

# New algorithms for finite density QCD

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

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

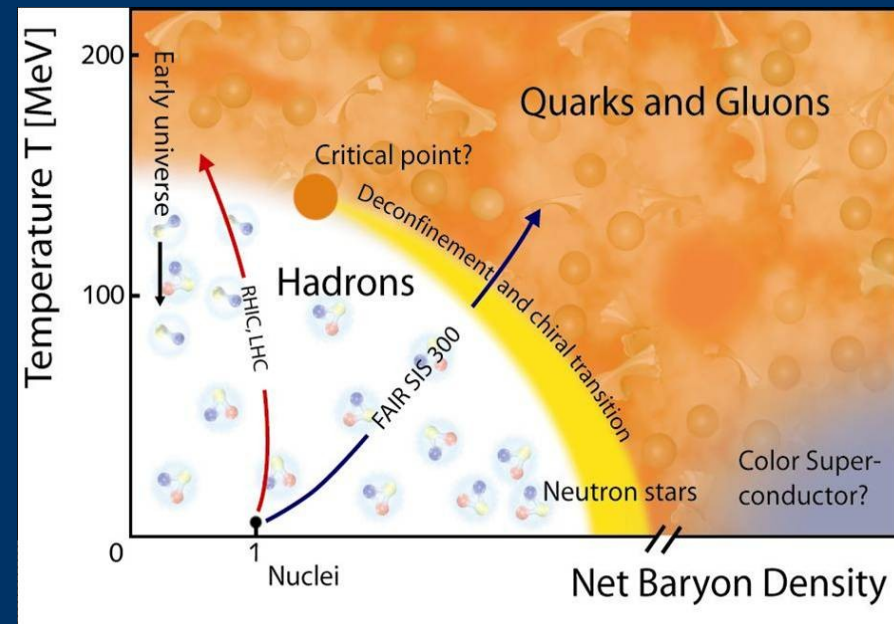
for  $\det(M(U)) > 0$  Importance sampling is possible

## 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  $\mu$

Lombardo '00; de Forcrand, Philipsen '02; D'Elia Sanfilippo '09; Cea et. al. '08-,...

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

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

## Direct Methods:

Use analyticity, 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 model:	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:

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

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  $\longrightarrow$  non-compact

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

Analytically continued observables

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

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

“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

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

measure has zeros ( $\text{Det } M = 0$ )  
complex logarithm has a branch cut  
——► 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 $S = F_{\mu\nu} F^{\mu\nu} + i\Theta \epsilon^{\mu\nu\theta\rho} F_{\mu\nu} F_{\theta\rho}$

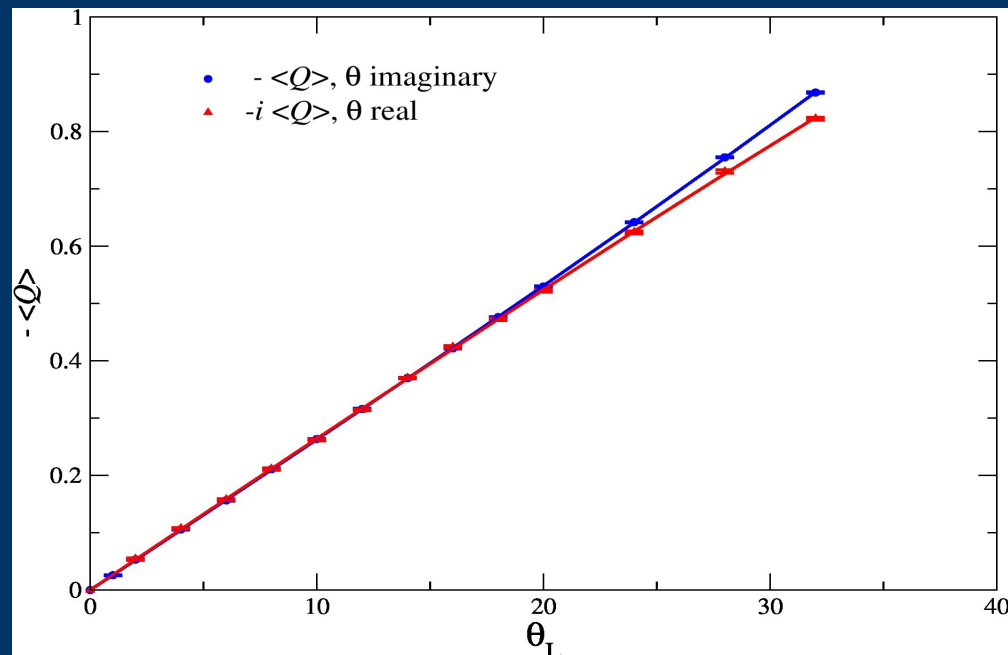
[Bongiovanni, Aarts, Seiler, Sexty, Stamatescu (2013)+in prep.]

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

comparing real  $\Theta$   
with imaginary  $\Theta$

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

$e^{\operatorname{Re}(S(z(t)))}$	peak + fast decay
$e^{i\operatorname{Im}(S(z(t)))}$	milder sign problem than original

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

Thanks to Cauchy-Riemann equations

Lefschetz thimble is a contour which  
starts from saddle points  $\partial_z S(z_0) = 0$

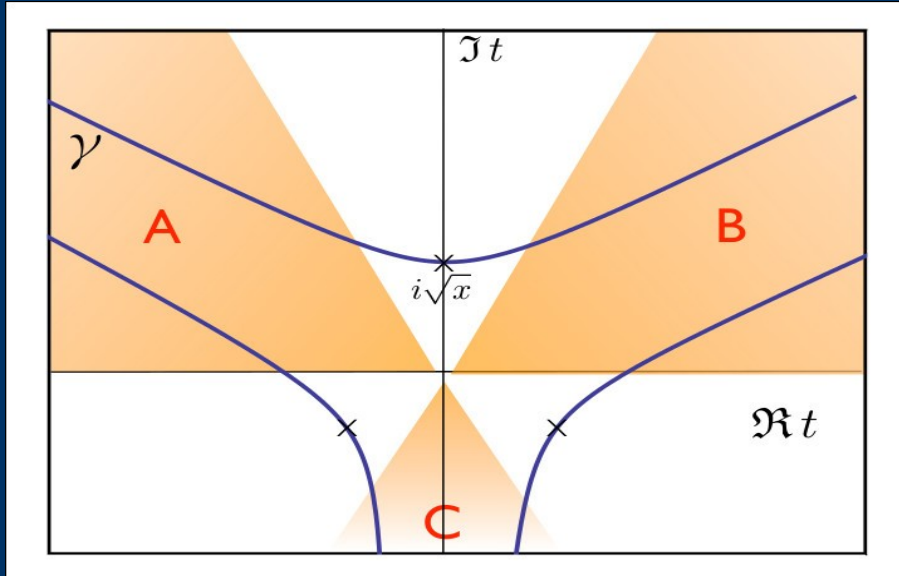
$$\frac{\partial z}{\partial t} = \pm \overline{\partial_z S(z)}$$

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

+ : stable thimble  $\longleftrightarrow$  steepest descent  
- : unstable thimble  $\longleftrightarrow$  steepest ascent

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

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:  $\sum_k m_k T_k \rightarrow T_0$

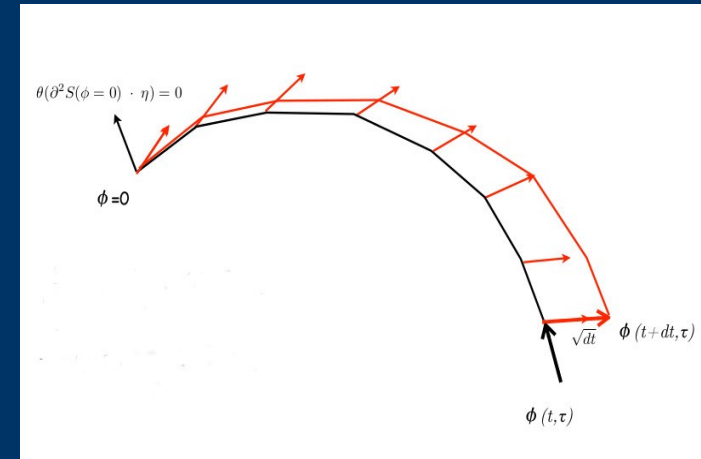
Choose thimble with the global minimum  
Regularisation of QFT  
Resurgence

# Numerical Simulations on the Lefschetz Thimble

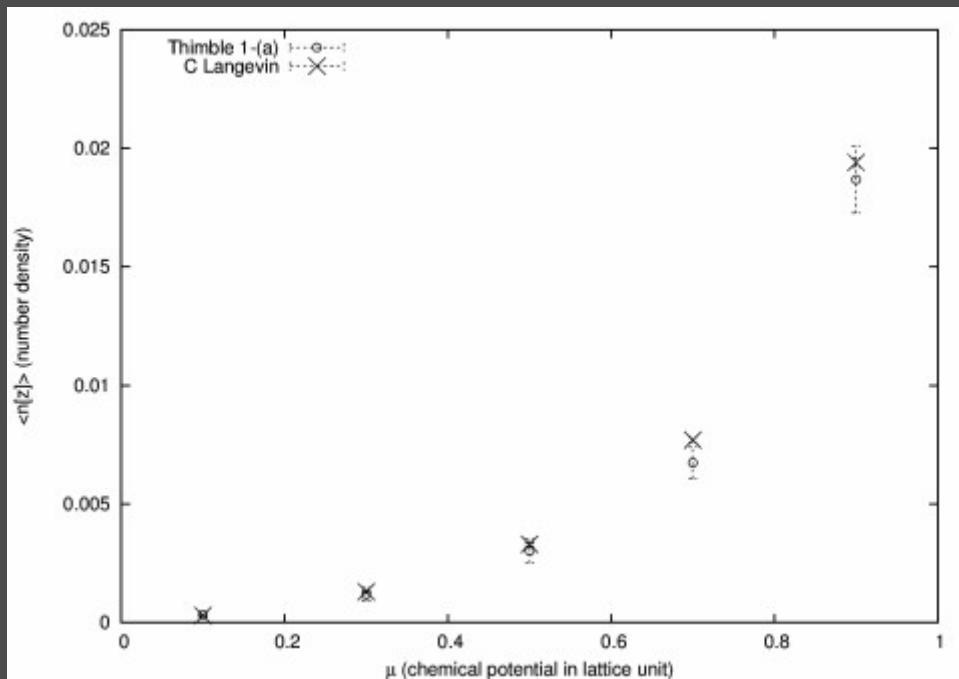
Algorithm needed to keep configurations on the thimble

