Testing dynamical stabilization of Complex Langevin simulations of QCD

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1. Introduction to complex Langevin
2. QCD and complex Langevin
3. dynamical stabilization

Importance Sampling

We are interested in a system
Described with the partition sum:

$$Z = \int D\phi\, e^{-S} = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \sum_C W[C]$$

Typically exponentially many configurations,
no direct summation possible.

If the Weight is positive, build a Markov chain with the Metropolis algorithm

$$\ldots \rightarrow C_{i-1} \rightarrow C_i \rightarrow C_{i+1} \rightarrow \ldots$$

Probability of visiting C $\quad p(C) \sim W[C]$

$$\langle X \rangle = \frac{1}{Z} \mathrm{Tr}\, X e^{-\beta(H-\mu N)} = \frac{1}{Z} \sum_C W[C] X[C] = \frac{1}{N} \sum_i X[C_i]$$

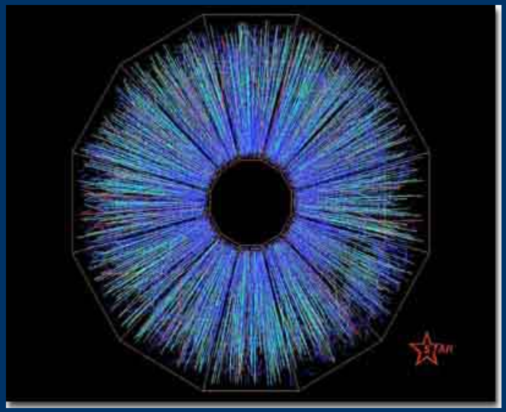
This works if we have $\quad W[C] \geq 0$

Otherwise we have a Sign problem

Sign problems

Real-time evolution in QFT

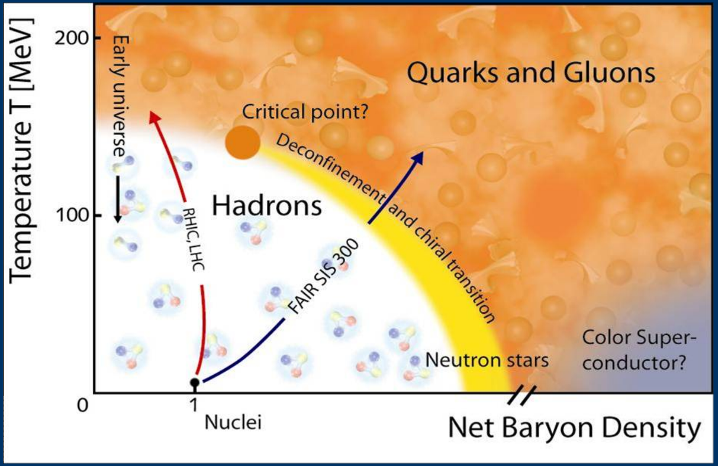
"strongest" sign problem e^{iS}



Non-zero density

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \int DU\, e^{-S[U]} \det(M[U])$$

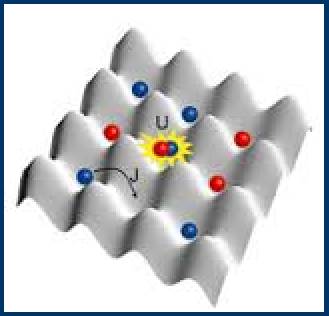
Many systems: Bose gas
XY model
SU(3) spin model
Random matrix theory
QCD



Theta therm

$$S = F_{\mu\nu} F^{\mu\nu} + i\Theta\, \epsilon^{\mu\nu\theta\rho} F_{\mu\nu} F_{\theta\rho}$$

Inbalanced Fermi gas



And everything else with complex action

$w[C] = e^{-S[C]}$ $\qquad$ $w[C]$ is positive $\leftrightarrow$ $S[C]$ is real

Langevin Equation (aka. stochatic quantisation)

Given an action $S(x)$

Stochastic process for x: $$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

Gaussian noise

$$\langle \eta(\tau) \rangle = 0$$
$$\langle \eta(\tau)\eta(\tau') \rangle = \delta(\tau - \tau')$$

Random walk in configuration space

Averages are calculated along the trajectories:

$$\langle O \rangle = \lim_{T\to\infty} \frac{1}{T}\int_0^T O(x(\tau))\,d\tau = \frac{\int e^{-S(x)} O(x)\,dx}{\int e^{-S(x)}\,dx}$$

Numerically,
results are extrapolated to $\Delta\tau \to 0$

Complex Langevin Equation

Given an action $S(x)$

Stochastic process for x: $\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$

Gaussian noise

$\langle \eta(\tau) \rangle = 0$

$\langle \eta(\tau)\eta(\tau') \rangle = \delta(\tau - \tau')$

$$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

The field is complexified

real scalar ⟶ complex scalar

link variables: SU(N) ⟶ SL(N,C)

compact / non-compact

$\det(U) = 1, \quad U^{+} \neq U^{-1}$

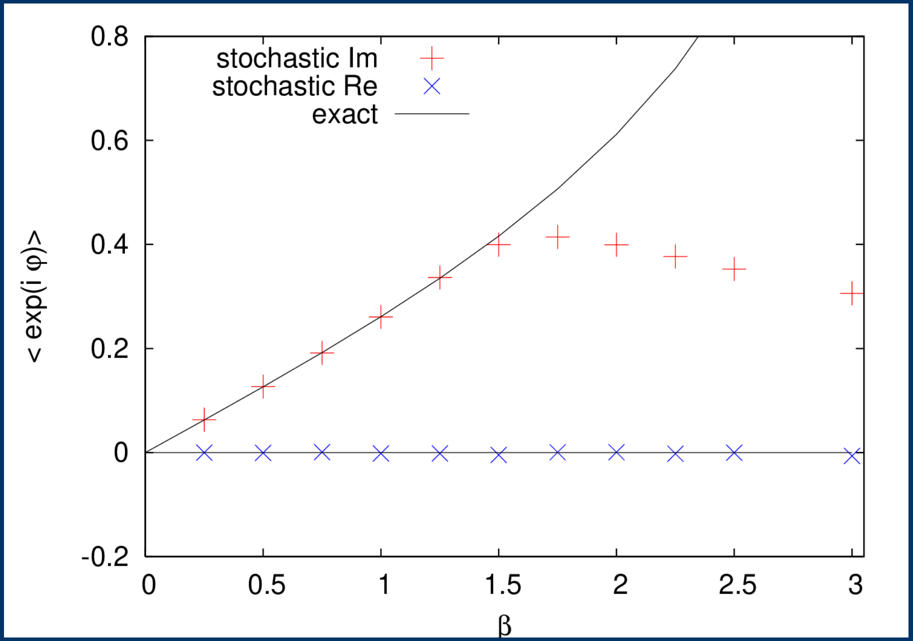
Analytically continued observables are calculated along the trajectories:

$$\langle O \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T O(x(\tau) + iy(\tau))\, d\tau$$

$$\langle x^2 \rangle_{real} \rightarrow \langle x^2 - y^2 \rangle_{complexified}$$

$$\frac{1}{Z} \int P_{comp}(x) O(x)\, dx = \frac{1}{Z} \int P_{real}(x, y) O(x + iy)\, dx\, dy \quad ?$$

For nontrivial models CLE may or may not give a correct answer



$$S(\varphi) = i\beta\cos\varphi + i\varphi$$

Do we know if it's correct?

Reasons for incorrect results: slowly decaying distributions (Boundary terms)
different cycles contributing [See talk of Michael Mandl]
non-holomorphic actions

Diagnostic observables: boundary terms
certain non-holomorphic observables, histograms

What can we do if it's incorrect?

Change variables
Use a kernel [See talk of Enno Carstensen]
Use a "regularization" (see below)

Can we apply Complex Langevin to QCD?

Yes, but there are some hurdles along the way:

1. respect group manifold

2. complexified gauge group is non-compact - gauge cooling

3. rough lattices – gauge cooling inefficient

4. Include light fermions

5. low beta (low temperature?) - system more instable
   Dynamical stabilization

1st problem: respect group manifold

$$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

In lattice gauge theory, we have link variables: $U_\gamma(x) \in \mathrm{SU}(N)$

First idea: use a map

$$U_\gamma(x) = U(\phi_i, \theta_j) \quad 0 \le \phi_i < 2\pi,\ 0 \le \theta_j < \pi,\ \ 1 \le i \le 5,\ 1 \le j \le 3 \text{ for SU}(3)$$

$$\int DU\, e^{-S(U)} \rightarrow \int d\phi_i\, d\theta_j\, H(\phi_i, \theta_j)\, e^{-S(\phi_i, \theta_j)}$$

→ Langevin eq. for ϕ_i, θ_j

$$K_i = -\partial_i S + \partial_i \ln H(\phi_i, \theta_j)$$

Con: Too cumbersome (already for real Langevin)

Map has singular points

Pro(?): potentially different complexifications

1st problem: respect group manifold

$$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

In lattice gauge theory, we have link variables: $U_\gamma(x) \in \mathrm{SU}(N)$

Better idea: use the map $U_\gamma(x) = e^{i\lambda_a \alpha_a} U_0$ locally, only for the update eq.

