Progress in finite density lattice QCD

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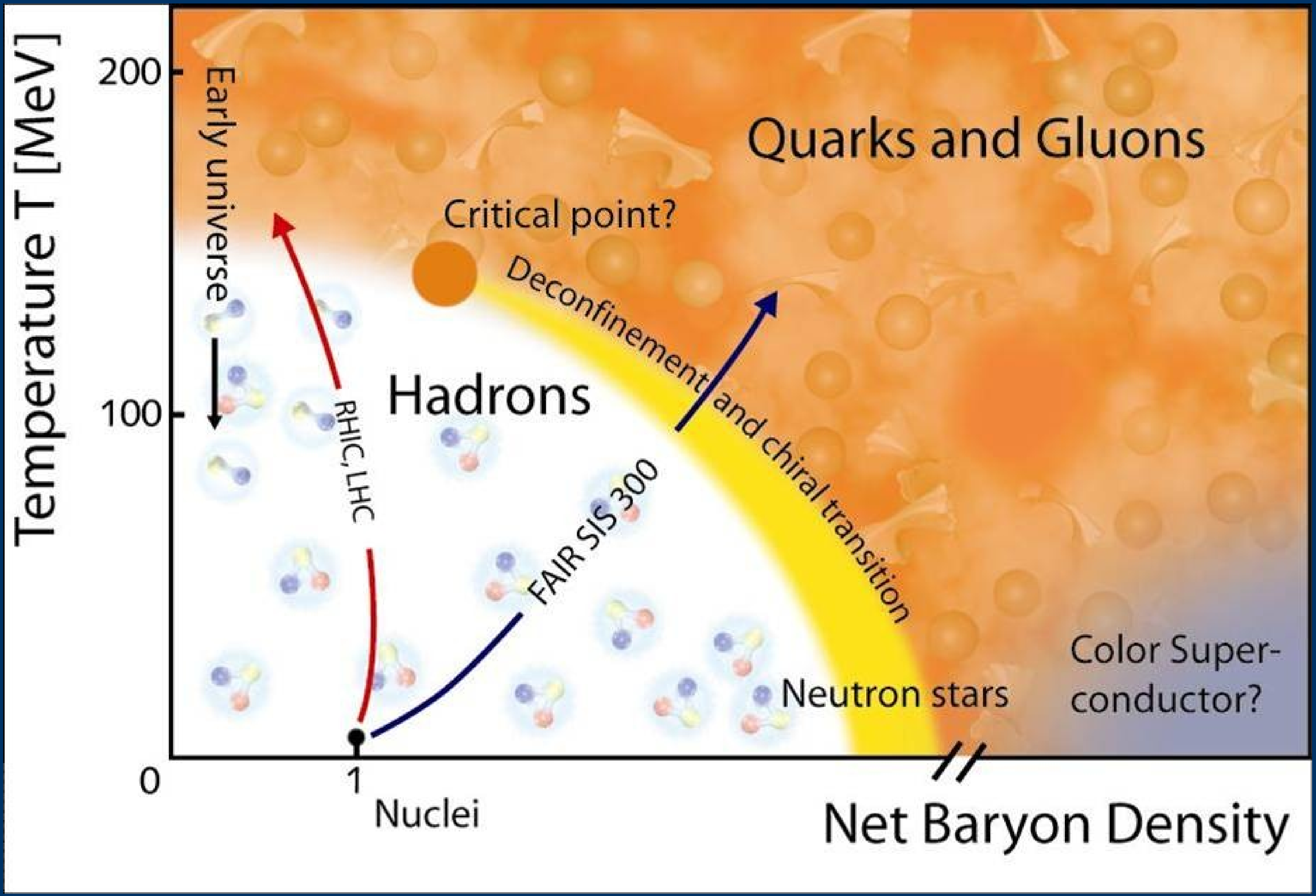
1. Sign problem
2. Complex Langevin
3. Gauge cooling
4. HDQCD → full QCD
5. CLE results for QCD

Motivations

Phase diagram of QCD matter



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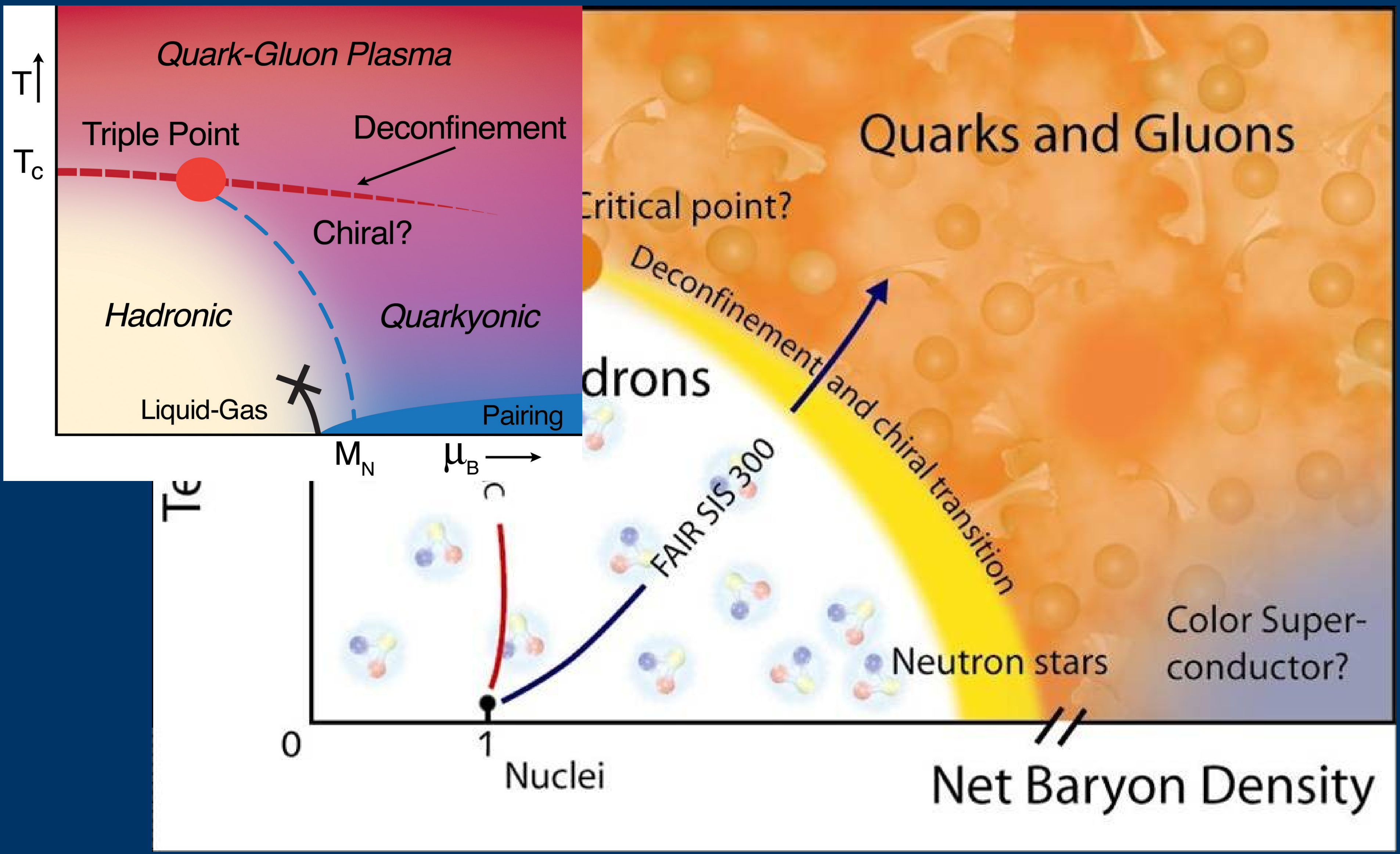

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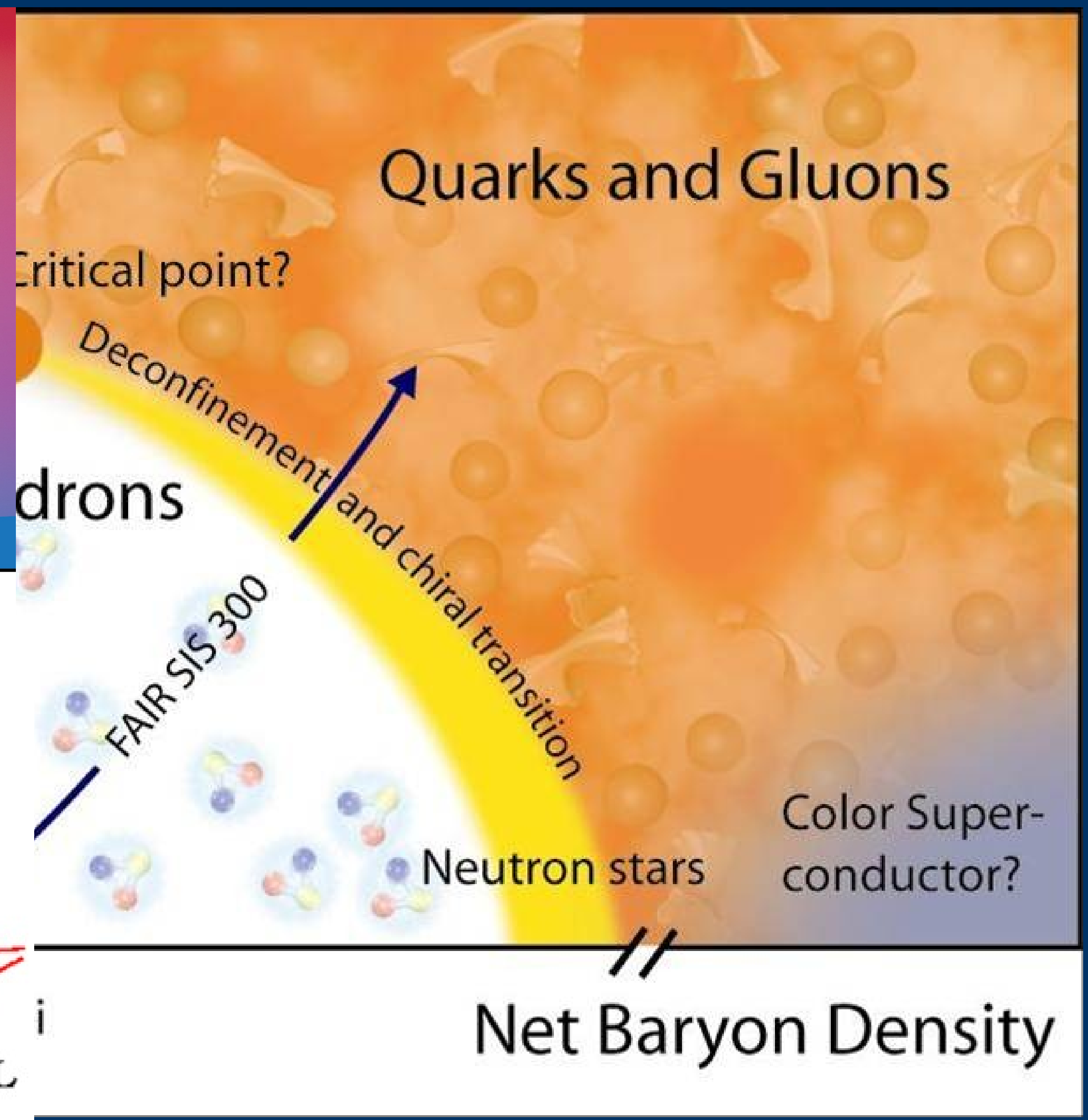

