A new look at the deconfinement transition with parallel tempering

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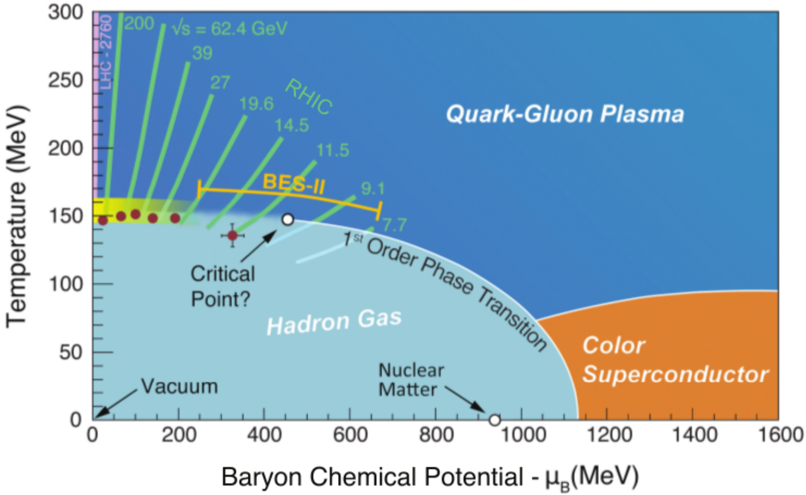
ECT*, Trento, May 25, 2022
Gauge Topology, Flux Tubes and Holographic Models



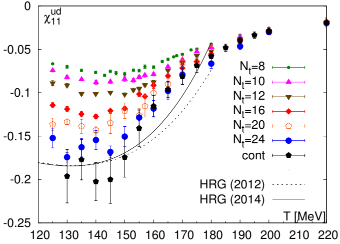
BES-II: chemical potentials of interest: $\mu_B/T = 1.5\ldots4$

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)]

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

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



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

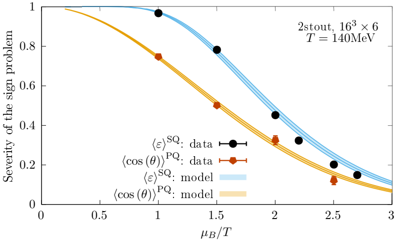
[Wuppertal-Budapest 1507.04627]

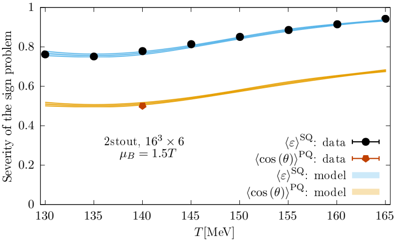
Idea: *sign quenched simulations:* $\mathrm{Re}\, e^{i\theta} = \underbrace{\pm}_{\text{reweighting}} \underbrace{|\cos(\theta)|}_{\text{simulation}}$

[Budapest 2004.10800]

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

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





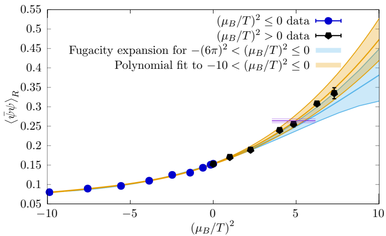
The data points are actual simulations!

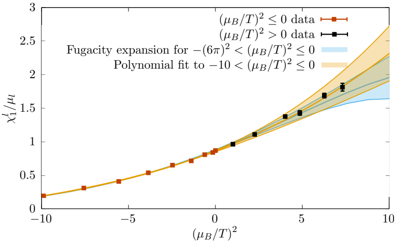
[Wuppertal-Budapest 2108.09213]

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 $0 < \mu_B \leq 380\ \mathrm{MeV}$





The direct result has the smallest errors.

[Wuppertal-Budapest 2108.09213]

Direct simulations at $\mu_B > 0$

Simulation in two steps:

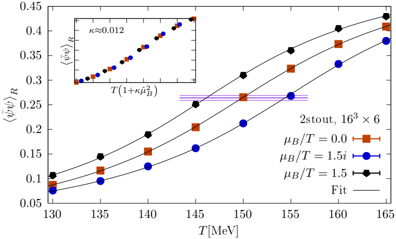
1. Simulate the real (sign quenched) action
2. Reweight each configuartion with the correct sign

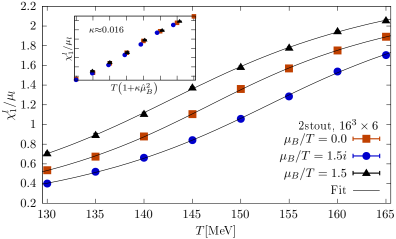
Feasible as long as the sign problem is not too severe.

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).





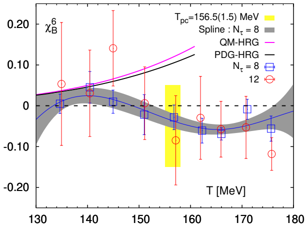
The plots show the matching imaginary μ_B results for comparison.

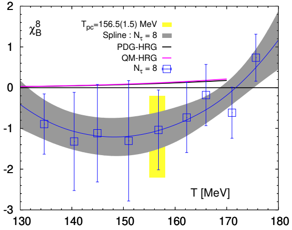
Inset plots: the scaling with temperature survives to real μ_B !

