Lattice QCD and physics at FAIR
(concerning thermodynamics)

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1. Sign problem (of lattice QCD)
2. Ideas to solve it
3. Some results extrapolating from $\mu=0$
4. Complex Langevin equation
   Toy models
   Lattice models – HDQCD and full QCD

From action to phenomenology

$$S = -\frac{1}{4}\,\mathrm{Tr}\,F_{\mu\nu}F^{\mu\nu} + \sum_1^6 \bar{\psi}_f\left(i\gamma^\mu D_\mu + m_f\right)\psi_f$$

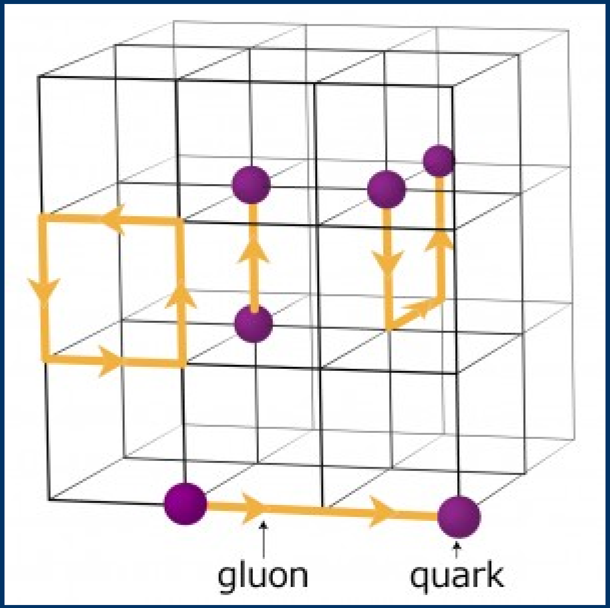
7 parameters

Confinement mechanism?
Mass of hadrons?
Scattering cross sections?
Phases transition to Quark-gluon plasma?
  Critical point at nonzero density?
  Equation of state?
Compressibility of quark matter? (in neutron stars)
Exotic phases:
  Color superconducting phases?
  Quarkyonic phase?
QCD in magnetic fields?
.... and so on

How?

Perturbation theory
Kinetic theory
Effective models (NJL, Polyakov-NJL, SU(3) spin model, ...)
Functional methods (FRG, 2PI, Dyson-Schwinger eq.)
Lattice

Lattice QCD



Discretise action on a cubic-space time lattice $N^3 N_T$

Gauge fields

$$A_\mu^a(x) \rightarrow U_\mu(x) = \exp\left(i \int dx\, A_\mu^a(x) \lambda_a\right)$$

Link variables $U_\mu(x) \in SU(3)$

Quark fields $\psi(x)$

Discretised action: $-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \rightarrow \sum_{plaquettes} Tr\left(U_{\mu\nu} - U_{\mu\nu}^{+}\right)$

Plaquette variables $U_{\mu\nu}(x) = U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^{-1}(x+\hat{\nu}) U_\nu^{-1}(x)$

$$i\gamma^\mu D_\mu + m \rightarrow 1 + \kappa \sum_{\pm\mu} (1+\gamma_\mu) U_\mu(x) \delta_{y,x+\hat{\mu}}$$

Wilson fermions
(or staggered, overlap...)

We want continuum and thermodynamical limit $a \rightarrow 0,\ V \rightarrow \infty$
at the physical point $m_\pi = 135\,\mathrm{MeV}$

Path integral formulation of QCD

Euclidean SU(3) gauge theory with fermions:

4d lattice   Temporal extent = inverse temperature

$$Z = \int DA_\mu^a D\bar{\Psi} D\Psi \exp\left(-S_E[A_\mu^a] - \bar{\Psi} D_E(A_\mu^a)\Psi\right)$$

$$A_\mu^a(x) \rightarrow U_\mu(x)$$

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

Integrating out fermions

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

Haar measure of SU(3) group

SU(N) is compact → Finite volume of gauge orbits

No gauge fixing neccesary
No Fadeev-Popov complication

We are interested in a system
Described with the partition sum:

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \sum_C W[C]$$

Typically exponentially many configurations,
no direct summation possible.

If the Weight is positive, build a Markov chain with the Metropolis alg.

$$\ldots \rightarrow C_{i-1} \rightarrow C_i \rightarrow C_{i+1} \rightarrow \ldots$$

Probability of visiting C $\quad p(C) = \frac{1}{N_W} W[C]$

$$\langle X \rangle = \frac{1}{Z} \mathrm{Tr}\, X e^{-\beta(H-\mu N)} = \frac{1}{N_W} \sum_C W[C] X[C] = \frac{1}{N} \sum_i X[C_i]$$

This works if we have $\quad W[C] \geq 0$

Otherwise we have a Sign problem

QCD sign problem

Euclidean SU(3) gauge theory with fermions:

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

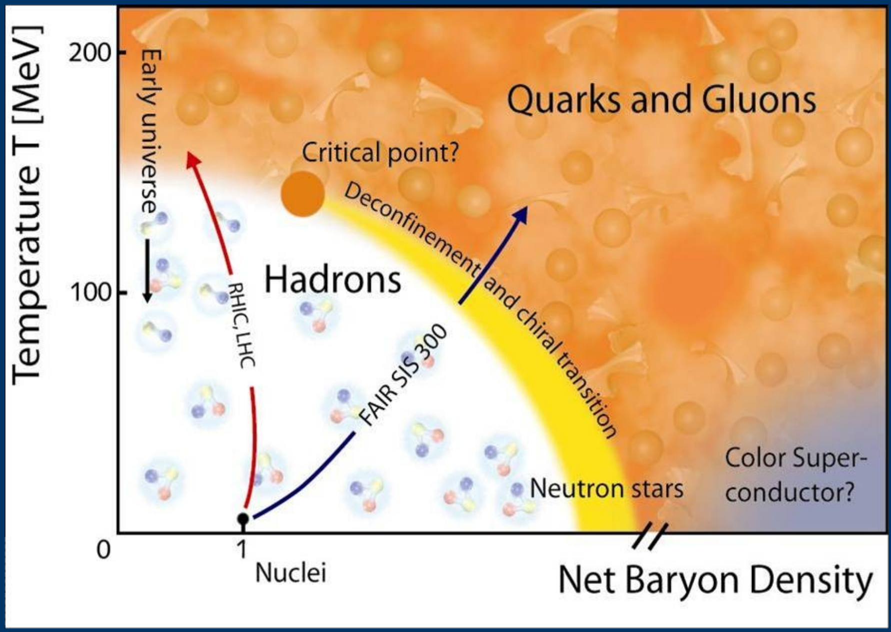
for $\det(M(U))>0$ Importance sampling is possible → Hadron masses, EOS, ...

Non-zero chemical potential

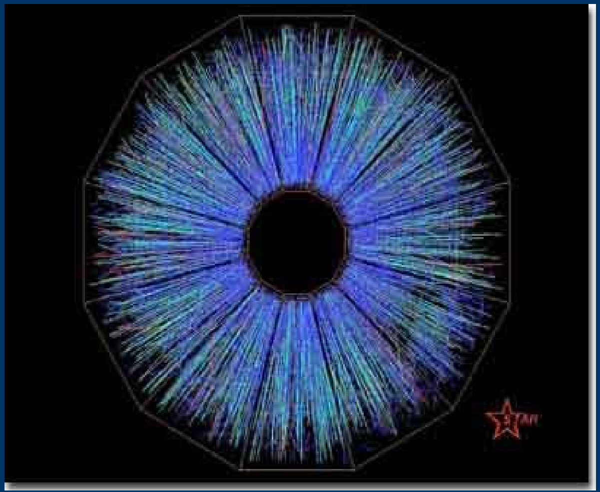
For nonzero chemical potential, the fermion determinant is complex

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

Sign problem → Naive Monte-Carlo breaks down



Sign problems in high energy physics

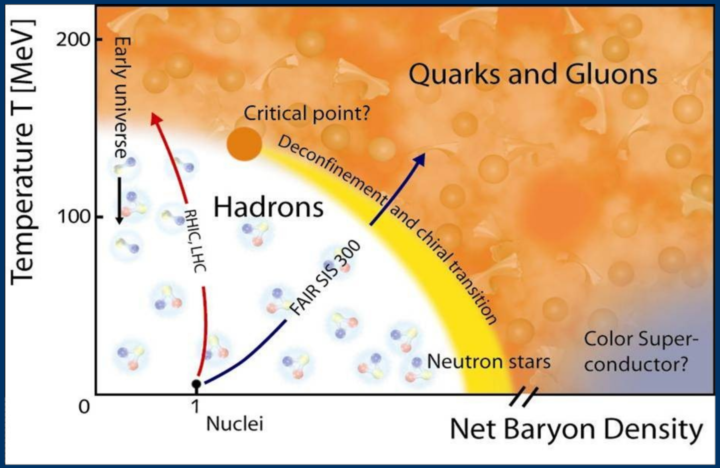


Real-time evolution in QFT

"strongest" sign problem e^{iS_M}

Non-zero density (and fermionic systems)

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \int DU\, e^{-S[U]} \det(M[U])$$



Many systems: Bose gas
XY model
SU(3) spin model
Random matrix theory
QCD

Theta therm

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

And everything else with complex action

$w[C] = e^{-S[C]}$ $w[C]$ is positive ←→ $S[C]$ is real

How to solve the sign problem?

Probably no general solution – There are sign problems which are NP hard

[Troyer Wiese (2004)]

Many solutions for particular models with sign problem exist

Transforming the problem to one with positive weights

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \sum_C W[C] = \sum_D W'[D]$$

Dual variables
Worldlines

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \sum_n Z_n e^{\beta\mu n}$$

Canonical ensemble

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \int dE\, \rho_\mu(E)\, e^{-\beta E}$$

Density of states

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \sum_C W[C] = \sum_S \left(\sum_{C\in S} W[C] \right)$$

Subsets

How to solve the sign problem?

Extrapolation from a positive ensemble

Reweighting $\langle X\rangle_W = \frac{\sum_c W_c X_c}{\sum_c W_c} = \frac{\sum_c W'_c (W_c/W'_c) X_c}{\sum_c W'_c (W_c/W'_c)} = \frac{\langle (W/W') X\rangle_{W'}}{\langle W/W'\rangle_{W'}}$

Taylor expansion $Z(\mu) = Z(\mu=0) + \frac{1}{2}\mu^2 \partial_\mu^2 Z(\mu=0) + \ldots$

Analytic continuation from imaginary sources
(chemical potentials, theta angle,..)

Using analyticity (for complexified variables)

Complex Langevin

Complexified variables – enlarged manifolds

Lefschetz thimble

Integration path shifted onto complex plane

In QCD direct simulation only possible at $\mu=0$

Taylor extrapolation, Reweighting, continuation from imaginary μ, canonical ens.
all break down around

$$\frac{\mu_q}{T}\approx 1-1.5 \qquad \frac{\mu_B}{T}\approx 3-4.5$$

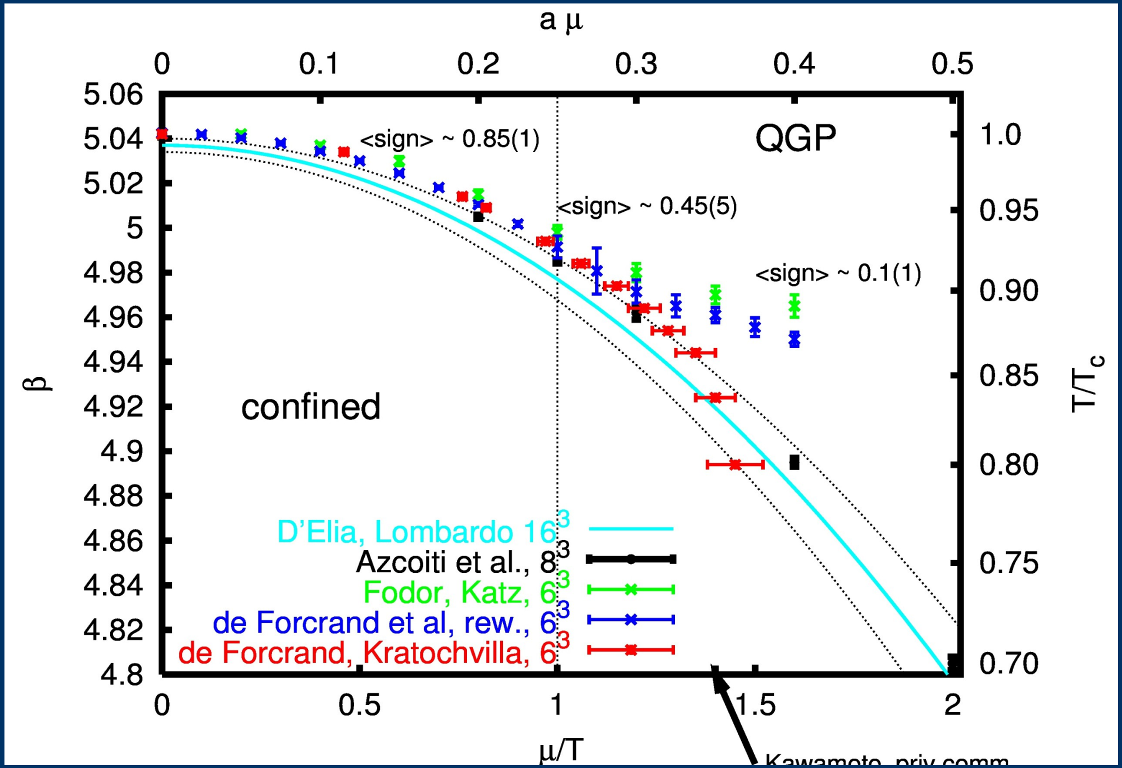
Around the transition temperature
Breakdown at

$$\mu_q\approx 150-200\,\mathrm{MeV} \qquad \mu_B\approx 450-600\,\mathrm{MeV}$$

Results on

$$N_T=4, N_F=4, ma=0.05$$

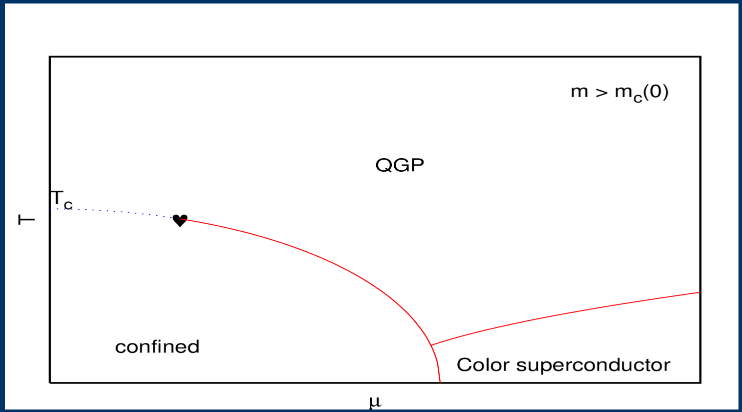
using
Imaginary mu,
Reweighting,
Canonical ensemble



