Simulating full QCD at nonzero density using the Complex Langevin Equation

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1. Introduction
2. Gauge symmetry and gauge cooling
3. HQCD with gauge cooling
4. Extension to Full QCD

Seiler, Sexty, Stamatescu PLB (2012)
Aarts, Bongiovanni, Seiler, Sexty, Stamatescu EPJA (2013)
Sexty, arXiv:1307.7748

Non-zero chemical potential

Euclidean gauge theory with fermions: $Z = \int dU \exp(-S_E) \, det(M)$

For nonzero chemical potential, the fermion determinant is complex

Sign problem → Naïve Monte-Carlo breaks down

Methods going around the problem work for $\mu = \mu_B/3 < T$

(Multi parameter) reweighting

Barbour et. al. '97; Fodor, Katz '01

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 $(\mu/T)^2$

de Forcrand et al. '99; Hart, Laine, Philipsen '00; Gavai and Gupta '08;
de Forcrand, Philipsen '08

Stochastic quantisation

Aarts and Stamatescu '08
Bose Gas, Spin model, etc. Aarts '08, Aarts, James '10 Aarts, James '11
QCD with heavy quarks: Seiler, Sexty, Stamatescu '12

Stochastic Quantization

Parisi, Wu (1981)

Weighted, normalized average: $\langle O \rangle = \frac{\int e^{-S(x)} O(x) dx}{\int e^{-S(x)} dx}$

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

Gaussian noise $\langle \eta(\tau) \rangle = 0 \quad \langle \eta(\tau) \eta(\tau') \rangle = 2 \delta(\tau - \tau')$

Averages are calculated along the trajectories:

$$\langle O \rangle = \frac{1}{T} \int_0^T O(x(\tau)) d\tau$$

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

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

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

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

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

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

Analytic observables

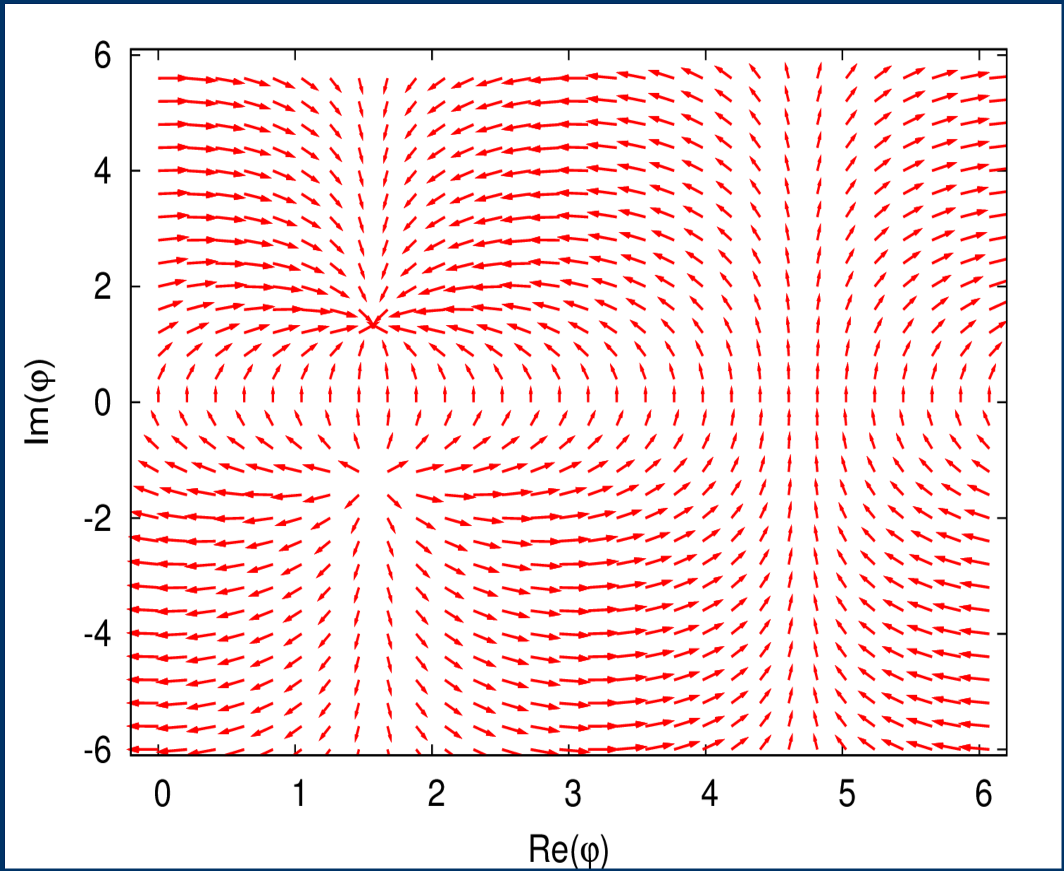
$$\frac{1}{Z} \int P_{comp}(x) O(x) dx = \frac{1}{Z} \int P_{real}(x, y) O(x + iy)\, dx\, dy$$

No general proof of convergence for complex axtion

But Schwhinger-Dyson eqs. are fulfilled

Runaway trajectories present

Typical drift structure



Noise is real "horizontal"

Runaway if field stays at $\frac{3}{2}\pi$

In continuum probabilty of a runaway=0

Discretised: getting far away

Numerical problem
drift proportional to field

Solution: small stepsize
Adaptive stepsize control

Gaugefixing in SU(2) one plaquette model

Berges, Sexty '08

SU(2) one plaquette model: $S = i\beta\, Tr\, U \qquad U \in SU(2)$

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

exact averages by numerical integration: $\langle f(U) \rangle = \frac{1}{Z} \int_0^{2\pi} d\phi \int d\Omega \sin^2 \frac{\phi}{2} e^{i\beta \cos \frac{\phi}{2}} f(U(\phi, \hat{n}))$

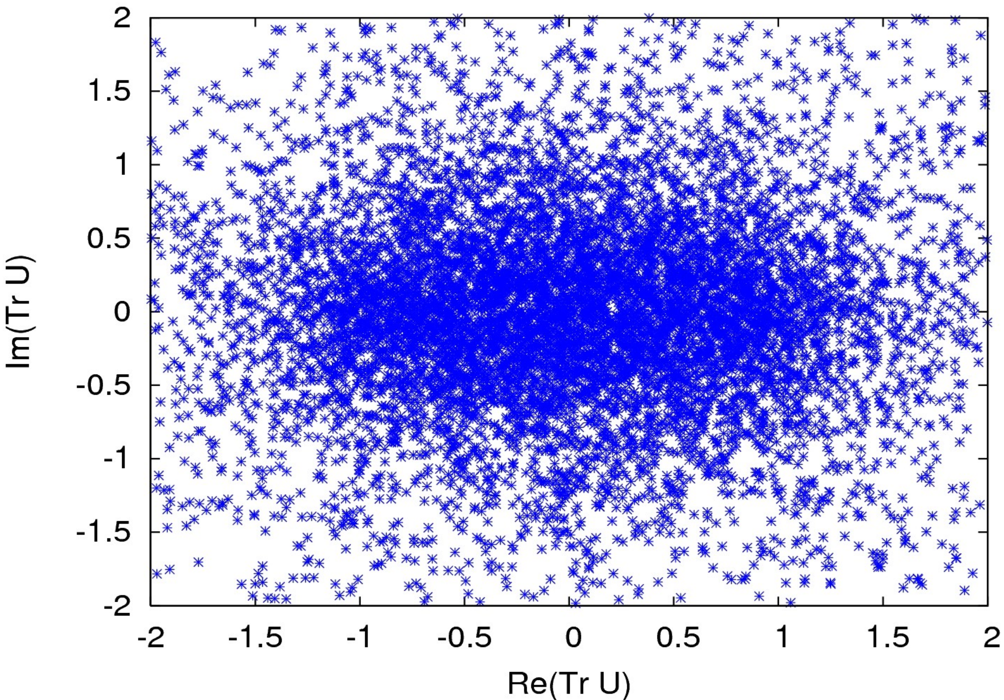
"gauge" symmetry: $U \rightarrow W U W^{-1}$ complexified theory: $U, W \in SL(2, \mathbb{C})$

