Selected topics at non-zero temperature and density

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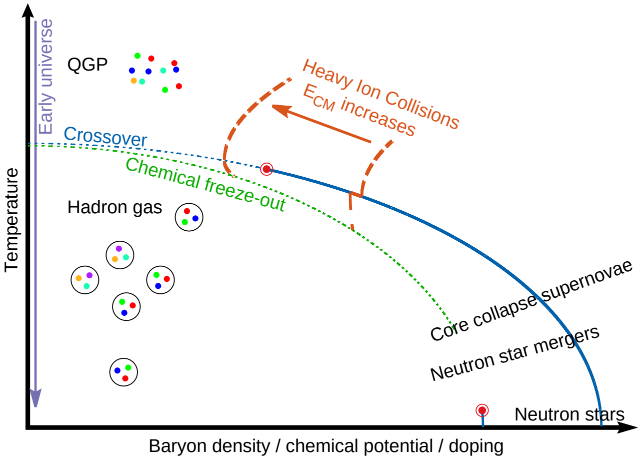
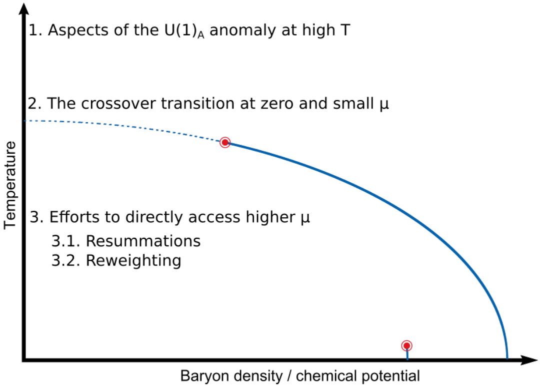
LATTICE 2023, FERMILAB

The conjectured phase diagram of QCD



A rough outline of my talk



Effective restoration of $U(1)_A$ at high T?

- Idea: towards chiral limit the determinant might suppress topology so that some observables related by $U(1)_A$ become degenerate
- Banks-Casher relation (assumes analyticity at $\lambda = 0$):

$$\frac{1}{V}\langle\bar{\psi}\psi\rangle \underset{V\to\infty}{\to} \int_0^\infty \rho(\lambda)\frac{m}{\lambda^2+m^2} \underset{m\to 0}{\to} \pi\rho(0)$$

- Naive expectation: $\rho(0) = 0$ at $T > T_c$ (chiral symmetry restoration)
- Small m (see e.g. [Kanazawa & Yamamoto PRD 91 (2015)]):

$$f = f_0 - f_2(m_u^2 + m_d^2) - f_A m_u m_d \cos\theta + \ldots$$

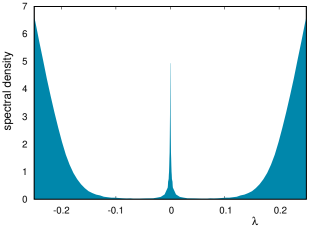
$$\text{as } m\to 0 \quad \chi_\pi - \chi_\delta \sim f_A \ \text{ and } \ \chi_{top} = \frac{1}{V}\langle Q_{top}^2\rangle \sim f_A m_u m_d$$

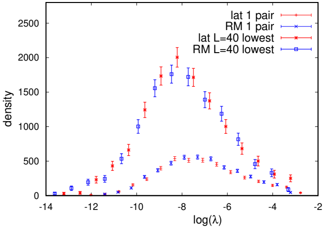
- Contrast: $T \ll T_c$: $\chi_{top} \propto m$ with $T \gg T_c$ $\chi_{top} \propto m^{N_f}$
- [Aoki et al, PRD86 (2012)]: analyticity in m and of $\rho(\lambda)$ at $\lambda = 0 \to f_A = 0$
- [Azcoiti, PRD107 (2023)]: analyticity in m and $f_A \neq 0$ $m \to \rho \underset{m\to 0}{\sim} m^2\delta(\lambda)$

$\to$ near zero modes of D are key

Weakly interacting instantons at high T

RM model of the physics of NZMs [T. Kovács: Tuesday 13:30]





- Peak near zero related to topology
- Here: overlap on quenched
- Overlap on staggered looks similar

  [Alexandru & Horváth, PRD100 (2019)]

