New algorithms for finite density QCD

Dénes Sexty

Heidelberg University

Lattice 2014, New York , 27th of June, 2014.

1. Complex Langevin
2. Lefschetz Thimble
3. connection of Langevin and Lefschetz
4. CLE results for QCD

Contributions to Lattice 2014

Complex Langevin equation

Complex Langevin dynamics for SU(3) gauge theory in the presence of a theta term
Lorenzo Bongiovanni

Exploring the phase diagram of QCD with complex Langevin simulations
Benjamin Jäger

The onset of the baryonic density in HD-QCD at low temperature
Ion-Olimpiu Stamatescu

Effective Polyakov-line actions, and their solutions at finite chemical potential
Jeff Greensite

Lefschetz thimble

An algorithm for thimble regularization of lattice field theories
Francesco Di Renzo

Solution of simple toy models via thimble regularization of lattice field theory
Giovanni Eruzzi

QCD sign problem

Euclidean SU(3) gauge theory with fermions:

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

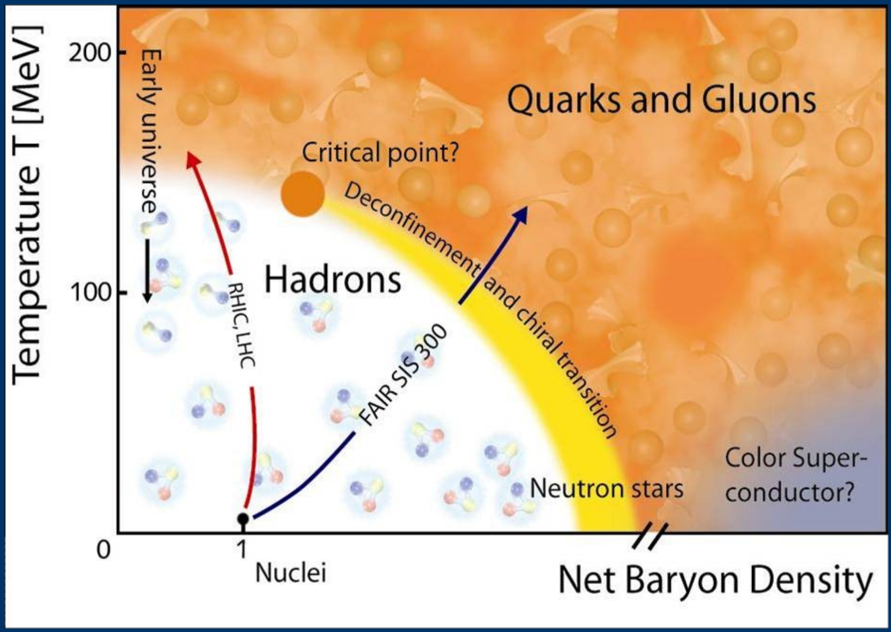
for $\det(M(U)) > 0$ Importance sampling is possible

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



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, ...

Direct Methods:

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
Full QCD with light quarks:	Sexty '14

Lefschetz thimble

Theory:	Witten '10 Cristoforetti et al. (Aurora) '12
Toy models, Bose gas, etc.:	Cristoforetti, Scorzato, Di Renzo '12
	Cristoforetti, Di Renzo, Mukherjee, Scorzato '13
	Mukherjee, Cristoforetti, Scorzato '13,
	Cristoforetti et. al. '14
	Fujii, Honda, Kato, Kikukawa, Komatsu, Sano '13
Hubbard modell:	Mukherjee, Cristoforetti '14

thimble and stochastic quantisation

Aarts '13

Aarts, Bongiovanni, Seiler, Sexty, Stamatescu, in prep.

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)]

Parallel 9A: Effective polyakov line actions with CLE
Jeff Greensite

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

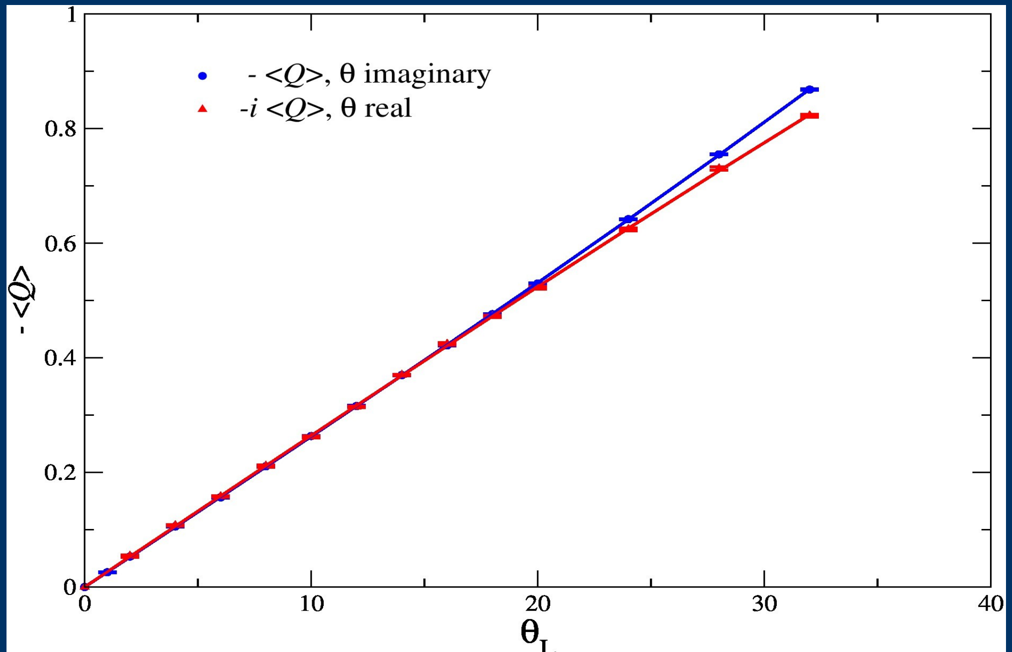
   [Bongiovanni, Aarts, Seiler, Sexty, Stamatescu (2013)+in prep.]

Parallel 4A: Complex Langevin dynamics for SU(3) gauge theory
in the presence of a theta term
Lorenzo Bongiovanni

comparing real Θ
with imaginary Θ

Analyticity

linear coeff. should agree



Lefschetz Thimble

Transform integral by shifting contour

$$\int_{-\infty}^{\infty} dx\, e^{S(x)} F(x) = \int_C dz\, e^{S(z)} F(z) = \int dt \left(\frac{dz}{dt}\right) e^{S(z(t))} F(z(t))$$

Better than the original contour if

$e^{\mathrm{Re}(S(z(t)))}$ peak + fast decay

$e^{i\,\mathrm{Im}(S(z(t)))}$ milder sign problem than original

$\mathrm{Im}(S(z(t))) =$ const $\longleftrightarrow$ steepest descent of $\mathrm{Re}(S(z(t)))$

Thanks to Cauchy-Riemann equations

Lefschetz thimble is a contour which

starts from saddle points $\partial_z S(z_0) = 0$

$$\frac{\partial z}{\partial t} = \pm \overline{\partial_z S(z)}$$

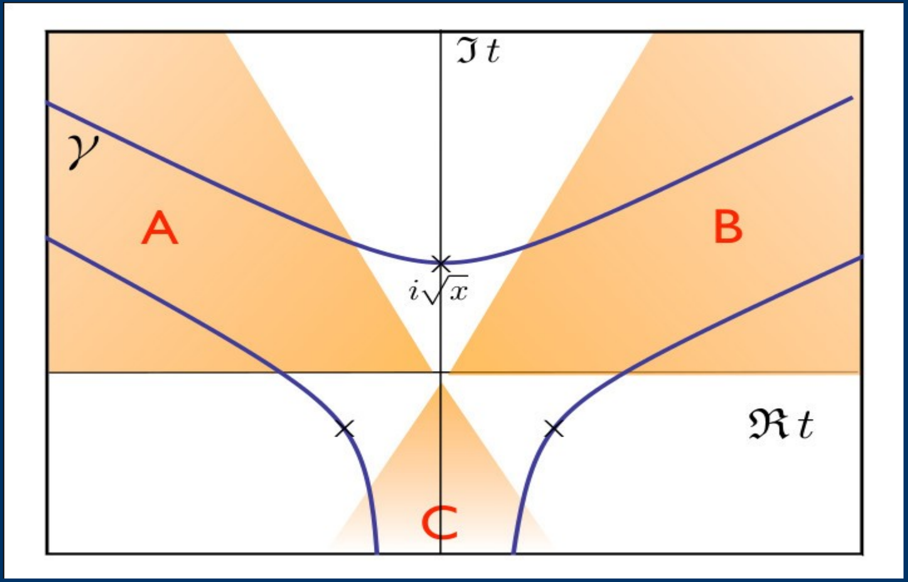
$$z \to z_0 \text{ for } t \to \infty$$

+: stable thimble $\longleftrightarrow$ steepest descent

-: unstable thimble $\longleftrightarrow$ steepest ascent

$$Z=\sum_k m_k e^{-\mathrm{Im}\,S(z_k)} \int_{T_k} dz\, e^{\mathrm{Re}\,S(z)} = \sum_k m_k e^{-\mathrm{Im}\,S(z_k)} \int_{T_k} dt\, \frac{dz}{dt} e^{\mathrm{Re}\,S_k(t)}$$

Intersection number (Morse theory)



[Fig: Scorzato]

Residual sign problem
from curvature of thimble
Is it mild?
Is it exponential in the volume?

Global sign problem
Easy as long as few thimbles contribute

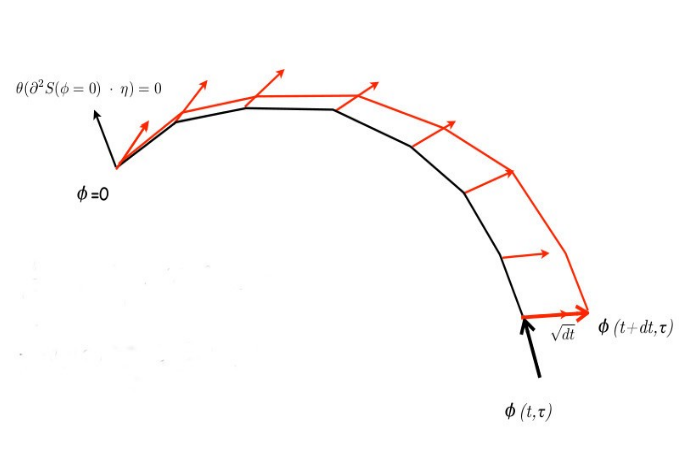
For large systems: $\sum_k m_k T_k \rightarrow T_0$