[Wuppertal-Budapest 2108.09213]

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

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

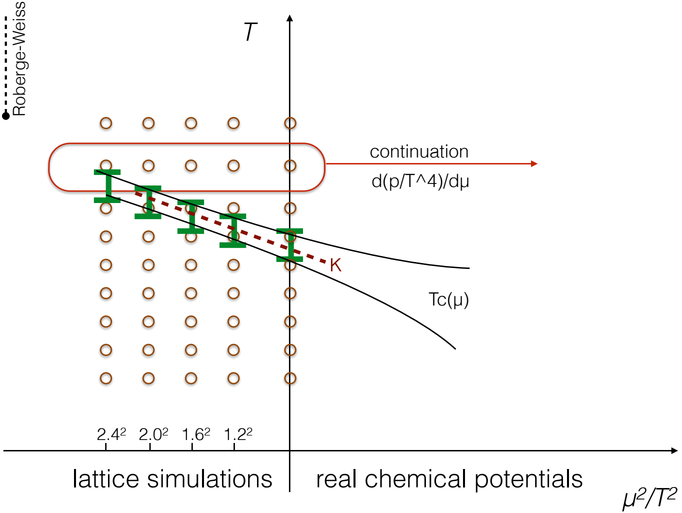




$N_\tau = 8$		$N_\tau = 12$	
T[MeV]	#conf.	T[MeV]	#conf.
134.64	1,275,380	134.94	256,392
140.45	1,598,555	140.44	368,491
144.95	1,559,003	144.97	344,010
151.00	1,286,603	151.10	308,680
156.78	1,602,684	157.13	299,029
162.25	1,437,436	161.94	214,671
165.98	1,186,523	165.91	156,111
171.02	373,644	170.77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

[Lattice results: HotQCD 2001.08530]

Analytic continuation



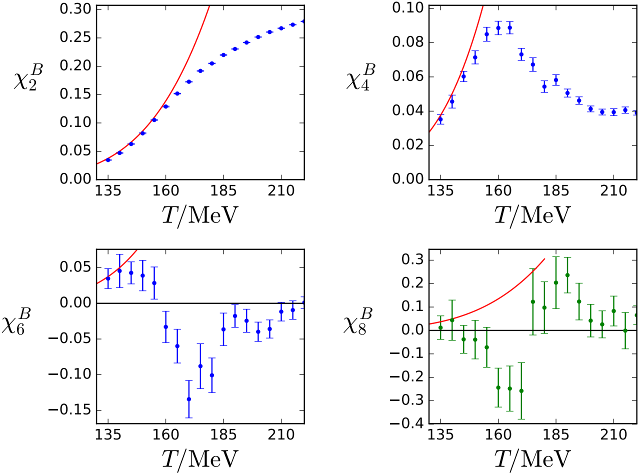
Many exploratory studies: [de Forcrand & Philipsen hep-lat/0205016]

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

[Wuppertal 1607.02493] [D'Elia et al 1611.08285]

Higher order χ_B from imaginary μ_B

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

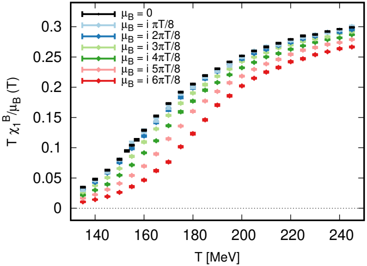


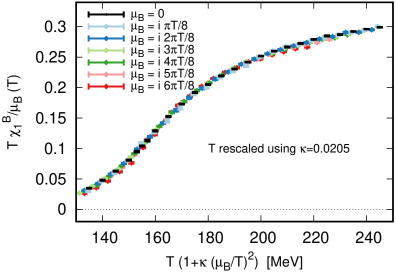
This structure is already known from chiral effecive models. [Friman et al 1103.3511]

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

Observations at imaginary μ_B

Normalized baryon density: $\chi_1^B(T,\hat{\mu}_B)/\mu_B = n_B/\mu_B$





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

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

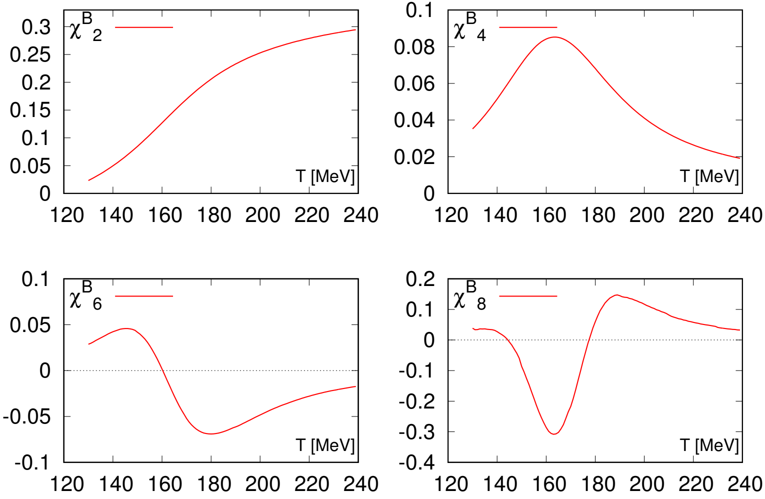
Expand both sides in μ_B:

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

[Wuppertal Budapest 2102.06660]

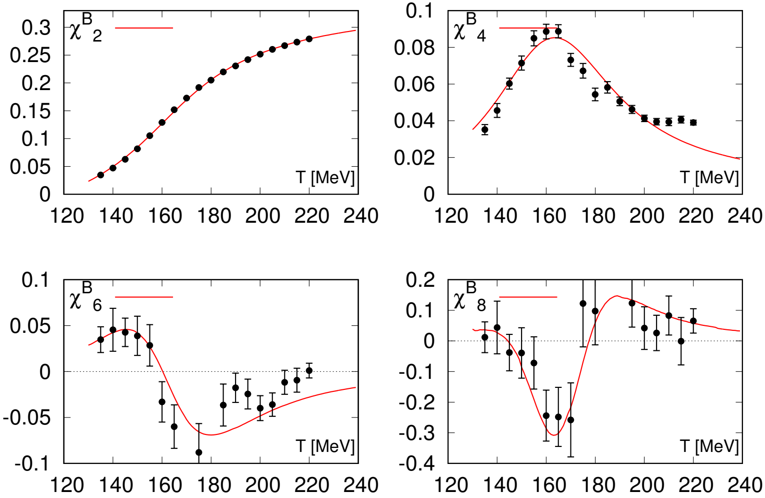
Higher order χ_B in the simple model

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 observation (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

