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, PLB (2014)

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

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

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

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

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

Non-zero chemical potential

For nonzero chemical potential, the fermion determinant is complex

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

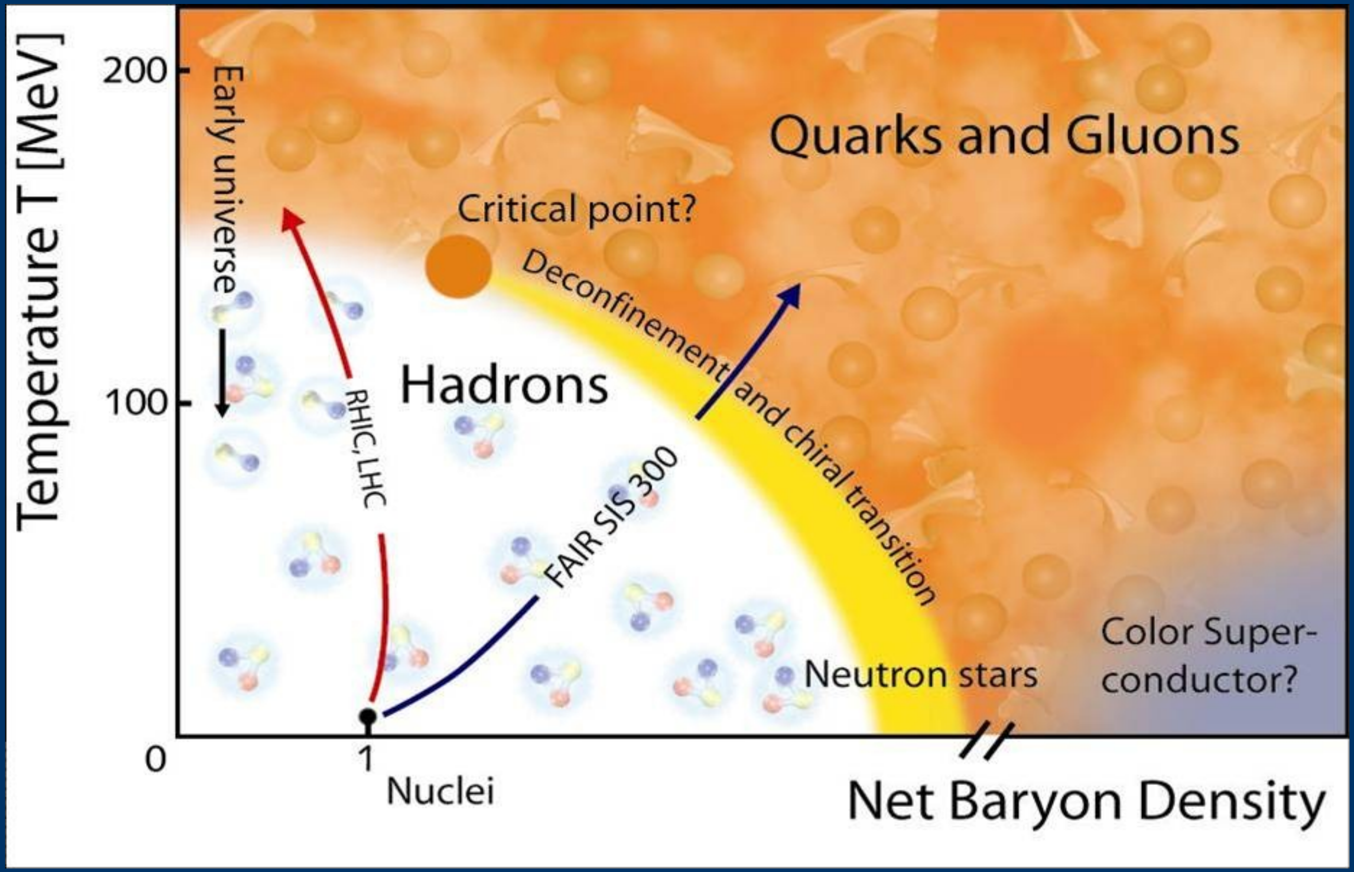
Sign problem ⟶ Naïve Monte-Carlo breaks down

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

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

$$= \frac{\langle F \det M(\mu)/R \rangle_R}{\langle \det M(\mu)/R \rangle_R}$$

$$R = \det M(\mu = 0),\ |\det M(\mu)|, \text{ etc.}$$

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

$\Delta f(\mu, T)$ =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 $(\mu/T)^2$

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

Canonical Ensemble, denstity of states, ...

Stochastic quantisation   Works also for large chemical potential

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
Full QCD with light quarks: Sexty '13

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, ...

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

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

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

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

Non-real action problems and CLE

1. Real-time physics

“Hardest” sign problem e^{iS_M}

Studies on Oscillator, pure gauge theory

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

2. Theta-Term

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

see Lorenzo Bongiovanni's talk

[Bongiovanni et al, (2013)]

3. Non-zero density

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

Bose Gas, SU(3) spin model, HQCD, full QCD with light quarks

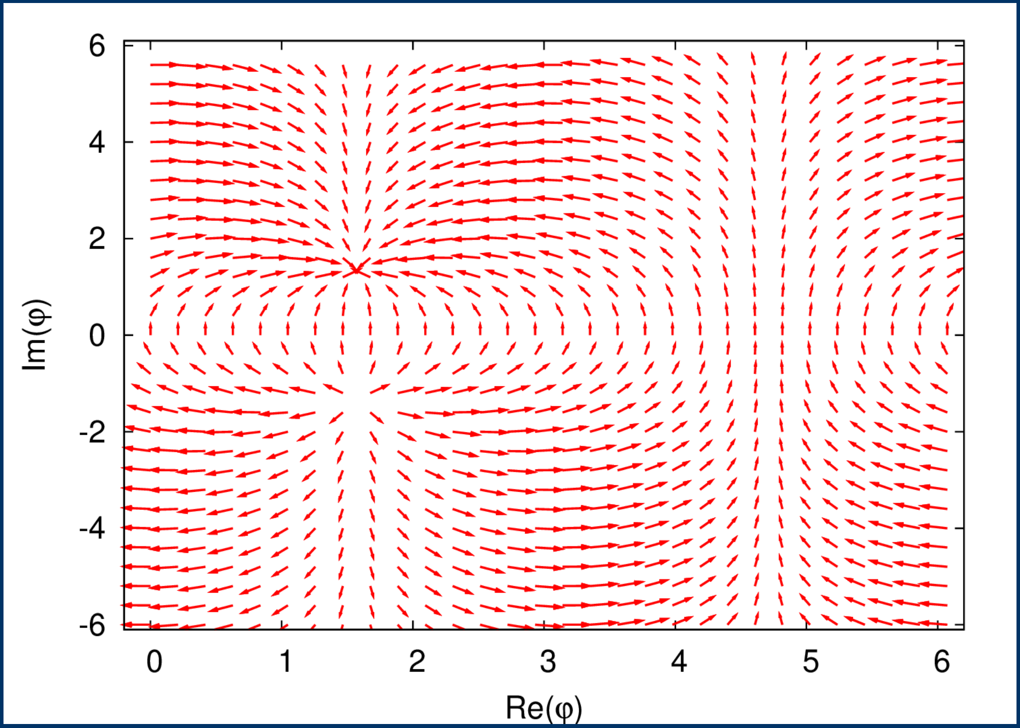
[Aarts, Stamatescu (2008), Aarts(2008), Aarts and James (2010)]
[Seiler, Sexty, Stamatescu (2013), Sexty (2014)]

Proof of convergence

Assuming fast decay
and a holomorphic action

see Erhard Seiler's talk

Typical drift structure



Runaway trajectories present

Runaway if $\mathrm{Im}\,\varphi$ stays at $\frac{3}{2}\pi$

In continuum probabilty of a runaway=0

Solution: small stepsize
Adaptive stepsize control

Non-holomorphic action

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

complex logarithm has a branch cut
meromorphic drift
Is it a problem?
see Kim Splittorff's talk
Erhard Seiler's talk