Choose thimble with the global minimum
Regularisation of QFT
Resurgence

Numerical Simulations on the Lefschetz Thimble

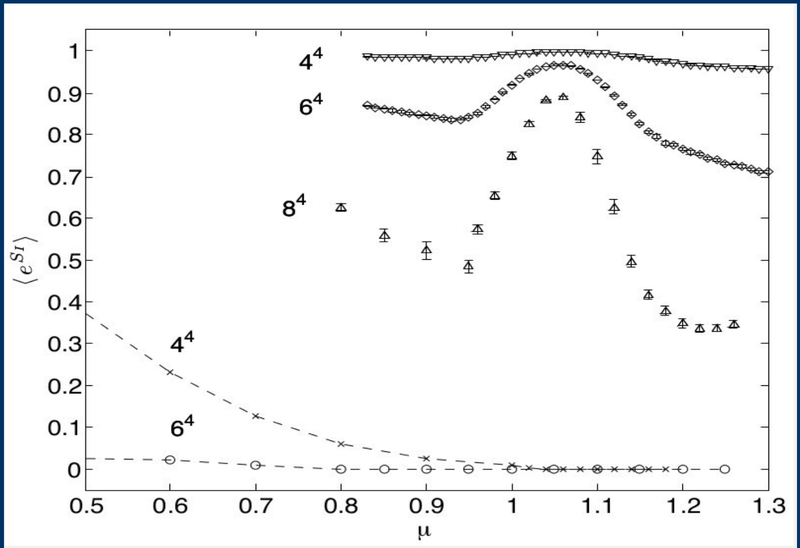
Algorithm needed to keep configurations on the thimble

φ^4 theory with nonzero μ

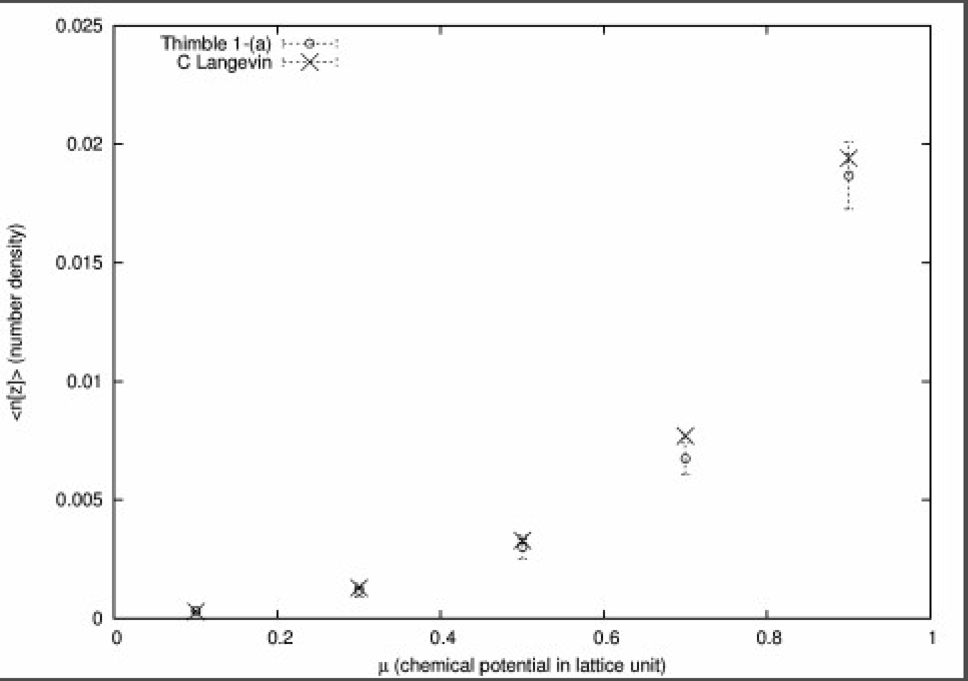


(real) Langevin eq. on the thimble

[Cristoforretti, Di Renzo, Scorzato (2012)]



HMC on the thimble



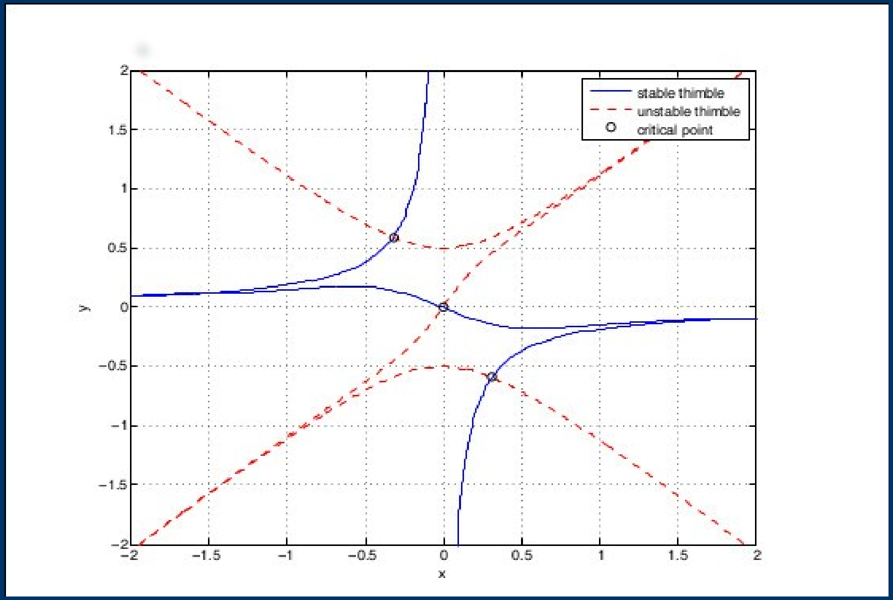
[Fujii, Honda, Kato, Kikukawa, Komatsu, Sano (2013)]

Parallel 4A: Solution of simple toy models via thimble regularization of lattice field theory
Giovanni Eruzzi

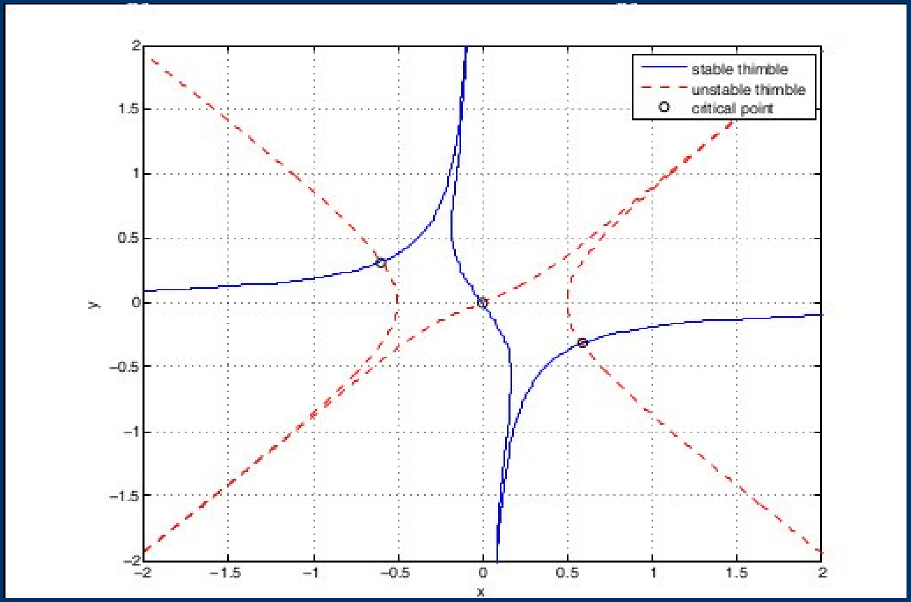
A number of algorithms tested to sample the thimble

$$S=\frac{1}{2}\sigma x^2+\frac{1}{4}x^4$$

$\mathrm{Re}\,\sigma>0$



$\mathrm{Re}\,\sigma<0$



Parallel 8F: An algorithm for thimble regularization of lattice field theories
Francesco Di Renzo

"Ideal sampling" on the thimble

Langevin and Lefschetz

Both use analiticity and complexifcation
Direct simulation of complex actions is possible

Complex Langevin Eq.

Allow complex drift in Langevin eq.

Complexify the field manifold
Dimensions are doubled

Check for convergence

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

Lefschetz thimble

Shift integration contour into complex plane

Look for critical points,
Find contributing thimbles

Reweight the residual sign problem

$$\frac{1}{Z}\int P_{comp}(x)O(x)dx=$$
$$\frac{1}{Z}\int_{T} P_{comp}(z)O(z)dz$$

Gaussian Example

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

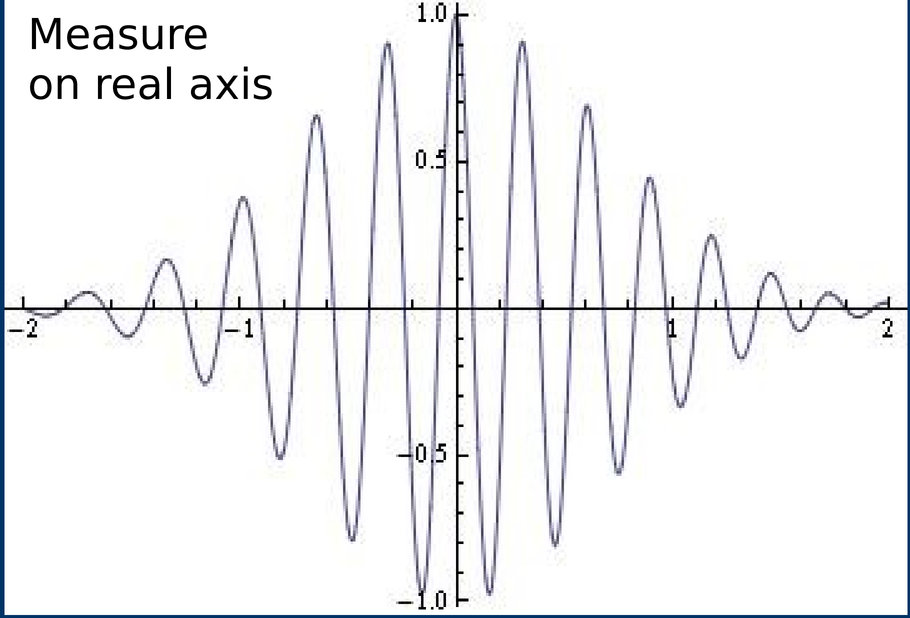
CLE

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

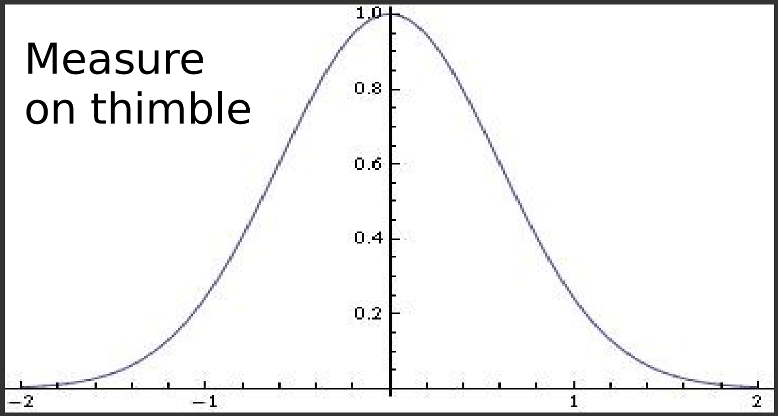
$$P(x,y)=e^{-a(x-x_0)^2-b(y-y_0)^2-c(x-x_0)(y-y_0)}$$