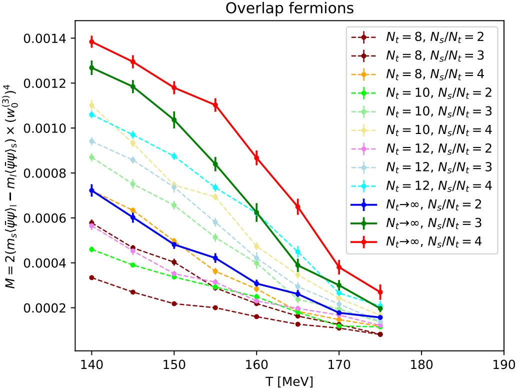
  [Alexandru & Horváth, PRL127 (2021)]
- Staggered: peak less pronounced

  [Ding et al, PRL126 (2021)]
- **Caveat:** JLQCD doesn't see the peak for overlap on DW (small V) [H. Fukaya, Monday, 15:30]

- 2 params describe I-AI mixing
- $\rho \to \lambda^{-\alpha}$ with $\alpha < 1$
- $\alpha \nearrow$ as $m \searrow$
- Eigenvectors have fractal structure
- $N_{NZM} \propto m^{N_f}$
- $\chi_\pi - \chi_\delta \neq 0$ for $N_f = 2$ χ limit
- $\chi_\pi - \chi_\delta \to 0$ for $N_f = 3$ χ limit
- instanton-aniinstanton molecules (?)

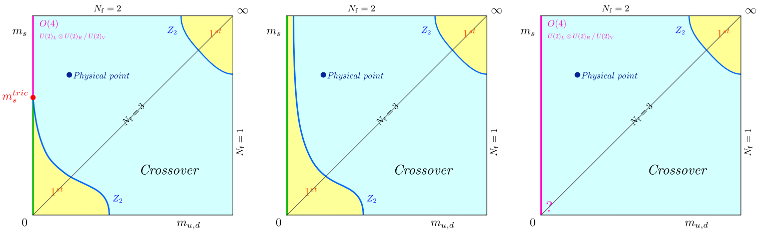
Ideally, one should look at the NZM peak with dynamical chiral fermions

Dynamical overlap fermions with physical quark masses



- [Monday: A. Kotov (13:30)]
- Dynamical overlap with standard Wilson kernel and 2steps of hex smearing
- Large finite volume effects (probably due to fixed topology)
- Large cut-off effects (???)

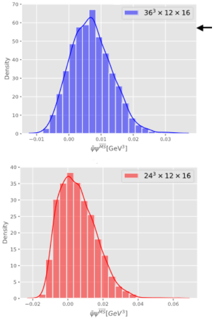
The Columbia plot and the anomaly

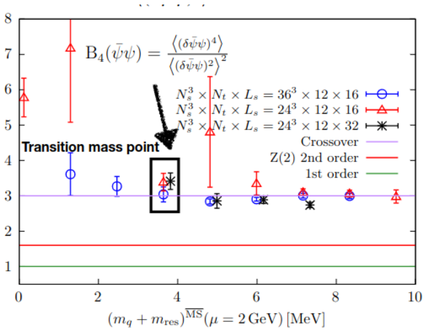


Plots from [Cuteri et al, JHEP11(2021)141]

- Perturbative RG (ϵ expansion) [Pisarski & Wilczek PRD89 (1984)]
  - If $U(1)_A$ effectively restored at T_c: $N_f = 2, 3$ cannot be 2nd order
  - If not: $N_f = 2$ can be second order, $N_f = 3$ cannot
- If correct, then left: phase diagram without anomaly, middle: with anomaly
- Recent work by Frankfurt group (staggered): new scenario on the right (see also [Dini et al, PRD 105(2022)])
- pRG not always reliable ($N_f = 3$ FP with no anomaly in [Fejős, PRD105 (2022)])
- [Ding et al, PRL 123 (2019)]: $N_f = 2$ consistent with $O(4)$
- Consistent with $T > T_c$ instantons: $U(1)_A$ eff. restored for $N_f = 3$ but not $N_f = 2$

MDW fermions for $N_f = 3$





- From the talk of [Y. Zhang, Mo 14:30]
- Domain wall, $N_\tau = 12$, $N_f = 3$, $LT = 2$ and 3
- Scan in the quark mass for fixed $T = 121$MeV:
  heavier → confined; lighter → deconfined
- Binder cumulants → crossover (Gaussian $\bar\psi\psi$)
- When the strange quark is as light as the up and down → crossover