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

λ_a Gellmann matrices

complexified link variables

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

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

Gaugefixing in SU(2) one plaquette model

Berges, Sexty '08

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

See Gert Aarts' talk for connection with thimbles

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

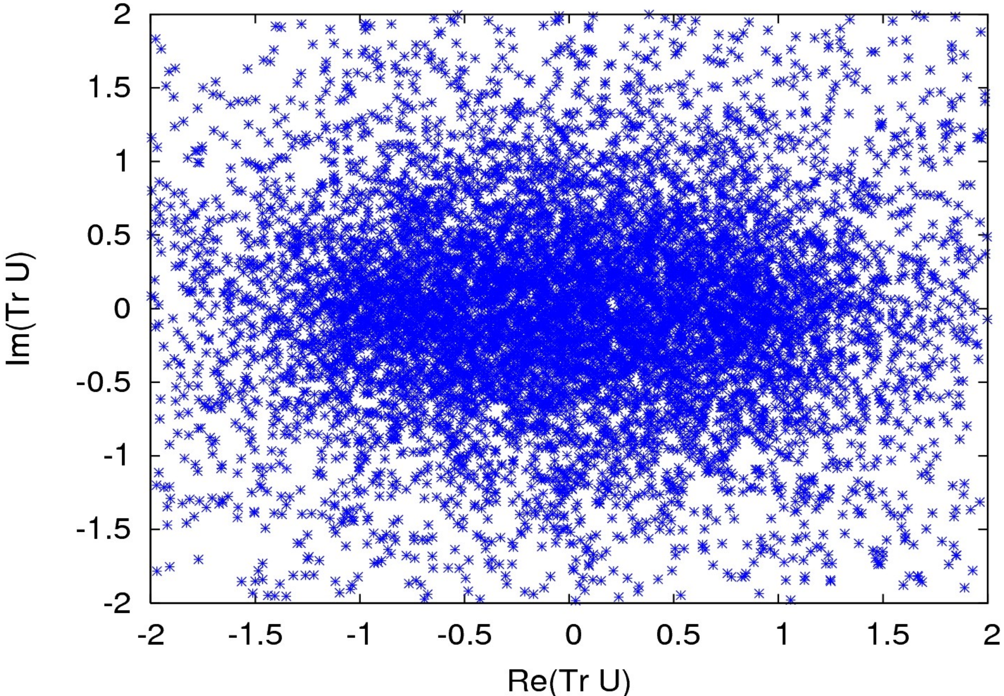
“gauge” symmetry: $U \rightarrow W U W^{-1}$ complexified theory: $U, W \in SL(2, \mathbb{C})$

After each Langevin timestep: fix gauge condition

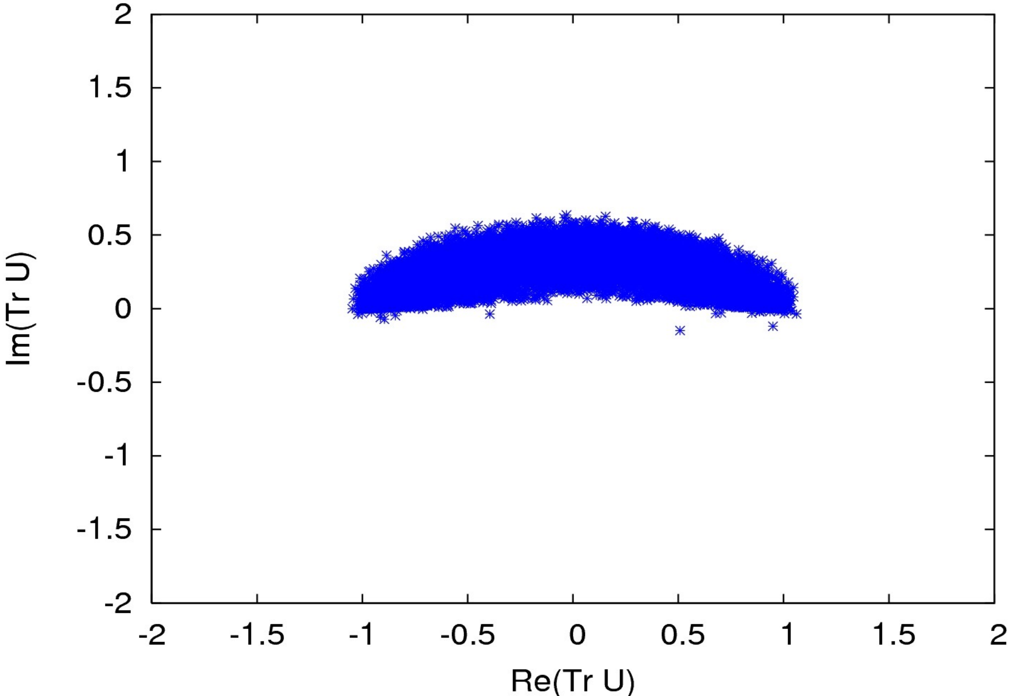
$U = a\mathbf{1} + i\sqrt{1-a^2}\,\sigma_3 \qquad b_i = (0,0,\sqrt{1-a^2})$

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 to wrong results

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

Using gauge transformations in SL(N,C)

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

$v_a(x)$ 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

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

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

Dynamical steps are interspersed with several gauge cooling steps

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

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

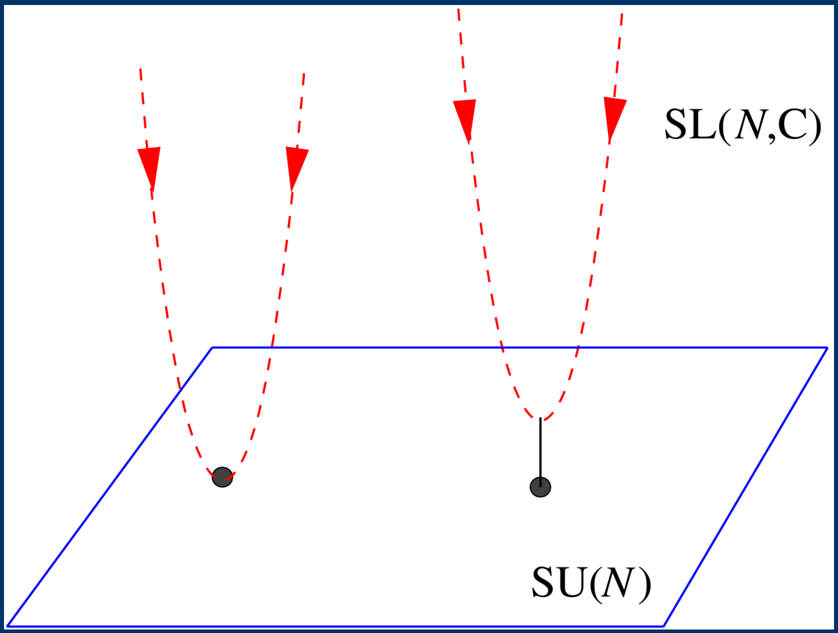
Empirical observation:
Cooling is effective for $\beta > \beta_{min}$

