Simulating full QCD at nonzero baryon density using the complex Langevin equation

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Workshop on QCD at high density
Tata Institute, Mumbai , 27th of January, 2015.

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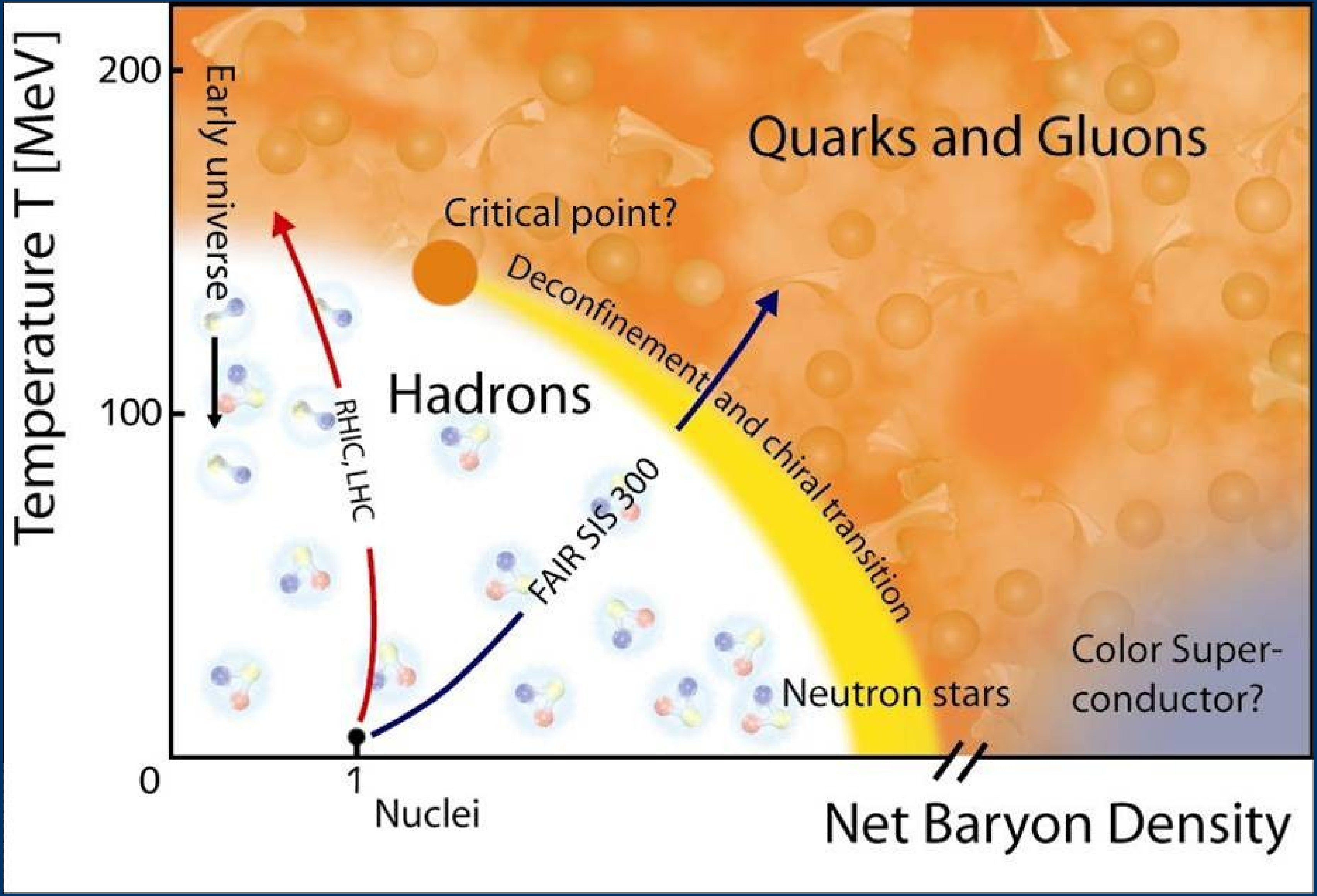
1. Sign problem in lattice QCD
2. complex Langevin equation and gauge cooling
3. phase diagram of HDQCD
4. kappa and kappa_s expansion
5. full QCD

Motivations

Phase diagram of QCD matter



QCD sign problem

Euclidean SU(3) gauge theory with fermions:

$$Z=\int DA_\mu^a D\bar{\Psi} D\Psi \exp(-S_E[A_\mu^a]-\bar{\Psi} D_E(A_\mu^a)\Psi)$$

Integrate out fermionic variables, perform lattice discretisation

$$A_\mu^a(x,\tau) \rightarrow U_\mu(x,\tau)\in SU(3) \text{ link variables}$$

$$D_E(A) \rightarrow M(U) \text{ fermion matrix}$$

$$Z=\int DU \exp(-S_E[U]) det(M(U))$$

$\det(M(U))>0 \rightarrow$ Importance sampling is possible

Non-zero chemical potential

For nonzero chemical potential, the fermion determinant is complex

$$\det(M(U,-\mu^*))=(\det(M(U),\mu))^*$$

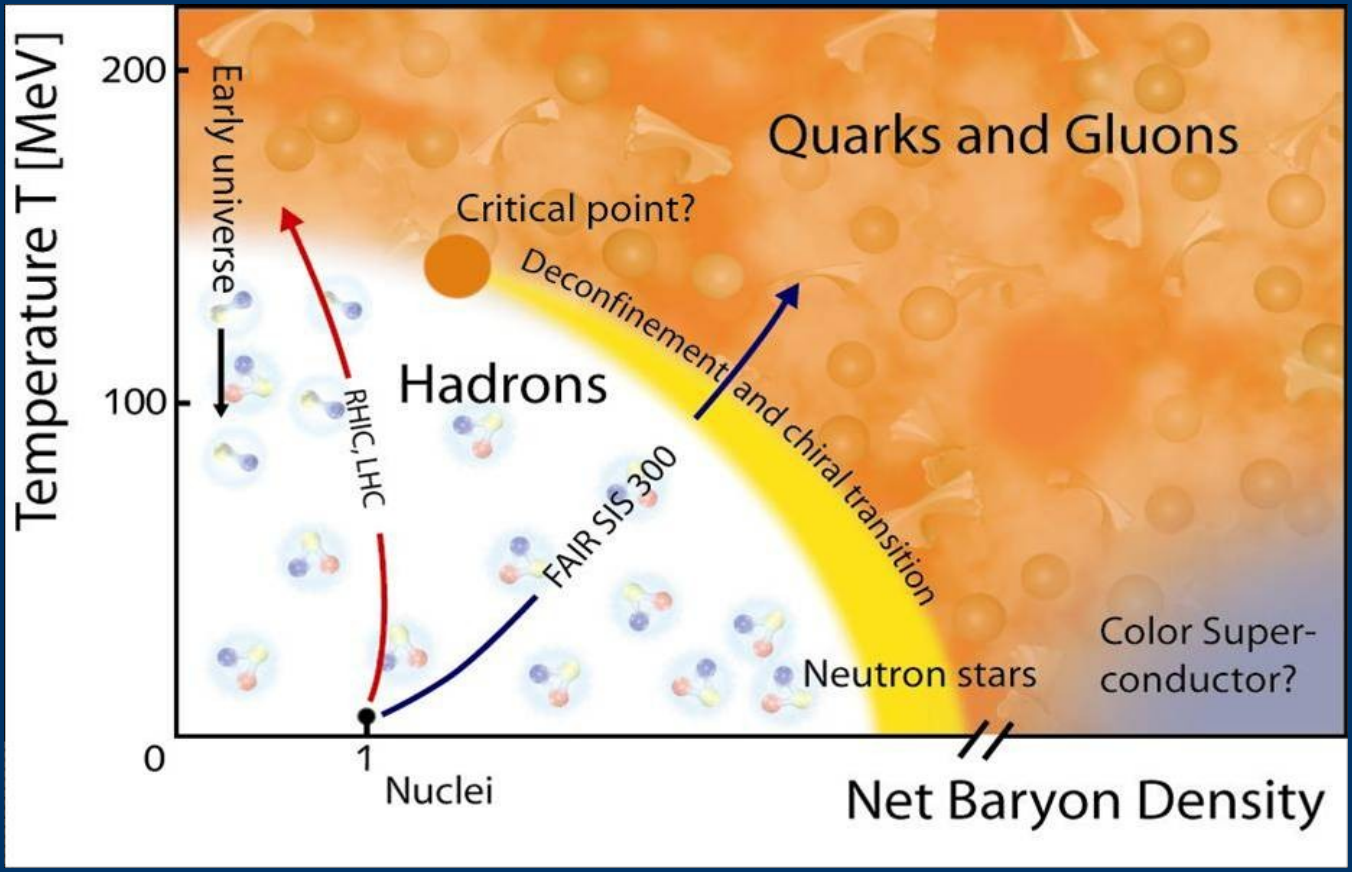
Sign problem → Naïve Monte-Carlo breaks down

QCD sign problem

$$\det(M(U,\mu)) \in \mathbb{C} \text{ for } \mu > 0$$

$$Z = \int DU \exp(-S_E[U]) det(M(U))$$

Path integral with complex weight



Only the zero density axis is directly accessible
to lattice calculations using importance sampling

Reweighting

$$\langle F \rangle_\mu = \frac{\int DU\, e^{-S_E} \det M(\mu)\, F}{\int DU\, e^{-S_E} \det M(\mu)} = \frac{\int DU\, e^{-S_E} R \dfrac{\det M(\mu)}{R} F}{\int DU\, e^{-S_E} R \dfrac{\det M(\mu)}{R}}$$

$$= \frac{\langle F \det M(\mu)/R \rangle_R}{\langle \det M(\mu)/R \rangle_R} \qquad R = \det M(\mu=0),\ |\det M(\mu)|, \text{ etc.}$$

$$\left\langle \frac{\det M(\mu)}{R} \right\rangle_R = \frac{Z(\mu)}{Z_R} = \exp\left(-\frac{V}{T} \Delta f(\mu, T) \right)$$

$\Delta f(\mu, T)$ =free energy difference

Exponentially small as the volume increases $\langle F \rangle_\mu$ → $0/0$

Reweighting works for large temperatures and small volumes

Sign problem gets hard at $\mu/T \approx 1$

Evading the QCD sign problem

Most methods going around the problem work only for $\mu = \mu_B/3 < T$

(Multi parameter) reweighting — Barbour et. al. '97; Fodor, Katz '02

Analytic continuation of results obtained at imaginary μ — Lombardo '00; de Forcrand, Philipsen '02; D'Elia Sanfilippo '09; Cea et. al. '08

Taylor expansion in $\left(\mu/T\right)^2$

de Forcrand et al. (QCD-TARO) '99; Hart, Laine, Philipsen '00;
Allton et al. '05; Gavai and Gupta '08; de Forcrand, Philipsen '08,...

Canonical Ensemble, denstity of states, curvature of critical surface, subsets, fugacity expansion, SU(2) QCD, G2 QCD, dual variables, worldlines, ...

A Direct Method: Complex Langevin

Use analiticity, expand integrals to the complex plane

Stochastic quantisation

Recent revival:	Aarts and Stamatescu '08
Bose Gas, Spin model, etc.	Aarts '08, Aarts, James '10 Aarts, James '11
Proof of convergence:	Aarts, Seiler, Stamatescu '11
QCD with heavy quarks:	Seiler, Sexty, Stamatescu '12
Kappa Expansion:	Aarts, Seiler, Sexty, Stamatescu 1408.3770
Full QCD with light quarks:	Sexty '14

Stochastic Quantization

Parisi, Wu (1981)

Given an action $S(x)$

Stochastic process for x:

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

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

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

Averages are calculated along the trajectories:

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

Fokker-Planck equation for the probability distribution of P(x):

$$\frac{\partial P}{\partial \tau} = \frac{\partial}{\partial x}\left(\frac{\partial P}{\partial x} + P \frac{\partial S}{\partial x}\right) = -H_{FP} P$$

Real action $\rightarrow$ positive eigenvalues

for real action the
Langevin method is convergent

Langevin method with complex action

Klauder '83, Parisi '83, Hueffel, Rumpf '83,
Okano, Schuelke, Zeng '91, ...
applied to nonequilibrium: Berges, Stamatescu '05, ...

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

<u>The field is complexified</u>

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

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

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

“troubled past”: Lack of theoretical understanding
Convergence to wrong results
Runaway trajectories

Proof of convergence

If there is fast decay $P(x, y) \rightarrow 0$ as $y \rightarrow \infty$

and a holomorphic action $S(x)$

then CLE converges to the correct result
[Aarts, Seiler, Stamatescu (2009)
Aarts, James, Seiler, Stamatescu (2011)]

Non-holomorphic action for nonzero density

$$S = S_W[U_\mu] + \ln \mathrm{Det}\, M(\mu)$$

measure has zeros $(Det\ M = 0)$
complex logarithm has a branch cut
$\longrightarrow$ meromorphic drift
Is it a problem for QCD?

[see also: Mollgaard, Splittorff (2013), Greensite(2014)]

[QCD and poles: Aarts, Seiler, Sexty, Stamatescu 2014]

Non-real action problems and CLE (besides nonzero density)

1. Real-time physics

   "Hardest" sign problem e^{iS_M}

[Berges, Stamatescu (2005)]
[Berges, Borsanyi, Sexty, Stamatescu (2007)]
[Berges, Sexty (2008)]

Studies on Oscillator, pure gauge theory

2. Theta-Term $S = F_{\mu\nu} F^{\mu\nu} + i\Theta \epsilon^{\mu\nu\theta\rho} F_{\mu\nu} F_{\theta\rho}$

[Bongiovanni, Aarts, Seiler, Sexty, Stamatescu (2013)+in prep.]

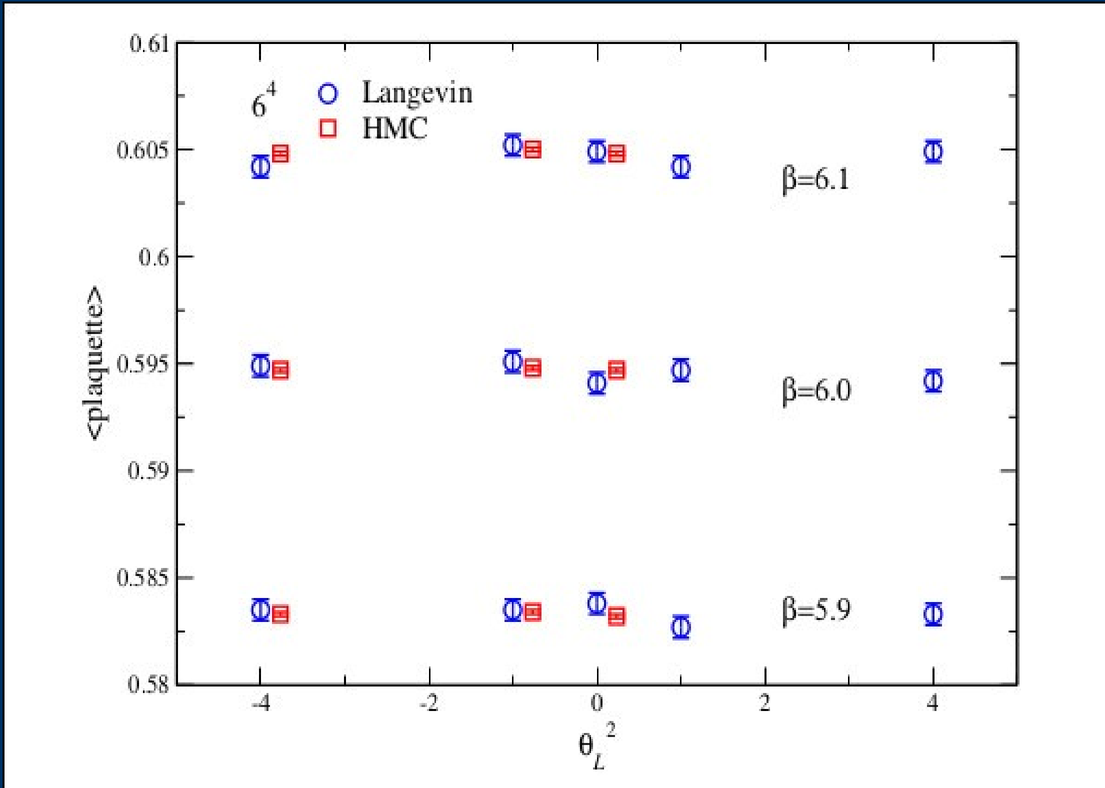
Θ real → complex action, $\langle Q \rangle$ imaginary

Θ imaginary → real action, $\langle Q \rangle$ real

On the lattice

$$Q = \epsilon^{\mu\nu\theta\rho} F_{\mu\nu} F_{\theta\rho} \rightarrow \sum_x q(x)$$

