result

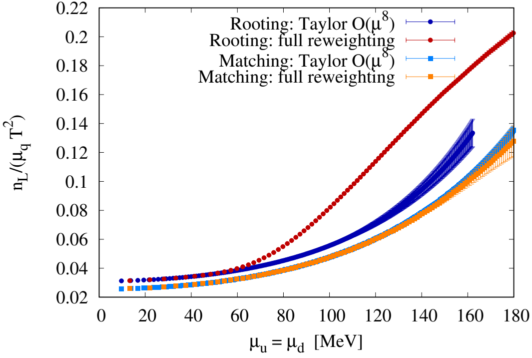


– The unphysical effect diminises with decreasing lattice spacing
– The effect hints for an essential singularity: $\sim \exp(-C/\mu^2)$

Golterman et al: combine quartets once quartets are formed

Budapest group: Geometric matching of doublets [2003.04355]





The unphysical behaviour is eliminated.

But this changes the definition of the chemical potential (can modify the theory away from the continuum).

What is the problem with real density simulations?

- Expansion schemes
  - Great progress
  - Taylor, Im μ have limitations : extrapolations have unknown systematics
- A two-step reweighting procedure exists for simulating at real μ_B

  Expensive, not impossible

  overlap problem has been mitigated
- Staggered fermions are ill-defined at $\mu_q \lesssim m_\pi/2$ and $T < T_c$

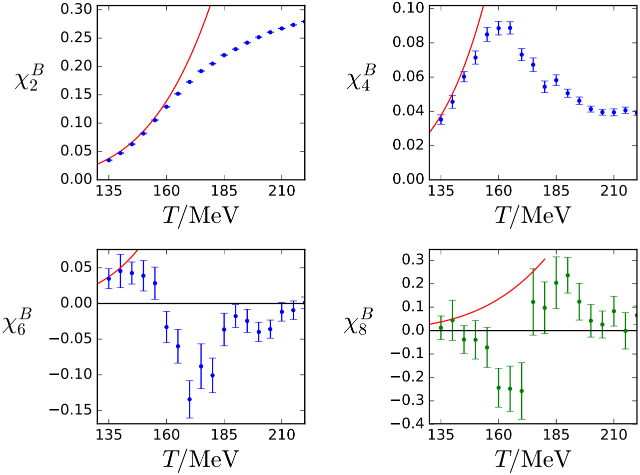
  Remedies:
  - Non-trivial continuum limit
  - Matching eigenvalues
  - Non-staggered action

    Candidate: minimally doubled fermions

    Two flavor simulations with staggered-like chiral symmetry. Light quarks are not rooted.

backup

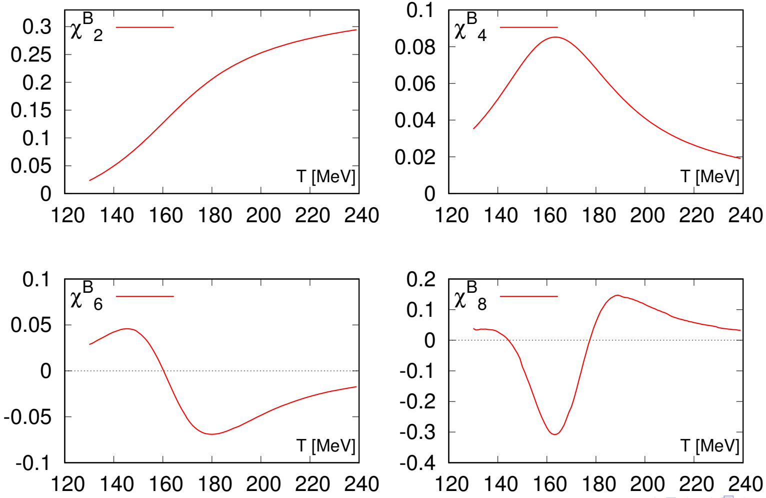
"Numerical derivatives" from $\mu_B^2 \leq 0$ simulations: [WB 1805.04445]



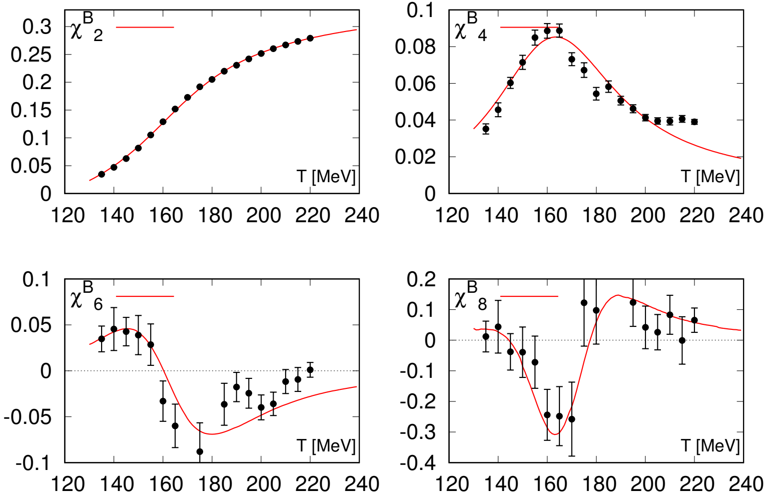
This structure is already known from chiral effecive models. [Friman et al 1103.3511]

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]:



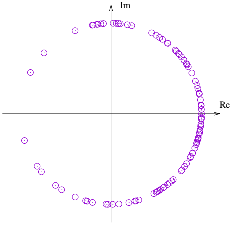
Comparing the simple model with our lattice result:

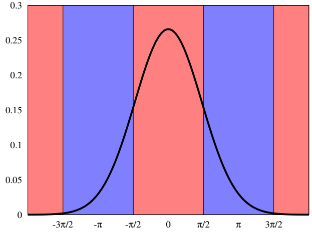


Simple model describes lattice result surprisingly well.

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:

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;

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

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

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

- 4 steps of HEX smearing + DBW2 gauge action
- Physical point defined by $m_\pi/f_\pi = 1.0337$, $m_s/m_{\mathrm{light}} = 27.63$
- m_{light} tuned in the a range: $0.22 \ldots 0.072$ fm
- Thermodynamics runs: cca 80000 configurations / ensemble
  10 Temperatures $130 \ldots 175$ MeV
  3 lattice spacings $16^3 \times 8$, $20^3 \times 10$, $24^3 \times 12$

Taste breaking
(smaller is better)
show relative quadratic discretization error on M_π^2

(HISQ: thanks to Peter Petreckzy)