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

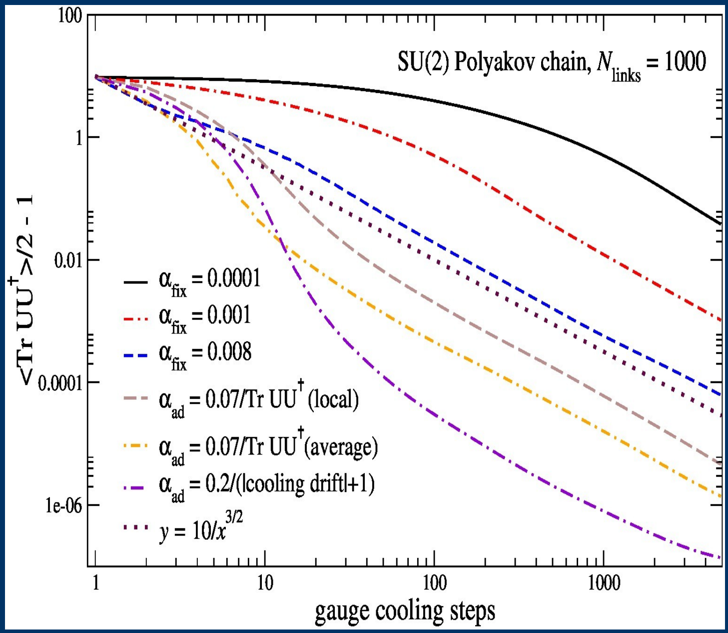
See also Nucu Stamatescu's talk

Adaptive cooling, Fourier accelerated cooling

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

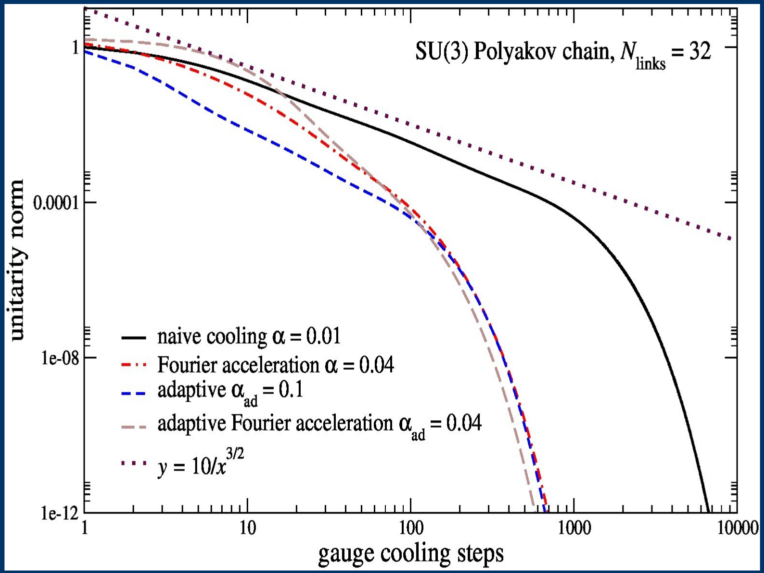


Get to minimum quickest



Stepsize dependent on gradient
Adaptive cooling

Low momentum modes cool slower
Fourier accelerated cooling



Heavy Quark QCD at nonzero chemical potential

Hopping parameter expansion of the fermion determinant
Spatial hoppings are dropped

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

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

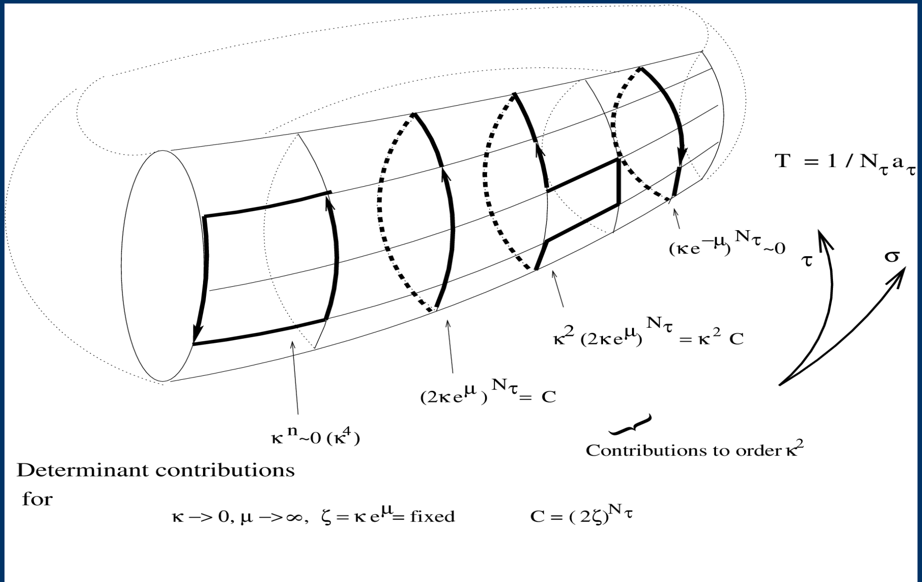
$$S = S_W[U_\mu] + \ln \mathrm{Det}\, M(\mu)$$

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

$$R = |\mathrm{Det}\, M|$$

CLE study using gaugecooling

[Seiler, Sexty, Stamatescu (2012)]



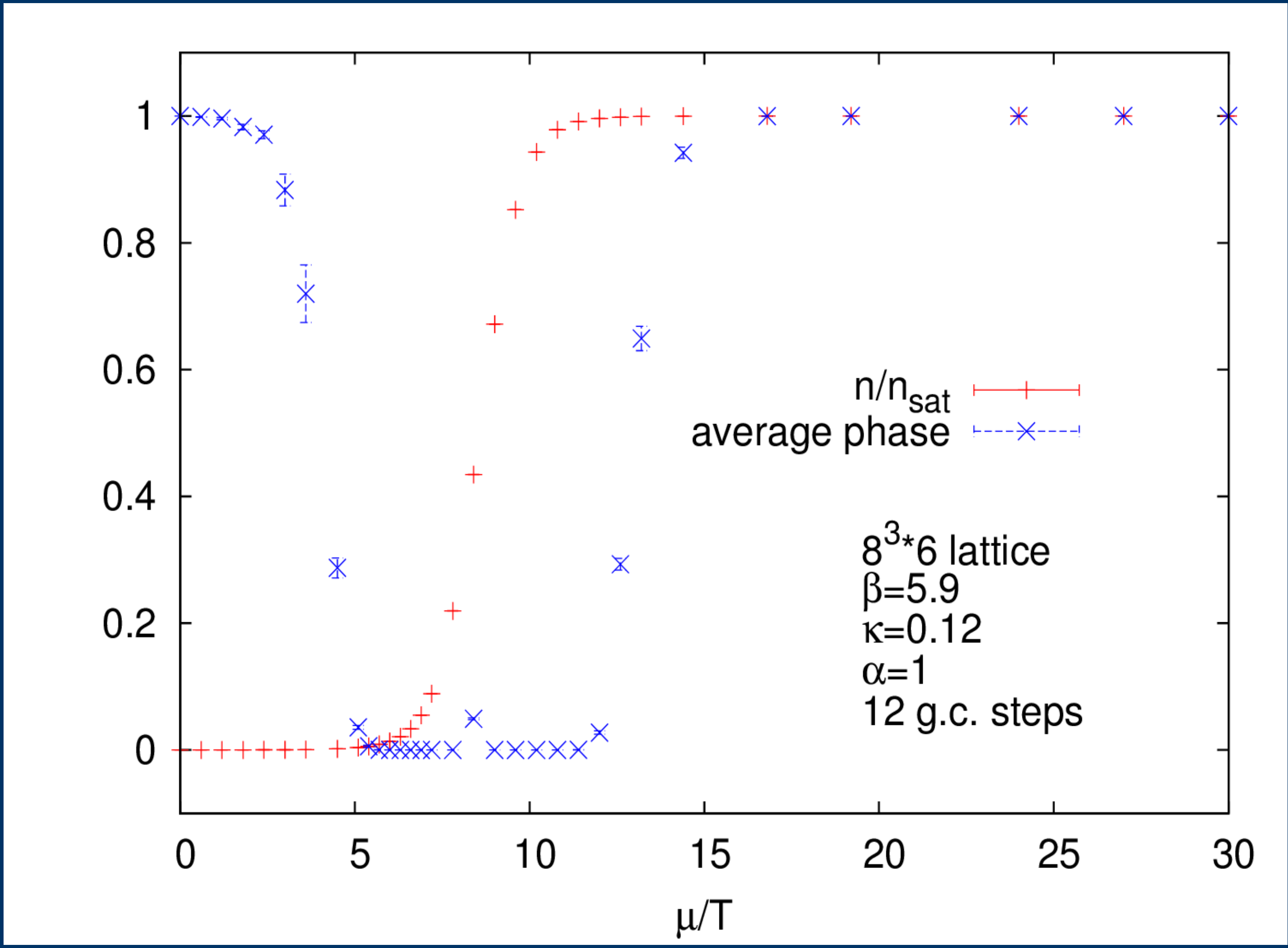
See Nucu Stamatescu's talk
for more details

Fermion density:

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

average phase:

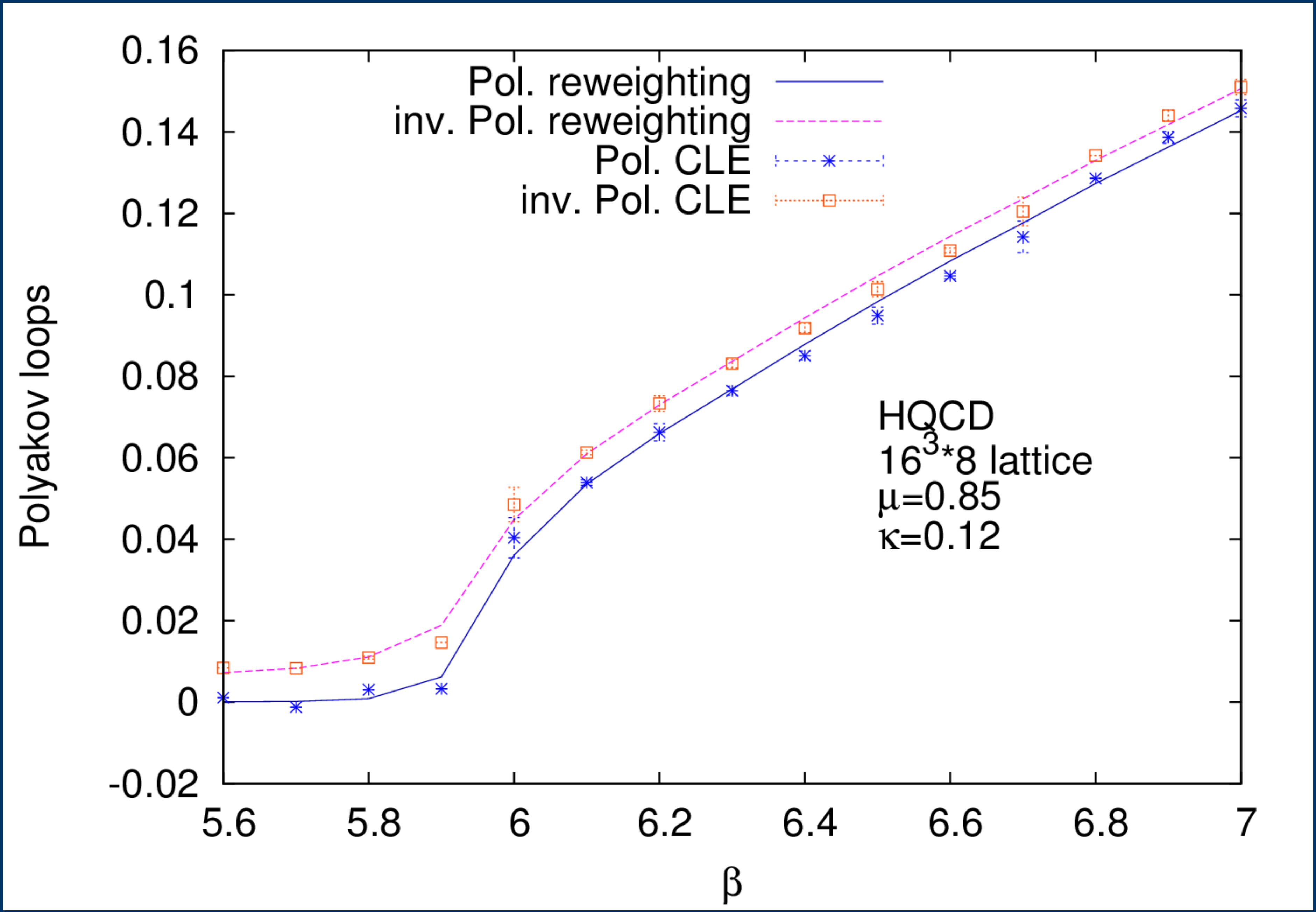
$$\langle \exp(2 i \varphi) \rangle = \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle$$



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

Sign problem is absent at small or large μ

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



Large lattice:
phase transition clearly visible

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

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

Langevin equation

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

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

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

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

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

Noisy inversion

Choose random vector with Gaussian (real) random numbers

η_i, satisfying $\quad \langle \eta_i \rangle = 0, \ \ \langle \eta_i \eta_j \rangle = \delta_{ij}$

Solve (with CG)

$$\psi = (M^+)^{-1} \eta$$

Build the product

$$\psi^+ M' \eta = \eta^+ M^{-1} M' \eta$$

Using many random vectors, the average is:

$$\langle \eta^+ M^{-1} M' \eta \rangle = \langle \eta_i \eta_j \rangle M^{-1}_{ik} M'_{kj} = \mathrm{Tr}\left(M^{-1} M' \right)$$

In $\epsilon \to 0$ limit infinitely many estimators in every $\Delta\epsilon$ step

↓

1 noisy vector is enough to estimate the inverse

1 CG step per gauge update (main cost of the simulation)

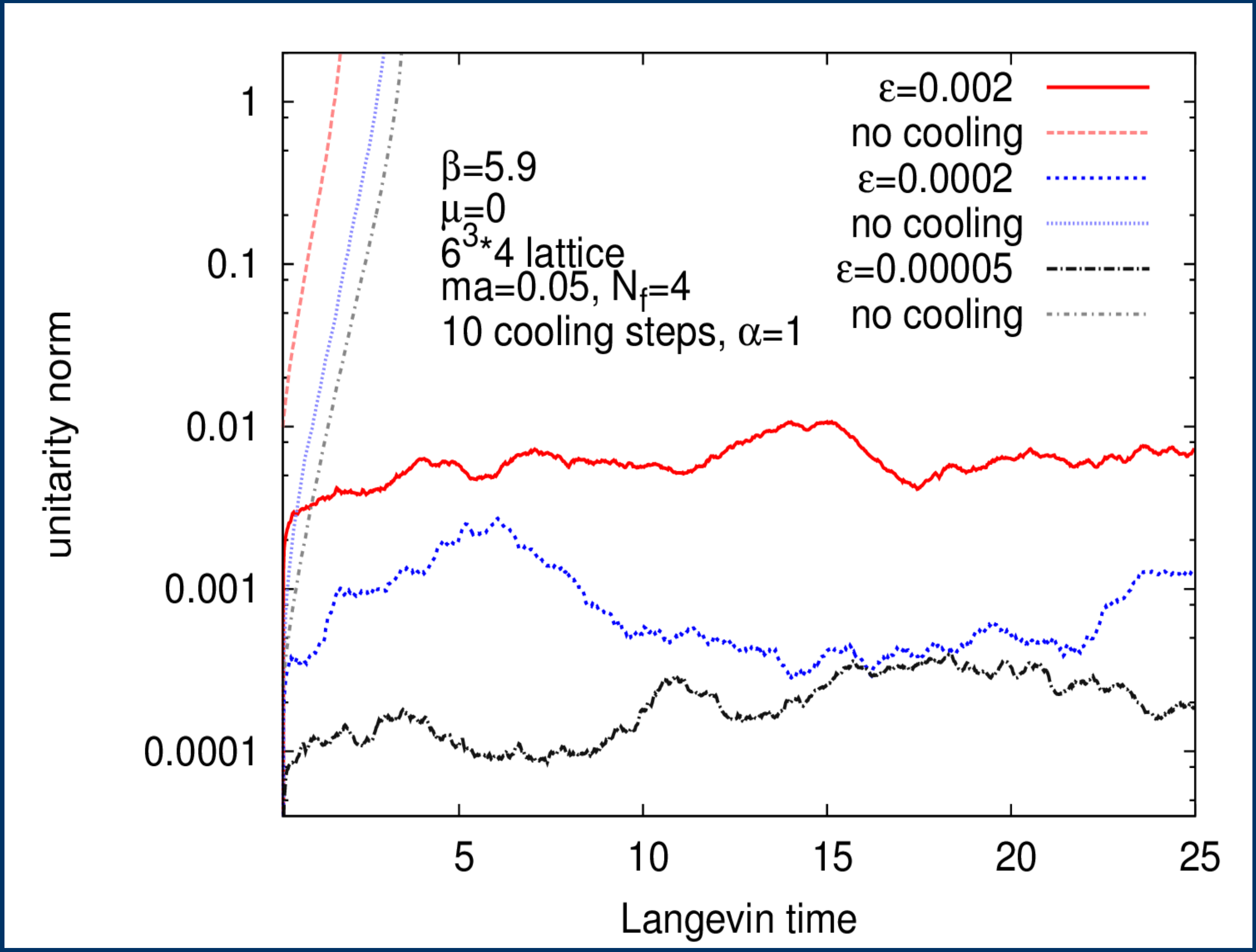
Can also be formulated as pseudofermion algorithm

[Batrouni et al. (1985), Fukugita et al. (1986)]