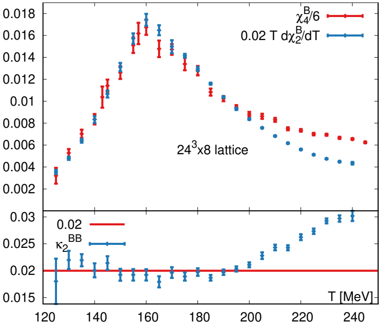
- $\chi_2^B(T)$: baryon number susceptibility (known precisely)
- $\kappa_2(T),\kappa_4(T)$ a series of slowly varying functions

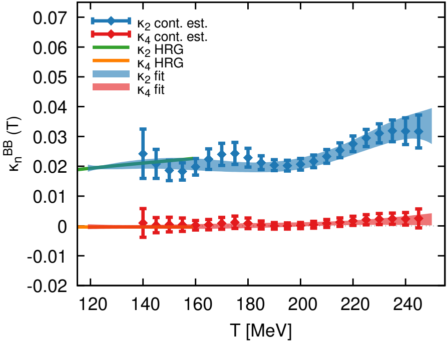
These functions are directly related to the Taylor coefficients:

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

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

Fairly constant $\kappa_2(T)$ over a large T-range, $\kappa_4(T)$ is less by an order of magnitude.

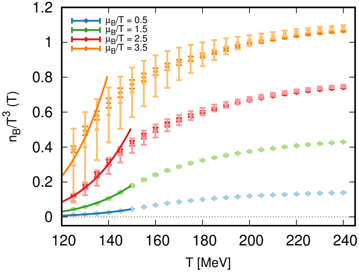


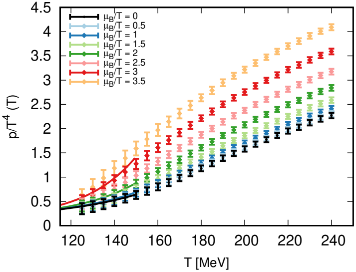


$$\kappa_2(T)\, T \frac{d\chi_2^B}{dT} = \chi_4^B(T)/6$$

[Wuppertal Budapest 2102.06660]

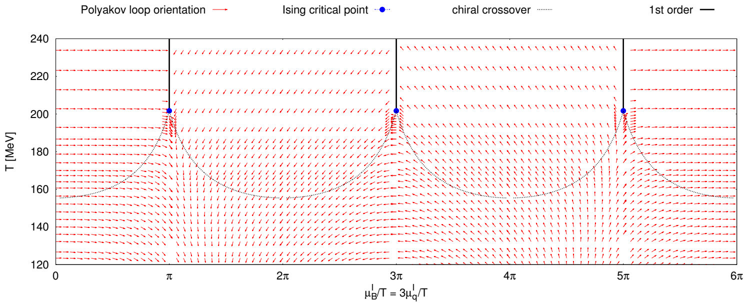
- We reconstruct thermodynamic quantities up to $\hat{\mu}_B \simeq 3.5$ with uncertainties well under control
- Agreement with HRG model calculations at small temperatures
- No pathological (non-monotonic) behavior is present





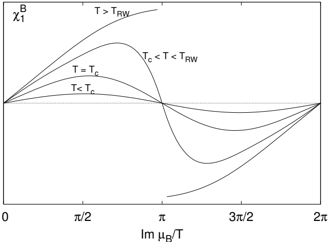
[Wuppertal Budapest 2102.06660]

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] [Bonati et al 1602.01426]



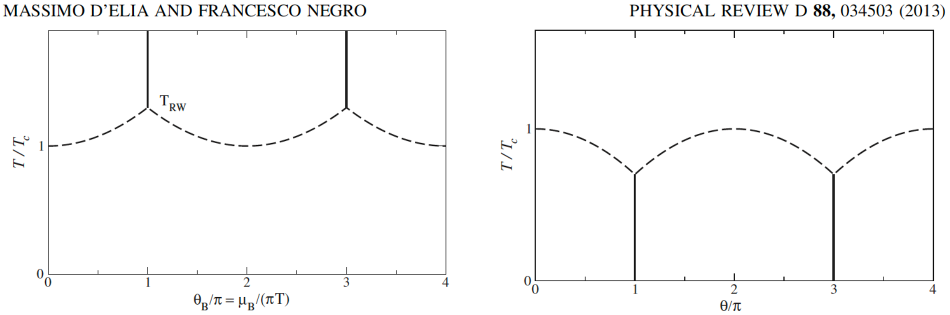
At low T only B states contribute:

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

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

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

Analogous phase diagrams $\mathrm{Im}\mu_B - T$ vs. $\Theta - T$

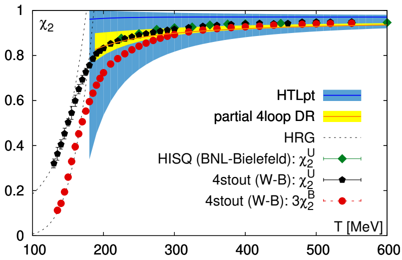


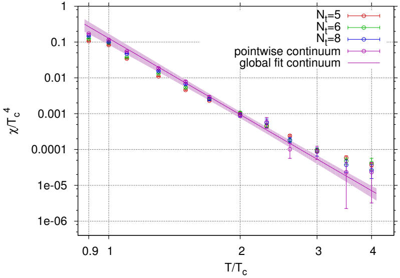
- Perodicity: integer baryon number and topological charge
- Suppressed fluctuations
  μ_B: heavy hadrons $T < T_c$; θ: dilute instantons [Yaffe&Gross (1981)]
- 1st order transition:
  μ_B: weak coupling $T > T_c$; θ: $\chi \sim N^0$ in large-N $T > T_c$ [Witten (1998)]
- Sign problem on the lattice for real μ_B and real θ
- 2nd μ_B or θ derivative: susceptibilities $\chi(T)$