QCD in the grand canonical ensemble

$$p = \frac{T}{V}\log \mathrm{Tr}\left[e^{-(H_{QCD}-\mu_u N_u-\mu_d N_d-\mu_s N_s)/T}\right] = \frac{T}{V}\log \mathrm{Tr}\left[e^{-(H_{QCD}-\mu_B B-\mu_Q Q-\mu_S S)/T}\right]$$

Generalized susceptibilities:

$$\chi^{BSQ}_{i,j,k} = \frac{\partial^{i+j+k}(\hat{p})}{(\partial\hat{\mu}_B)^i(\partial\hat{\mu}_S)^j(\partial\hat{\mu}_Q)^k} \qquad \chi^{uds}_{i,j,k} = \frac{\partial^{i+j+k}(\hat{p})}{(\partial\hat{\mu}_u)^i(\partial\hat{\mu}_d)^j(\partial\hat{\mu}_s)^k}$$

where $\hat{\mu} = \mu/T$ and $\hat{p} = p/T^4$.

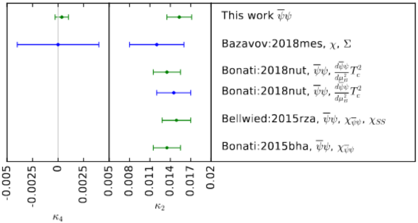
$$\mu_u = \frac{1}{3}\mu_B + \frac{2}{3}\mu_Q \quad \mu_d = \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q \quad \mu_s = \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q - \mu_S$$

$$\chi^B_1 \sim \langle B\rangle \quad \chi^B_2 \sim \left\langle B^2\right\rangle - \langle B\rangle^2 \quad \chi^{BQ}_{11} \sim \langle BQ\rangle - \langle B\rangle\langle Q\rangle$$

Higher orders are crucial for methods based on analytic continuation:
DATA ($\mathrm{Im}\,\mu_B$ or derivatives at $\mu_B = 0$) and ANSATZ (Taylor, Padé, ...)

The phase diagram for $LT = 4$

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



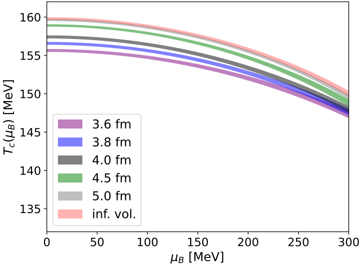
[Borsanyi et al, PRL 125(2020)]

Continuum extrapolated ✔

Fixed volume ✗

Strangeness neutrality ✔

Finite volume effects



[R. Kara: Tuesday 14:50]

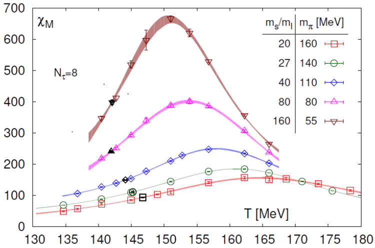
Fixed spacing $N_\tau = 12$ (4stout) ✗

Several volumes, inf.vol. extrap. ✔

Strangeness neutrality ✔

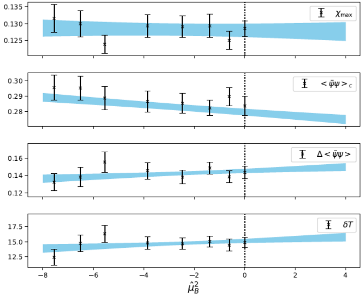
The strength of the crossover

When decreasing m_{ud}



[Ding et al, PRL 123 (2019)]

When increasing μ_B



[Borsanyi et al, PRL 125(2020)]

[R. Kara: Tuesday 14:50]

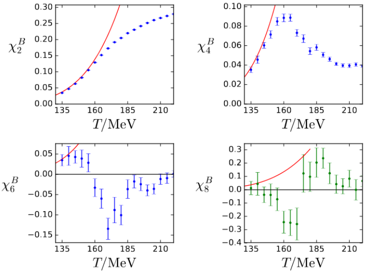
See also: [W-P Huang, Wednesday 9:00]
$N_f = 2$ 2nd order $\leftrightarrow$ D eigenvalues

Apparently, the system at $\mu_B = 0$ is only sensitive to $O(4)$ criticality ($O(2)$ for staggered at finite spacing) in the $N_f = 2$ chiral limit

