

Simulating full QCD at nonzero density using the Complex Langevin Equation

Dénes Sexty
Heidelberg University

QM2014, Darmstadt, 20th of May, 2014.

Collaborators:

Gert Aarts (Swansea), Lorenzo Bongiovanni (Swansea), Benjamin Jäger (Swansea), Erhard Seiler (MPI München), Ion Stamatescu (Heidelberg)

1. Introduction
2. 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:

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

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

Non-zero chemical potential

For nonzero chemical potential, the fermion determinant is complex

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

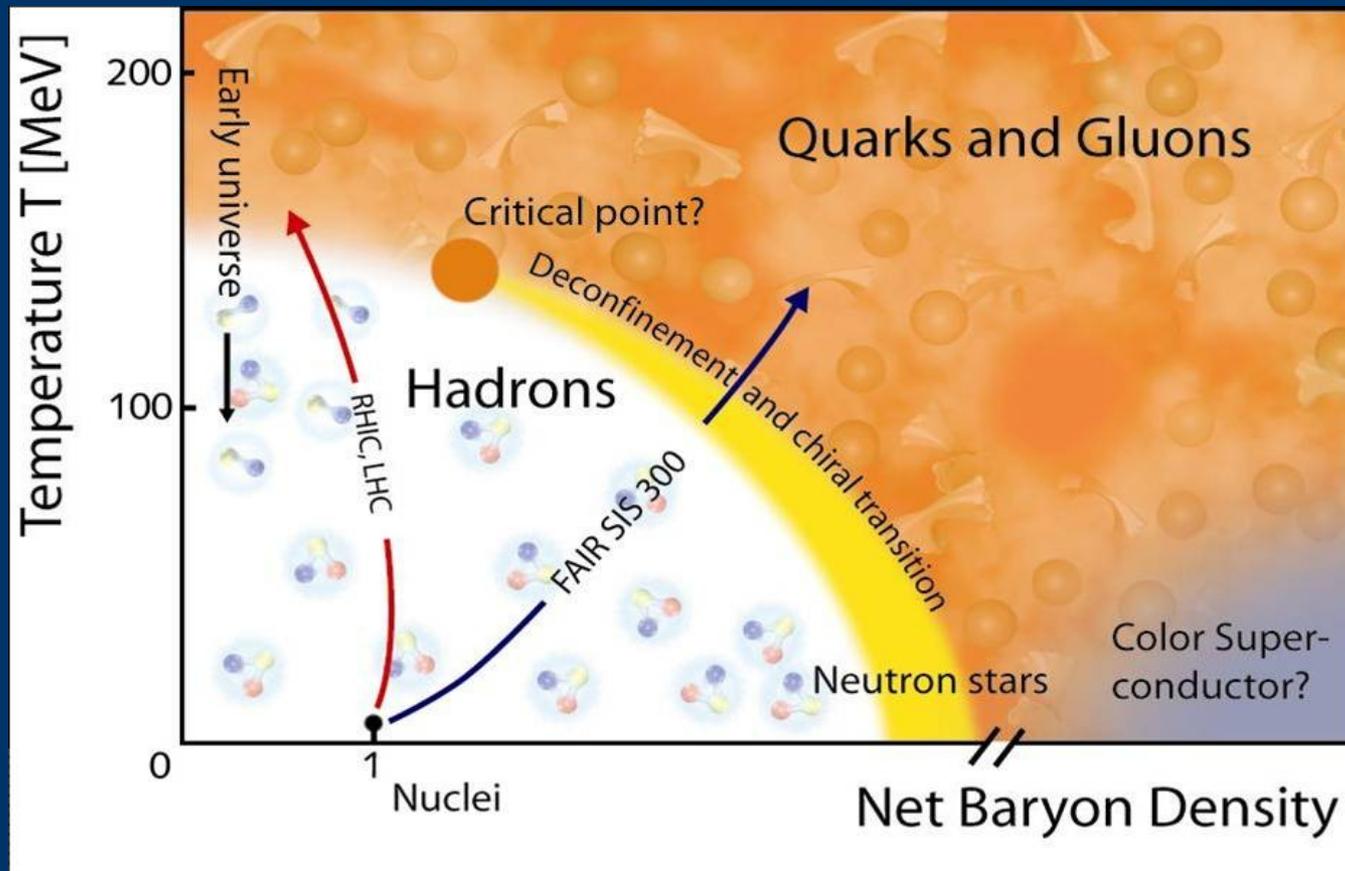
Sign problem \longrightarrow Naïve Monte-Carlo breaks down

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

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, density 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)

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:

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

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, ...

The field is complexified

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

real scalar \longrightarrow complex scalar

link variables: SU(N) \longrightarrow SL(N,C)
compact non-compact

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

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

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

[Bongiovanni et al, (2013)]

3. Non-zero density

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

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

[Aarts, Seiler, Stamatescu (2010)]

Runaway trajectories present

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

In continuum probability of a runaway=0

Solution: small stepsize
Adaptive stepsize control

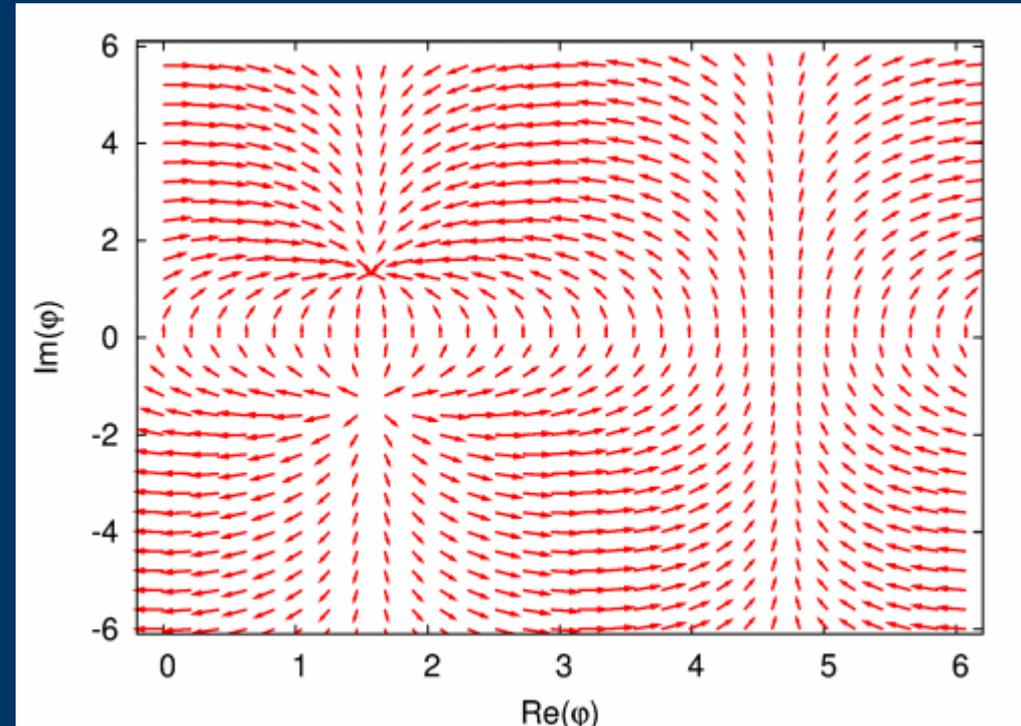
Non-holomorphic action

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

complex logarithm has a branch cut
meromorphic drift
Is it a problem?

[see also: Mollgaard, Splittorff (2013)]

Typical drift structure



Gauge cooling

complexified distribution with slow decay \longrightarrow convergence to wrong results

Minimize unitarity norm: $\sum_i \text{Tr}(U_i U_i^+)$
Distance from SU(N) $\sum_{ij} |(U U^+ - 1)_{ij}|^2$
 $\text{Tr}(U U^+) + \text{Tr}(U^{-1} (U^{-1})^+) \geq 2N$
For SU(2): $(\text{Im Tr } U)^2$

Using gauge transformations in SL(N,C)

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

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

Gradient of the unitarity norm gives steepest descent

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

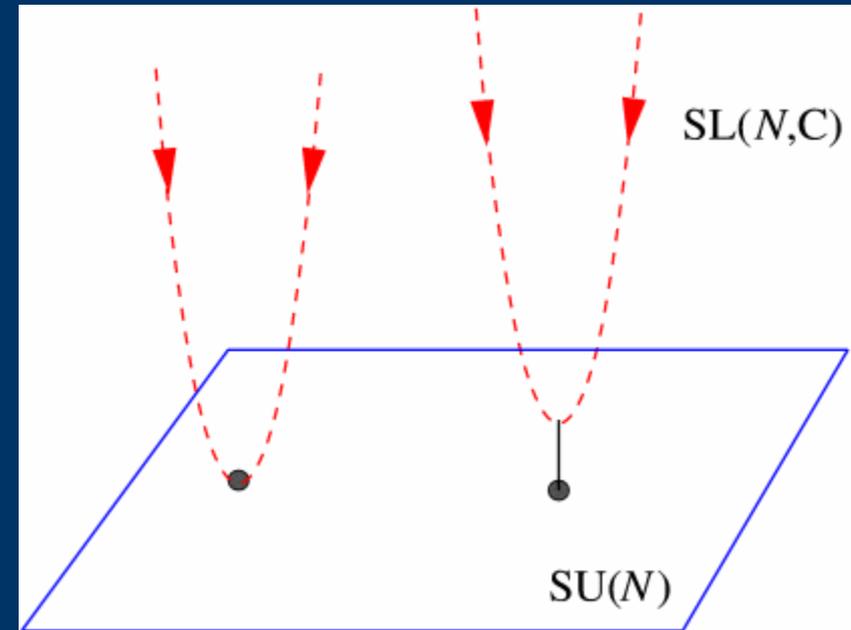
Gauge transformation at x changes 2d link variables