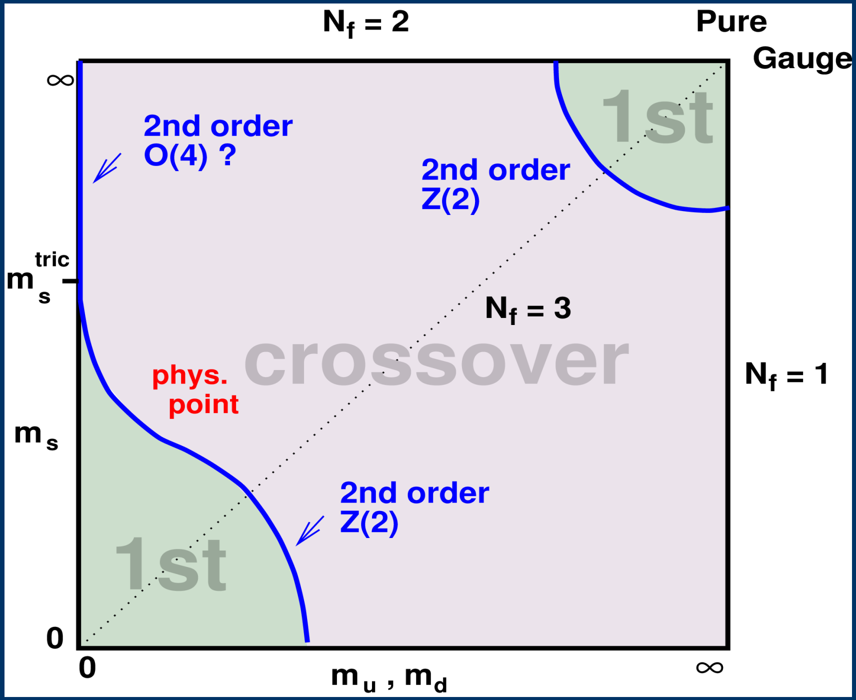
Agreement only at $\mu/T<1$

Is there a critical point?

$$\text{Critical point in } (T, \mu) \text{ plane} \rightarrow$$
$$\text{Critical surface in } (T, \mu, m_{ud}, m_s) \text{ space}$$

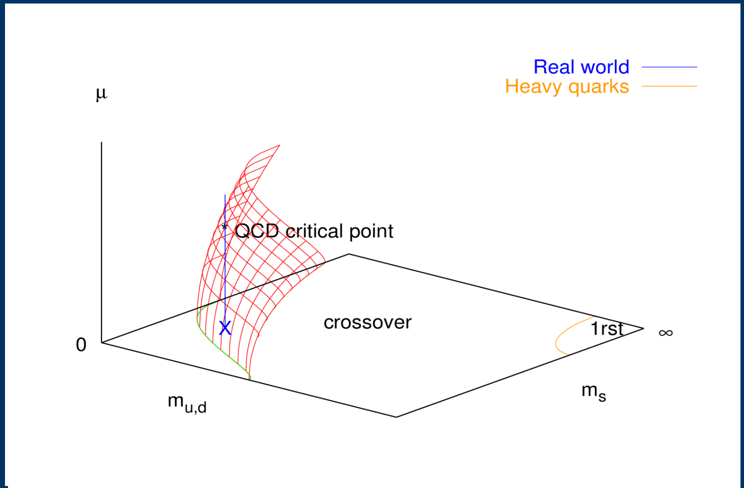


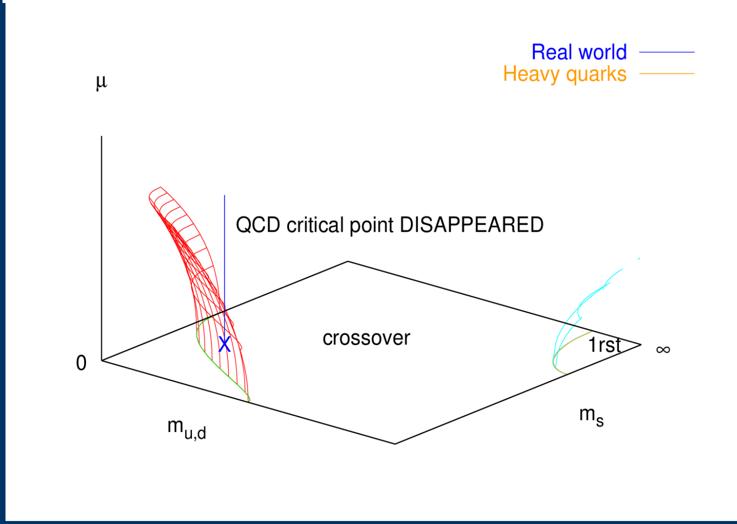
Order of the transition at $\mu = 0$



Which Scenario?

Calculate curvature at $\mu = 0$





[de Forcrand, Philipsen 2007...]

Taylor expansion of the EOS

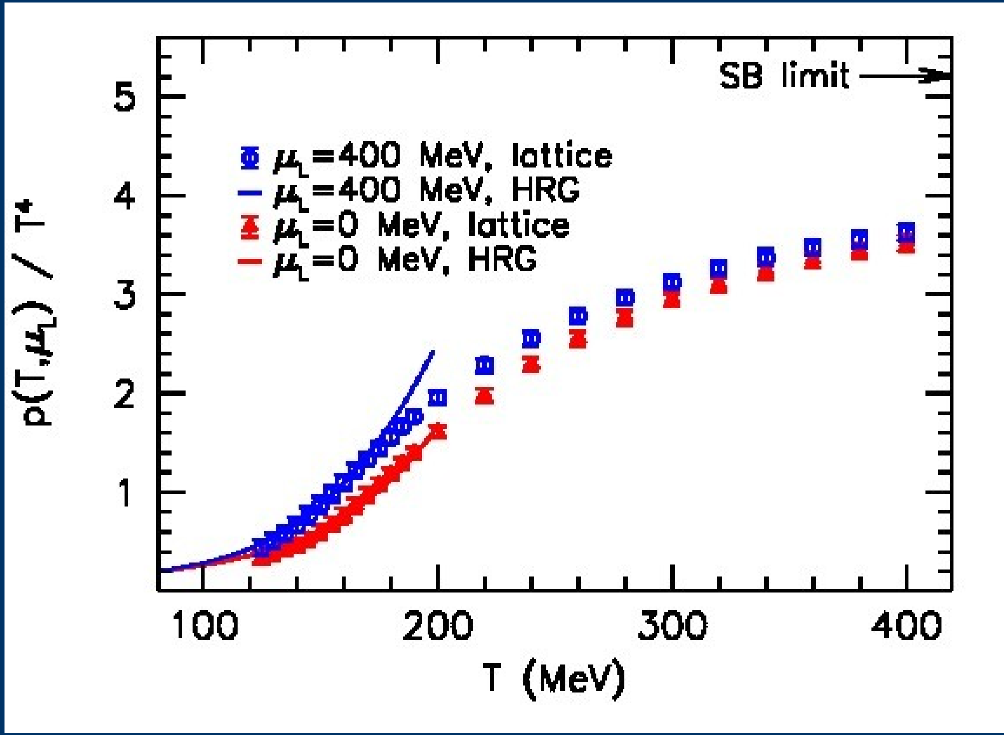
[Wu.-Bp. collaboration 2012]

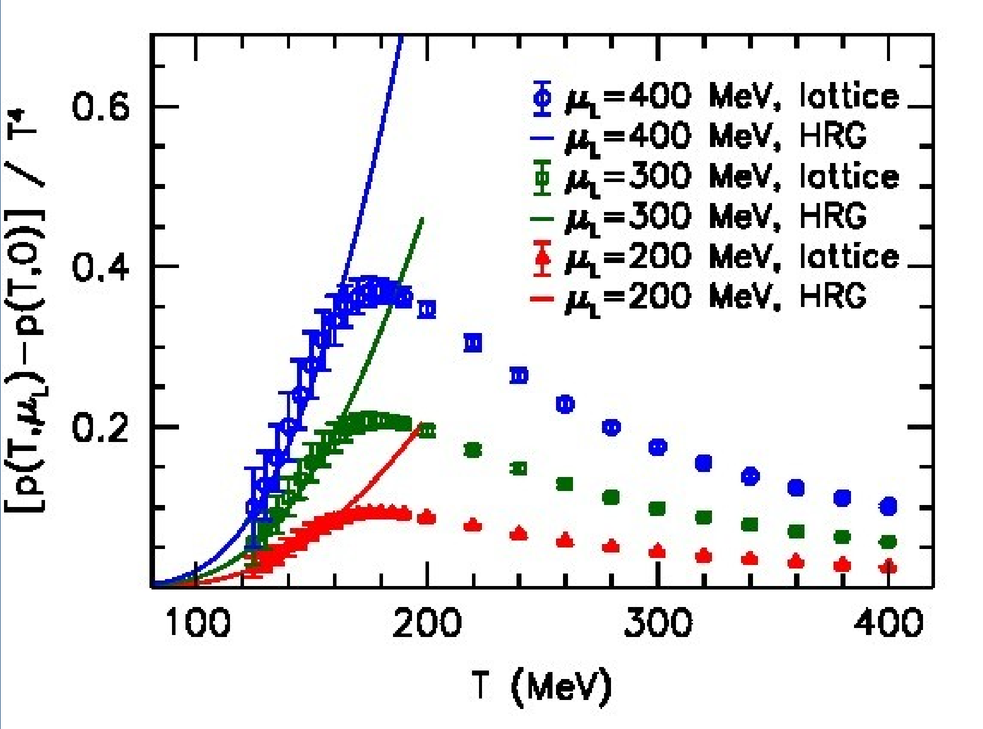
$$p(T,\mu_i) = p(T,0) + \frac{T^2}{2}\chi_2^{ij}\mu_i\mu_j \qquad \chi_2^{ij} = \frac{1}{TV}\frac{\partial^2 \log Z(\mu=0)}{\partial\mu_i\partial\mu_j} \qquad i,j=u,d,s$$

χ_4 is used to estimate errors

Continuum estimate, physical quark masses, zero strangeness

At constant μ





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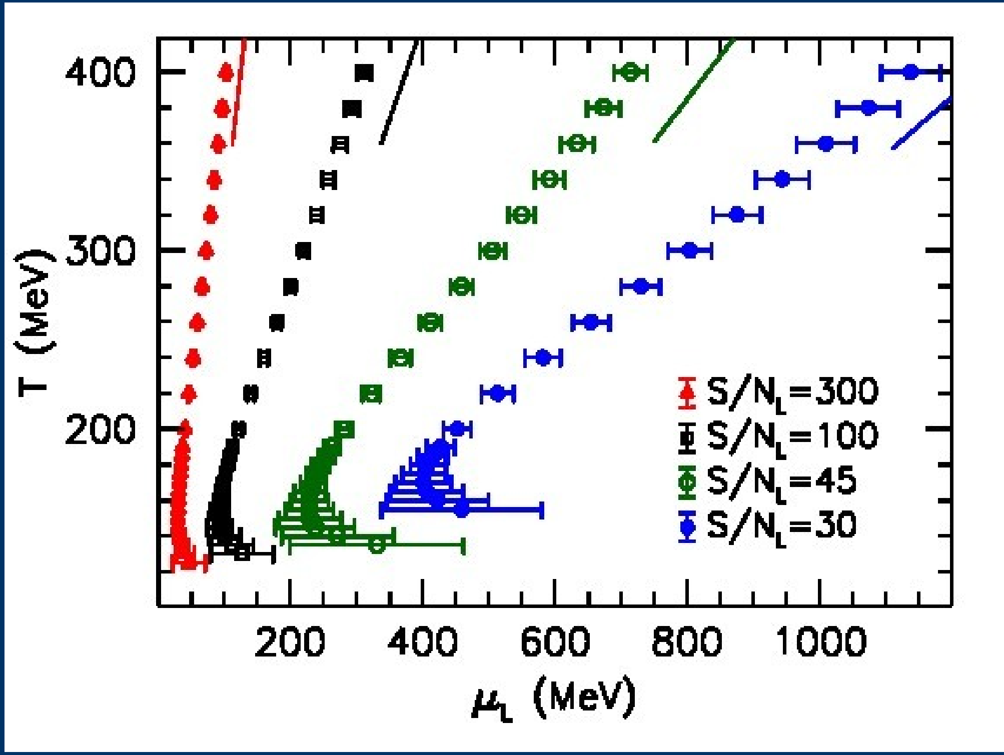
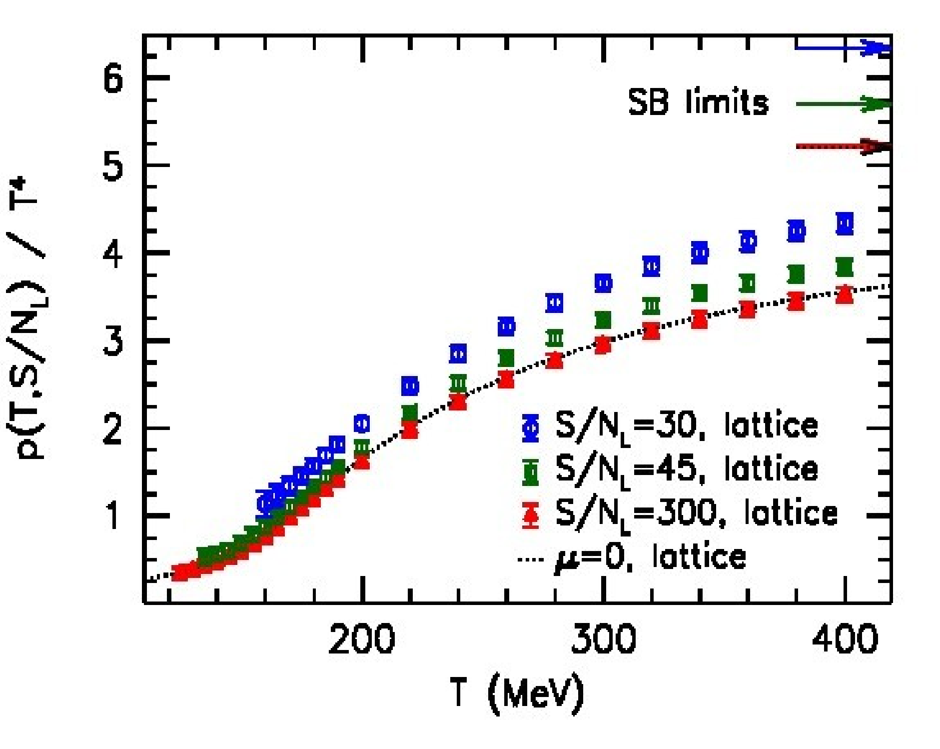
Continuum estimate, physical quark masses, zero strangeness

At constant entropy/particle number





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

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

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

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

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

"troubled past": Lack of theoretical understanding
Convergence to wrong results
Runaway trajectories

Klauder '83, Parisi '83, Hueffel, Rumpf '83, Karsch. Wyld '84, Gausterer, Klauder '86.
Matsui, Nakamura '86, ...