Not topological
Cooling is needed
Θ_L bare parameter needs renormalisation



Θ imaginary → use real Langevin or HMC

Θ real → use complex Langevin

Gaussian Example

$$S[x]=\sigma x^2+i\lambda x$$

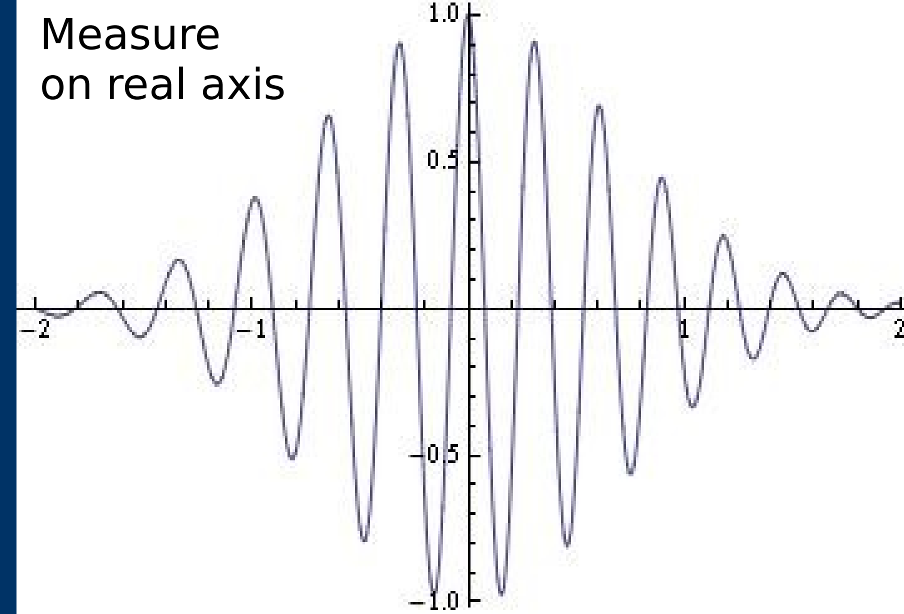
CLE

$$\frac{d}{d\tau}(x+iy)=-2\sigma(x+iy)-i\lambda+\eta$$

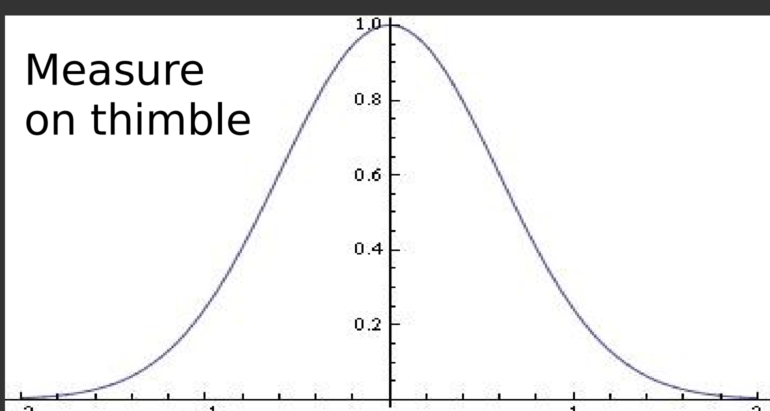
$$P(x,y)=e^{-a(x-x_0)^2-b(y-y_0)^2-c(x-x_0)(y-y_0)}$$

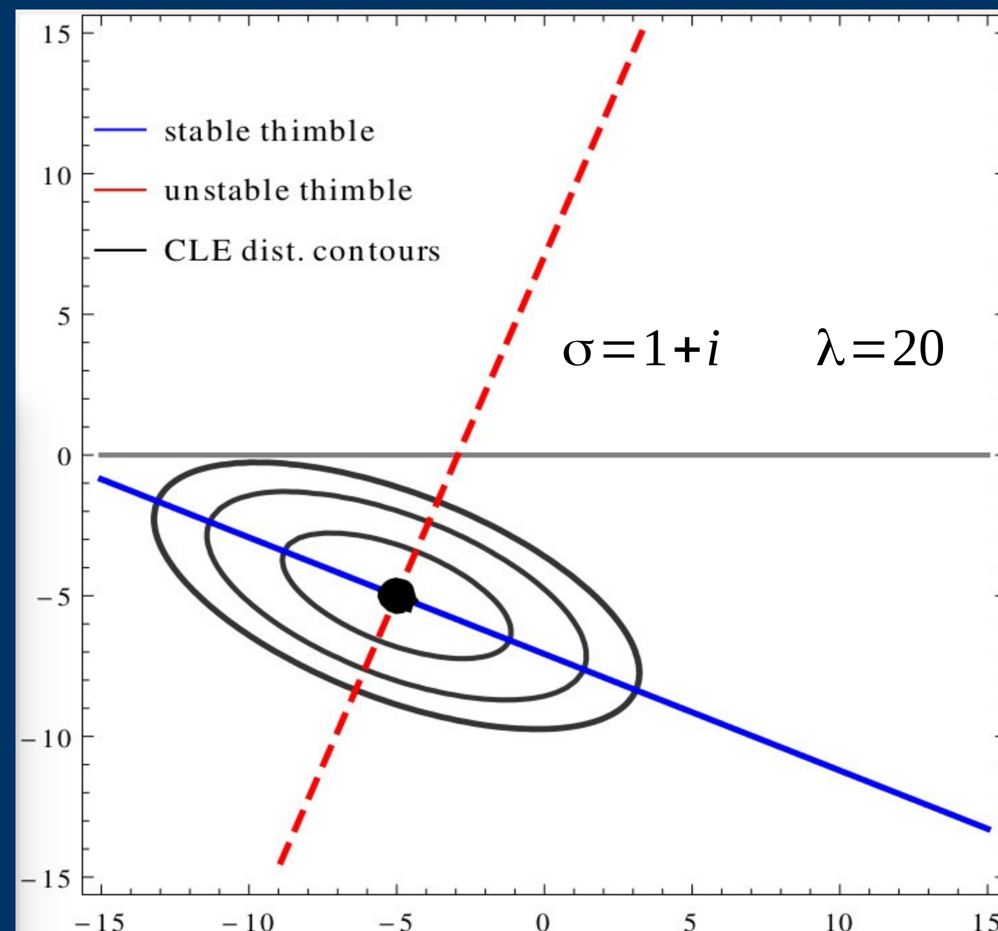
Gaussian distribution around critical point

$$\left.\frac{\partial S(z)}{\partial z}\right|_{z_0}=0$$



Thimble $\dot{z}=-\overline{\partial_z S(z)}$ Straight lines starting from z_0





Stochastic quantisation on the group manifold

Updating must respect the group structure:

$$\langle \eta_{ia} \rangle = 0$$

$$U'_i = \exp\left(i\lambda_a\left(-\epsilon D_{i,a} S[U] + \sqrt{\epsilon}\,\eta_{i,a}\right)\right) U_i$$

$$\langle \eta_{ia} \eta_{jb} \rangle = 2\,\delta_{ij}\,\delta_{ab}$$

Left derivative: $D_a f(U) = \left(\frac{\partial}{\partial \alpha} f\left(e^{i\lambda_a \alpha} U\right) \right)\Big|_{\alpha=0}$

λ_a Gellmann matrices

complexified link variables

SU(N) → SL(N,C) $det(U) = 1, \quad U^{+} \neq U^{-1}$

compact → non-compact

Distance from SU(N) $\sum_{ij} \left| \left(U U^{+} - 1 \right)_{ij} \right|^2$

Unitarity Norms: $Tr\left(U U^{+} \right) \geq N$

$$Tr\left(U U^{+} \right) + Tr\left(U^{-1} \left(U^{-1} \right)^{+} \right) \geq 2N$$

For SU(2): $\left(Im \;\; Tr\, U \right)^2$

Gauge theories and CLE

link variables: SU(N) → SL(N,C)

compact → non-compact

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

Gauge degrees of freedom also complexify

→ Infinite volume of irrelevant, unphysical configurations

Process leaves the SU(N) manifold exponentially fast already at $\mu \ll 1$

Unitarity norm: $\sum_i Tr(U_i U_i^{+})$

Distance from SU(N) $\sum_{ij} \left| (U U^{+} - 1)_{ij} \right|^2$

$$Tr(U U^{+}) + Tr(U^{-1}(U^{-1})^{+}) \geq 2N$$

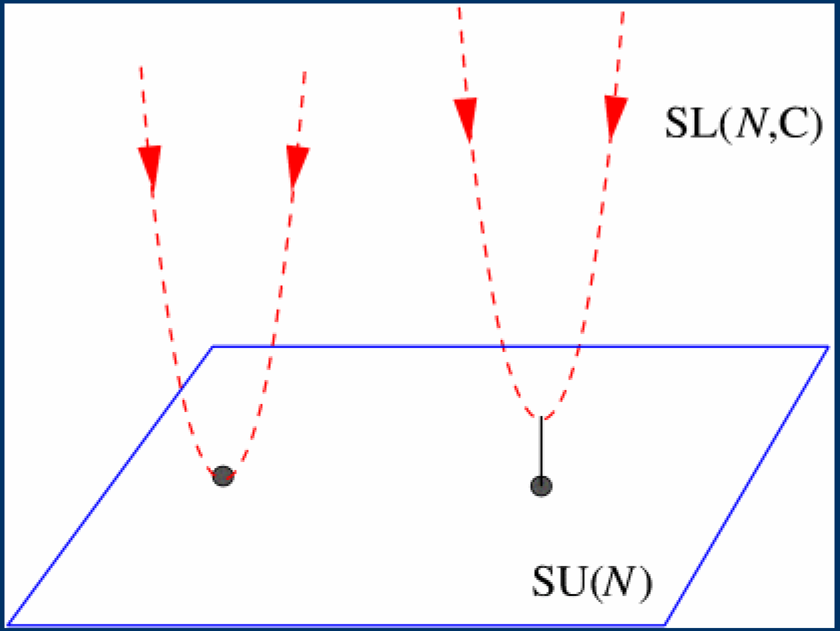
Gauge transformation at x changes 2d link variables

$$U_\mu(x) \to \exp(-\alpha \epsilon \lambda_a G_a(x)) U_\mu(x)$$

$$U_\mu(x-a_\mu) \to U_\mu(x-a_\mu) \exp(\alpha \epsilon \lambda_a G_a(x))$$

Dynamical steps are interspersed with several gauge cooling steps

The strength of the cooling is determined by
- cooling steps
- gauge cooling parameter α



Empirical observation:
Cooling is effective for $\beta > \beta_{min}$, $a < a_{max}$

but remember, $\beta \to \infty$ in cont. limit

Heavy Quark QCD at nonzero chemical potential (HDQCD)

Hopping parameter expansion of the fermion determinant
Spatial hoppings are dropped

$$\mathrm{Det}\, M(\mu) = \prod_x \det(1 + C\, P_x)^2 \det(1 + C'\, P_x^{-1})^2$$

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

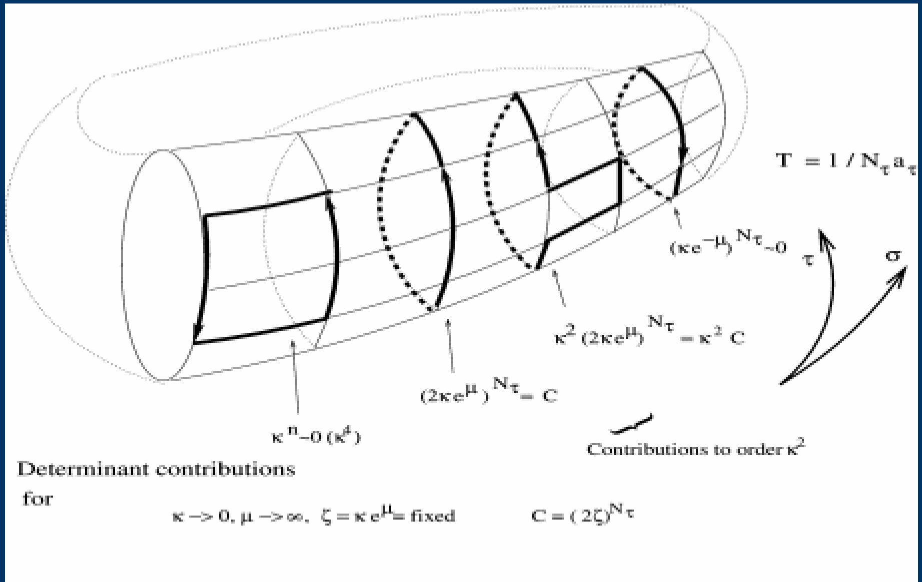
$$S = S_W[U_\mu] + \ln \mathrm{Det}\, M(\mu)$$

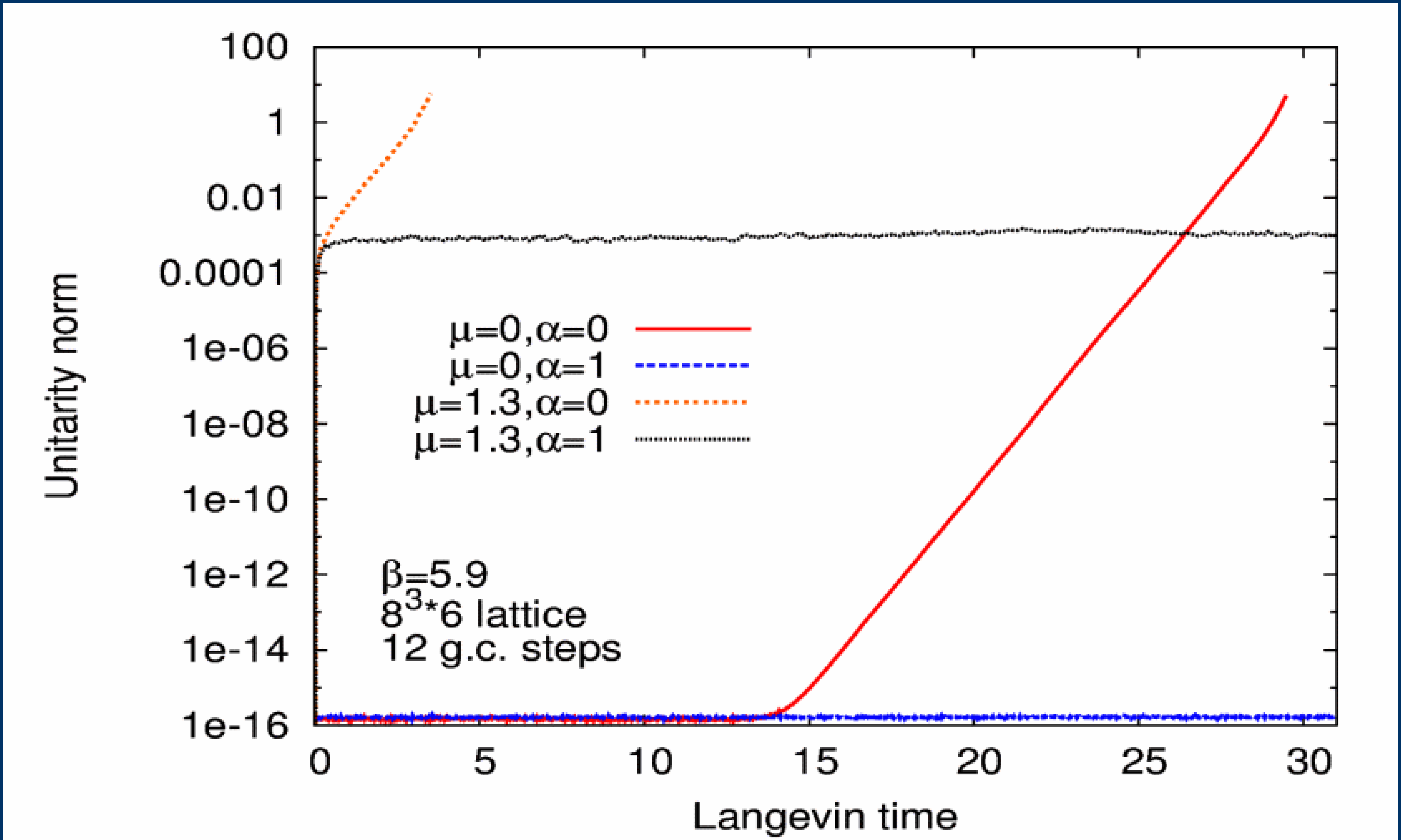
Studied with reweighting De Pietri, Feo, Seiler, Stamatescu '07

$$R = e^{\sum_x C\, \mathrm{Tr}\, P_x + C'\, \mathrm{Tr}\, P^{-1}}$$

CLE study using gaugecooling

[Seiler, Sexty, Stamatescu (2012)]





