Towards a reliable lower bound on the location of the critical endpoint

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Introduction

- I will focus on conceptual issues about calculating **the radius of convergence** or the **position of the leading singularity** of the pressure around $\mu_B = 0$
- Important issues the knowledge this would tell us about:
  - How far is the EoS from Taylor exp. trustworthy?
  - If limiting singularity is $\notin$ real axis $\rightarrow$ rigorous lower bound on CEP location
  - If limiting singularity is $\in$ real axis $\rightarrow$ prediction for a phase transition
- Standard methods (Taylor and analytic continuation) are standard for a reason, but they can't seem to handle this problem well

Plan of the talk

Two parts:

(1) Issues related to finite volume
M. Giordano, A. Pásztor, hep-lat/1904.01974, PRD99 (2019) no.11, 114510
- General and rigorous arguments about statistical mechanical systems in a finite volume
- Generic features are illustrated on a toy lattice: $N_f = 4$ unimproved staggered, $6^3 \times 4$
- Suggests an approach to attacking the problem

(2) Convergence radius from lattice QCD using an improved action
M. Giordano, K. Kapás, S. Katz, D. Nógrádi, A. Pásztor, hep-lat/1911.00043
- We follow the approach outlined in (1)
- Analyticity issues of rooted staggered fermions make this non-trivial, but we propose a sol.n
- Results on $N_t = 4$ lattices using 2+1 flavors of stout improved staggered fermions

High-order behavior of the coefficients in a finite volume - 1

In a "typical" stat. mech. system the grand canonical part. fn.:

$$Z(\hat{\mu}) = \sum_{n=-kV}^{n=+kV} Z_n e^{n\hat{\mu}} = e^{-2kV\hat{\mu}} \sum_{m=0}^{2kV} Z_{m-kV} e^{m\hat{\mu}}$$

where the Z_n are the canonical partition functions with the quark number fixed to n.

- k is a model dependent constant, $\hat{\mu} = \mu_q/T$
- Polynomial $\rightarrow$ has $2kV$ complex roots in $e^{\hat{\mu}}$: **Lee-Yang zeros**(LY0) z_i
- Accumulation of the LY0s to some real μ as $V \rightarrow \infty$ signals a phase transition
- Z has $\mu \rightarrow -\mu$ symmetry (CP)
- $Z_n \in \mathbf{R} \rightarrow$ Lee-Yang zeros come in complex conjugate pairs
- The high order terms in $\log Z = \sum c_n \mu^{2n}$ are dominated by 4 logarithmic singularities(LY0s) at the same distance from 0 and are given by:

$$c_k \sim \frac{-2}{k} \frac{\cos(2k\theta)}{r^{2k}} \quad \text{as} \quad k \rightarrow \infty \qquad \text{leading LY0s} : \mu = re^{\pm i\theta}, re^{\pm i(\pi-\theta)}$$

High-order behavior of the coefficients in a finite volume - 2

$$c_k \sim \frac{-2}{k} \frac{\cos(2k\theta)}{r^{2k}} \quad \text{as} \quad k \to \infty$$

Consequences:

- The **ratio estimator does not converge**:

$$\left| \frac{c_k}{c_{k+1}} \right| = r^2 \frac{k+1}{k} \left| \frac{\cos(2k\theta)}{\cos(2(k+1)\theta)} \right|$$

- The **asymptotically high order fluctuations are strongly correlated** on any gauge ensemble, since they are all given by r and θ
- Even if the ensemble is enough to determine r and θ accurately, **the errorbars of the high order fluctuations will always blow up** (linear error propagation applied to the above formula)

High-order behavior of the coefficients in a finite volume - 3

- If the correlations between the c_n are kept, even if they have $> 100\%$ errorbars, the leading LY0 position can still be recovered several ways, e.g. by taking one of these **new estimators for the radius of convergence** as $k \to \infty$:

modified Mercer-Roberts estimator:

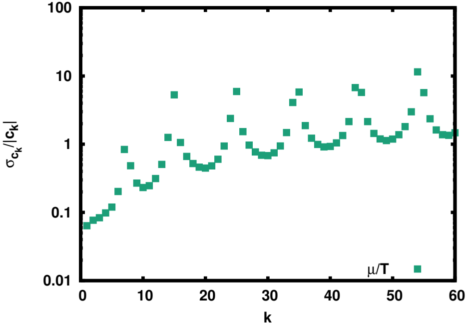
$$r_k^{(\mathrm{MMR})} = \left| \frac{(k+1)(k-1)c_{k+1}c_{k-1} - k^2 c_k^2}{(k+2)k c_{k+2} c_k - (k+1)^2 c_{k+1}^2} \right|^{\frac{1}{2}}$$

doubled index estimator:

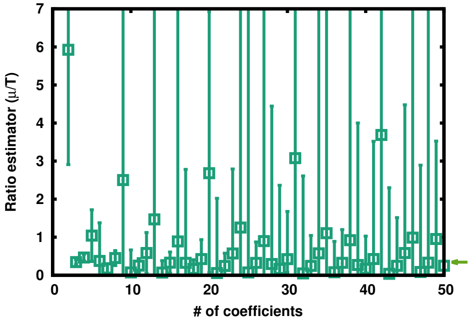
$$r_k^{(2\mathrm{i})} = \left| \frac{2}{2k c_{2k} + k^2 c_k^2} \right|^{\frac{1}{2k}}$$

- These are by definition exact for a single (quartet of) LY0(s)
- Original Mercer-Roberts and Cauchy-Hadamard also work, but they converge slower
- Can also construct estimators for the angle $\cos\theta$
- So far I didn't really use anything QCD specific, this is generic stat. mech.
- To illustrate these issues I use a toy lattice: $N_f = 4$ unimproved, where there is a specific construction that allows for the calculation of the c_n to arbitrary order (most of them will have $> 100\%$ errors though)

Toy lattice results: $N_f = 4$ unimproved, $6^3 \times 4$

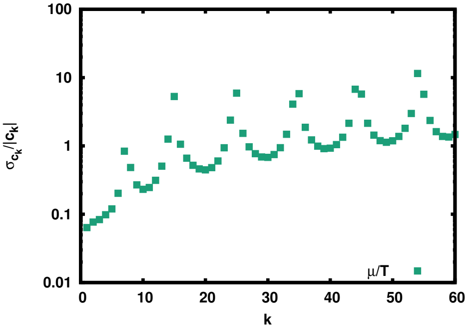


Relative errors

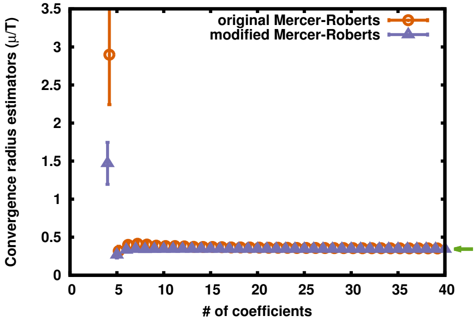


Ratio estimator

Toy lattice results: $N_f = 4$ unimproved, $6^3 \times 4$



Relative errors



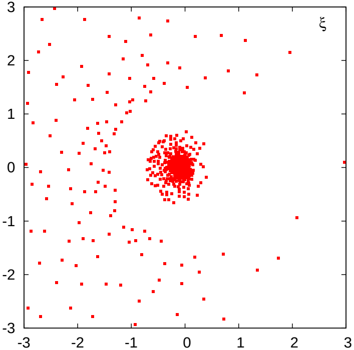
Mercer-Roberts type estimators

Towards a more physical situation: rooted staggered fermions

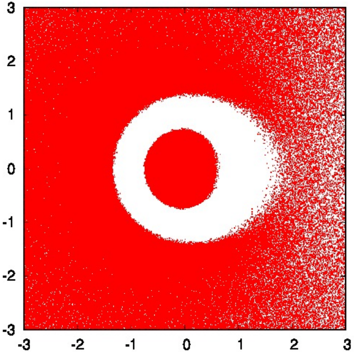
$$Z = \int \mathcal{D}U (\det M)^{N_f/4} e^{-S_G[U]}$$