Interest went down as difficulties appeared

Renewed interest in connection of otherwise unsolvable problems

applied to nonequilibrium: Berges, Stamatescu '05, ...

aimed at nonzero density QCD: Aarts, Stamatescu '08 ... many important results since revival

New results about complex Langevin in the last decade or so

1. Study many exactly solvable toy models to gain more understanding
   one-plaquette model, random matrices, thirring model,
   few variable models, Polyakov chain

2. Theoreretical discussion and practical methods
   Proof of convergence
   Gauge cooling
   Non-holomorphic actions

3. Lattice models
   Non-equilibrium QFT (scalar field theory, pure gauge theory)
   XY model, SU(3) spin models, Bose gas
   Applications also in condensed matter: Bose gas in rotating frame,
   Imbalanced Fermi gas

4. Approximations to QCD
   HDQCD, kappa expansion

5. full QCD

Proof of convergence

If there is fast decay $P(x, y) \to 0 \text{ as } y \to \infty$

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
→ meromorphic drift

[Mollgaard, Splittorff (2013), Greensite(2014)]

Gaussian Example

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

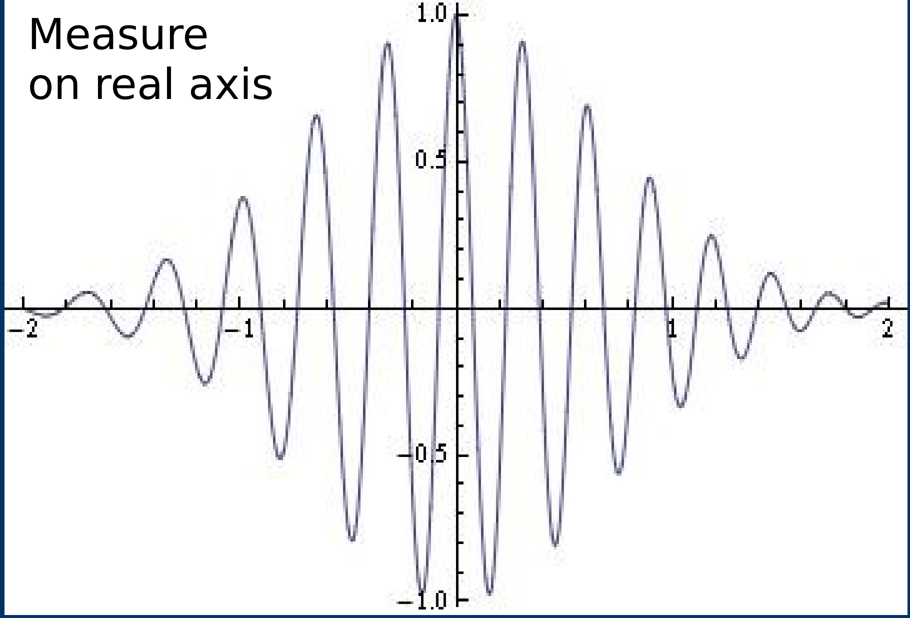
CLE

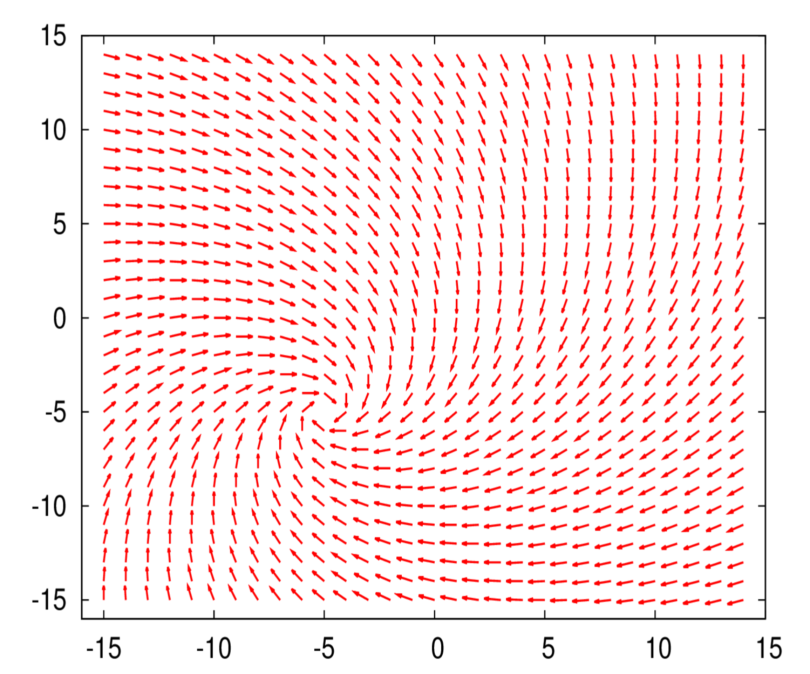
$$\frac{d}{d\tau}(x+iy)=-2\sigma(x+iy)-i\lambda+\eta$$

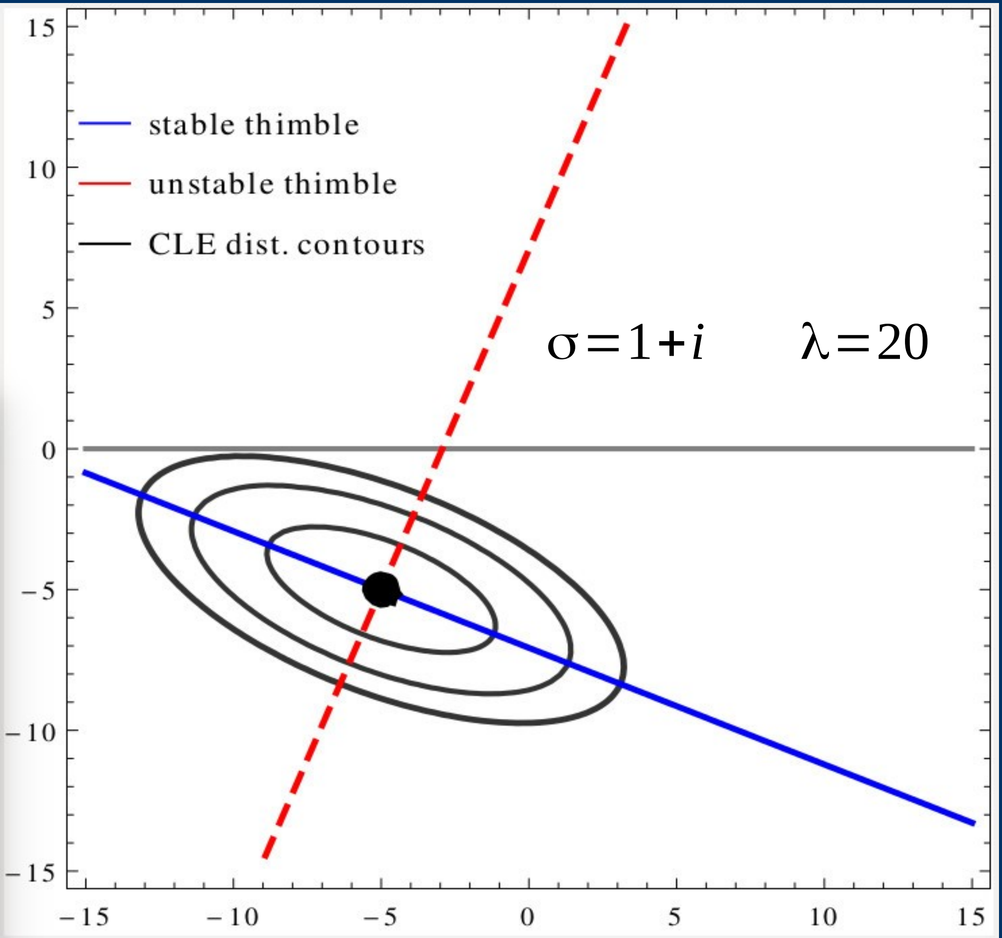
$$P(x,y)=e^{-a(x-x_0)^2-b(y-y_0)^2-c(x-x_0)(y-y_0)}$$

Gaussian distribution
around critical point

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







Simple model of QCD with finite chemical potential

Euclidean U(1) One plaquette model with "fermion determinant"

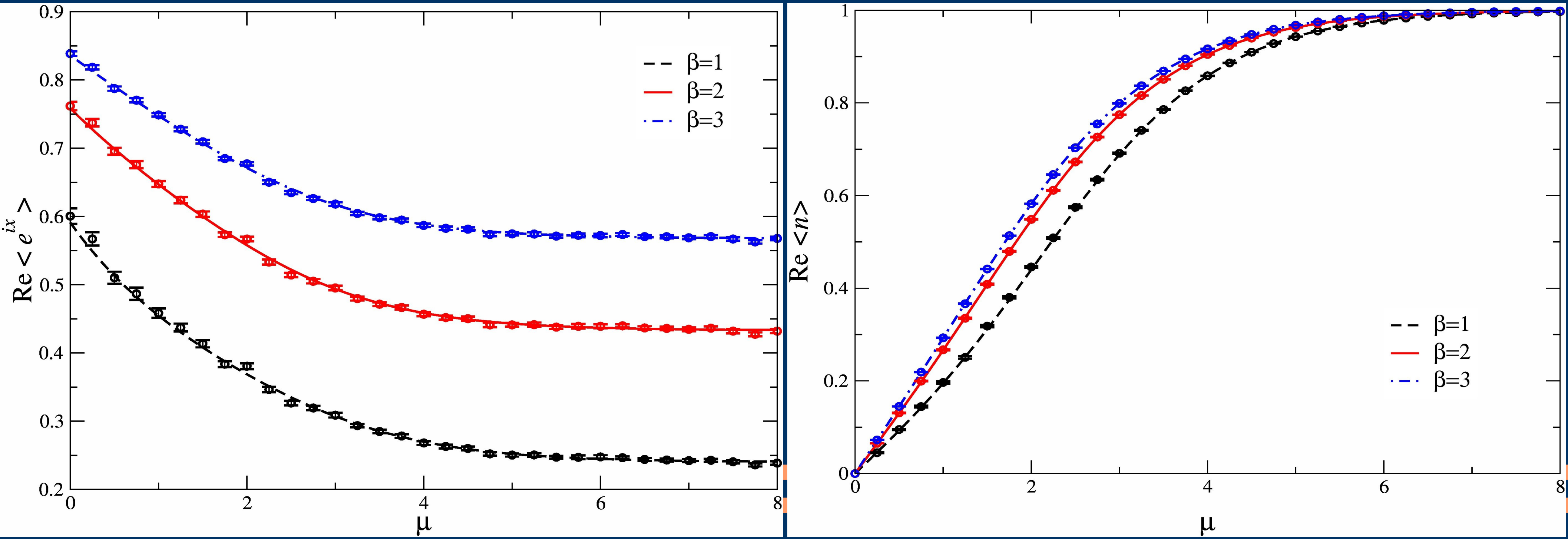
$$Z = \int_0^{2\pi} dx\, e^{-S_B} \det M \qquad S_B = -\frac{\beta}{2}(U + U^{-1}) = -\beta \cos(x) \qquad U = e^{ix}$$

$$\det M = 1 + \frac{1}{2}\kappa (e^{\mu} U + e^{-\mu} U^{-1}) = 1 + \kappa \cos(x - i\mu)$$

Similar to QCD fermion determinant:

$$\det M(\mu) = [\det M(-\mu)]^* \qquad \det M(i\mu_I) \text{ is real}$$

Exact averages calculated by numerical integration



Fixedpoint structure

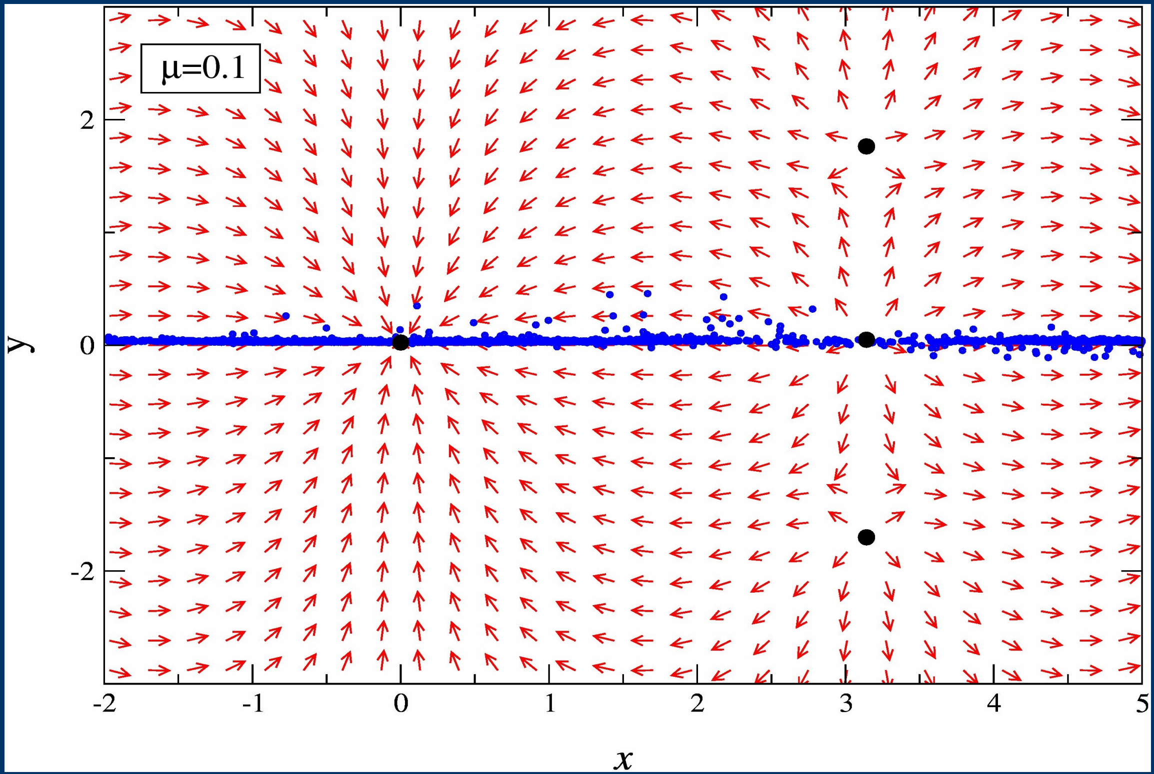
Distribution centered
around attractive fixedpoints
of the flow