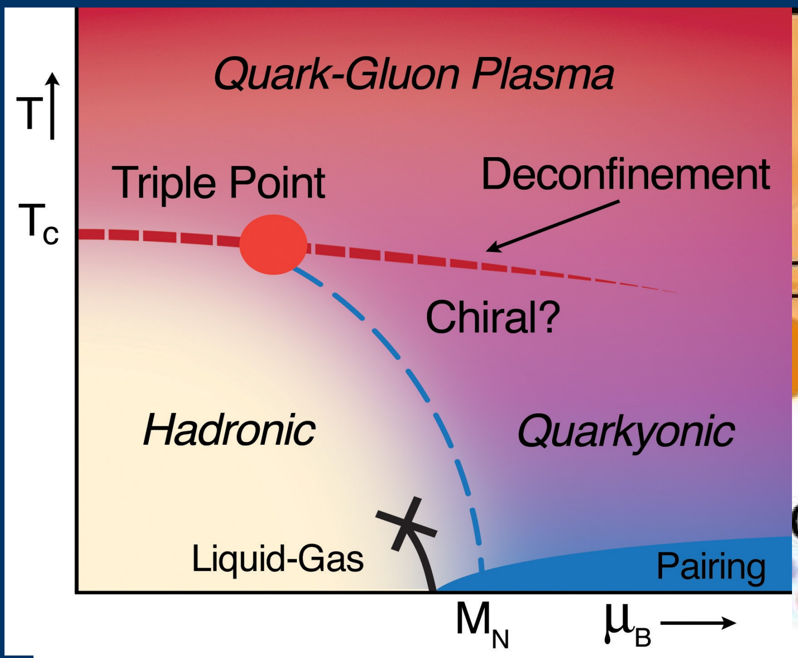

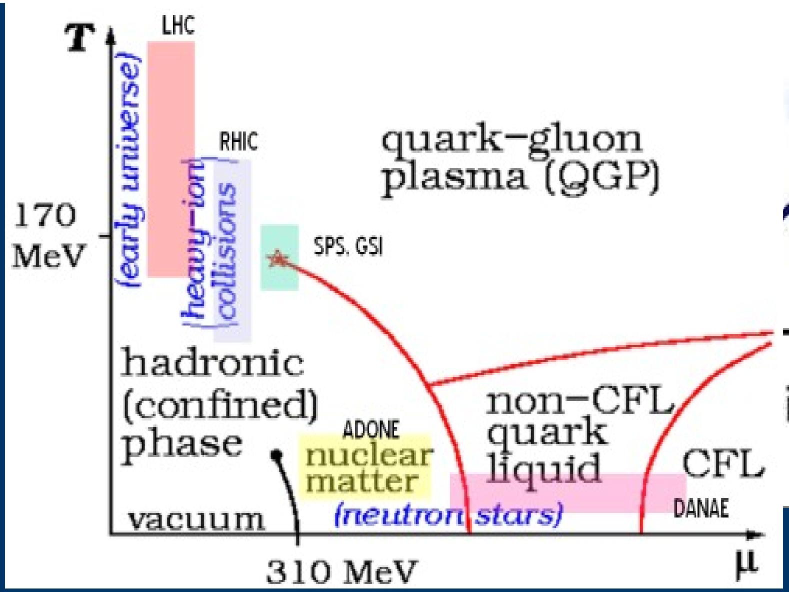

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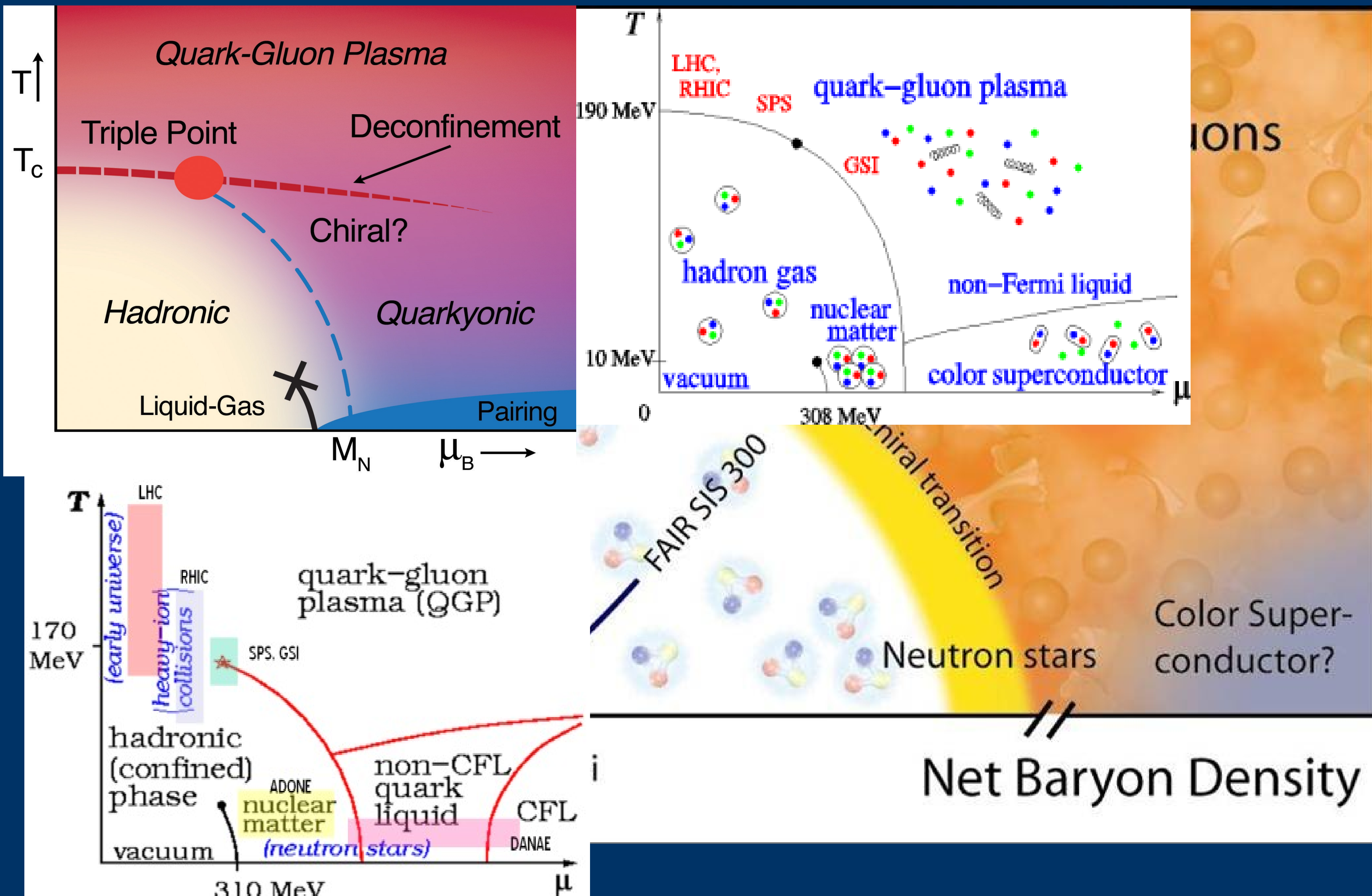