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

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

Dynamical steps are interspersed with several gauge cooling steps

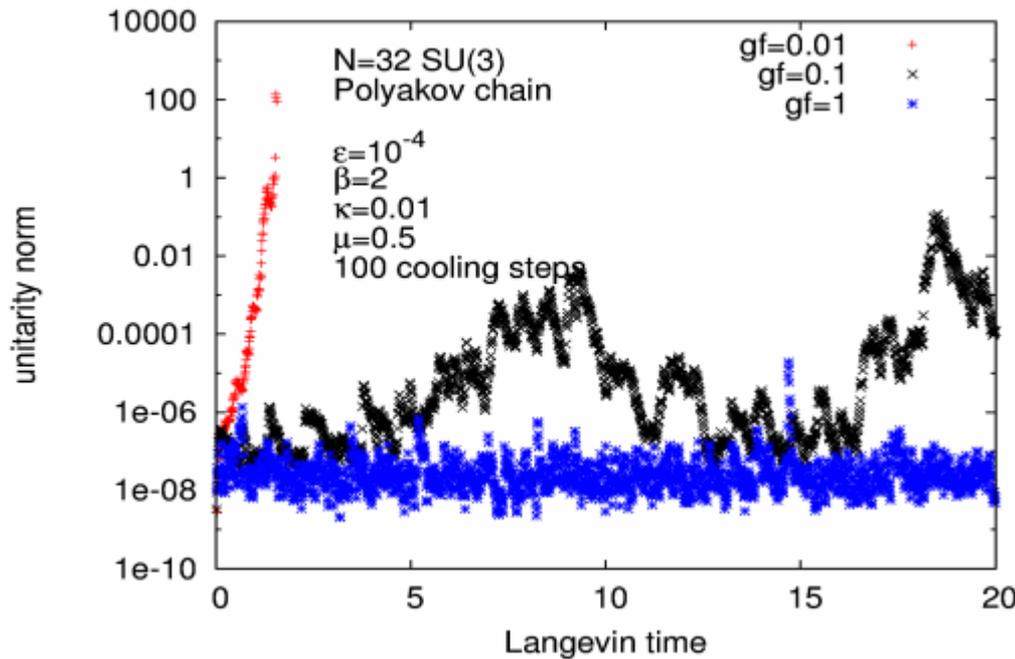
The strength of the cooling is determined by
cooling steps
gauge cooling parameter α



Empirical observation:
Cooling is effective for

$$\beta > \beta_{\min}$$

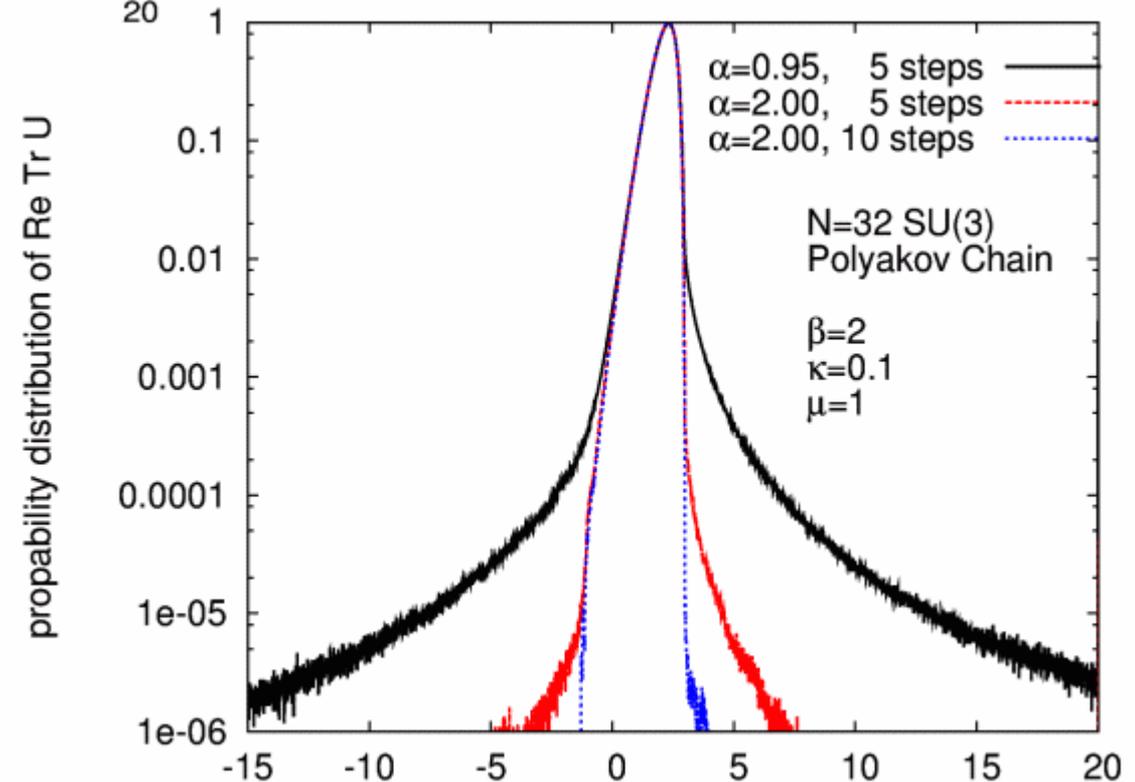
but remember, $\beta \rightarrow \infty$
in cont. limit



Smaller cooling

excursions into complexified manifold

“Skirt” develops
small skirt gives correct result



Heavy Quark QCD at nonzero chemical potential

Hopping parameter expansion of the fermion determinant
Spatial hoppings are dropped

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

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

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

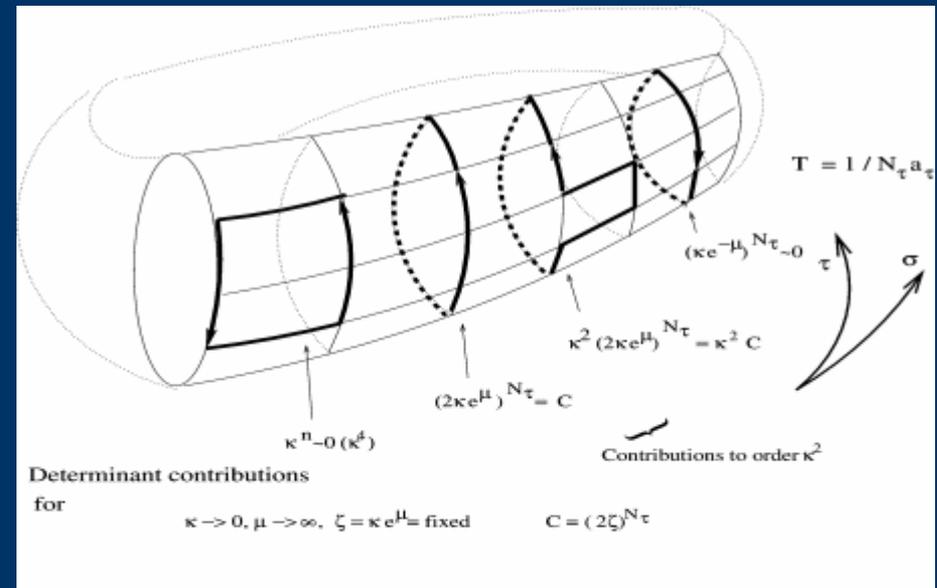
Studied with reweighting

De Pietri, Feo, Seiler, Stamatescu '07

$$R = |\text{Det } M|$$

CLE study using gaugecooling

[Seiler, Sexty, Stamatescu (2012)]

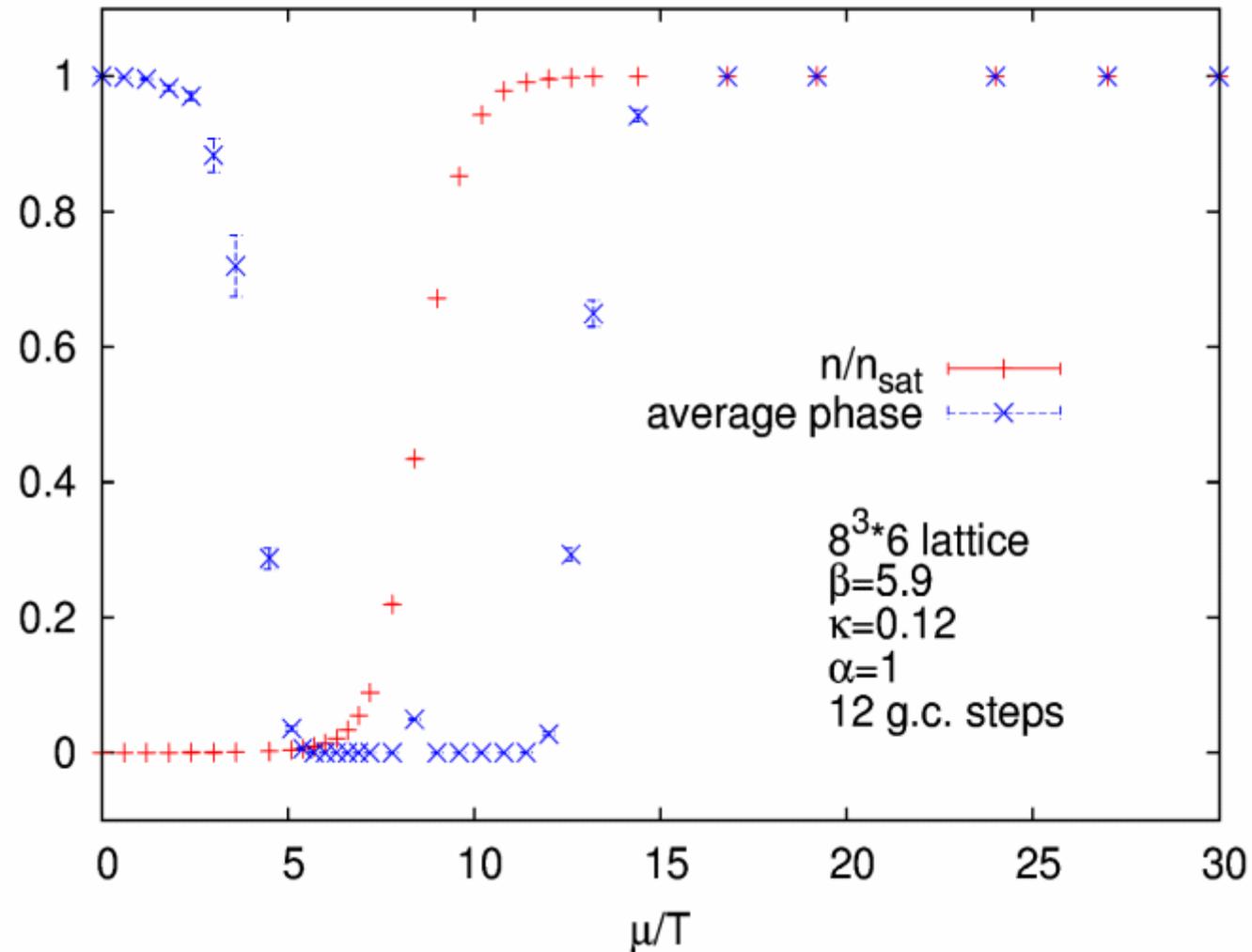


Fermion density:

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

average phase:

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

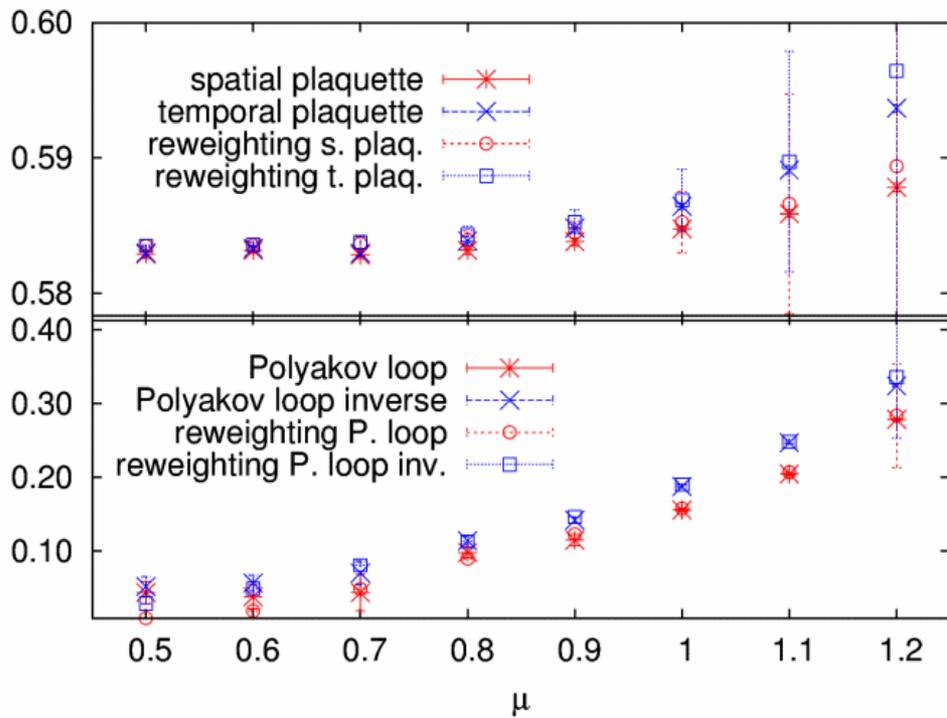


$$\det(1 + CP) = 1 + C^3 + C \text{Tr} P + C^2 \text{Tr} P^{-1}$$

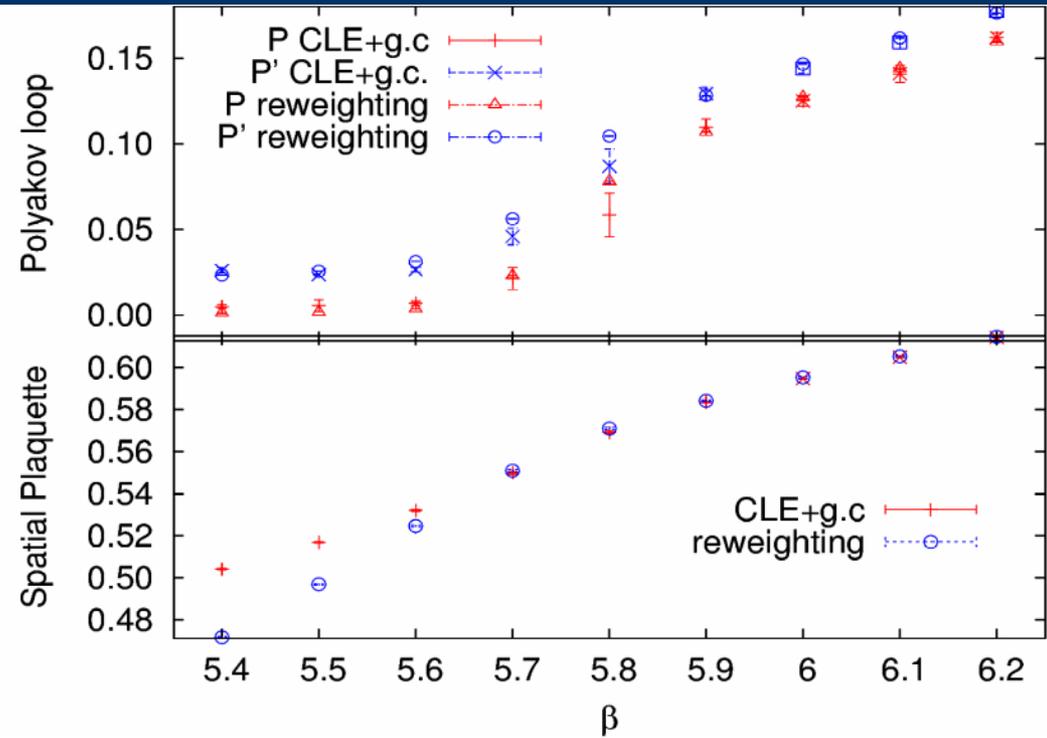
Sign problem is absent at
small or large μ

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

Comparison to reweighting

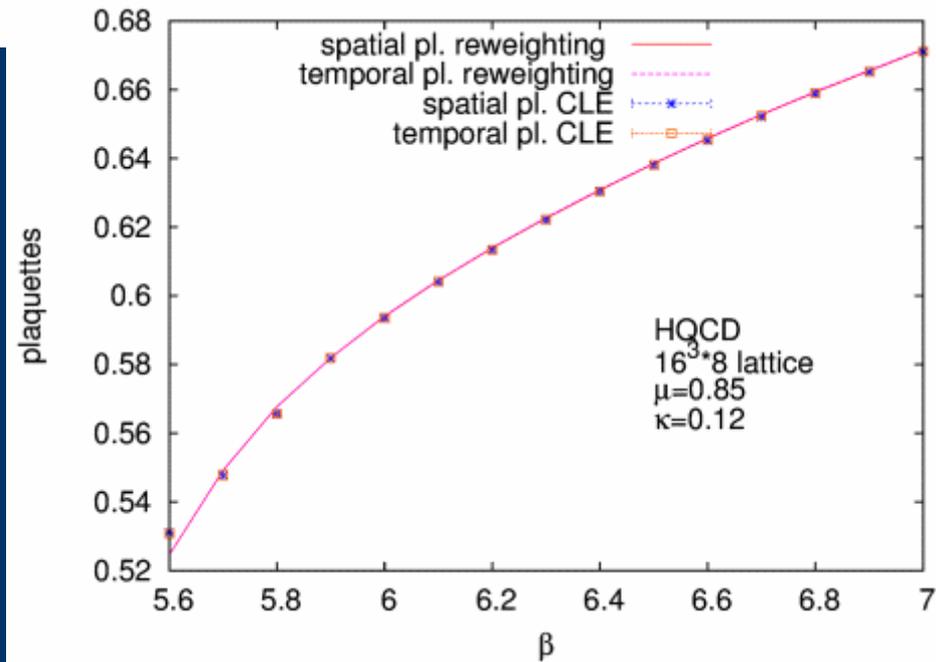
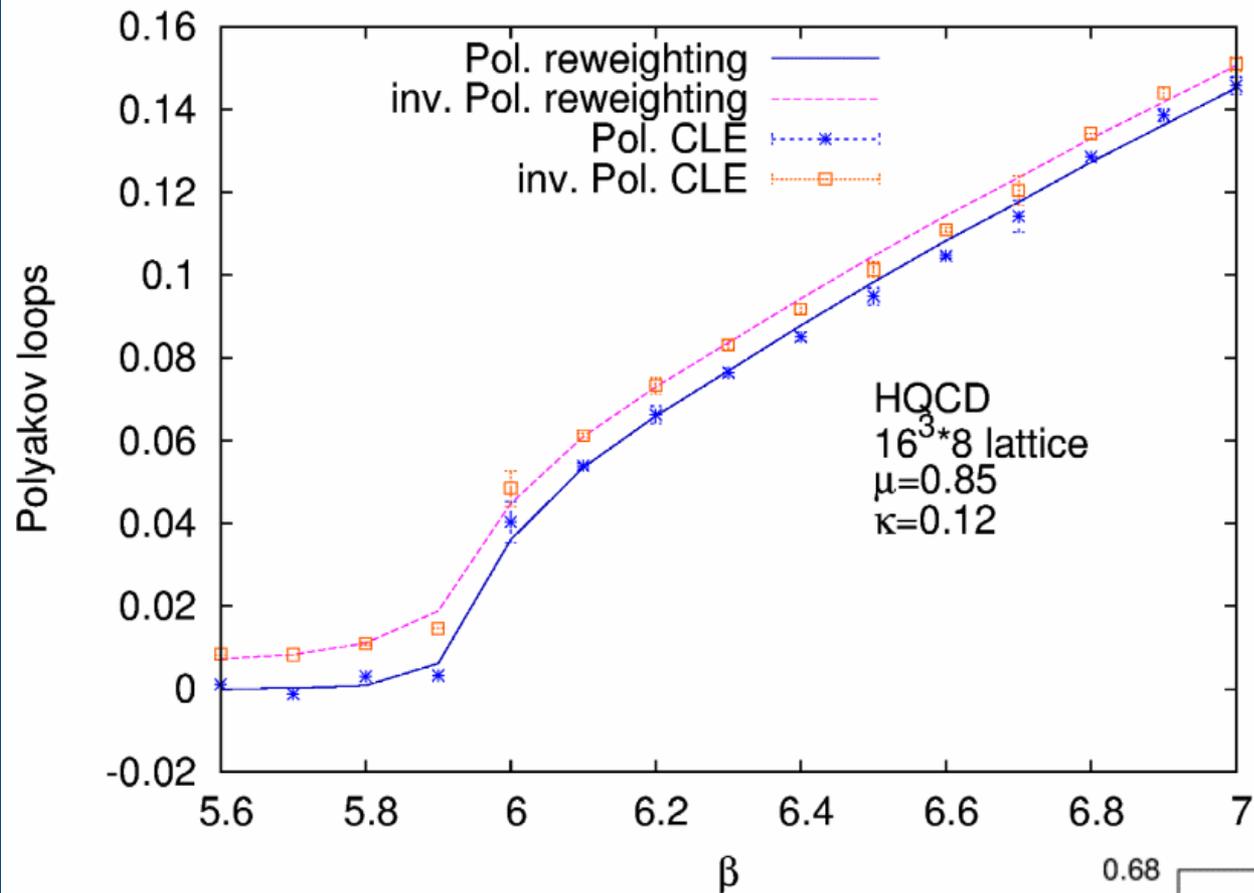