- $\mu_B \neq 0 \rightarrow \det M \in \mathbf{C}$. How do we choose the sign of the sqrt for $N_f = 2$?
- Standard methods (analytic continuation and Taylor expansion) use the root that continuously connects to the positive sqrt at $\mu_B = 0$
- Consequence: **The partition function is non-analytic everywhere on the support of the density of the zeros of the unrooted staggered det**
- Sol.n with standard methods: calculate the cont. lim. of the individual c_n first, and only later study the high order behavior of the series
- I would rather not do that, because this washes out the correlations between the c_n
- We propose a specific construction that reduces to the standard prescription in the continuum limit, but gives the "rooted" determinant as a polynomial in the fugacity already at finite a. (Involves grouping eigenvalues of the reduced fermion matrix: **geometric matching**)

Zeros of the unrooted staggered determinant

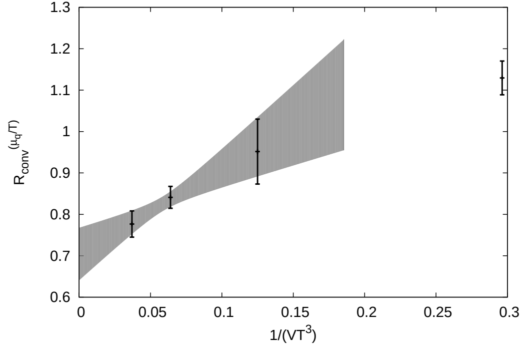


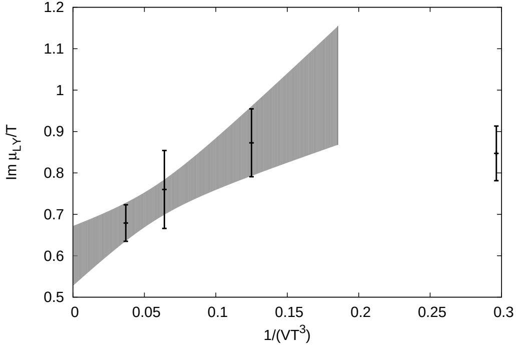
1 configuration



3000 configurations

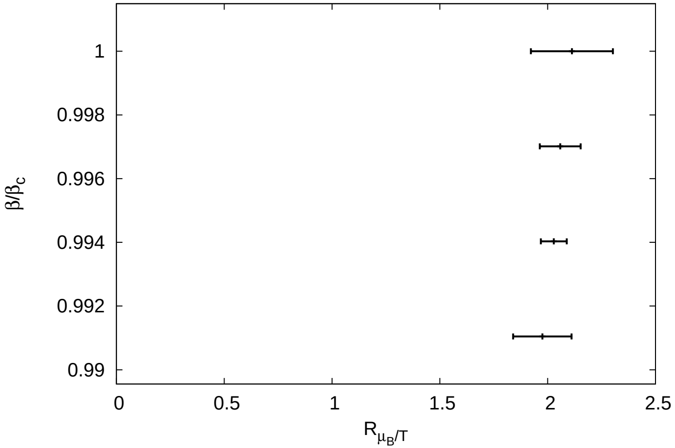
Numerical results for 2-stout improved $N_f = 2+1$, $N_t = 4$





The LY0s we find are in the region analytically inaccessible with the standard methods

Numerical results for 2-stout improved $N_f = 2+1$, $N_t = 4$



vertical axis: gauge coupling, I did not convert it to T on purpose, as it is a coarse lattice