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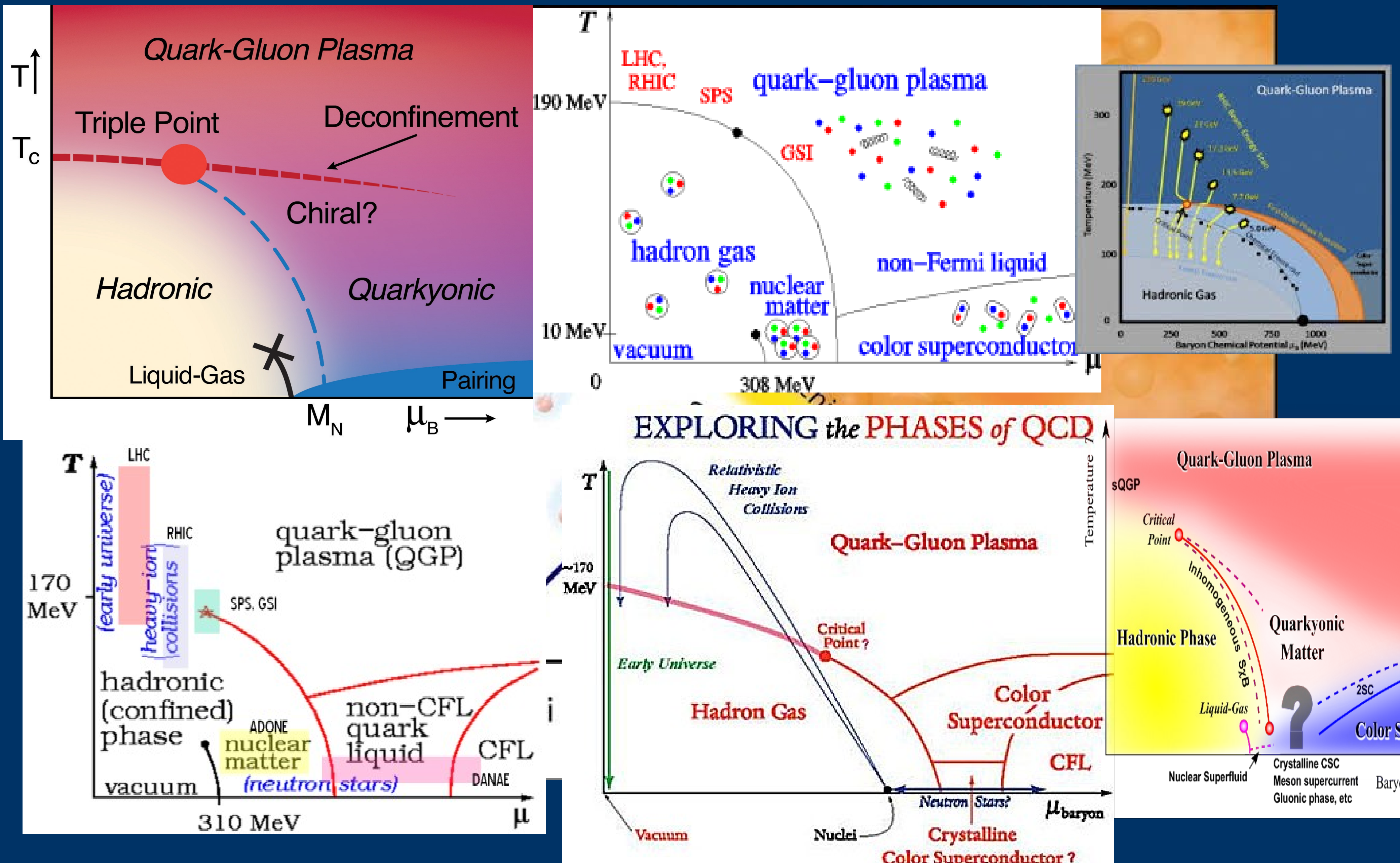


QCD sign problem

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

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

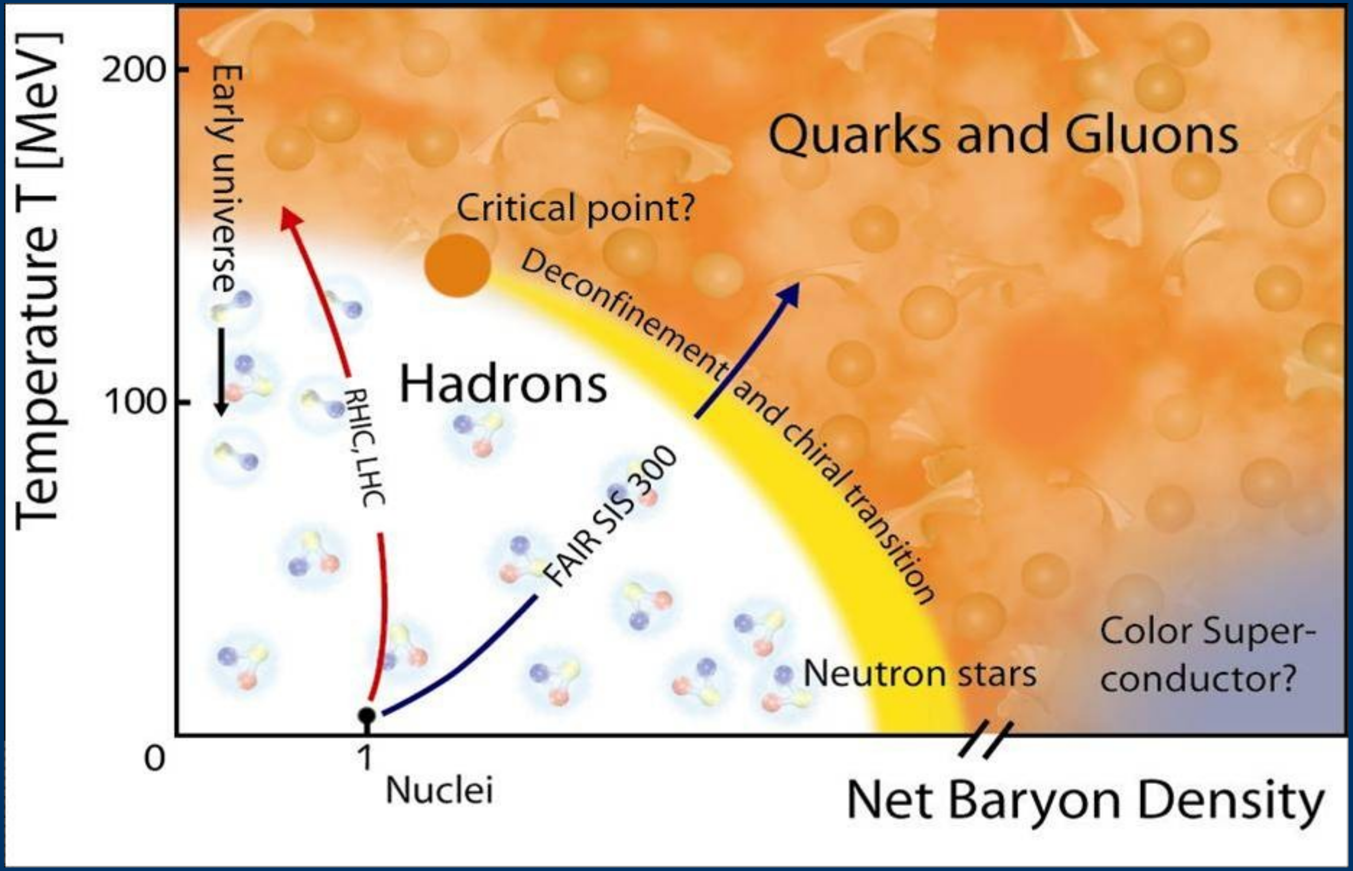
Sign problem → Naïve Monte-Carlo breaks down

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

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

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

$R = \det M(\mu = 0)$, $|\det M(\mu)|$, 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. (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

Euclidean theory	Parisi and Wu '81
Complex Langevin	Klauder '83, Parisi '83, Hüffel, Rumpf '83, ...
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
Gauge cooling,	
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, Di Renzo, Mukherjee, Scorzato '13
	Mukherjee, Cristoforetti, Scorzato '13,
	Cristoforetti et. al. '14
	Fujii, Honda, Kato, Kikukawa, Komatsu, Sano '13

thimble and stochastic quantisation

Aarts '13

Aarts, Bongiovanni, Seiler, Sexty '14

See talk of Gert Aarts

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, ...

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

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

$$\frac{1}{Z}\int P_{comp}(x) O(x) dx = \frac{1}{Z}\int P_{real}(x, y) O(x+iy) dx\, dy \qquad \left(= \frac{1}{T}\int O(z(\tau)) d\tau \right)$$

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

"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
→ meromorphic drift
Is it a problem for QCD?

[see also: Mollgaard, Splittorff (2013)]

Gaussian Example

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

CLE

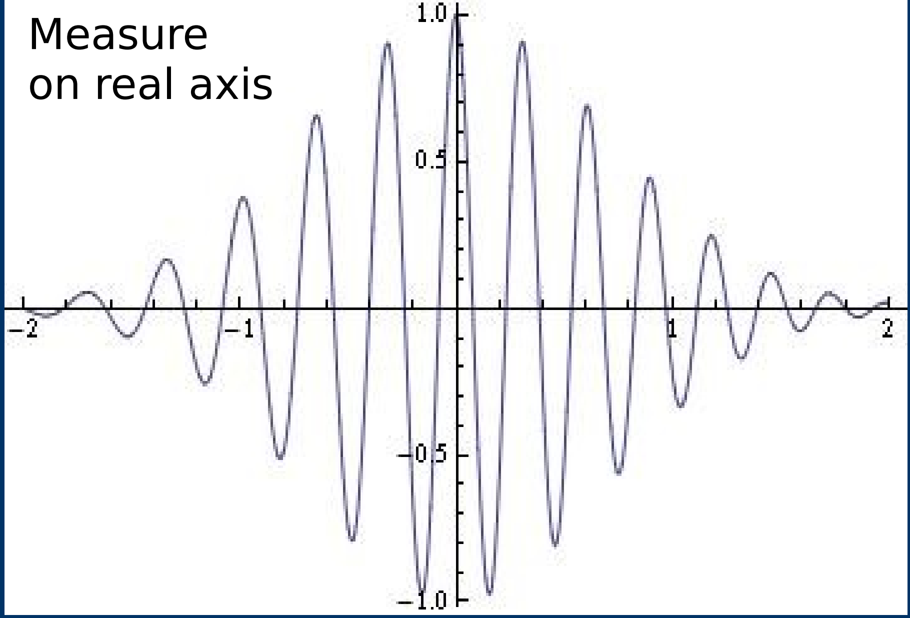
$$\frac{d}{d\tau}(x+iy)=-2\sigma(x+iy)-i\lambda+\eta$$