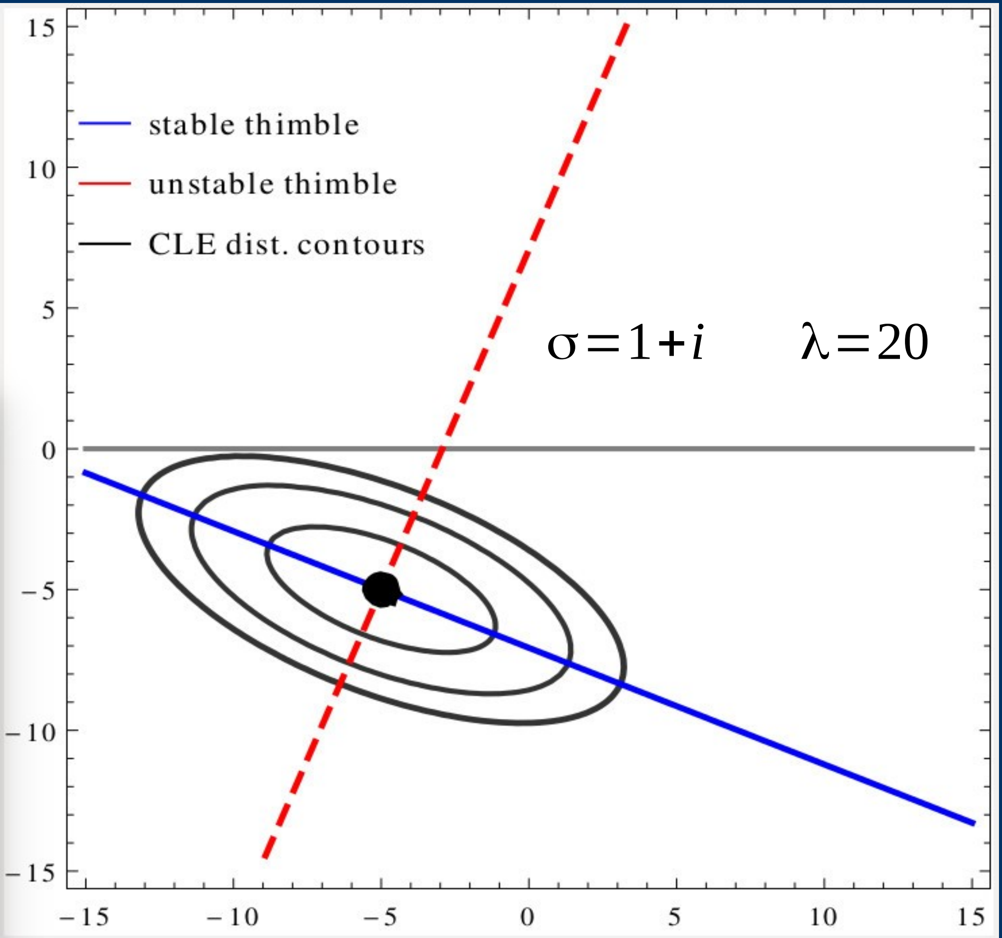
Gaussian distribution around critical point

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



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



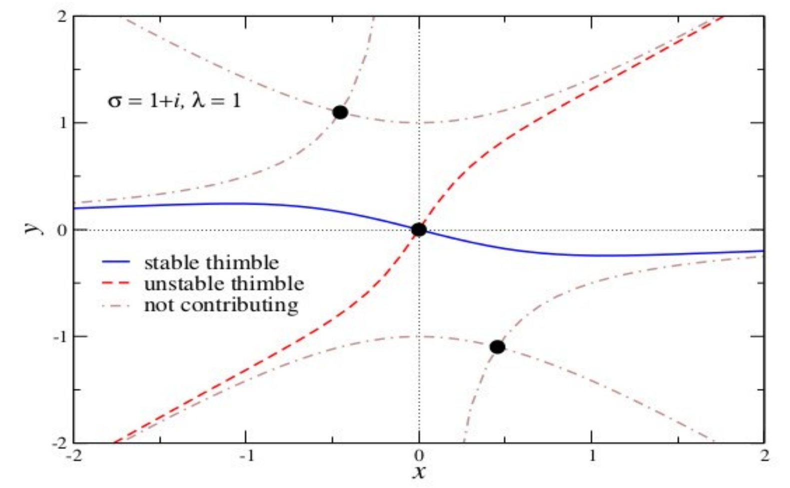


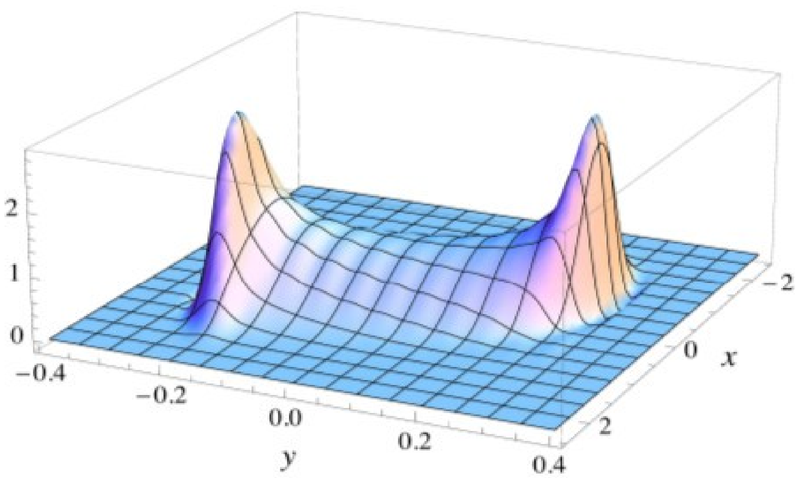
Quartic model

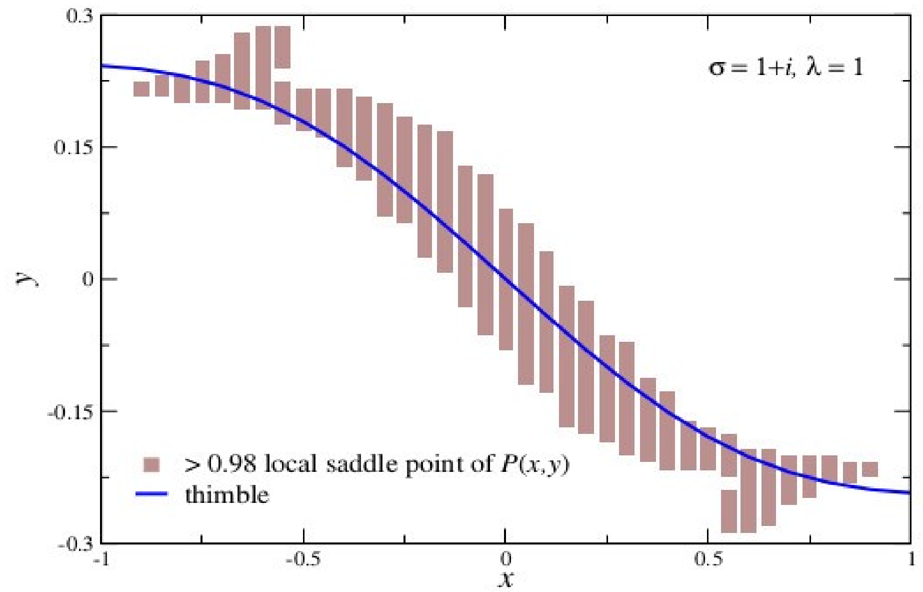
[Aarts (2013)]

$$Z = \int dx\, e^{-S(x)}$$

$$S(x) = \frac{\sigma}{2} x^2 + \frac{\lambda}{4} x^4 \quad \text{with} \quad \sigma \in \mathbb{C}$$







CLE distributions follow thimble

Deeper connection?

Gauge theories and CLE

link variables: SU(N) $\longrightarrow$ 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:

Distance from SU(N)

$$\sum_i Tr(U_i U_i^+)$$

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

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

Gauge cooling

[Seiler, Sexty, Stamatescu (2012)]

complexified distribution with slow decay $\longrightarrow$ convergence to wrong results

Keep the system from trying to explore the complexified gauge degrees of freedom

Minimize unitarity norm

Distance from SU(N)

$$\sum_i Tr\left(U_i U_i^+ - 1\right)$$

Using gauge transformations in SL(N,C)

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

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

Gradient of the unitarity norm gives steepest descent

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

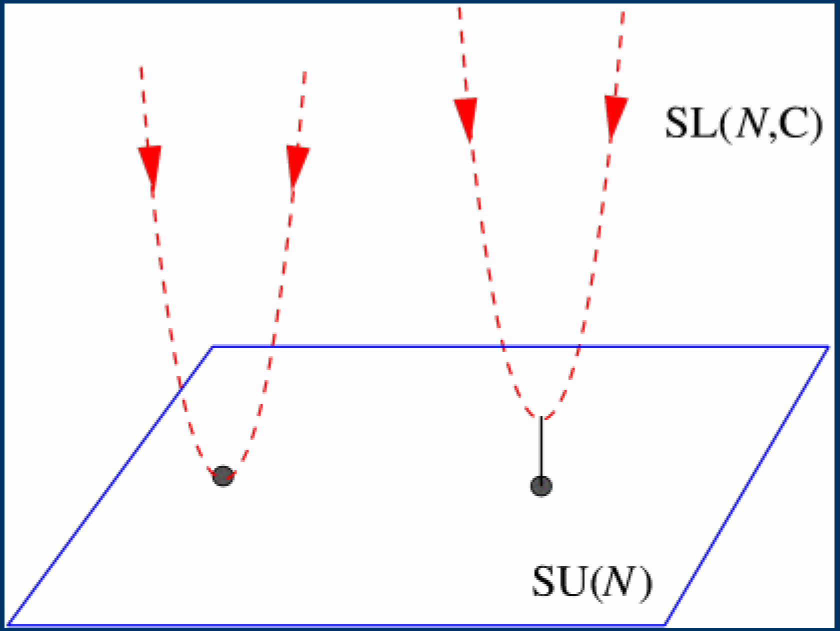
Gauge transformation at x changes 2d link variables

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

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

Dynamical steps are interspersed with several gauge cooling steps

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



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

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

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

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

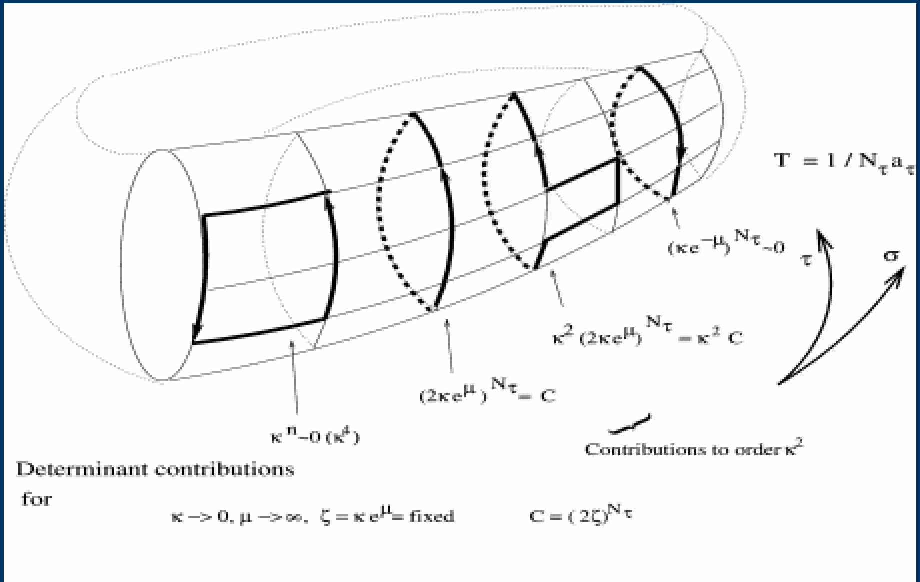
$$S = S_W[U_\mu] + \ln \mathrm{Det}\, M(\mu)$$