Taylor coefficients of the pressure at $\mu_B = 0$

- Up to 4th order in μ_B and μ_S in the continuum ✔
- χ_4^Q challenging: taste breaking effects large ✗
- χ_6^B and χ_8^B at finite N_τ

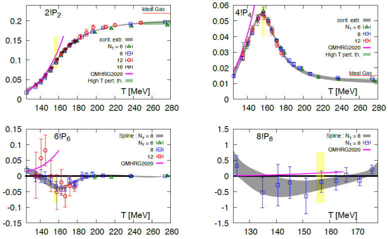
From Im μ_B simulations



[Borsanyi et al, JHEP 10 (2018)]

strangeness chemical potential $\mu_S = 0$

From $\mu_B = 0$ simulations



[Bollweg et al, PRD108 (2023)]

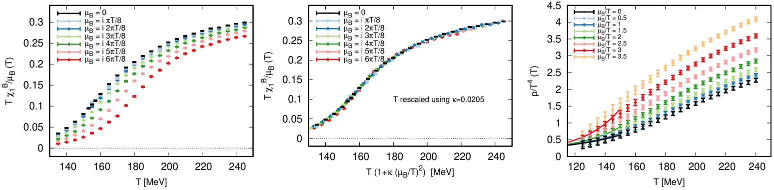
strangeness density $\chi_1^S(T, \mu_B) = 0$

Resummed equation of state

- At $\mathrm{Im}\,\mu_B$ we *observe*: $\frac{\chi_1^B(T,\hat{\mu}_B)}{\hat{\mu}_B} \approx \chi_2^B\left(T\left(1+\kappa\hat{\mu}_B^2\right),0\right)$
- Can be turned into a systematically improvable ansatz:

$$F(T,\mu_B) = F(T',0) \quad T' = T(1-\kappa_2(T)\hat{\mu}^2 - \kappa_4(T)\hat{\mu}^4 + \ldots)$$

- A choice of the observable F together with this ansatz defines an extrapolation scheme (a resummation of the Taylor series in μ_B)
- Analysis becomes similar to the extrapolation of $T_c(\mu_B)$



$\mu_S = 0$: [Borsányi et al, PRD106 (2021)]

$\chi_1^S = 0$: [Borsányi et al, PRD105 (2022)]

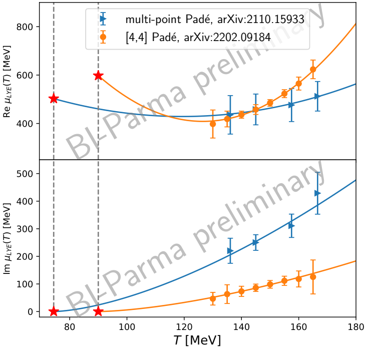
Analytic structure: Lee-Yang zeros

$$\mathcal{Z} = \mathrm{Tr}\left(e^{-(H-\mu_B B)/T}\right) = \sum_{n=-kV}^{+kV} e^{n\mu/T}\,\mathrm{Tr}_n(e^{-H/T}) = \sum_n Z_n e^{n\mu_B/T}$$

- (up to a factor) a polynomial in $e^{\mu/T}$ → zeros [Lee, Yang PR87 (1952)]
- $Z_n \in \mathbf{R}$ → Lee-Yang zeros come in complex conjugate pairs
- LY zeros → $p \propto \log Z$ has a branch point → $R_{conv} = (\limsup_{n\to\infty} |\chi_n^B/n!|^{1/n})^{-1}$
- Finite volume scaling → order of transition [Itzykson et al, NPB (1983)]
- $V = \infty$: analytic cont of RG scaling → $h_{LY} \sim |T - T_c|^{\Delta}$ (near a crit. pt)
  - Chiral limit: $m_{ud} \sim h$
  - Roberge-Weiss: $\mathrm{Im}\,\mu_B - \pi \sim h$
  - Critical endpoint: $\mu - \mu_{CEP} \sim h$
- LY zeros determine the large order behavior of series expansions
- In the context of QCD, the asymptotic behavior is discussed in:
  - Taylor (μ_B), $V = \infty$ [Stephanov, PRD73 (2006)]
  - Taylor (μ_B), $V < \infty$ [Giordano & Pásztor, PRD99 (2019)]
  - Fugacity ($e^{\mu_B/T}$), $V = \infty$ [Almási et al, PLB 793 (2019)]
  - Fugacity ($e^{\mu_B/T}$), $V < \infty$ [C. Schmidt, Friday 9:40]
- Rooted staggered → no LY polynomial: [Giordano et al, PRD99 (2019)]