After each Langevin timestep: fix gauge condition

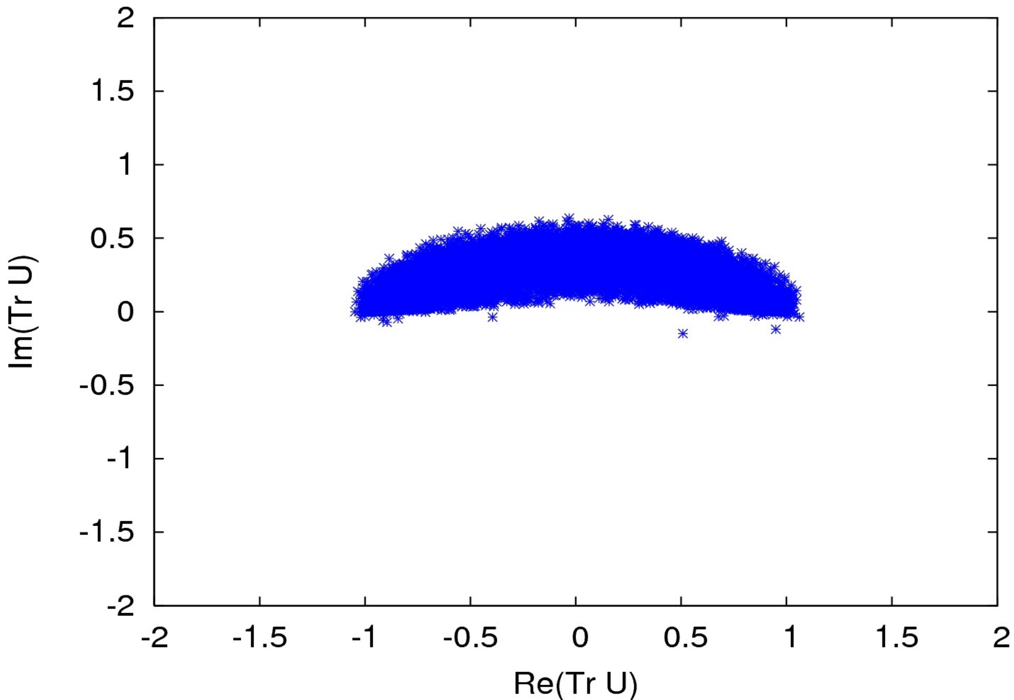
$U = a\mathbf{1} + i\sqrt{1-a^2}\,\sigma_3$ $b_i = (0, 0, \sqrt{1-a^2})$

SU(2) one-plaquette model

Distributions of Tr(U) on the complex plane



Without gaugefixing



With gaugefixing

Exact result from integration: $\langle Tr\, U \rangle = i\, 0.2611$

From simulation:

$(-0.02 \pm 0.02) + i\,(-0.01 \pm 0.02)$

$(-0.004 \pm 0.006) + i\,(0.260 \pm 0.001)$

With gauge fixing, all averages are correctly reproduced

Gauge cooling

complexified distribution with slow decay → convergence wrong results

Minimize unitarity norm: $\sum_i Tr\left(U_i U_i^{+}\right)$

Using gauge transformations in SL(N,C)

$$U_\mu(x) \to V(x) U_\mu(x) V^{-1}(x+a_\mu) \qquad V(x) = \exp\left(i \lambda_a v_a(x)\right)$$

$v_a(x)$ is imaginary (for real $v_a(x)$, unitarity norm is not changed)

Gradient of the unitarity norm gives steepest descent

$$G_a(x) = 2\,Tr\left[\lambda_a\left(U_\mu(x) U_\mu^{+}(x) - U_\mu^{+}(x-a_\mu) U_\mu(x-a_\mu)\right)\right]$$

Gauge transformation at x changes 2d link variables

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

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

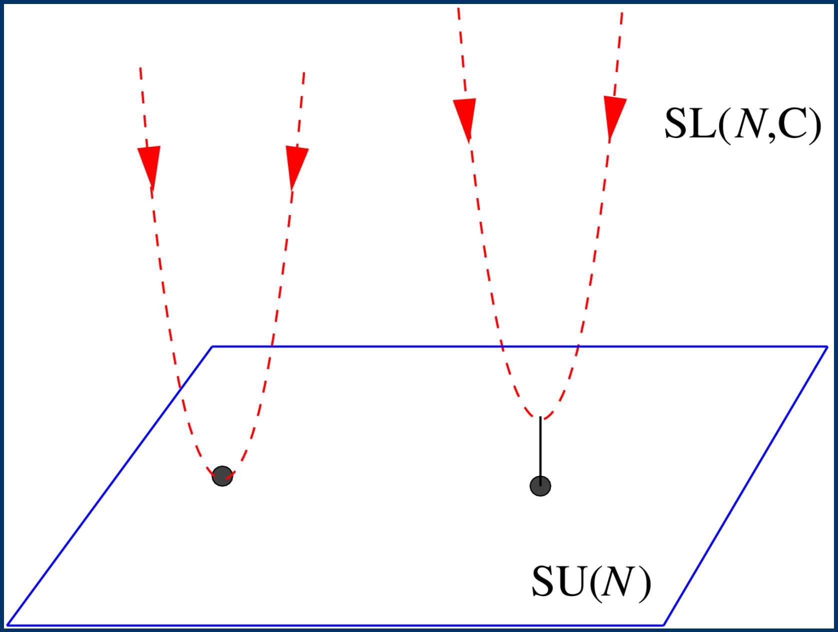
Dynamical steps are interspersed with several gauge cooling steps

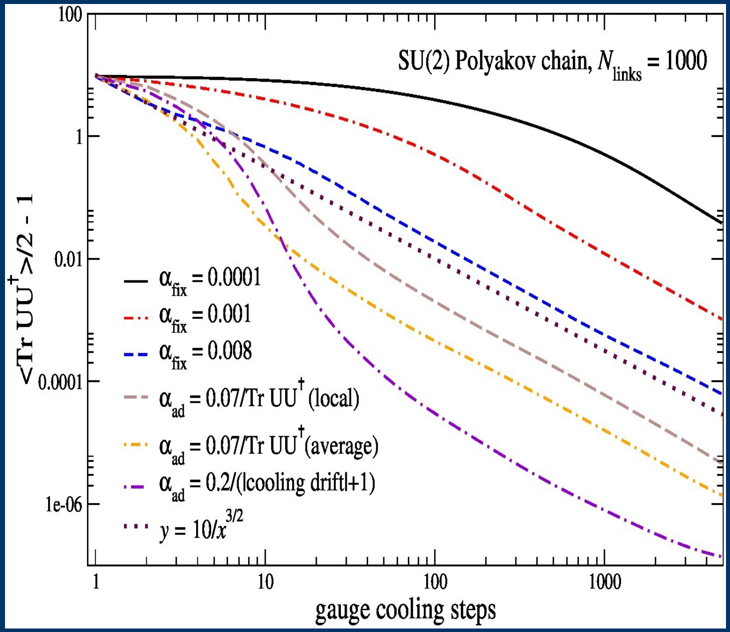
The strength of the cooling is determined by
- cooling steps
- gauge cooling parameter α

During cooling, unitarity norm decays to a minimum with a power law behaviour

Adaptive cooling, Fourier accelerated cooling

[Aarts, Bongiovanni, Seiler, Sexty, Stamatescu (2013)]

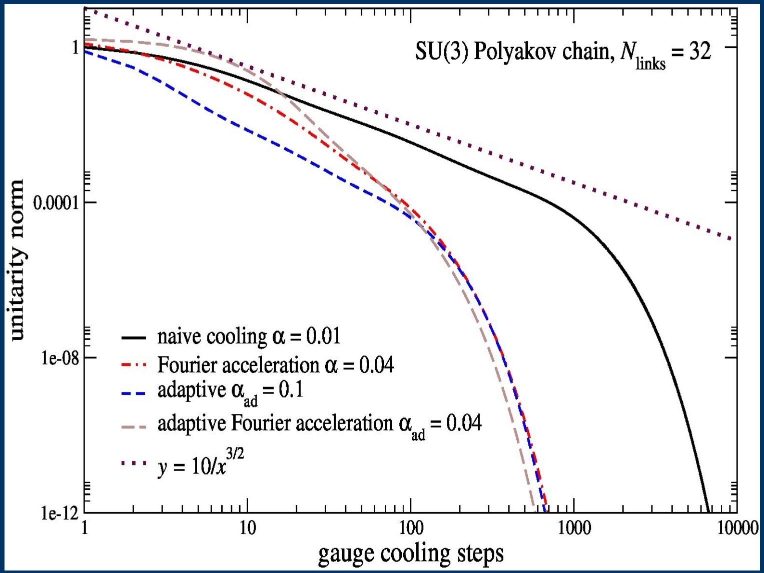




Get to minimum quickest

Stepsize dependent on gradient
Adaptive cooling

Low momentum modes cool slower
Fourier accelerated cooling



Polyakov chain model

[Seiler, Sexty, Stamatescu (2012)]