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)]

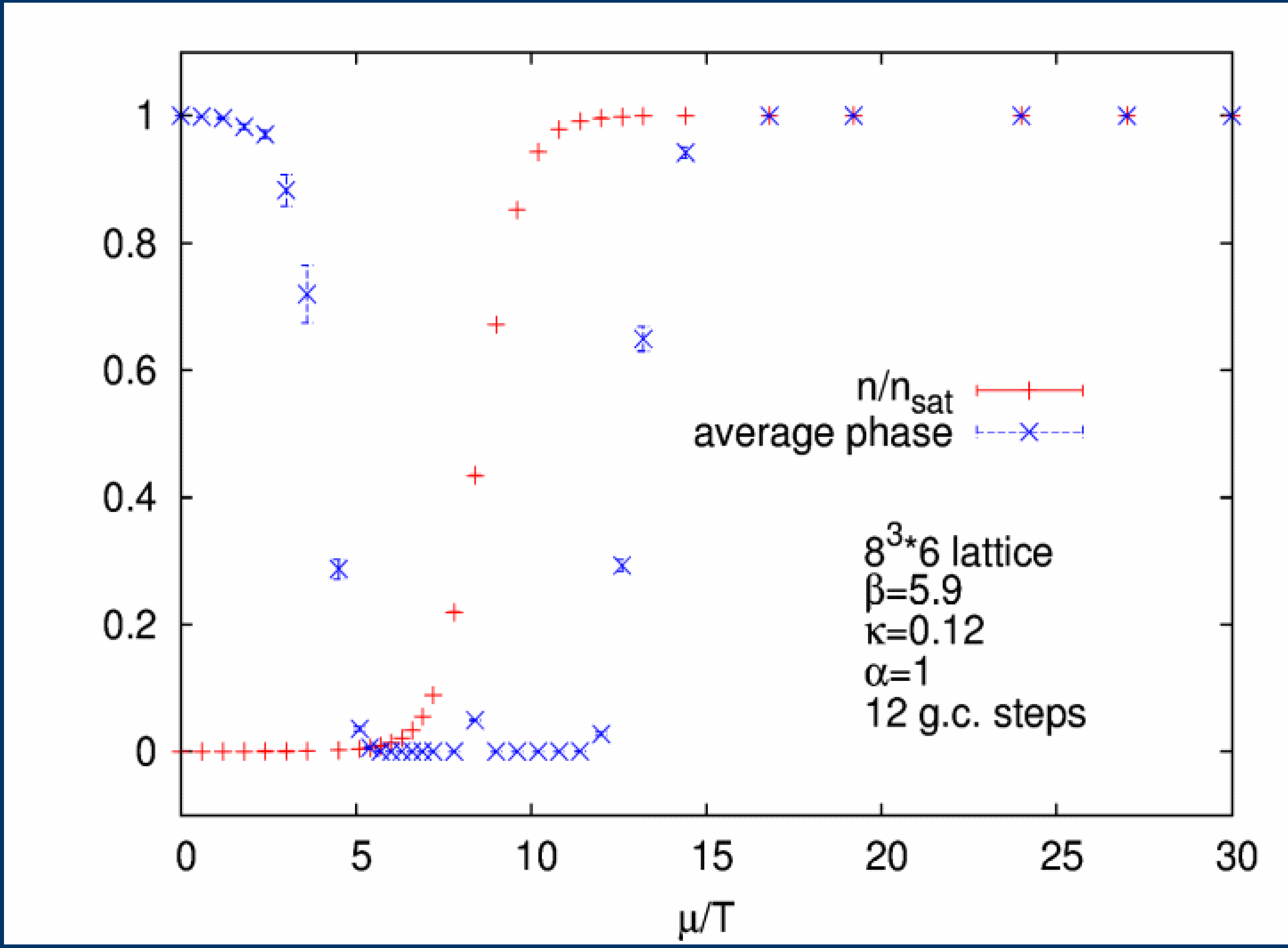


Fermion density:

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

average phase:

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

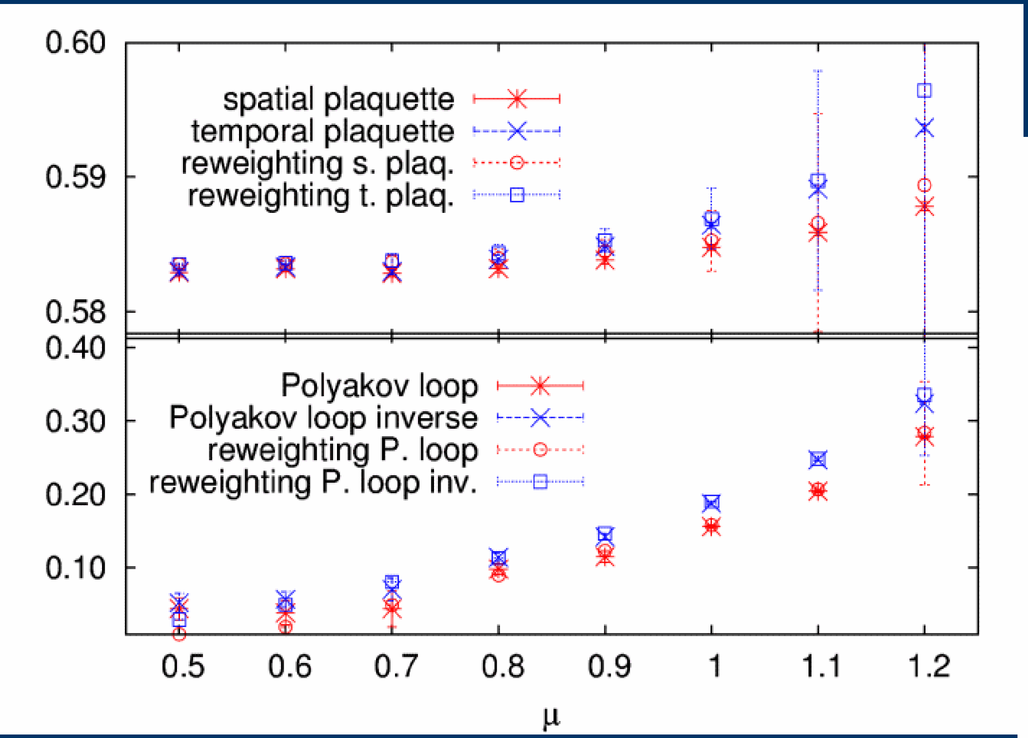


$$\det(1 + C\,P) = 1 + C^3 + C\,\mathrm{Tr}\,P + C^2\,\mathrm{Tr}\,P^{-1}$$

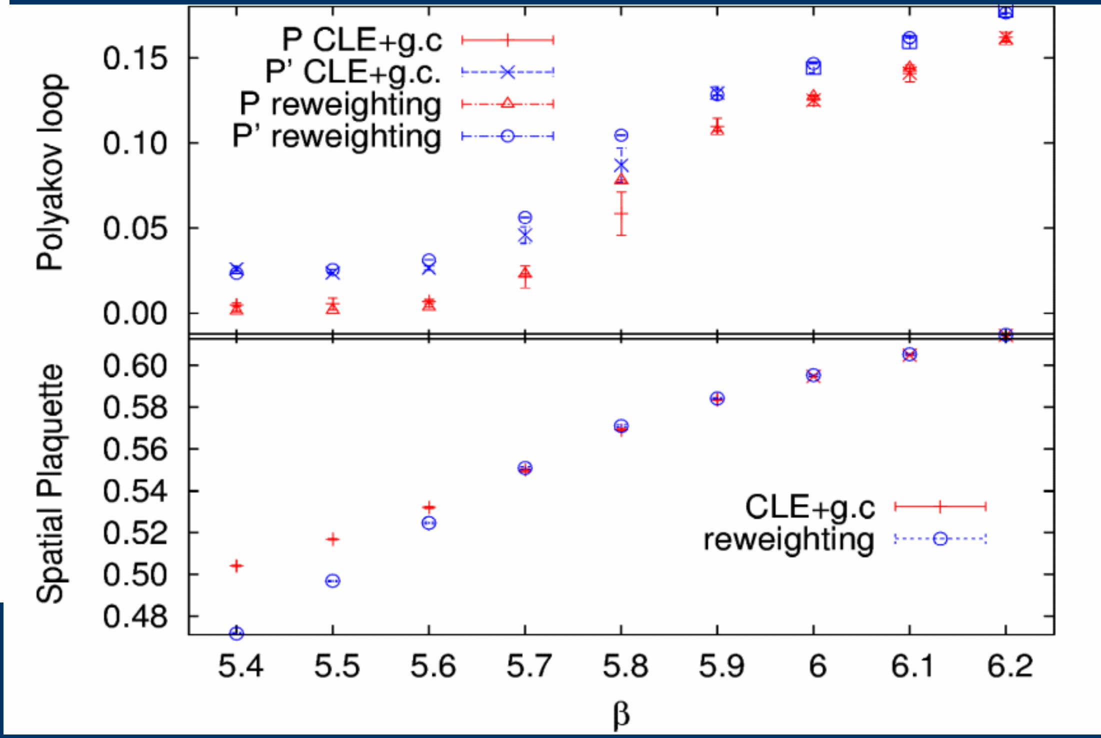
Sign problem is absent at small or large μ