Gauge cooling stabilizes the distribution

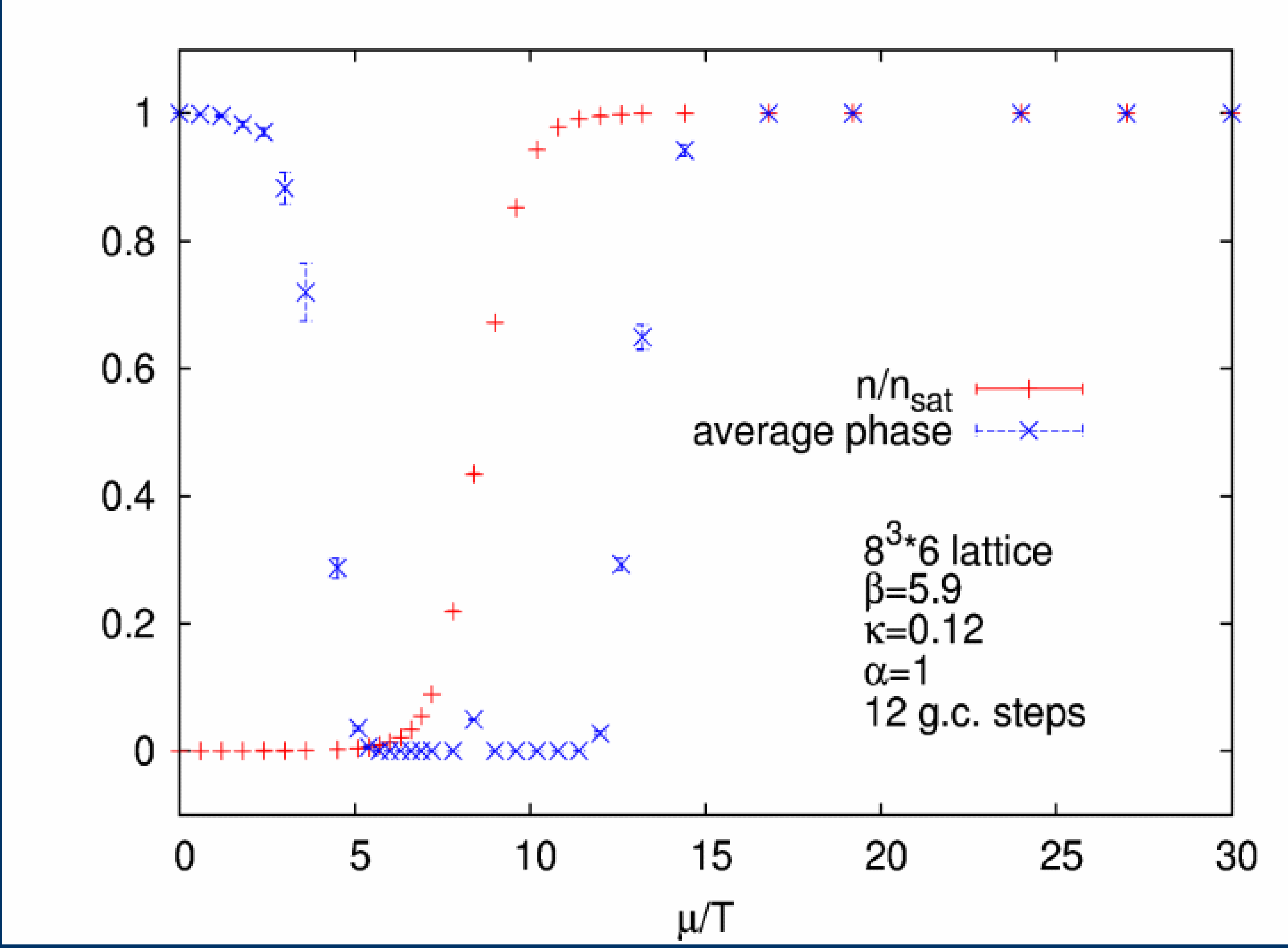
SU(3) manifold instable even at $\mu = 0$

Fermion density:

$$n = \frac{1}{N_\tau} \frac{\partial \ln Z}{\partial \mu}$$

average phase:

$$\langle \exp(2 i \varphi) \rangle = \left\langle \frac{\mathrm{Det}\, M(\mu)}{\mathrm{Det}\, M(-\mu)} \right\rangle$$

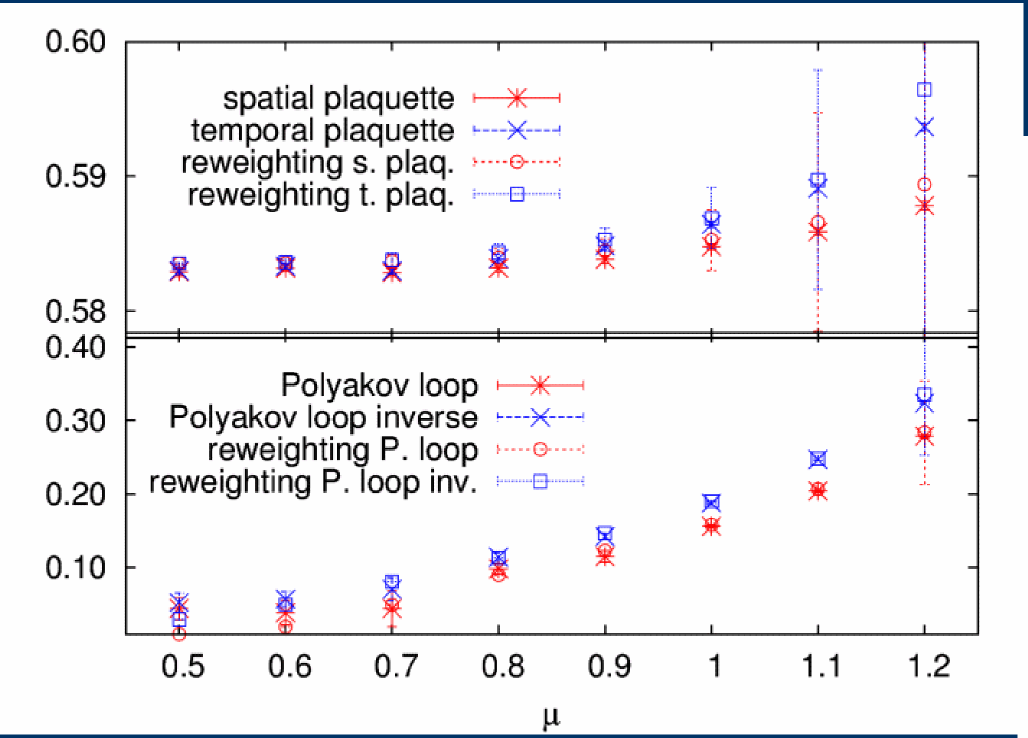


$$\det(1 + C P) = 1 + C^3 + C\, \mathrm{Tr}\, P + C^2\, \mathrm{Tr}\, P^{-1}$$

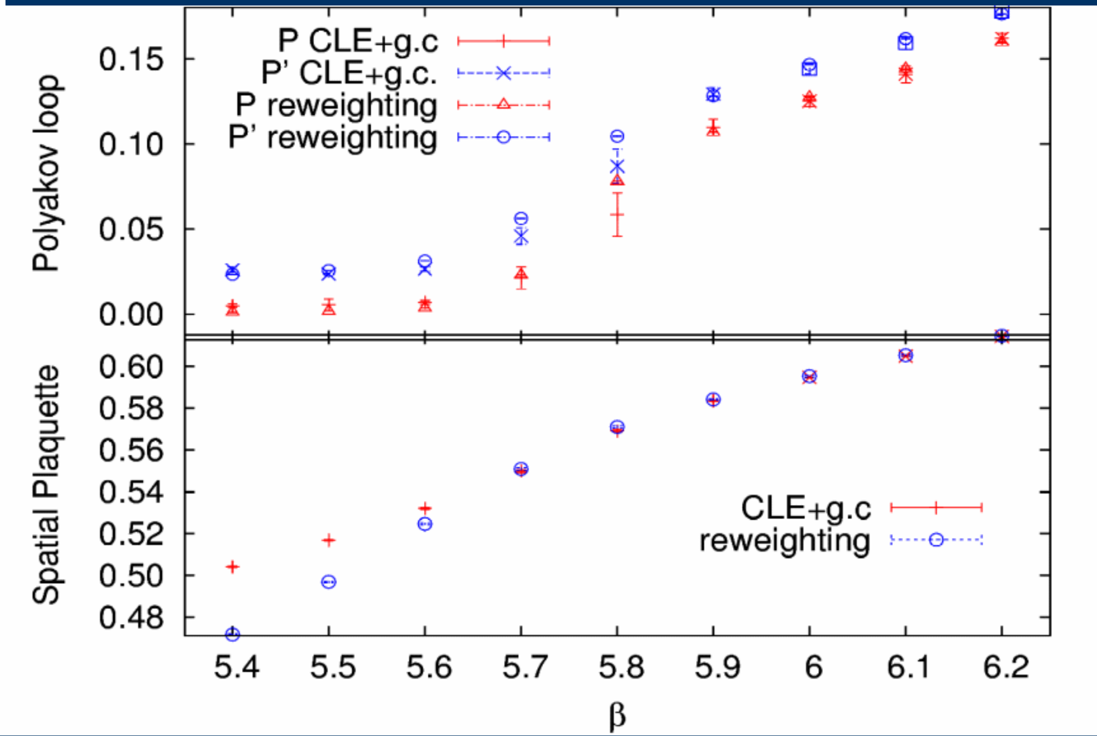
Sign problem is absent at small or large μ

Reweigthing is impossible at $6 \le \mu / T \le 12$, CLE works all the way to saturation