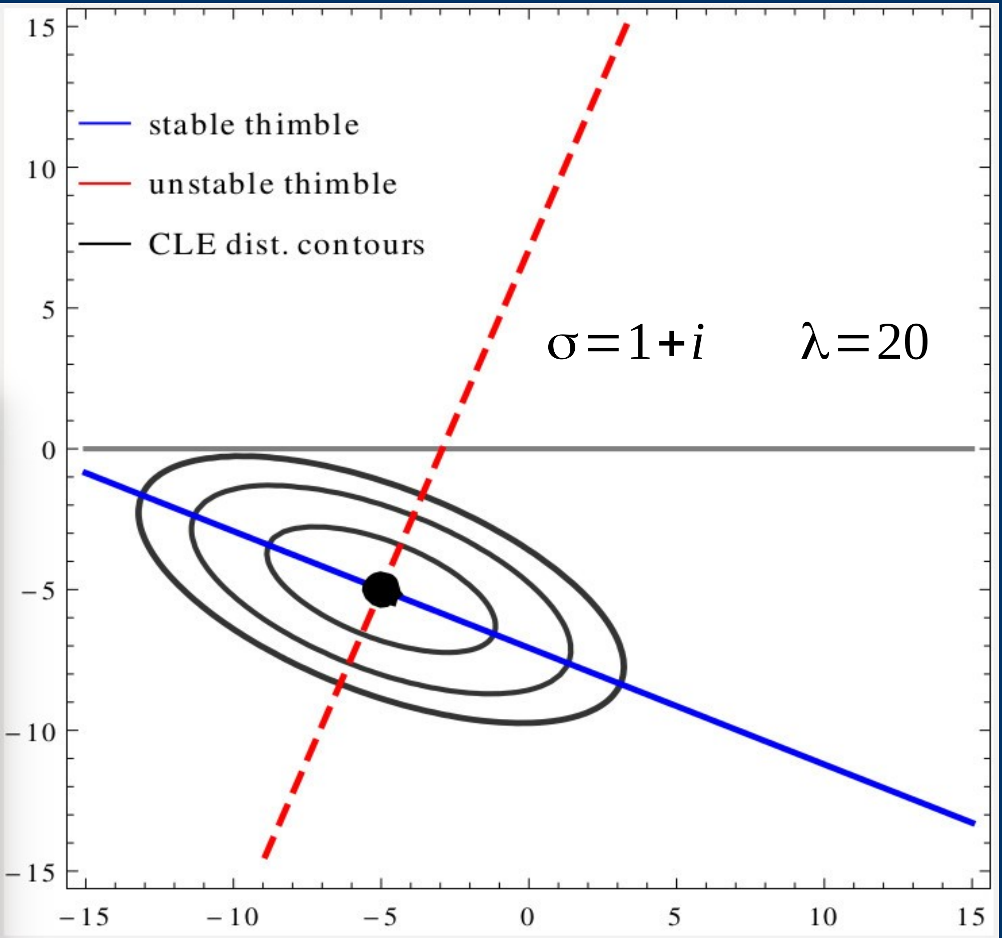
$$P(x,y)=e^{-a(x-x_0)^2-b(y-y_0)^2-c(x-x_0)(y-y_0)}$$

real and positive
Gaussian distribution

$$\frac{1}{Z}\int P_{comp}(x)O(x)\,dx=$$

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





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.]

Θ real → complex action, $\langle Q \rangle$ imaginary

Θ imaginary → real action, $\langle Q \rangle$ real

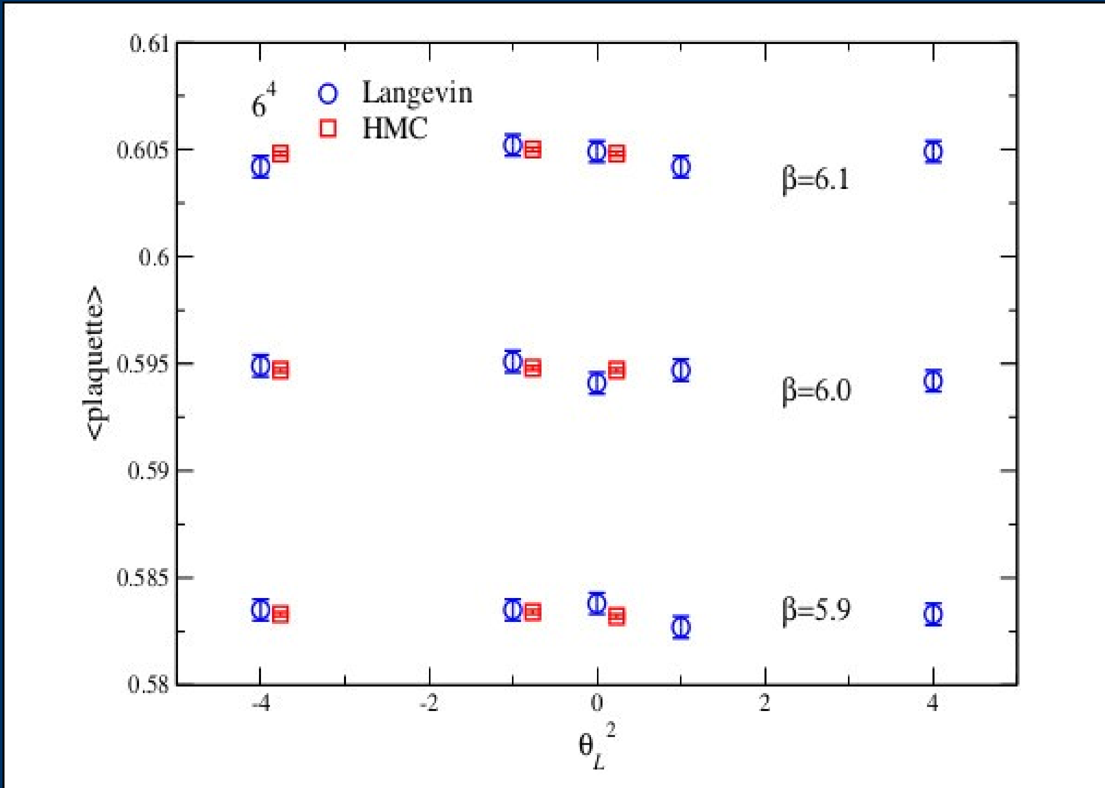
On the lattice

$$Q = \epsilon^{\mu\nu\theta\rho} F_{\mu\nu} F_{\theta\rho} \rightarrow \sum_x q(x)$$

Not topological

Cooling is needed

Θ_L bare parameter needs renormalisation



Θ imaginary → use real Langevin or HMC

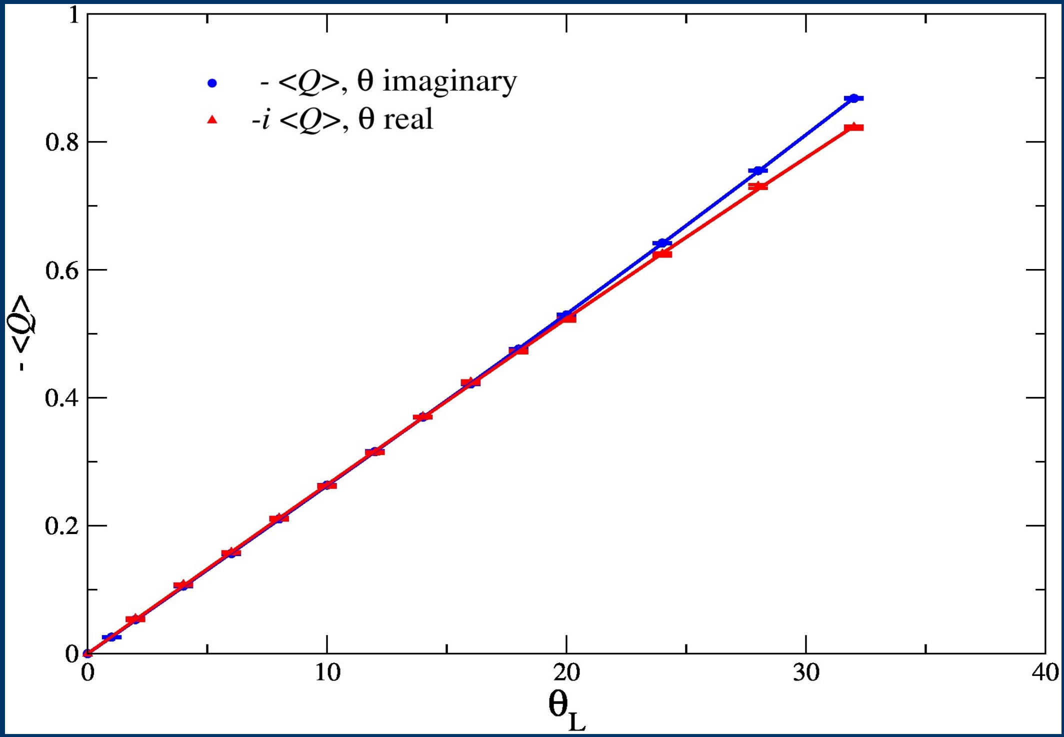
Θ real → use complex Langevin

comparing real Θ
with imaginary Θ

$$-i\langle Q\rangle_{\Theta_R}=\frac{\partial \ln Z}{\partial \Theta_R}=\Omega\chi_L\Theta_R(1+2b_2\Theta_R^2+3b_4\Theta_R^4+\ldots)$$