$\varphi^4$  theory with nonzero  $\mu$

(real) Langevin eq. on the thimble

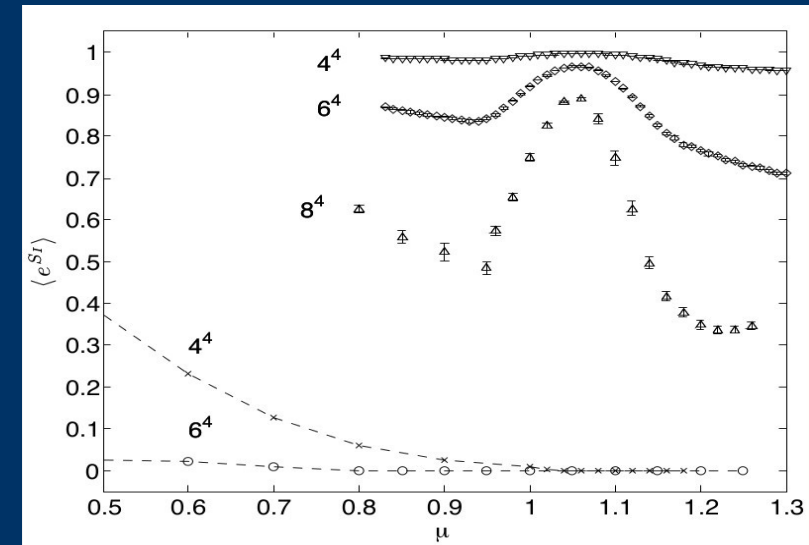


## HMC on the thimble



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

[Cristoforretti, Di Renzo, Scorzato (2012)]



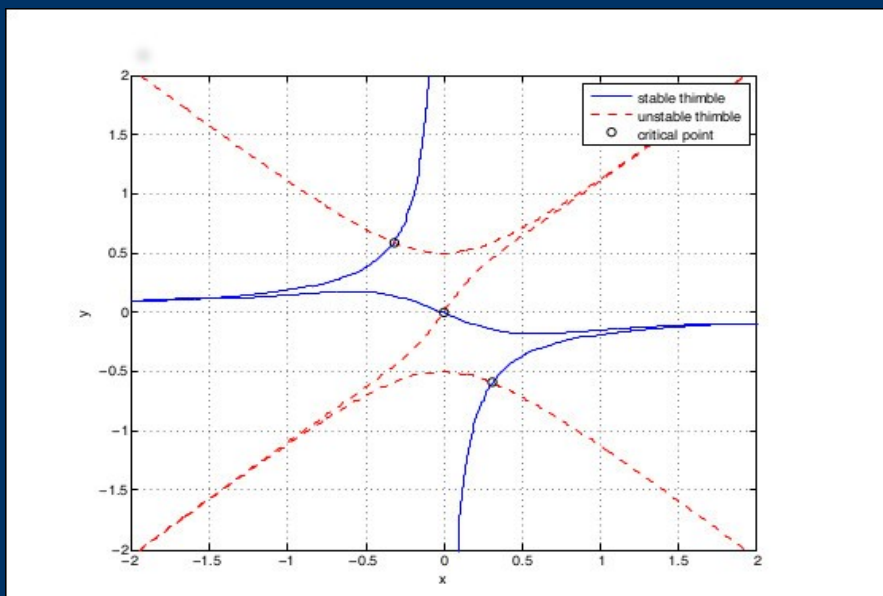
# Parallel 4A: Solution of simple toy models via thimble regularization of lattice field theory

Giovanni Eruzzi

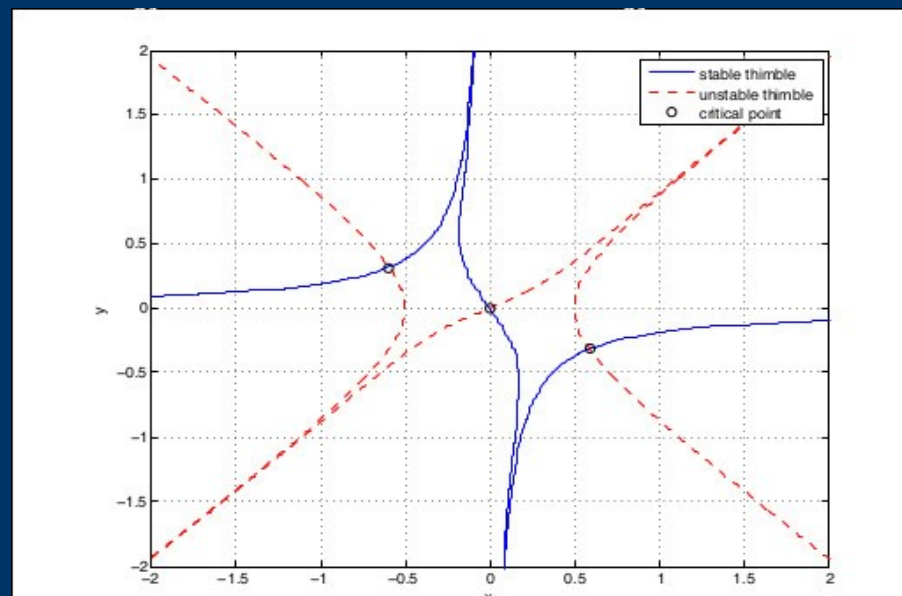
A number of algorithms tested to sample the thimble

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

$\text{Re } \sigma > 0$



$\text{Re } \sigma < 0$



# Parallel 8F: An algorithm for thimble regularization of lattice field theories

Francesco Di Renzo

“Ideal sampling” on the thimble

# Langevin and Lefschetz

Both use analyticity and complexification

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

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

# 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

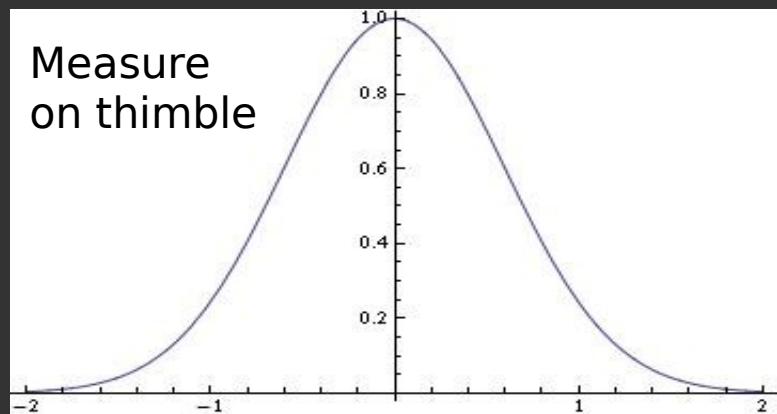
$$\left. \frac{\partial S(z)}{\partial z} \right|_{z_0} = 0$$

Thimble

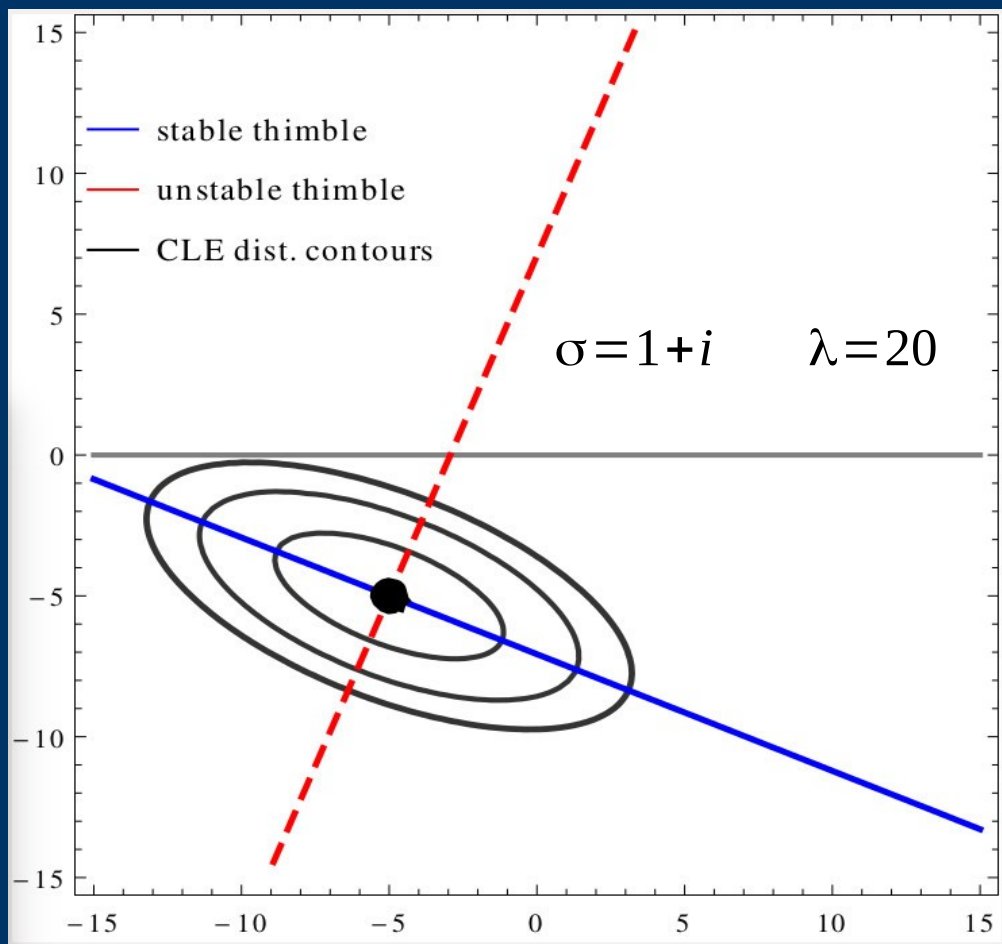
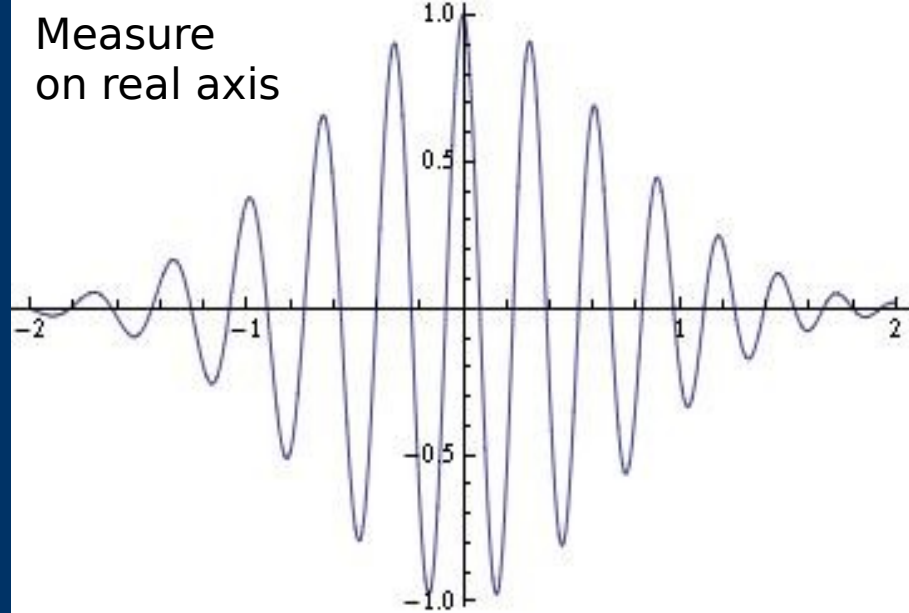
$$\dot{z} = -\overline{\partial_z S(z)}$$