6^4 lattice, $\beta=5.9$



6^4 lattice, $\mu=0.85$

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



Large lattice:
phase transition clearly visible

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

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

$$M(x, y) = m \delta(x, y) + \sum_v \frac{\eta_v}{2a_v} (e^{\delta_{v4}\mu} U_v(x) \delta(x+a_v, y) - e^{-\delta_{v4}\mu} U_v^{-1}(x-a_v, y) \delta(x-a_v, y))$$

Still doubling present $N_F=4$

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

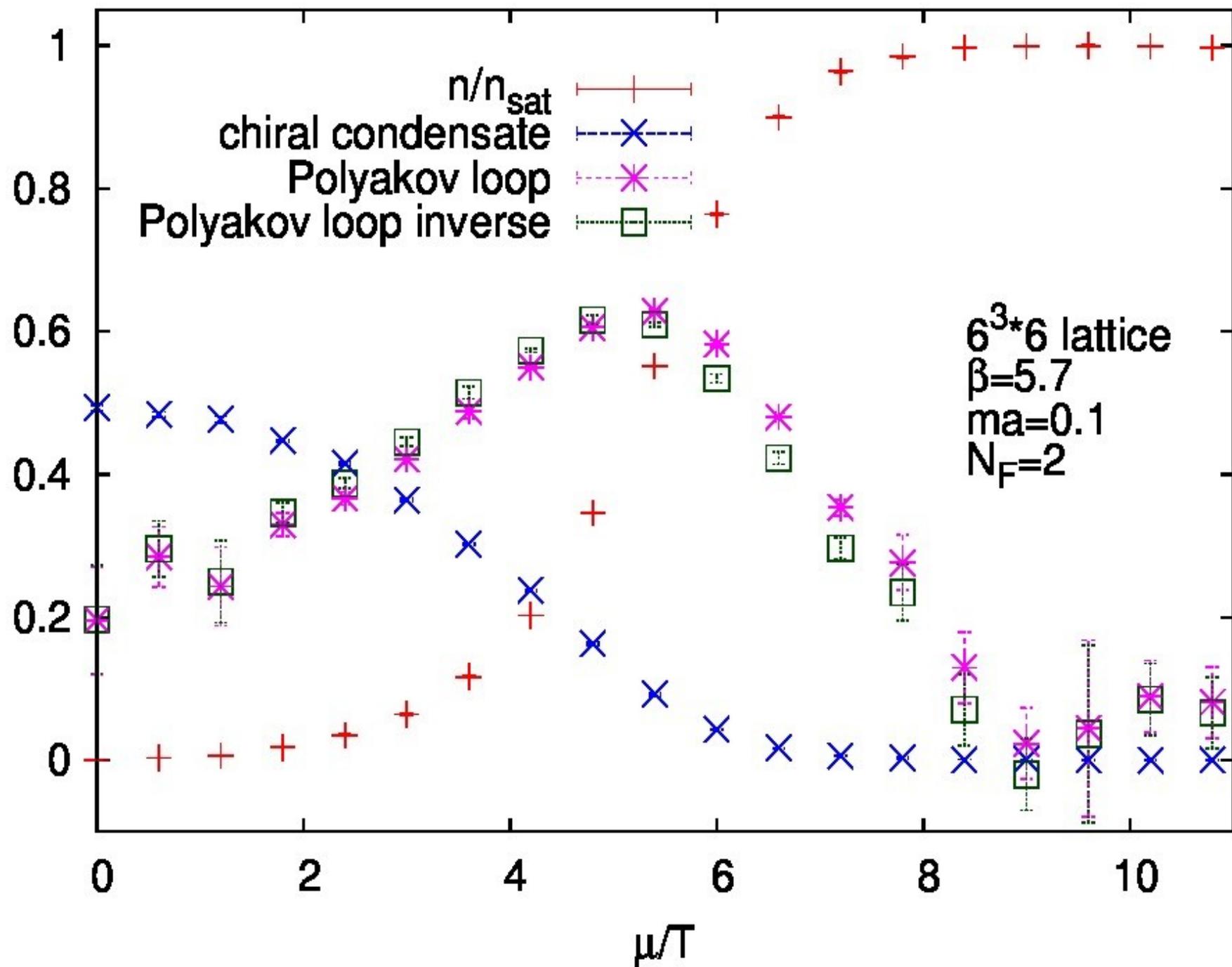
Langevin equation

$$U' = \exp(i\lambda_a (-\epsilon D_a S[U] + \sqrt{\epsilon} \eta_a)) U \quad \text{Drift term: } -D_a S[U] = K^G + K^F$$

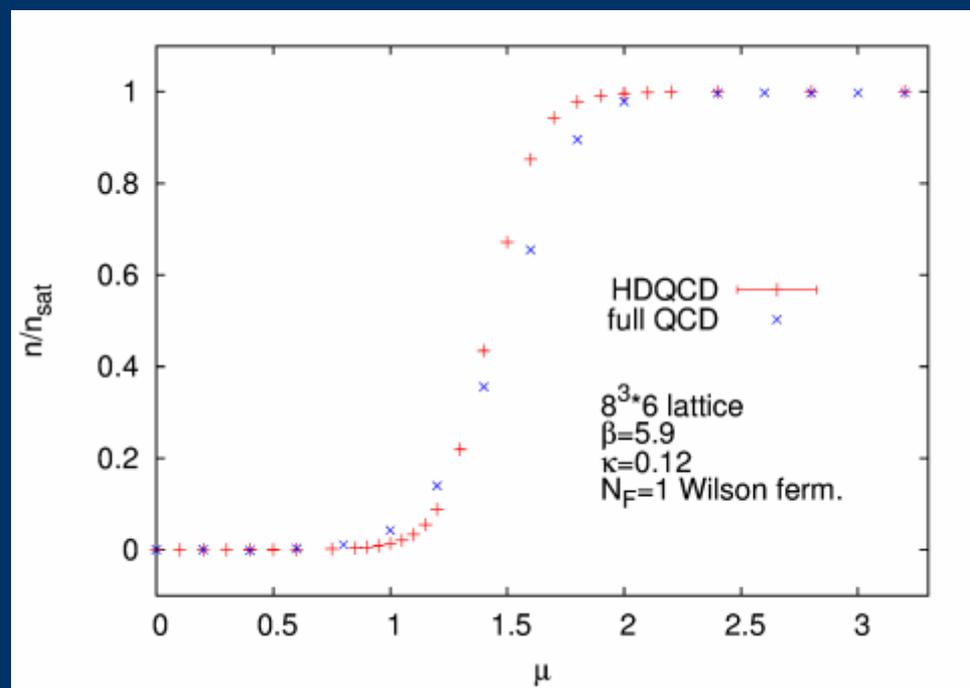
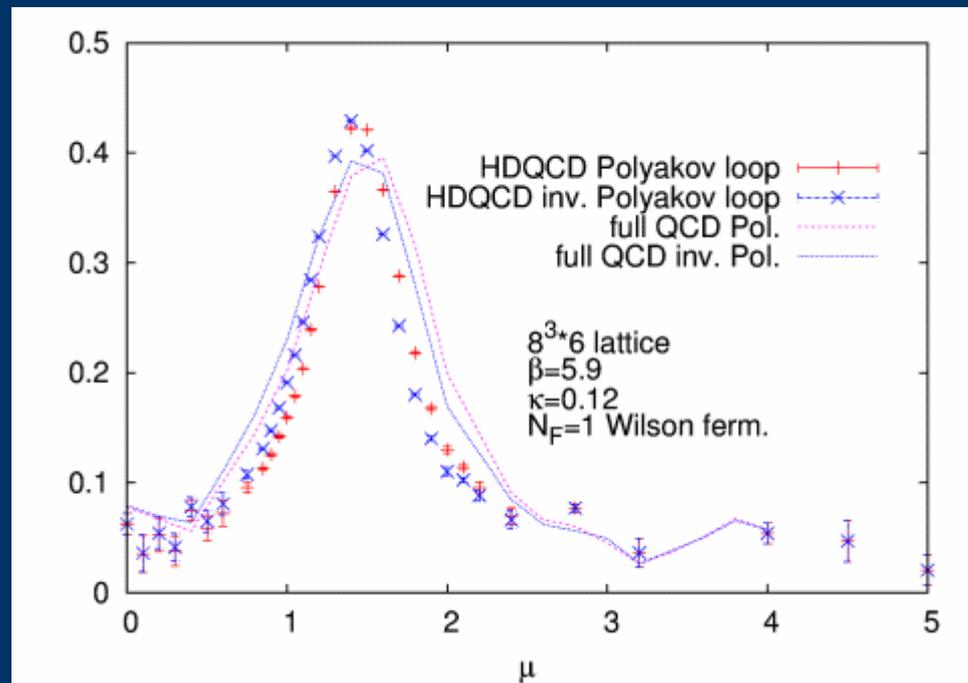
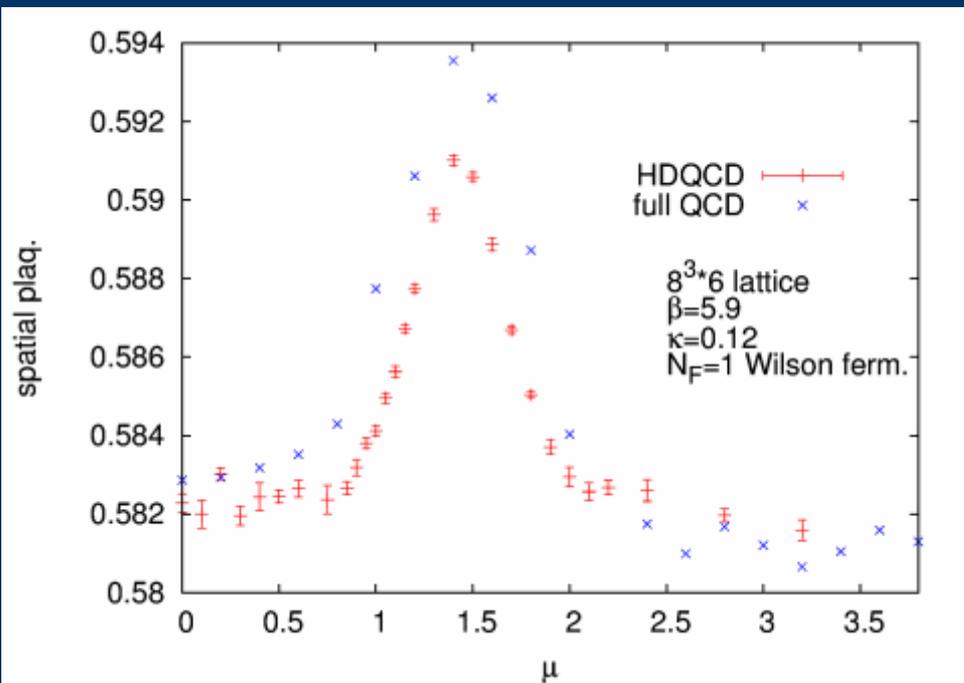
$$K_{axv}^G = -D_{axv} S_G[U]$$