[Batrouni, Kawai, Rossi (1985)]

update eq.: $U(\tau + \Delta\tau) = \exp\left[i\lambda_a \left(K_a \Delta\tau + \eta_a \sqrt{2\Delta\tau}\right)\right] U(\tau)$

Drift term: $K_a = D_a S(U) = \left(\frac{\partial}{\partial \alpha_a} S(e^{i\lambda_a \alpha_a} U)\right)\Big|_{\alpha_a = 0}$ Left derivative

Complexification: $K_a \in \mathbb{C}$ $U \in \mathrm{SU}(N) \rightarrow U \in \mathrm{SL}(3, \mathbb{C})$

Unitarity norm: distance from the real manifold

$N_U = Tr(U U^+ - 1)^2$ $\approx \sum \mathrm{Im}\,\phi^2$ for scalars

2^{nd} problem: Gauge degrees of freedom also complexify

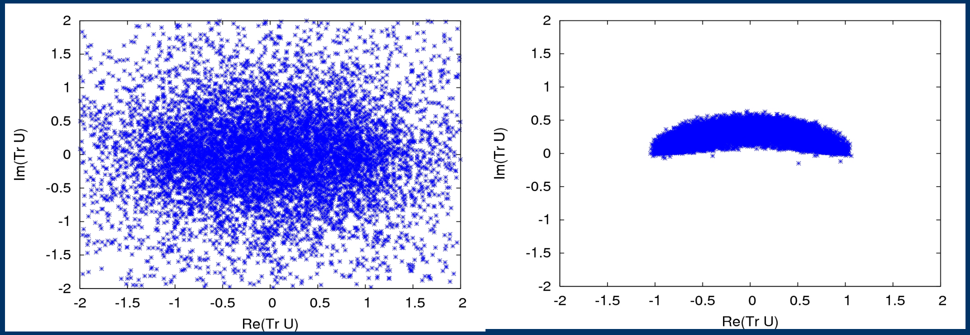
$SL(N, \mathbb{C})$ is a non-compact group

In SU(N) simulations, gaugefixing is not needed, as gauge freedom is a compact group.

In Complex Langevin, this gives a non-compact group to be explored by the simulations.

Gauge fixing

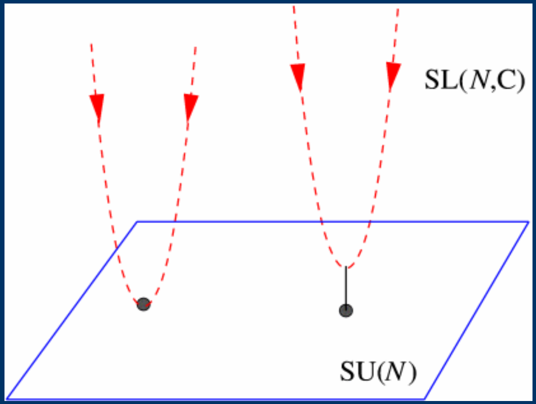
SU(2) one-plaquette



[Berges, Sexty (2008)]

Gauge cooling

Decrease N_U using gauge transformations



[Seiler, Sexty Stamatescu (2013)]

Heavy Quark QCD at nonzero chemical potential (HDQCD)

Hopping parameter expansion of the fermion determinant
Spatial hoppings are dropped ⟶ unmovable quarks

$$\mathrm{Det}\, M(\mu) = \prod_x \det(1 + C P_x)^2 \det(1 + C' P_x^{-1})^2 \qquad S = S_W[U_\mu] + \ln \mathrm{Det}\, M(\mu)$$

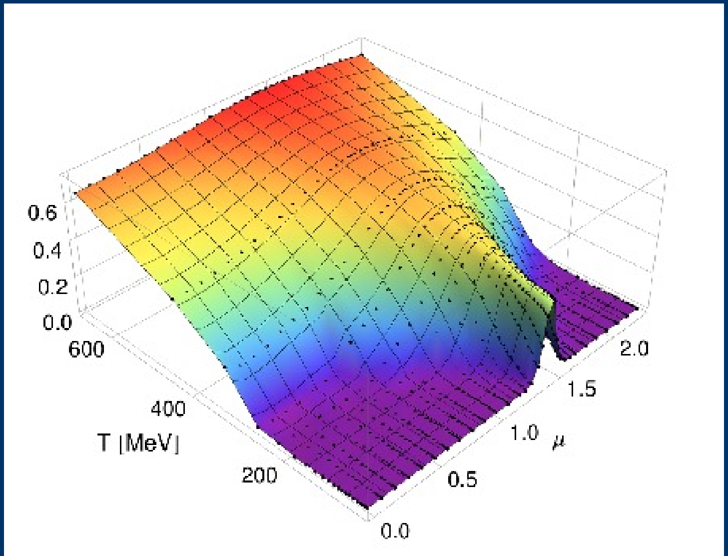
$$P_x = \prod_\tau U_0(x + \tau a_0) \qquad C = [2\kappa \exp(\mu)]^{N_\tau} \qquad C' = [2\kappa \exp(-\mu)]^{N_\tau}$$

CLE study using gaugecooling

[Seiler, Sexty, Stamatescu (2013)]

Phase diagram mapped out

[Aarts, Attanasio, Jaeger, Sexty (2016)]



At large lattice spacings
Gauge cooling inefficient

Use small lattice spacings

(Use large N_t for small temperatures)

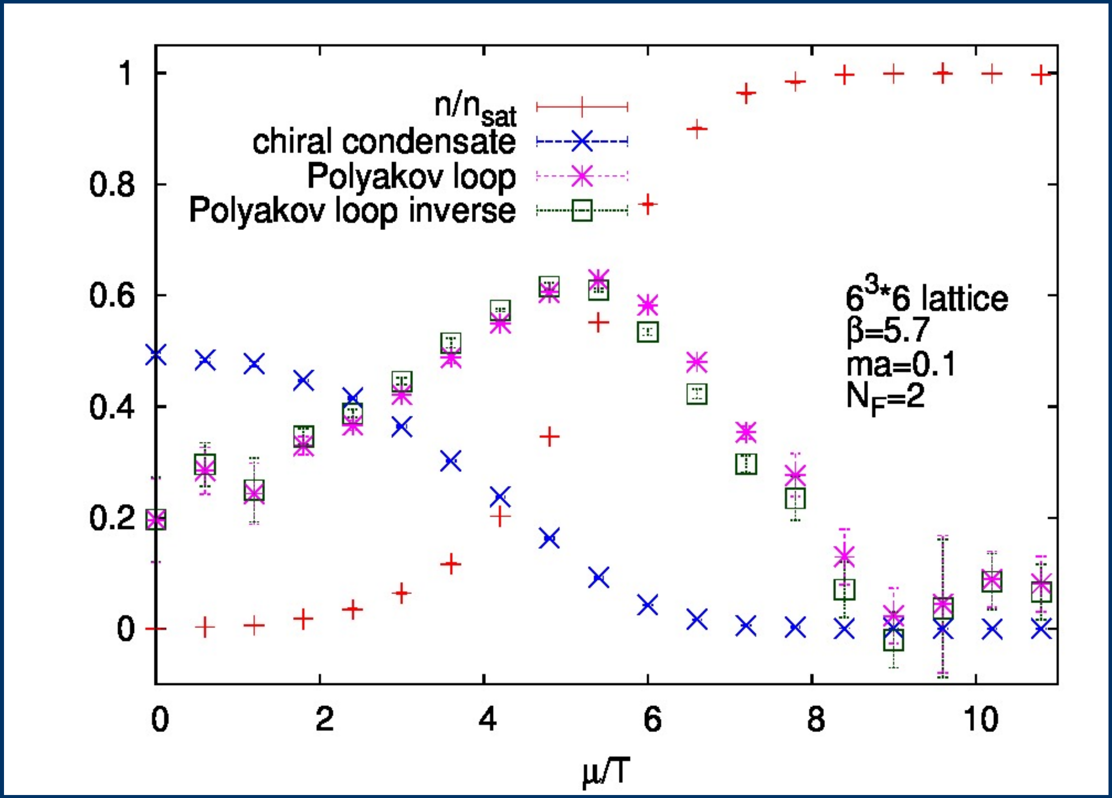
CLE and full QCD with light quarks

$$Z=\int DU\, e^{-S} \det M$$

Fermionic drift:

$$K_F = D_a \ln \det M = \mathrm{Tr}\left(M^{-1} D_a M\right)$$

Exact drift terms only for tiny Lattices.
Partial reduction of the matrix allows also small lattices



[Sexty (2014)]

Large lattices: noisy estimator

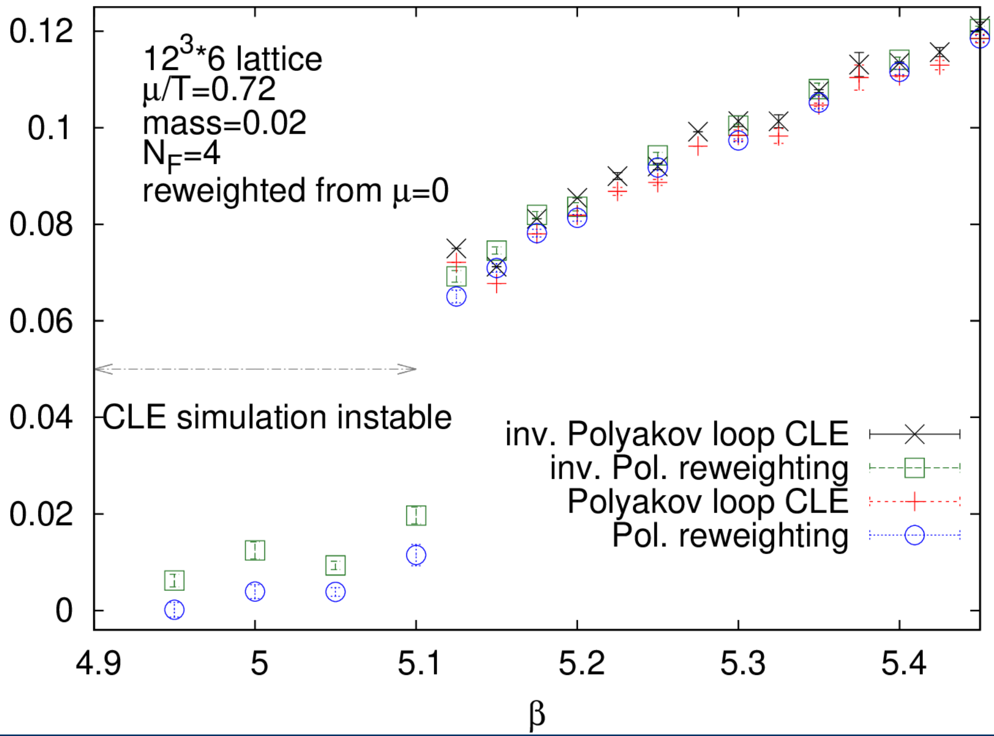
$$\mathrm{Tr}\left(M^{-1} D_a M\right) = \langle s^+ M^{-1} D_a M s \rangle$$
$$s = \text{noise field}$$