Comparison to reweighting



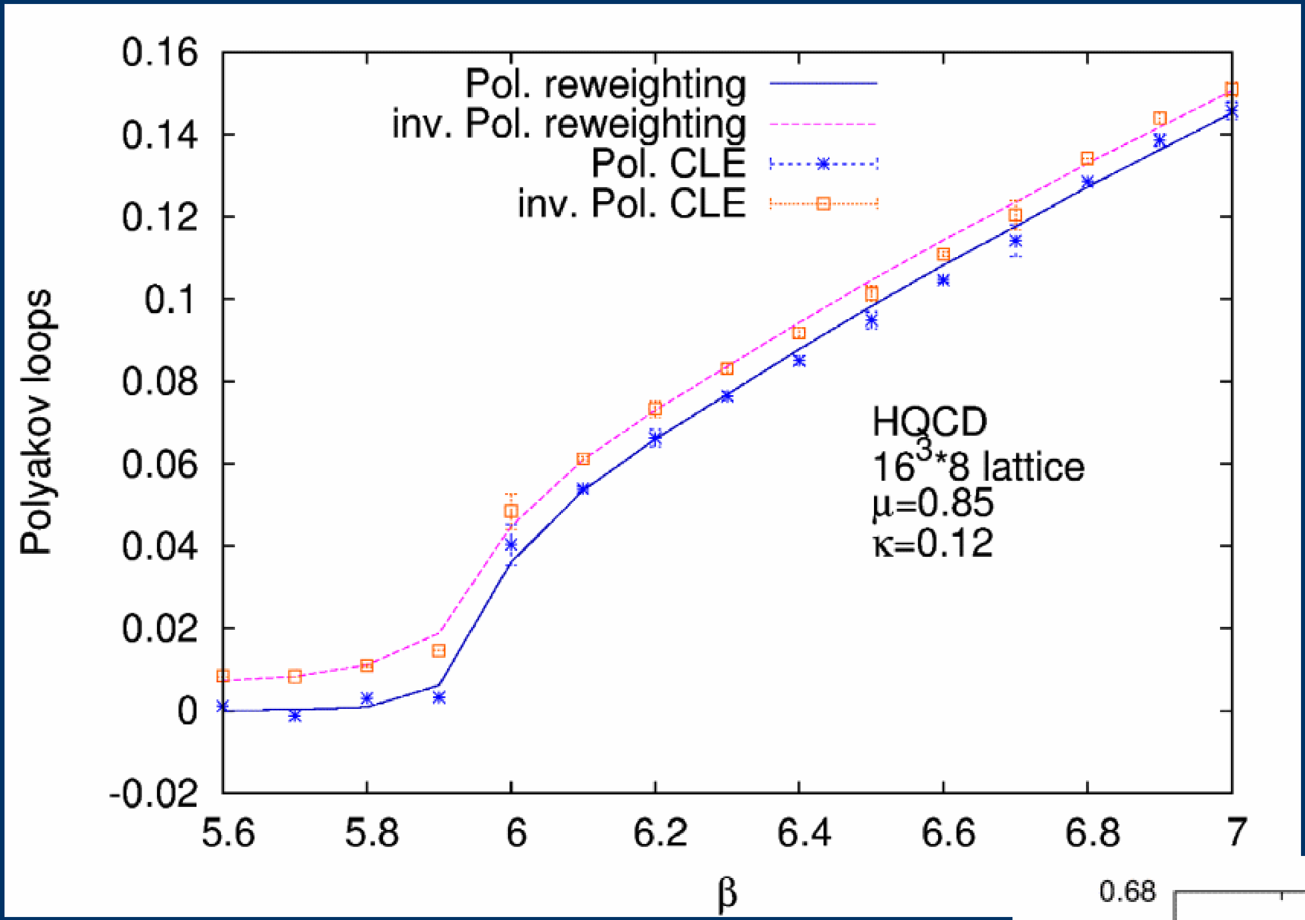
6^4 lattice, $\beta = 5.9$

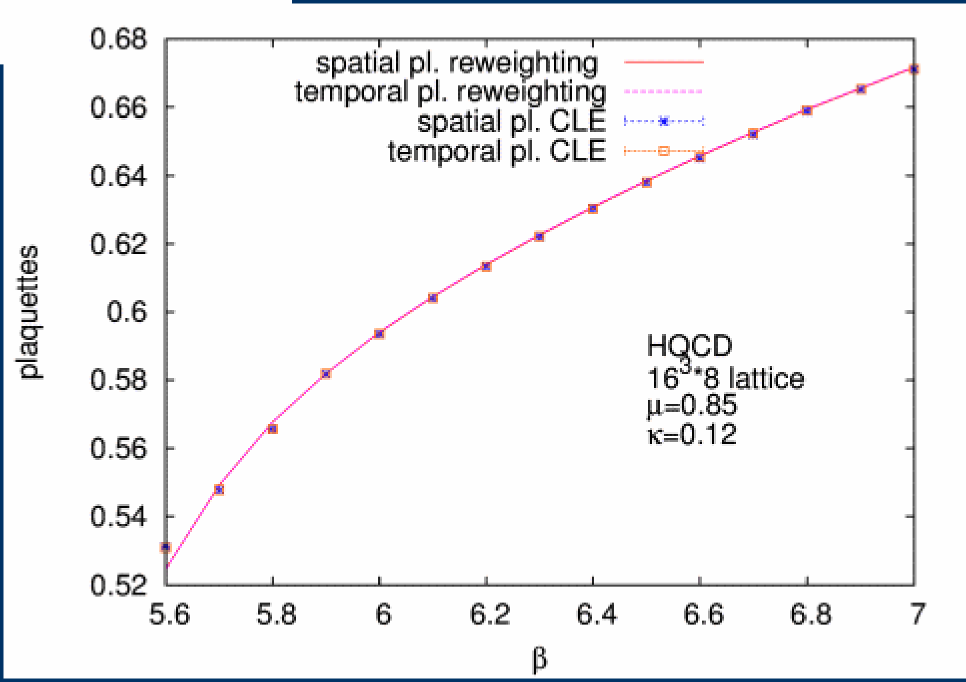


6^4 lattice, $\mu = 0.85$

Discrepancy of plaquettes at $\beta \leq 5.6$
a skirted distribution develops

$$a(\beta = 5.6) = 0.2\,\mathrm{fm}$$



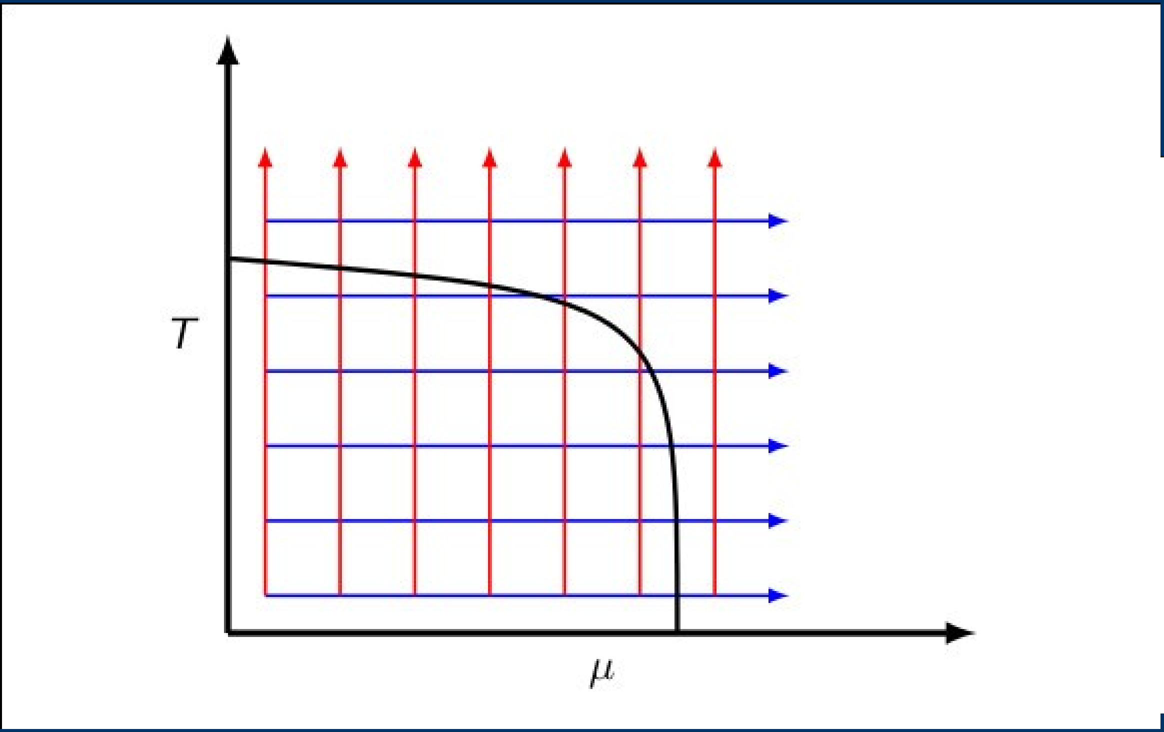


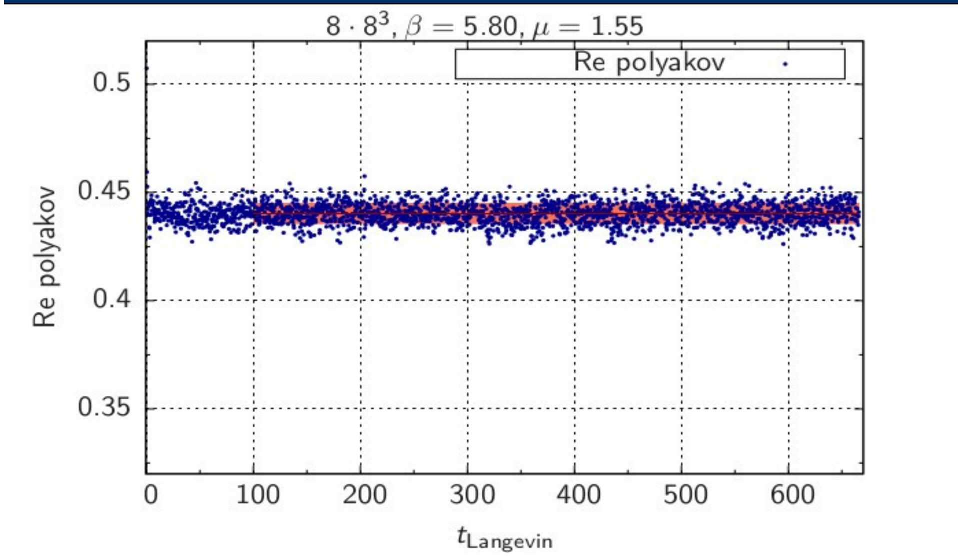
Large lattice:
phase transition clearly visible

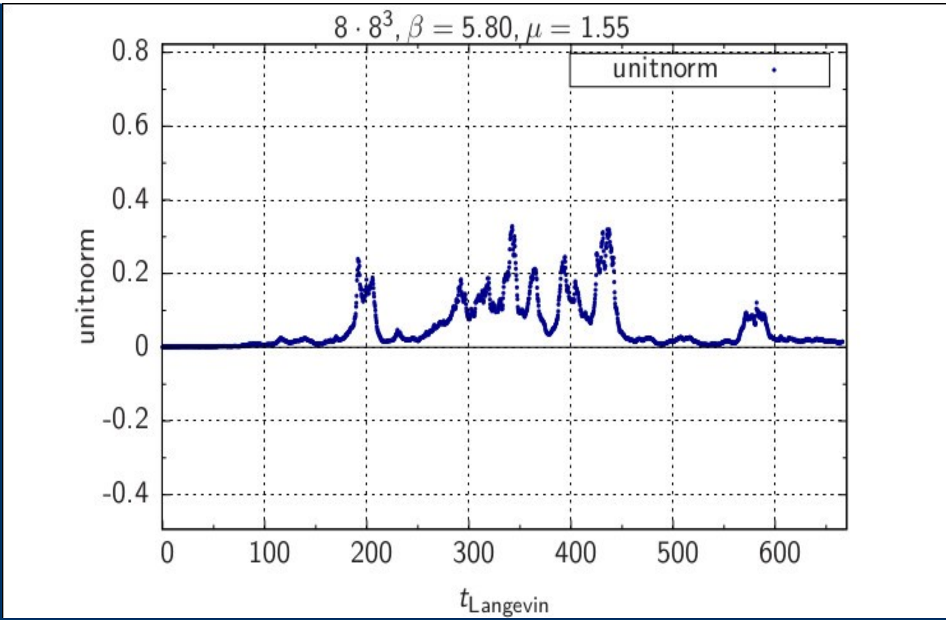
for $\beta > \beta_{min}$

Mapping the phase diagram

[Aarts, Attanasio, Jäger, Seiler, Sexty, Stamatescu, in prep.]







fixed $\beta = 5.8 \rightarrow a \approx 0.15\,\text{fm}$

$\kappa = 0.12$

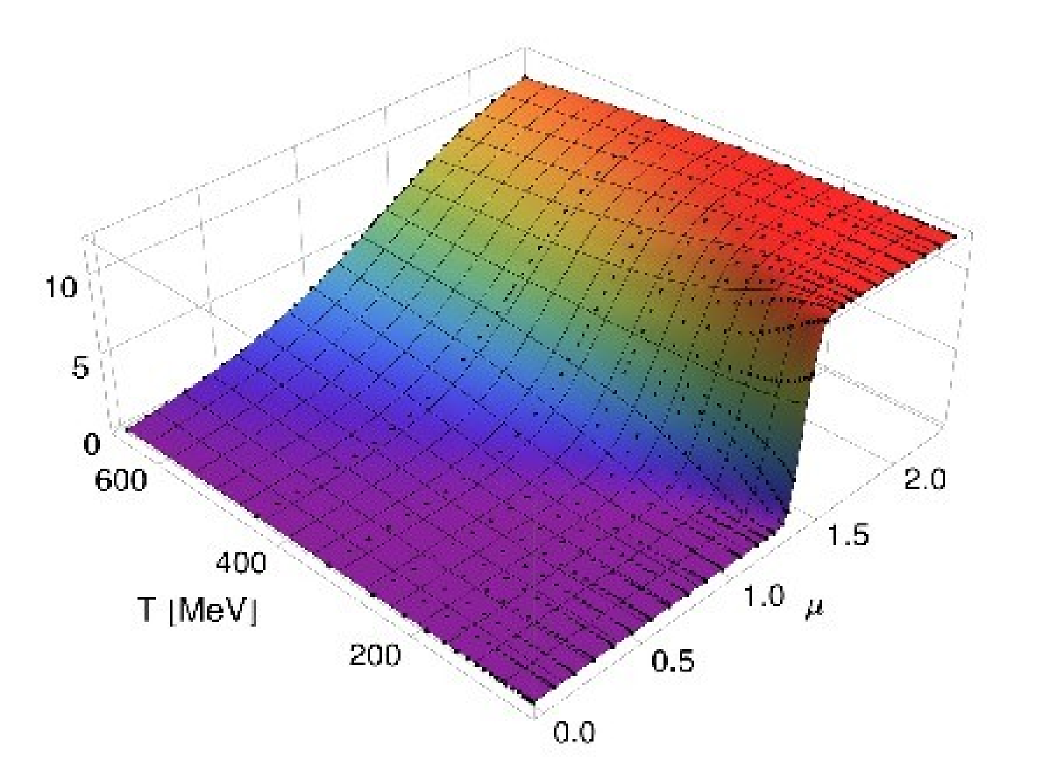
onset transition at $\mu = -\ln(2\kappa) = 1.43$

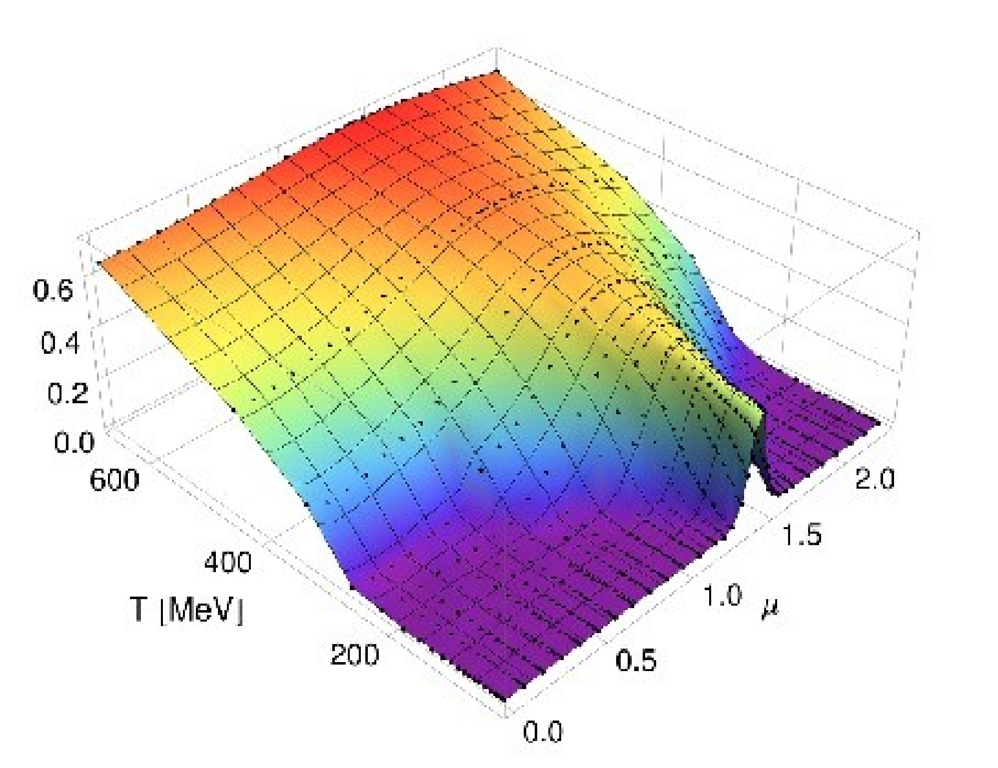
$N_t * 8^3$ lattice

$N_t = 2..28$

Temperature scanning

Exploring the phase diagram of HDQCD



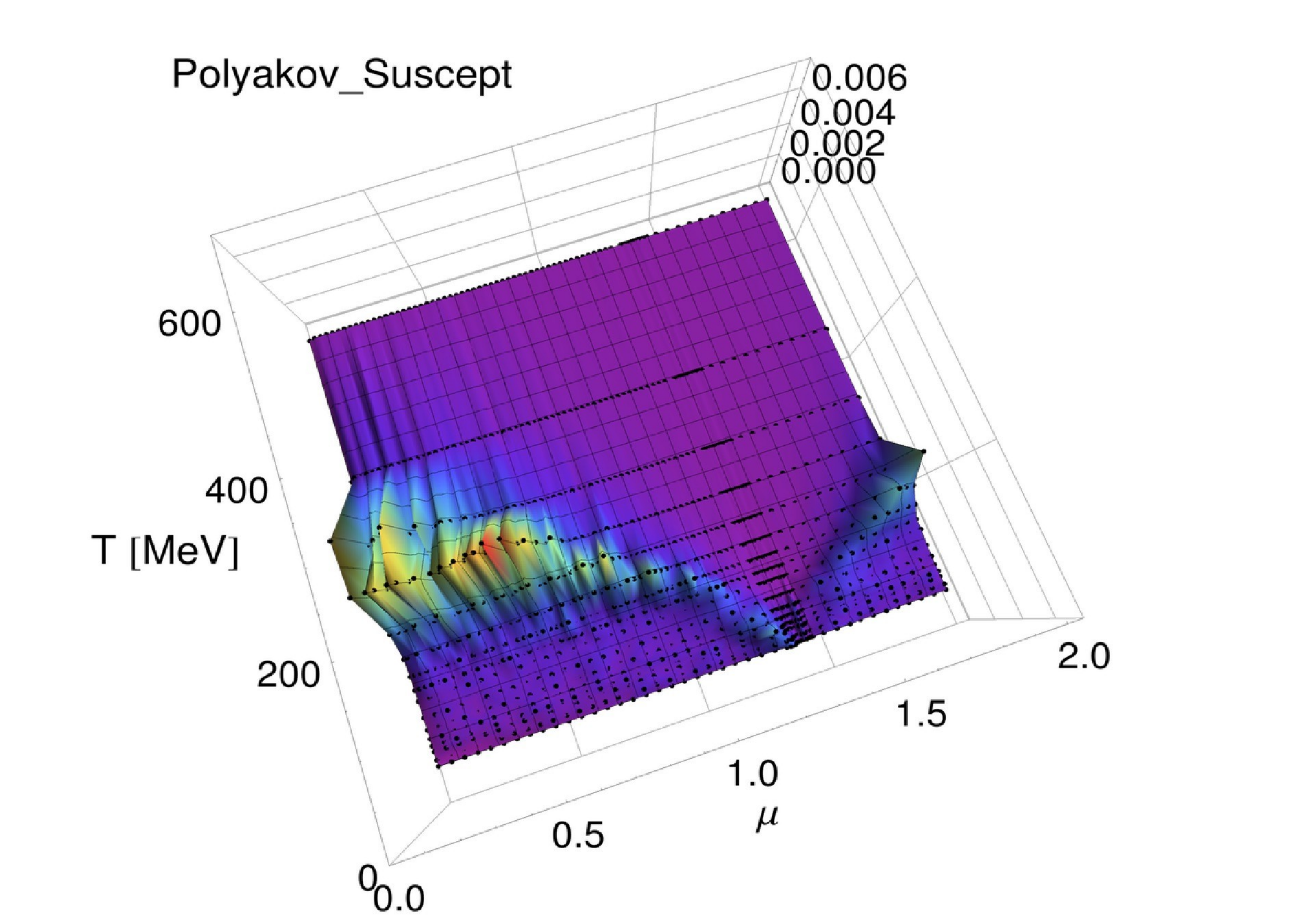


Onset in fermionic density
Silver blaze phenomenon

Polyakov loop
Transition to deconfined state

$\beta = 5.8 \quad \kappa = 0.12 \quad N_f = 2 \quad N_t = 2 \ldots 24$

Polyakov loop susceptibility



Hint of first order deconfinement and first order onset transition

κ Expansion using the loop expansion

$$M = 1 - \kappa Q = 1 - R - \kappa_s S$$ Wilson fermions

$$S = \sum_i 2\Gamma_i^- U_i(x)\delta_{y,x+i} + 2\Gamma_i^+ U_i^{-1}(y)\delta_{y,x-i}$$ Spatial hoppings

$$R = 2\kappa e^{\mu}\Gamma_4^- U_4(x)\delta_{y,x+4} + 2\kappa e^{-\mu}\Gamma_4^+ U_4^{-1}(y)\delta_{y,x-4}$$ Temporal hoppings

$$\mathrm{Det}\, M = \exp(\mathrm{Tr}\ln M) = \exp\left(-\mathrm{Tr}\sum \frac{\kappa^n}{n} Q^n\right) = \exp\left(-\mathrm{Tr}\sum_C \frac{\kappa^{ls}}{s} L_c^s\right)$$