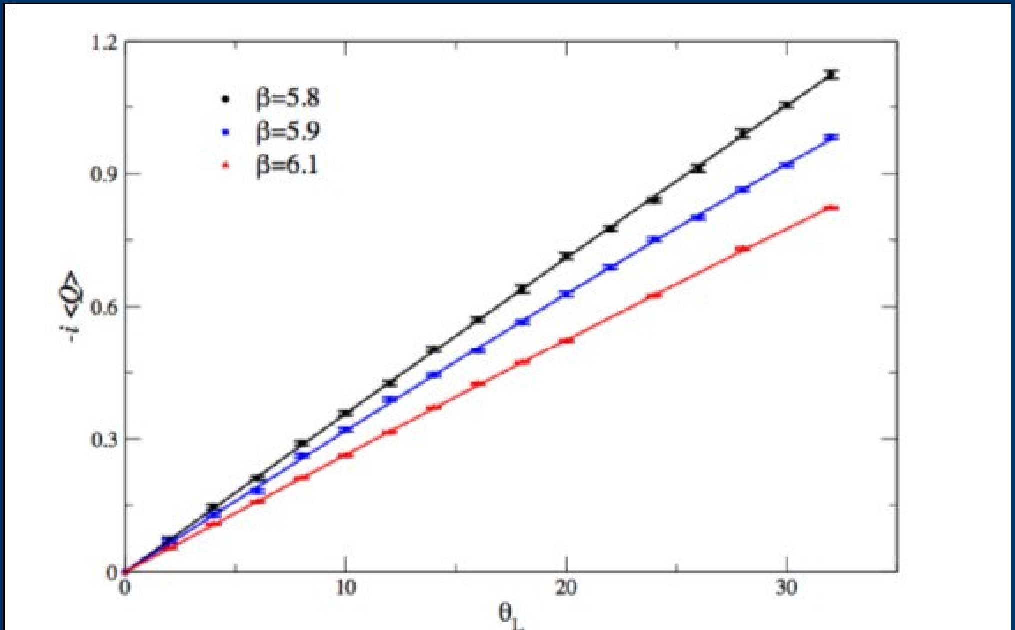
Using analyticity

$$\langle Q\rangle_{\Theta_I}=-\frac{\partial \ln Z}{\partial \Theta_I}=\Omega\chi_L\Theta_I(1-2b_2\Theta_I^2+3b_4\Theta_I^4+\ldots)$$



Expected dependence

χ_L drops at higher temperature



No renormalisation yet

Gaugefixing in SU(2) one plaquette model

Berges, Sexty '08

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

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

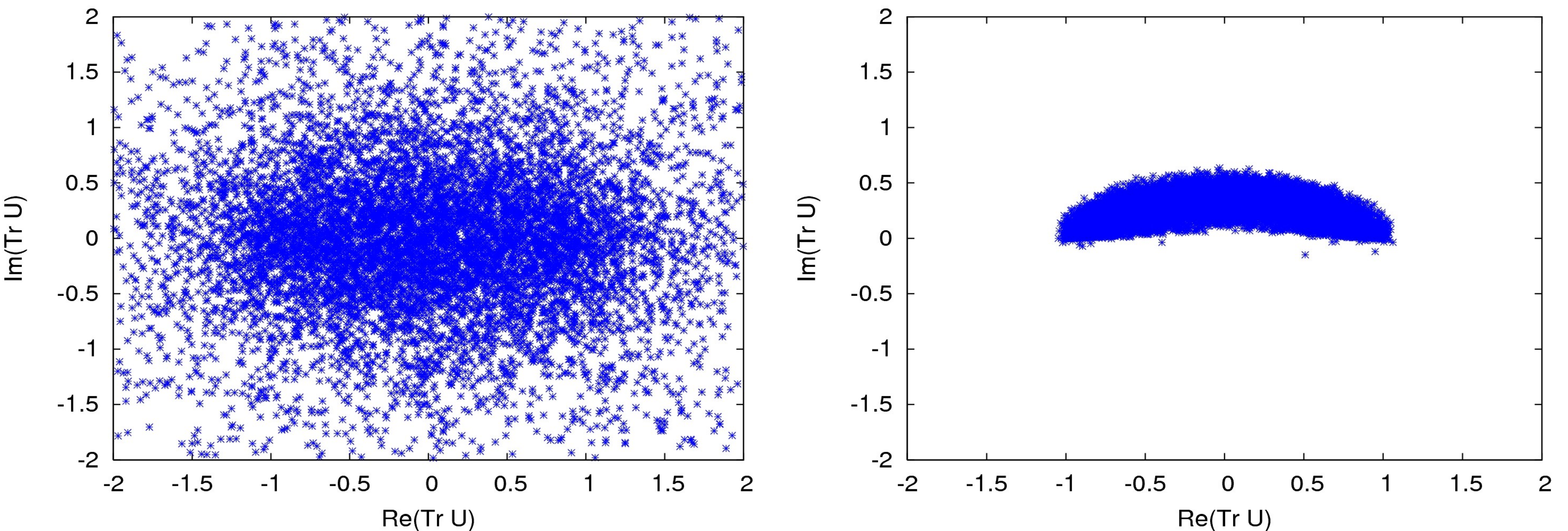
"gauge" symmetry: $U \rightarrow W U W^{-1}$ complexified theory: $U, W \in SL(2, \mathbb{C})$

Using gauge symmetry
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 theories and CLE

link variables: SU(N) → 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)

$$\sum_i Tr(U_i U_i^{+}) \geqslant N$$

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

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

Gauge cooling

[Seiler, Sexty, Stamatescu (2012)]

complexified distribution with slow decay ⟶ 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)

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

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

Gradient of the unitarity norm gives steepest descent

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

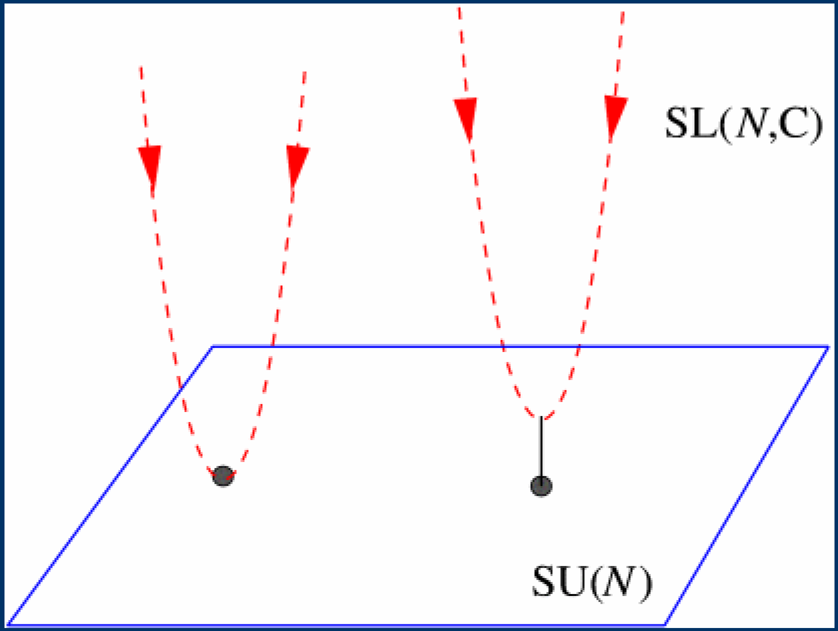
Gauge transformation at x changes 2d link variables

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

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

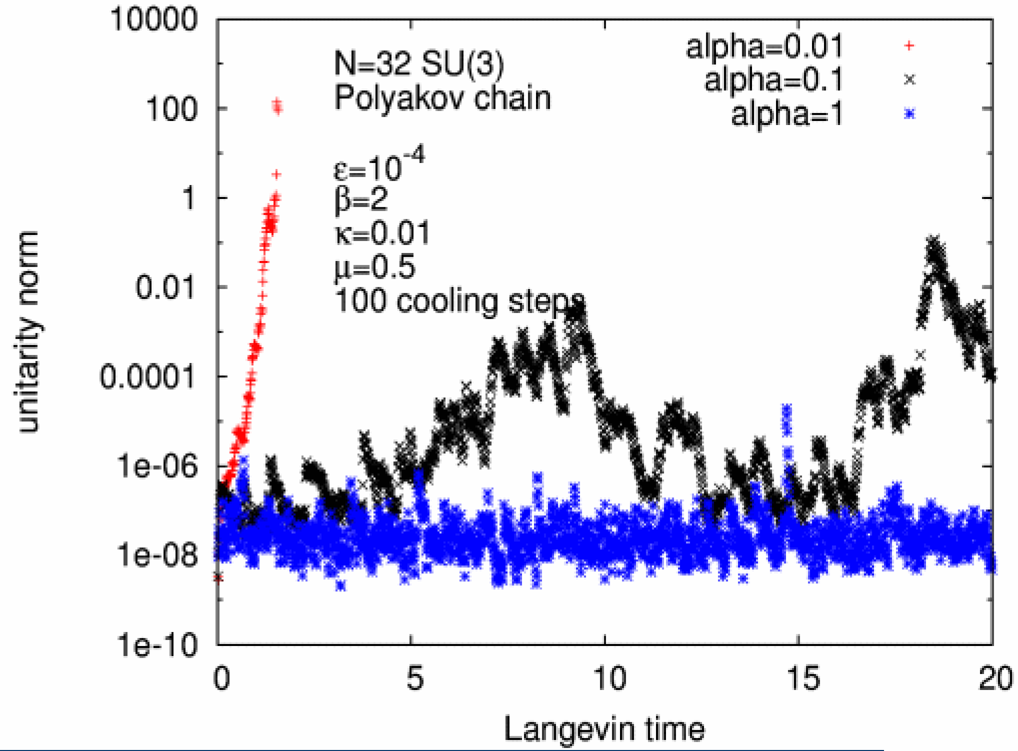
Dynamical steps are interspersed with several gauge cooling steps