CEP extrapolation from the Parma-Bielefeld group

[F. di Renzo, Friday 9:20] [C. Schmidt, Friday 9:40] [D. Clarke, Friday 10:00]



$$\mathrm{Im}\,\mu_{LY} = c(T - T_{CEP})^{\Delta}$$

$$\mathrm{Re}\,\mu_{LY} = \mu_{CEP} + a(T - T_{CEP}) + b(T - T_{CEP})^2$$

The basic approach:

- Padé → estimated $\mu_{LY}(T)$
- Orange: Taylor data, $N_\tau = 8$ (HISQ)
- Blue: $\mathrm{Im}\,\mu_B$ data, $N_\tau = 6$ (HISQ)
- An extrapolation

Comments:

- Inconsistent data for $\mathrm{Im}\,\mu_B$
- $b = 0$: scaling close to CEP
- Tension with the idea that near $\mu = 0$ QCD is mostly sensitive to $O(4)$ crit
- Similar ballpark to other approaches:
  DS: [J. Bernhardt et al, PRD 104 (2021)]
  FRG: [Fu et al, PRD 104 (2021)]
- Best case scenario: this observable is mainly sensitive to CEP, and finds it
- Worst case: once all systematics are considered, the signal disappears

Reweighting: in general

Fields: ϕ Target theory: Z_t Simulated theory: Z_s

$$Z_t = \int \mathcal{D}\phi \; w_t(\phi) \qquad w_t(\phi) \in \mathbb{C}$$

$$Z_s = \int \mathcal{D}\phi \; w_s(\phi) \qquad w_s(\phi) > 0$$

$$\frac{Z_t}{Z_s} = \left\langle \frac{w_t}{w_s} \right\rangle_s$$

$$\langle O \rangle_t = \frac{\int \mathcal{D}\phi \; w_t(\phi) O(\phi)}{\int \mathcal{D}\phi \; w_t(\phi)} = \frac{\int \mathcal{D}\phi \; w_s(\phi) \frac{w_t(\phi)}{w_s(\phi)} O(\phi)}{\int \mathcal{D}\phi \; w_s(\phi) \frac{w_t(\phi)}{w_s(\phi)}} = \frac{\left\langle \frac{w_t}{w_s} O \right\rangle_s}{\left\langle \frac{w_t}{w_s} \right\rangle_s}$$

Two problems that are exponentially hard in the volume can arise:

- $\frac{w_t}{w_s} \in \mathbb{C} \rightarrow$ the complex action problem became a **sign problem** $\rightarrow$ noise
- Tails of $\rho(\frac{w_t}{w_s})$ long $\rightarrow$ **overlap problem** $\rightarrow$ potentially incorrect results
- Important to choose a "good" w_s
- If the overlap problem is avoided $\rightarrow$ reliable results on a fixed lattice setup

Phase and sign reweighting

$w_t / w_s \in$ compact space → no tails, no overlap problem (at least in the pressure)

Phase reweighting

$$\begin{aligned} w_t &= e^{-S_g} \det M = e^{-S_g} |\det M| e^{i\theta} \\ w_s &= e^{-S_g} |\det M| \quad \text{phase quenched ensemble} \end{aligned} \quad \Rightarrow \quad \frac{w_t}{w_s} = e^{i\theta}$$

- $N_f = 2$ equiv. to isospin $\det M(\mu) \det M(-\mu) = |\det M(\mu)|^2$
- At non-zero isospin, a Goldstone mode appears at $\mu = m_\pi/2$
- Hard to simulate PQ ensemble, prev. used $\det(M^\dagger M + \lambda^2)$ (not compact)