Summary

- The only info in c_n as $n \to \infty$ in a finite vol. is the location of the leading LY0
- This implies the c_n on a given gauge ensemble will be strongly correlated
- Want to keep these correlations, so the errors can cancel in certain combinations and we can obtain a radius of convergence
- For this we want a useful definition of the radius of convergence that works at finite a, so that the c_n can come from the same ensemble
- Rooting at finite a introduces extra singularities that decrease the radius of convergence to an unphysical value. $\to$ With standard methods, it is important to take cont. lim. of the individual c_n, before trying to infer the singularity structure.
- To fix the analyticity issues, we introduce a construction to make Z a polynomial already at finite a (geometric matching)
- This allows for a numerical study of LY0s
- We demonstrated this whole procedure numerically on $N_t = 4$ staggered lattices with 2-stout improvement and obtained the **position of the leading singularity without relying on a finite order Taylor-expansion**

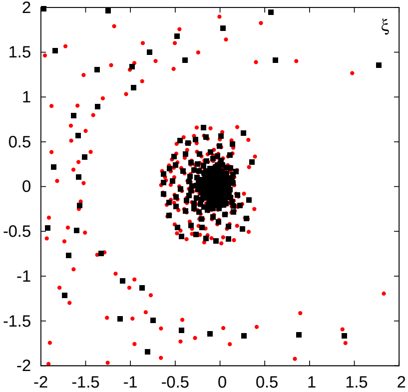
Backup

The Lee-Yang polynomial in lQCD: $N_f = 4$ staggered

$$Z = \int \mathcal{D}U \det M[U] e^{-S_G[U]}$$

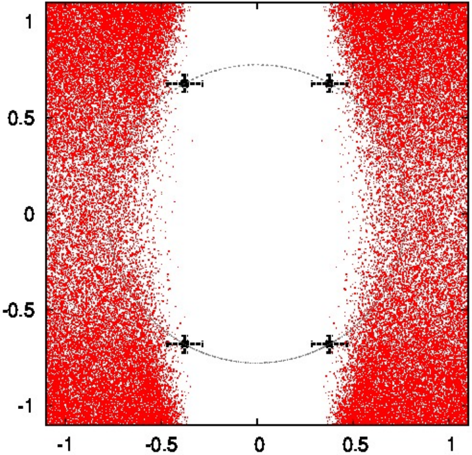
- Hasenfratz, Touissaint '91: for this discretization, the fermionic determinant can be written as:
$$\det M(\hat{\mu}) = e^{-3V\hat{\mu}} \prod_{i=1}^{6V} \left(\xi_i - e^{\hat{\mu}}\right) = e^{-3V\hat{\mu}} \mathcal{P}_\xi \left(e^{\hat{\mu}}\right)$$
- the ξ_i are the eigenvalues of the so-called **reduced matrix** P, which can be constructed from the original Dirac operator at $\mu = 0$
- The ξ_i depend only on the gauge fields, and not μ
- The Lee-Yang polynomial is $\langle \mathcal{P}_\xi \rangle_U$
- Knowing the Lee-Yang polynomial I can calculate all fluctuations to arbitrary order on my ensemble (most of them will have $> 100\%$ stat. errors though)

Geometric matching



- Do not actually take the square root
- Find close pairs of eigenvalues of P and take their geom. mean: $\tilde{\xi} = \sqrt{\xi_1 \xi_2}$
- The new "rooted" determinant is def. to be prop. to $\prod_{n=1}^{3V} (\tilde{\xi}_n - e^{\hat{\mu}})$
- OK in the continuum, where the unrooted staggered op. describes 4 degenerate flavors, but is a polynomial already at finite a
- Can again utilize the power of the LY polynomial

LY0 vs determinant zeros



LY0 with new method (full statistics) vs zeros of the unrooted det on 3000 config.s

Possible objections

(1) This geometric matching procedure is a **non-local modification of the theory**
Yes, and so is the standard staggered rooting.

(2) You have an **overlap problem**
Yes, and so do the two standard methods (analytical continuation and Taylor expansion)

(3) **Diagonalization of P is expensive**, you won't be able to do it for say $N_t = 12$ or 16
Probably true. Let us try.