sum for distinct paths

$$= \prod_C \det(1 - \kappa^l L_c)$$

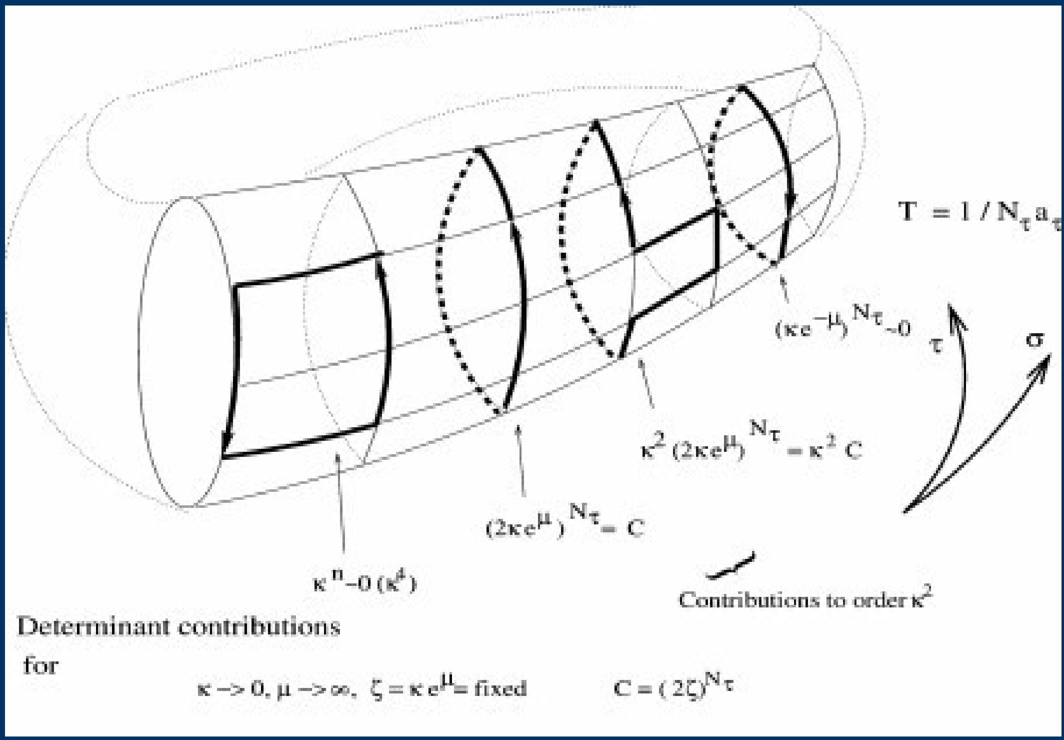
Static limit

$$\kappa \to 0,\ \mu \to \infty,\ \zeta = 2\kappa e^{\mu} = \mathrm{const}$$

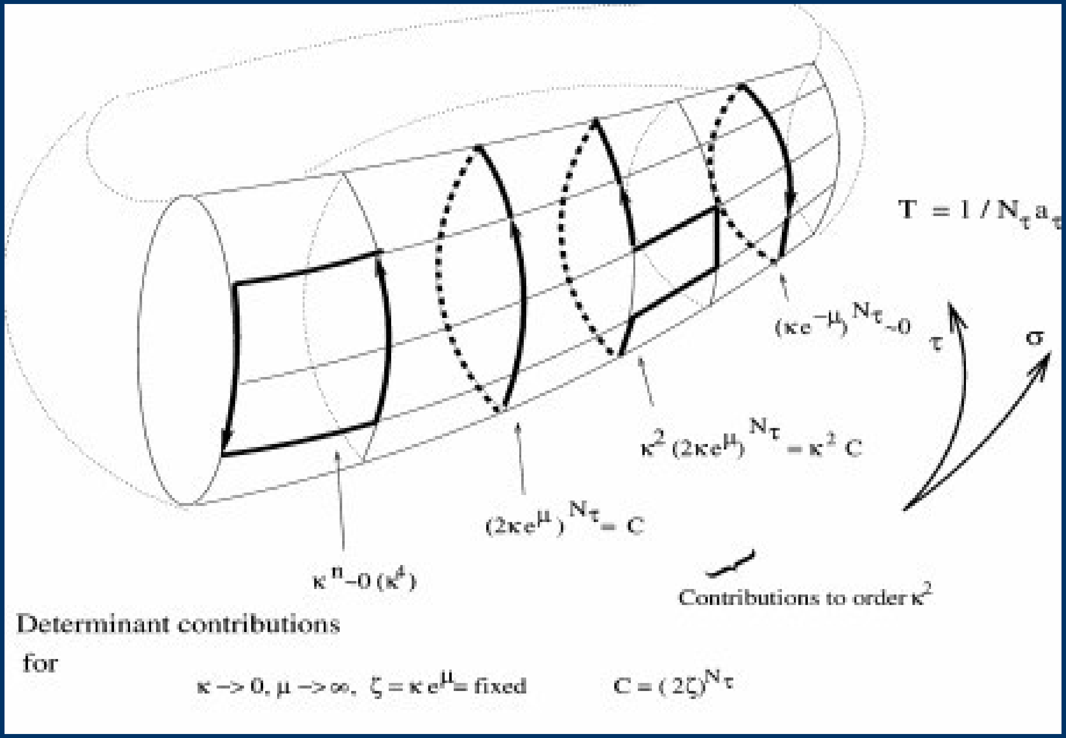
Only Polyakov loops contribute

Wilson fermions

$$\Gamma_\nu^+ \Gamma_\nu^- = 0$$ → no backtracking



Caculation of the first few orders
Is possible using loop expansion



with full gauge action

[Bender et al. (1992)]
[Aarts et al. (2002)]
[De Pietri, Feo, Seiler, Stamatescu (2007)]

κ^2 corrections

with strong coupling expansion

[Fromm, Langelage, Lottini, Philipsen (2012)]
[Greensite, Myers, Splittorff (2013)]
[Langelage, Neuman, Philipsen (2014)]

κ^4 corrections

expansions with complex Langevin

[Aarts, Seiler, Sexty, Stamatescu 1408.3770]

κ expansion

$$M = 1 - \kappa Q = 1 - R - \kappa_s S$$

$$\mathrm{Det}\, M = \exp(\mathrm{Tr} \ln M) = \exp\left(-\mathrm{Tr} \sum \frac{\kappa^n}{n} Q^n \right)$$

Contribution to Drift term: $K_{\mu,x,a} = \mathrm{Tr}\left(\sum \kappa^n Q^{n-1} D_{\mu,x,a} Q \right)$

noise vector η $\quad K_{\mu,x,a} = \eta^* D_{\mu,x,a} Q s \quad$ with $s = -\sum \kappa^n Q^{n-1} \eta$

κ_s expansion

$$\mathrm{Det}\, M = \mathrm{Det}(1-R)\, \mathrm{Det}\left| 1 - \frac{\kappa_s S}{1-R} \right| = \mathrm{Det}(1-R) \exp\left| -\mathrm{Tr} \sum \frac{\kappa_s^n}{n} \frac{S^n}{(1-R)^n} \right|$$

Contribution to Drift term:

using noise vector

analitically (same as LO HDQCD)

κ expansion

$$\mathrm{Det}\, M = \exp\left(\mathrm{Tr} \ln M\right) = \exp\left(-\mathrm{Tr} \sum \frac{\kappa^n}{n} Q^n\right)$$

No poles!

Numerical cost: N multiplications with Q

$Q = R + \kappa S$ with $R^+ \propto e^{\mu}$ → bad convergence at high μ

κ_s expansion

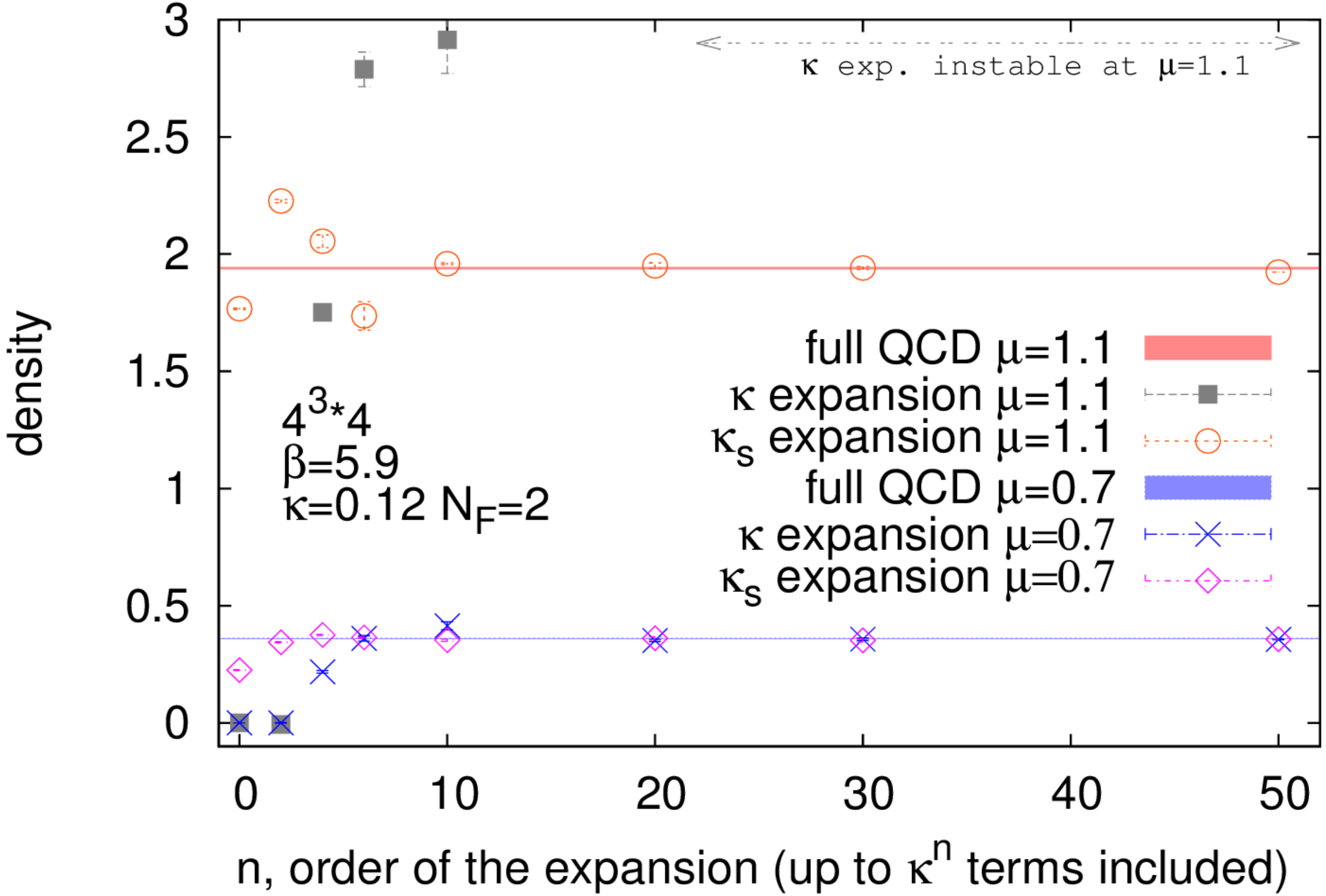
$$\mathrm{Det}\, M = \mathrm{Det}\left(1-R\right) \mathrm{Det}\left(1 - \frac{\kappa_s S}{1-R}\right) = \mathrm{Det}\left(1-R\right) \exp\left(-\mathrm{Tr} \sum \frac{\kappa_s^n}{n} \frac{S^n}{\left(1-R\right)^n}\right)$$

Numerical cost: N multiplications with S and $\left(1-R\right)^{-1}$

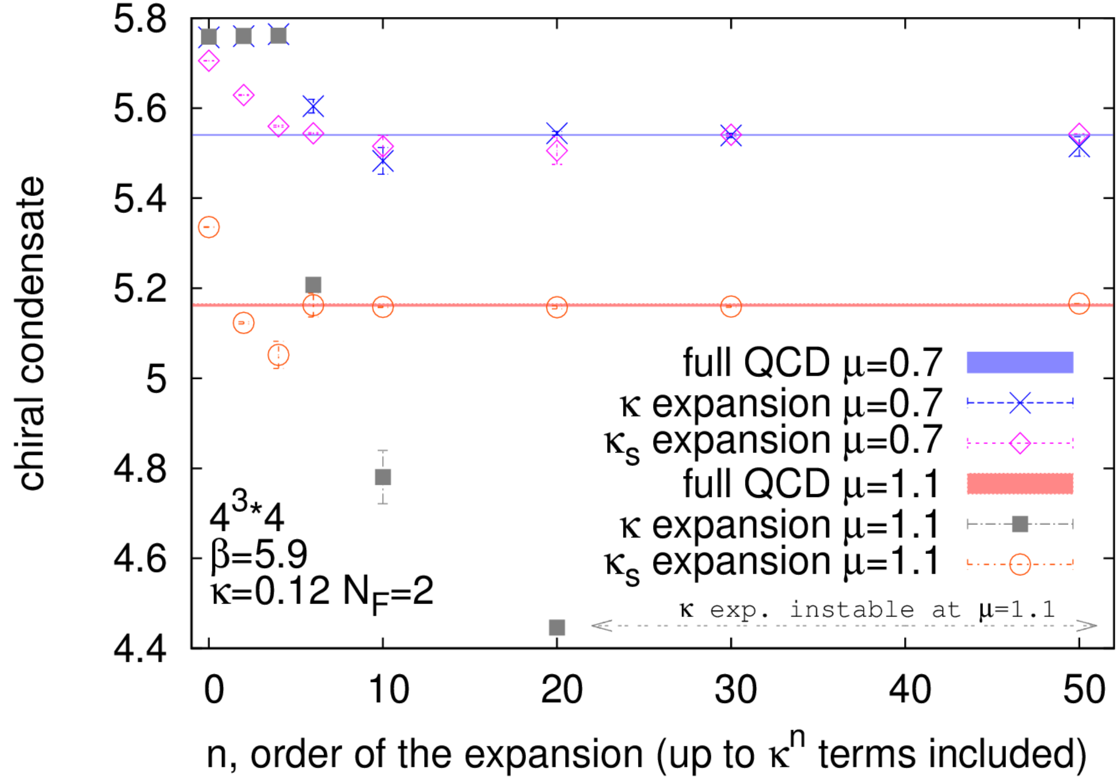
Temporal part analytically → better convergence properties

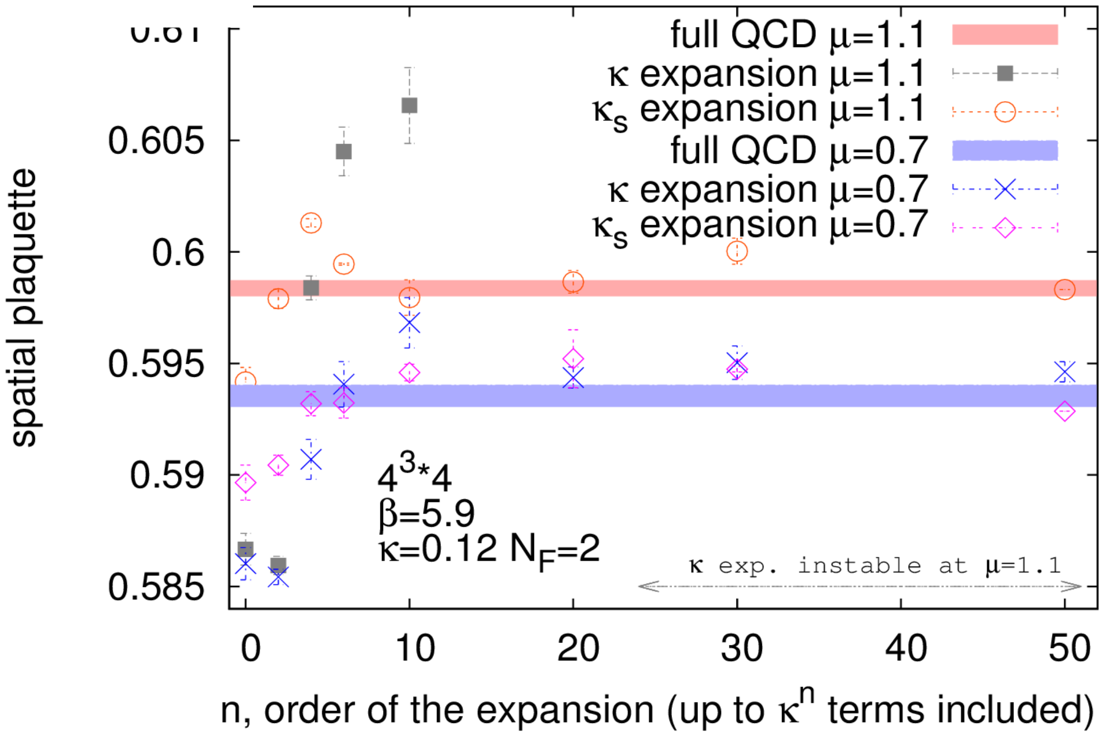
Calculation of high orders of corrections is easy
Explicit check of the convergence to full QCD