exactly solvable toy model with gauge symmetry

$$S = -\beta_1 Tr\, U_1 \ldots U_N - \beta_2 Tr\, U_N^{-1} \ldots U_1^{-1} \qquad U_i \in SU(3)$$

$$\beta_1 = \beta + \kappa e^{\mu} \qquad \beta_2 = \beta^* + \kappa e^{-\mu}$$

Complex action for $\kappa, \mu > 0$

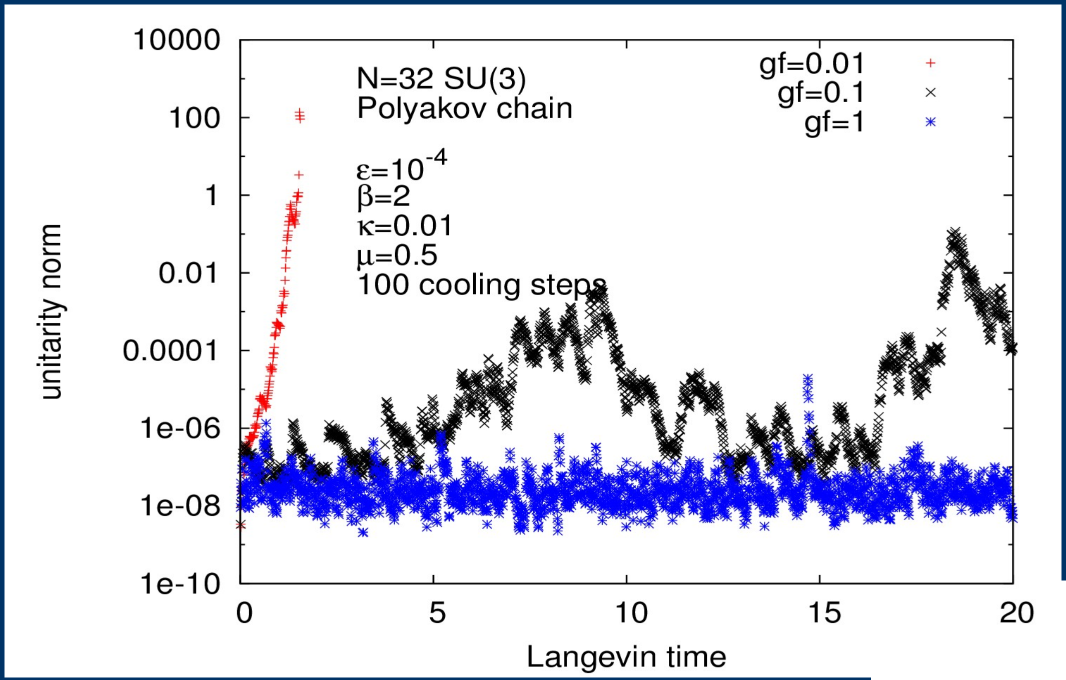
Observables: $Tr\, P^k$ *with* $P = U_1 \ldots U_N$

Averages independent of N

Calculated with numerical integration at $N = 1$

Gauge symmetry

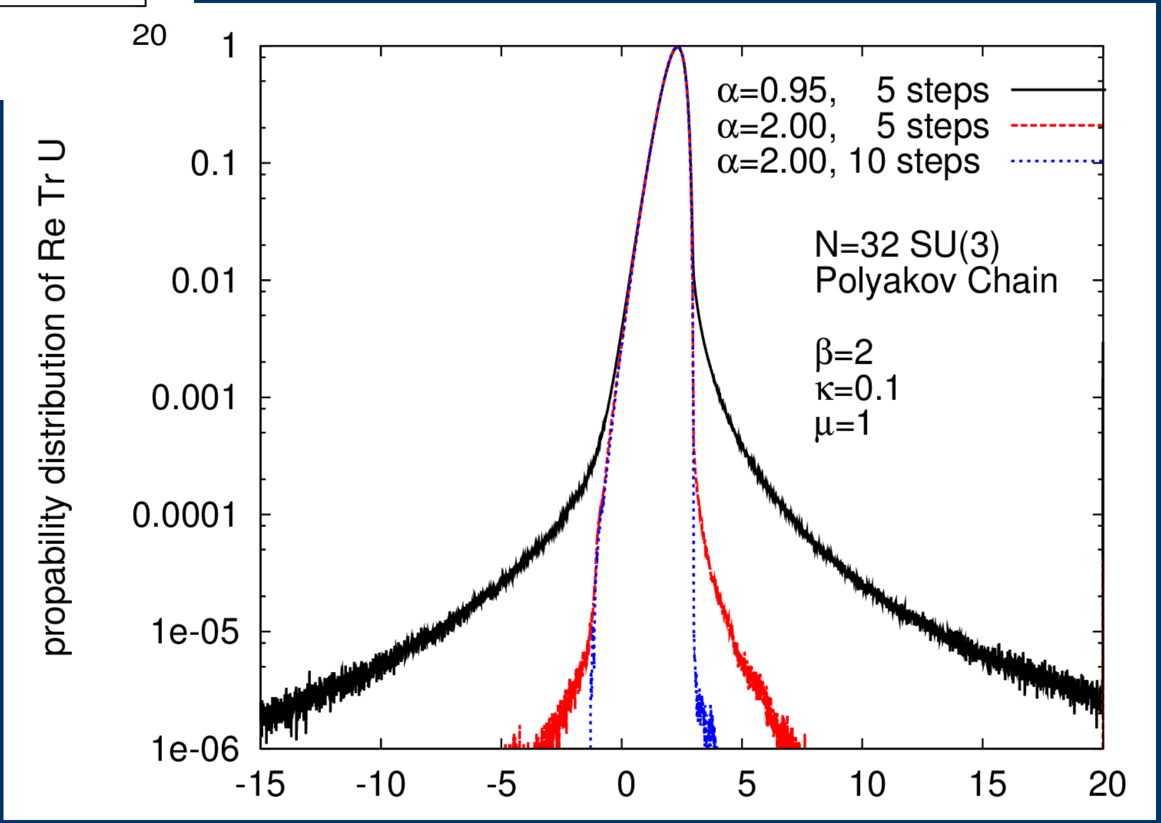
$$U_i \rightarrow V_i U_i V_{i+1}^{-1}$$

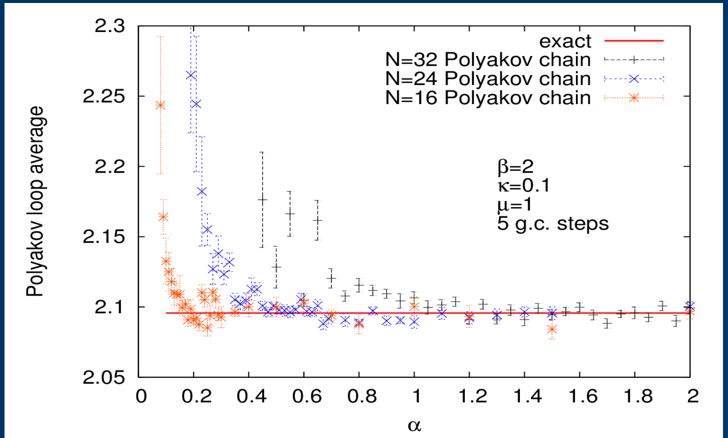


Smaller cooling → excursions

“Skirt” develops

small skirt gives correct result





Heavy Quark QCD

Hopping parameter expansion of the fermion determinant
Spatial hoppings are dropped