One CG solution per update step

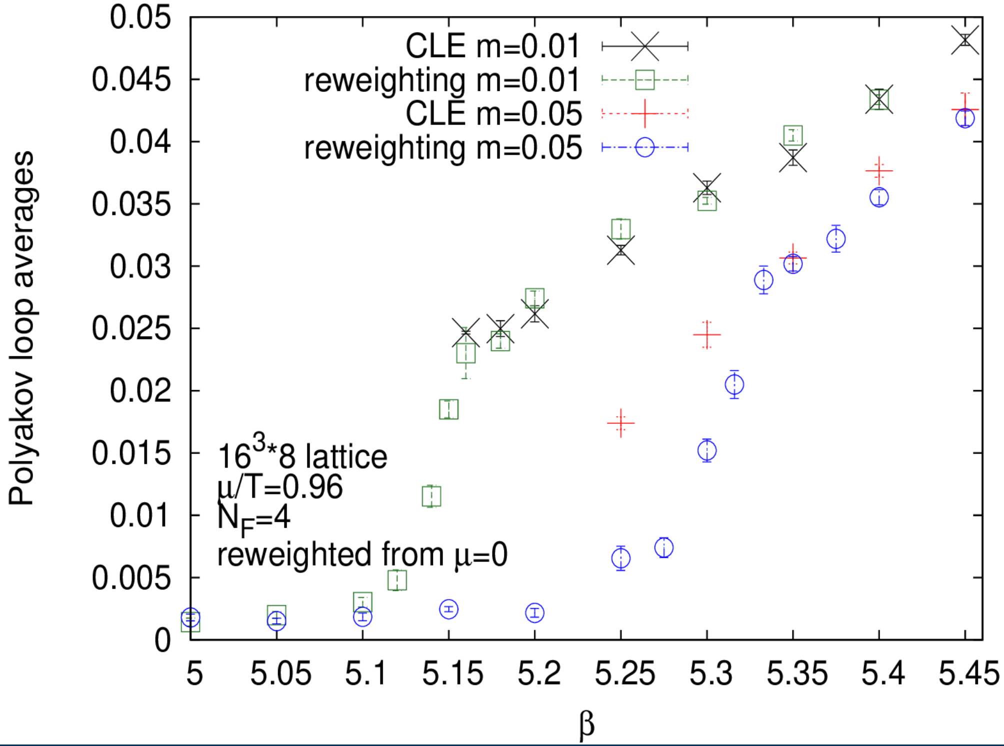
Direct simulations of full QCD at high densities possible for the first time

At low beta, CLE simulation instable

$N_T = 6$



$N_T = 8$



[Fodor, Katz, Sexty, Török (2015)]

Breakdown prevents simulations in the confined phase for staggered fermions with $N_T = 4,6,8$

→ Stay above the deconfinement temperature for now

Pressure of the QCD Plasma using CLE

[Sexty (2019)]

If we can simulate at $\mu > 0$

$$\Delta\left(\frac{p}{T^4}\right) = \frac{p}{T^4}(\mu = \mu_q) - \frac{p}{T^4}(\mu = 0) = \frac{1}{V\,T^3}\left(\ln Z(\mu) - \ln Z(0)\right)$$

$$\ln Z(\mu) - \ln Z(0) = \int_0^{\mu} d\mu \,\frac{\partial \ln Z(\mu)}{\partial \mu} = \int_0^{\mu} d\mu\, n(\mu)$$

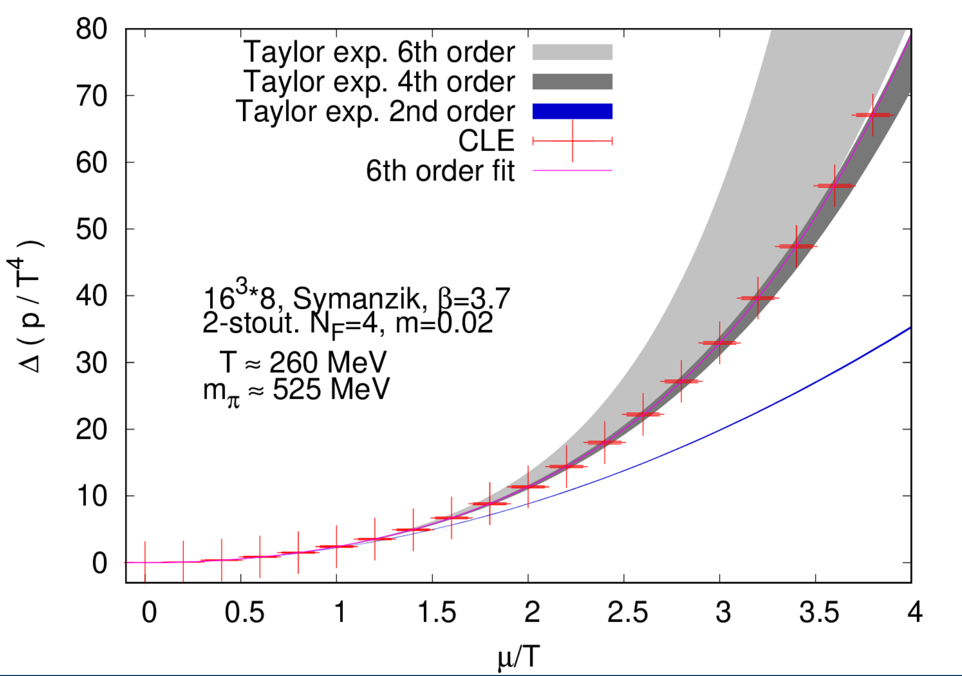
$$n(\mu) = \langle \mathrm{Tr}\left(M^{-1}(\mu)\,\partial_\mu M(\mu)\right)\rangle$$

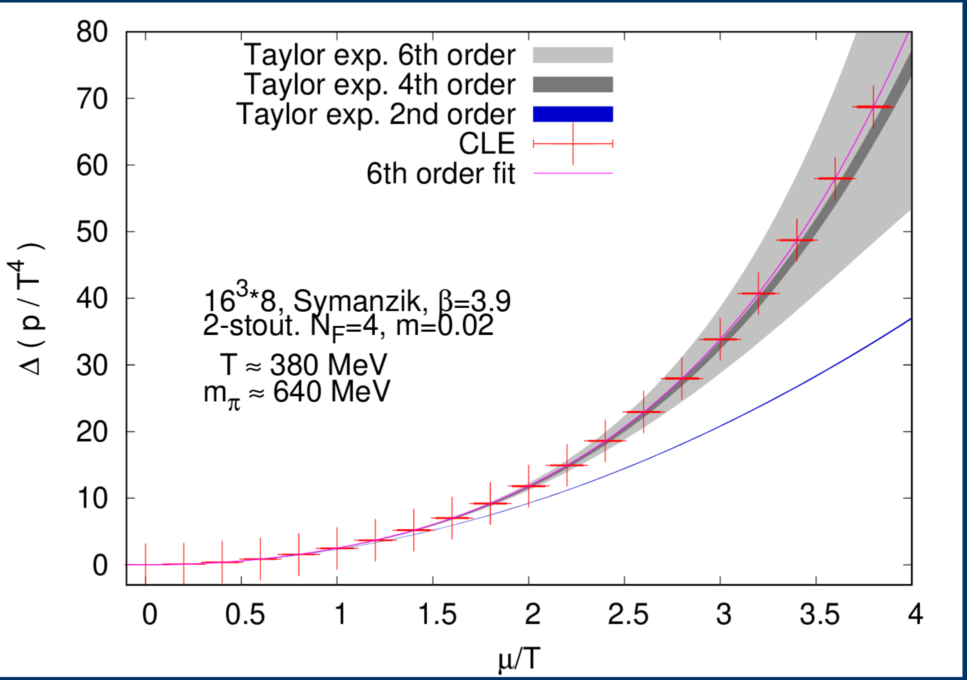
Using CLE it’s enough to measure the density
– much cheaper than Taylor expansion

Pressure with CLE and improved action

[Sexty (2019)]

In deconfined phase
Symanzik gauge action
stout smeared staggered fermions





β	c_2 Taylor exp.	c_4 Taylor exp.	c_6 Taylor exp.	c_2 CLE	c_4 CLE	c_6 CLE
3.7	2.206 ± 0.009	0.156 ± 0.016	0.016 ± 0.013	2.33 ± 0.1	0.13 ± 0.02	0.002 ± 0.001
3.9	2.312 ± 0.007	0.150 ± 0.007	0.001 ± 0.005	2.36 ± 0.04	0.14 ± 0.01	0.002 ± 0.001

Good agreement at small μ
CLE calculation is much cheaper

further interesting quantities: Energy density, quark number susceptibility, ...