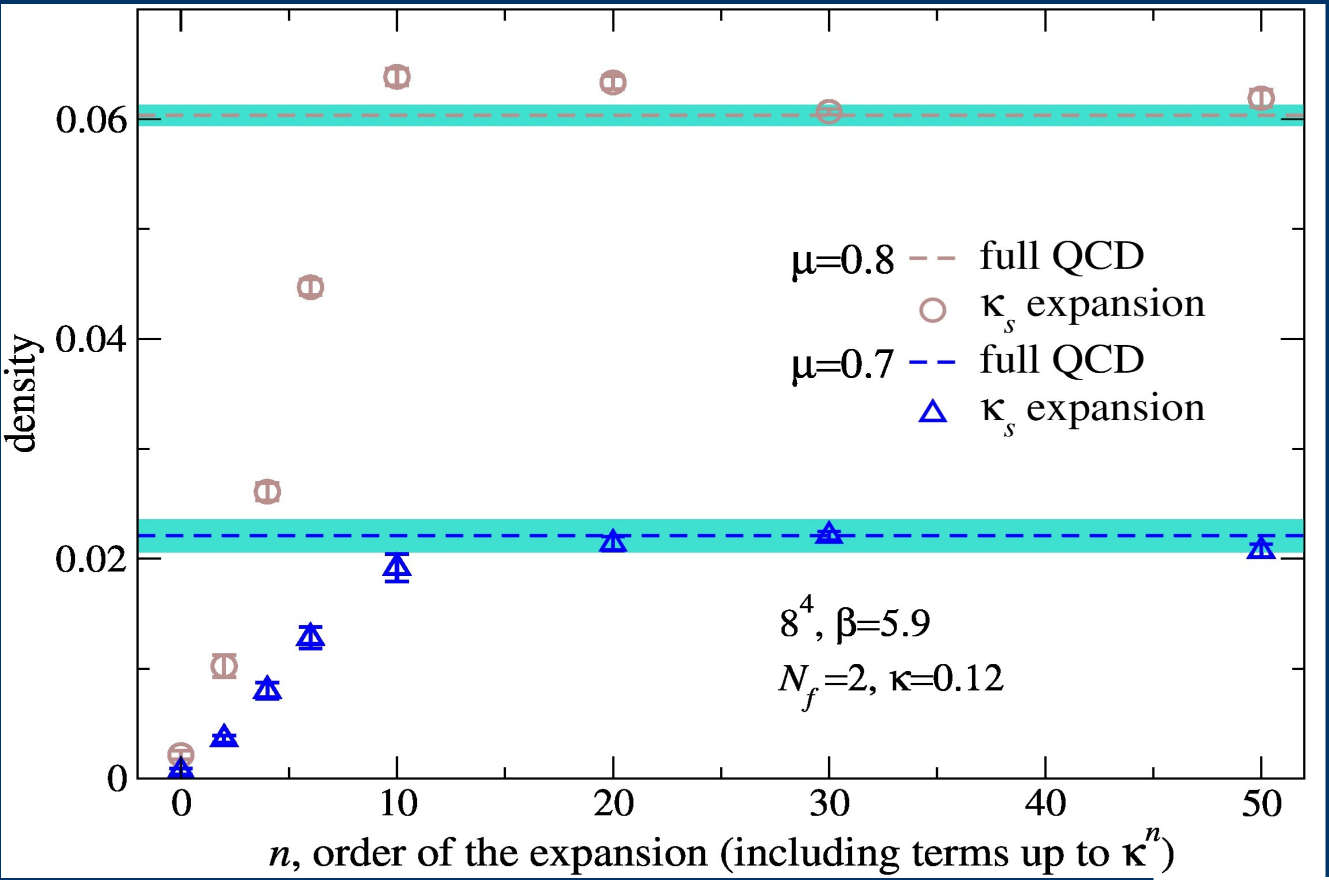
Convergence to full QCD with no poles → non-holomorphicity of the QCD action is not a problem

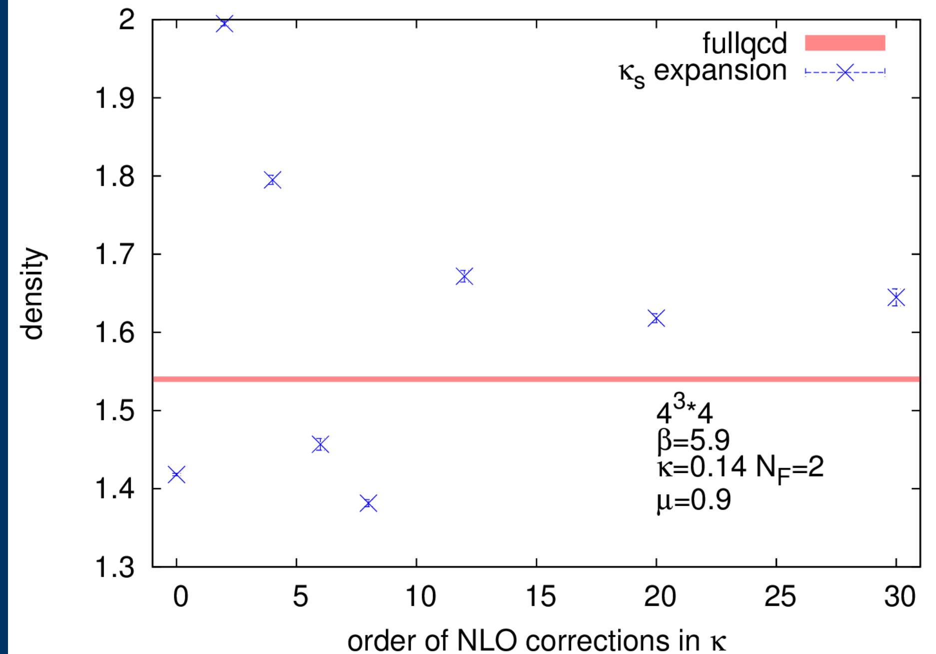


3
2.5
2
1.5
1
0.5
0
density
0
10
20
30
40
50
n, order of the expansion (up to κ^n terms included)
κ exp. instable at μ=1.1
4^3*4
β=5.9
κ=0.12 N_F=2
full QCD μ=1.1
κ expansion μ=1.1
κ_s expansion μ=1.1
full QCD μ=0.7
κ expansion μ=0.7
κ_s expansion μ=0.7


chiral condensate
5.8
5.6
5.4
5.2
5
4.8
4.6
4.4
0
10
20
30
40
50
n, order of the expansion (up to κ^n terms included)
full QCD μ=0.7
κ expansion μ=0.7
κ_s expansion μ=0.7
full QCD μ=1.1
κ expansion μ=1.1
κ_s expansion μ=1.1
4^3*4
β=5.9
κ=0.12 N_F=2
κ exp. instable at μ=1.1


spatial plaquette
0.605
0.6
0.595
0.59
0.585
0
10
20
30
40
50
n, order of the expansion (up to κ^n terms included)
full QCD μ=1.1
κ expansion μ=1.1
κ_s expansion μ=1.1
full QCD μ=0.7
κ expansion μ=0.7
κ_s expansion μ=0.7
4^3*4
β=5.9
κ=0.12 N_F=2
κ exp. instable at μ=1.1





Converges at low temperatures
(large lattices)

Convergence radius

$\kappa \approx 0.14$?

Extension to full QCD with light quarks [Sexty (2014)]

QCD with staggered fermions $Z=\int DU\, e^{-S_G} \det M$

$$M(x,y)=m\delta(x,y)+\sum_\nu \frac{\eta_\nu}{2a_\nu}\left(e^{\delta_{\nu 4}\mu} U_\nu(x)\delta(x+a_\nu,y)-e^{-\delta_{\nu 4}\mu} U_\nu^{-1}(x-a_\nu,y)\delta(x-a_\nu,y)\right)$$

Still doubling present N_F=4

$$Z=\int DU\, e^{-S_G}(\det M)^{N_F/4} \qquad S_{eff}=S_G-\frac{N_F}{4}\ln\det M$$

Langevin equation

$$U'=\exp\left(i\lambda_a(-\epsilon D_a S[U]+\sqrt{\epsilon}\eta_a)\right)U$$

Drift term: $-D_a S[U]=K^G+K^F$

$$K^G_{ax\nu}=-D_{ax\nu} S_G[U]$$

$$K^F_{ax\nu}=\frac{N_F}{4}D_{ax\nu}\ln\det M=\frac{N_F}{4}\mathrm{Tr}\left(M^{-1}M'_{\nu a}(x,y,z)\right)$$

$$M'_{\nu a}(x,y,z)=D_{az\nu}M(x,y)$$

Extension to full QCD with light quarks [Sexty (2014)]

QCD with fermions $Z=\int DU\, e^{-S_G} det\, M$

Additional drift term from determinant

$$K^F_{ax\nu}=\frac{N_F}{4}D_{ax\nu}\ln\det M=\frac{N_F}{4}\mathrm{Tr}\left(M^{-1}M'_{\nu a}(x,y,z)\right)$$

Noisy estimator with one noise vector
Main cost of the simulation: CG inversion

Inversion cost highly dependent on chemical potential
Eigenvalues not bounded from below by the mass
(similarly to isospin chemical potential theory)

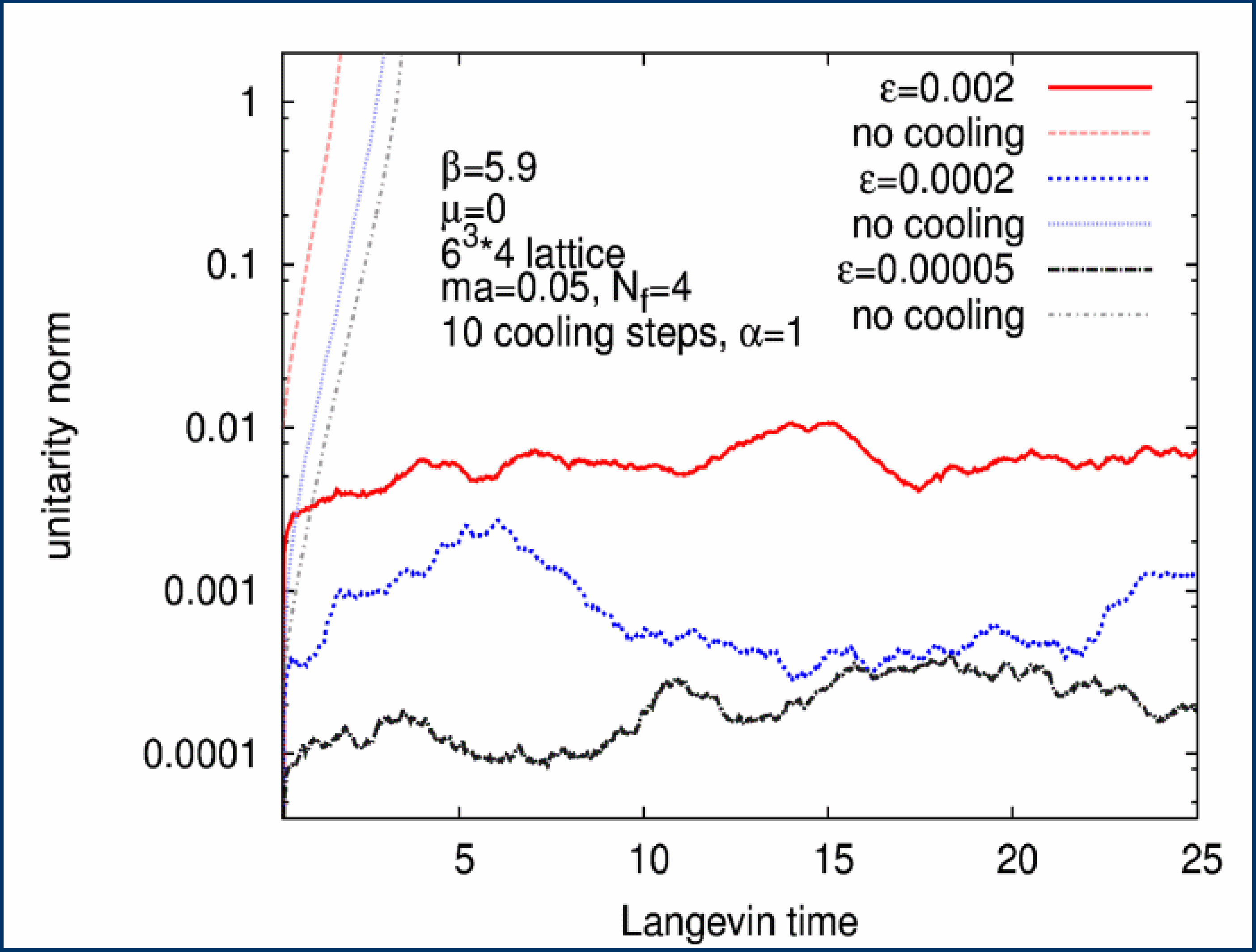
Unimproved staggered and Wilson fermions

Heavy quarks: compare to HDQCD
Light quarks: compare to reweighting

Zero chemical potential

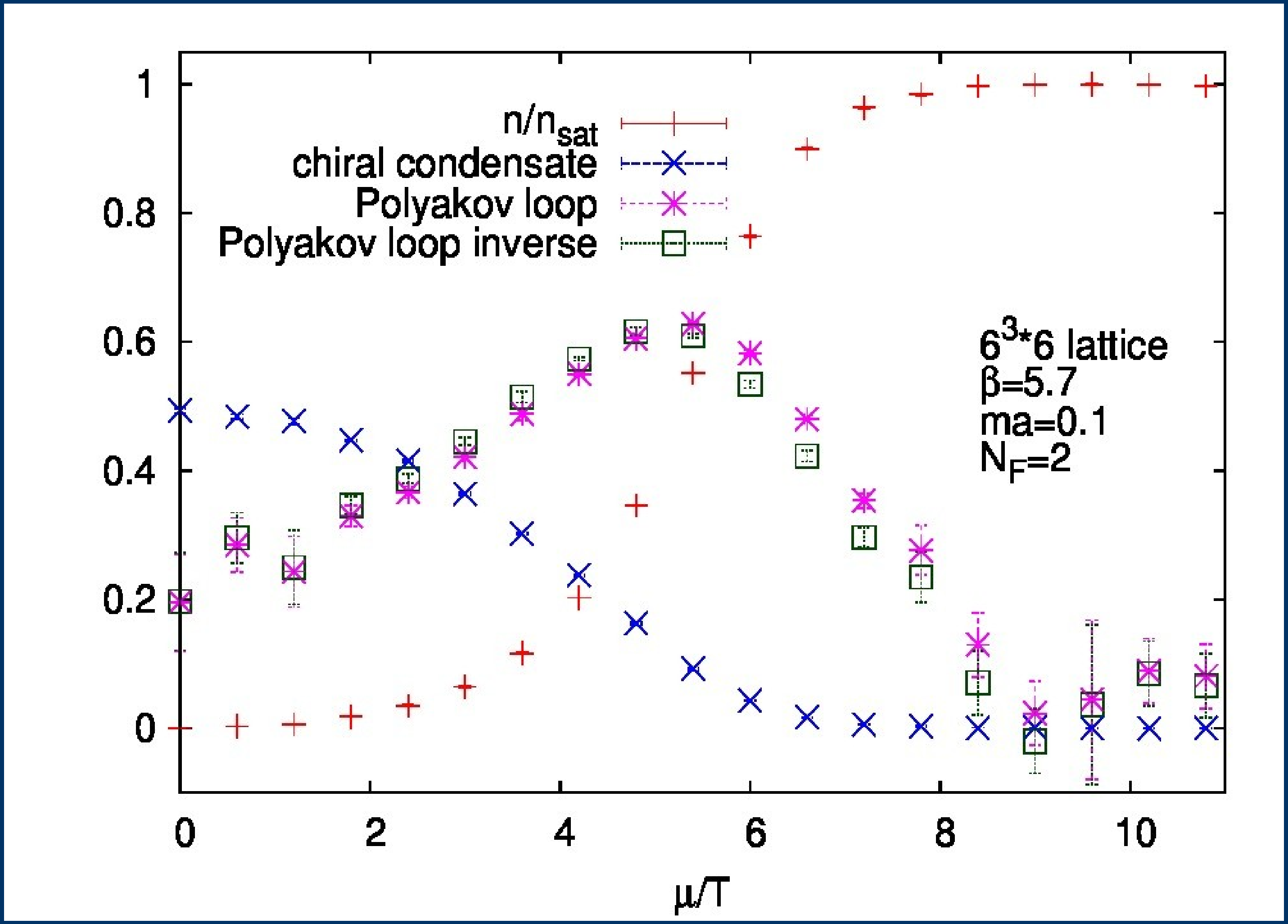
Drift is built from random numbers   real only on average

Cooling is essential already for small (or zero) mu



CLE and full QCD with light quarks [Sexty (2014)]

Physically reasonable results



Non-holomorphic action
poles in the fermionic drift

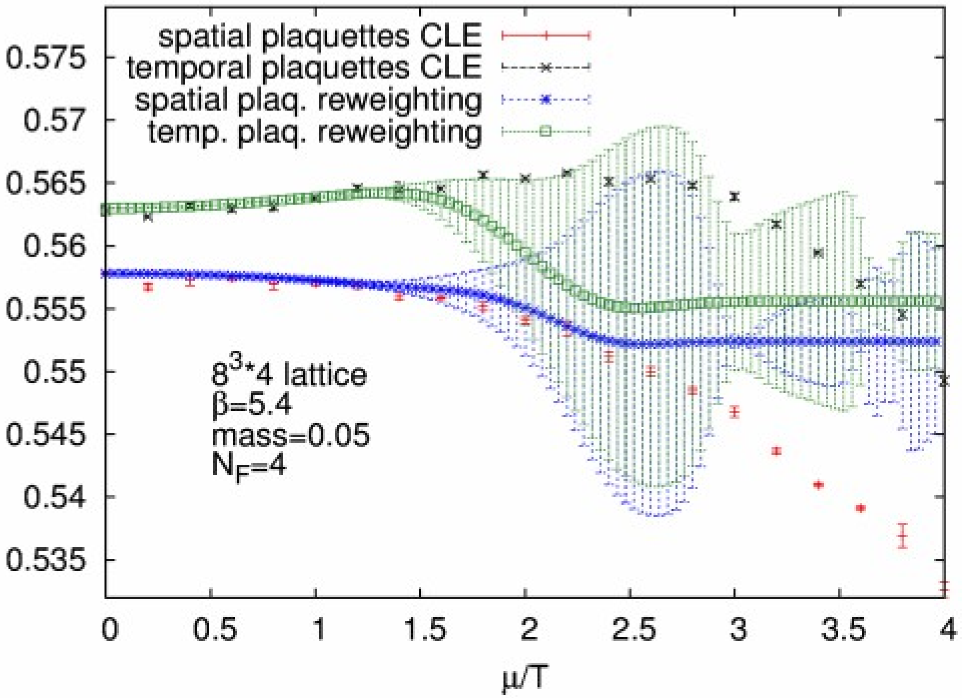
Is it a problem for full QCD?