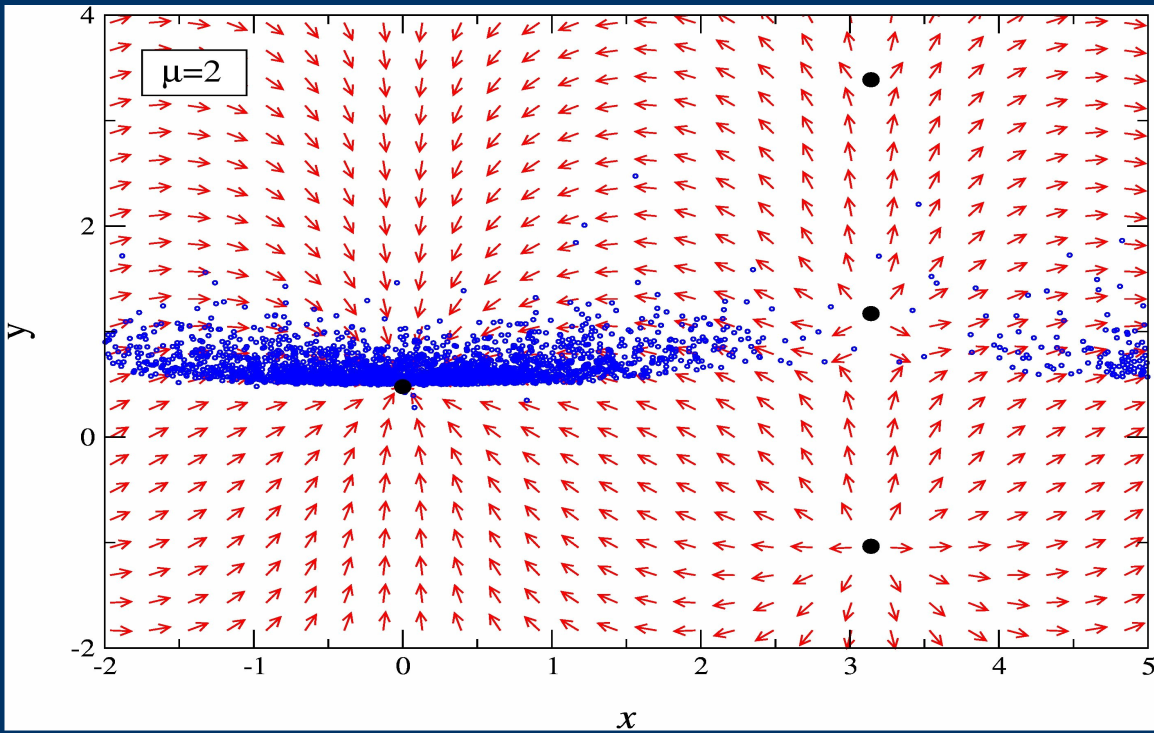
μ grows

↓

Fixed points move
no change in analytical structure

No breakdown,
Langevin works for high μ





Gauge theories and CLE

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

λ_a Gellmann matrices

complexified link variables

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

compact ⟶ non-compact

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

Gauge cooling

[Seiler,Sexty,Stamatescu '13]

Minimize unitarity norm $\sum_i Tr(U_i U_i^+ - 1)$

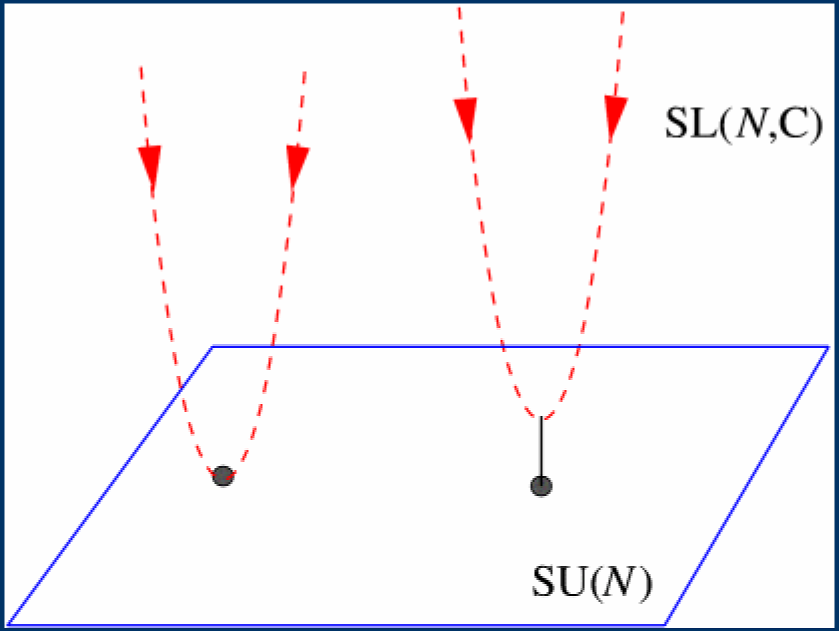
Distance from SU(N)

Gauge transformation at x changes 2d link variables

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

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

Steepest descent



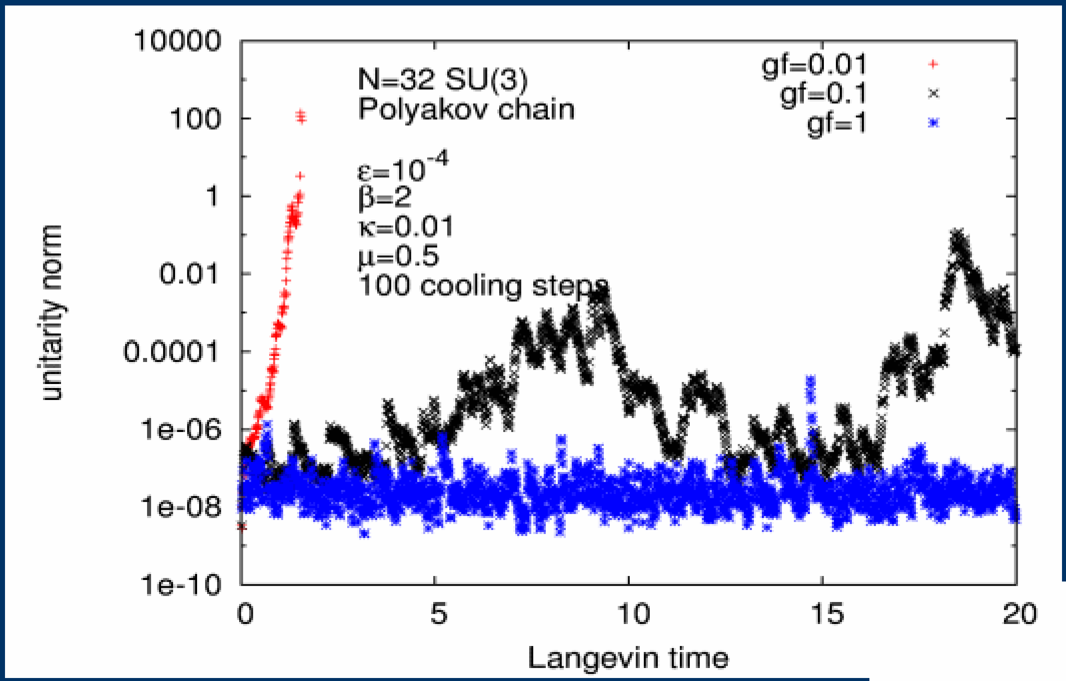
Dynamical steps are interspersed with several gauge cooling steps

Gauge cooling leaves Fokker-Planck eq. For gauge invariant quantities unchanged [Nagata, Nishimura, Shimasaki '15]

Empirical observation: Cooling is effective for $\beta > \beta_{min}$, $a < a_{max}$

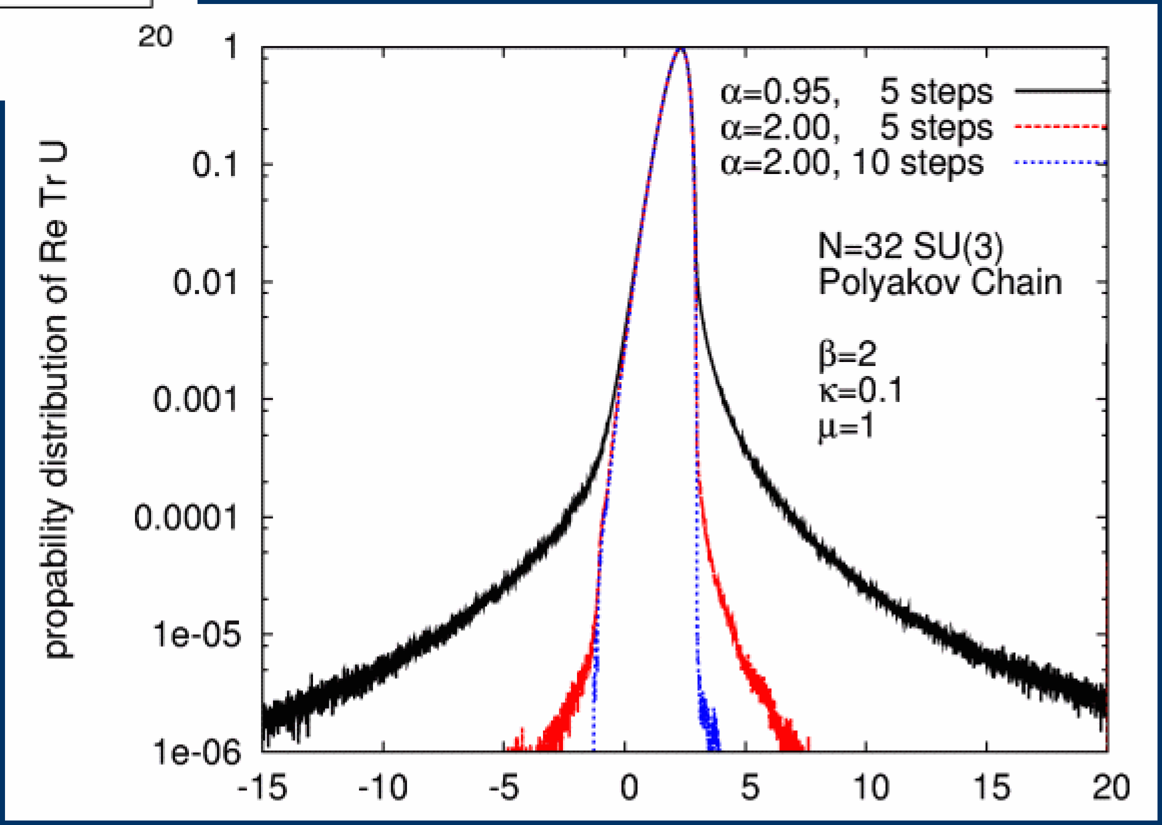
but remember, $\beta \rightarrow \infty$ in cont. limit

$$a_{max} \approx 0.1 - 0.2\, fm$$



Smaller cooling

excursions into complexified manifold



“Skirt” develops

small skirt gives correct result

Heavy Quark QCD at nonzero chemical potential (HDQCD)

Hopping parameter expansion of the fermion determinant
Spatial hoppings are dropped

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

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

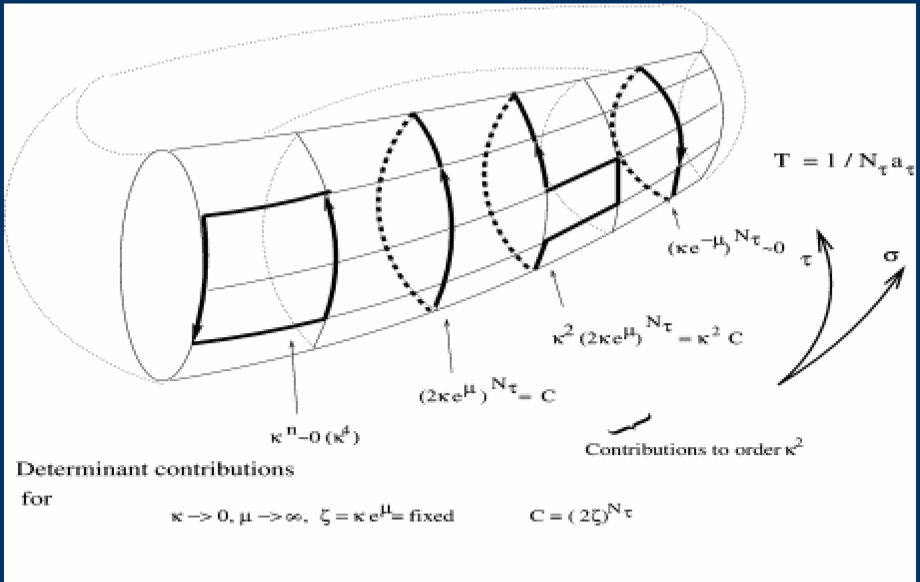
$$S = S_W[U_\mu] + \ln \mathrm{Det}\, M(\mu)$$

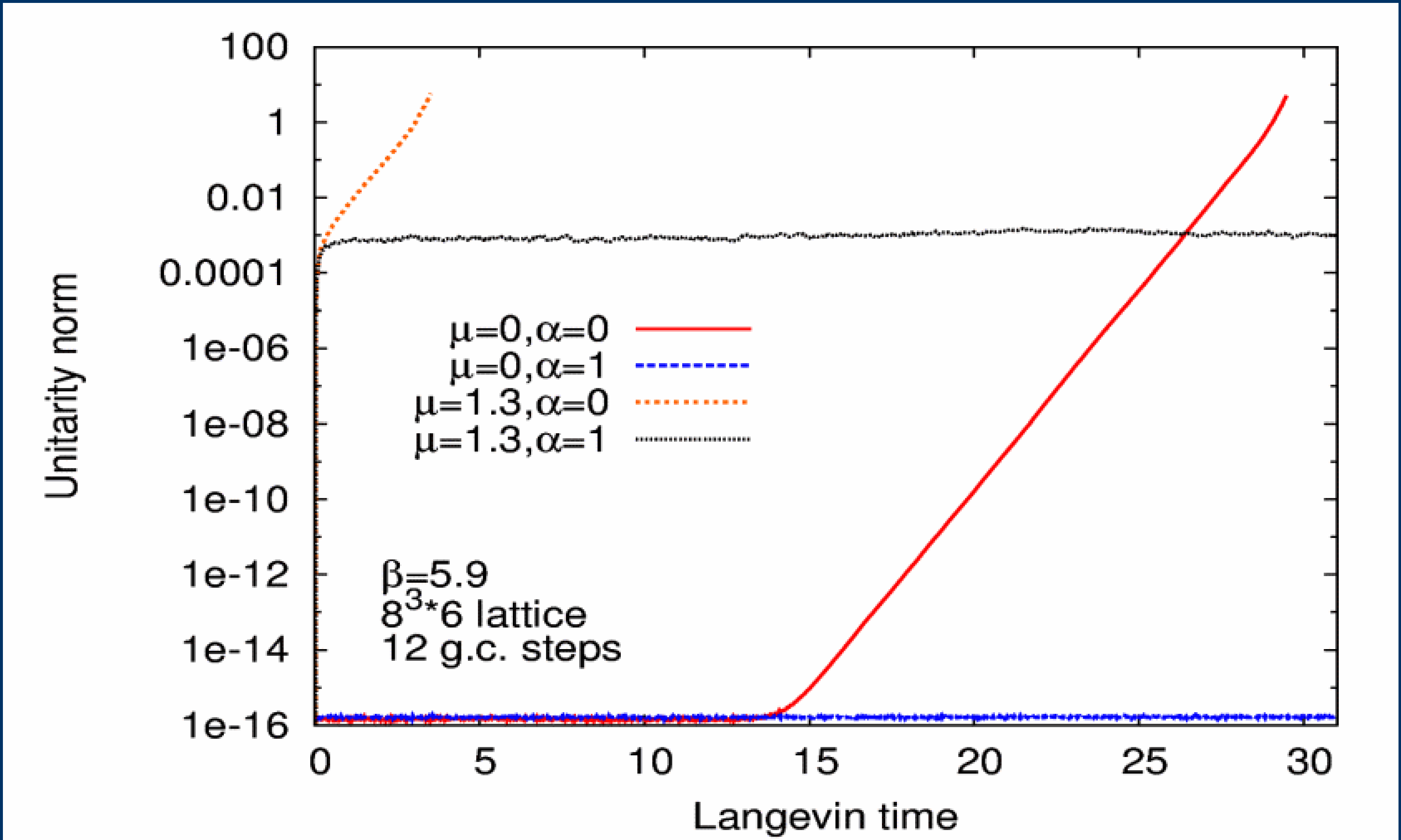
Studied with reweighting [De Pietri, Feo, Seiler, Stamatescu '07]