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



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

but remember, $\beta \to \infty$ in cont. limit $(a \to 0)$

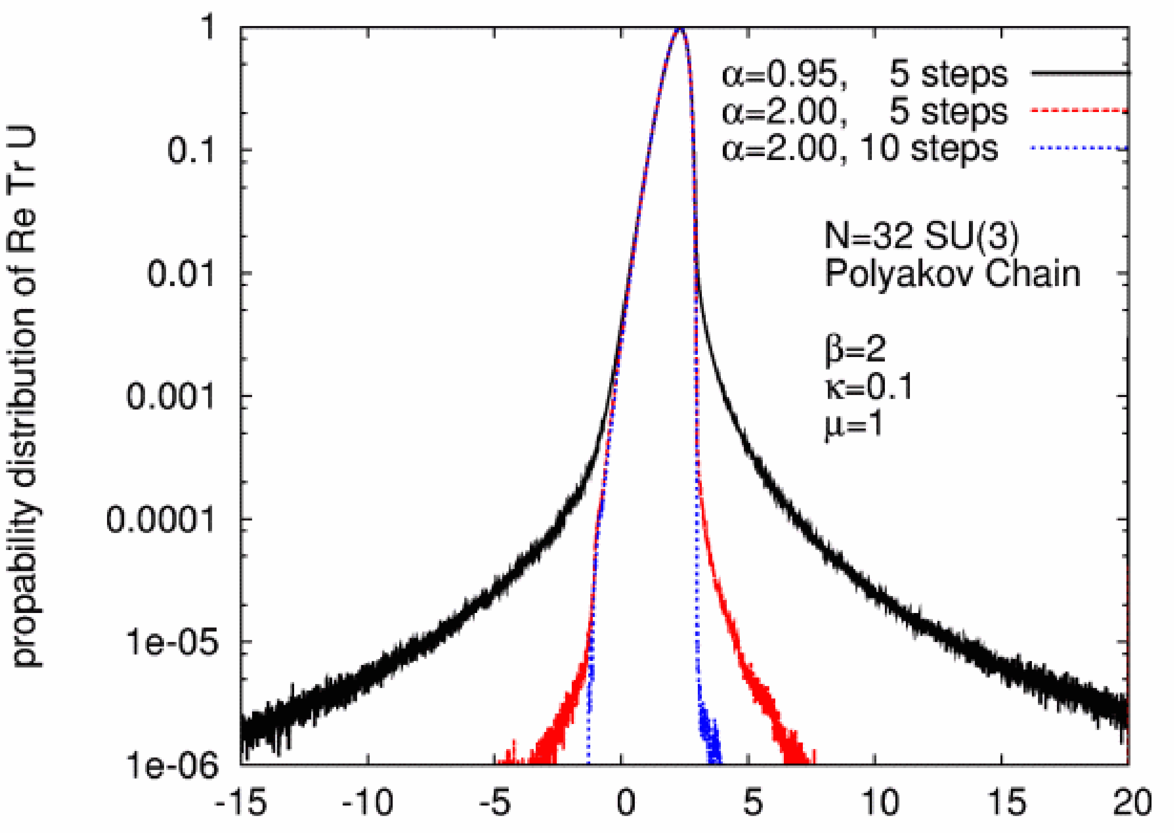


Smaller cooling

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

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

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

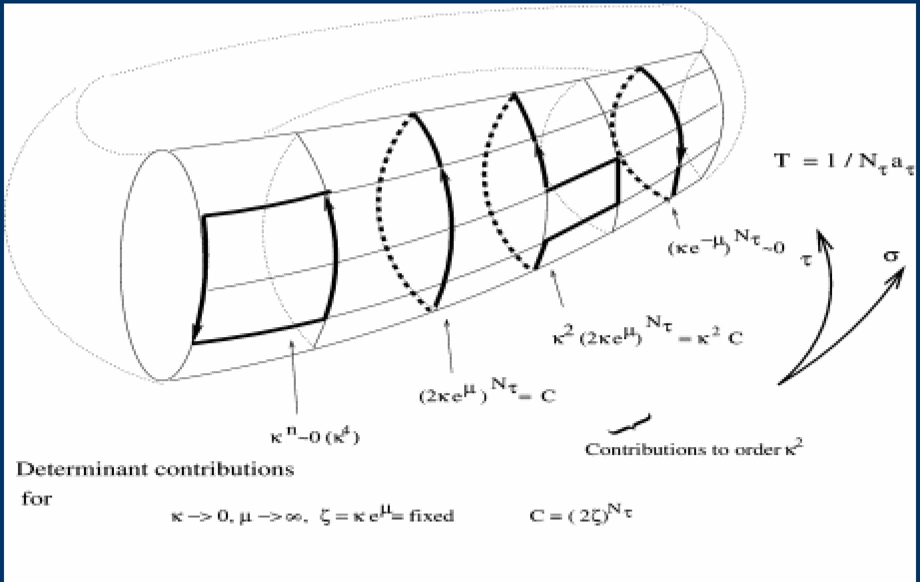
$$S = S_W[U_\mu] + \ln \mathrm{Det}\, M(\mu)$$

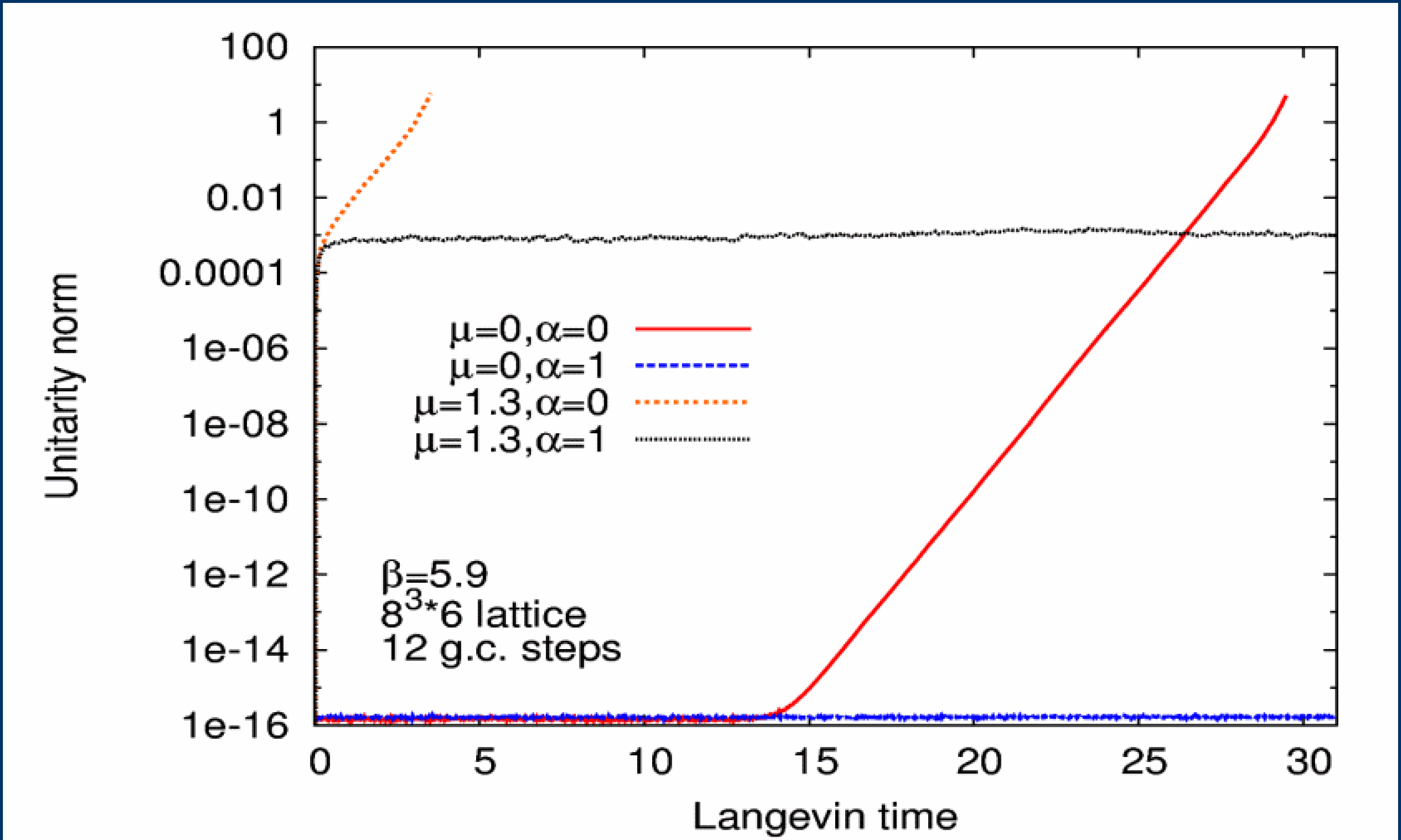
Studied with reweighting De Pietri, Feo, Seiler, Stamatescu '07

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

CLE study using gaugecooling

[Seiler, Sexty, Stamatescu (2012)]