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

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

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

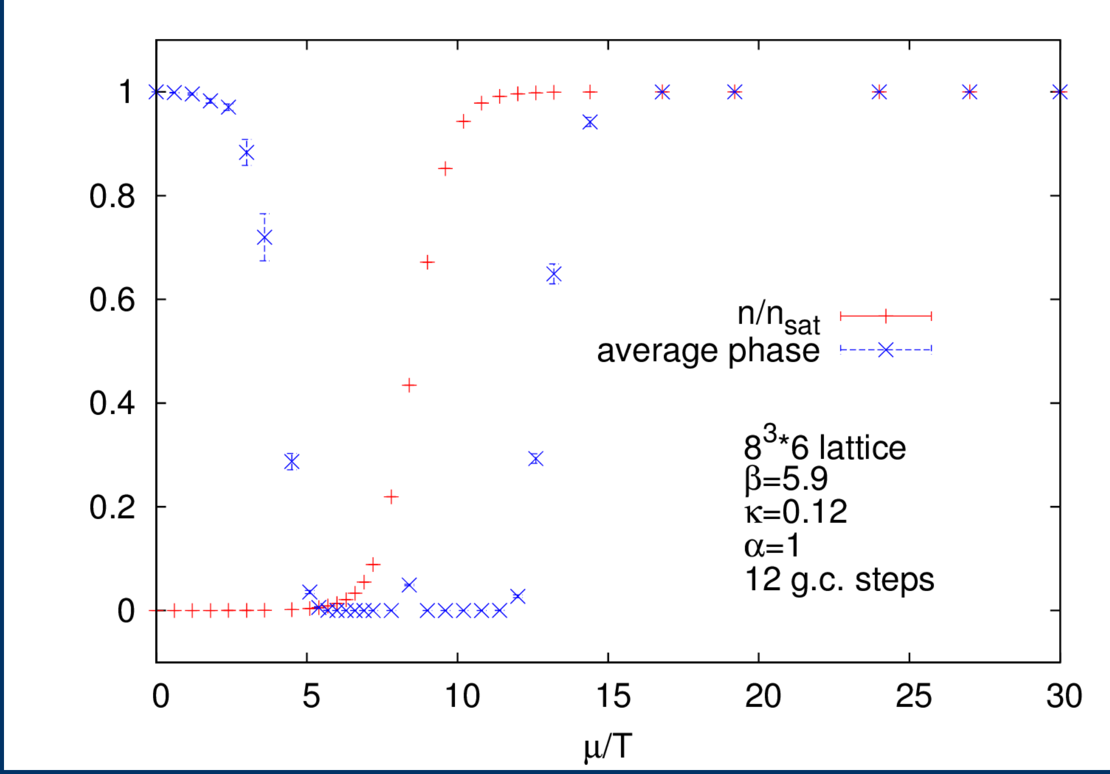
De Pietri, Feo, Seiler, Stamatescu '07

Studied with reweighting

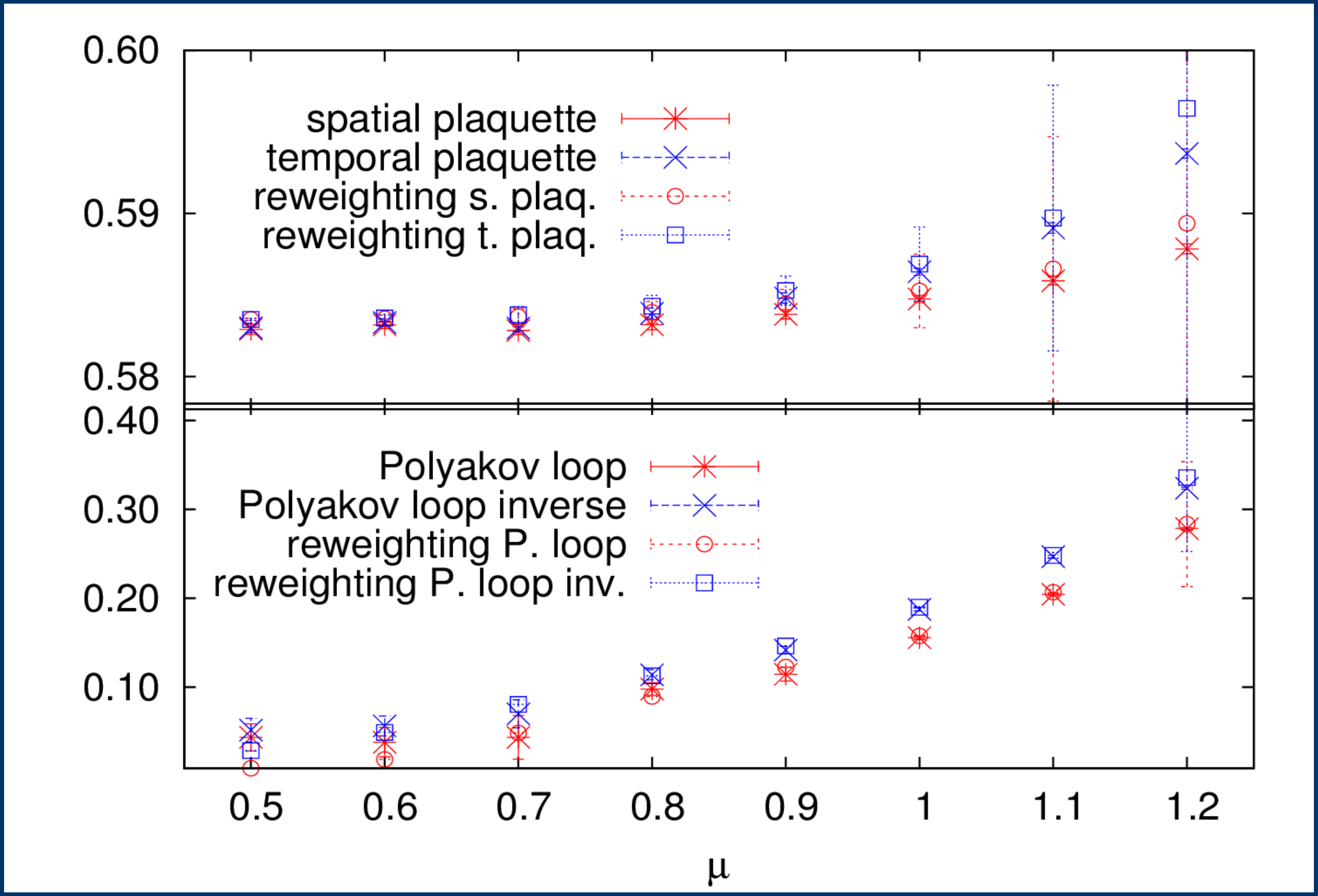
CLE study using gaugecooling

[Seiler, Sexty, Stamatescu (2012)]