Baryon fluctuations vs. topological susceptibility

- Left: $\chi_B(T)$, baryon fluctuations are suppressed by a Boltzmann factor at low T, high T: Stefan-Boltzmann limit
- Right: $\chi_t(T)$, topological fluctuations are suppressed at high T:

$$\chi(T) \sim T^4 e^{-2\pi/\alpha_s} \sim T^{4-11} \sim T^{-7} \sim T^{-b}$$





$N_f = 0$, χ_t lattice data: [Wuppertal 1508.06917]

$N_f = 2+1+1$, χ_B lattice data: [Wuppertal 1507.04627]

Many methodical improvements to lattice $\chi_t(T)$

- Simulations at imaginary θ

  [Panagopoulos&Vicari 1109.6815]

- Pisa group: Analytical contiuation from imaginary θ

  [D'Elia et al 1306.2919], [Bonati et al 1512.01544, 1607.06360,1807.06558]

  Extract χ, b_2, $dT_c/d\theta^2$, (+ effect of $\mathrm{Tr}\, P = 0$)

- Integral method, analogous to equation of state with $\epsilon - 3p$
  Frison et al [1606.07175], Wuppertal [1606.07494]

  Relative weight of $Q = 0$ and $Q = 1$ sectors are calculated

- Darmstadt: Metadynamics with reweighting

  [Jahn et al 1805.11511, 2002.01153]

  Metropolis step to enhance disclocations

- Pisa group: Multicanonical approach

  [Bonati et al 1807.07954]

  Topology enhancement term in built into the HMC force

- Density of states approach

  [Gattringer&Orasch 2101.03383], [Borsanyi&Sexty 2101.03383]

  Explore a broad range in Q with constrained simulations

$$Z = \int D\Phi e^{-S[\Phi]}.$$

The Gaussian integral $\int_{-\infty}^{\infty} dc \ e^{-\frac{P}{2}(c-a)^2} = \sqrt{\frac{2\pi}{P}}$ is a-independent.

$$Z = \int D\Phi \int_{-\infty}^{\infty} dc \ e^{-\frac{P}{2}(c-F[\Phi])^2} e^{-S[\Phi]},$$

where $F[\Phi]$ is an arbitrary functional of the fields. Swapping the order of the integrations we can write

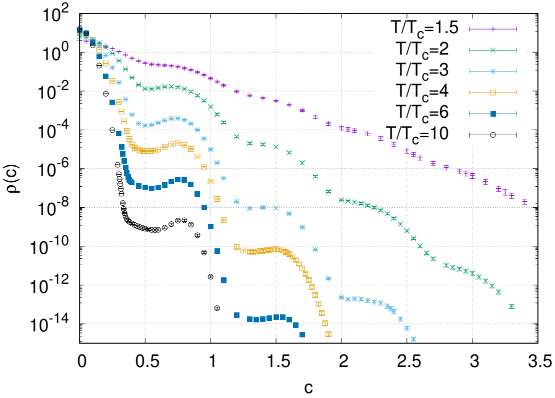
$$Z = \int_{-\infty}^{\infty} dc \ \rho(c)$$

where we defined the $\rho(c)$ as the 'density of states':

$$\rho(c) = \int D\Phi e^{-S[\Phi]-\frac{P}{2}(c-F[\Phi])^2}.$$

$\rho(c)$ can be calculated with from a mesh of c-ensembles:

$$\frac{\partial \ln \rho(c)}{\partial c} = \frac{1}{\rho(c)} \int D\Phi e^{-S[\Phi]-\frac{P}{2}(c-F[\Phi])^2} \left(-P(c-F[\Phi])\right) = \langle -P(c-F[\Phi]) \rangle_c,$$



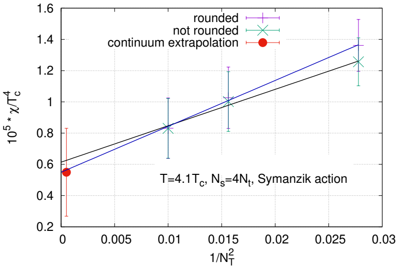
In our work $F[\Phi]$ is the stout-smeared $Q_{\text{proxy}} \sim \int \tilde{F} F dV$

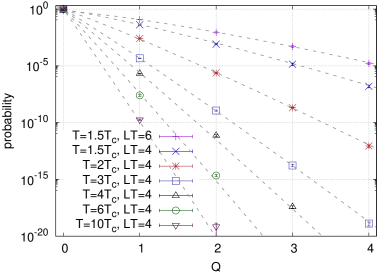
Density of states method for the topological charge