$$K_{axv}^F = \frac{N_F}{4} D_{axv} \ln \det M = \frac{N_F}{4} \text{Tr} (M^{-1} M'_{va}(x, y, z))$$

$$M'_{va}(x, y, z) = D_{azv} M(x, y)$$



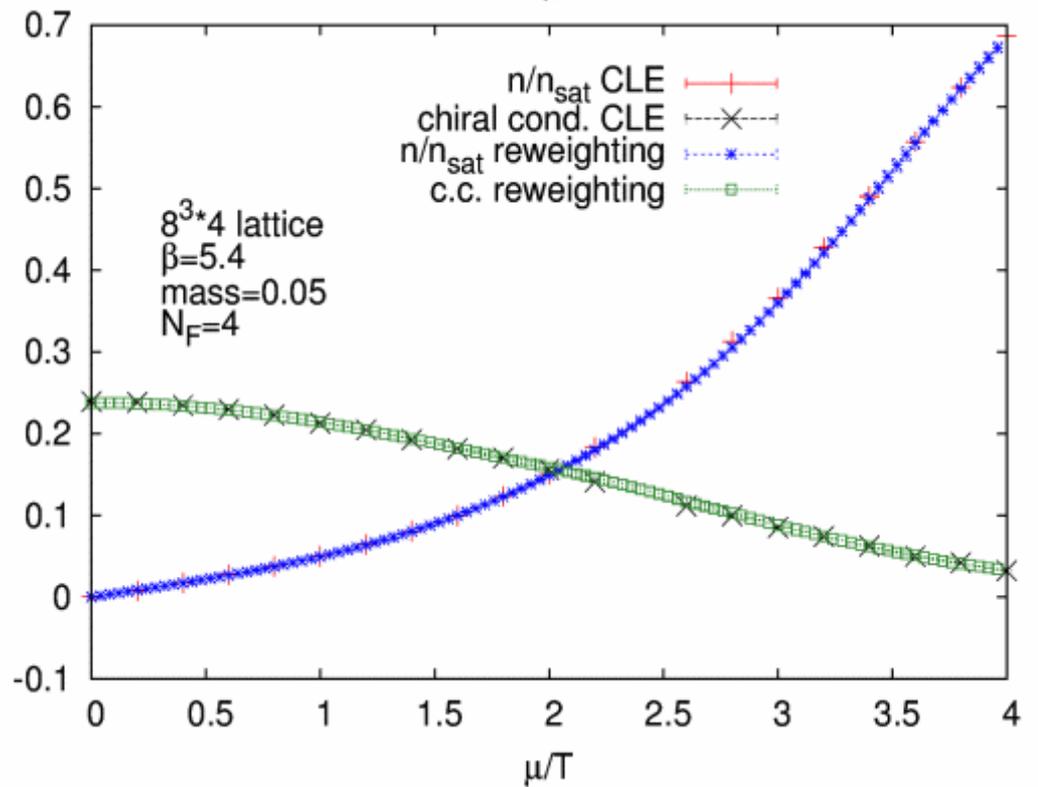
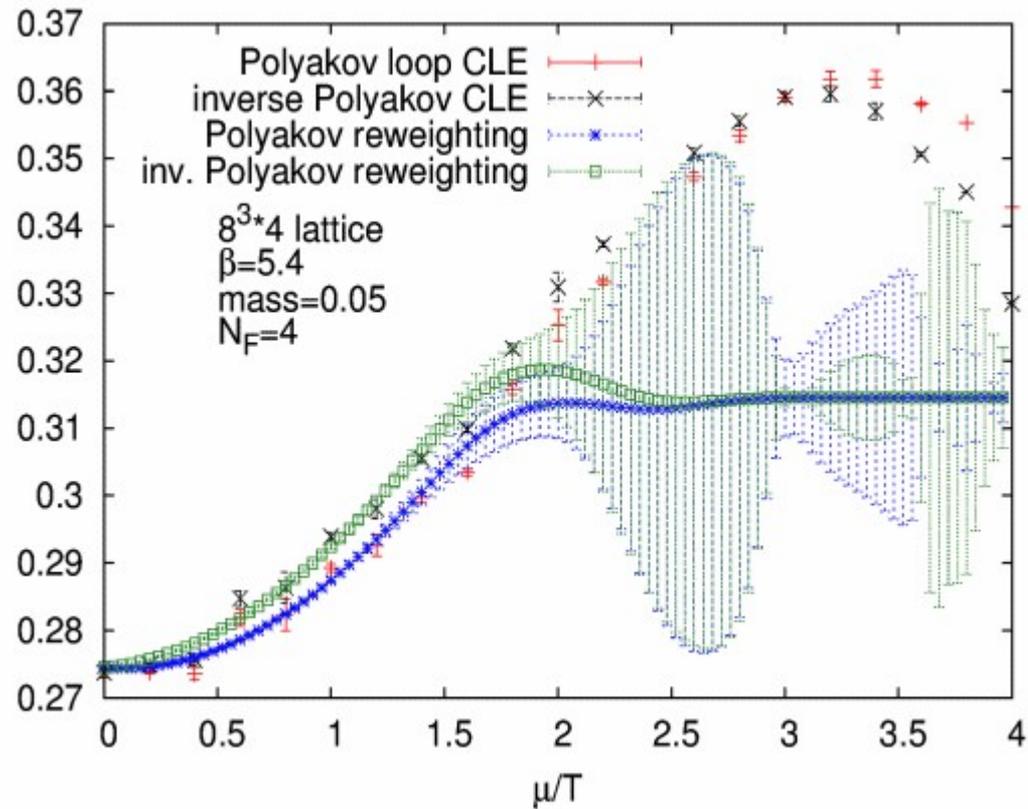
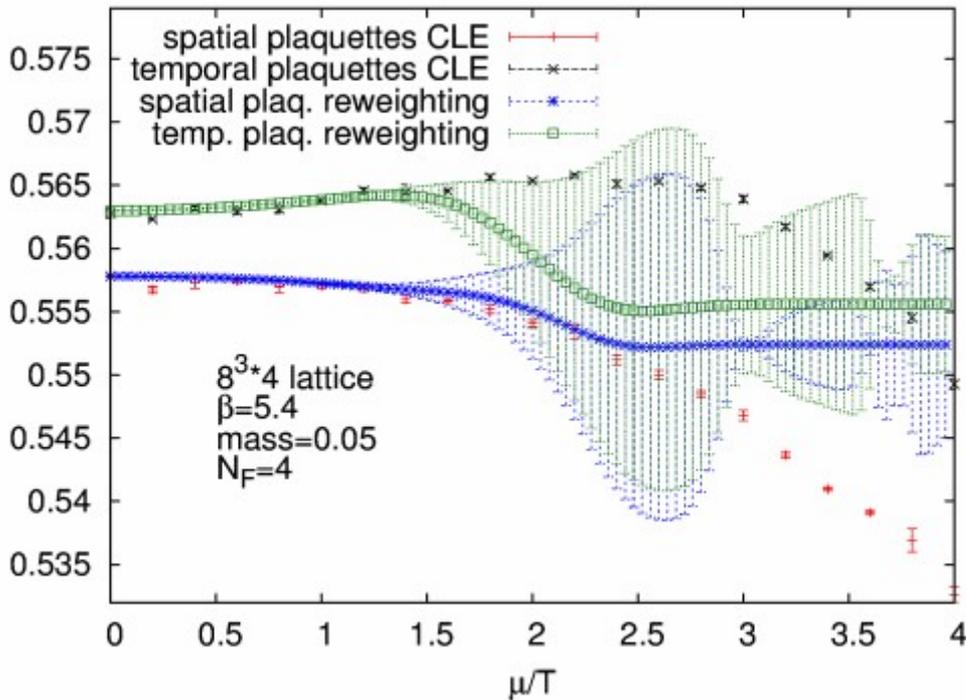
Comparison of HDQCD in LO and full QCD