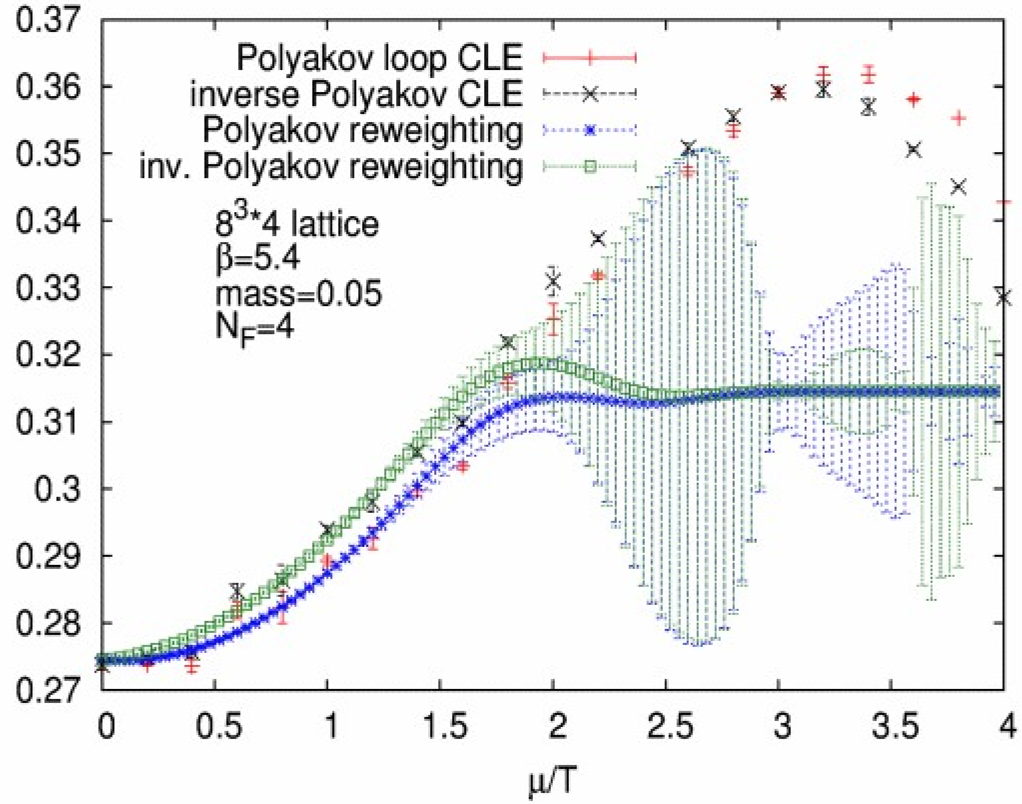
So far, it isnt:
Comparison with reweighting
Study of the spectrum
Hopping parameter expansion

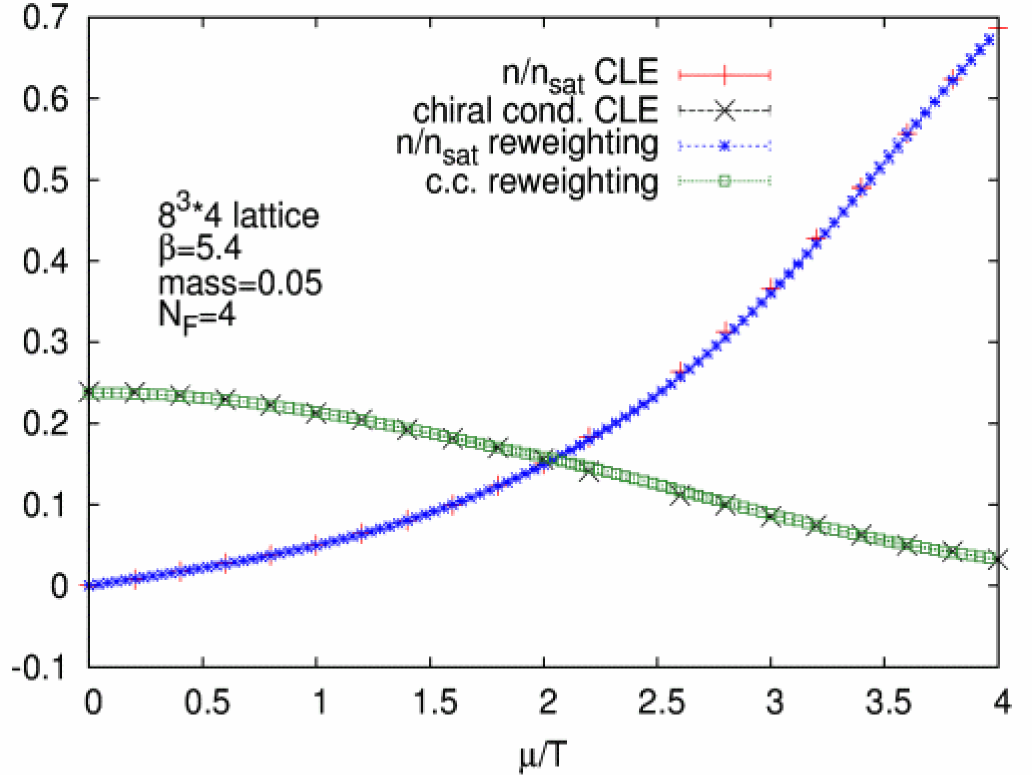
Comparison with reweighting for full QCD

Reweighting from ensemble at

$$R = \mathrm{Det}\, M(\mu = 0)$$



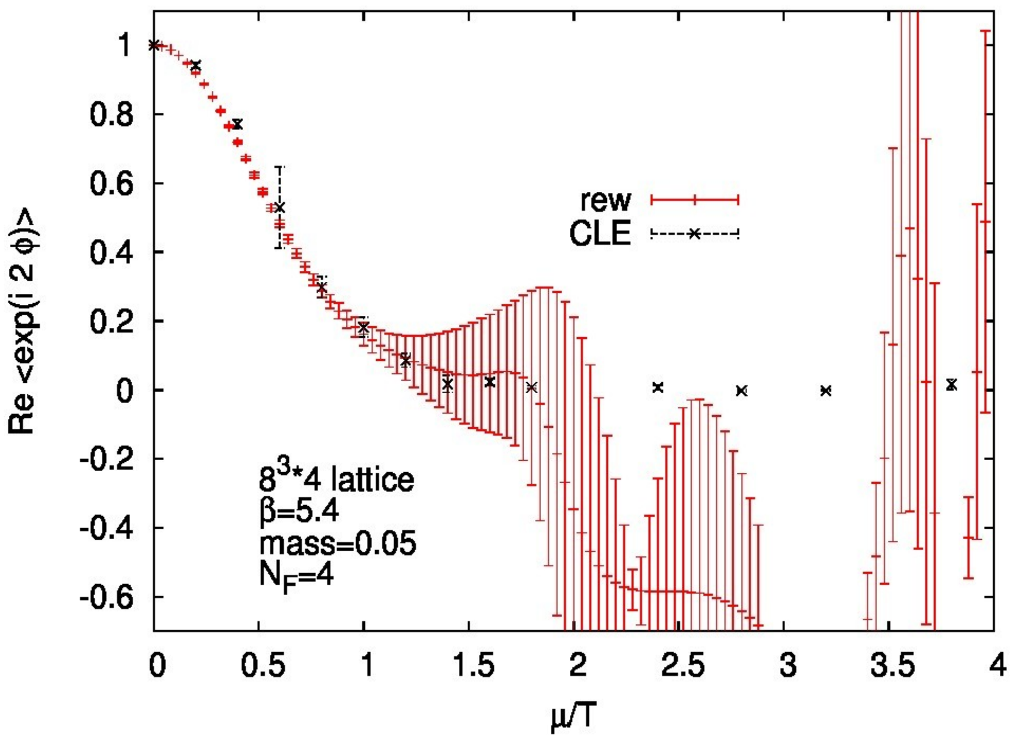


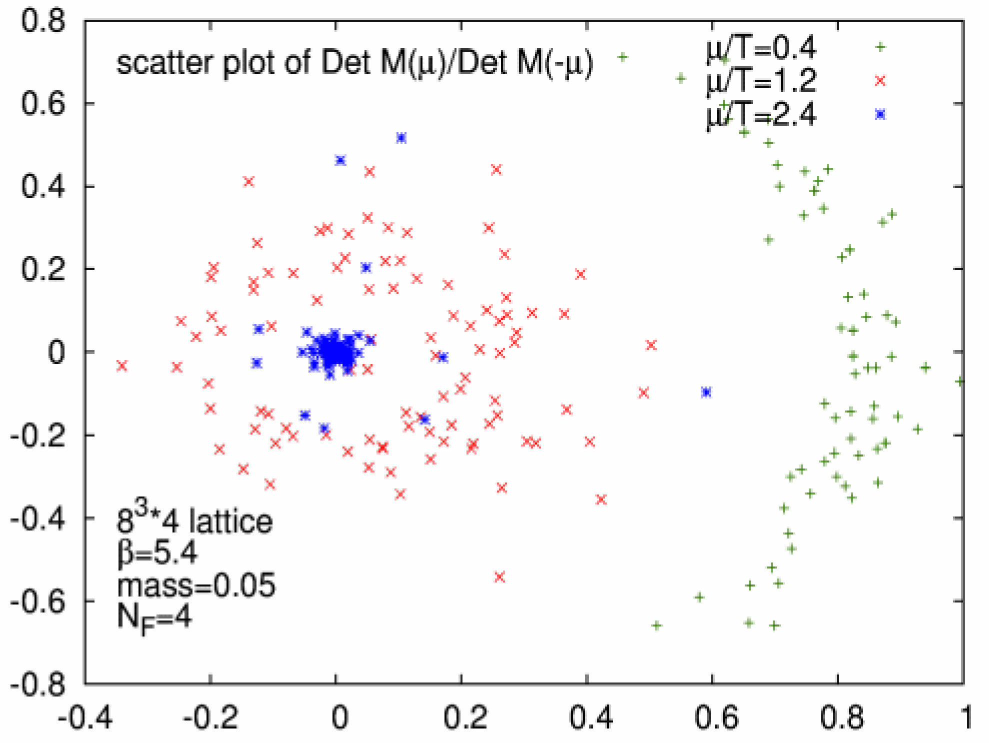


[Fodor, Katz, Sexty (in prep.)]