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

CLE study using gaugecooling

[Seiler, Sexty, Stamatescu (2012)]





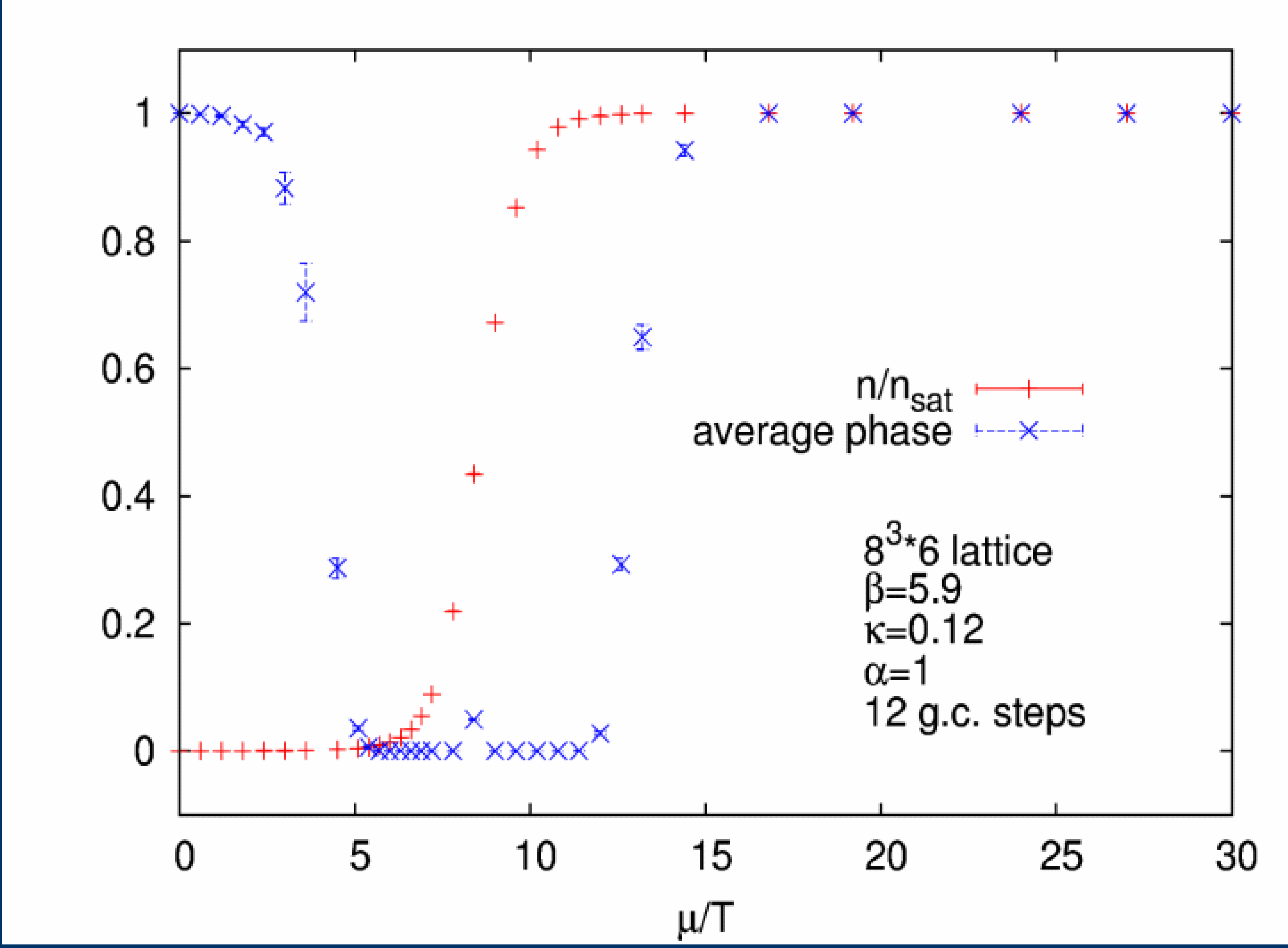
Gauge cooling stabilizes the distribution
SU(3) manifold instable even at $\mu=0$

Fermion density:

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

average phase:

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

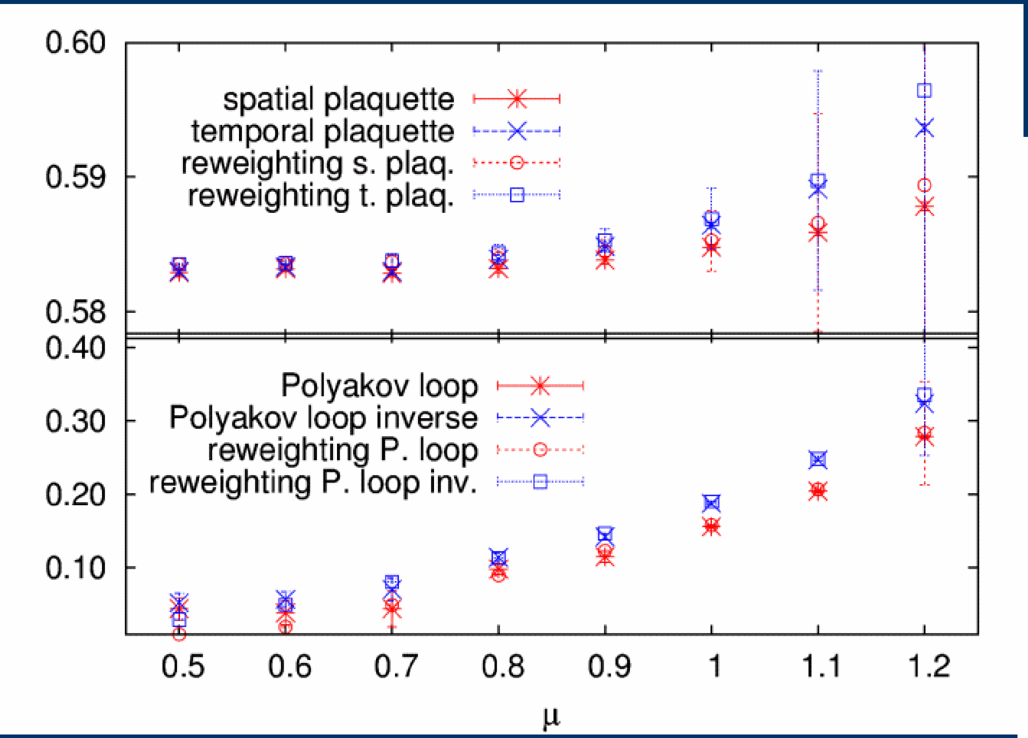


$$\det(1 + C P) = 1 + C^3 + C\, \mathrm{Tr}\, P + C^2\, \mathrm{Tr}\, P^{-1}$$

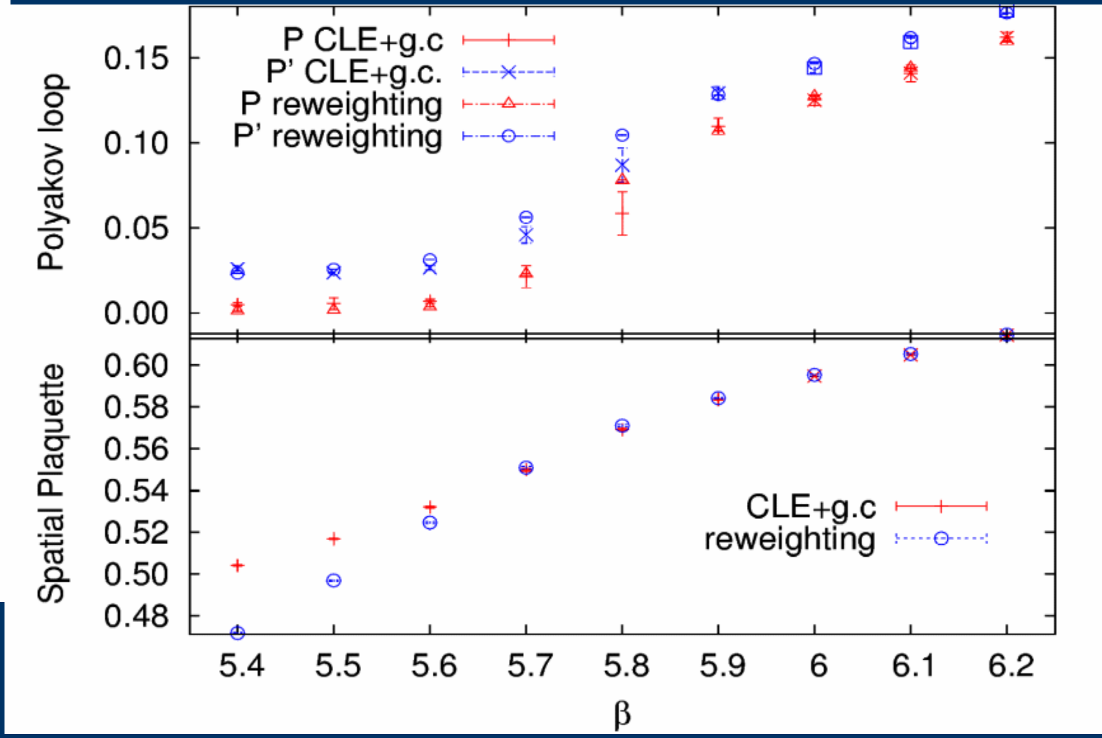
Sign problem is absent at small or large μ

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

Comparison to reweighting



6^4 lattice, $\beta = 5.9$



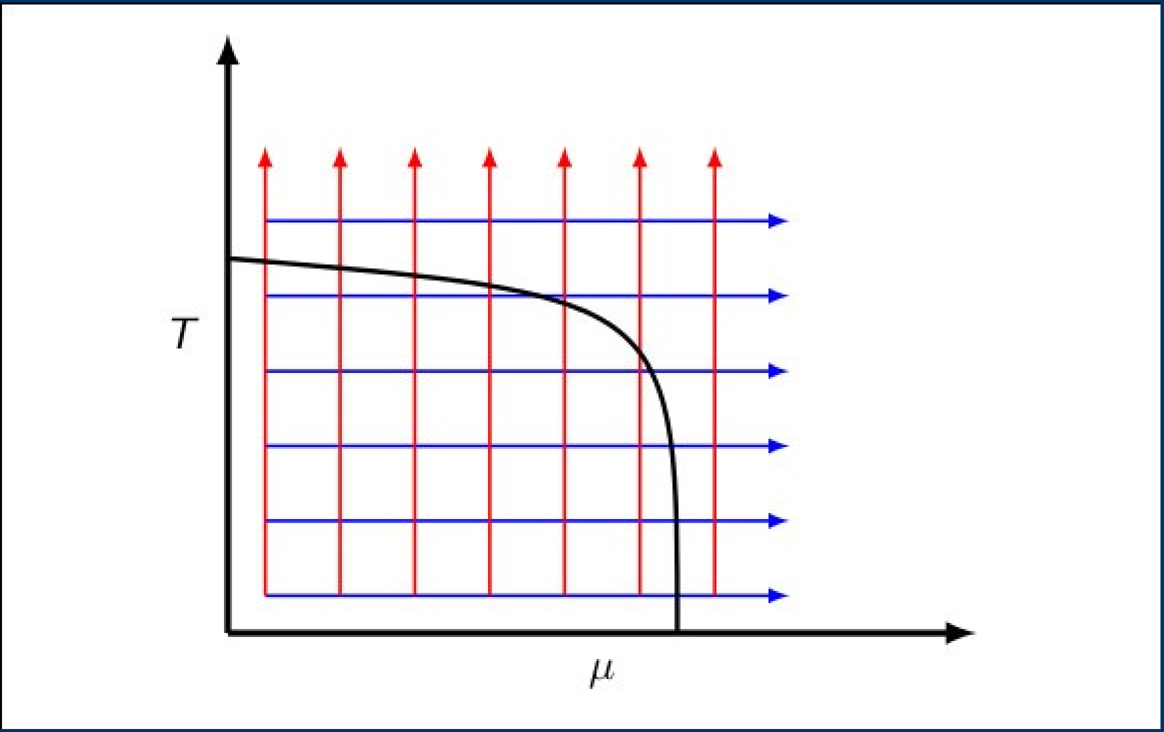
6^4 lattice, $\mu = 0.85$

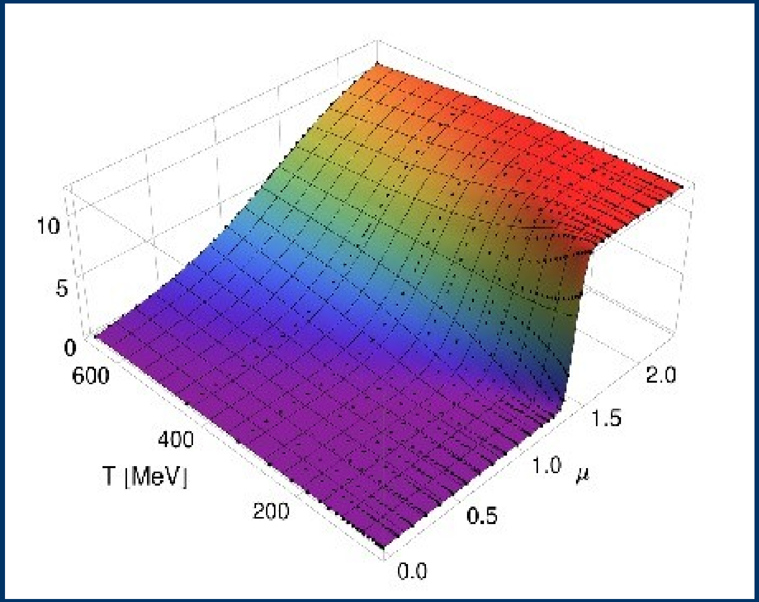
Discrepancy of plaquettes at $\beta \leq 5.6$
a skirted distribution develops