Dynamical Stabilization [Attanasio, Jäger (2018)]

Prevent growth of Unitarity norm

"Soft cutoff" in the imaginary directions of SL(3,C)

New term in drift

$$K^a_{x,\nu} \rightarrow K^a_{x,\nu} + i\,\alpha_{\mathrm{DS}}\,M^a_x$$

$$M^a_x = i\,b^a_x \left(\sum_c b^c_x b^c_x\right)^3 \qquad b^a_x = Tr\left[\lambda^a \sum_\nu U_{x,\nu} U^+_{x,\nu}\right]$$

New term is SU(3) gauge invariant (not SL(3,C))
Not a derivative of an action
Not holomorphic
Gauge cooling is still used with DS on top
α_{DS} controls strength of attraction to SU(3)

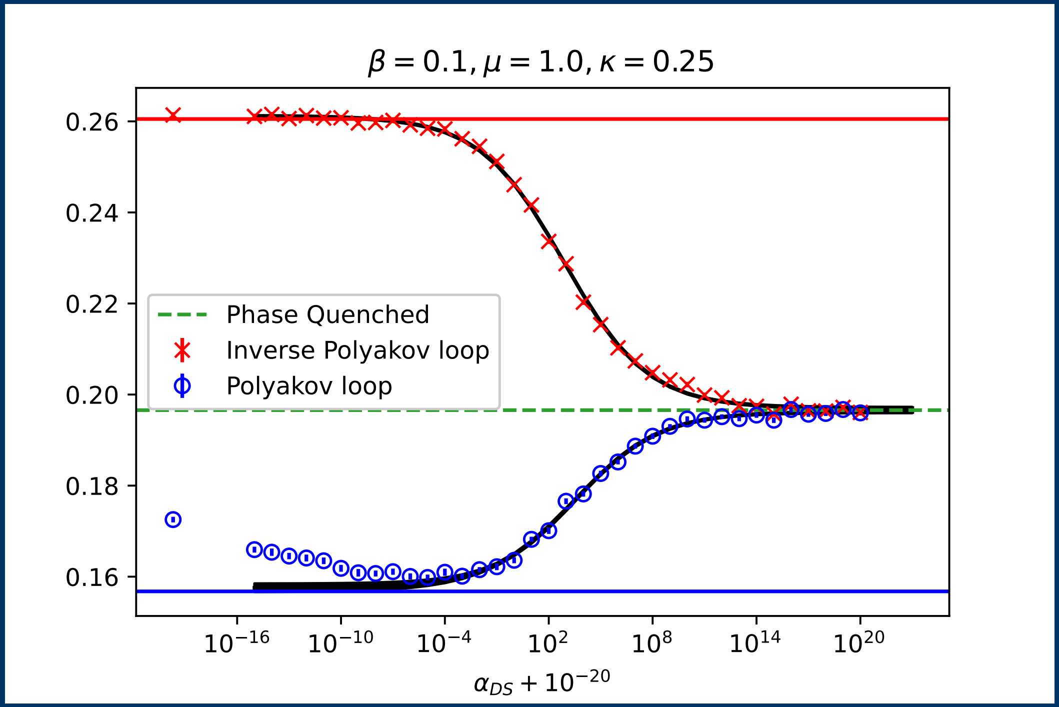
Dynamical Stabilization of a toy model

[Hansen, Sexty (2024)]

$$S = -(\beta + \kappa e^{\mu})\,\mathrm{Tr}\,U - (\beta + \kappa e^{-\mu})\,\mathrm{Tr}\,U^{-1}$$

one Polyakov line of QCD

Complex Langevin + dynamical stabilization



large α_{DS}

system confined to real manifold

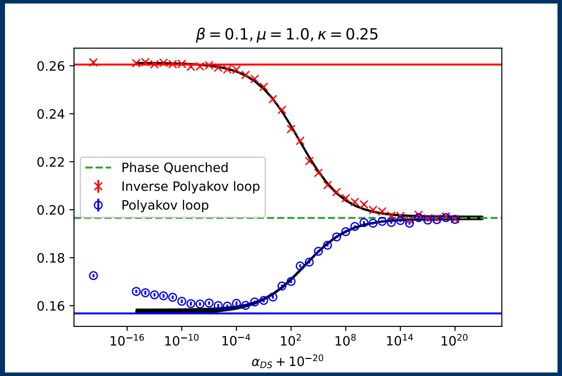
phasequenched simulation

$$Z_{PQ} = \int DU \left| e^{-S(U)} \right| = \int DU\, e^{-\mathrm{Re}\, S(U)}$$

fit function: $f(\alpha_{DS}) = A + \dfrac{B - A}{1 + C\,\alpha_{DS}^{D}}$

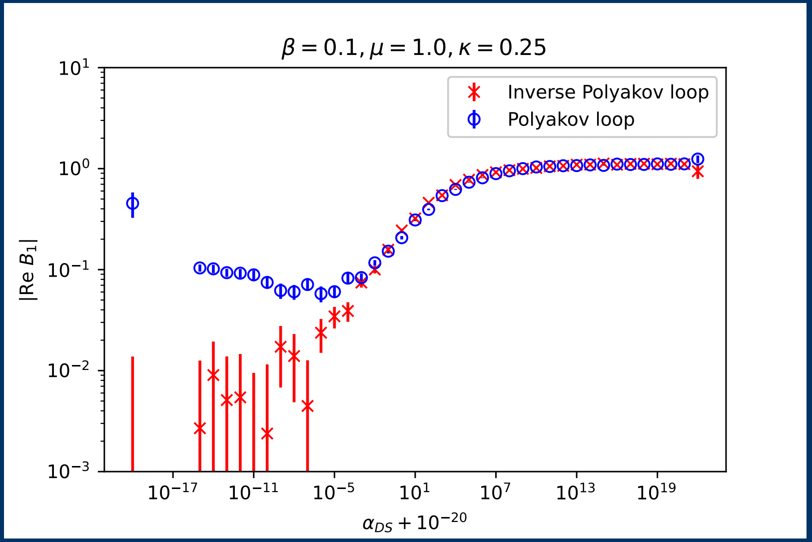
extrapolated to $\alpha_{DS} = 0$

Dynamical Stabilization of a toy model



Fit range?

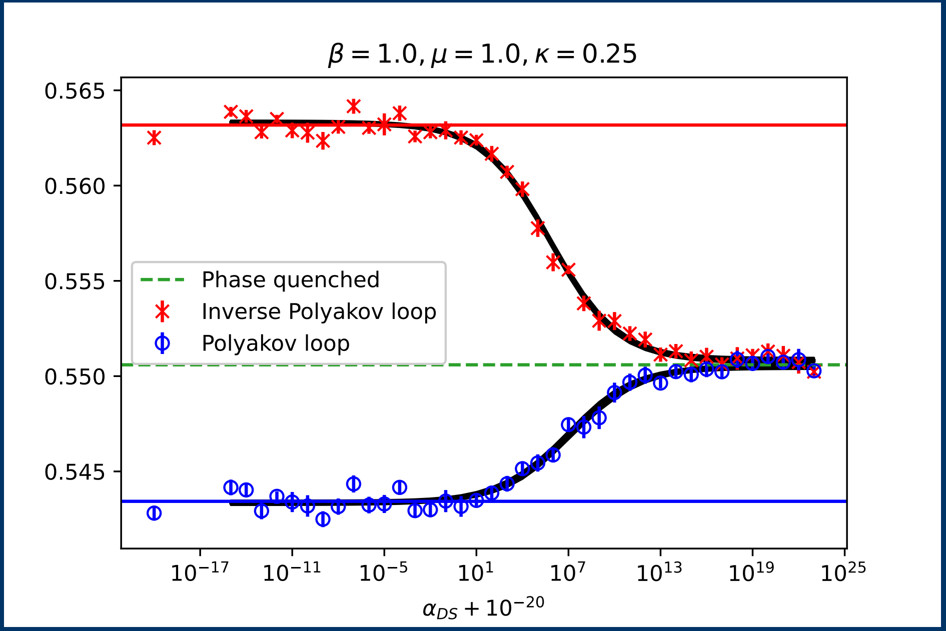
Boundary terms:

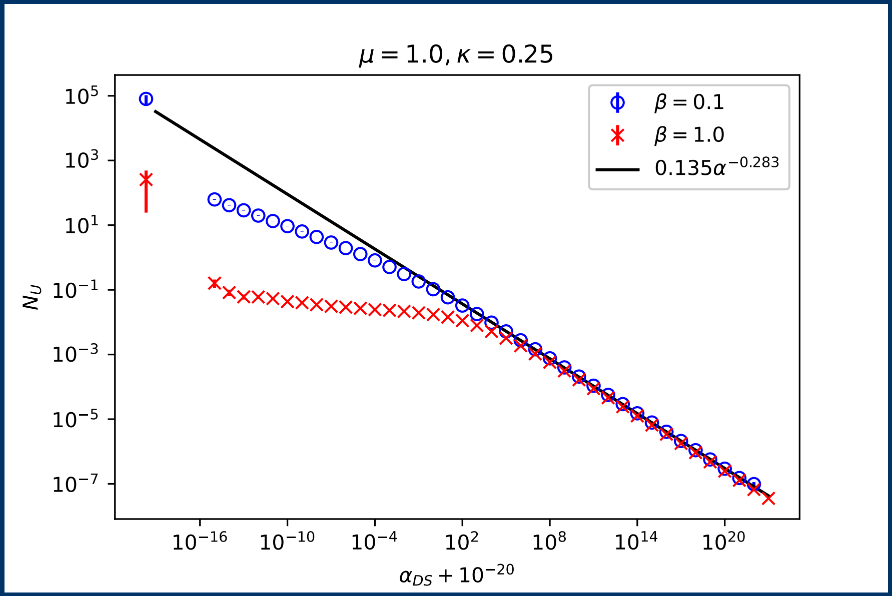


"large temperature"