Zero chemical potential

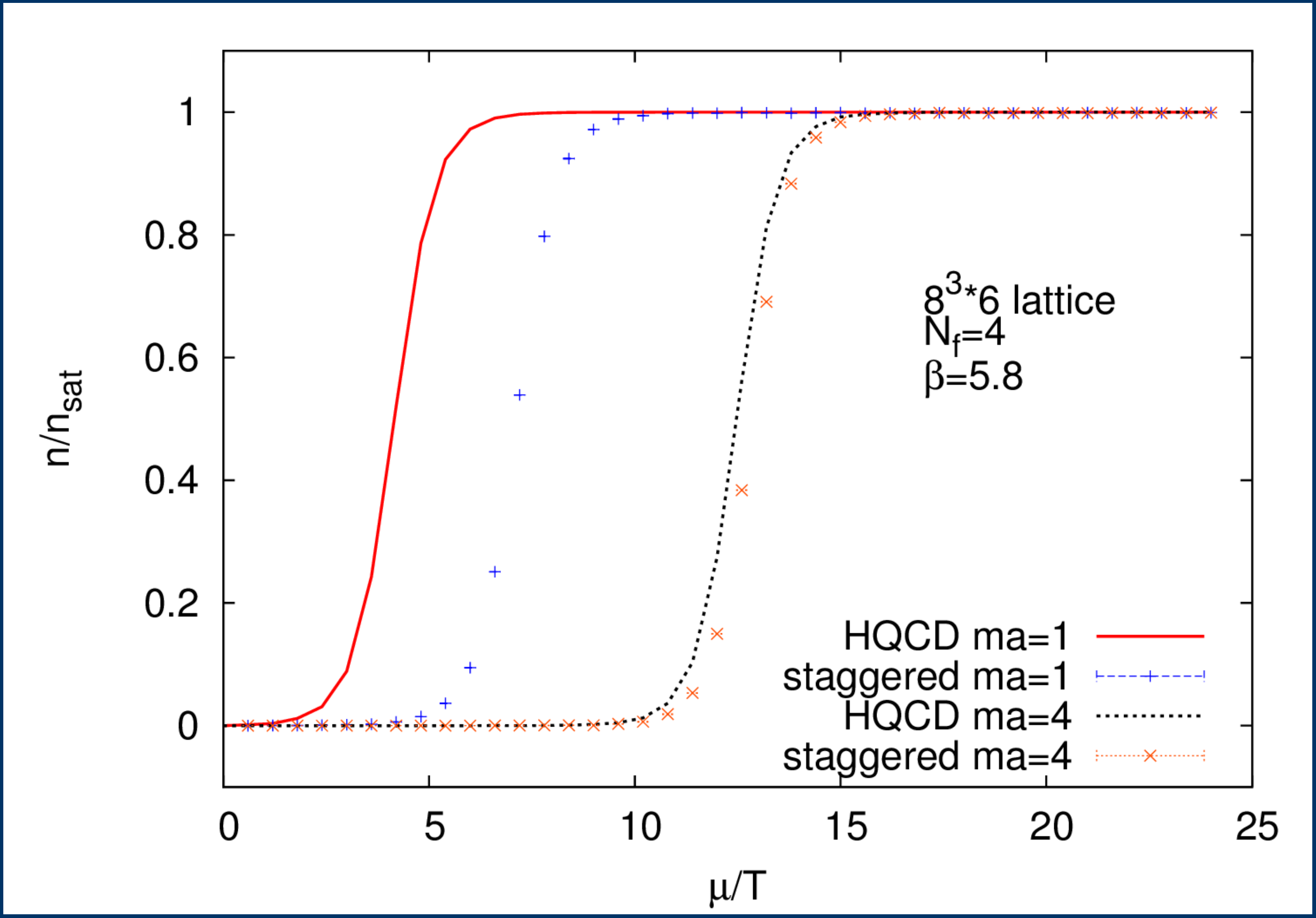
Drift is built from random numbers   real only on average

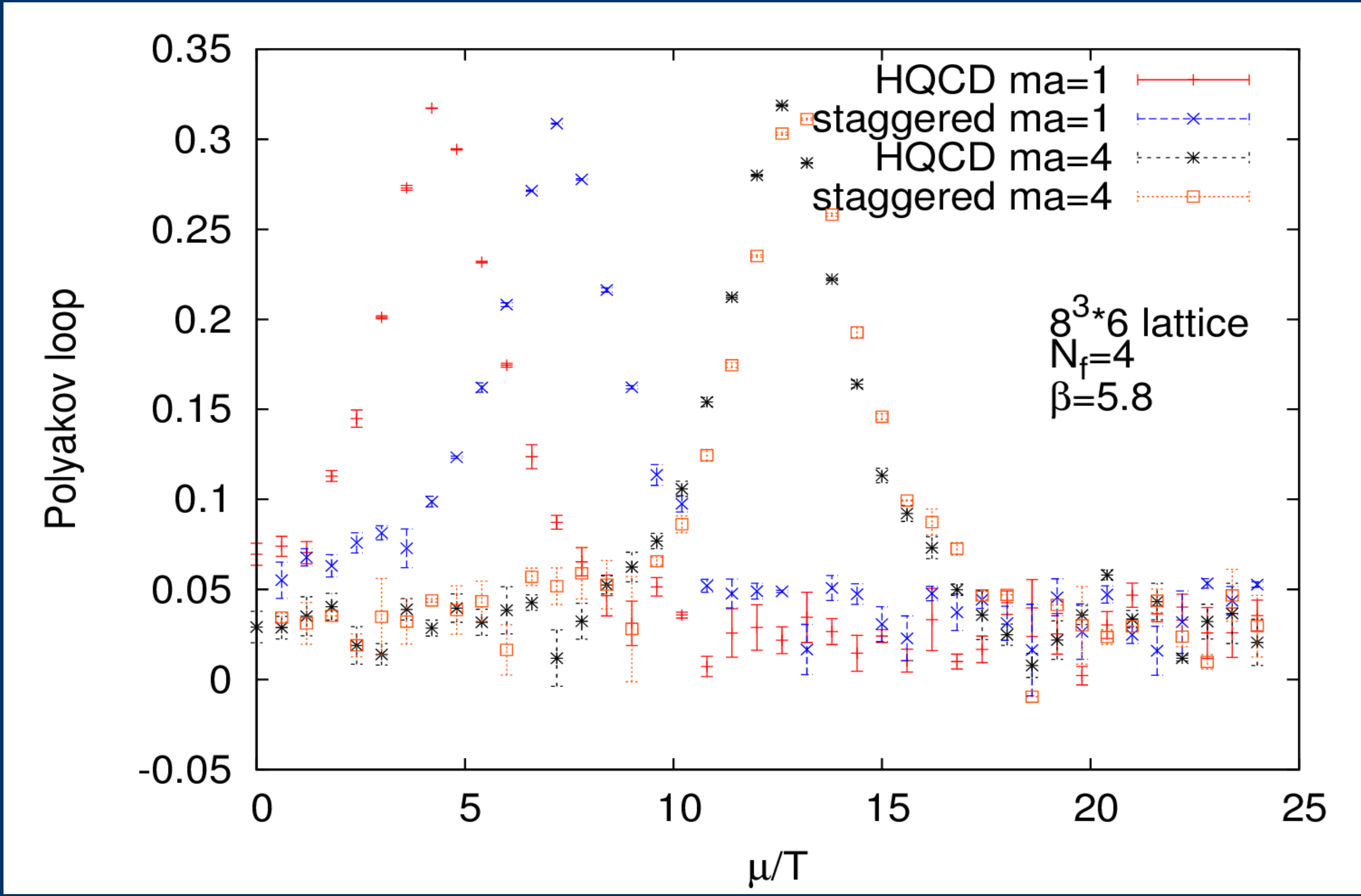
Cooling is essential already for small (or zero) mu



Comparison of HQCD to full QCD

Qualitatively similar, chemical potential "rescaled"