Comparison with reweighting for full QCD

Reweighting from ensemble at

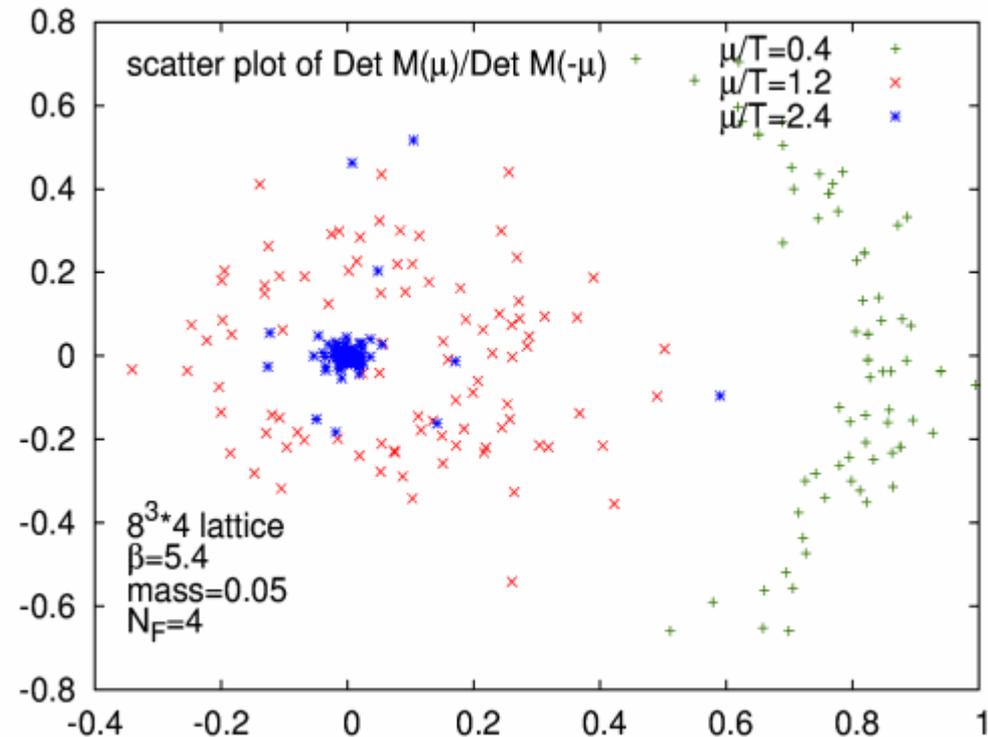
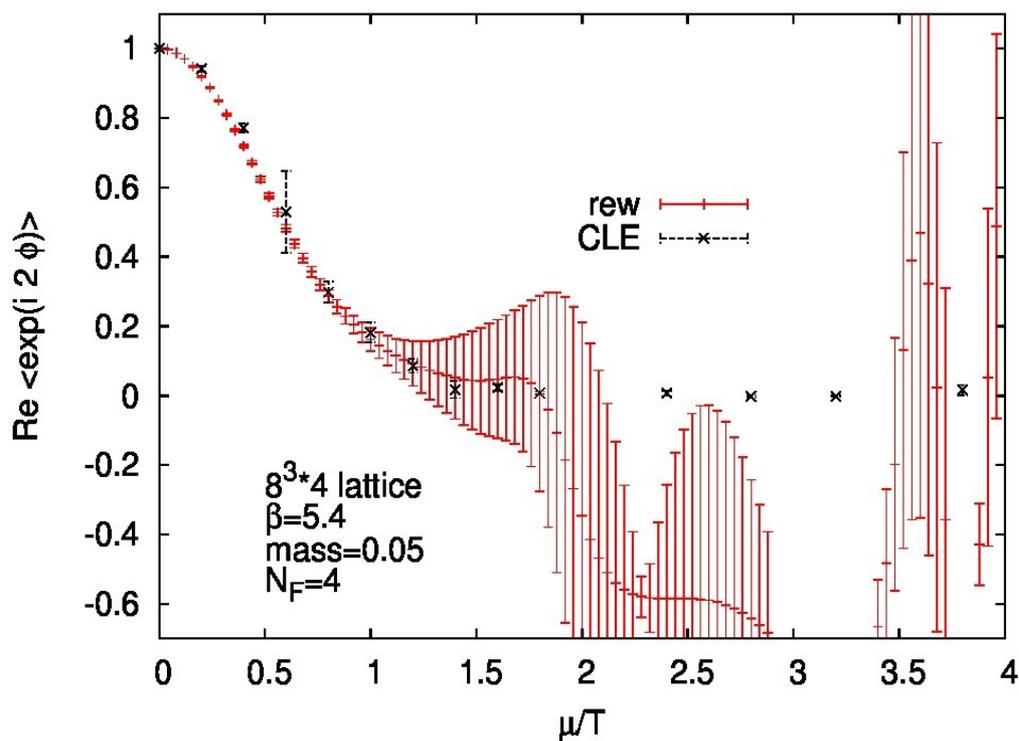
$$R = \text{Det } M(\mu=0)$$