No dynamical stabilization needed

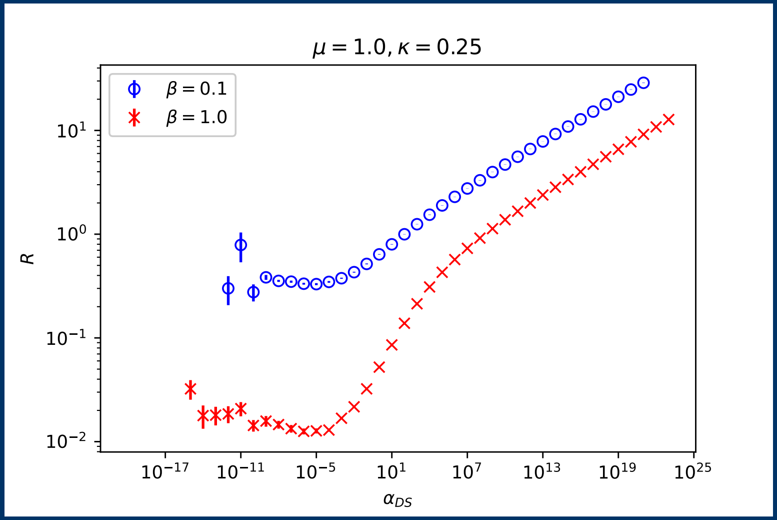
Fit still works





stronger stabilization drift
squeezes distribution to real manifold

$$N_u \sim \alpha^{-1/4}$$



Relatively small contribution to drift

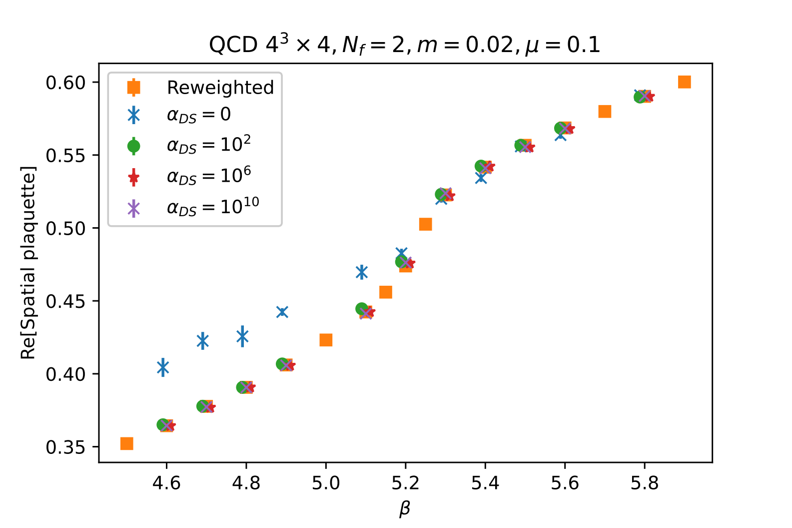
Except for high α_{DS}
where system is close to phasequenched

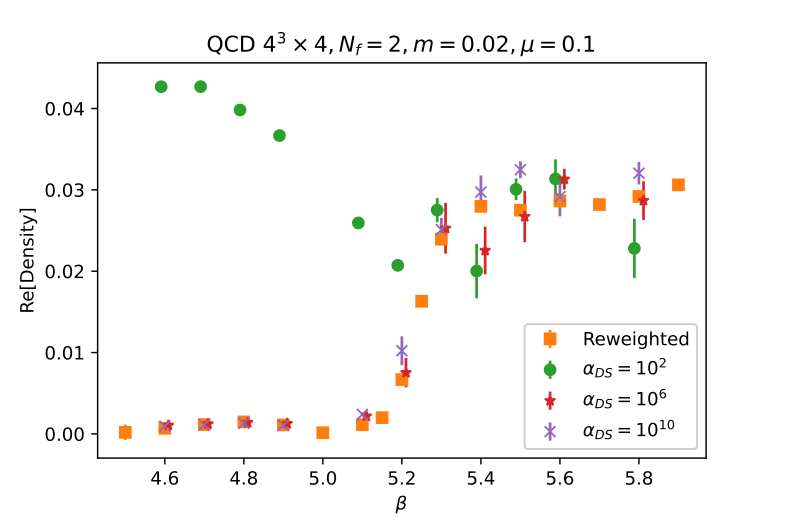
$$R = \frac{\text{Norm of DS drift}}{\text{Norm of drift from action}}$$

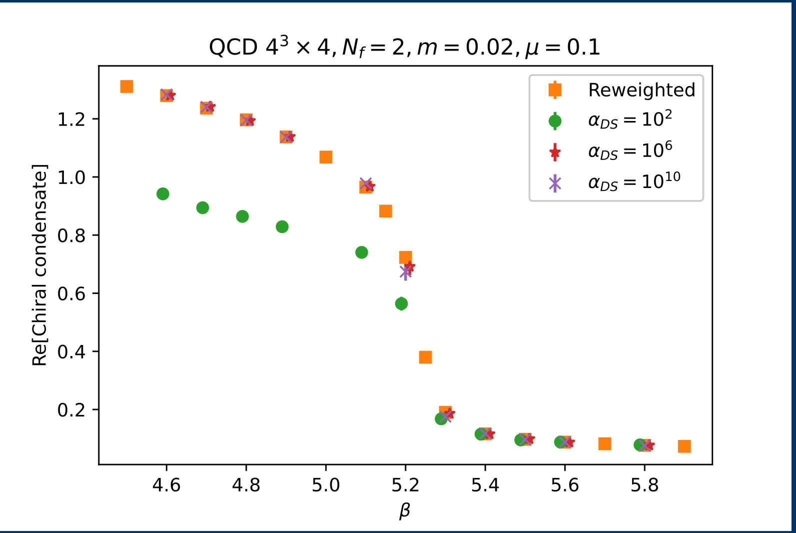
Dynamical Stabilization in QCD

[Hansen, Sexty (2024)]

At low temperatures stabilization needed
high temperatures, naive simulation is fine







From far away, dyn.stab. seems
to correct give results also at low T

Let’s take a closer look!

Two versions of Dynamical stabilization

Original proposal

[Jager, Attanasio (2018)]

$$K^a_{x\nu} \rightarrow K^a_{x\nu} - i\,\alpha_{DS}\, b^a_x \left(b^c_x b^c_x\right)^3 \qquad b^a_x = \mathrm{Tr}\left(\lambda_a \sum_{\nu=1}^{4} U^+_{x\nu} U_{x\nu}\right)$$

Mixes force of all 4 link variables attached to a site “Mixing version”

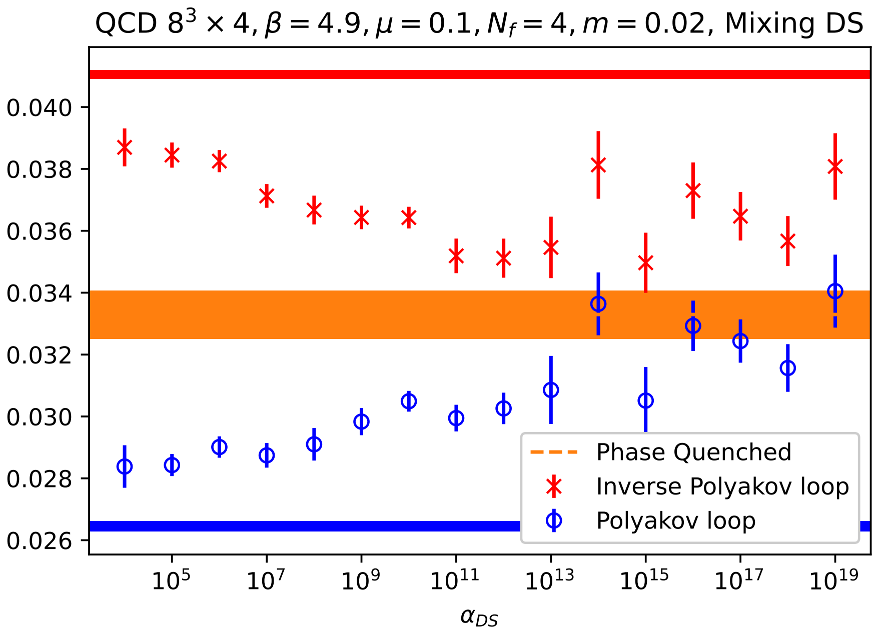
Modified proposal

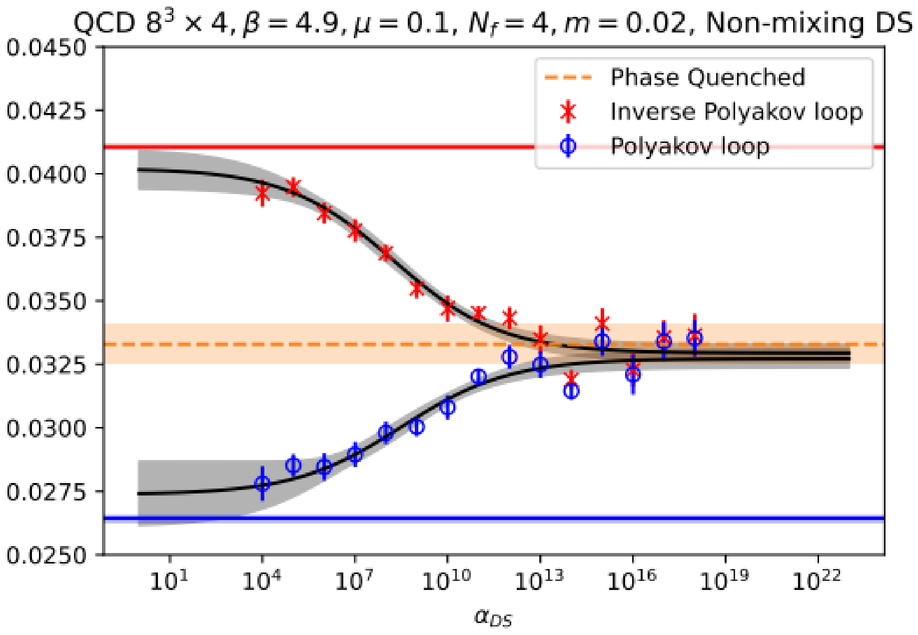
$$K^a_{x\nu} \rightarrow K^a_{x\nu} - i\,\alpha_{DS}\, b^a_{x\nu} \left(b^c_{x\nu} b^c_{x\nu}\right)^3 \qquad b^a_{x\nu} = \mathrm{Tr}\left(\lambda_a U^+_{x\nu} U_{x\nu}\right)$$

All 4 links have a separate stabilizing force “Non-Mixing version”