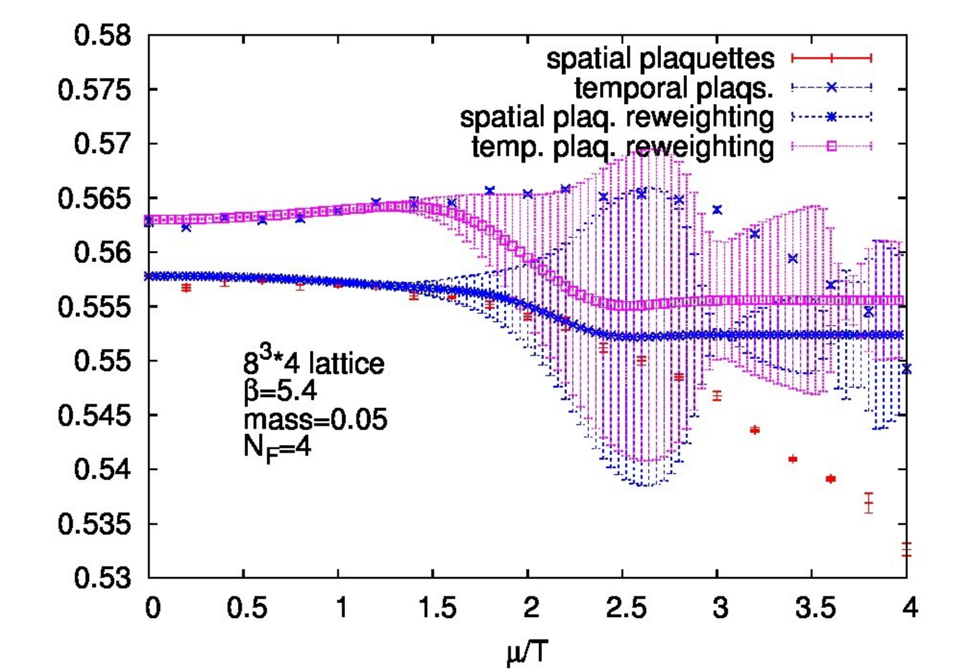
Conclusion

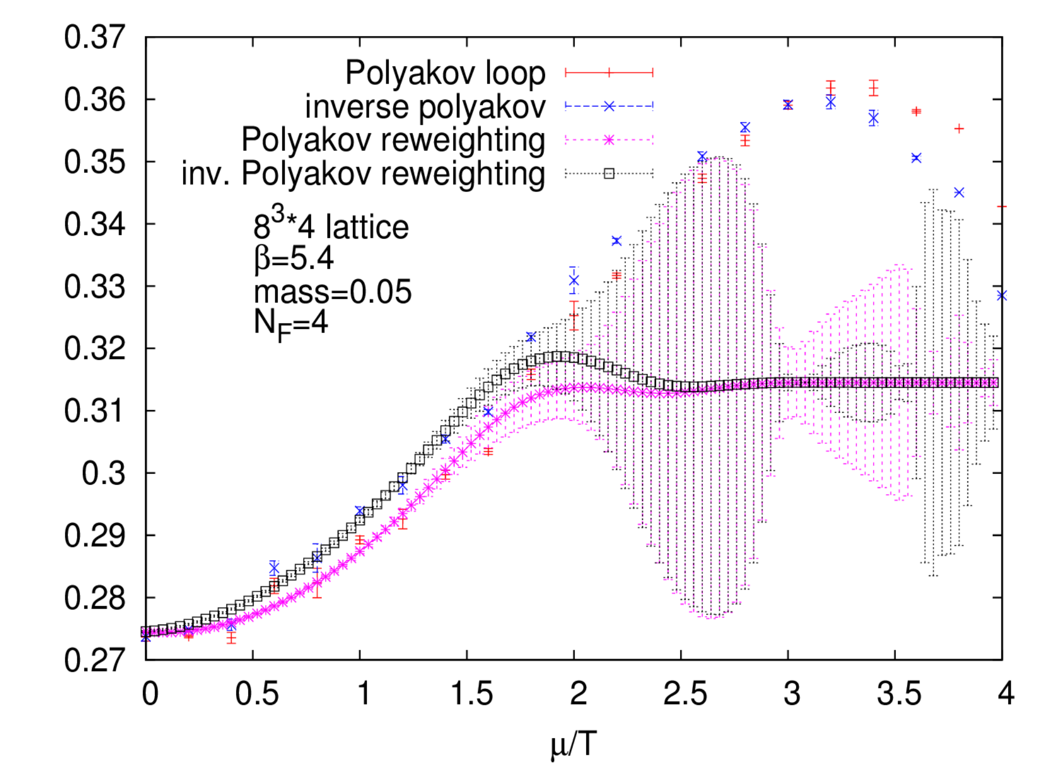
QCD = HQCD for quark mass > 4/a

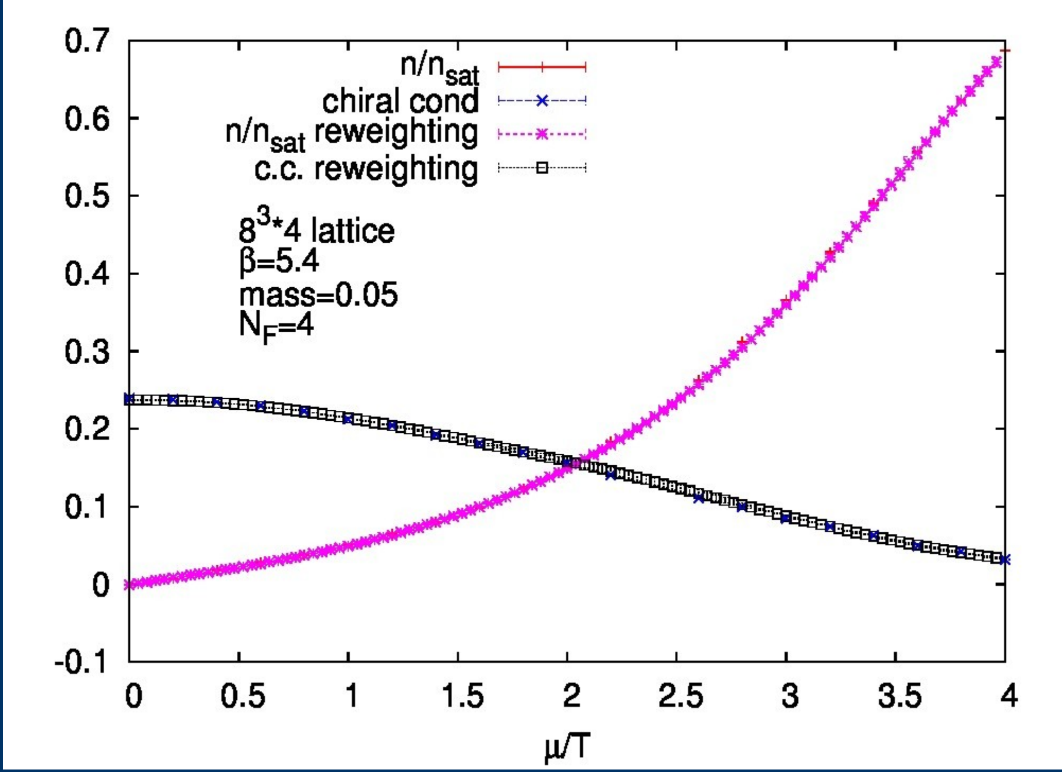
(For large mass) HQCD is qualitatively similar to QCD