Any observable A can be then expressed as

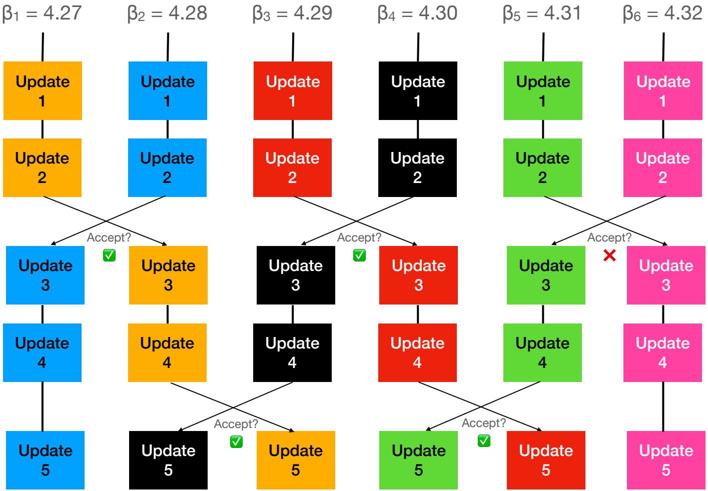
$$\langle A\rangle = \frac{1}{Z}\int_{-\infty}^{\infty} dc \int D\Phi A[\Phi] e^{-S[\Phi]-\frac{P}{2}(c-F[\Phi])^2} = \frac{\int_{-\infty}^{\infty} dc\ \rho(c)\langle A\rangle_c}{\int_{-\infty}^{\infty} dc\ \rho(c)}$$

Histogram of Q: $h(n) = \int dc\rho(c)\langle\delta_{Q,n}\rangle_c$.





The parallel tempering update



The tempering update fulfills detailed balance with the joint equilibrium distribution:

$$Z = \prod_i Z_i = \prod_i \int DU_i e^{-S_i(U_i)} = \int DU_1 \cdots DU_N e^{-S_1(U_1)\cdots - S_N(U_N)}$$

Swapping $(a \leftrightarrow b)$ is accepted with $P(a, b)$:

$$P(a, b)e^{-S_a(U_a)-S_b(U_b)} = P(b, a)e^{-S_b(U_a)-S_a(U_b)}$$

The corresponding Metropolis step:

$$P(a, b) = \min(1, e^{-\Delta H})$$

with

$$\Delta H = [S_b(U_a) + S_a(U_b)] - [S_a(U_a) + S_b(U_b)]$$

Technically:

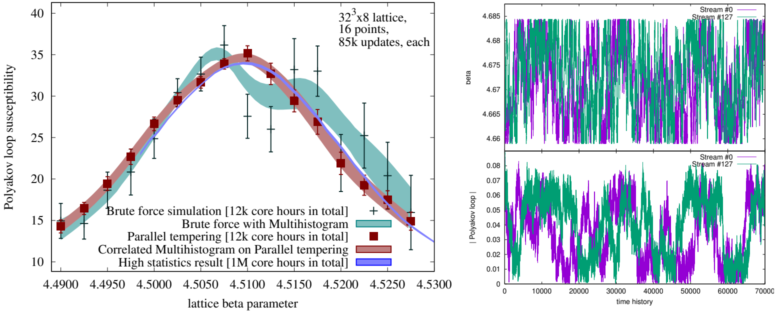
The node holding the U_a configuration calculates $S_a(U_a)$ and $S_b(U_a)$ and communicates to the master. The master works out all swaps.

Many uses of parellel tempering

- [Swendsen&Wang Phys.Rev. Lett. 57 (1986) 2607]
  Replica Monte Carlo simulation of spin-glasses
  Introduce temperature as a new dimension.
- [Marinari&Parisi Europhys. Lett. 19 (1992) 451]
  Simulated tempering: A New Monte Carlo scheme
  Add dynamics to the temperature parameter.
- [G. Boyd Necl. Phys. Proc. Suppl 60A (1998) 341], [E-M. Ilgenfritz et al. Phys. Rev. D65 (2002) 094506], [B. Joo et al Phys. Rev. D59 (1999) 114501]
  Application to lattice QCD with dynamical fermions (κ)
- [G. Burgio et al. Phys Rev D75 (2007) 014504]
  Lattice gauge theory near a phase boundary.
- [M. Hasenbusch et al. Phys.Rev. D96 (2017) 054504]
  [C. Bonani et al. JHEP 03 (2021) 111]
  Topological freezing $\rightarrow$ open boundary conditions $+$ tempering
- [Borsanyi&Sexty Phys. Lett. B815 (2021) 136148]
  Tempering combined with density of states: topological charge
- [R. Kara (Wupperal) Lattice'21]
  Seaching for the heavy critical mass in the Columbia plot...
- [Wuppertal: Phys. Rev. D. 105 (2022) 074513]
  SU(3) Yang Mills theory

Parallel tempering: a susceptibility peak

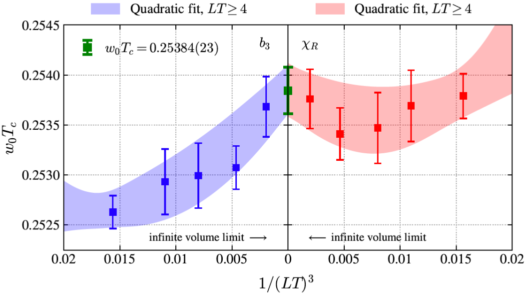
Let us simulate the transition in the SU(3) Yang-Mills theory. The susceptibility of the Polyakov loop exhibits a peak near β_c.



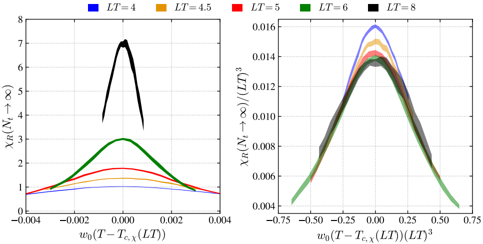
Tempering updates give the combining effect Ferrenberg&Swendsen's multihistogram reweighting.

In addition, the tempering updates allow a stream to thermalized with dynamically changing temperatures.

The continuum extrapolated transition temperature $w_0 T_c$ scales with $1/V$:



The renormalized Polyakov loop susceptibility converges to a scaling curve.