Polyakov loop in QCD

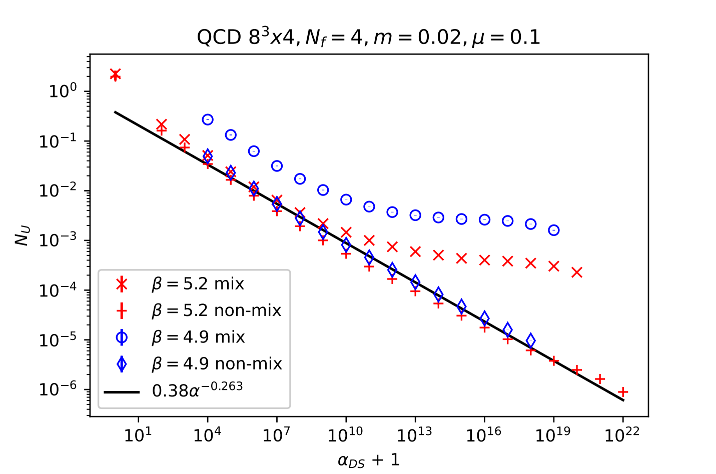
Low temperature





Non-mixing force has stronger effect

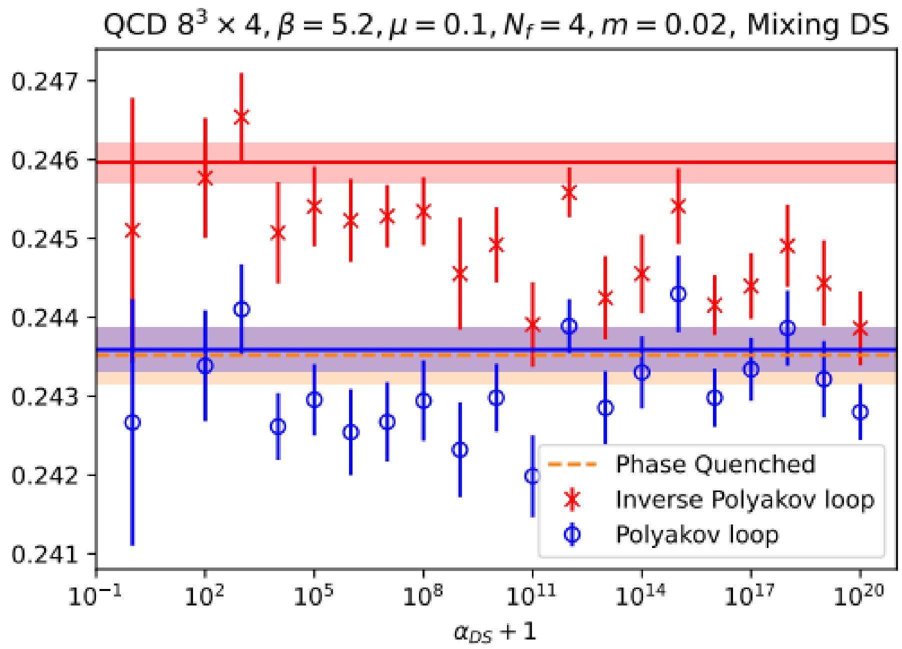
Strong stabilization drives to phasequenched →

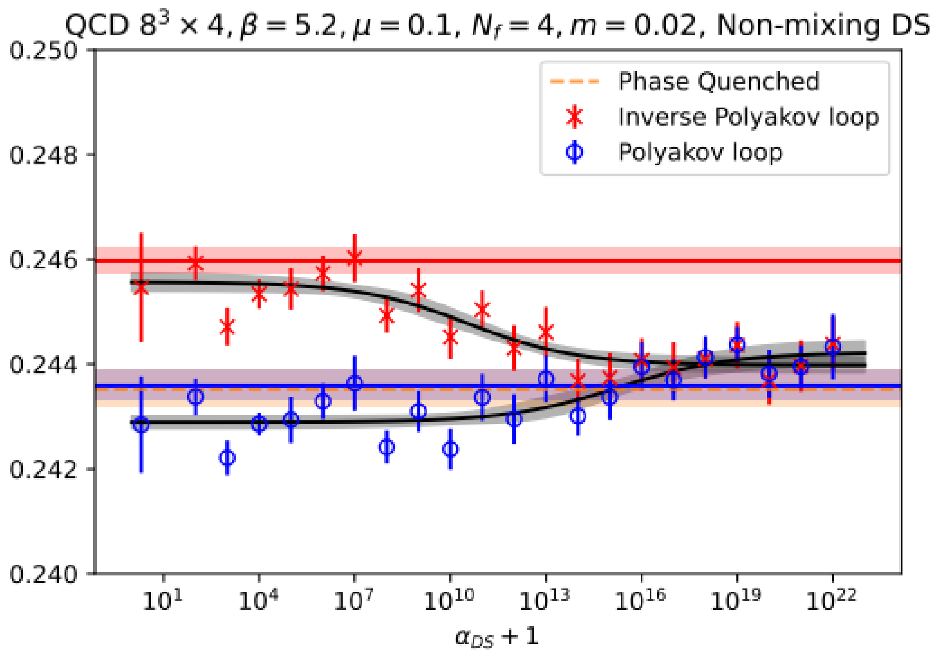


Sigmoid fit work reasonably well

Polyakov loop in QCD

High temperature





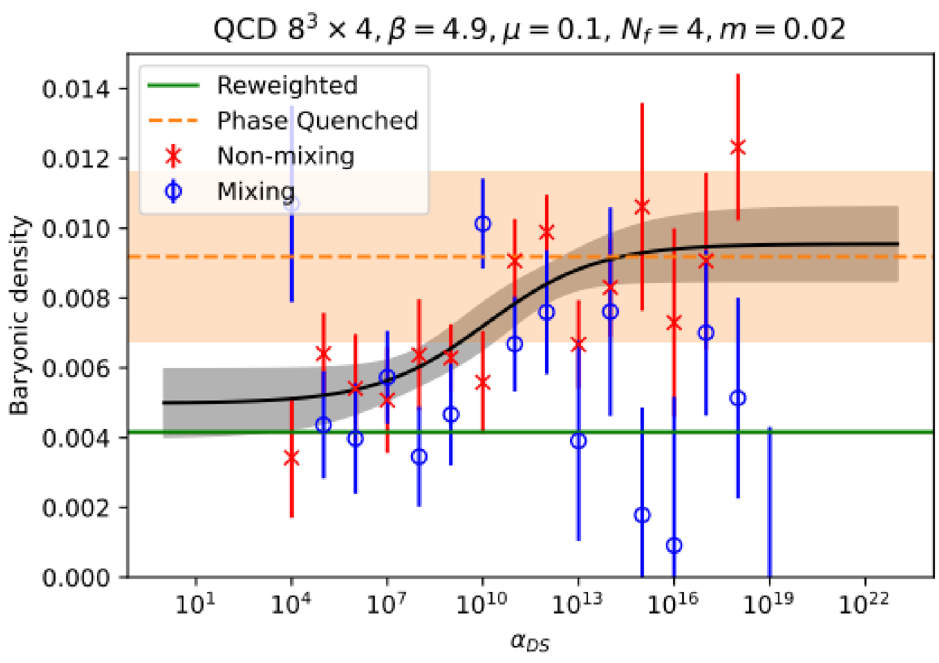
Non-mixing force has stronger effect

Strong stabilization still drives to phasequenched

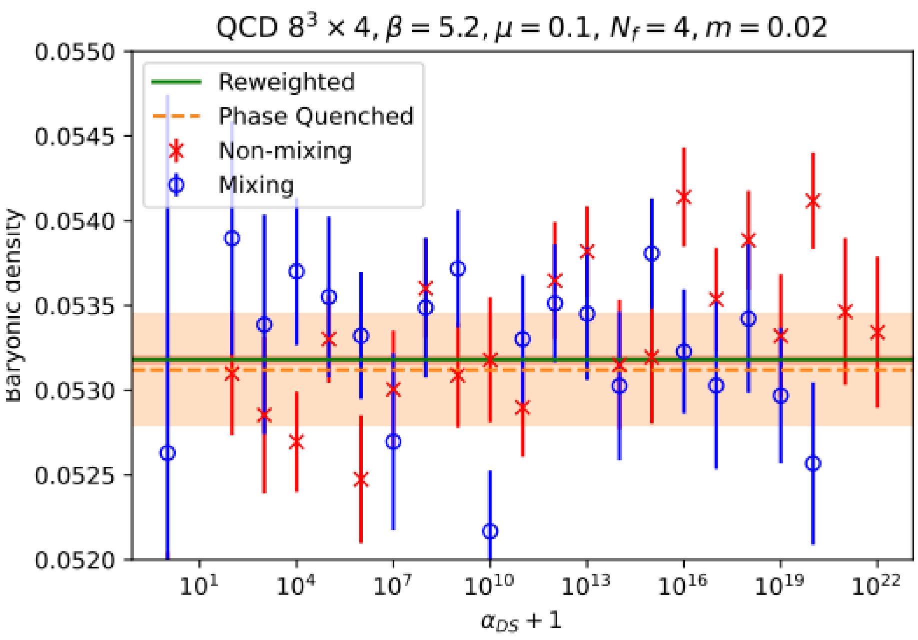
Dynamic stabilization was not really needed

Fermionic observable: density

low temperature



high temperature



low temperature: Sigmoid fit gives a reasonable extrapolation

High temperature: dynamical stabilization is not needed

Summary

Dynamical stabilization = soft cutoff in imaginary directions

Toy model: changing DS strength
Interpolate between full model and phasequenched
Sigmoid fit -- extrapolate to zero DS force