Straight lines  
starting from  $z_0$

Measure  
on thimble



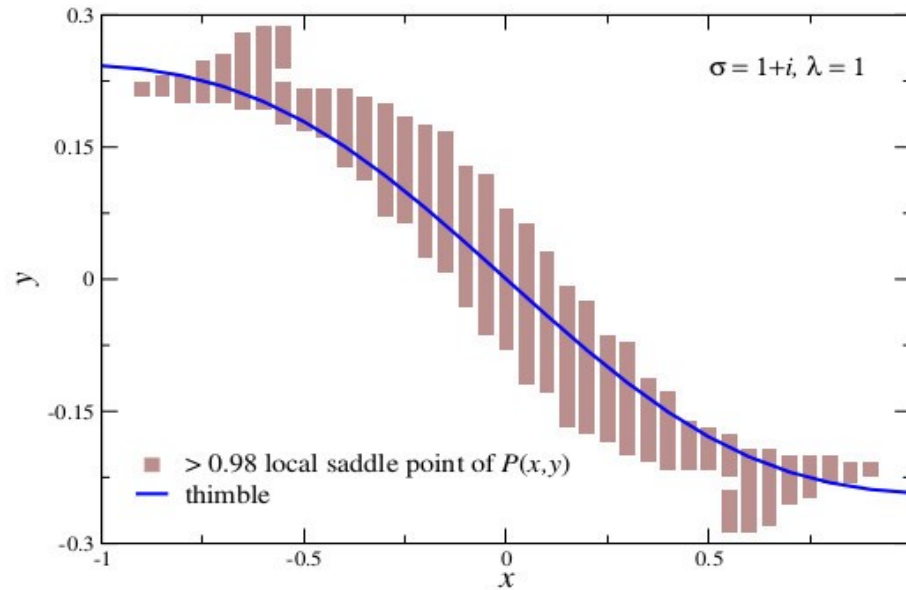
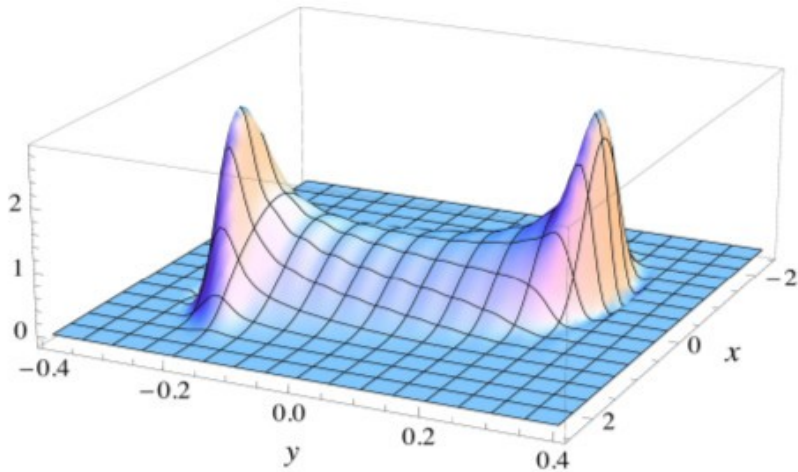
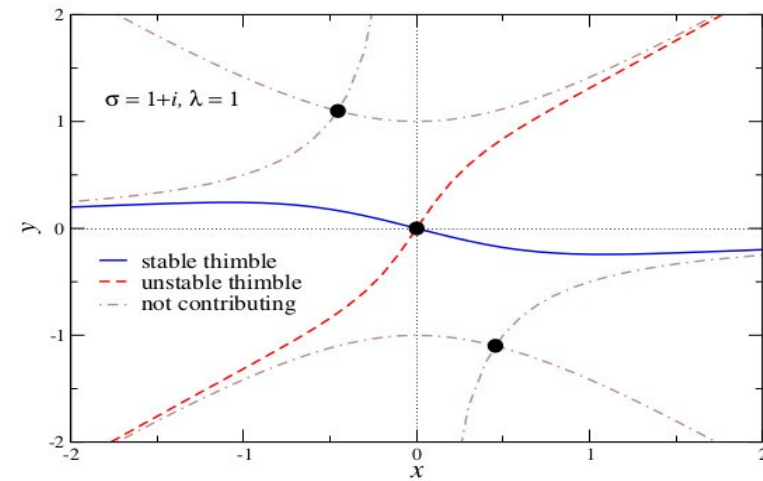
Measure  
on real axis



# Quartic model

[Aarts (2013)]

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



CLE distributions follow thimble

Deeper connection?



# Gauge theories and CLE

link variables:  $SU(N)$   $\longrightarrow$   $SL(N, \mathbb{C})$   
compact non-compact  
 $\det(U) = 1, \quad U^\dagger \neq U^{-1}$

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  $SU(N)$

$$\sum_i \text{Tr}(U_i U_i^\dagger)$$

$$\sum_{ij} |(U U^\dagger - 1)_{ij}|^2$$

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

# 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  $SU(N)$

$$\sum_i \text{Tr}(U_i U_i^\dagger - 1)$$

Using gauge transformations in  $SL(N, \mathbb{C})$

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

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

Gradient of the unitarity norm gives steepest descent

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

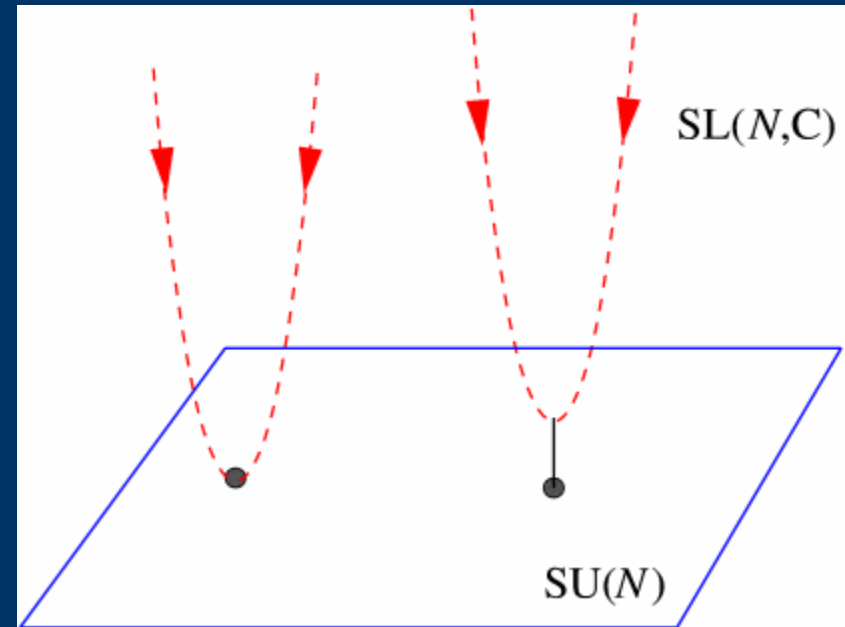
Gauge transformation at  $x$  changes 2d link variables

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

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

Dynamical steps are interspersed with several gauge cooling steps

The strength of the cooling is determined by  
cooling steps  
gauge cooling parameter  $\alpha$



Empirical observation:  
Cooling is effective for

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

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

# Heavy Quark QCD at nonzero chemical potential (HDQCD)

Hopping parameter expansion of the fermion determinant  
 Spatial hoppings are dropped

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

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

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

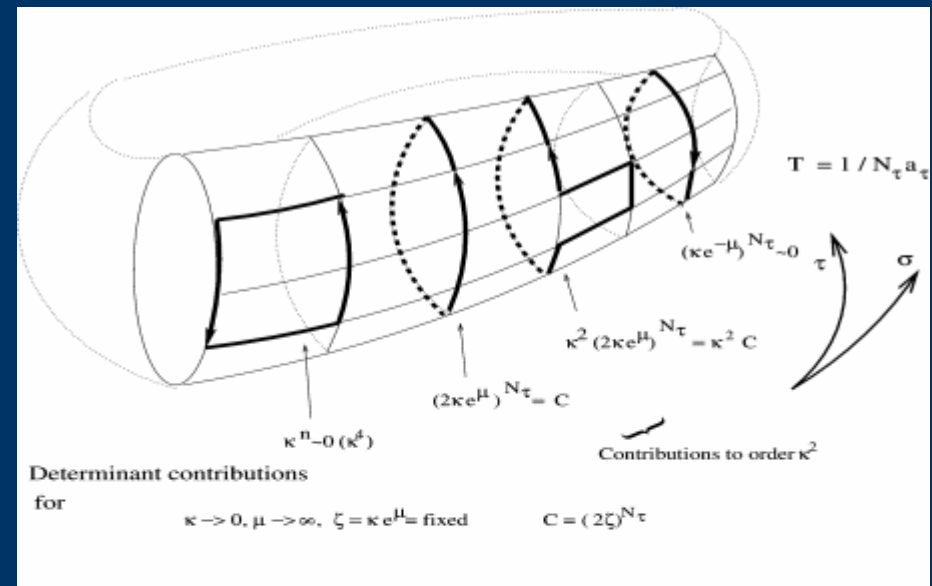
Studied with reweighting

De Pietri, Feo, Seiler, Stamatescu '07

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

CLE study using gaugecooling

[Seiler, Sexty, Stamatescu (2012)]

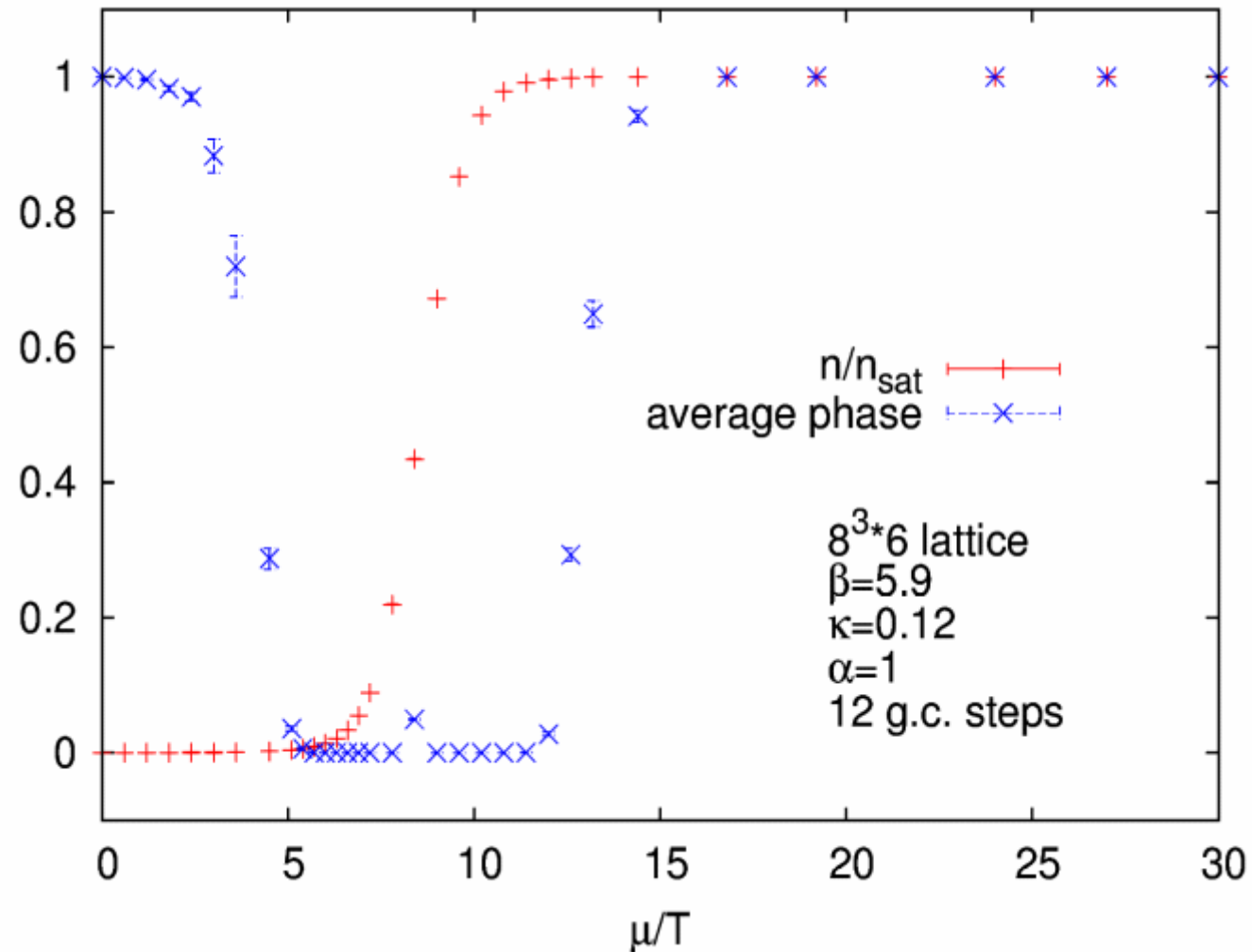


Fermion density:

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

average phase:

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

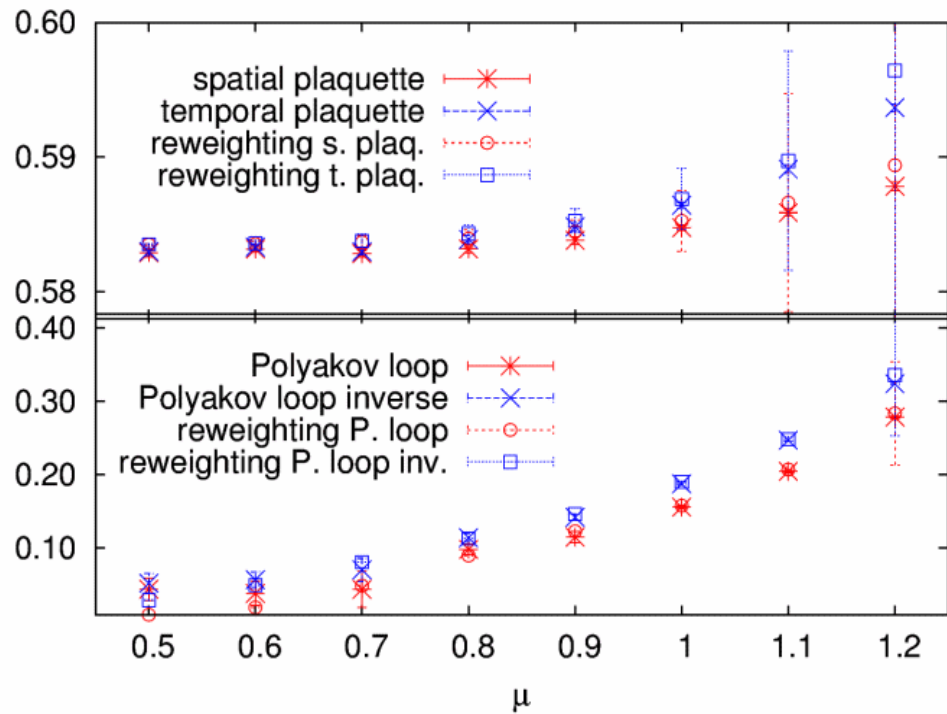


$$\det(1 + CP) = 1 + C^3 + C \text{Tr } P + C^2 \text{Tr } P^{-1}$$

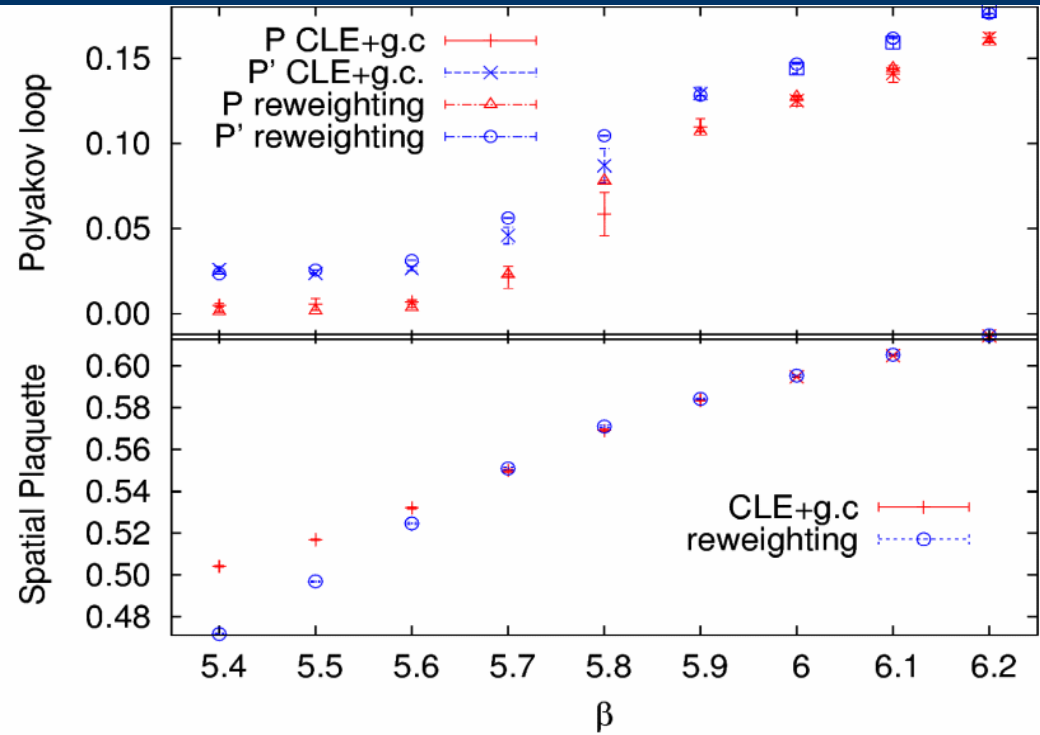
Sign problem is absent at  
small or large  $\mu$