$a(\beta = 5.6) = 0.2\,\mathrm{fm}$

Mapping the phase diagram

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





fermionic density

fixed $\beta=5.8 \rightarrow a\approx 0.15\,\mathrm{fm}$

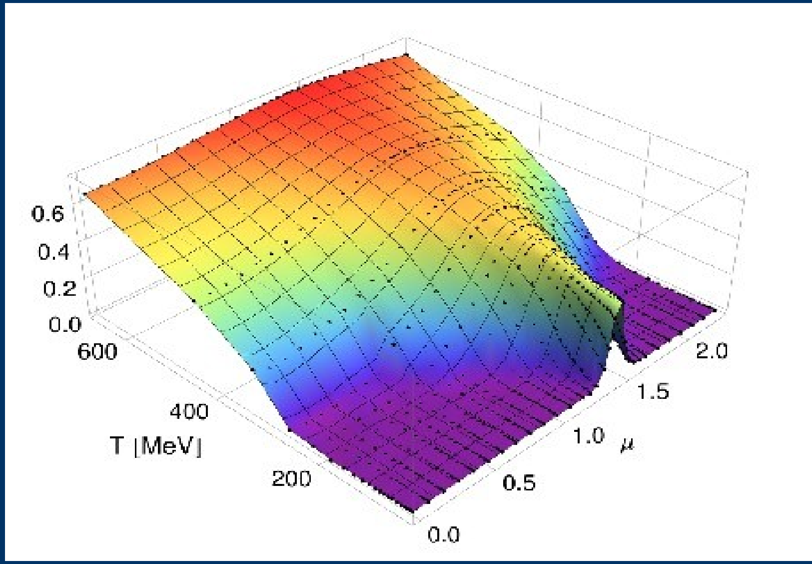
$\kappa=0.12$

onset transition at $\mu=-\ln(2\kappa)=1.43$

$N_t * 8^3$ lattice

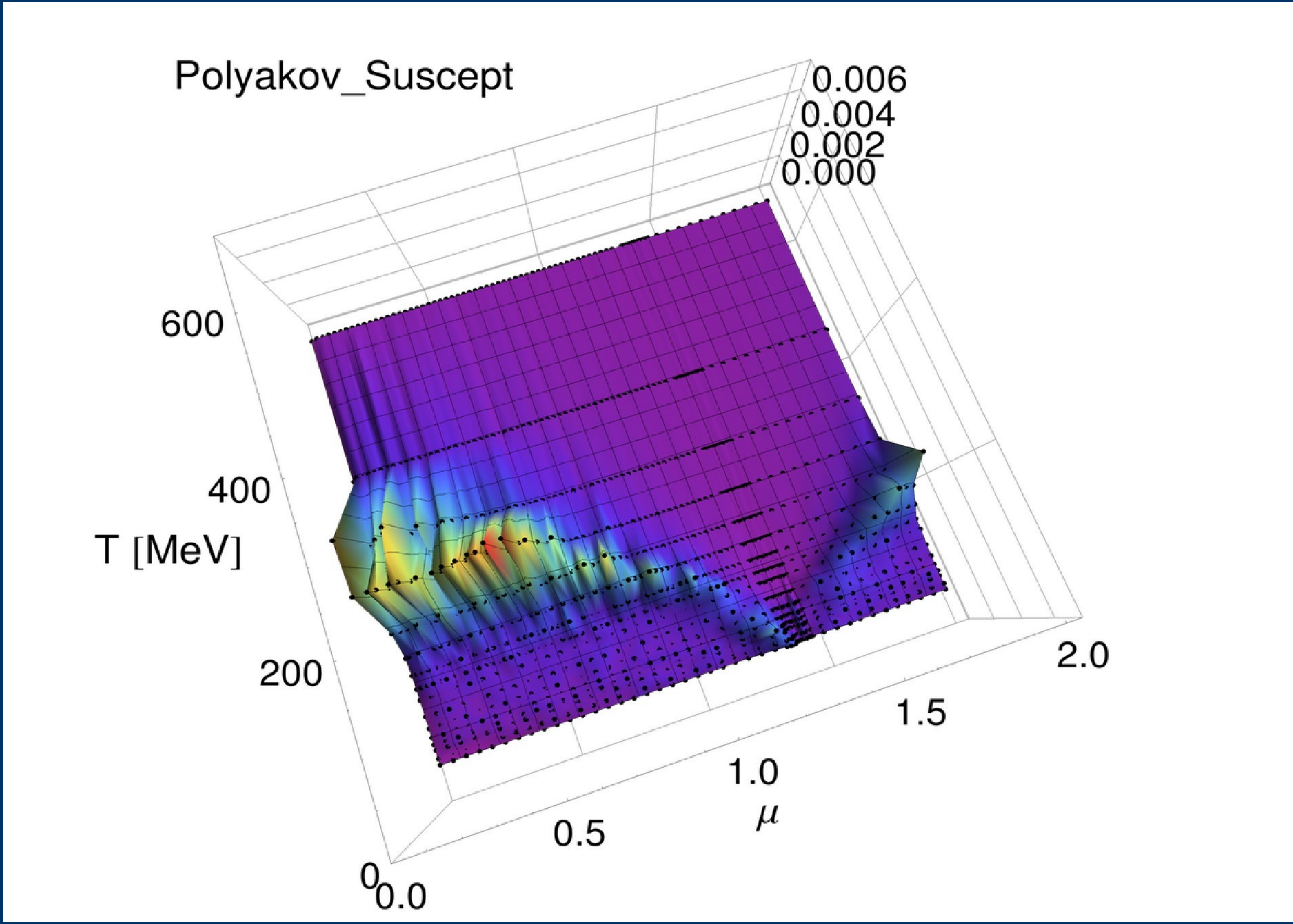
$N_t=2..28$

Temperature scanning



Polyakov loop

Polyakov loop susceptibility



Hint of first order deconfinement and first order onset transition

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

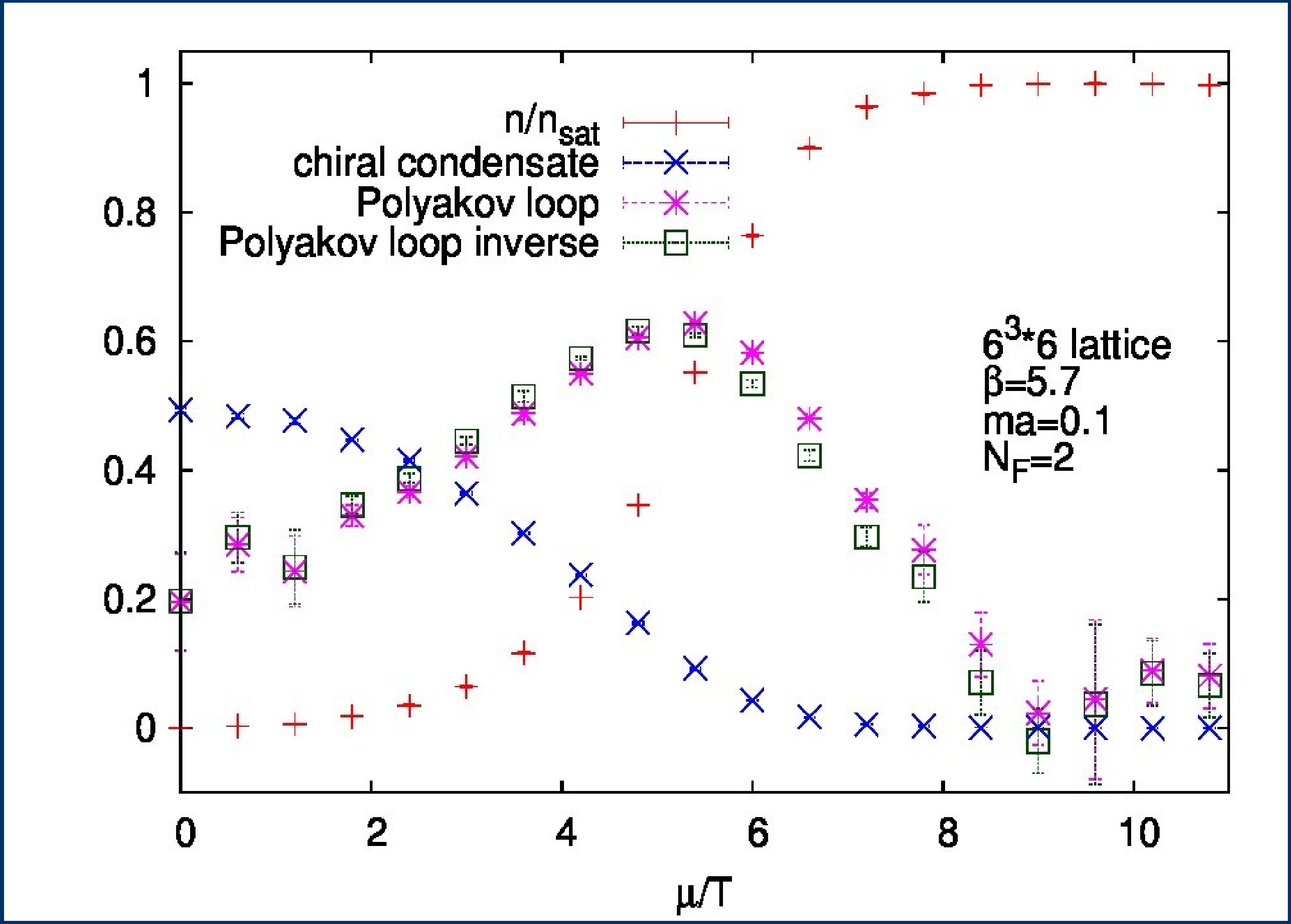
Inversion cost highly dependent on chemical potential
Eigenvalues not bounded from below by the mass
(similarly to isospin chemical potential theory)

Unimproved staggered and Wilson fermions

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

CLE and full QCD with light quarks [Sexty (2014)]

Physically reasonable results



Non-holomorphic action
poles in the fermionic drift

Is it a problem for full QCD?

So far (at high temperatures), it isn't:
Comparison with reweighting
Study of the spectrum
Hopping parameter expansion

Reweighting

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

$$= \frac{\langle F \det M(\mu)/R \rangle_R}{\langle \det M(\mu)/R \rangle_R} \qquad R = \det M(\mu=0),\ |\det M(\mu)|, \text{etc.}$$

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

$\Delta f(\mu, T)$ =free energy difference

Exponentially small as the volume increases $\langle F \rangle_\mu$ → $0/0$

Reweighting works for large temperatures and small volumes

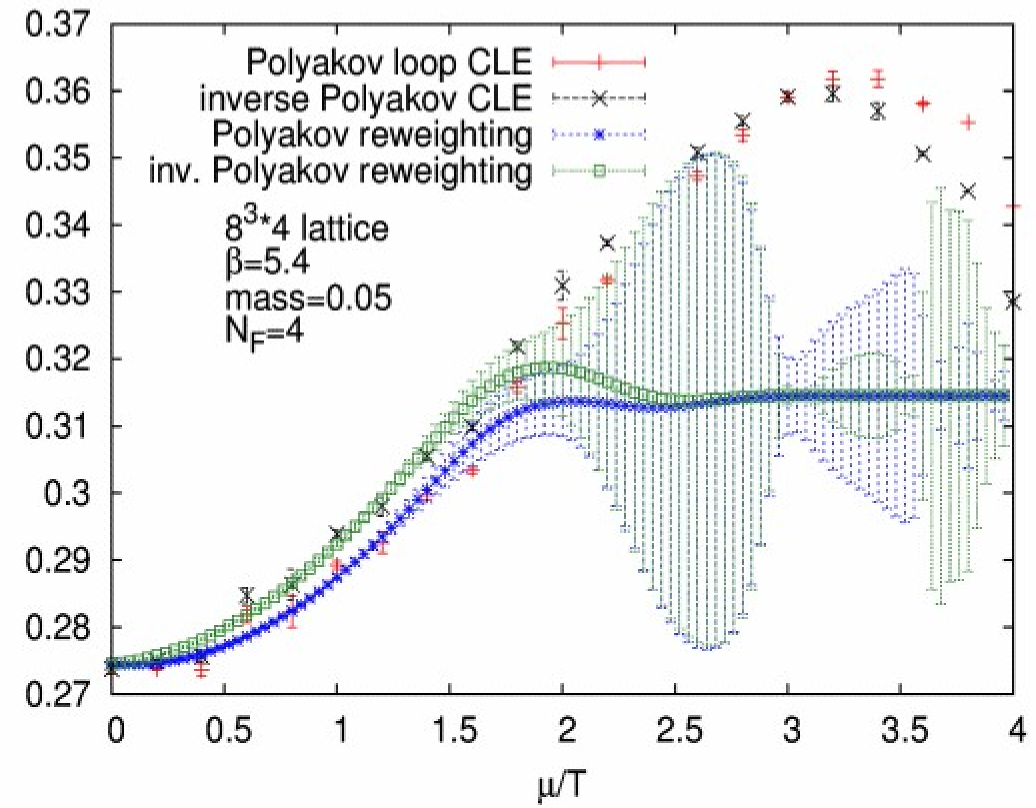
Sign problem gets hard at $\mu/T \approx 1$