Gauge cooling stabilizes the distribution

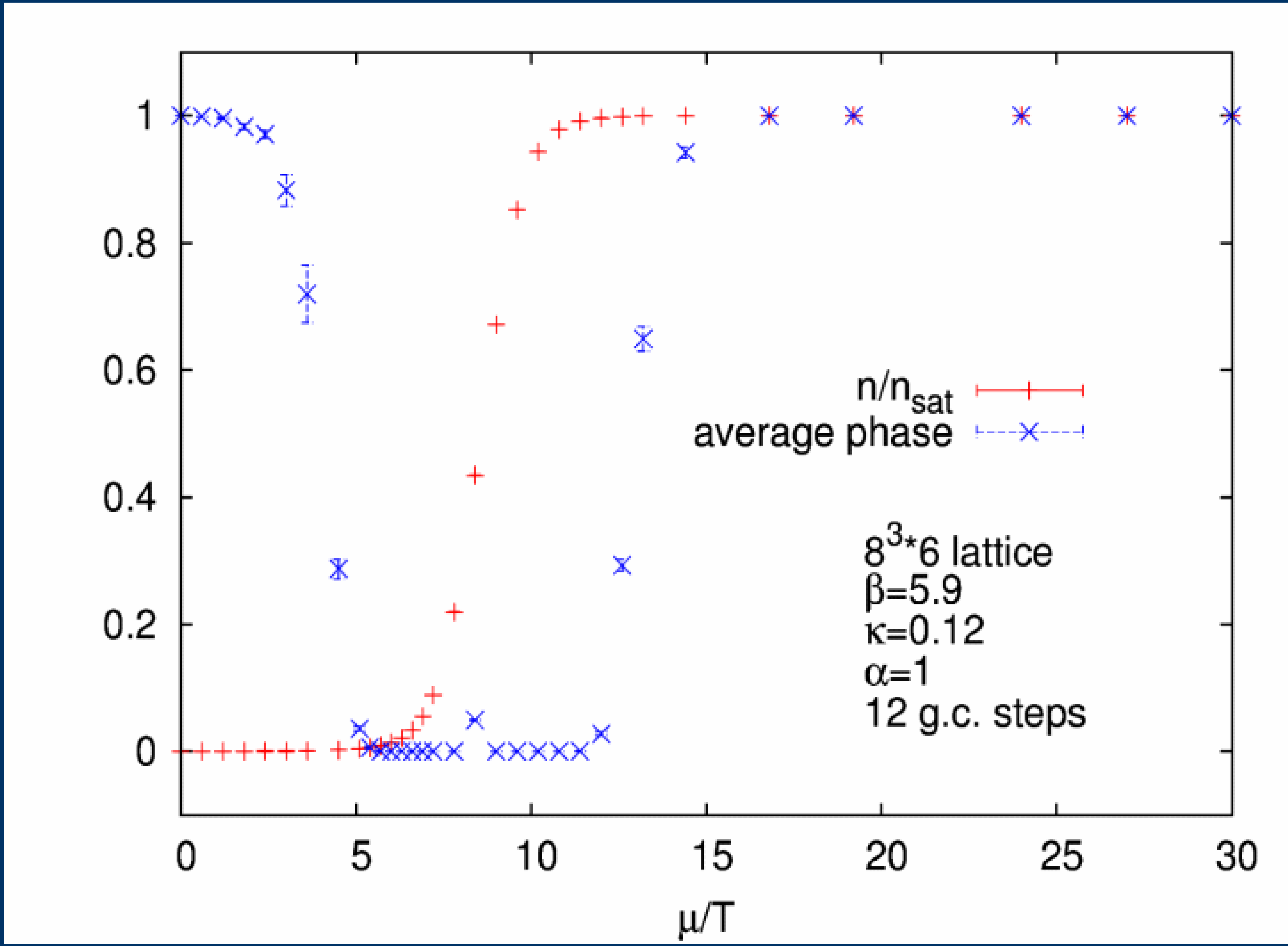
SU(3) manifold instable even at $\mu=0$

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

Saturation – "inverse" Silver Blaze behaviour

Polyakov loop at high densities

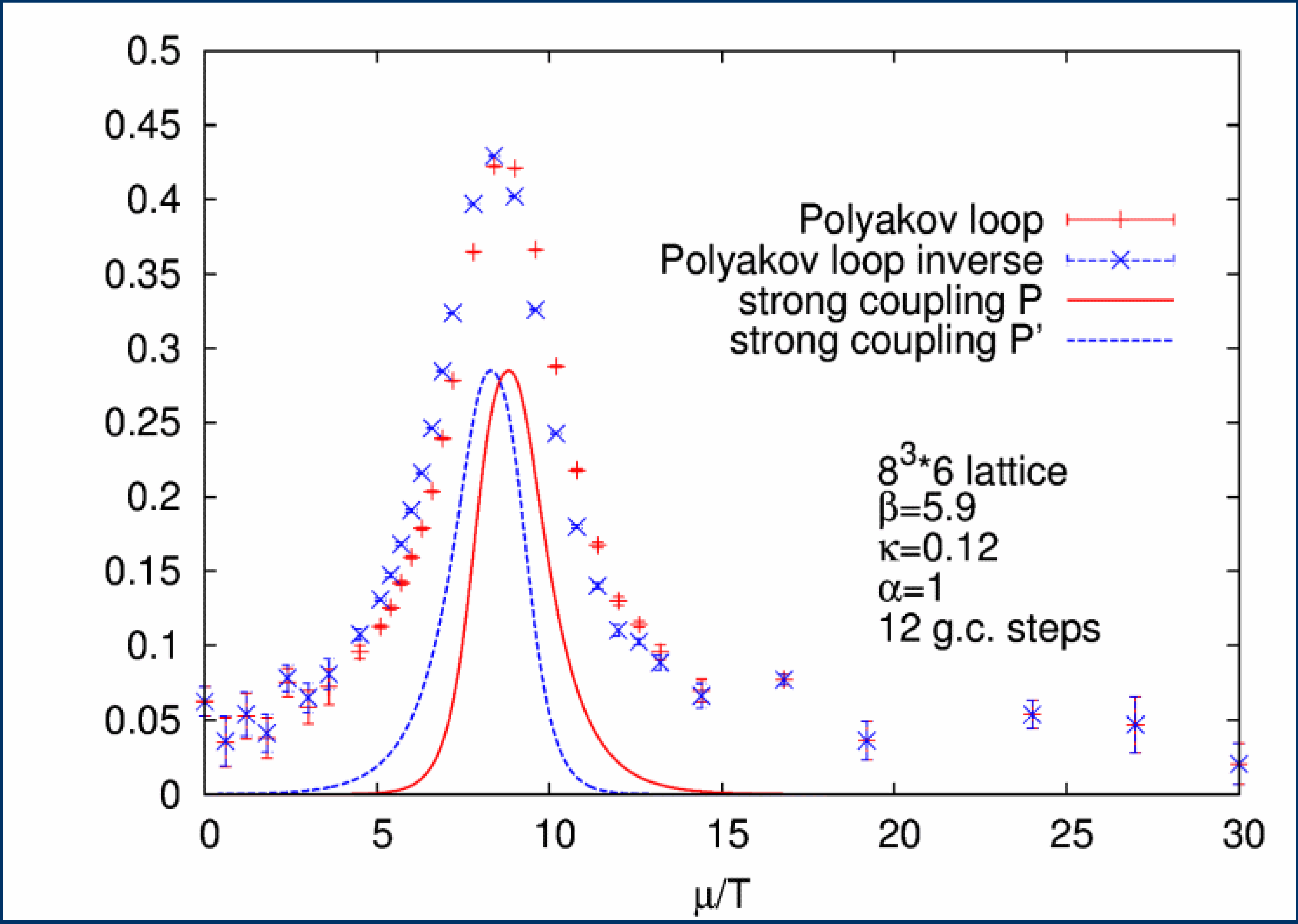
Nonzero value when: colorless bound states formed with P or P'

1 quark:
meson with P'

2 quark:
Baryon with P

↓

P' has a peak before P

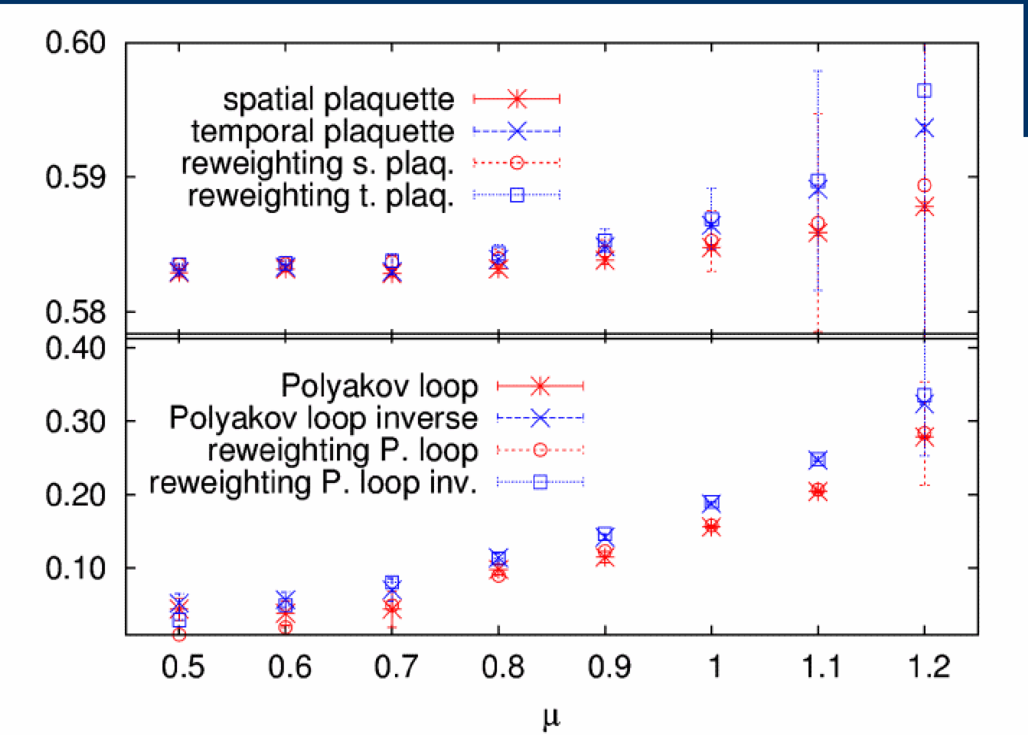


Large chemical potential: all quark states are filled
No colorless state can be formed