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

# Comparison to reweighting

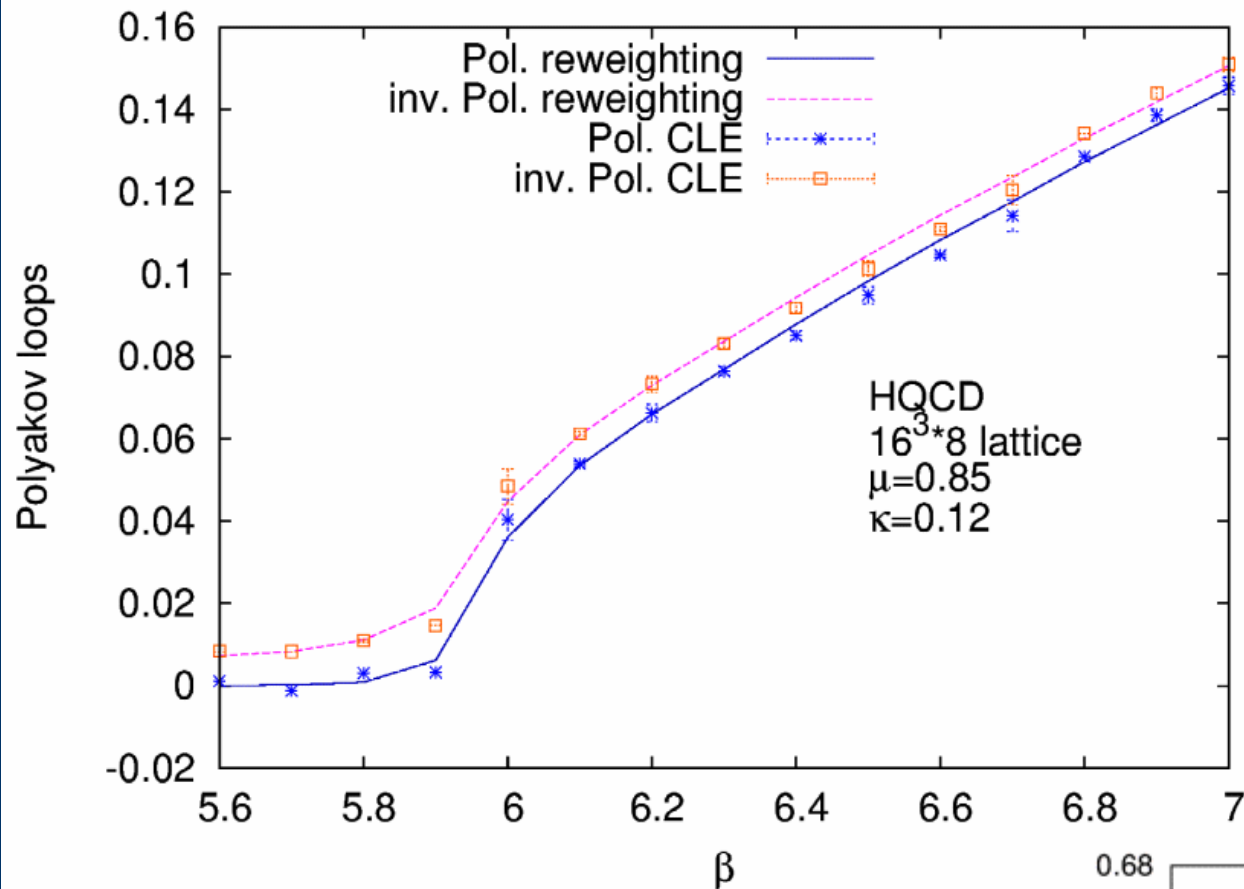


$6^4$  lattice,  $\beta=5.9$



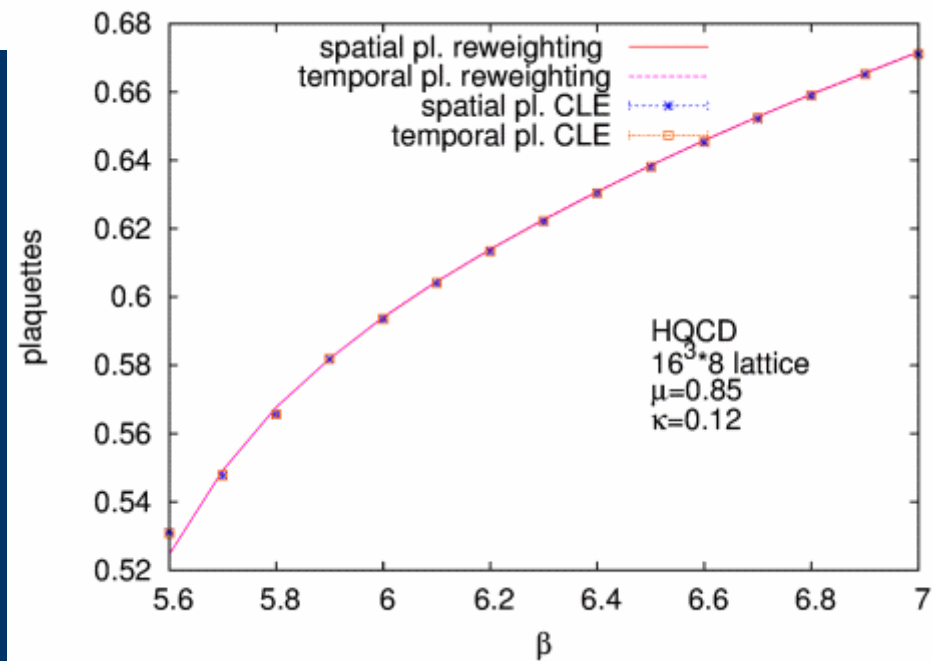
$6^4$  lattice,  $\mu=0.85$

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



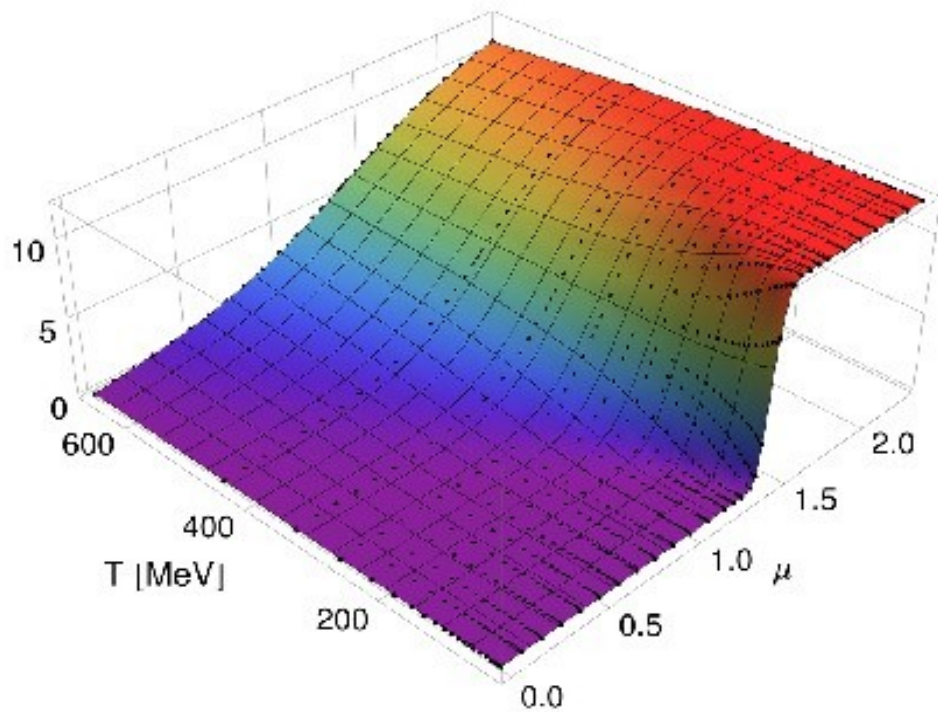
Large lattice:  
phase transition clearly visible

for  $\beta > \beta_{min}$

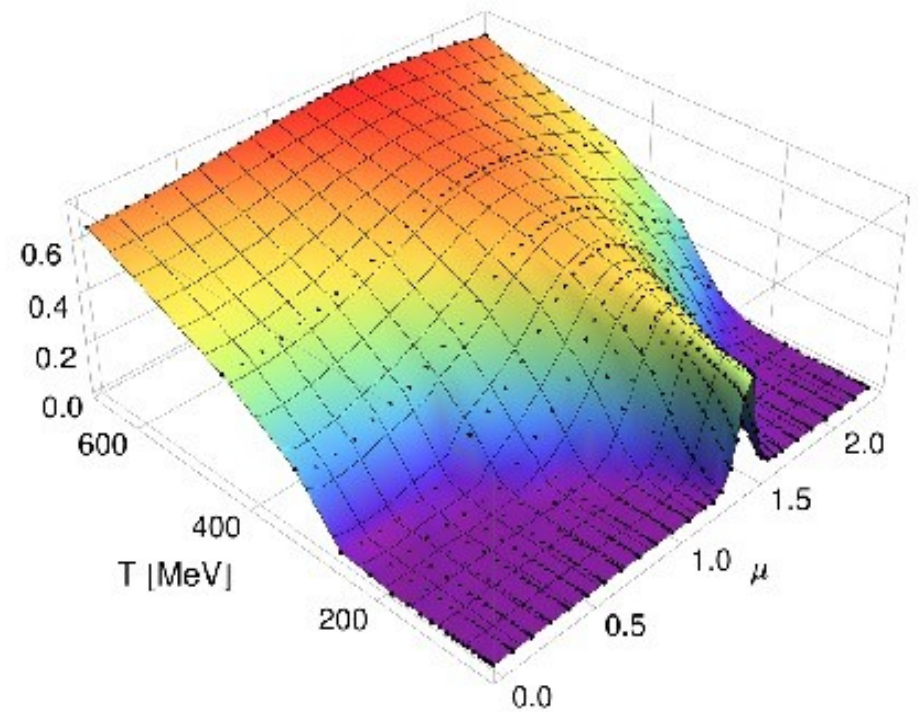


# Parallel 4A: Exploring the phase diagram of QCD with complex Langevin simulations Benjamin Jäger

Phase diagram in HDQCD



Onset in fermionic density  
Silver blaze phenomenon



Polyakov loop  
Transition to deconfined state

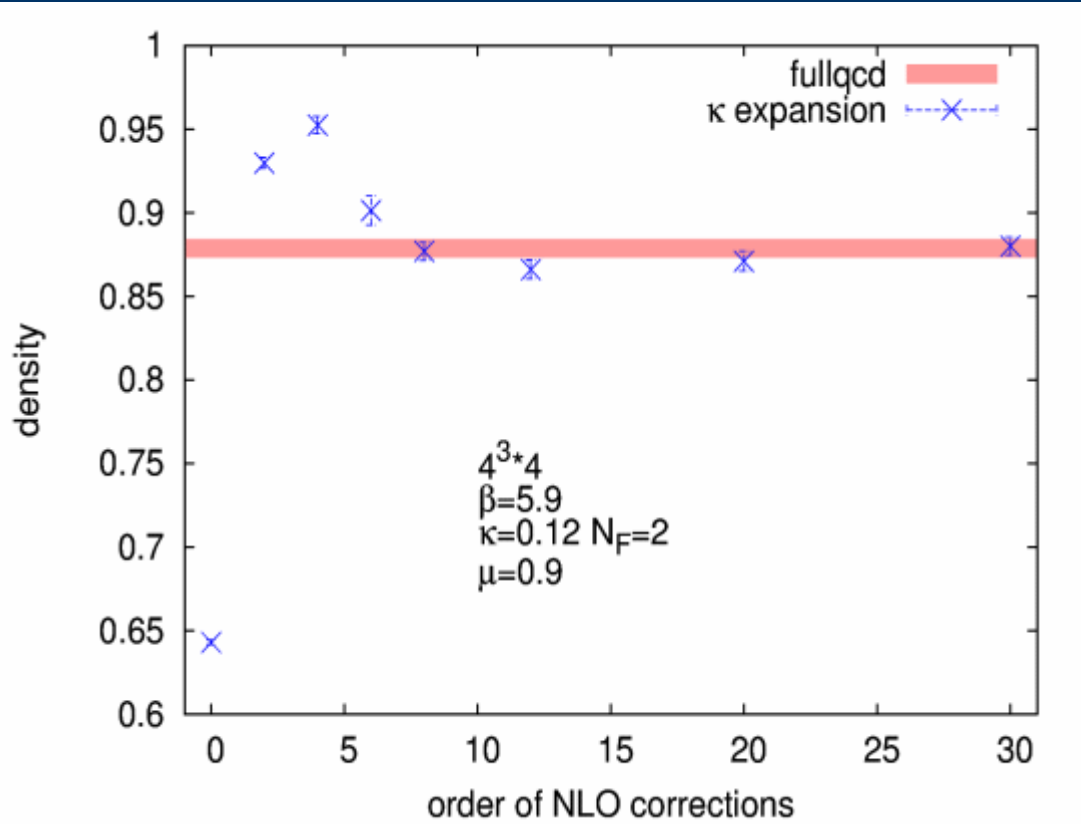
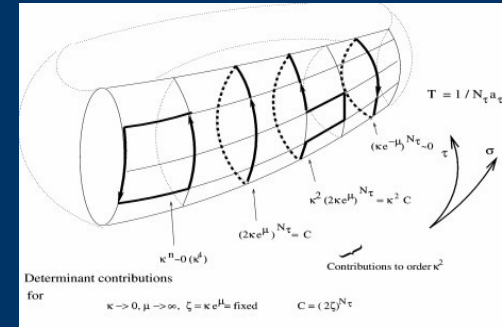
$$\beta=5.8 \quad \kappa=0.12 \quad N_f=2 \quad N_t=2\dots 24$$