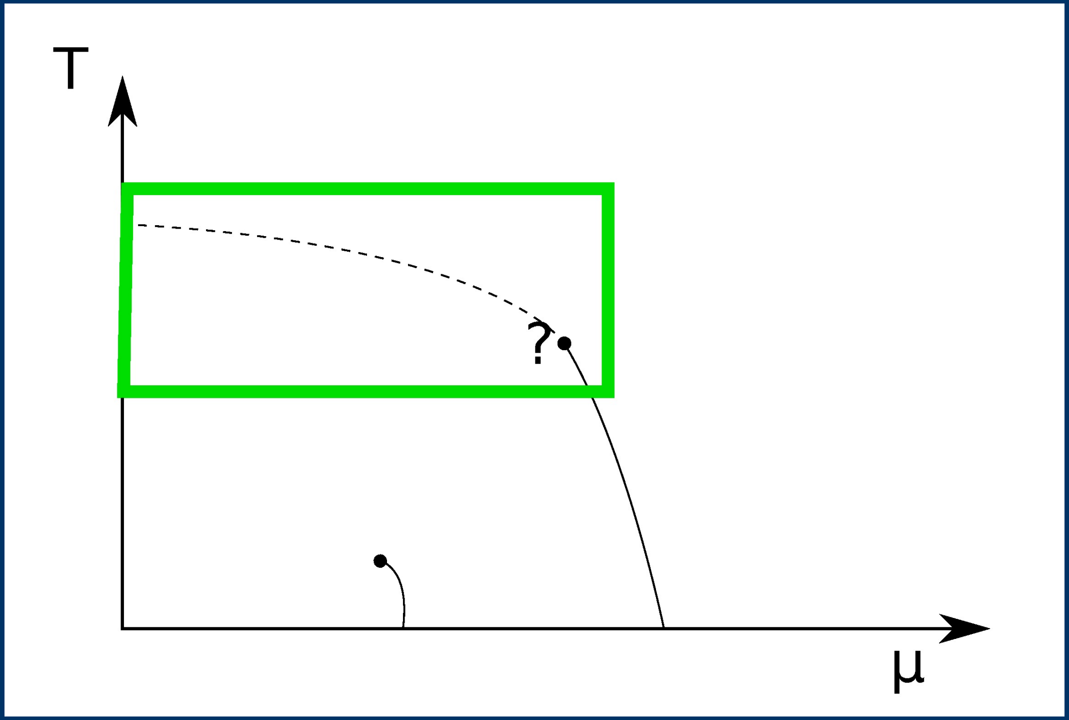
QCD test
mixing and non-mixing version
high temperature: stabilization unneeded
sigmoid fit and extrapolation works reasonably

Also: find a Kernel using Machine Learning,
Reformulate, etc.

TODO: can we get to thermodynamics at physical quark masses
and low temperatures?

Mapping out the phase transition line

[Scherzer, Sexty, Stamatescu (2020)]



Follow the phase transition line starting from $\mu = 0$

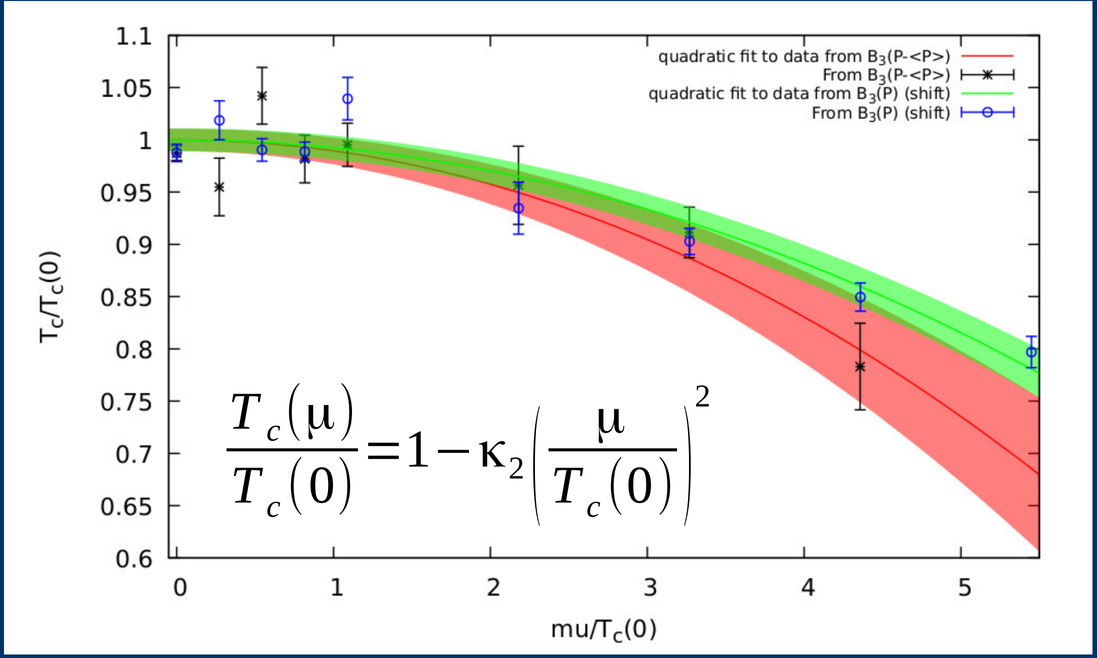
Using Wilson fermions

Fixed lattice spacing and spatial vol.
N_t scan

Lattice spacing: $a = 0.065$ fm

Pion mass: $m_\pi = 1.3$ GeV

Volumes: $8^3, 12^3, 16^3$



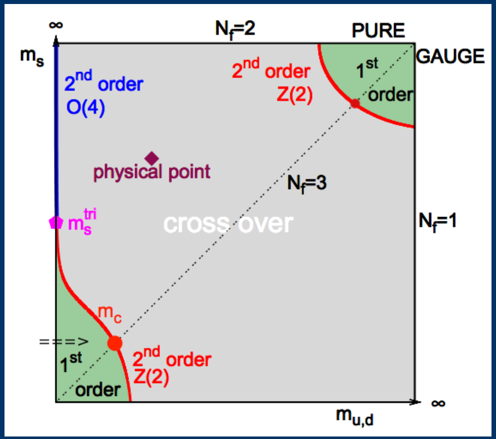
Finite size effects large

$\kappa_2 \approx 0.0012$

Consistent results

In literature
For physical pion mass
$\kappa_2 = 0.015$

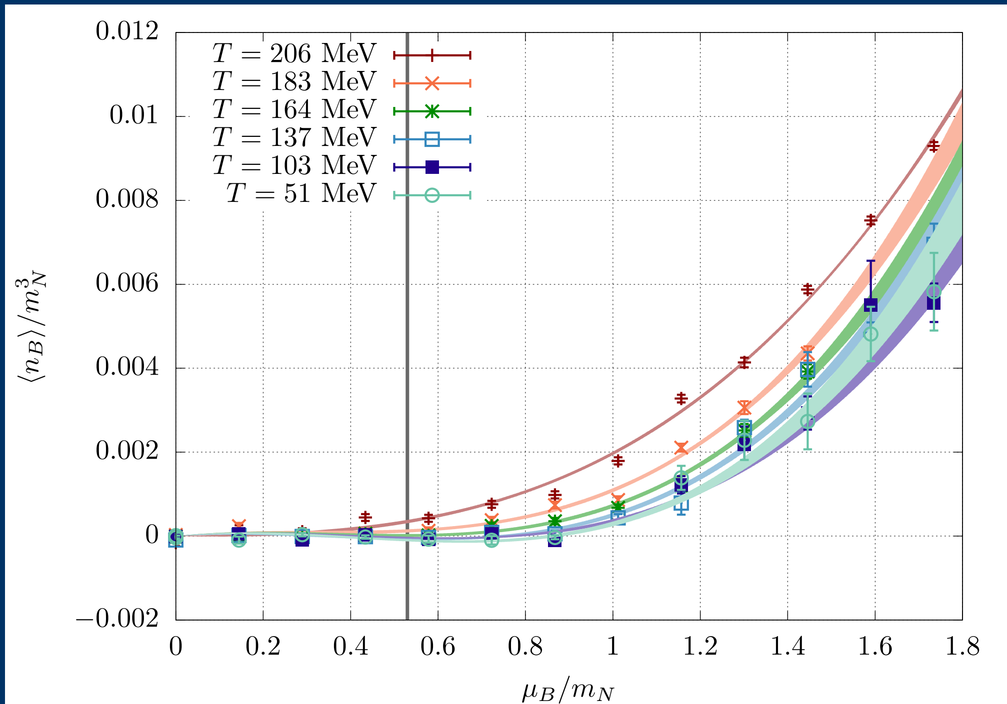
Can follow the line to
quite high μ/T



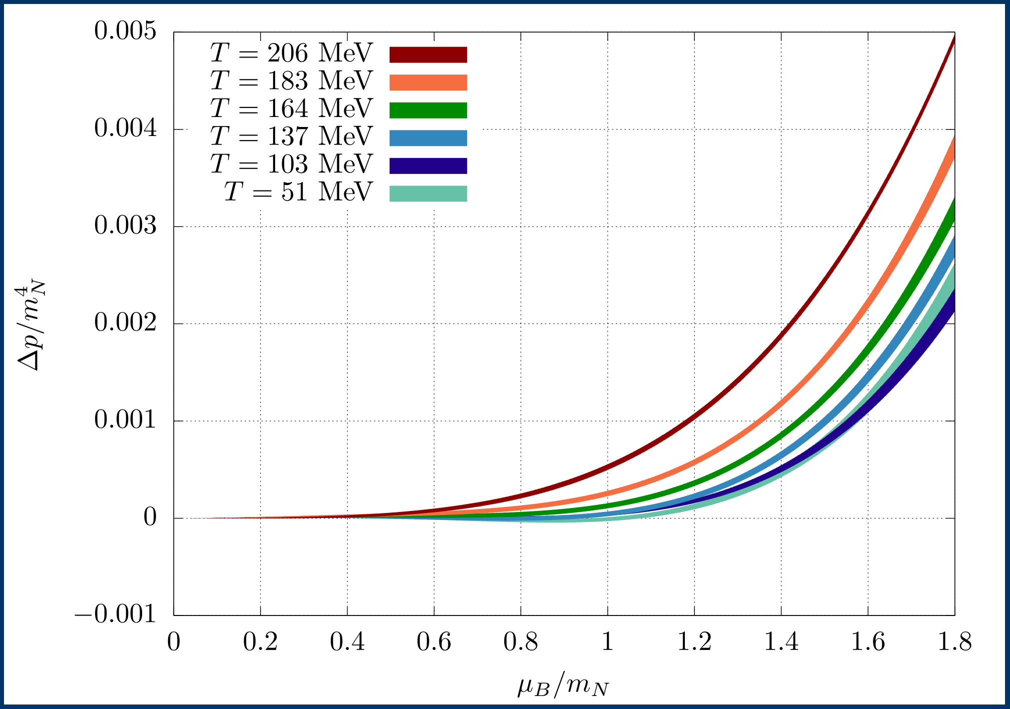
Open questions
Possible for lighter quarks?
Finite size scaling?
Where is the upper right corner of Columbia plot?
Critical point nearby?