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

Comparison to reweighting

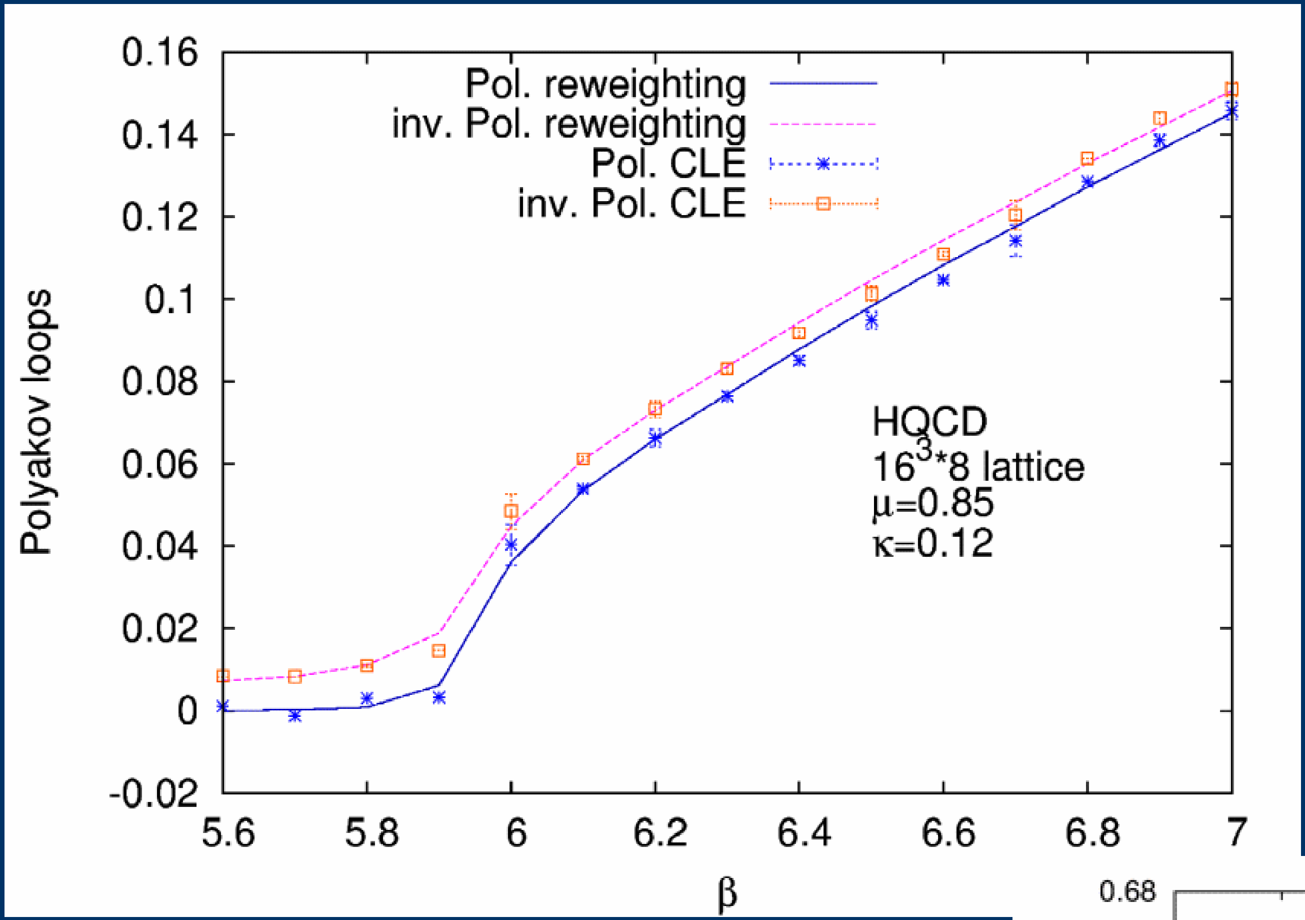


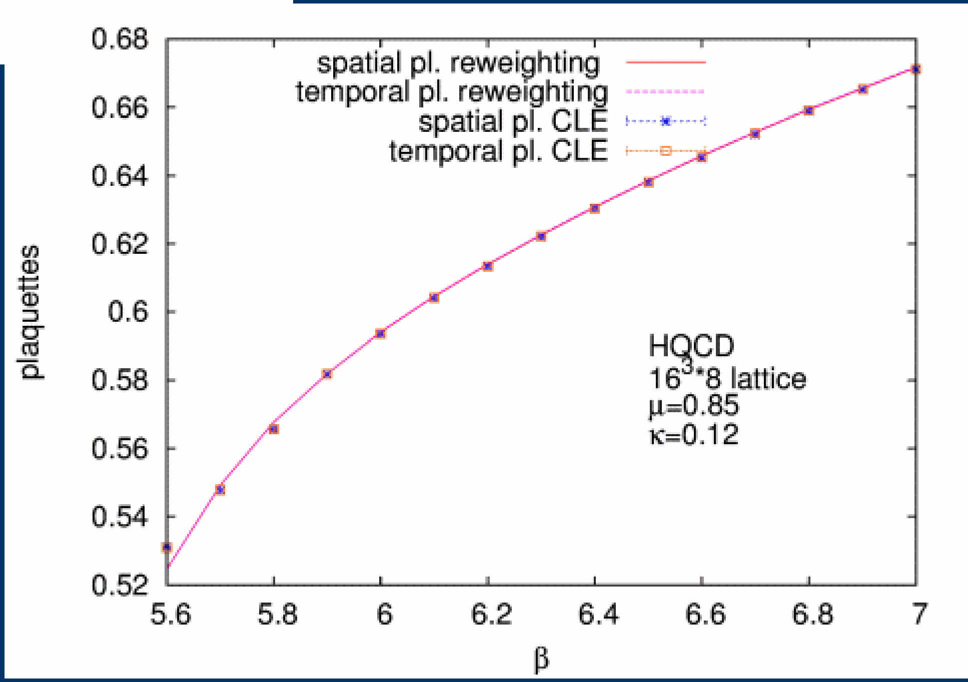
6^4 lattice, $\beta=5.9$



6^4 lattice, $\mu=0.85$

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





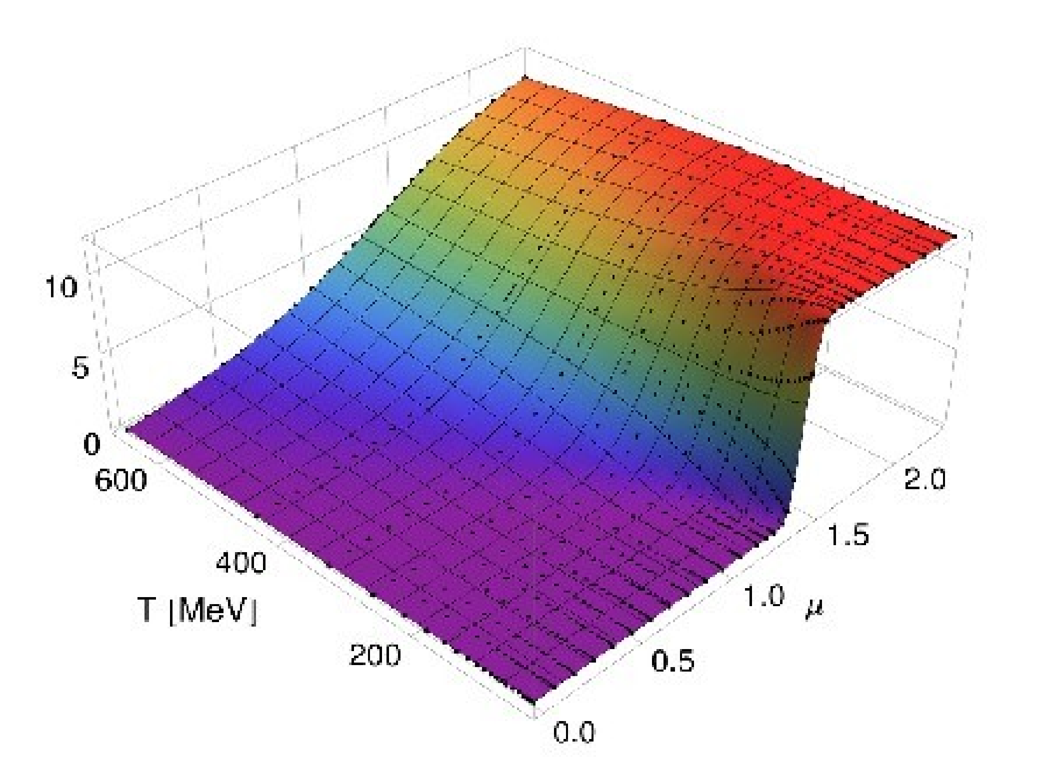
Large lattice:
phase transition clearly visible

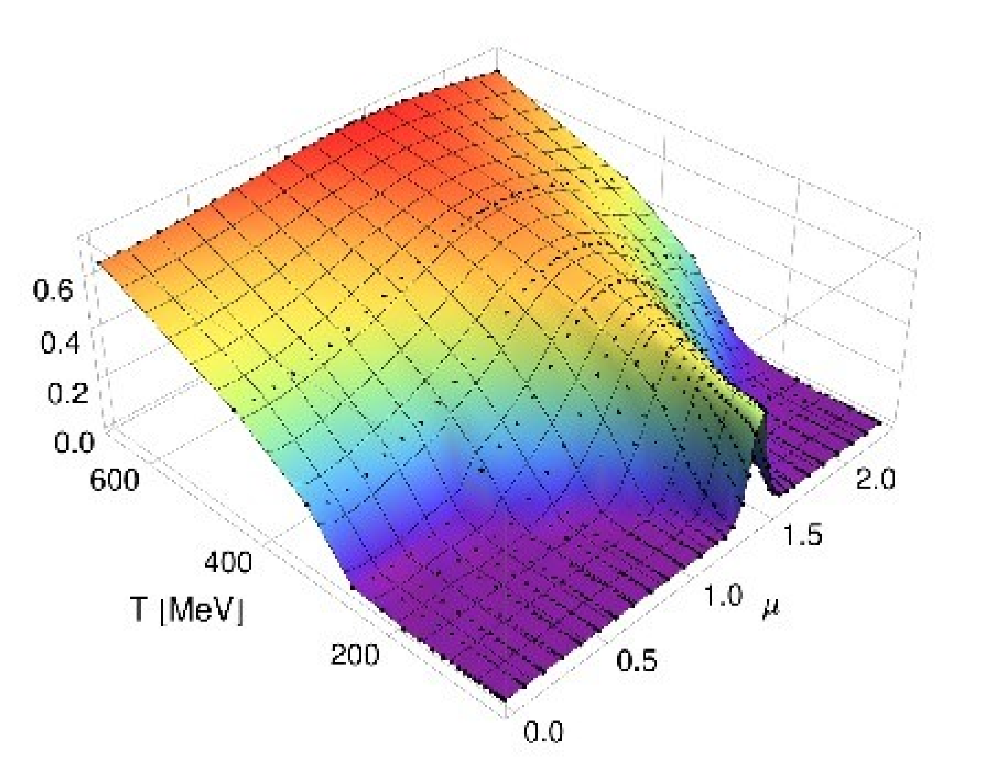
for $\beta > \beta_{min}$

Parallel 4A: Exploring the phase diagram of QCD with complex Langevin simulations

Benjamin Jäger

Phase diagram in HDQCD





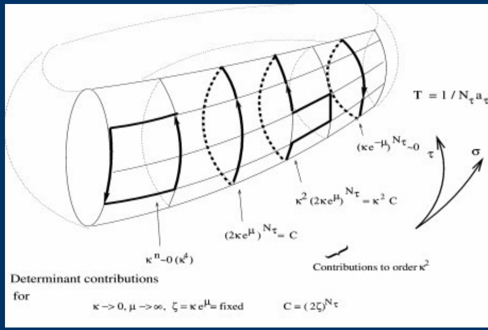
Onset in fermionic density
Silver blaze phenomenon