Comparison with reweighting

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



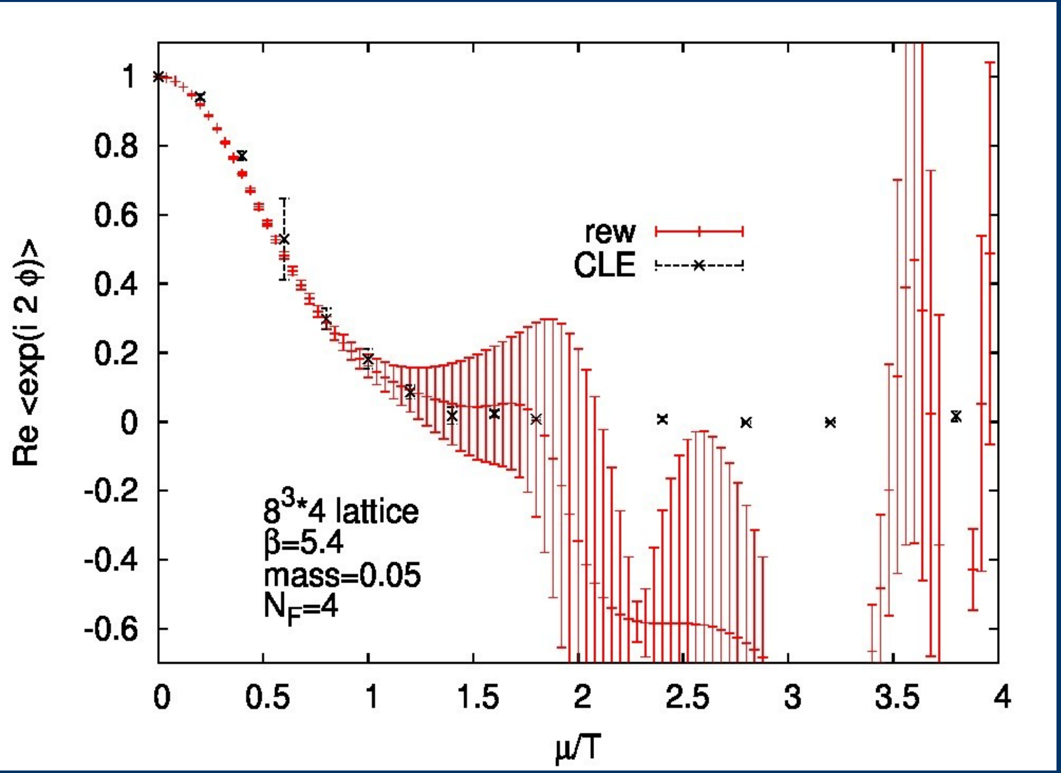


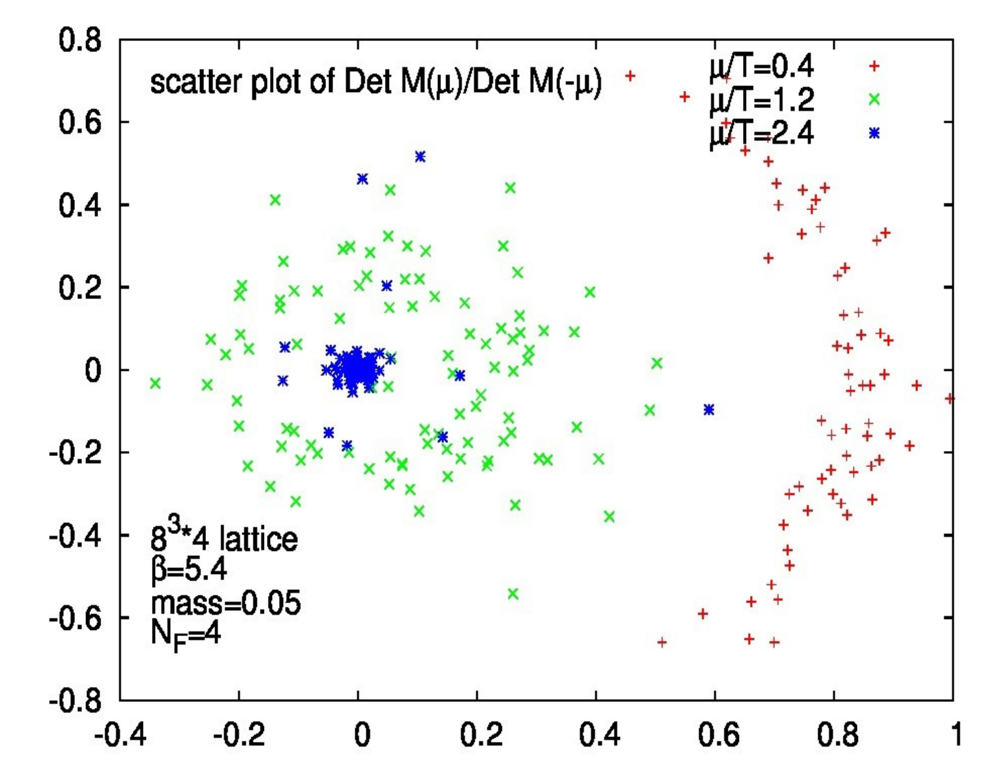


[Fodor, Katz, Sexty (in prep.)]