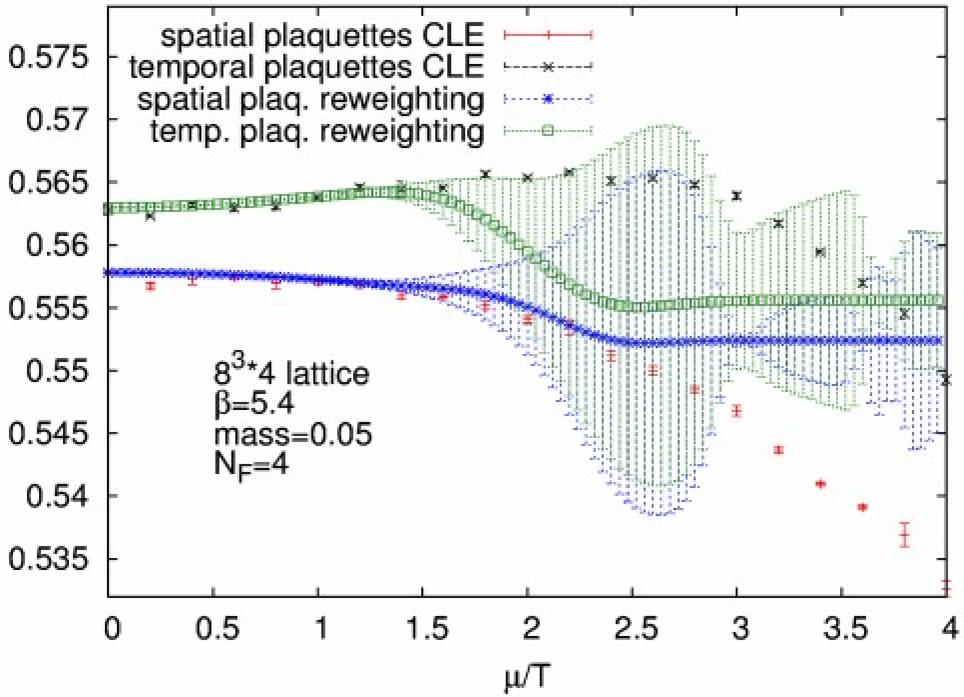
Comparison with reweighting for full QCD

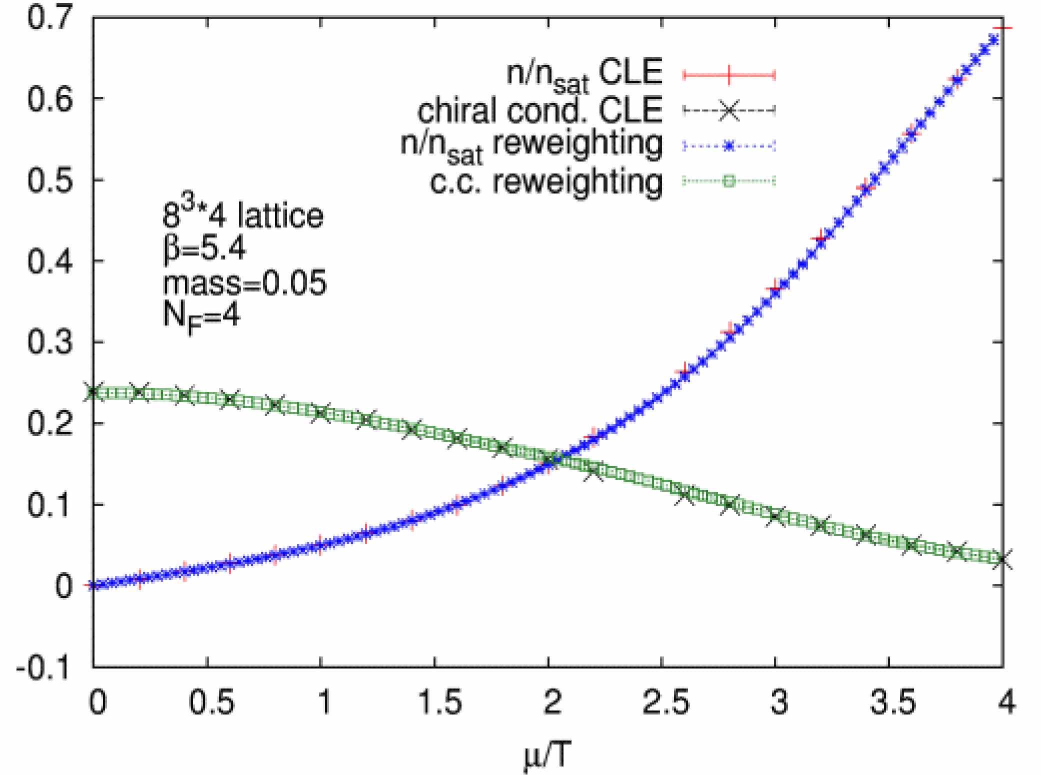
[Fodor, Katz, Sexty, Török 2015]

Reweighting from ensemble at

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





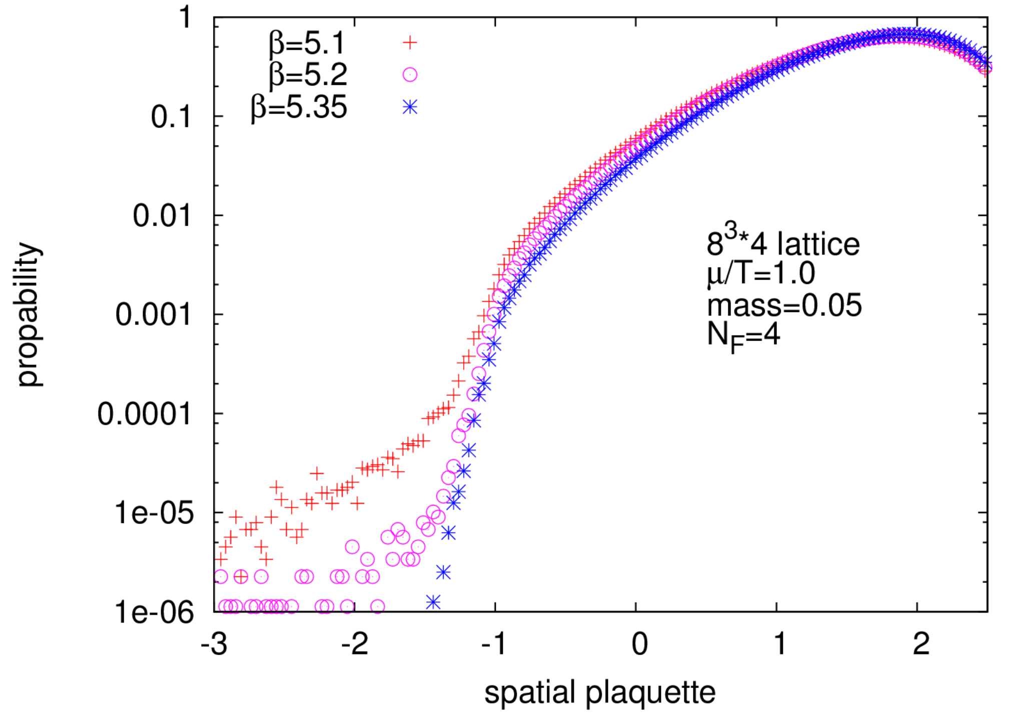


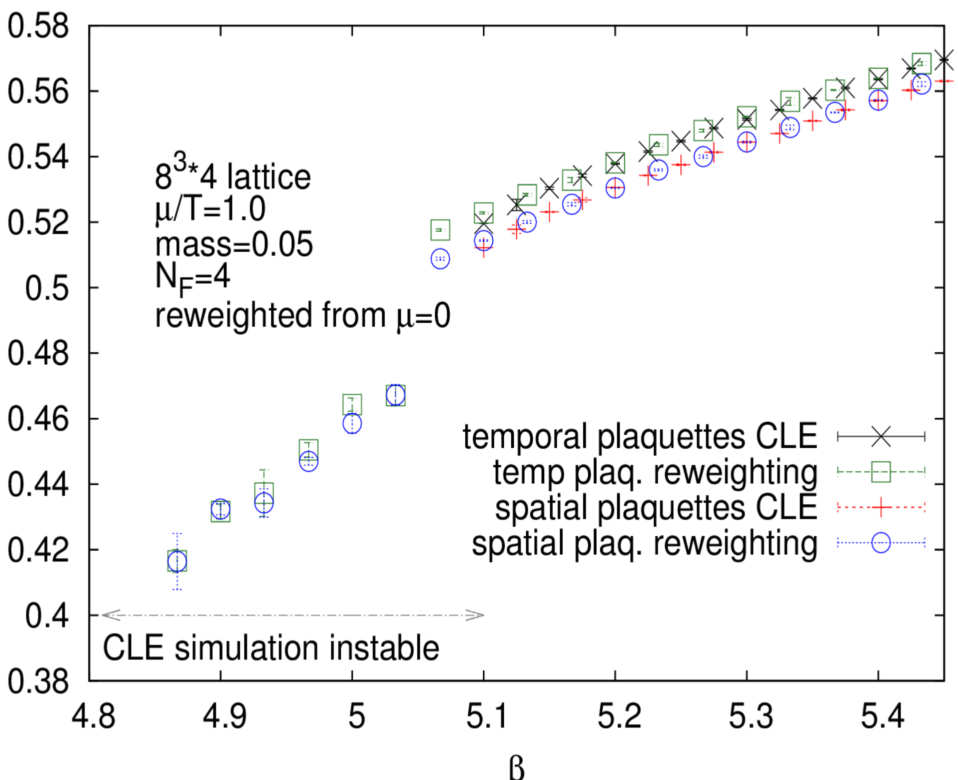
Comparisons as a function of beta

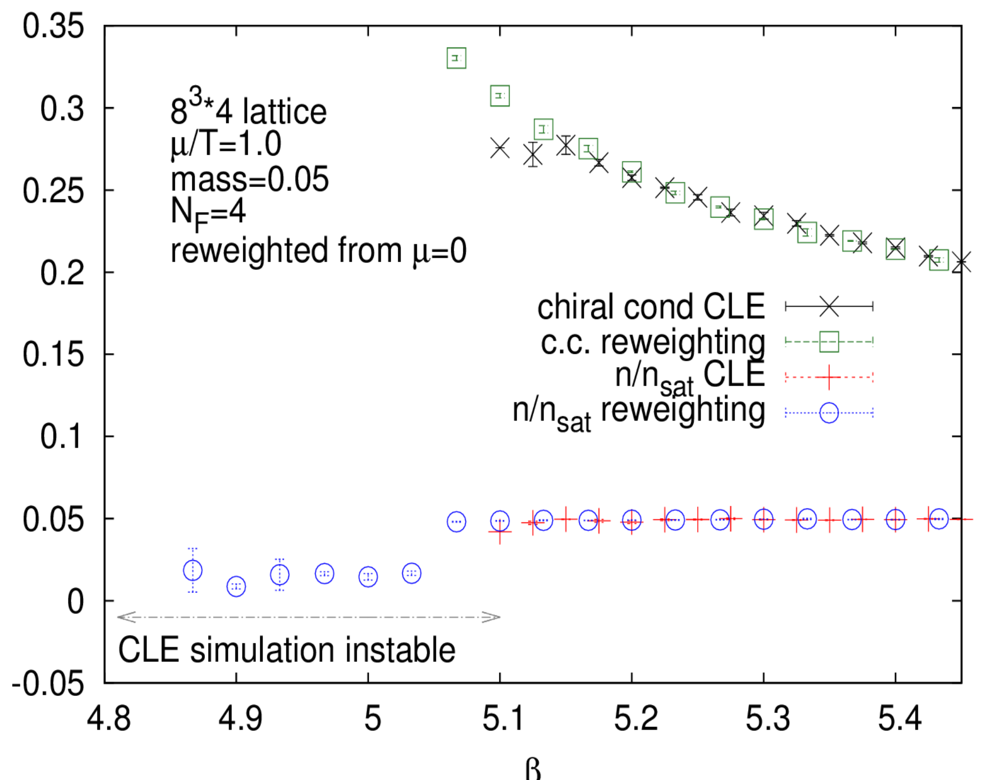
Similarly to HDQCD
Cooling breaks down at small beta

at $N_T = 4$ breakdown at $\beta = 5.1 - 5.2$

At larger N_T?

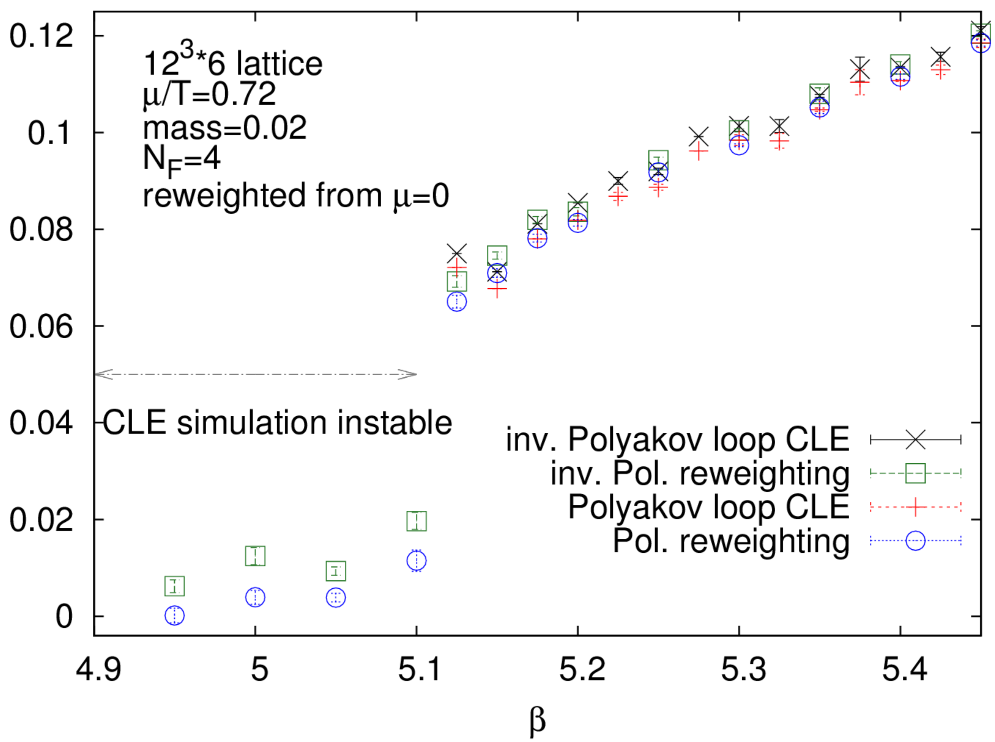


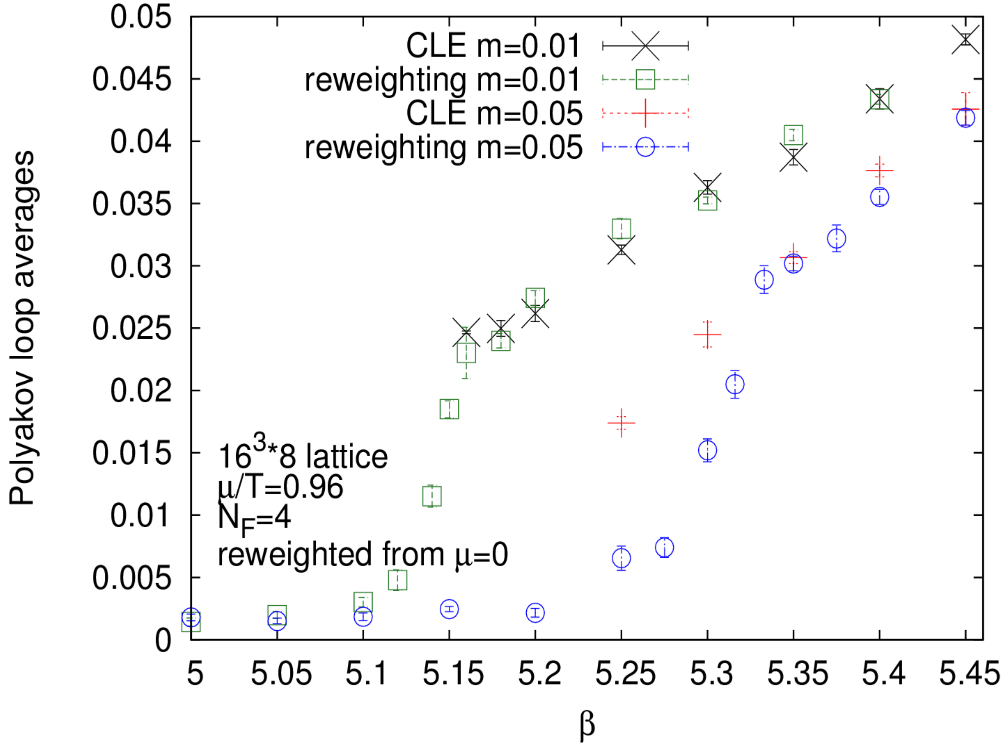




Comparisons as a function of beta

$N_T = 6$ $N_T = 8$





Breakdown prevents simulations in the confined phase for staggered fermions with $N_T = 4,6,8$