In a real transition susceptibilities diverge with the volume V

$$\chi \sim V(\langle O^2\rangle - \langle O\rangle^2)$$

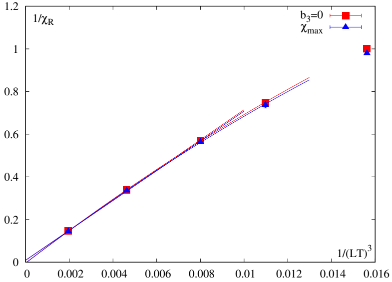
Left) Yang-Mills theory ($O \equiv$ Polyakov loop)

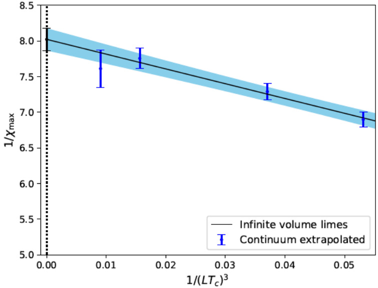
Right) QCD with physical quark masses ($O \equiv \bar{\psi}\psi$)

[Phys. Rev. D. 105 (2022) 074513]

[Nature 443 (2006) 675-678]

[Phys.Rev.Lett. 125 (2020) 5, 052001]

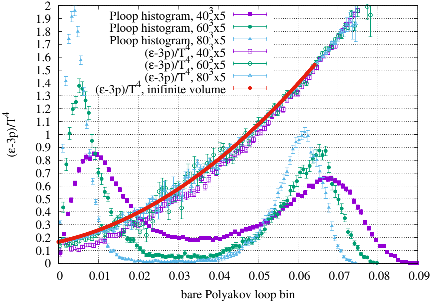


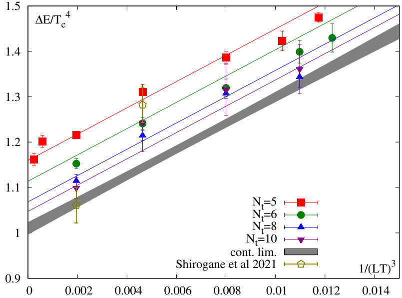


On both sides: continuum extrapolated results

Latent heat: the discontinuity of e.g. the trace anomaly

[Svetitsky (1983), Kogut (1983), Gottlieb (1987), Beinlich(1996) Shirogane (2016) and (2020)]





Observation: The trace anomaly is a continuous function of the Polyakov loop magnitude, and this function can be extrapolated to infinite volume.

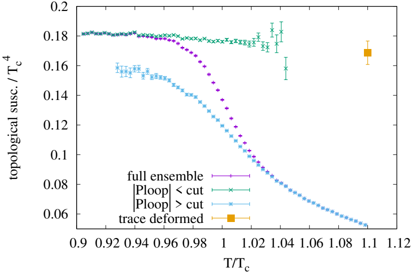
Standard procedure: split the ensemble into two by the Polyakov loop. Latent heat is the difference of $(\epsilon - 3p)/T_c^4$ between the two phases.

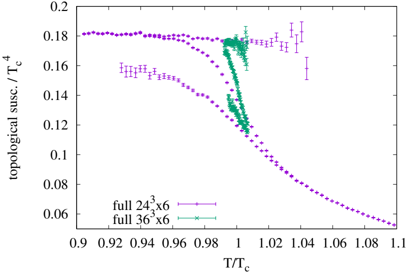
$$\frac{\Delta\epsilon}{T_c^4} = \Delta\left[\frac{\epsilon - 3p}{T^4}\right] = 1.025(21)_{(\mathrm{stat})}(27)_{(\mathrm{sys})}$$

[Wuppertal, PRD105 (2022) 074513]

$\chi_t(T)$ near T_c: coexistence of phases

We analyze on the distribution of the topological charge on a toy lattice at T_c.





[See Bonati et al 1807.06558 for more trace deformed simulations.]

What follows, the susceptiblity has a discontinuity $\Delta\chi$. This was, in fact, predicted by a Classius-Clapeyron-like equation [D'Elia&Negro 1205.0538]

$$\frac{T_c(\theta)}{T_c(0)} = 1 - \underbrace{\frac{\Delta\chi}{2\Delta\epsilon}}_{\kappa_\theta}\theta^2 + \mathcal{O}(\theta^4)$$

Continuum limit for the curvature $\kappa_\theta = 0.0178(5)$ [D'Elia&Negro 1306.2919]

Combined with the latent head this gives $\Delta\chi/T_c^4 = 0.0365(18)$.

Conclusions

Our recent lattice simulations have explored the QCD phase diagaram

- Transition line [2002.02821]
- Equation of state using an improved scheme [2102.06660]
- Equation of state with strangeness neutrality [2202.05574]
- with real-μ_B simulations [2108.09213]

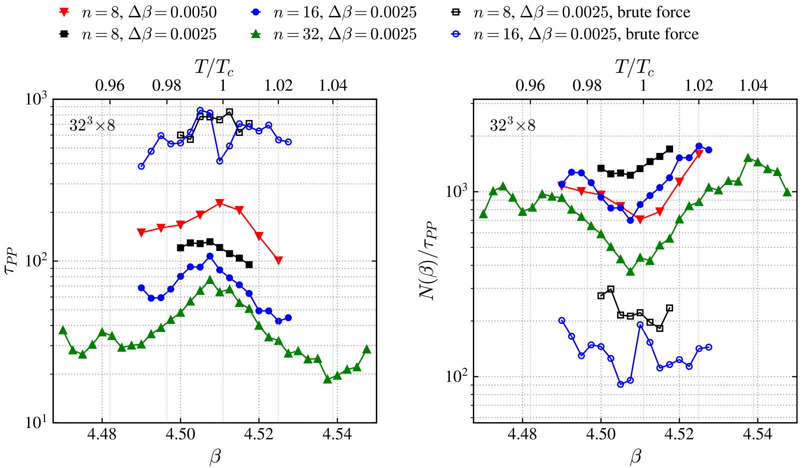
We also use the tool-box to study the $T - \theta$ phase diagram