Polyakov loop
Transition to deconfined state

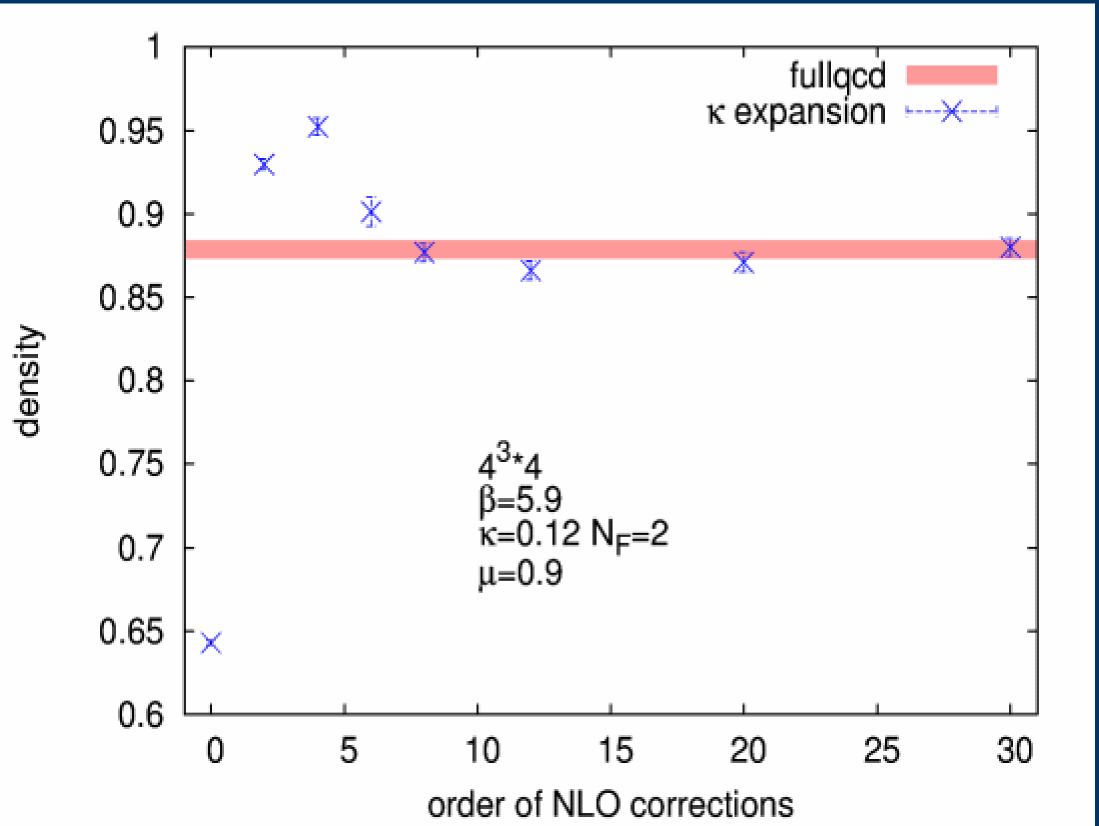
$\beta=5.8 \quad \kappa=0.12 \quad N_f=2 \quad N_t=2...24$

Poster: The onset of the baryonic density in HD-QCD at low temperature

Ion-Olimpiu Stamatescu



HDQCD $\kappa_s = 0$ → κ_s expansion → full QCD

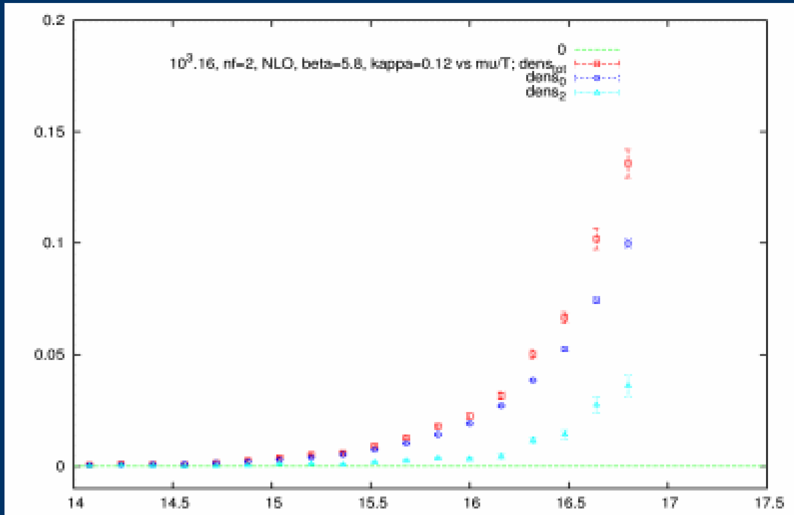


Systematic expansion in κ_s

Convergence can be checked explicitly

Cheaper alternative to full QCD
At heavier quark masses

Onset of the fermionic density
At low temperatures



[Sexty, Stamatescu, et al. in prep.]

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

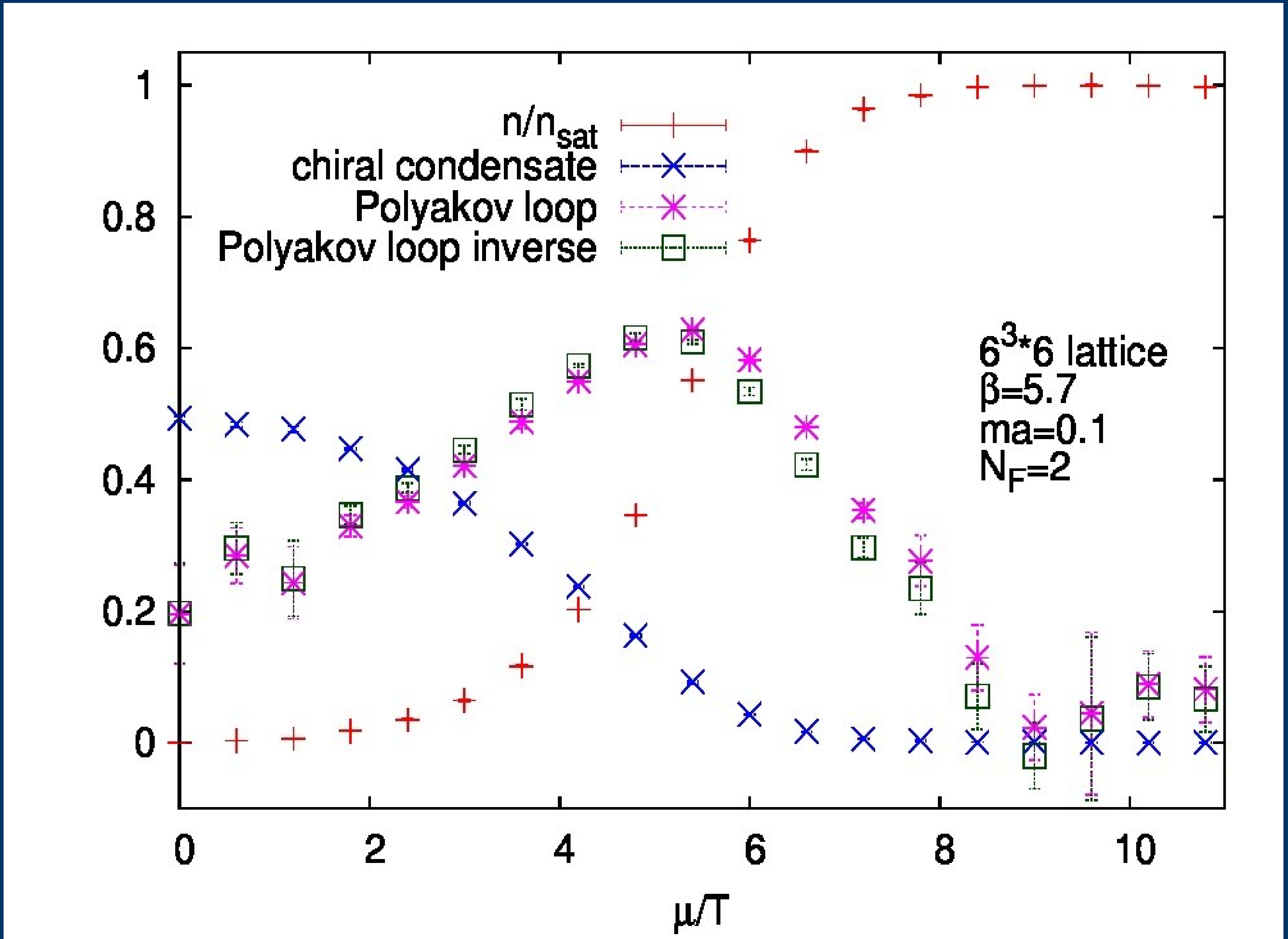
$$K^F_{ax\nu}=\frac{N_F}{4}D_{ax\nu}\ln\det M=\frac{N_F}{4}\mathrm{Tr}\left(M^{-1}M'_{\nu a}(x,y,z)\right)$$

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

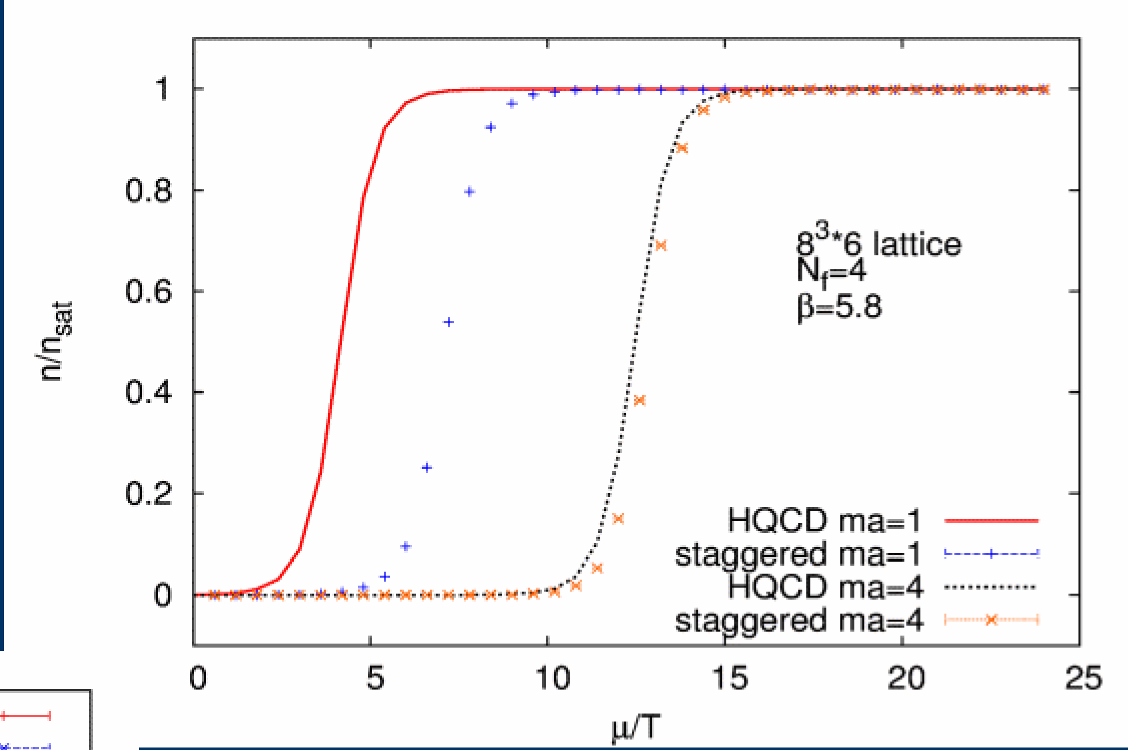
Heavy quarks: compare to HDQCD
Light quarks: compare to reweighting