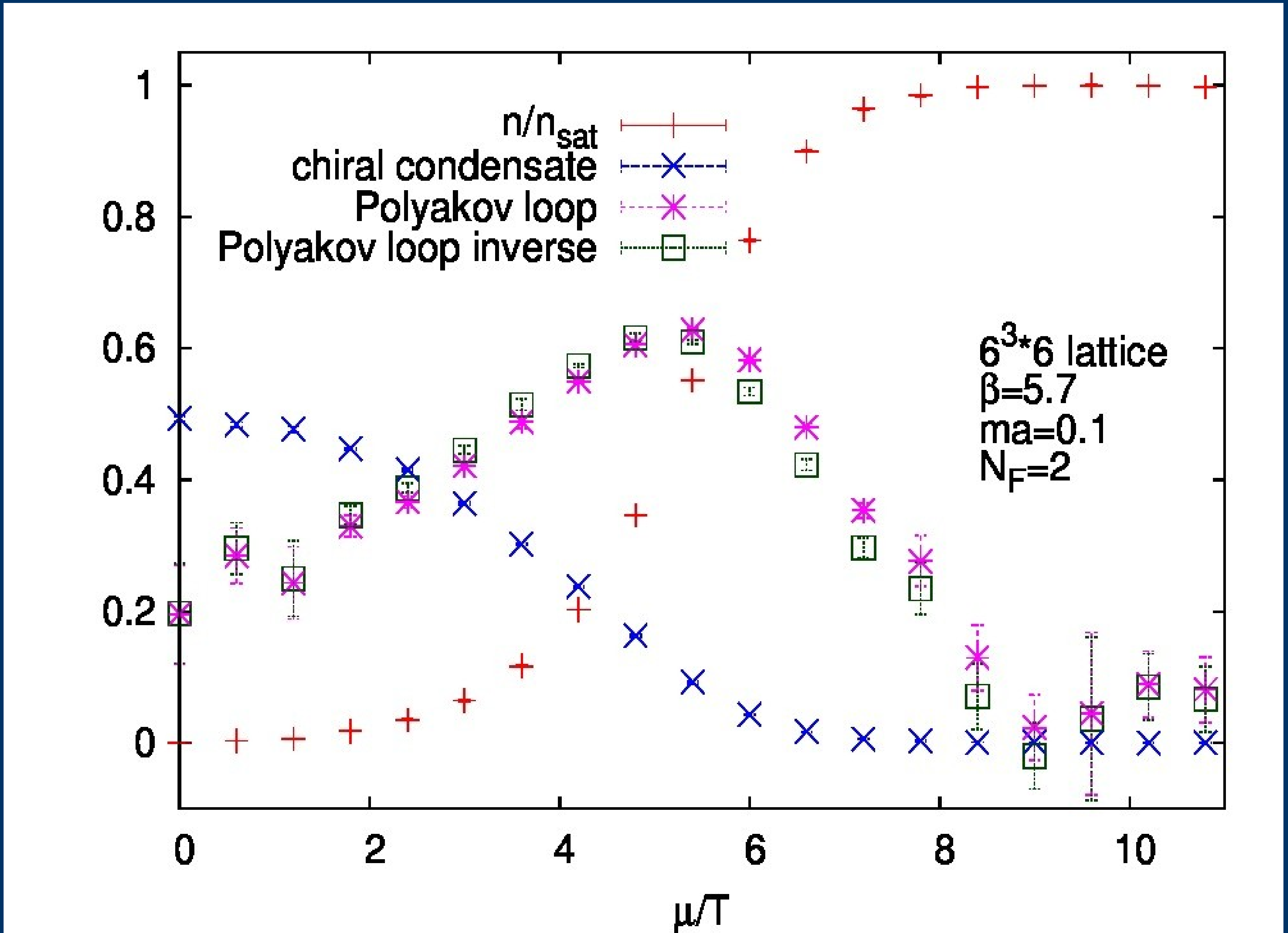
Sign problem

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



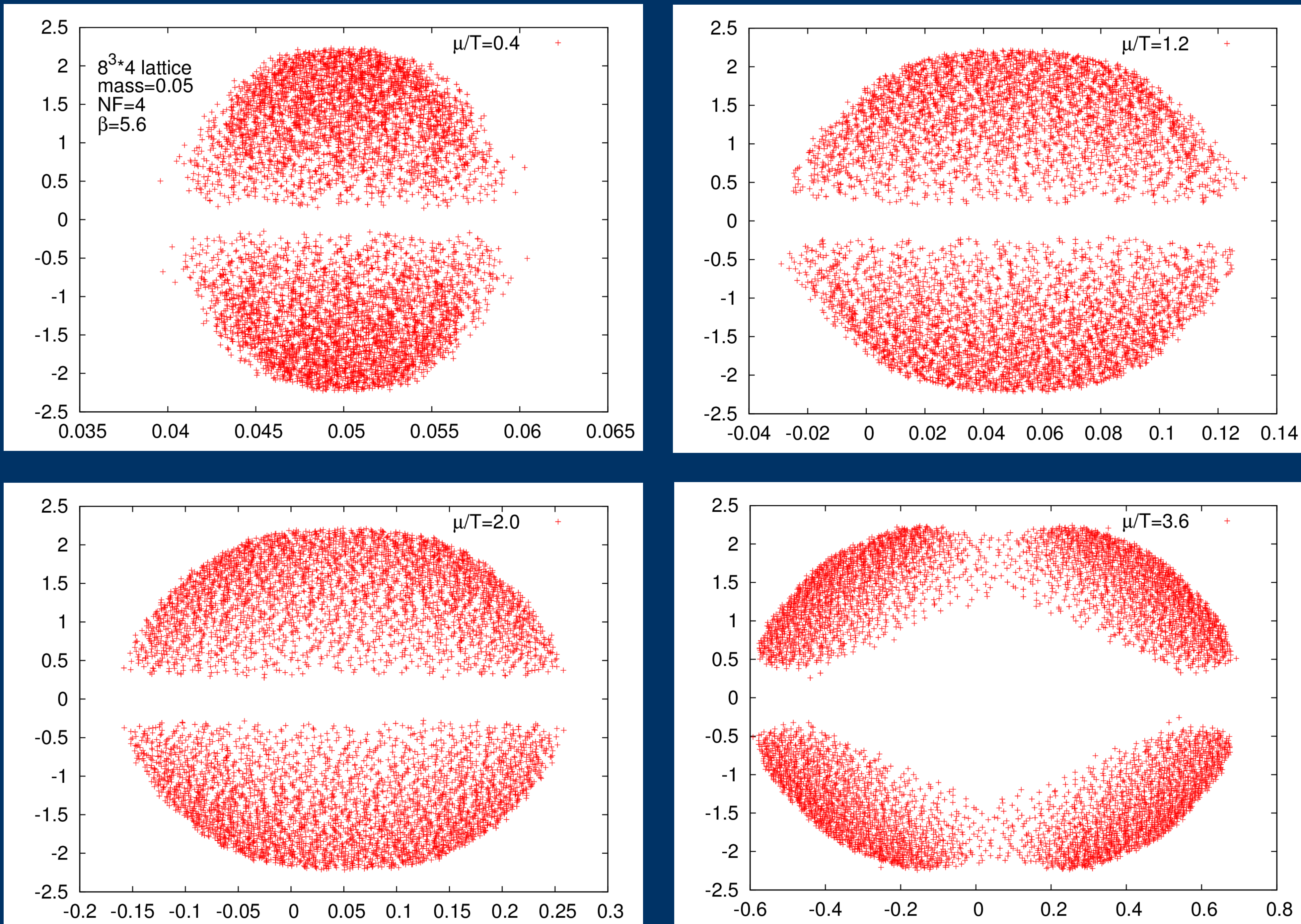


$$\langle \exp(2 i \varphi) \rangle = \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle$$



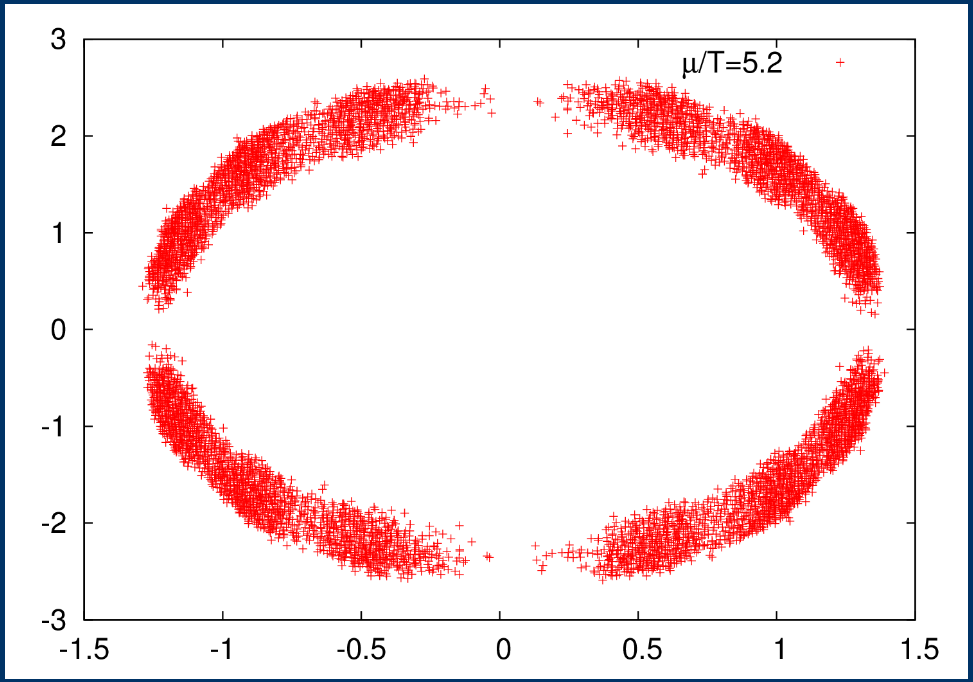
n/n_sat
chiral condensate
Polyakov loop
Polyakov loop inverse
6^3*6 lattice
β=5.7
ma=0.1
N_F=2
μ/T
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10

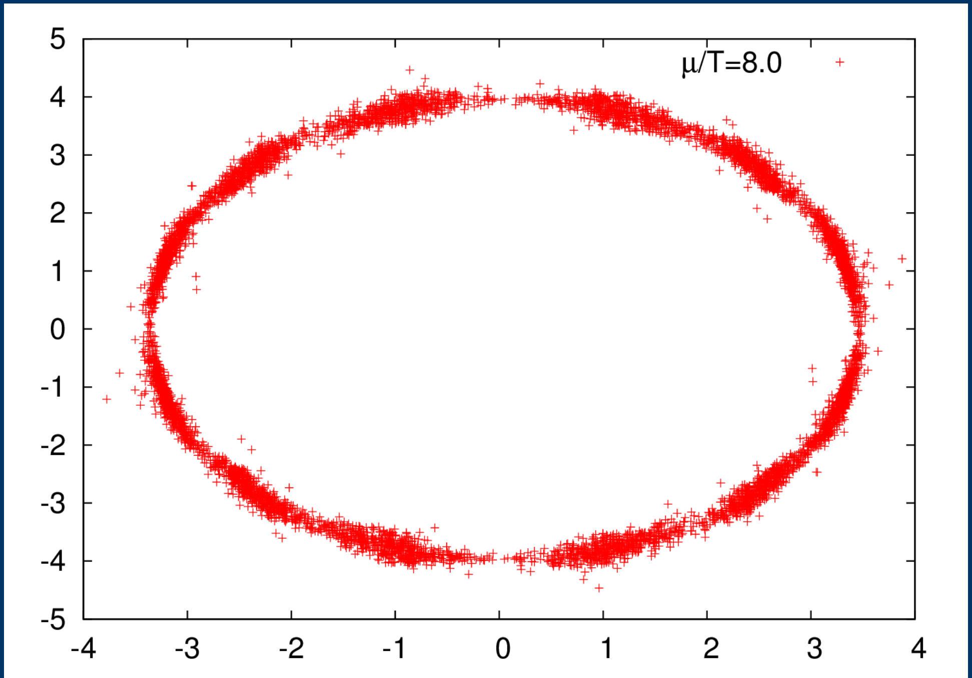
Spectrum of the Dirac Operator $N_F = 4$ staggered



Spectrum of the Dirac Operator

Large chemical potential, towards saturation





Conclusions

New algorithm for Complex Langevin of gauge theories:
- Gauge cooling

Tested on QCD 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
- Comparison with reweighting for small chem. pot.
- Low temperatures are more demanding