Sign problem

Sign problem gets hard around $\mu/T \approx 1 - 1.5$

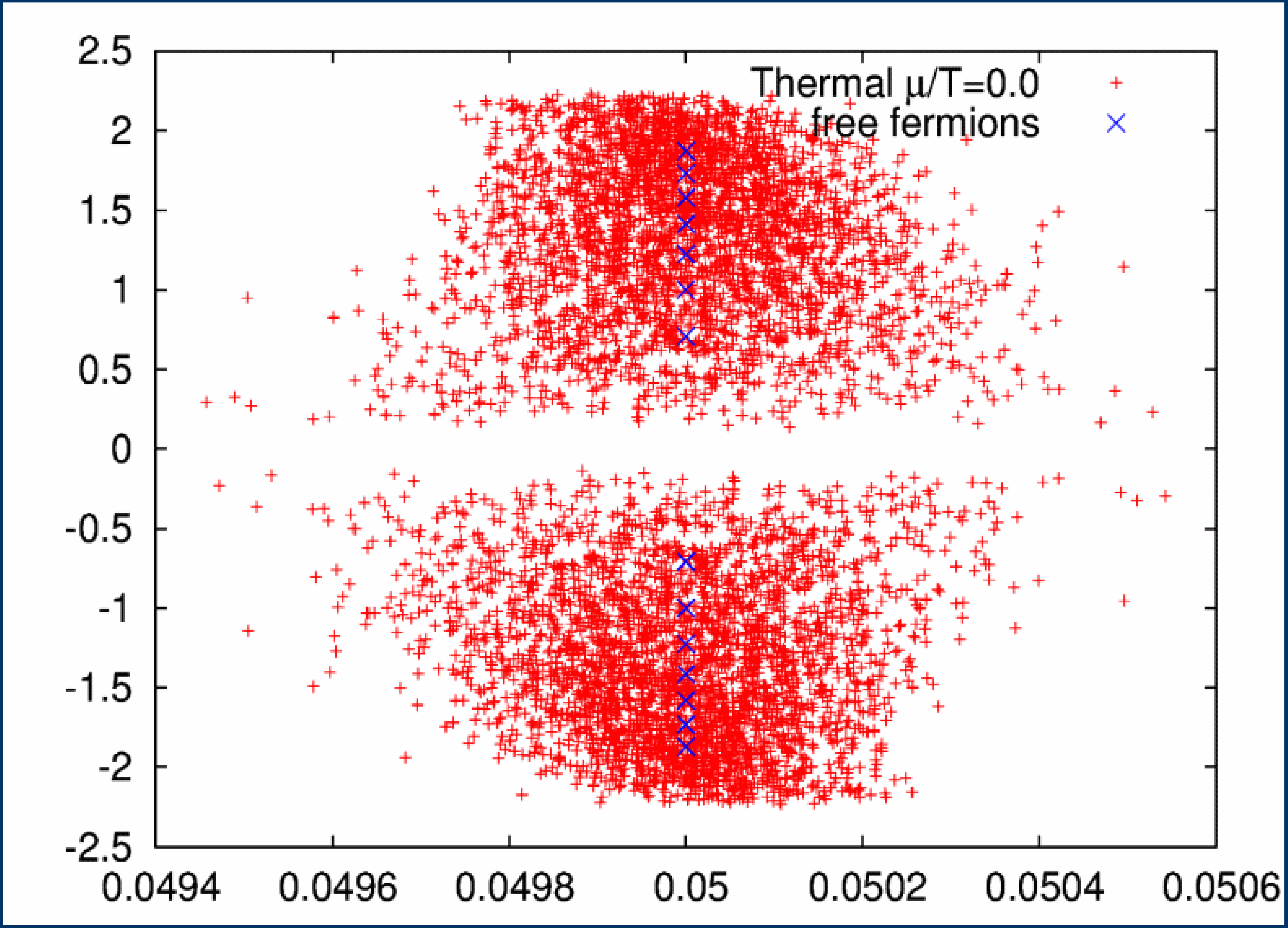




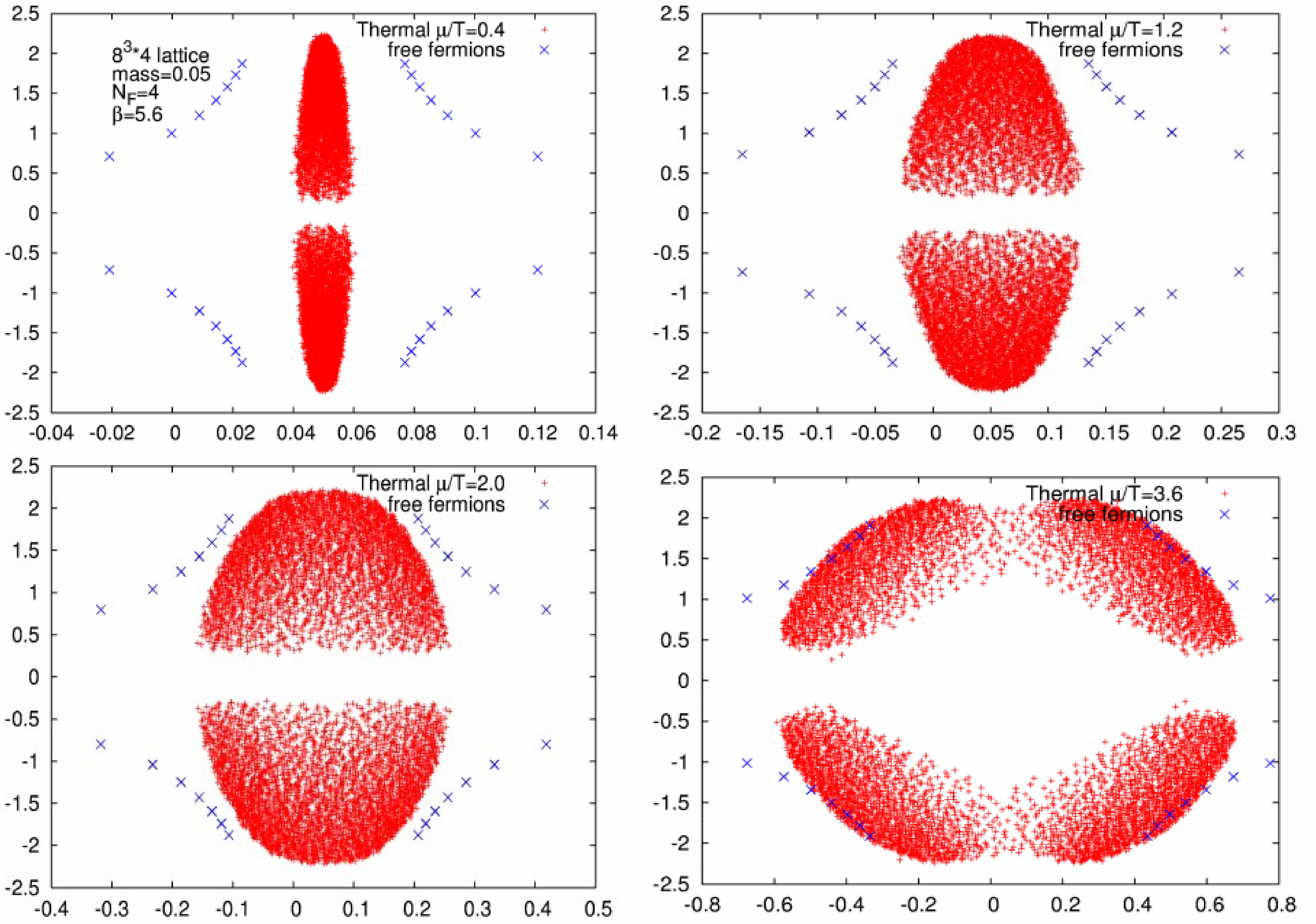
$$\langle \exp(2 i \varphi) \rangle = \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle$$

Spectrum of the Dirac Operator $N_F = 4$ staggered

Massless staggered operator at $\mu = 0$ is antihermitian



Spectrum of the Dirac Operator $N_F=4$ staggered



Conclusions

Direct simulations of QCD at nonzero density using complexified fields

Complex Langevin Equations

Recent progress for CLE simulations

- Better theoretical understanding (poles?)
- Gauge cooling

Kappa expansion

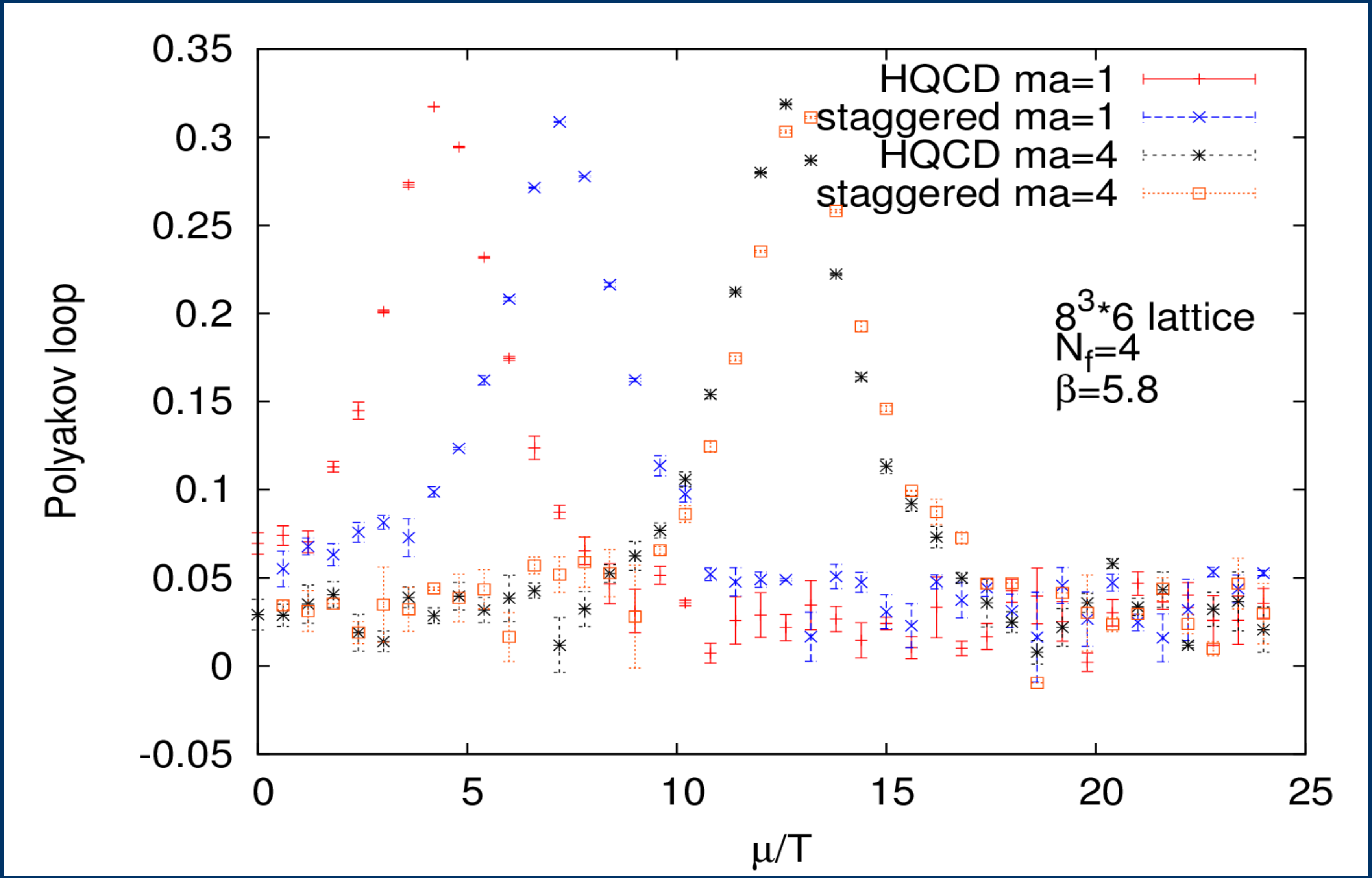
- Two novel implementations with CLE: kappa and kappa_s
- Calculations at very high orders are feasible
- Convergence checked explicitly
- Shows that poles give no problem in QCD

Phase diagram of HDQCD mapped out

First results for full QCD with light quarks

- No sign or overlap problem
- CLE works all the way into saturation region
- Comparison with reweighting for small chem. pot.
- Low temperatures are more demanding

Backup slides



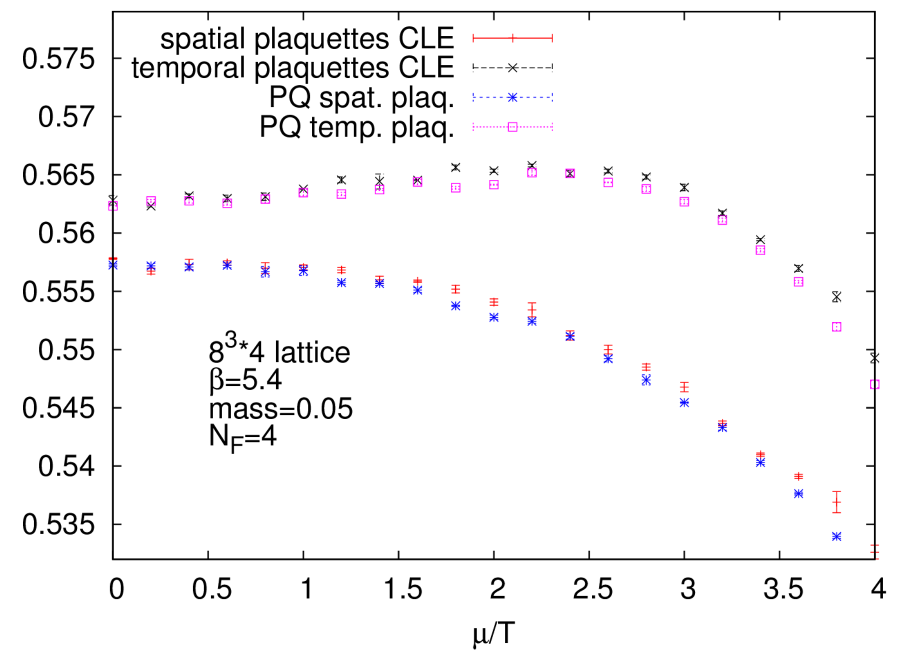
Conclusion

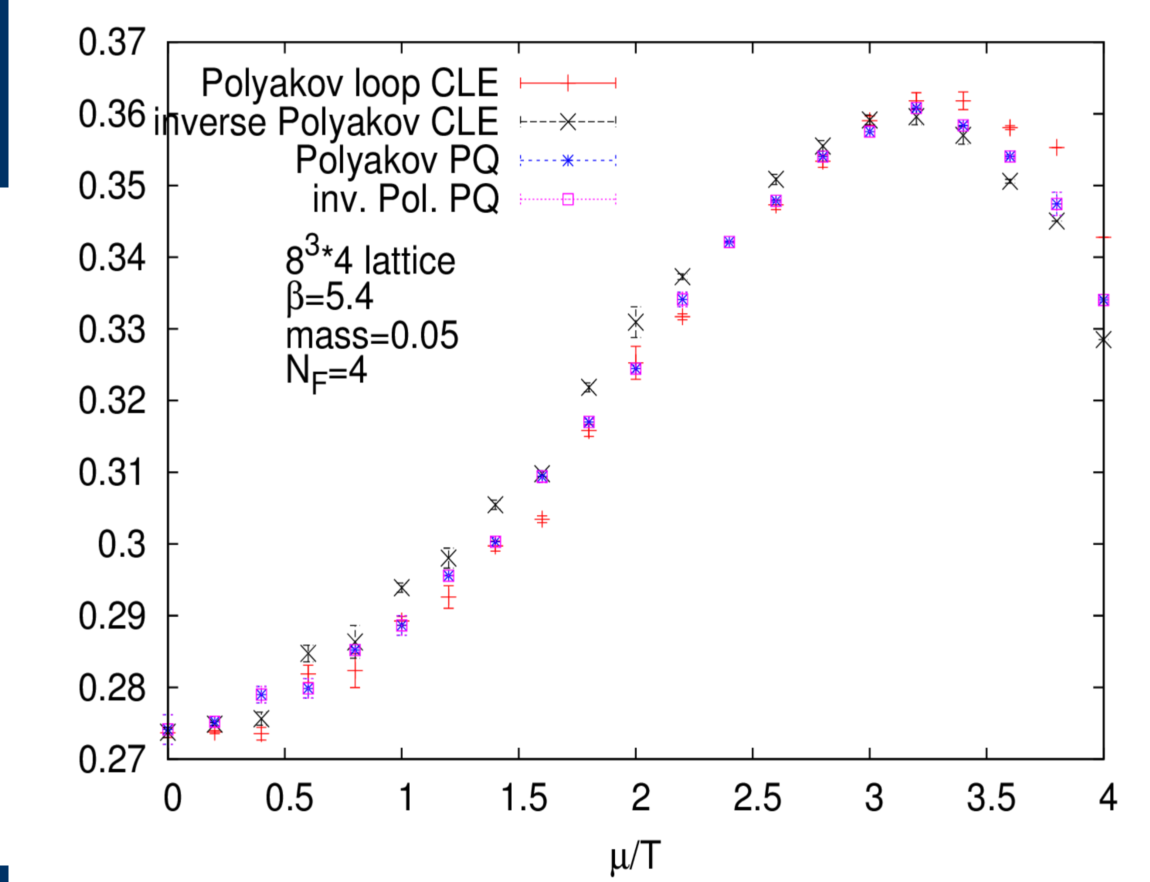
QCD = HQCD for quark mass > 4/a

(For large mass) HQCD is qualitatively similar to QCD

Phasequenched vs full

$$Z=\int dU\, e^{-S_g}|det\, M|$$





in phasequenched $P=P^{-1}$

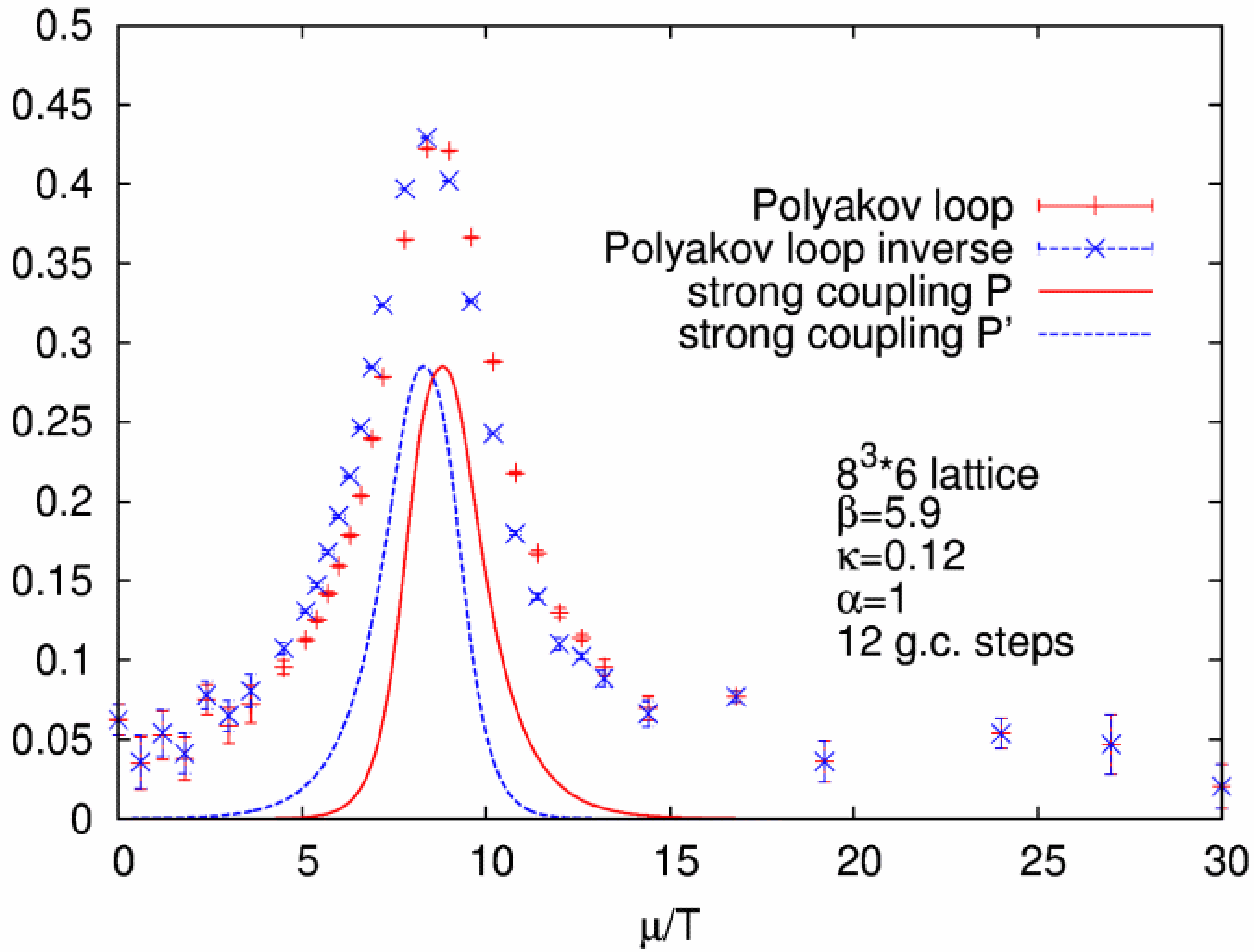
in full theory, inv. Polyakov loop rises first

Reweighting form PQ theory better than Reweighting from $\mu=0$?

Nonzero value when: colorless bound states formed with P or P'

1 quark:
meson with P'

2 quark:
Baryon with P



P' has a peak before P

Large chemical potential: all quark states are filled
No colorless state can be formed

P and P' decays again

Spectrum of the Dirac Operator

Large chemical potential, towards saturation

Fermions become "heavy"