Sign problem

Sign problem gets hard around

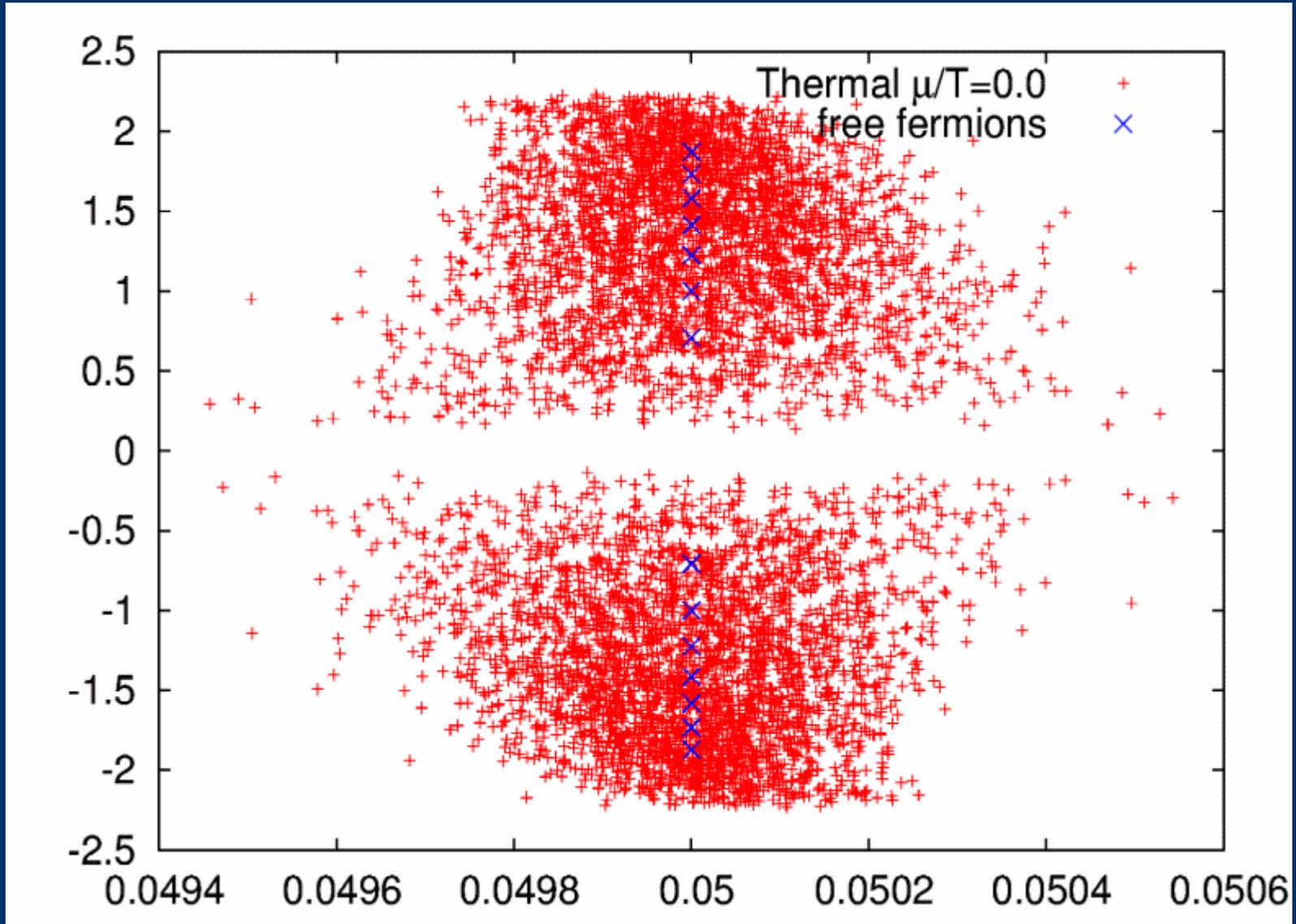
$$\mu/T \approx 1 - 1.5$$



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

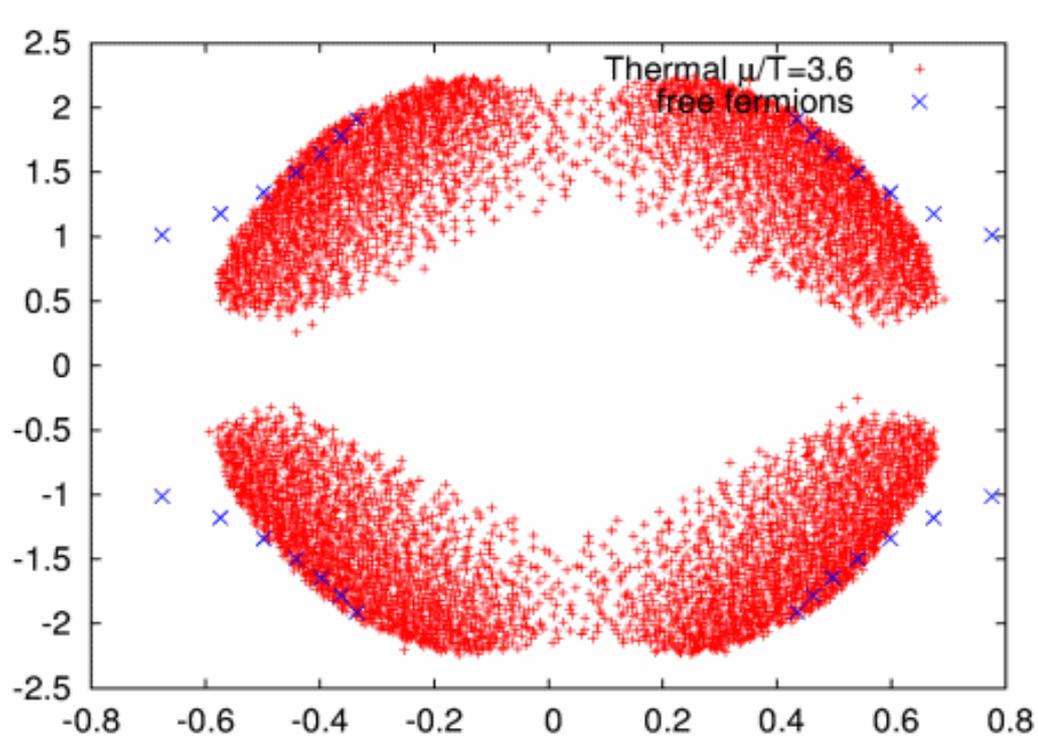
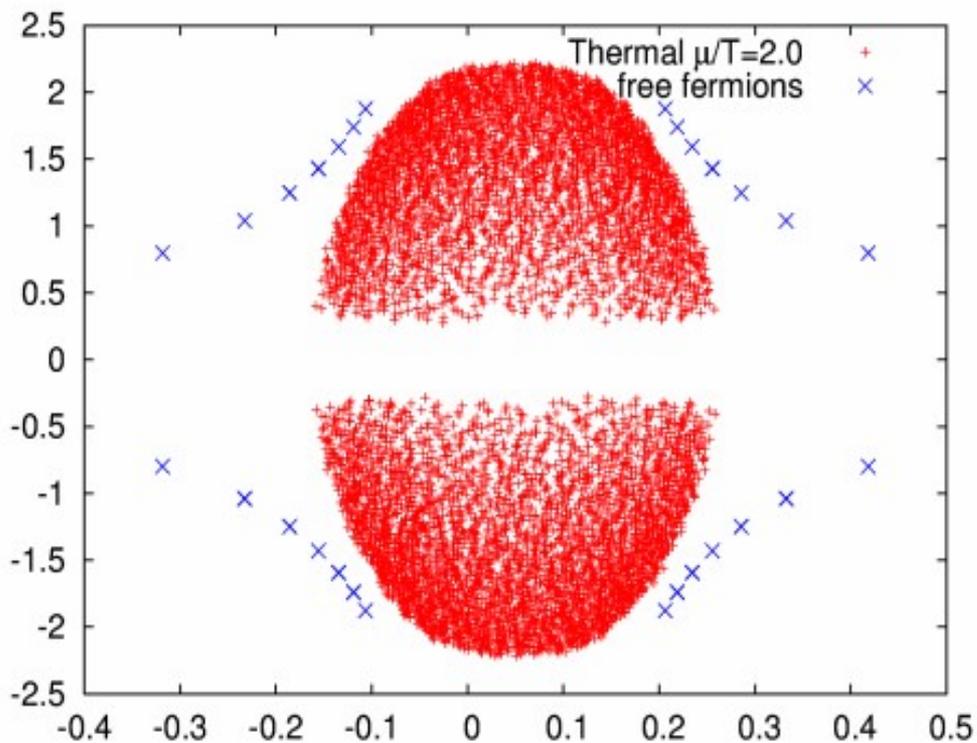
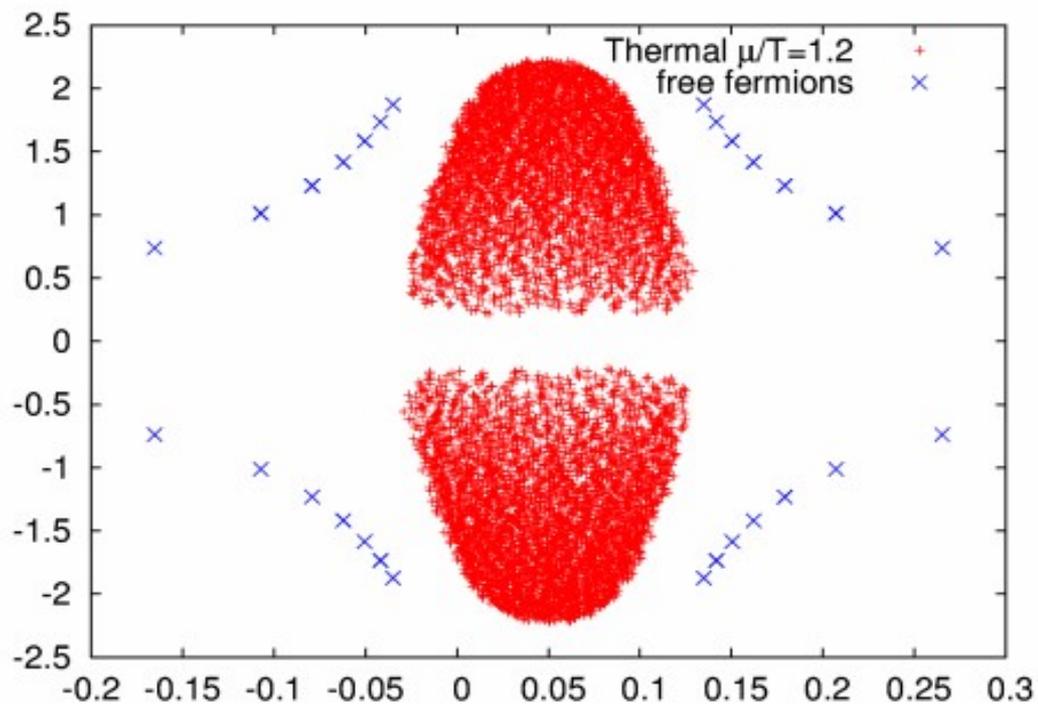
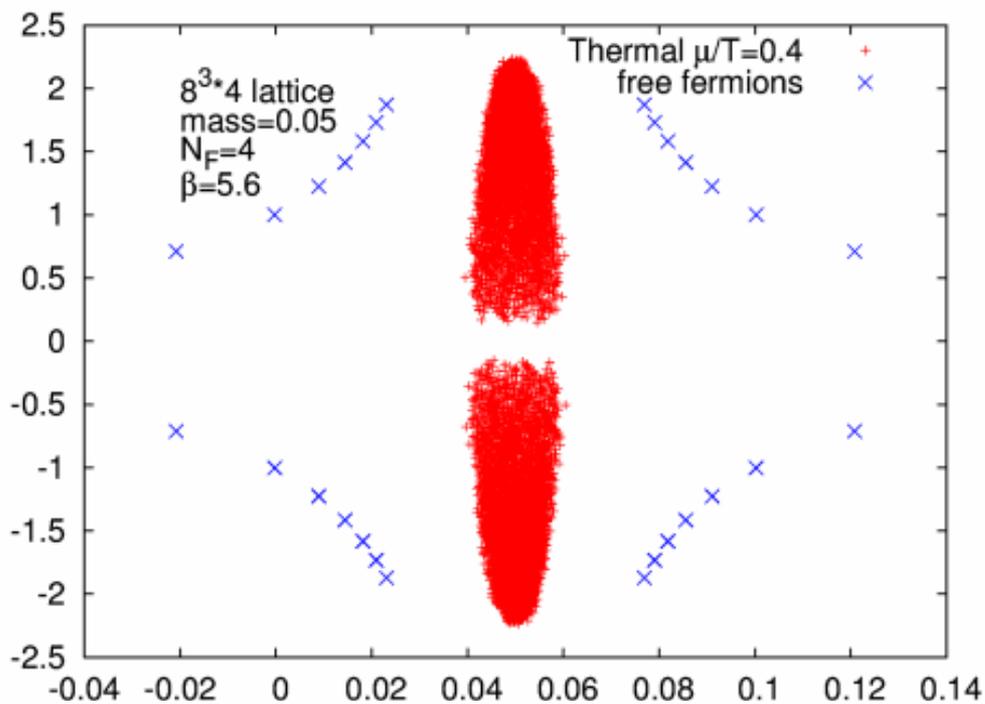
Spectrum of the Dirac Operator $N_F=4$ staggered