Thermo study of QCD with DS

[Attanasio, Jaeger, Ziegler (2022)]



density



pressure

Plaquette action + Wilson fermions $m_\pi \approx 480\,\mathrm{MeV}$

Simulations also at low temperatures - using dynamical stabilization

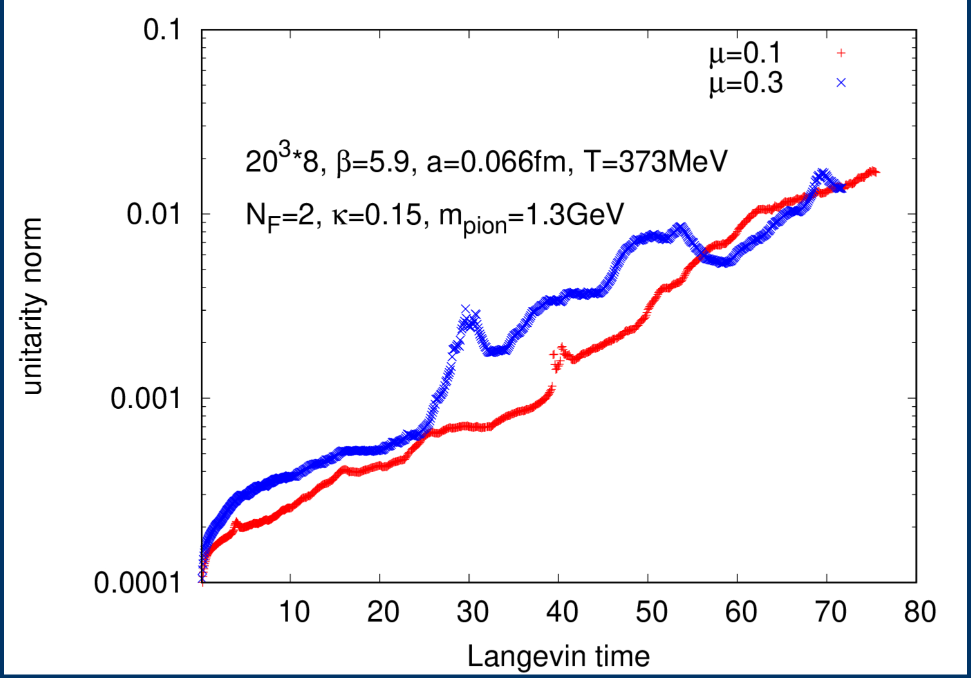
Long runs with CLE

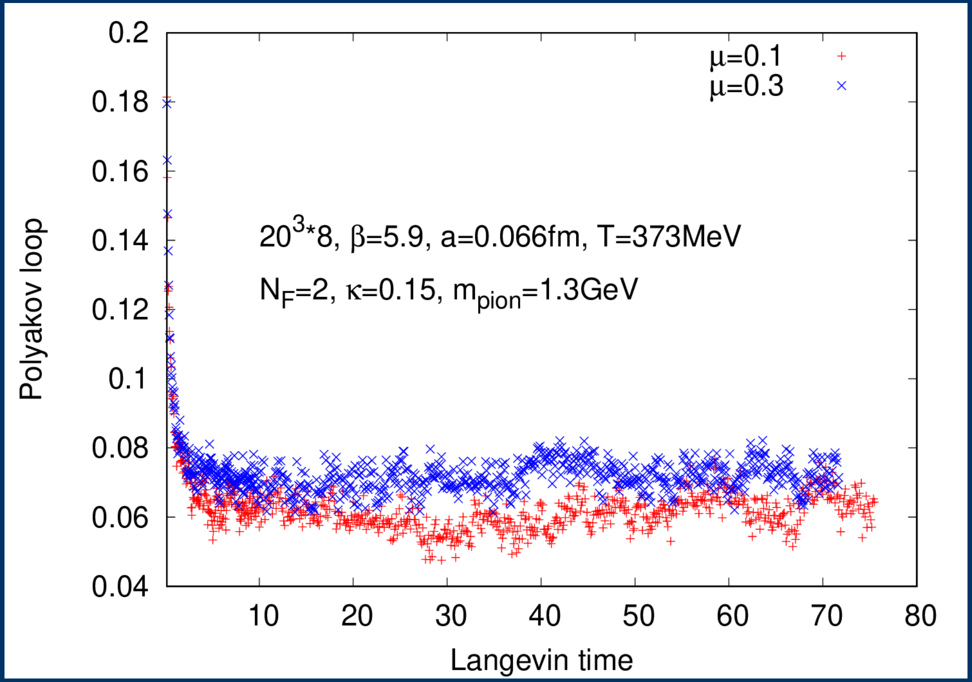
Unitarity norm has a tendency to grow slowly (even with gauge cooling)

$$UN = \sum_{x,\nu} Tr\left(U_{x\nu} U_{x\nu}^{+} - 1\right)$$

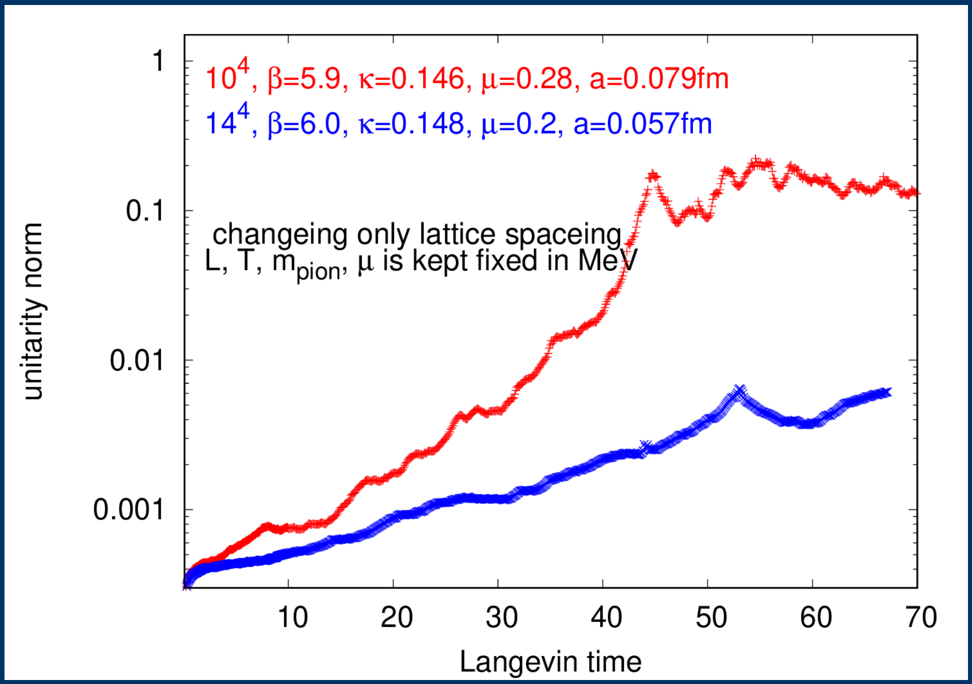
Runs are cut if it reaches ~ 0.1

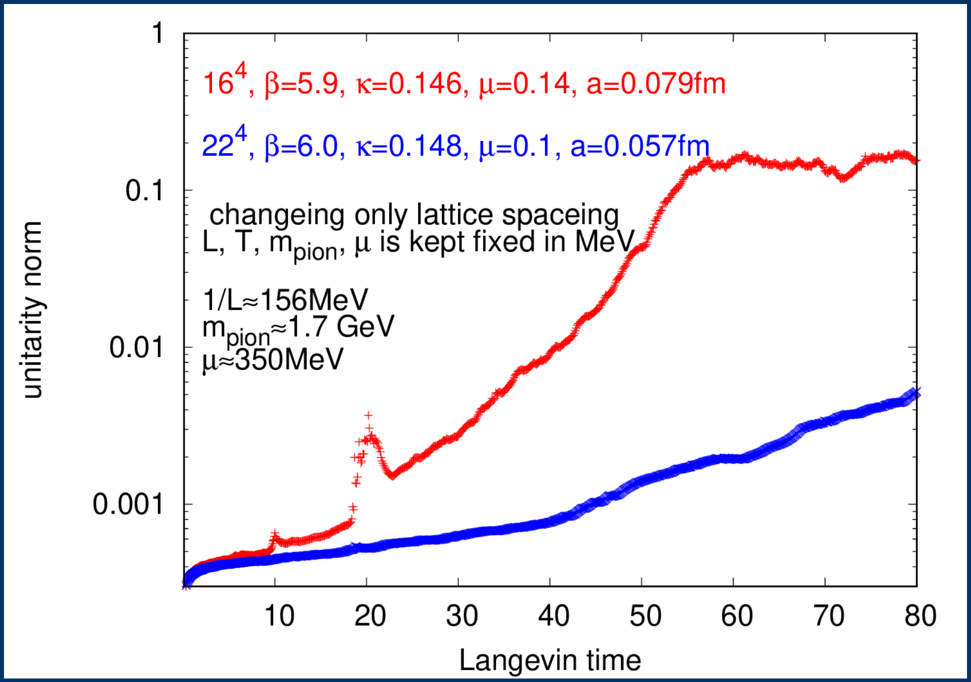
Thermalization usually fast
– might be problematic close to critical point or at low T





Getting closer to continuum limit





Test with Wilson fermions
Increase β by 0.1 – reduces lattice spacing by 30%
change everything else to stay on LCP

behavior of Unitarity norm improves
autocorrelation time decreases as lattice gets finer