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

Ion-Olimpiu Stamatescu

HDQCD  $\kappa_s = 0 \rightarrow \kappa_s$  expansion  $\rightarrow$  full QCD



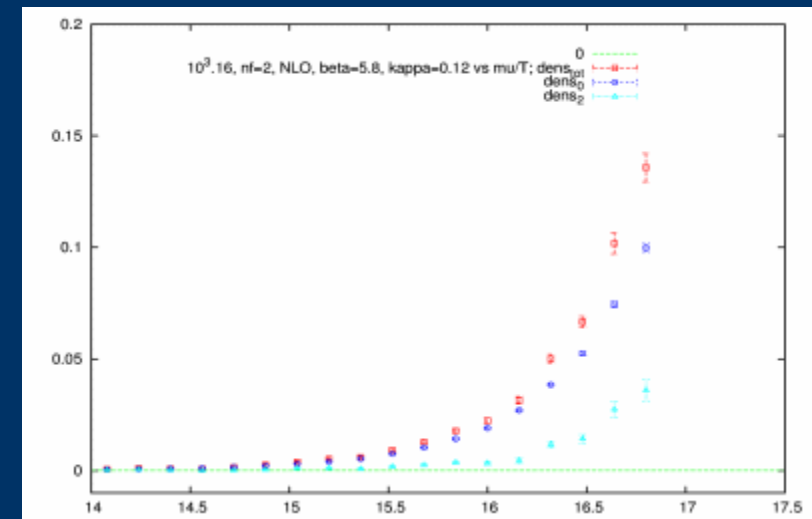
Systematic expansion in  $\kappa_s$

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

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

Noisy estimator with one noise vector

Main cost of the simulation: CG inversion

Inversion cost highly dependent on chemical potential

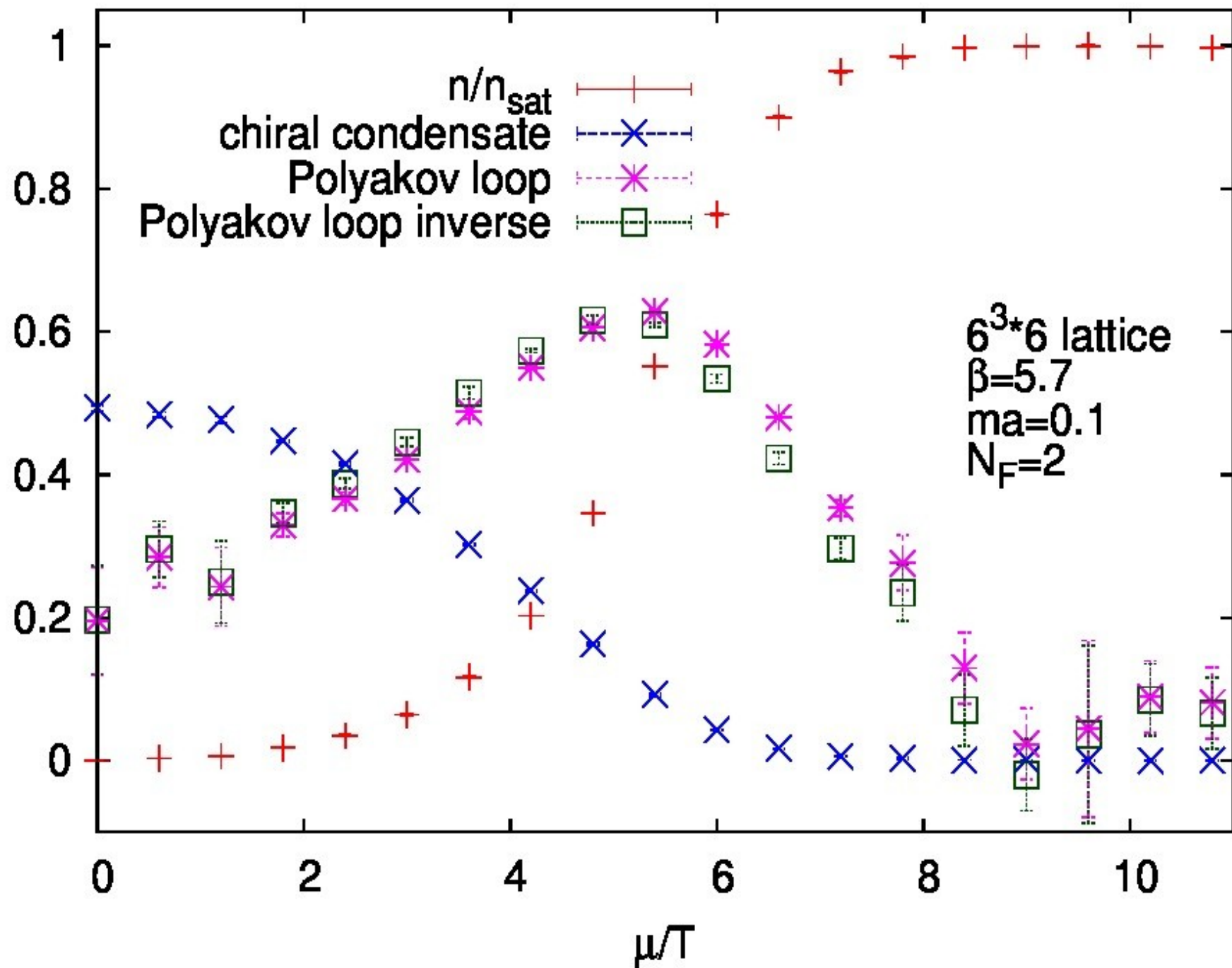
Eigenvalues not bounded from below by the mass

(similarly to isospin chemical potential theory)

Unimproved staggered and Wilson fermions

Heavy quarks: compare to HDQCD

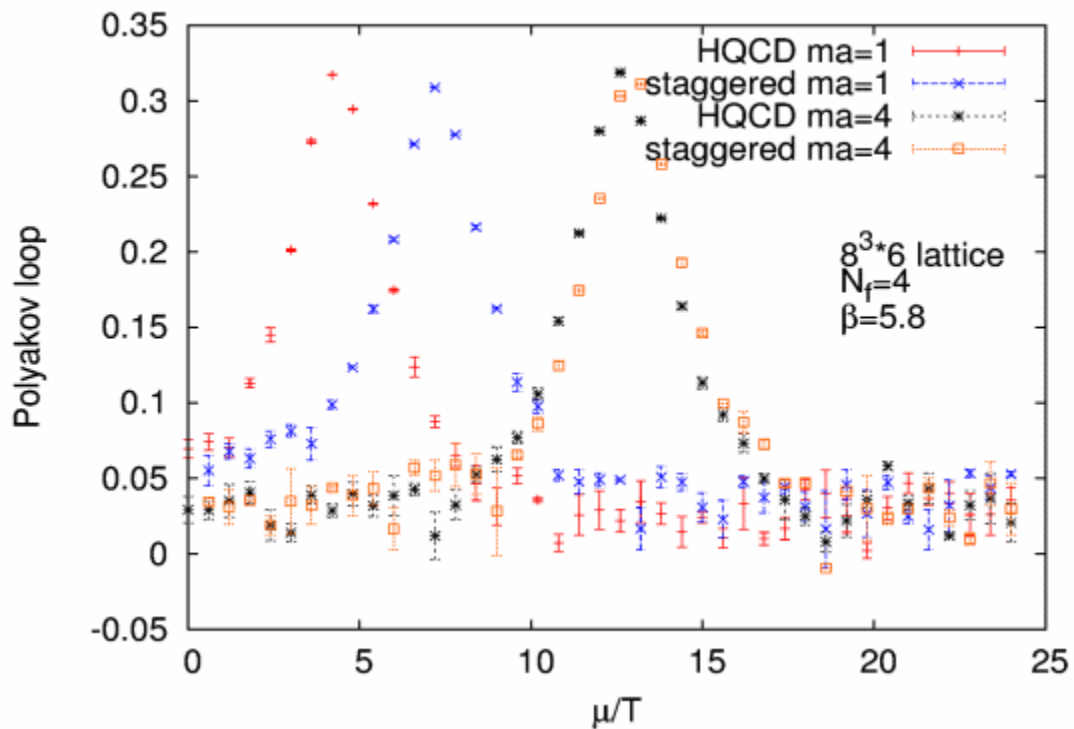
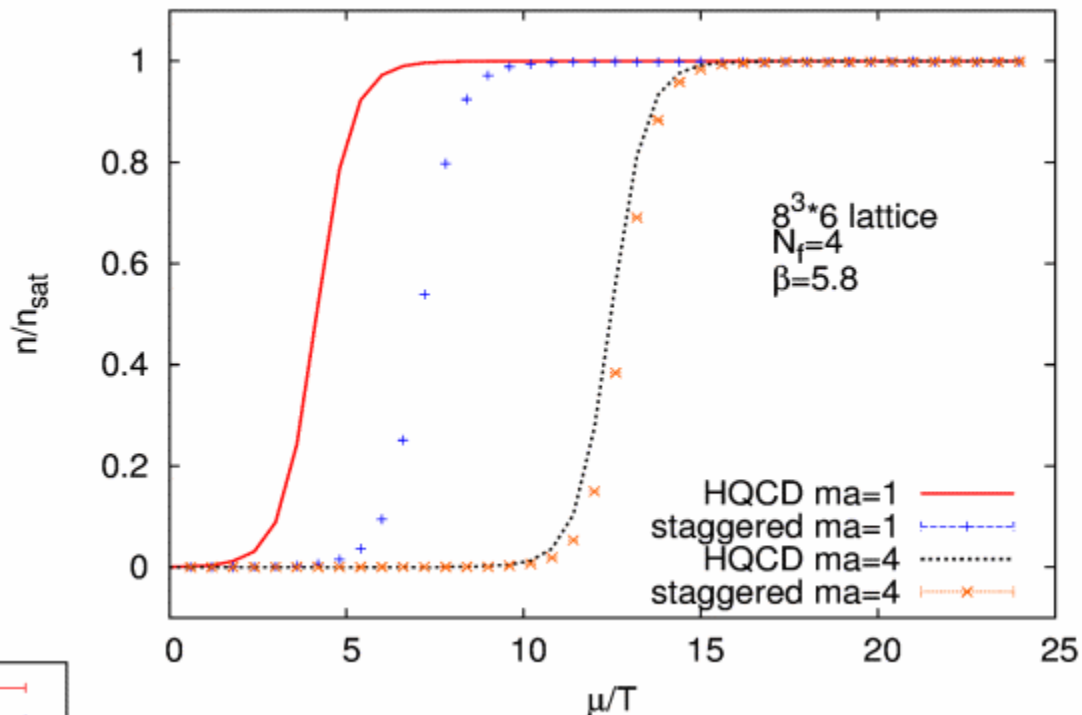
Light quarks: compare to reweighting