Sign reweighting

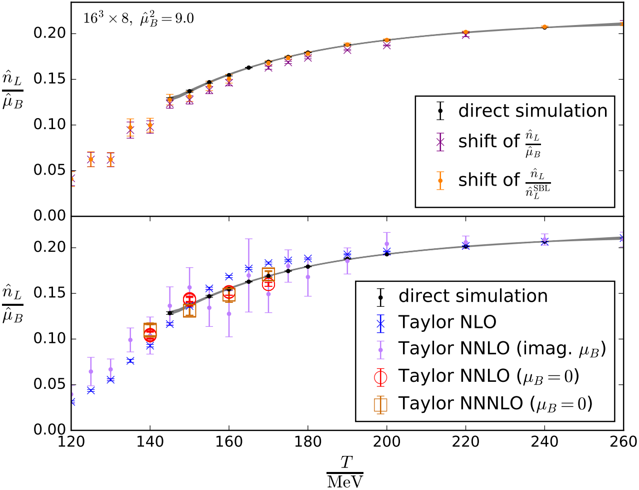
$$\begin{aligned} w_t &= e^{-S_g} \mathrm{Re} \det \mathrm{M} \\ w_s &= e^{-S_g} |\mathrm{Re} \det \mathrm{M}| \quad \text{sign quenched ensemble} \end{aligned} \quad \Rightarrow \quad \frac{w_t}{w_s} = \mathrm{sgn} \cos\theta = \pm 1$$

- $\det M \to \mathrm{Re} \det M$ can be done in Z but not in generic expectation values. E.g. things like $\frac{\partial^n \log Z}{\partial \mu_{ud}^n}$, $\frac{\partial^n \log Z}{\partial m_{ud}^n}$ and $\frac{\partial^n \log Z}{\partial \beta^n}$ can be calculated.
- Has a weaker sign problem than phase reweighting [de Forcrand et al, 2003]
- BUT: hard to simulate with weights $\propto |\mathrm{Re} \det \mathrm{M}|$

First true PQ and SQ studies (improved action): [Borsanyi et al, PRD (2022)]

Extrapolations vs direct results for the EoS

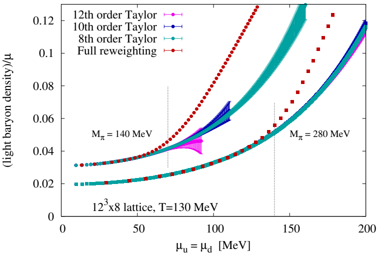
- Wuppertal-Budapest; PRD 107 (2023)
- $\mu_s = 0$, fixed volume $LT = 2$, fixed lattice spacing $N_\tau = 8$
- at the end of the RHIC range in μ_B

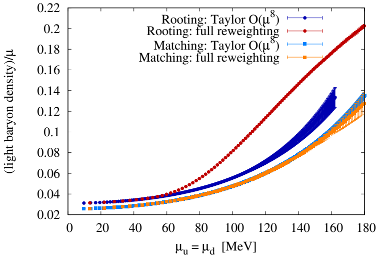


Troubles at low temperatures

At low T: cut-off effects related to rooting: [Goltermann et al, PRD75 (2006)]

$$Z_{N_f=2+1} = \int \mathcal{D}U (\det M_l(U,\mu_q))^{1/2} (\det M_s(U))^{1/4} e^{-S_G[U]}$$





[C.H. Wong, Friday] The rooted staggered free energy ($a \neq 0$) is non-analytic at $\mu = 0$. Only defined pertrubatively in μ. Before anything, we need a path integral that is worth trying to solve.

- Geometric matching of $\det M_{stagg}$ zeros [Giordano et al, PRD99 (2019)]
- Minimally doubled fermions?
  [R. Víg, Tue 16:40] [D. Godzieba, Tue 17:00] [J.H. Weber, Wed 9:20]

Summary

I talked about four topics:

- Near zero modes and topology at high T
- The crossover transition at small quark mass and small μ_B
- The equation of state and analytic structure from resummations
- More direct reweighting methods

And had to make some important omissions:

- Resummations: [Mondal+, PRL128 (2022)], [Dunne & Basar, PRD105 (2022)]
- Non-zero isospin density [W. Detmold Mo 16:20]
- Magnetic fields: [J.J. Hernandez We 10:00], [J.-B. Gu, We 10:20] [Marques Valois, Fri 10:20]
- Anomalous transport [E. Garnacho-Velasco Thu 13:30] [Brandt et al, JHEP 07 (2023)]
- Sign problem approaches: [Tuesday, finite μ], [Thursday, Algorithms and AI]
- Heavy quarks at non-zero temperature: [S. Sharma, Tue 16:40]
- ...