- Density of states [2101.03383]
- Parallel tempering [2202.05234]

For the quenched theory we have new results on $T_c w_0 = 0.25384(23)$ and the latent heat (1.025(21)(27)), which implicitly provides $\Delta\chi = 0.036(2)$.

backup

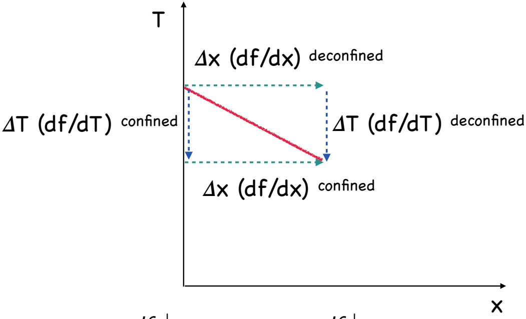
Parallel tempering: autocorrelation times



Runtime: 12000 core hours for each data set

Left: Autocorrelation time

Right: Number of updates / autocorrelation time



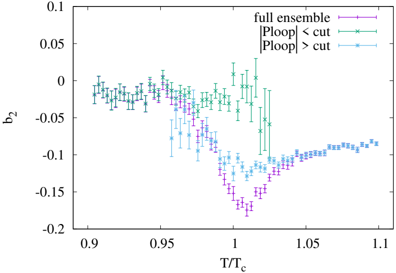
$$\Delta x \left.\frac{df}{dx}\right|_{\text{confined}} + \Delta T \left.\frac{df}{dT}\right|_{\text{confined}} = \Delta x \left.\frac{df}{dx}\right|_{\text{deconfined}} + \Delta T \left.\frac{df}{dT}\right|_{\text{confined}}$$

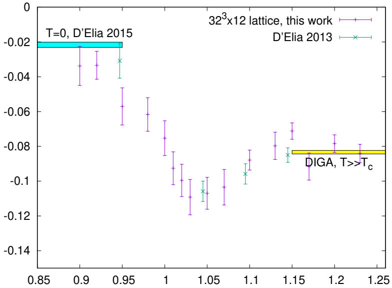
$$-T\Delta S = \left.\frac{df}{dT}\right|_{\text{deconfined}} - \left.\frac{df}{dT}\right|_{\text{confined}} \qquad \frac{1}{2}\Delta\chi = \left.\frac{df}{dx}\right|_{\text{deconfined}} - \left.\frac{df}{dx}\right|_{\text{confined}}$$

$$\kappa = -\frac{\Delta T}{T\Delta x} = \frac{\Delta\chi}{2\Delta S}$$

$b_2(T)$ near T_c: coexistence of phases

We analyze on the distribution of the topological charge on a toy lattice at T_c.

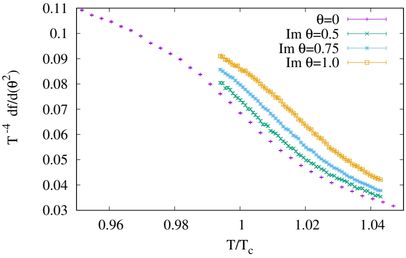


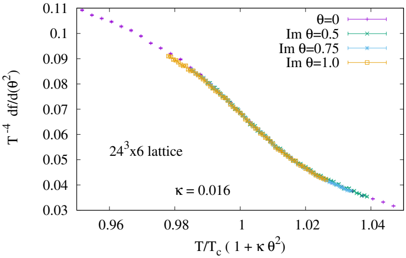


b_2 dips below the DIGA limit of -1/12 in the transition region. Phase coexistence drives this to very negative values $\sim -V$.

$$b_2 = -\frac{\langle Q^4\rangle - 3\langle Q^2\rangle^2}{12\langle Q^2\rangle} = -\frac{\mathcal{O}(V^2)}{\mathcal{O}(V)}$$

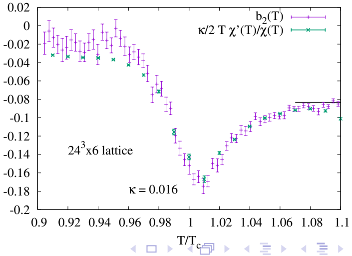
Let us repeat the trick we had in full QCD for $\chi_1^B(T,\mu_B)$.
We analyze the topological charge density at imaginary θ.





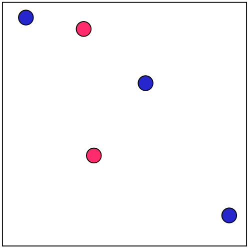
$$b_2 = -\frac{\chi_4}{12\chi_2}$$

$$\kappa(T) = \frac{1}{6T}\frac{\chi_4(T)}{\chi_2\prime(T)}$$



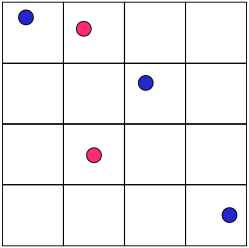
Axion potential from rare instantons

If instantons are dilute we neglect their interactions.



Axion potential from rare instantons

If instantons are dilute the universe can be split into sub-volumes.