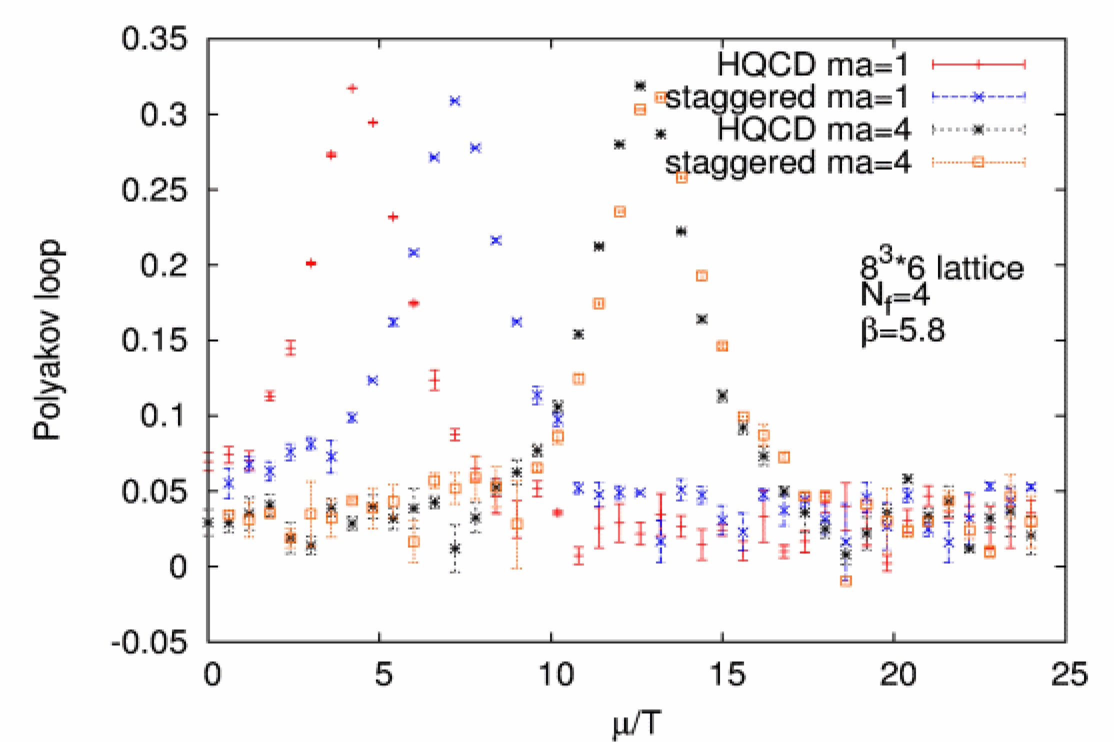

n/n_sat
chiral condensate
Polyakov loop
Polyakov loop inverse
6^3*6 lattice
β=5.7
ma=0.1
N_F=2
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10
μ/T

Comparison of HDQCD in LO and full QCD

Similar behaviour at intermediate masses

Quantative agreement at high masses

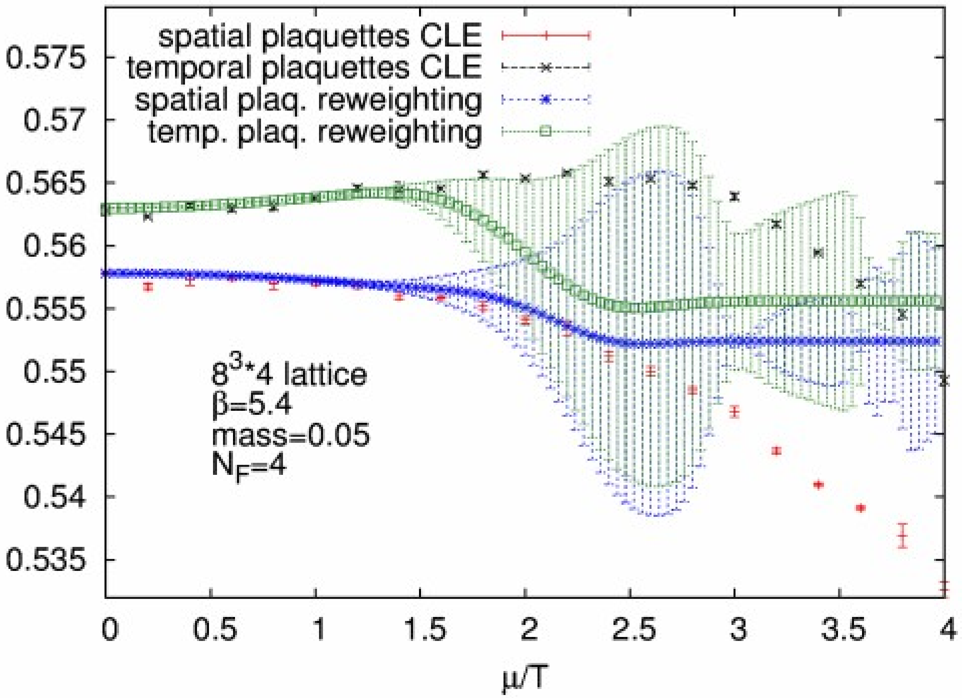


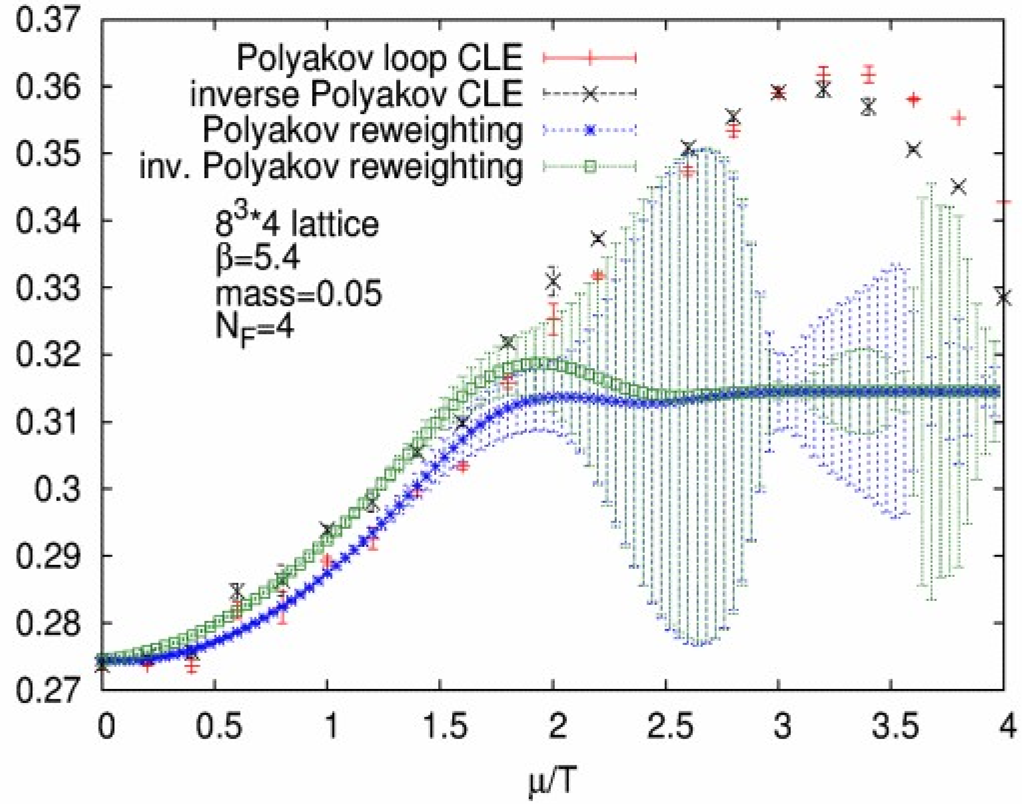


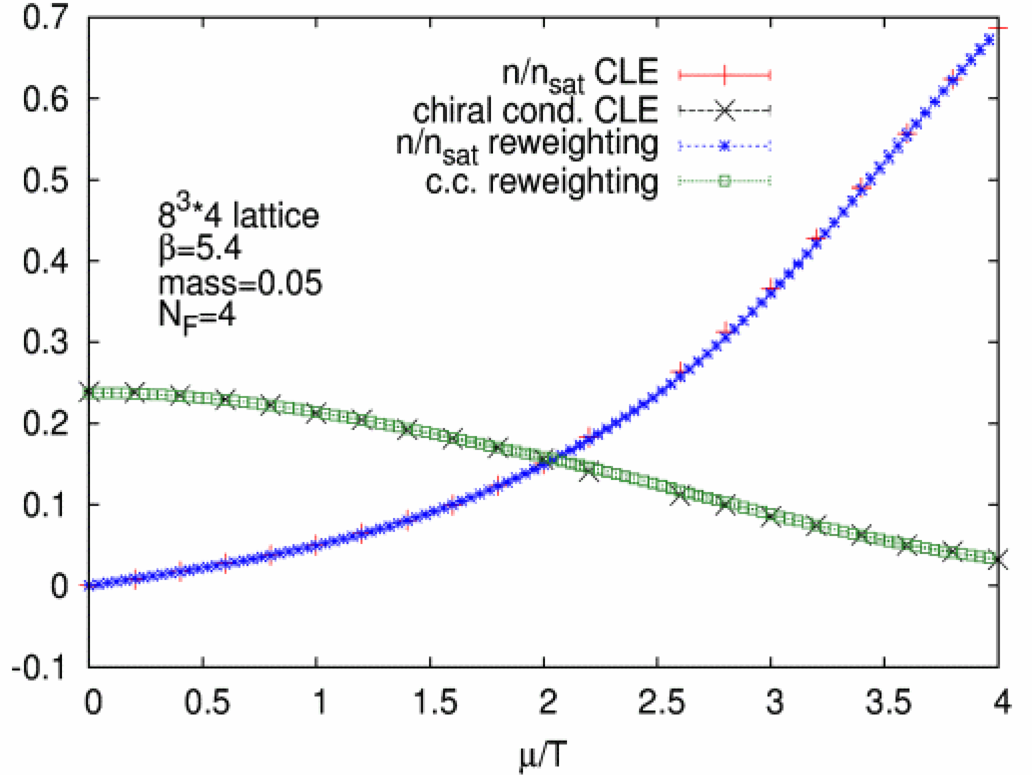
Comparison with reweighting for full QCD