# Comparison of HDQCD in LO and full QCD

Similar behaviour at intermediate masses

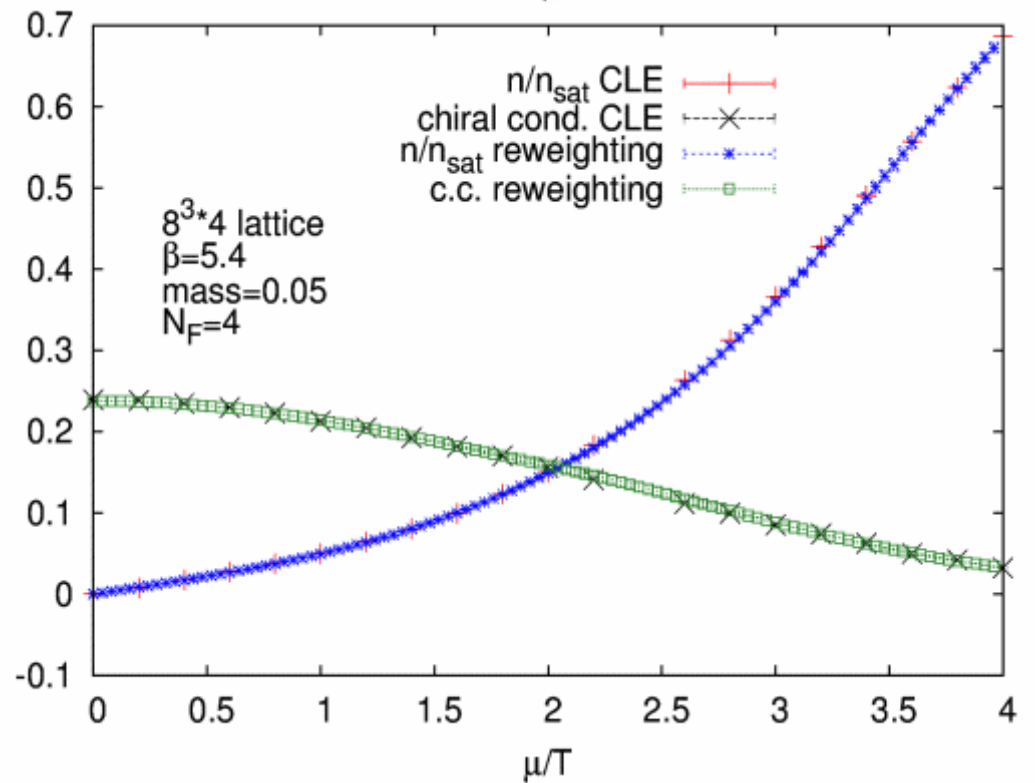
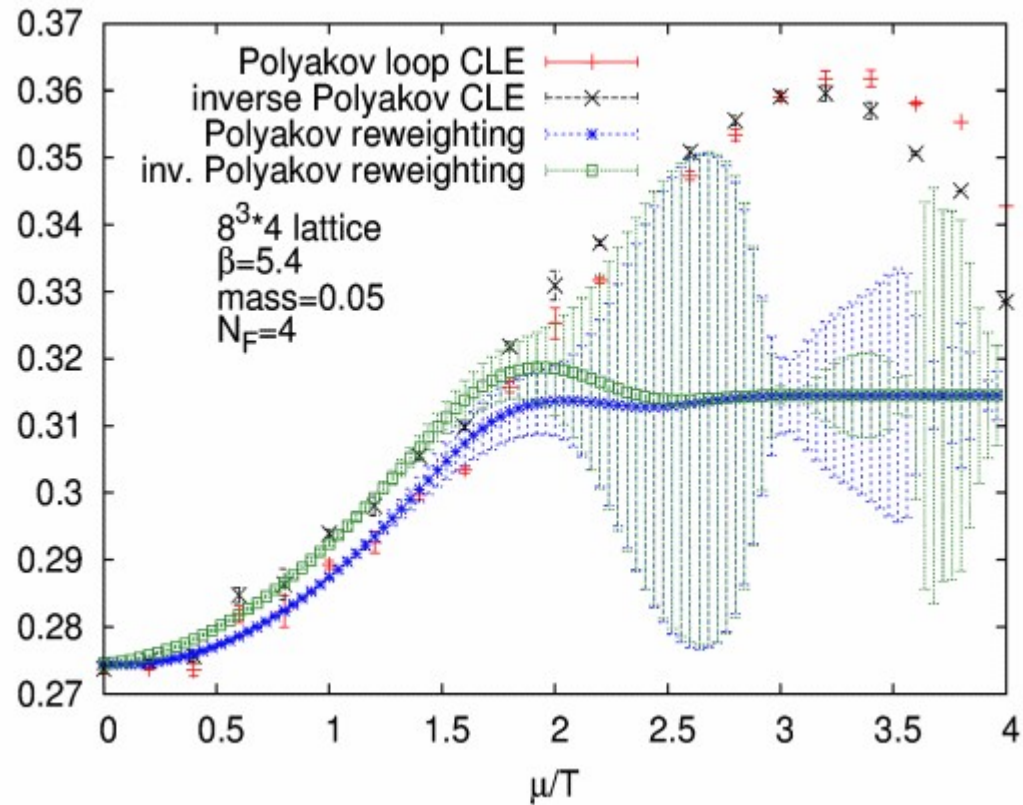
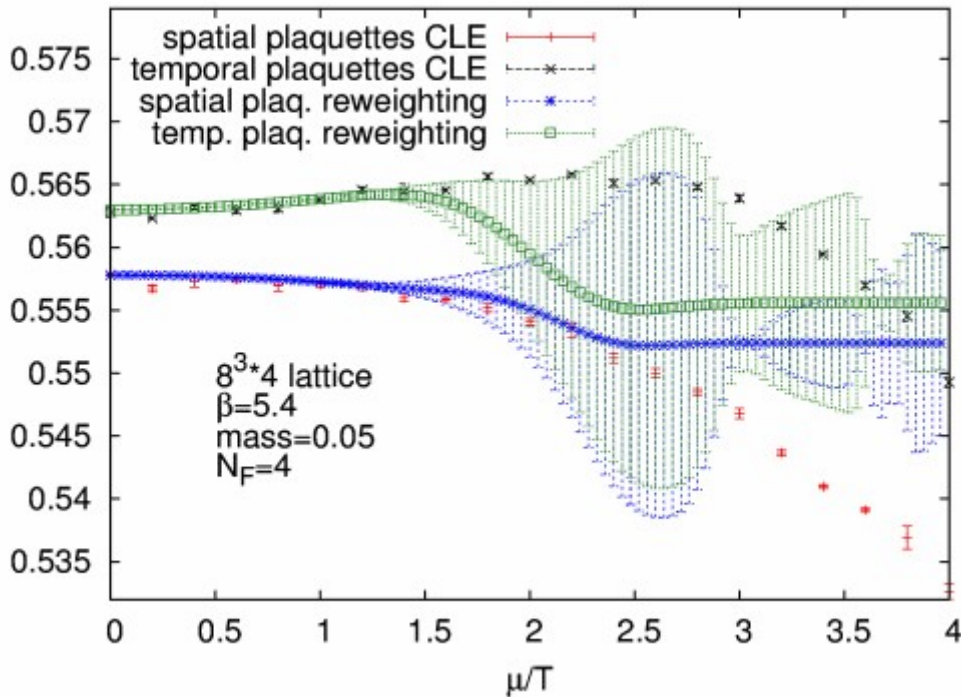
Quantitative agreement at high masses



# Comparison with reweighting for full QCD

Reweighting from ensemble at

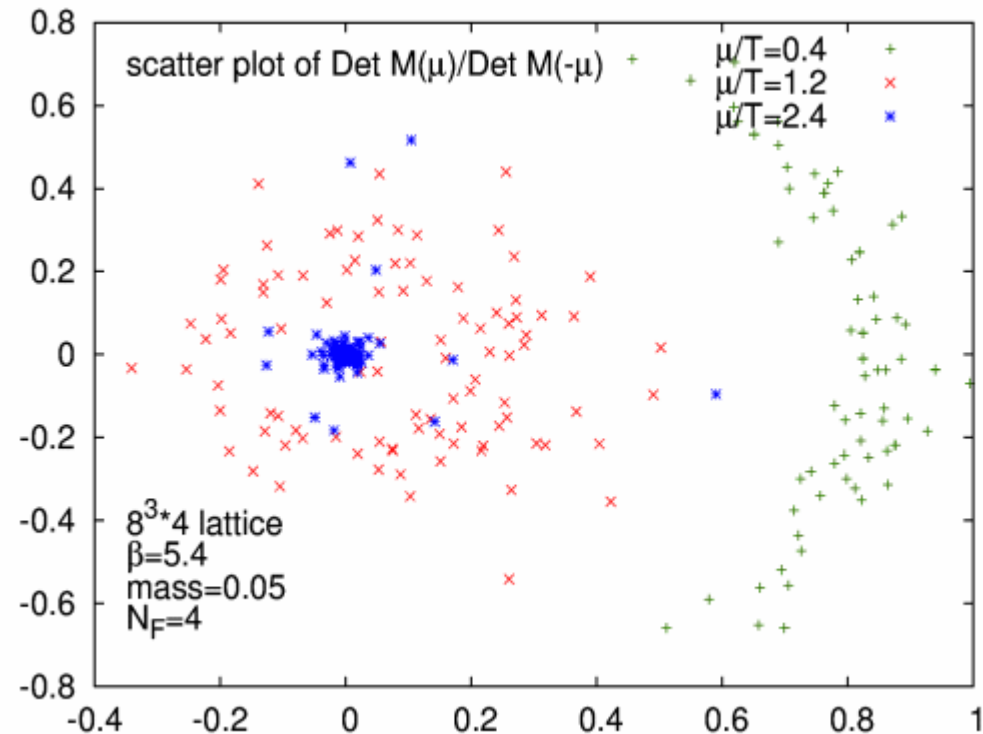
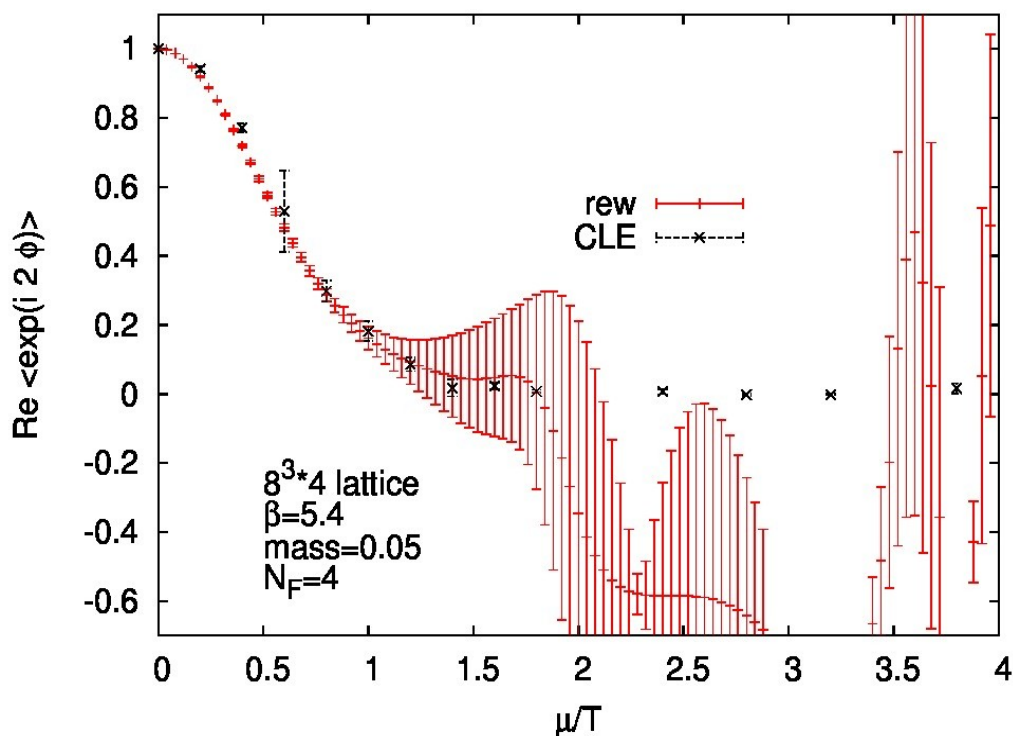
$$R = \text{Det } M(\mu=0)$$