See Nucu Stamatescu's poster



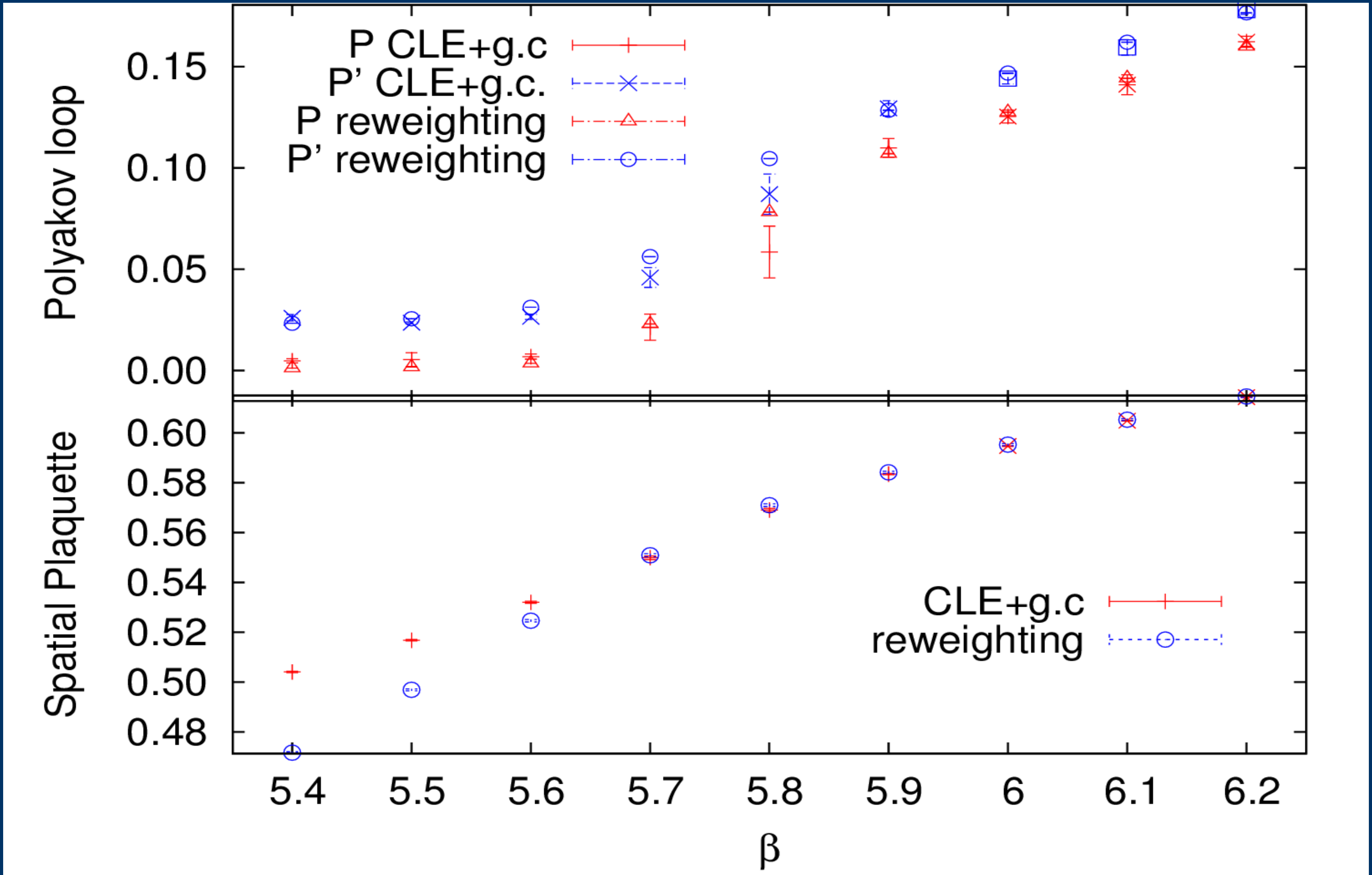
Comparison to reweighting



6^4 lattice, $\beta = 5.9$, $\alpha = 1$, 12 gaugecooling steps

Reweighting errors start to blow up at $\mu \approx 1.1$

Comparison to reweighting

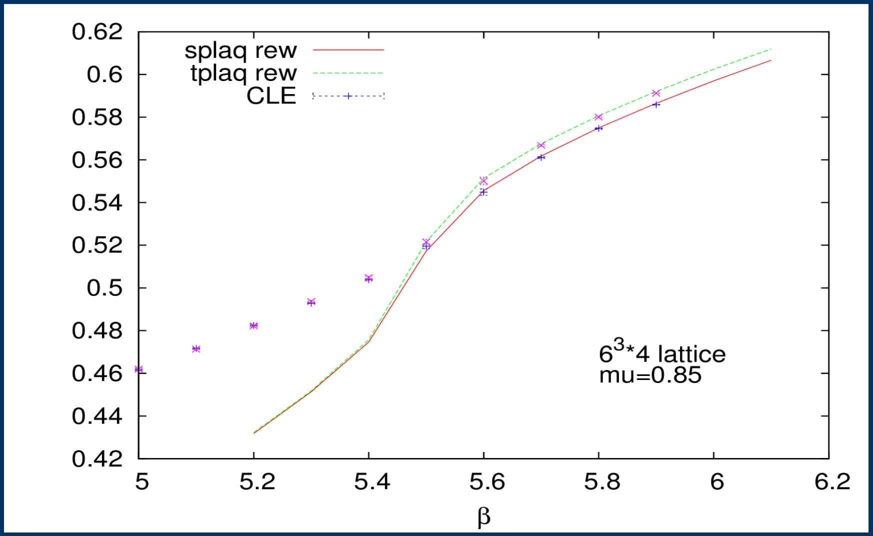


6^4 lattice, $\mu = 0.85$, $\alpha = 1$, adaptive step size

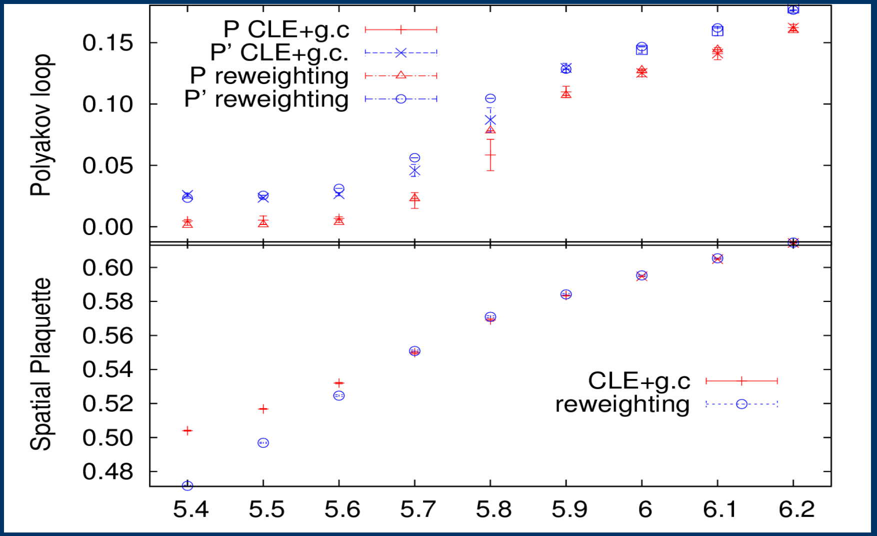
Discrepancy of plaquettes at $\beta \leq 5.6$
a skirted distribution develops

Lattice size dependence of the breakdown

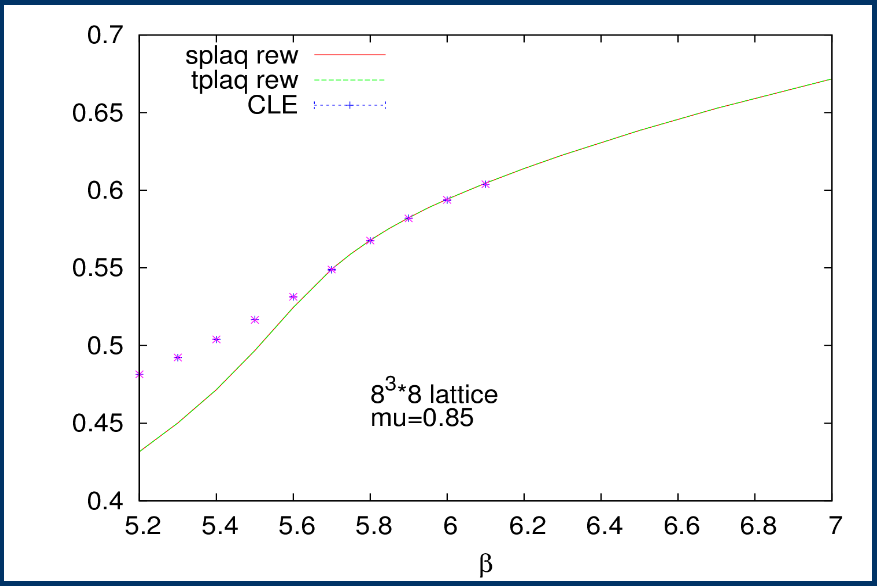
$6^3 4$



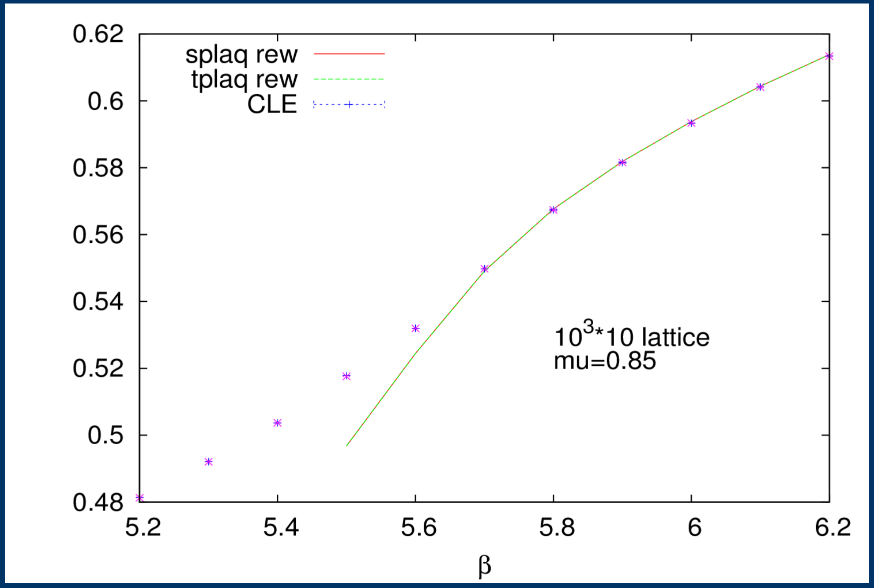
6^4



8^4



10^4



Cooling works deeper in confined phase as N increases

$\beta_{lim} = 5.6$ Going towards continuum limit → cooling is more effective

Extension to full QCD with light quarks [Sexty, arXiv:1307.7748]