Reweighting from ensemble at

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



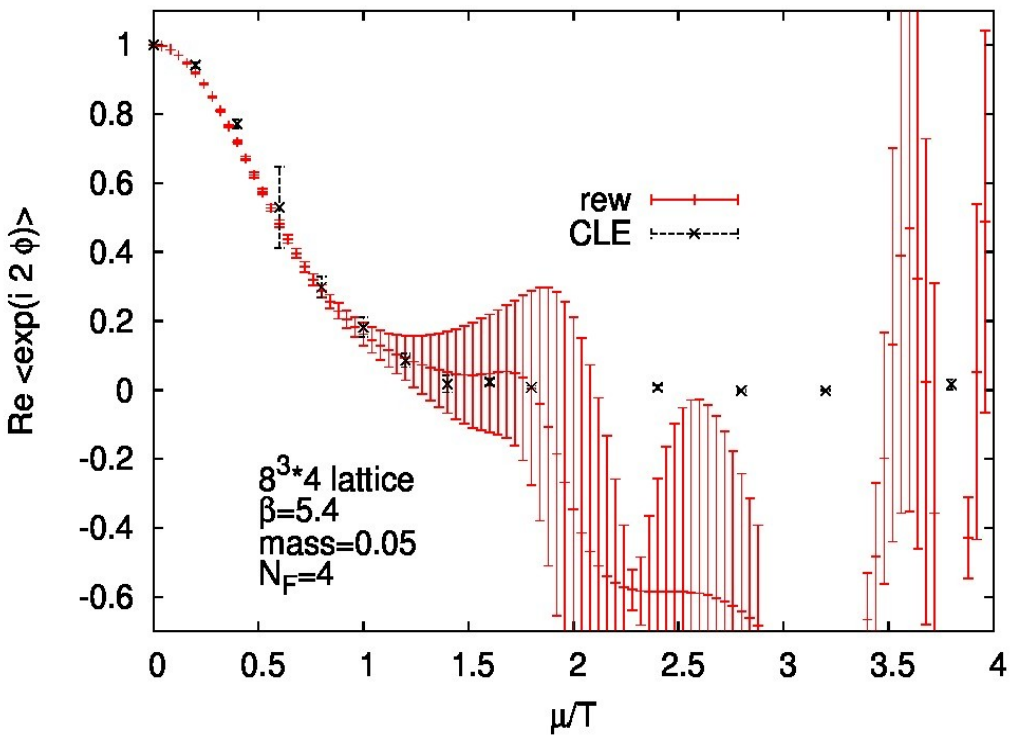


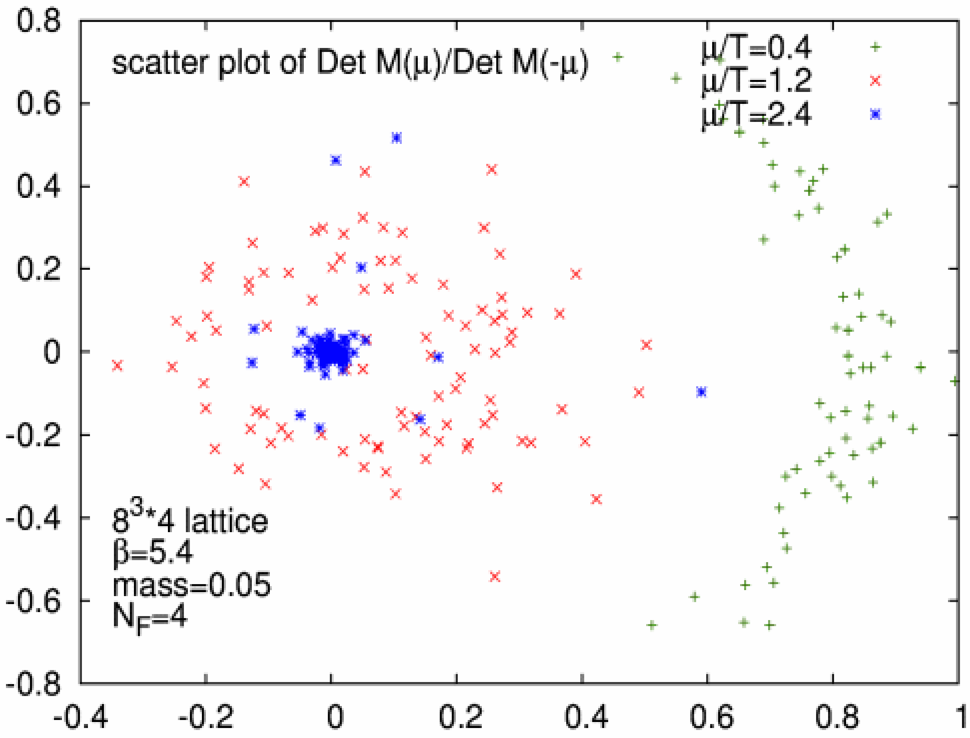


[Fodor, Katz, Sexty (in prep.)]

Sign problem

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





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

Conclusions

Direct simulations at nonzero density using complexified fields
- Complex Langevin Equations
- Lefschetz thimble

Numerical simulations on the Lefschetz thimble are feasible
- Extension to gauge theories?

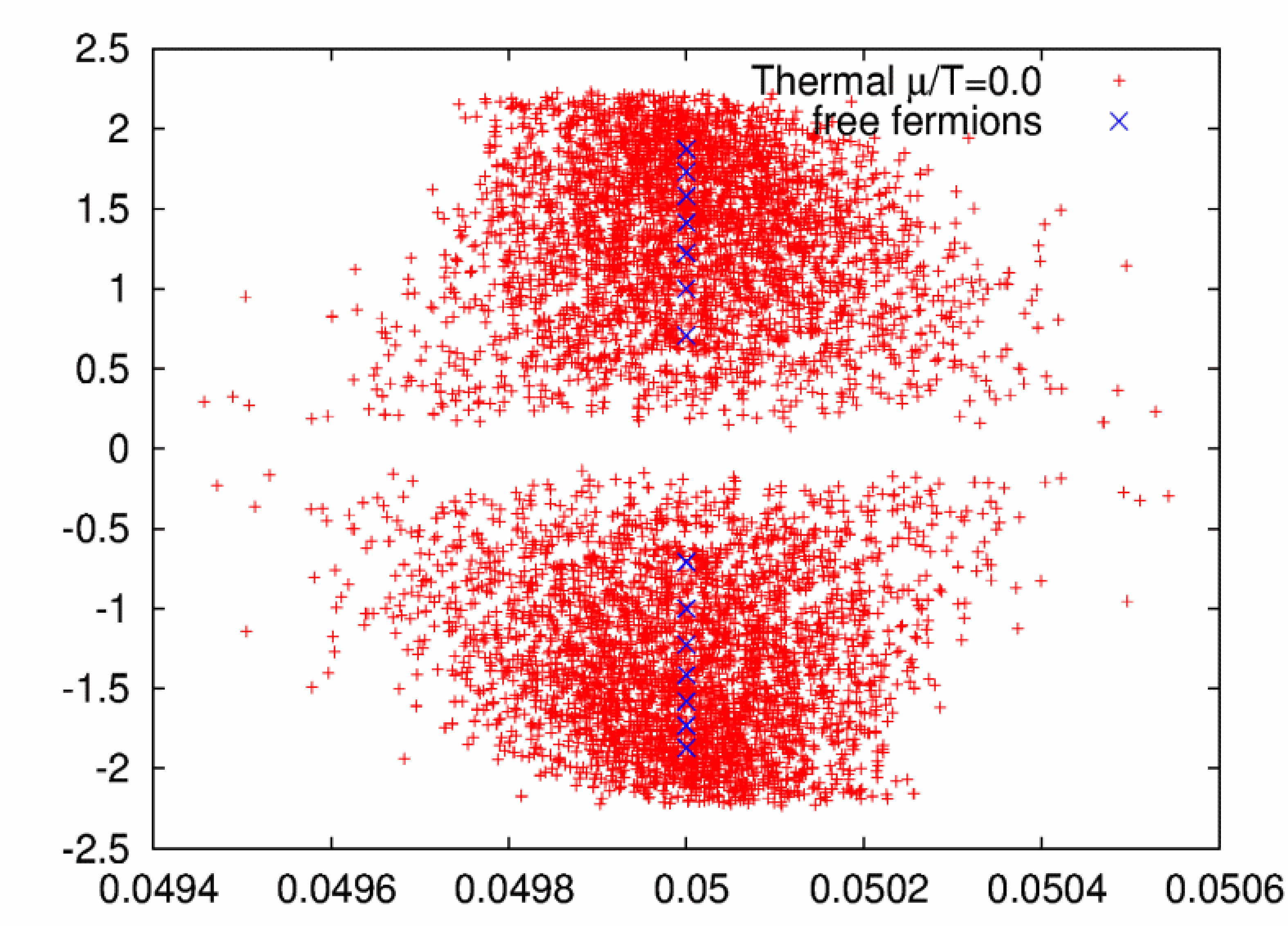
Recent progress for CLE simulations
- Better theoretical understanding (poles?)
- Gauge cooling

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
- First results for the phase diagram

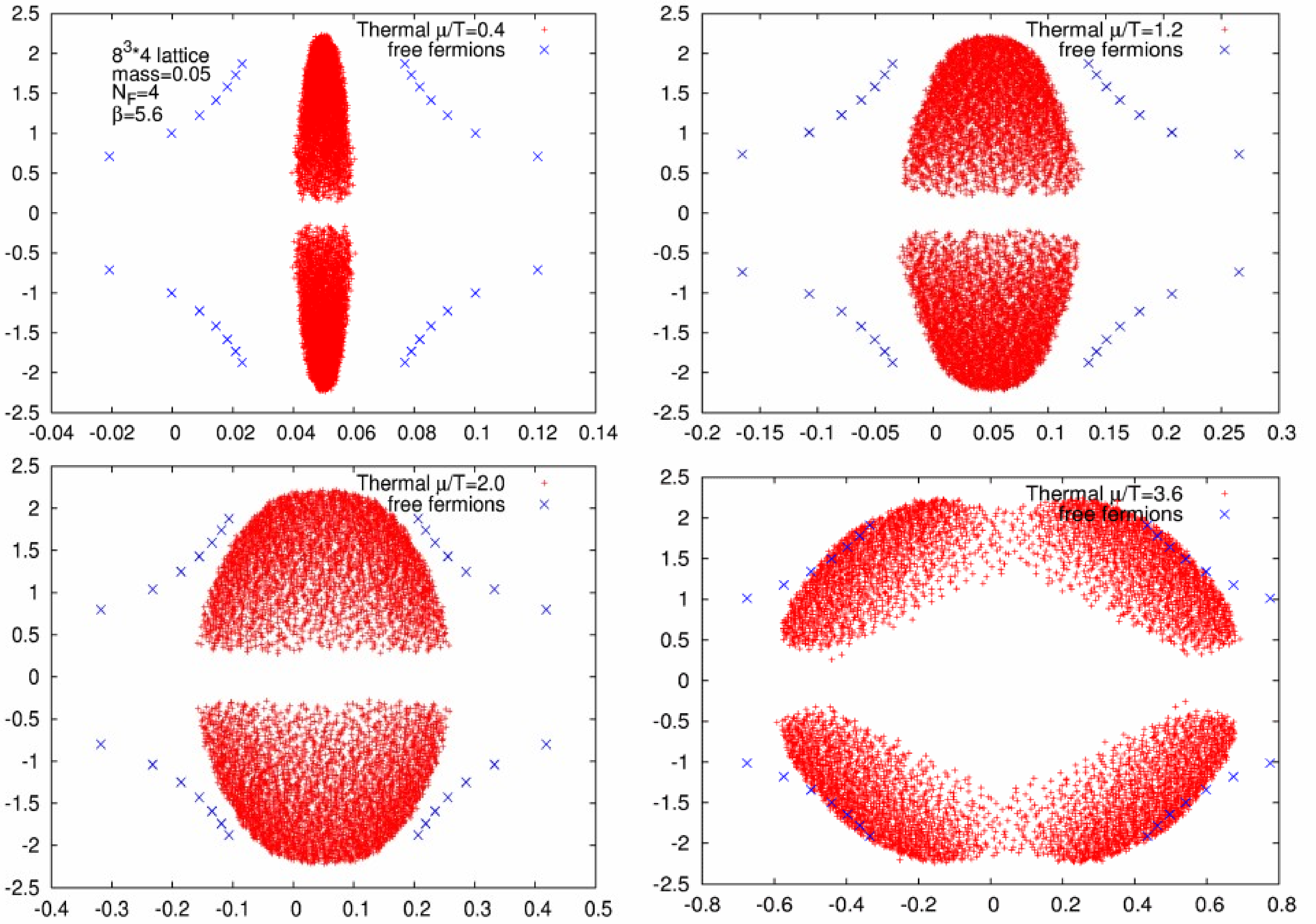
Backup slides

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"