Conclusions

Sign problem of lattice QCD solid results only below $\mu_q/T=1$

Evading the sign problem by direct simulations
using complexified fields in the Complex Langevin Equation

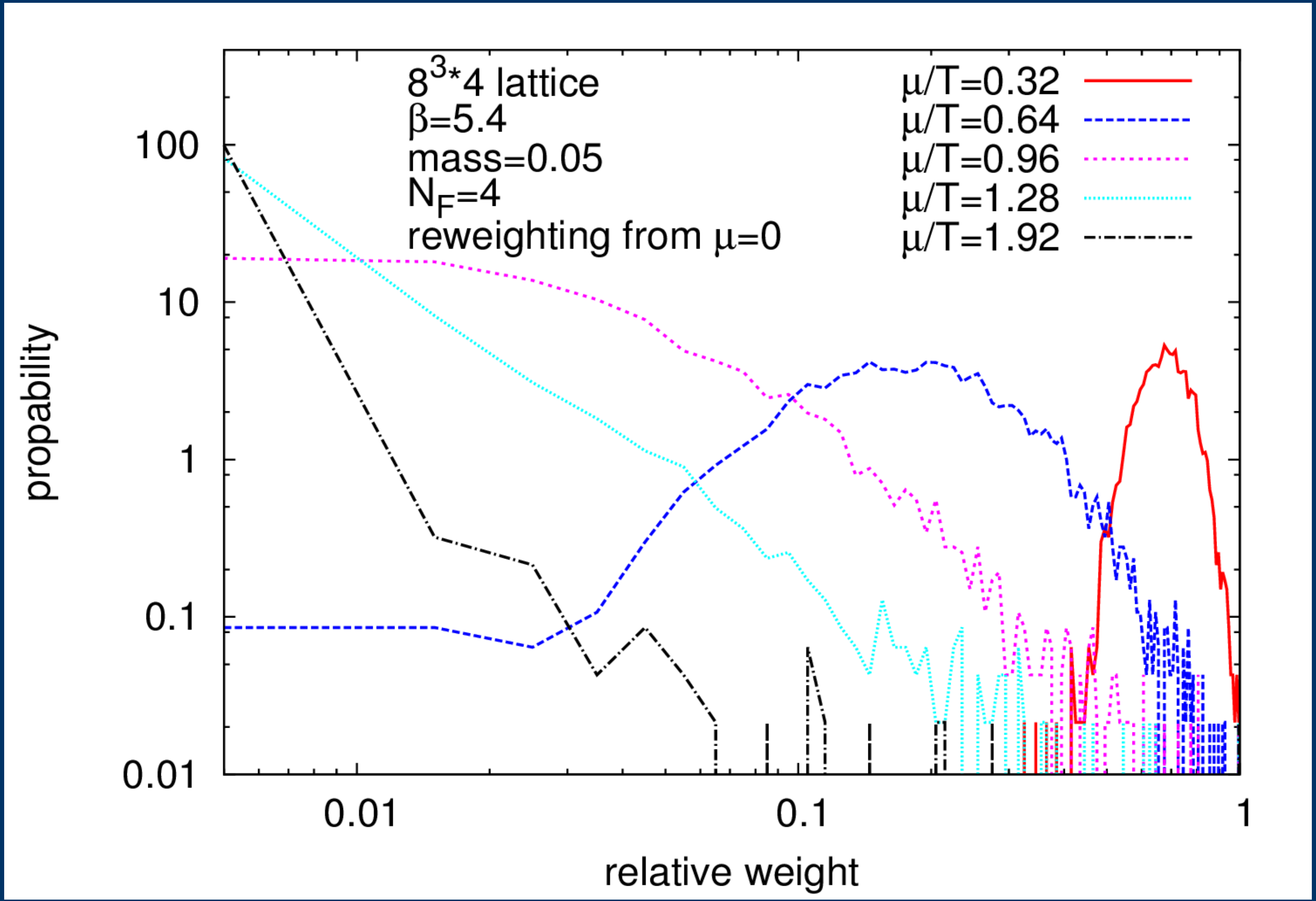
Recent progress for CLE simulations
Better theoretical understanding (poles?)
Gauge cooling

Solved models
Bose gas, SU(3) spin model, random matrix theory
Condensed matter applications

Phase diagram of HDQCD mapped out
Kappa expansion very high orders for QCD
full QCD with light quarks – only high temperatures so far

Outstanding issues
– What happens if the poles are problematic?
How to diagnose, how to solve the problem?
– is QCD at low temperatures an example for that?

Overlap problem

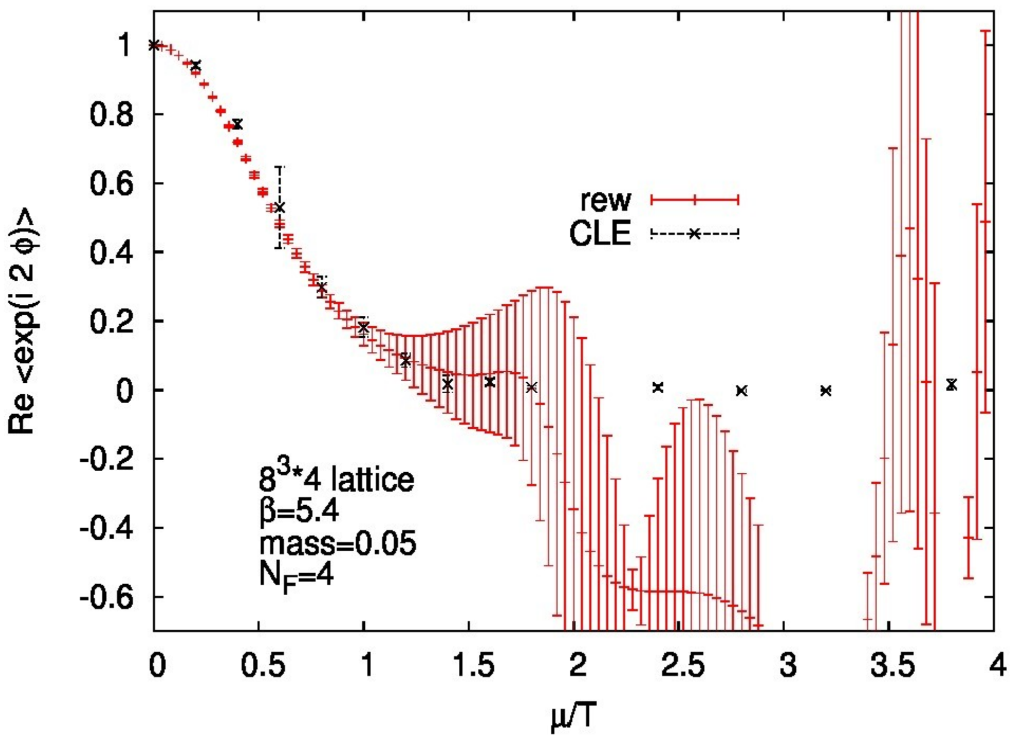


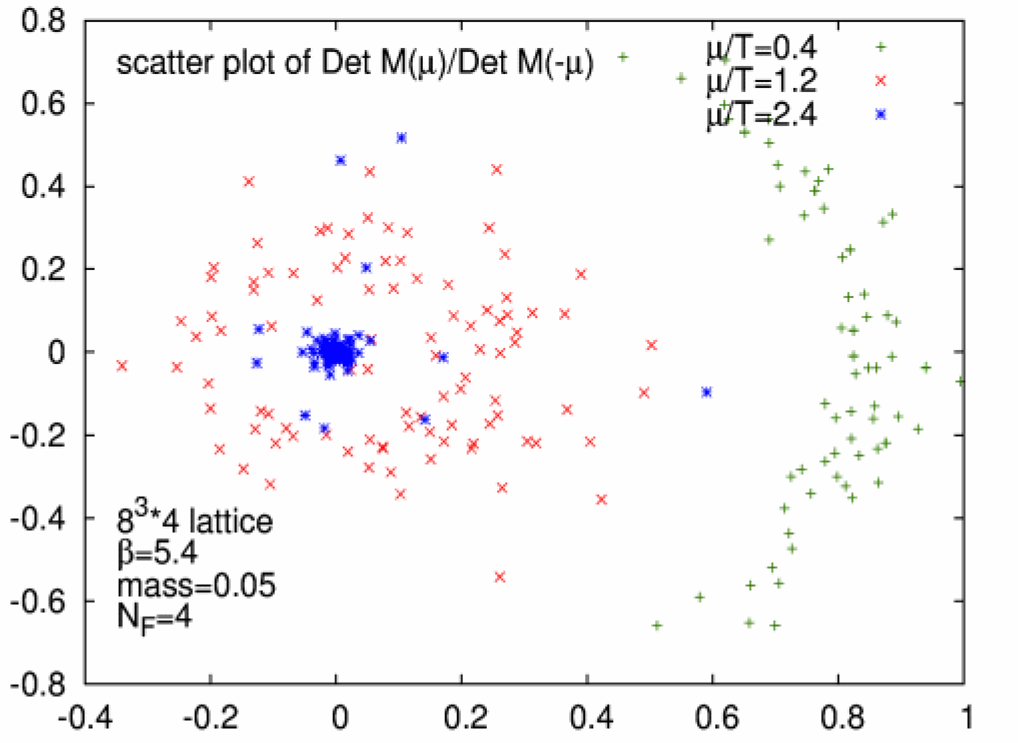
Histogram of weights
Relative to the largest weight in ensemble

Average becomes dominated by very few configurations

Sign problem

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

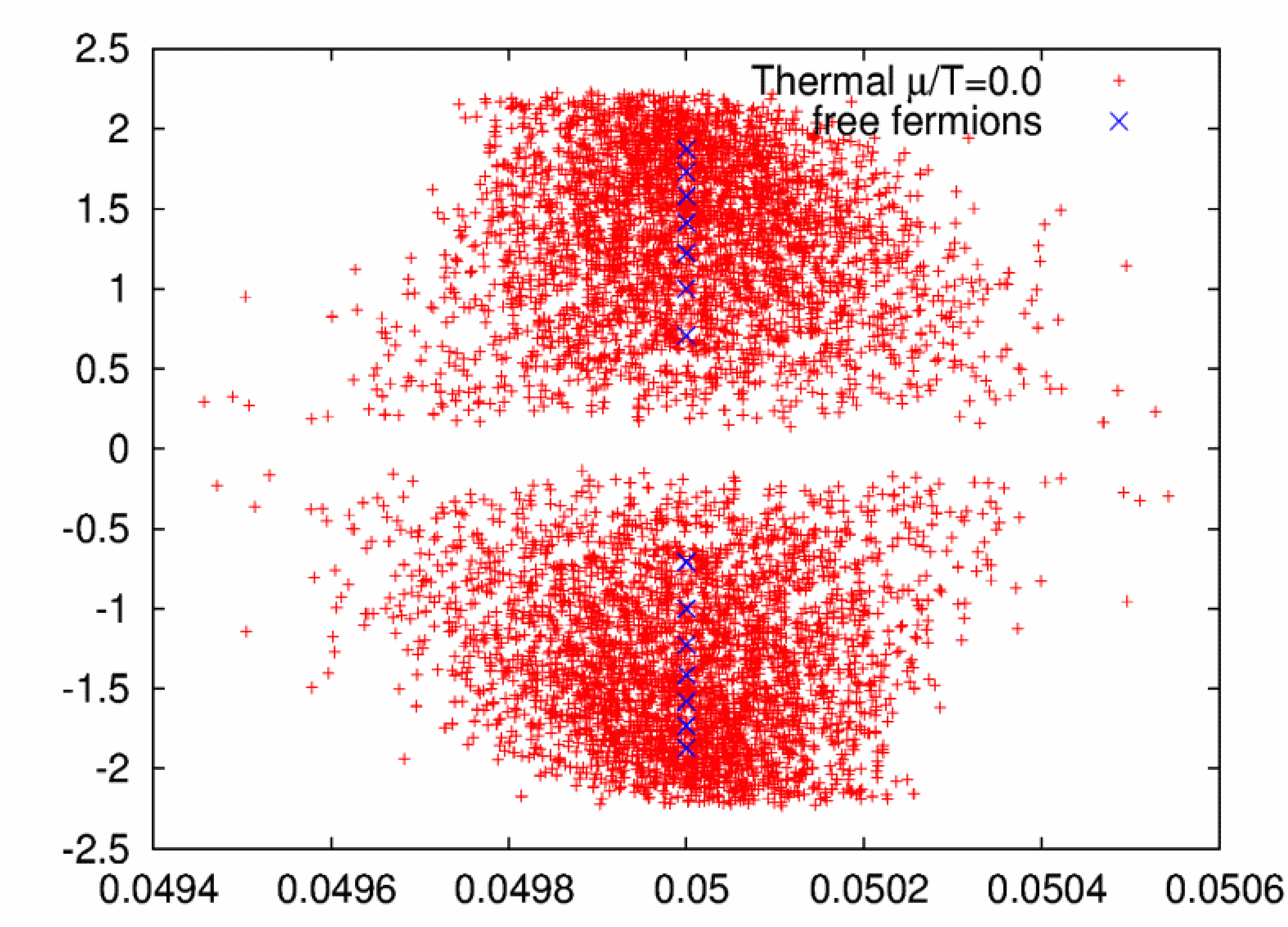




$$\langle \exp(2i\varphi) \rangle = \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle$$

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