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 doubleing present N_F=4

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

Langevin equation

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

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

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

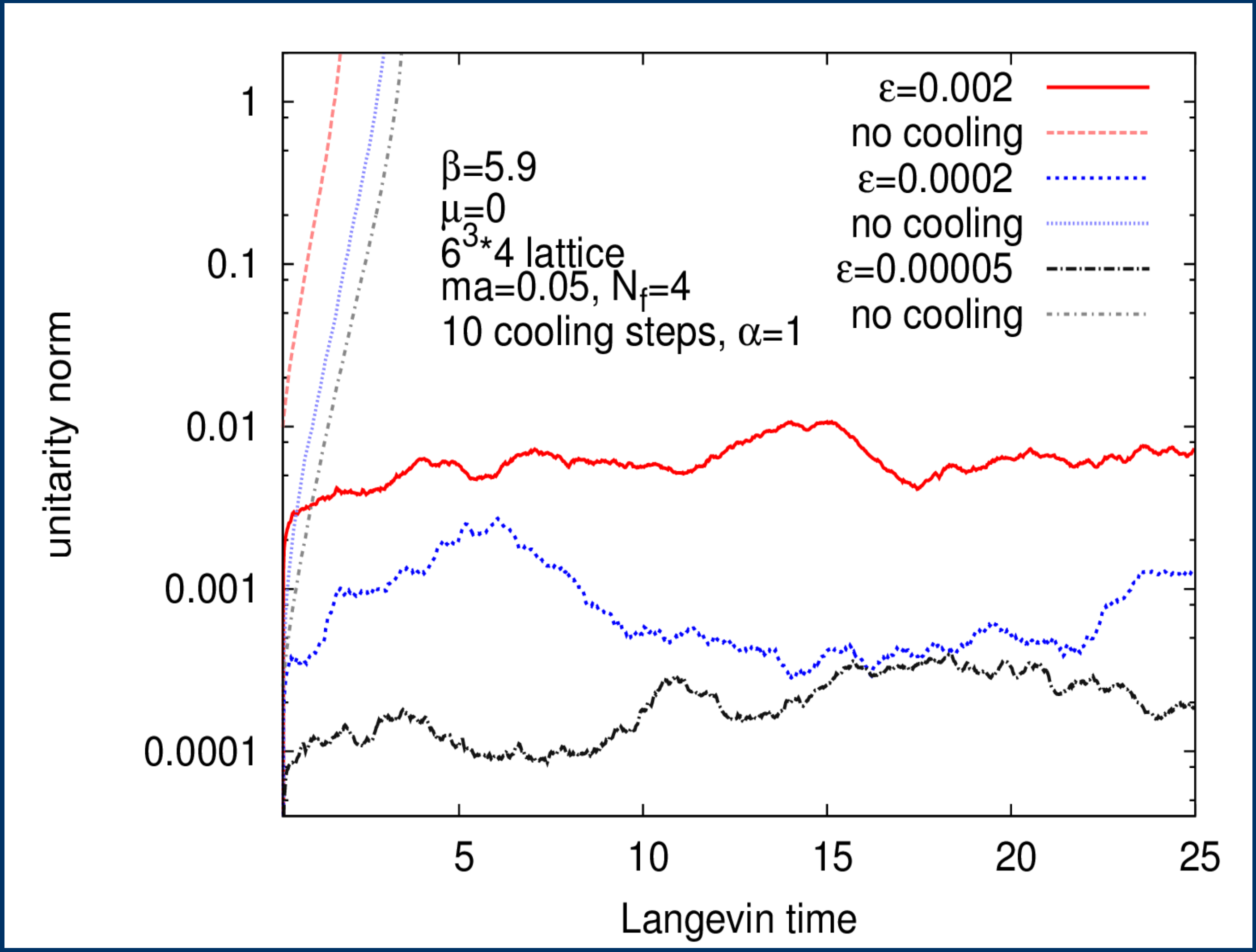
$$M'_{\nu a}(x,y,z)=D_{az\nu} M(x,y)$$

Estimated using random sources
1 CG solution per update

Zero chemical potential

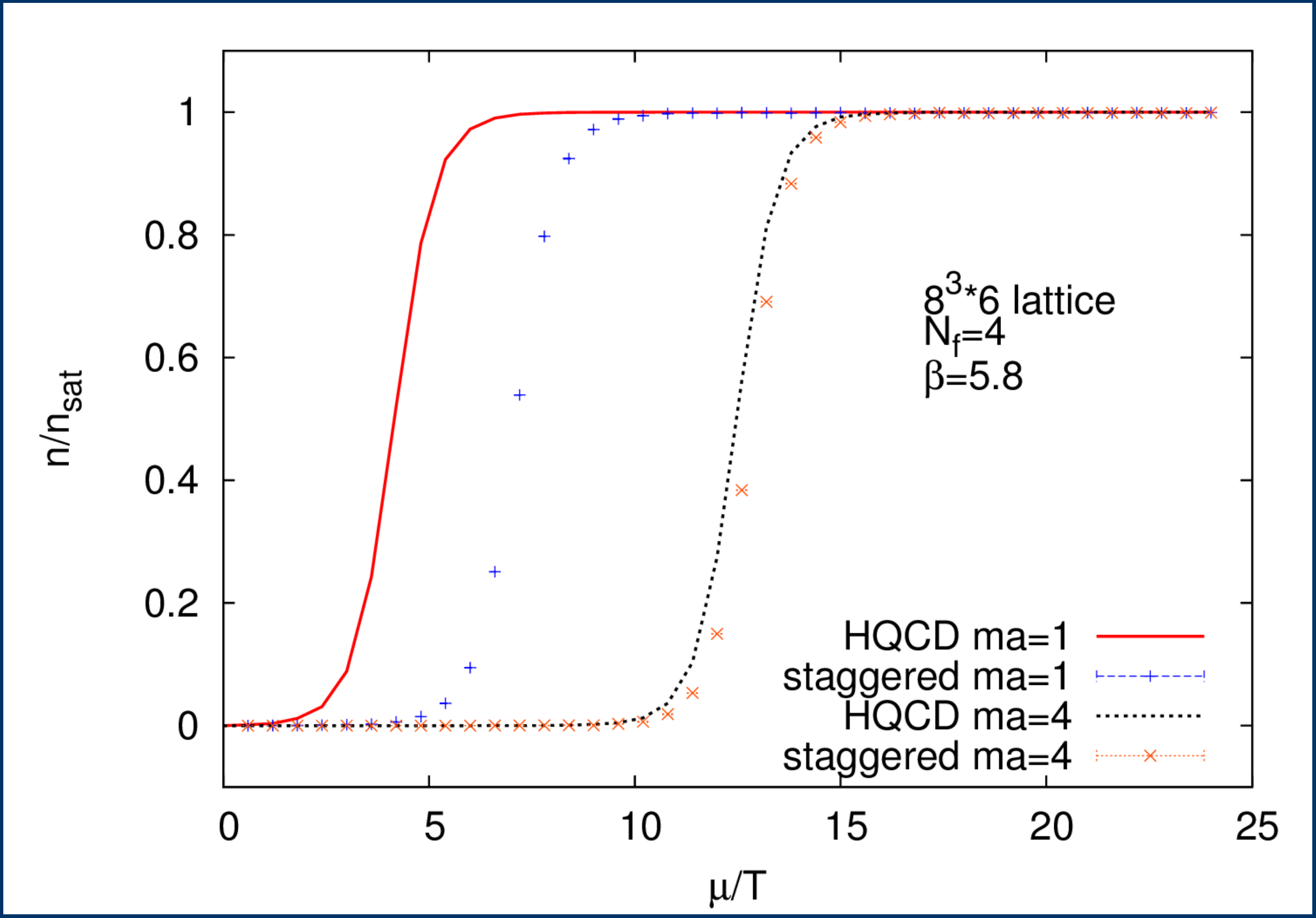
Drift is built from random numbers   real only on average