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



Spectrum of the Dirac Operator

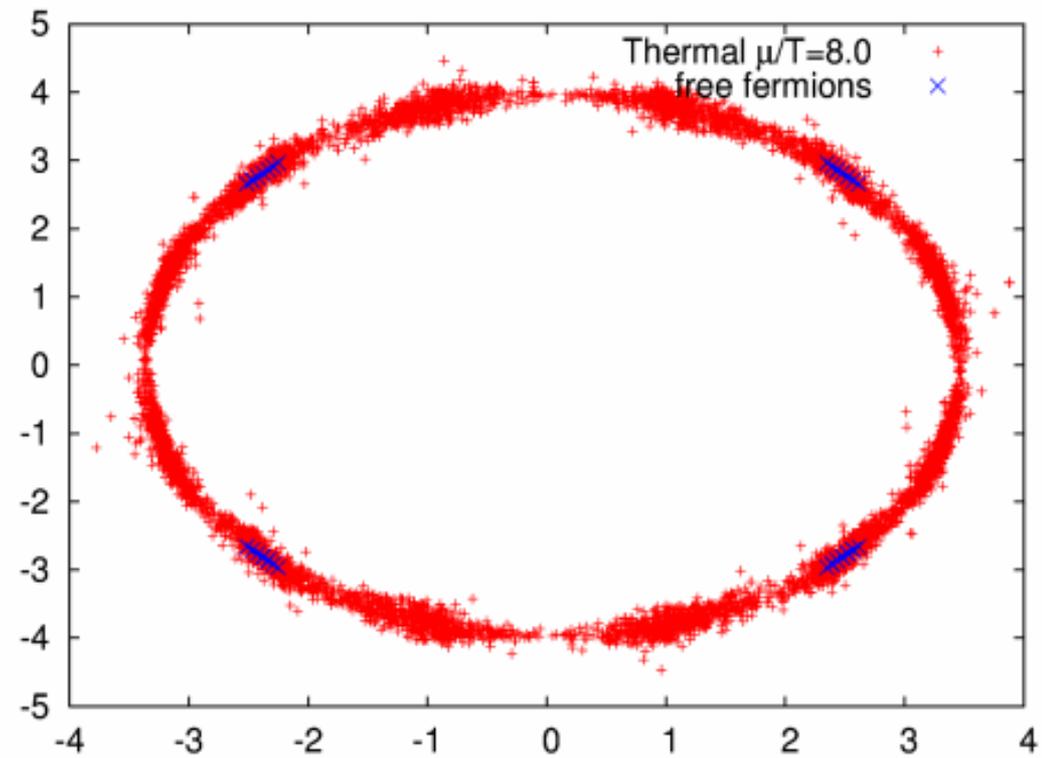
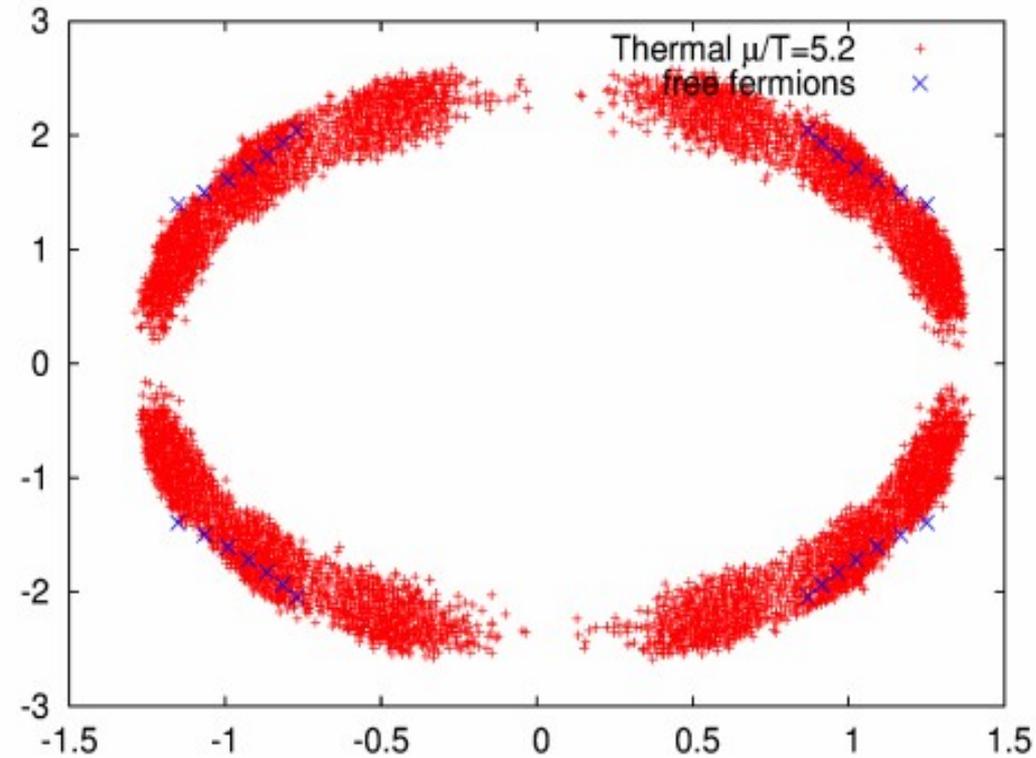
$N_F=4$ staggered



Spectrum of the Dirac Operator

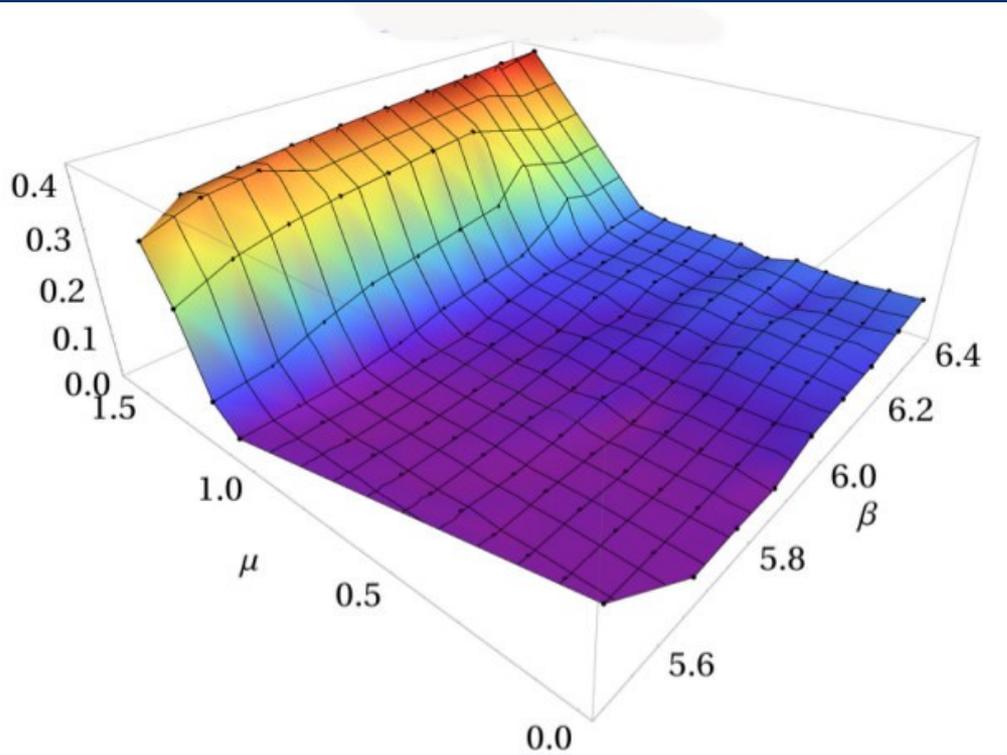
Large chemical potential, towards saturation

Fermions become “heavy”



Phase diagram

Polyakov loop

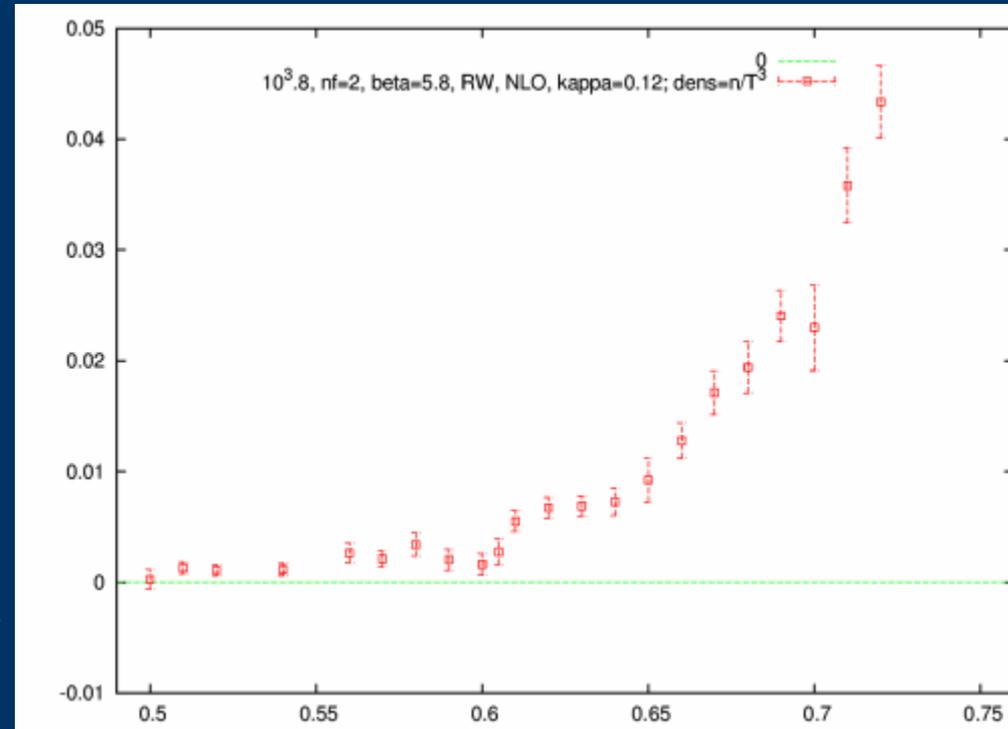


LO in κ_s expansion

NLO:
Nuclear matter ?

In LO deconfinement
and onset transition

NLO in κ_s expansion



Onset transition at low temperature
and high chemical potentials

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

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

First results for the phase diagram