- Subvolume is small enough: *only one instanton or anti-instanton*

$$Z^{\mathrm{sub}}(\theta) = Z_{Q=-1}e^{-i\theta} + Z_{Q=0} + Z_{Q=+1}e^{+i\theta}$$

- Subvolume is big enough: *large spatial separtion:*
  $\rightarrow$ no instanton interaction

$$Z(\theta) = \prod_i Z_i^{\mathrm{sub}}(\theta)$$

If the potential in one volume is

$$V_0^{\text{eff}}(\theta) = -\frac{1}{V_0}\log\left[Z_0 + Z_{+1}e^{-i\theta} + Z_{-1}e^{i\theta}\right] , \qquad Z_{+1} \overset{parity}{=} Z_{-1} = Z_0\frac{\chi_t V_0}{2}$$

We can extend this to the whole Universe with $V_4 = NV_0$, $N \to \infty$:

$$V^{\text{eff}}(\theta) = -\frac{1}{V_4}\log\left[Z_0 + 2Z_1\cos(\theta)\right]^N$$

Using $\chi_t = 2Z_1/Z_0V_0$ we can write $2Z_1 = Z_0\frac{1}{N}V_4\chi_t$, thus:

$$V^{\text{eff}}(\theta) = -\frac{1}{V_4}\log\left[Z_0 + Z_0\frac{1}{N}V_4\chi_t\cos\theta\right]^N = -\frac{1}{V_4}\log\left[1 + \frac{1}{N}V_4\chi_t\cos\theta\right]^N +\text{co}$$

In the limit $N \to \infty$ we recognize the exponetial function:

$$V^{\text{eff}}(\theta) = -\frac{1}{V_4}\log\exp V_4\chi_t\cos(\theta) + \text{const}$$

$$V^{\text{eff}}(\theta) = \chi(T)(1 - \cos\theta)$$

Higher moments of the topological susceptibility

The Taylor expansion coefficients of $V(\theta)$ determine the non-Gaussianity:

$$V(\theta, T) = \frac{1}{2}\chi(T)\theta^2\left[1 + b_2(T)\theta^2 + b_4(T)\theta^4 + \dots\right]$$

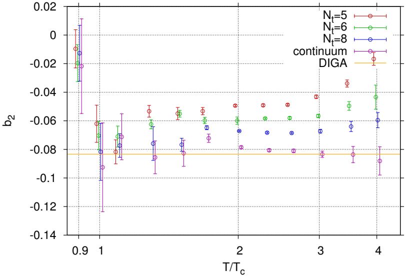
$$b_2 = \frac{\langle Q^4\rangle - 3\langle Q^2\rangle^2}{12\langle Q^2\rangle}$$

If the instanton gas is dilute $V(\theta, T) \approx \chi(T)(1 - \cos\theta)$

$$b_2 = -1/12, \; b_4 = 1/360$$

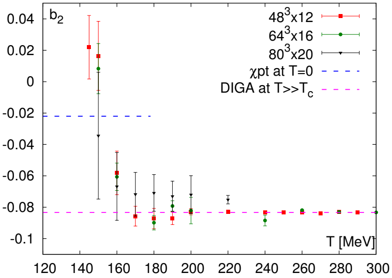
Chiral perturbation theory: $b_2 = -0.0022(1)$ (for $m_u = m_d$)

Yang-Mills theory:



[Wuppertal-Budapest 1508.06917]

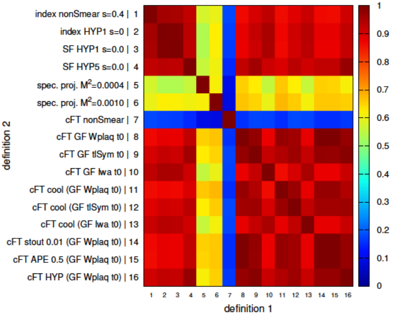
Full QCD:

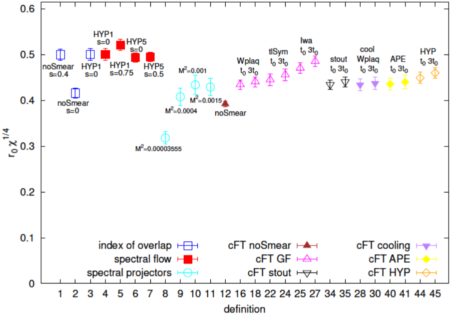


[Wuppertal-Budapest preliminary]
[See also Bonati et al 1512.06746]

Comparison of many definitions of Q

All fermionic and gluonic definitions of the topolocigal charge correlate – except for the unsmeared $\int G^{\mu\nu}\tilde{G}^{\mu\nu}$.

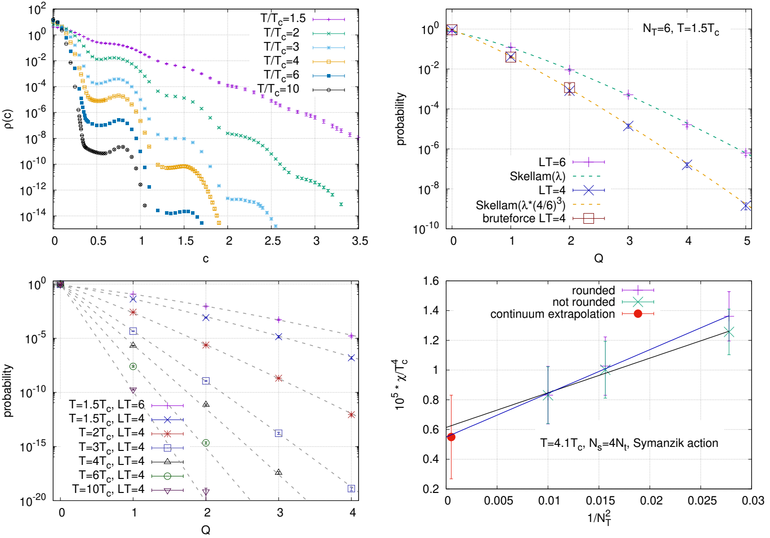




The discretization errors can be very different.

[Alexandrou et al 1708.00696]

DOS results for the distribution of the topological charge



[Borsanyi&Sexty 2101.03383]

The simulation of c-mesh was accelerated with parallel tempering.