BACKUP

Some recent results on topology and near zero modes

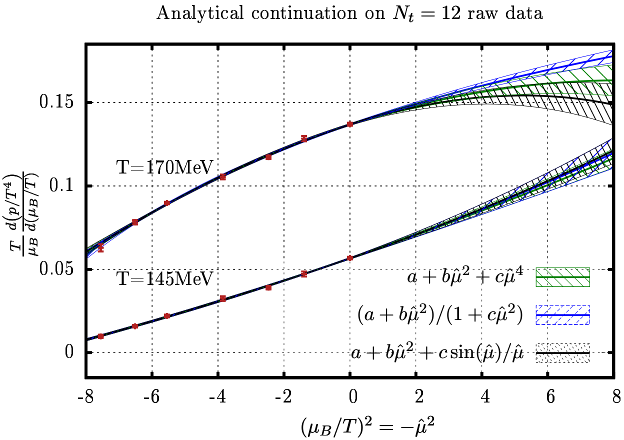
About instantons at high T

- [Víg & Kovács PRD103 (2021)]: free instantons ($T > T_c$) in pure YM
- [Borsányi et al, PRD107 (2023)]: χ_{top} discont at T_c in pure SU(3)
- [Borsányi et al, Nature (2016)]: χ_{top} in QCD at physical point
- Also [Petreczky et al, PLB762 (2016)], [Athenodorou et al, JHEP (2022)]
- Exponent compatible with free instantons above $T \gtrsim 2T_{pc}$
- With and without assuming free instanton gas: same result for $T \gtrsim T_c$

About near zero modes

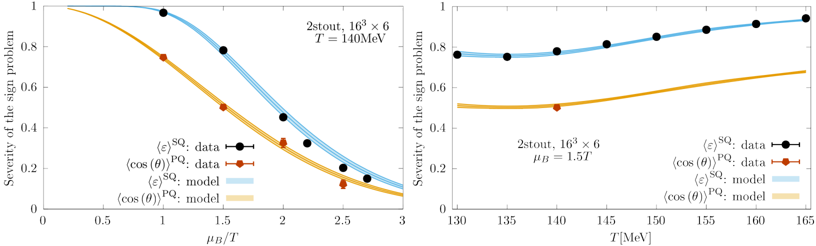
- [Ding et al, PRL126 (2021)]: $N_{NZM} \propto m_{ud}^2 \rightarrow f_A \neq 0$
- [Alexandru & Horváth, PRD100 (2019)]: $\rho(\lambda) \rightarrow \infty$ as $\lambda \rightarrow 0$
- [Alexandru & Horváth, PRL127 (2021)]: eigenvectors are fractals

The two uses of imaginary μ simulations



- Numerical differentiation at $\mu = 0$: relaitvely safe
- Extrapolation: relatively risky

Estimating the severity of the sign problem

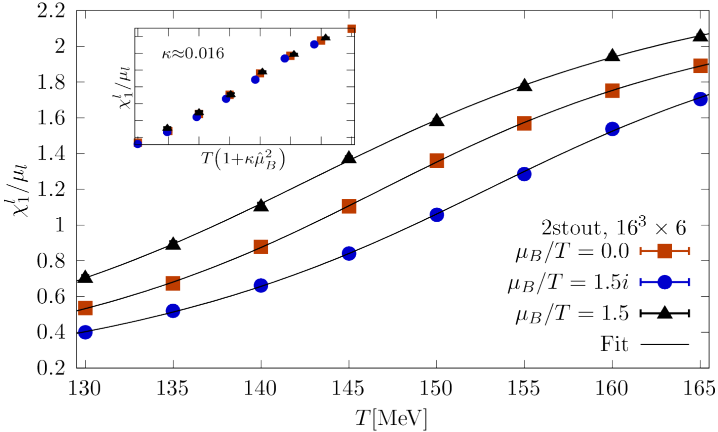


W-B: PRD 105 (2022) 5, L051506

- Statistics required $\propto 1/(\text{strength of the sign problem})^2$
- Gaussian model describes simulation data pretty well
- Const. strength of the sign problem for ≈ const. $(LT)^3 \left(\frac{\mu_B}{T}\right)^2$
- For $LT = 16/6 \approx 2.7$ ($T = 140\text{MeV} \rightarrow L \approx 4\text{fm}$) the sign problem is managable for the entire RHIC BES range

Does the rescaling work at real non-zero μ_B?

Yes, up to some point at least: PRD 105 (2022) 5, L051506 ($N_\tau = 6$)



Rescaling also works at real μ_B → no sign of a strengthening crossover