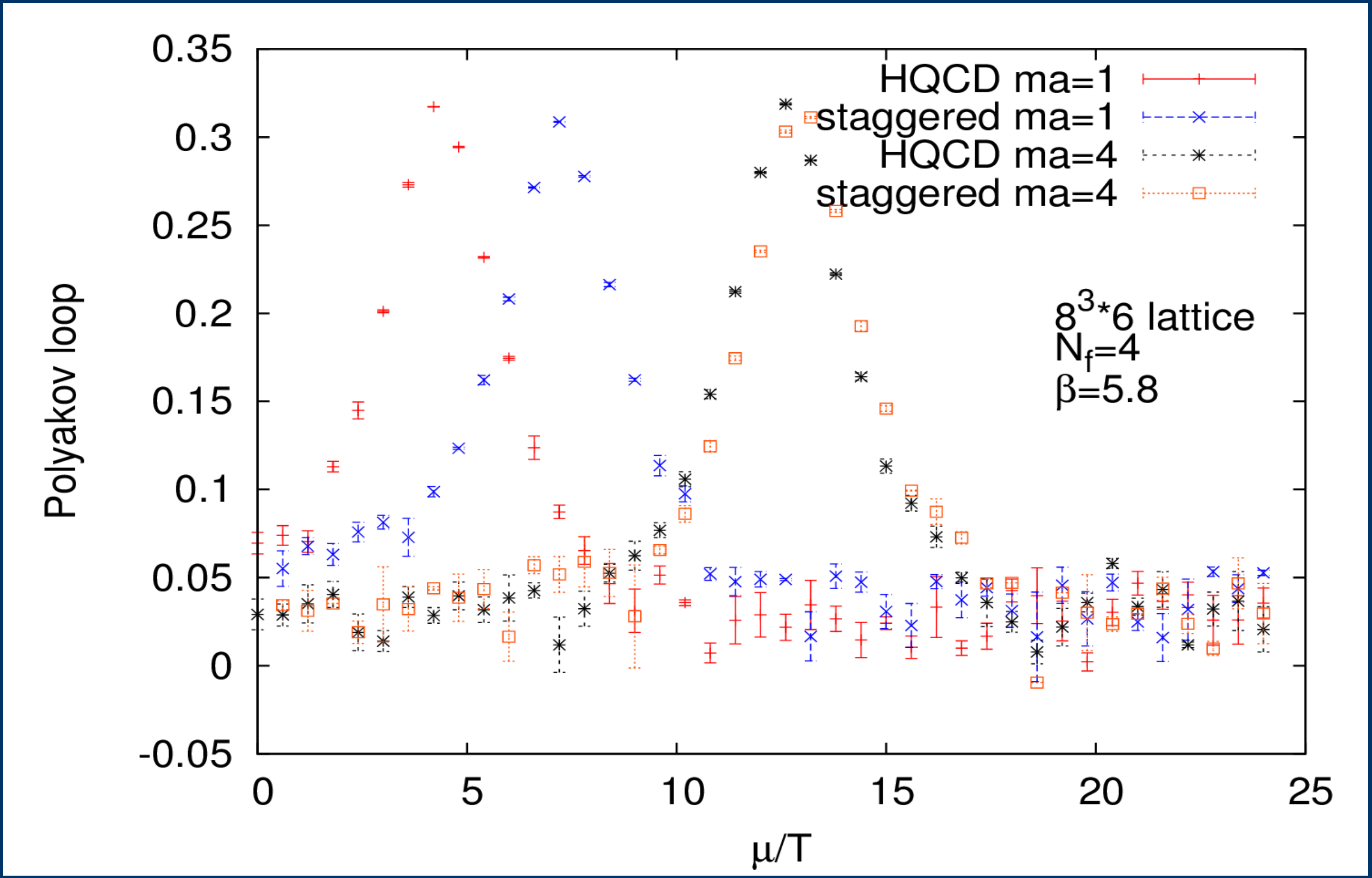
Cooling is essential already for small (or zero) mu



Comparison of HQCD to full QCD

Qualitatively similar, chemical potential “rescaled”





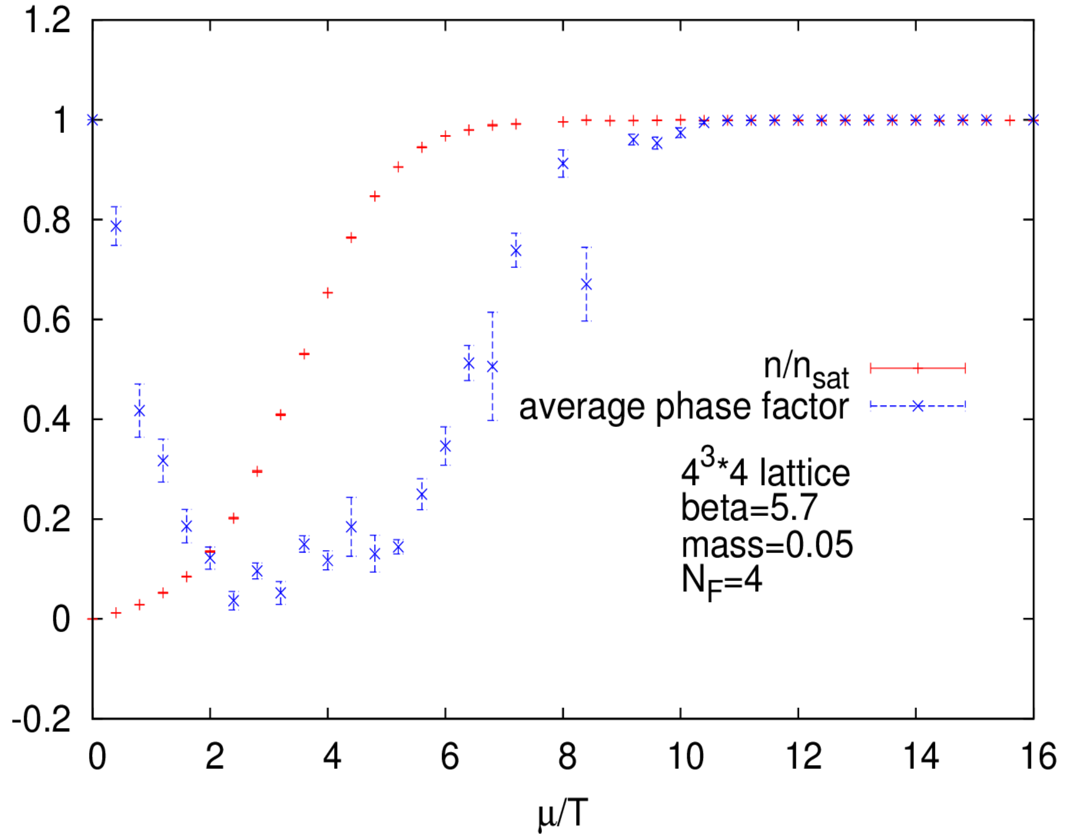
Conclusion

QCD = HQCD for quark mass > 4

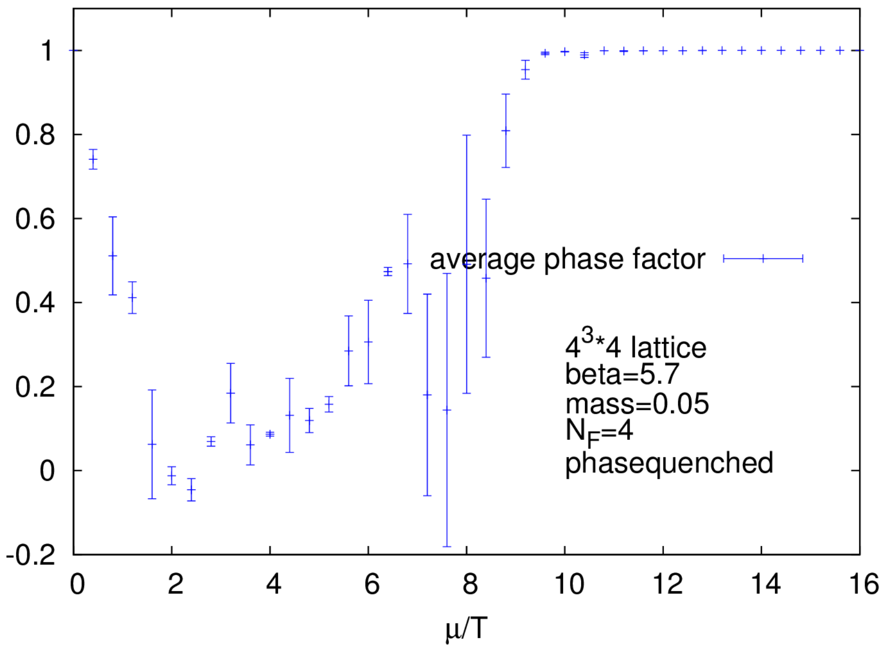
(For large mass) HQCD is qualitatively similar to QCD