# Sign problem

Sign problem gets hard around

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



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

# 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

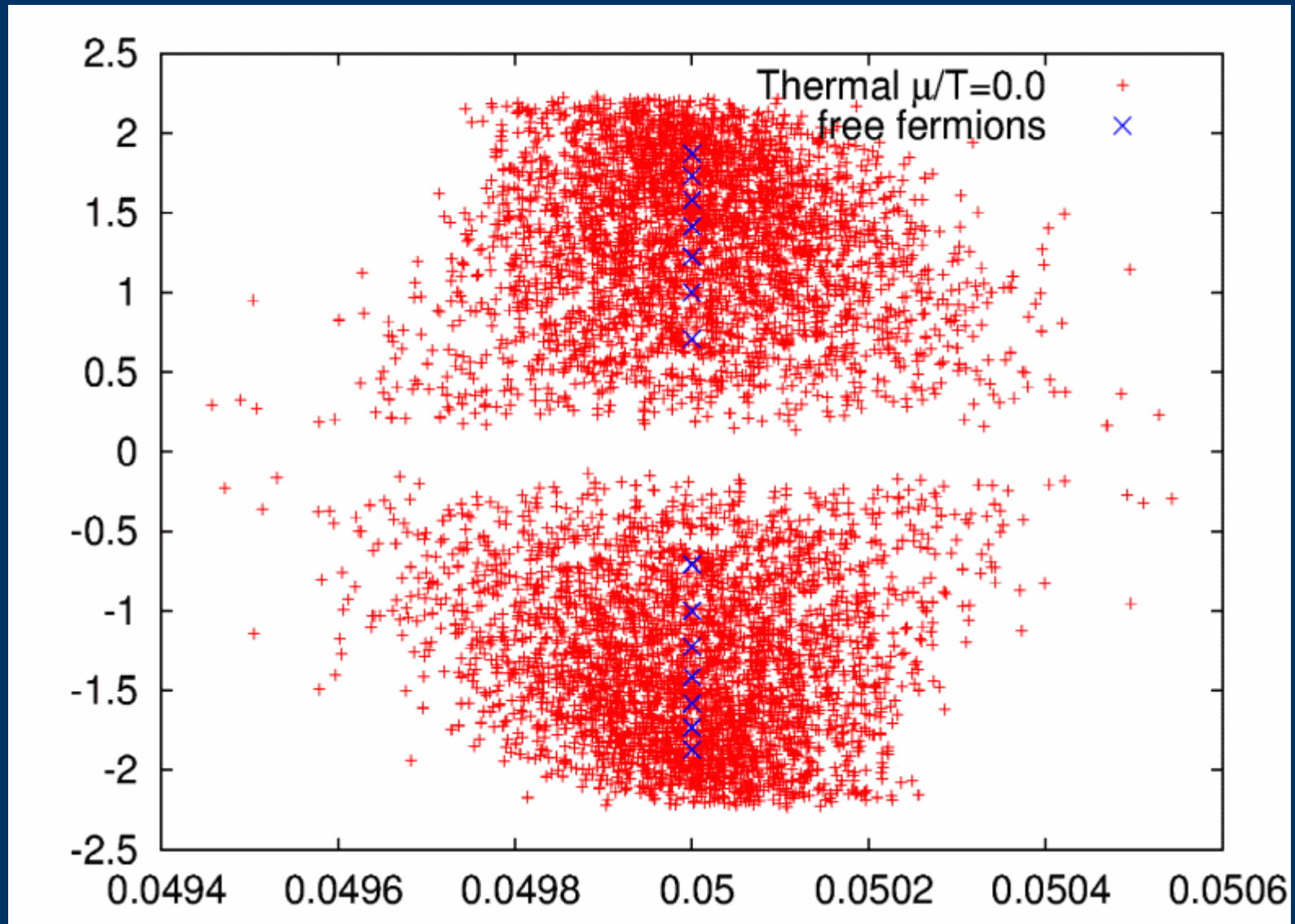
First results for full QCD with light quarks  
No sign or overlap problem  
CLE works all the way into saturation region  
Comparison with reweighting for small chem. pot.  
Low temperatures are more demanding  
First results for the phase diagram of HDQCD

Backup slides



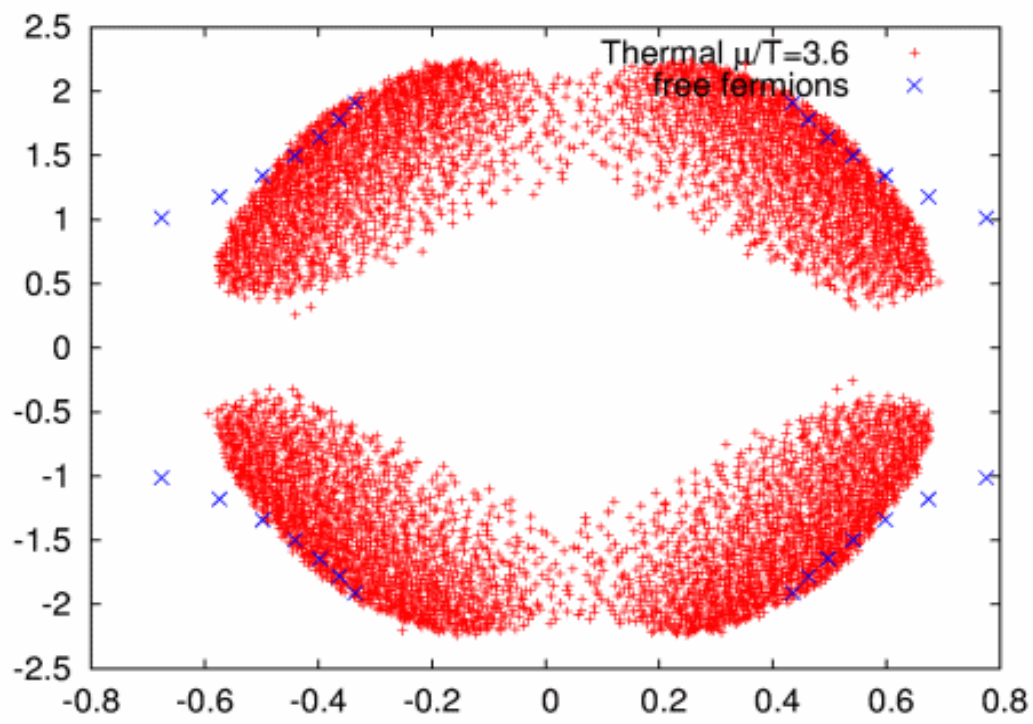
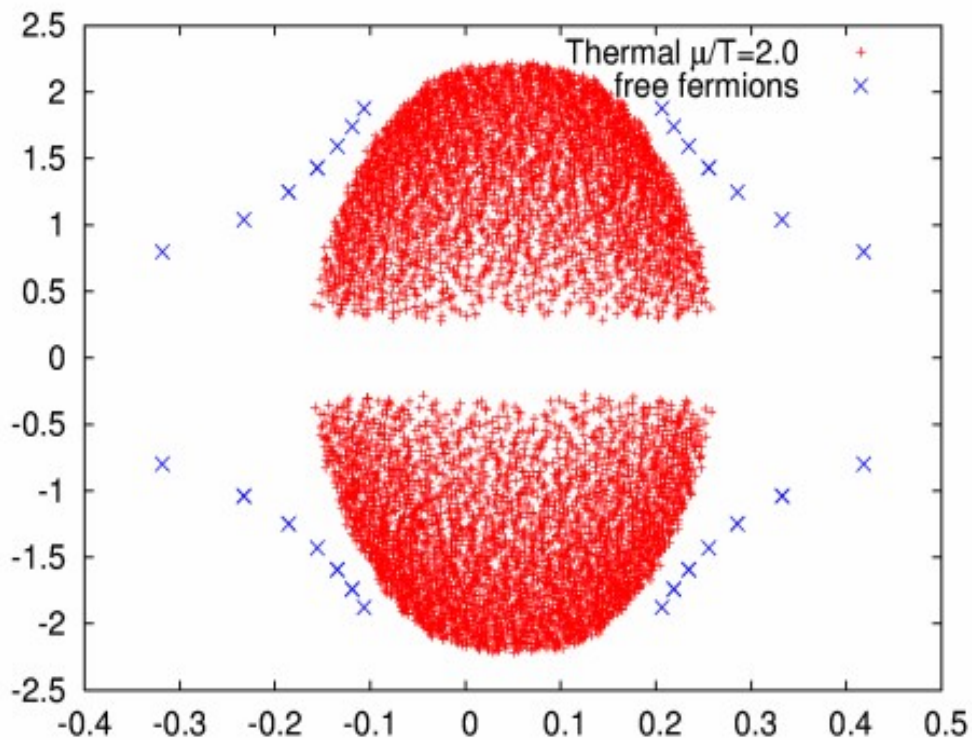
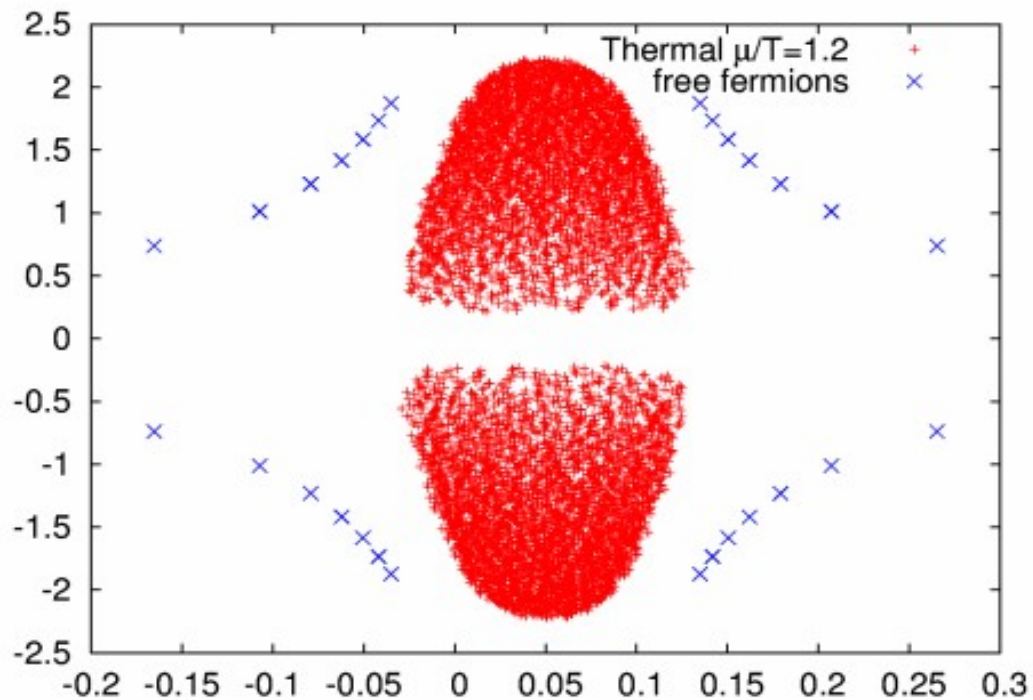
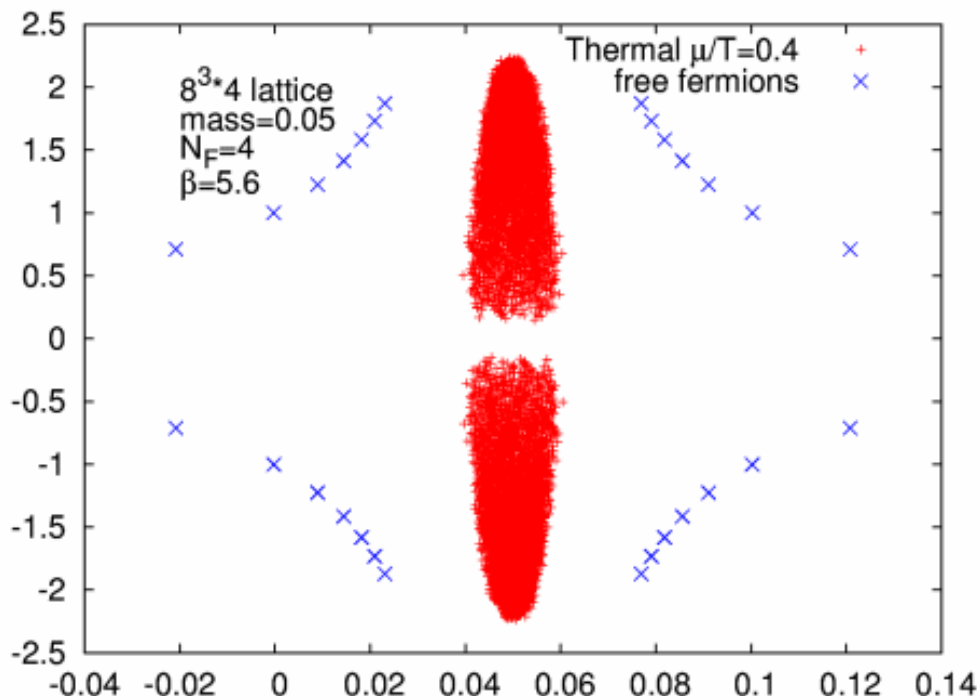
# Spectrum of the Dirac Operator $N_F=4$ staggered

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”