Average sign of the fermion determinant for small mass

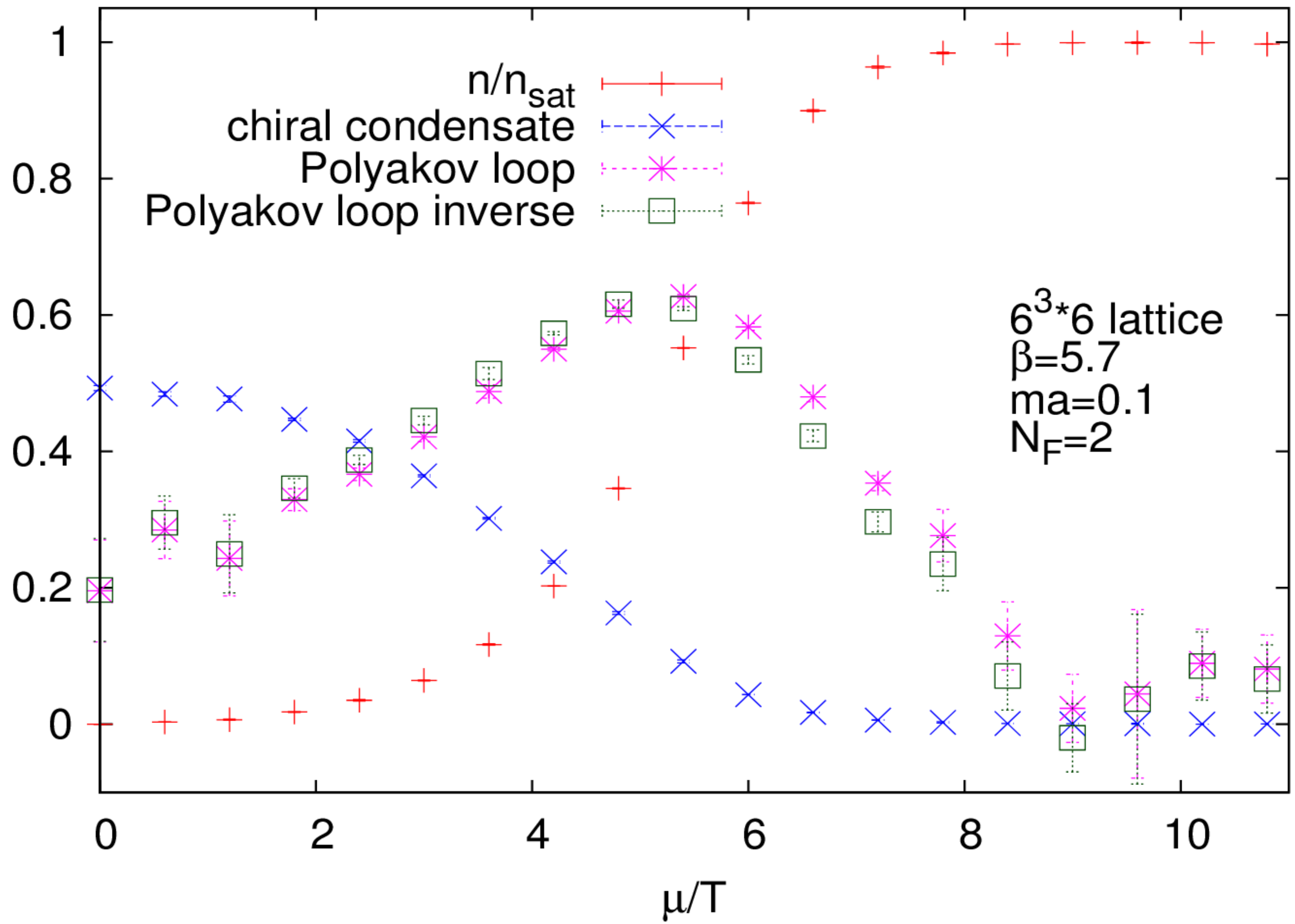
Costly observable, only on small latices possible



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



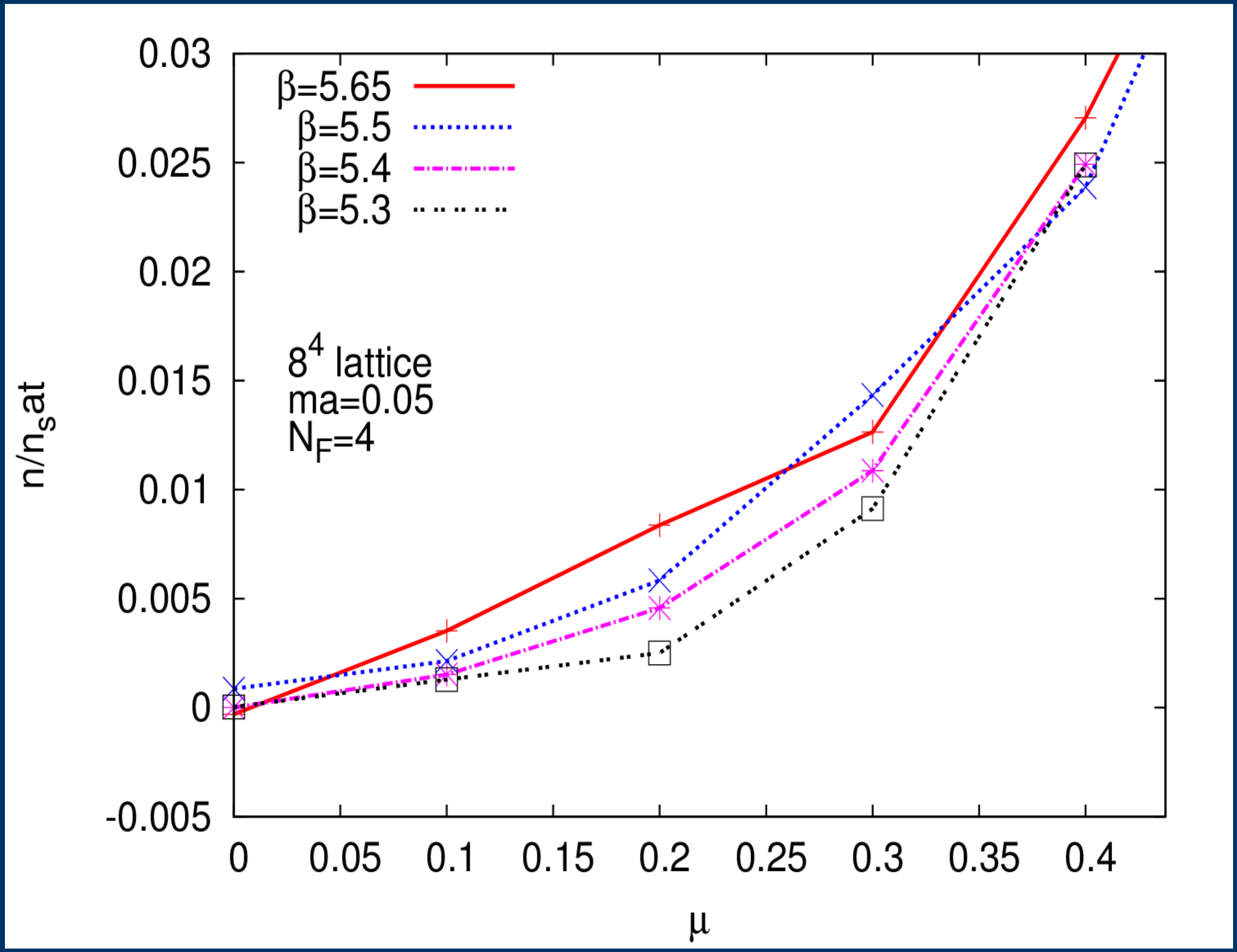
Horizontal slice of phase diagram



Silver Blaze phenomenon

No dependence on chemical potential for small chemical potential

Zero temperature physics



Finite size effects important

Consistent with Silver Blaze

Conclusions

New algorithm for Complex Langevin of gauge theories:
   Gauge cooling

Tested on exactly solvable toy model Polyakov chain
Results for HQCD with heavy quarks with chemical potential
     Validated with reweighting

Results for full QCD with light quarks
   No sign or overlap problem
   CLE works all the way into saturation region
   Low temperatures are more demanding