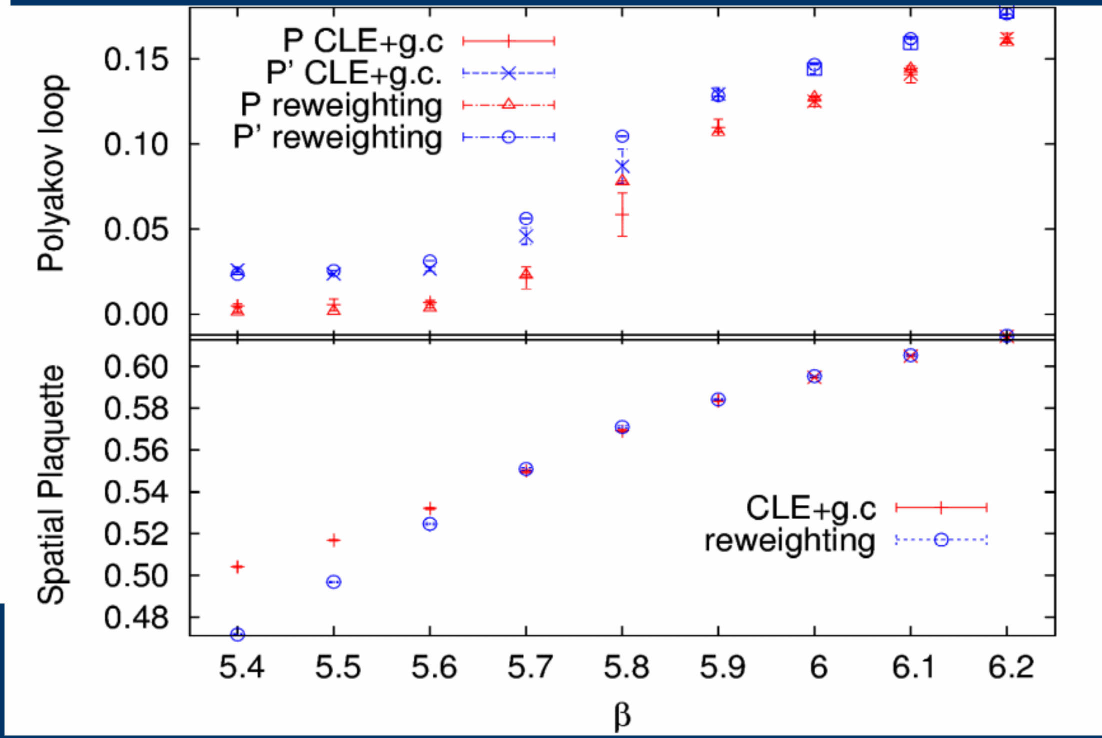
↓

P and P' decays again

Comparison to reweighting



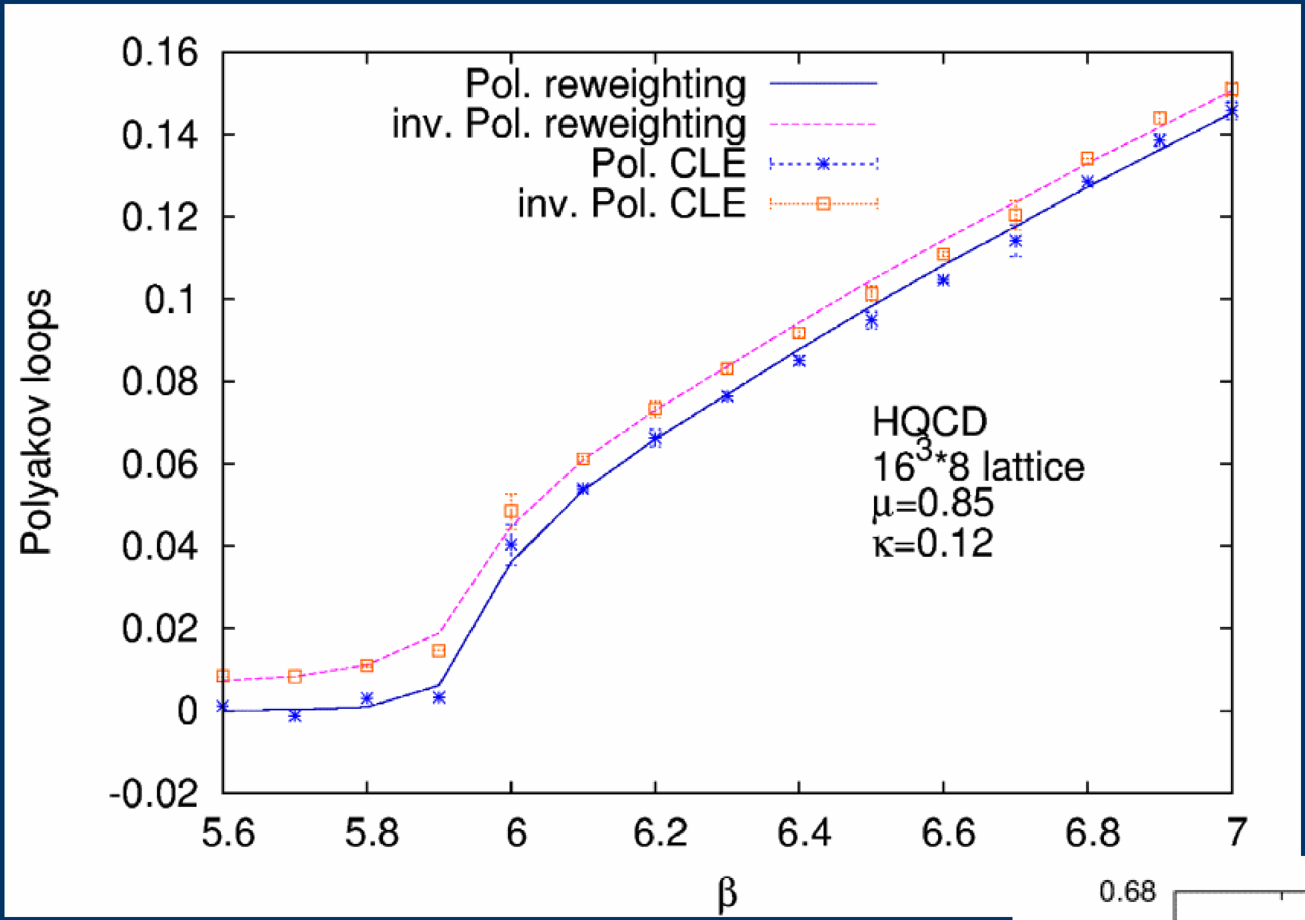
6^4 lattice, $\beta = 5.9$

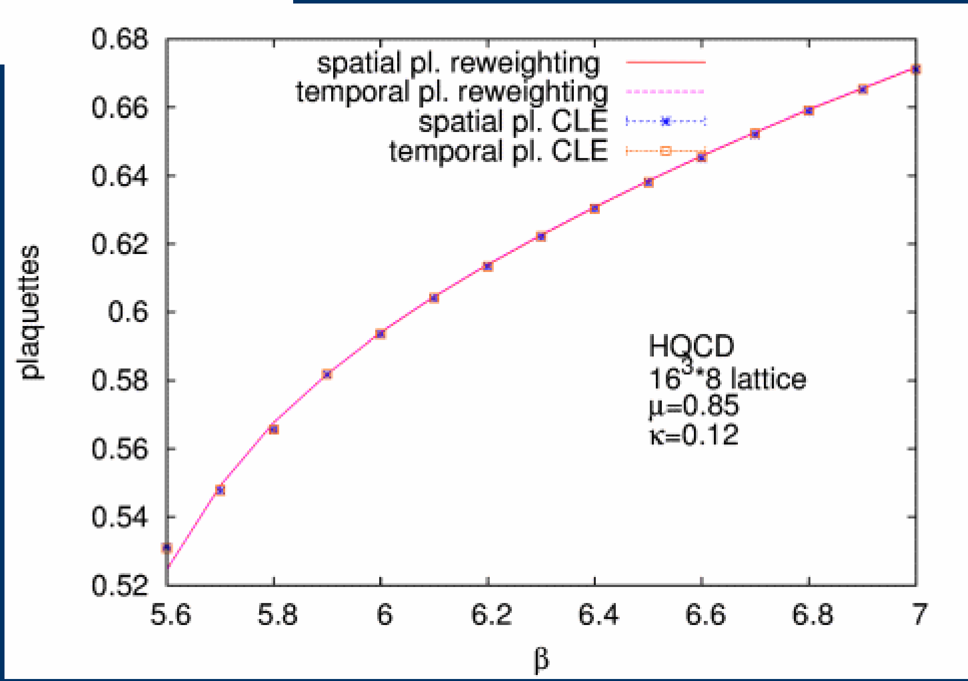


6^4 lattice, $\mu = 0.85$

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

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



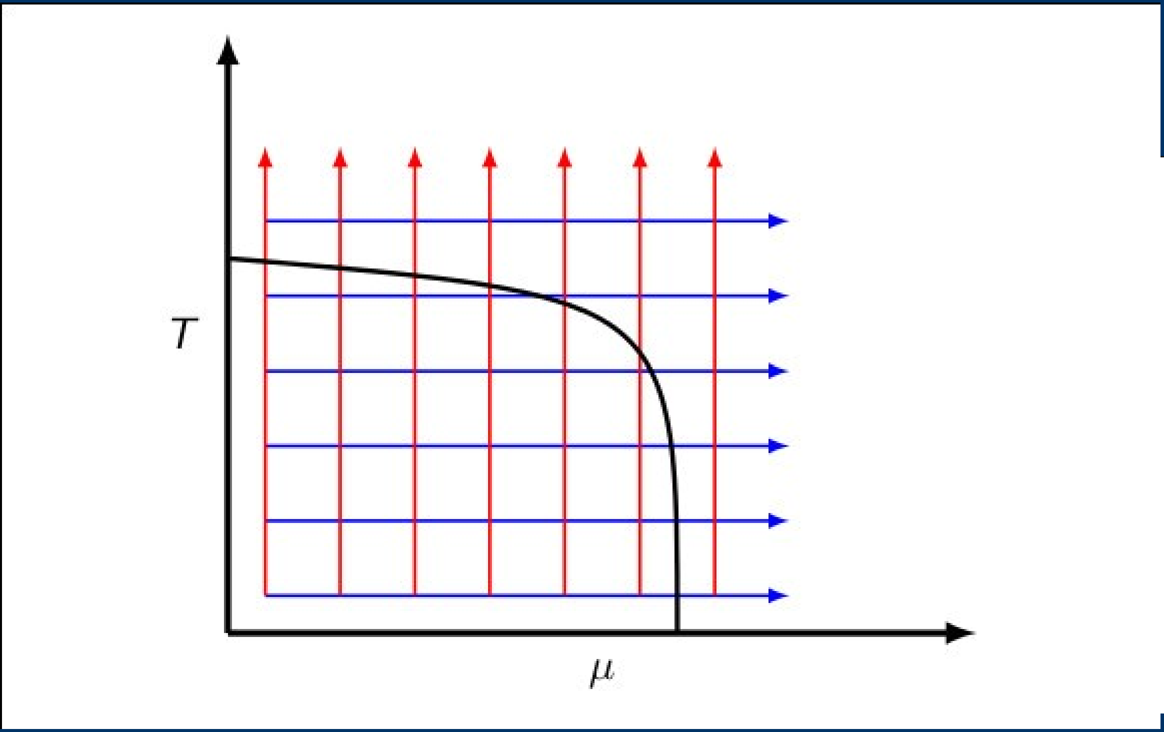


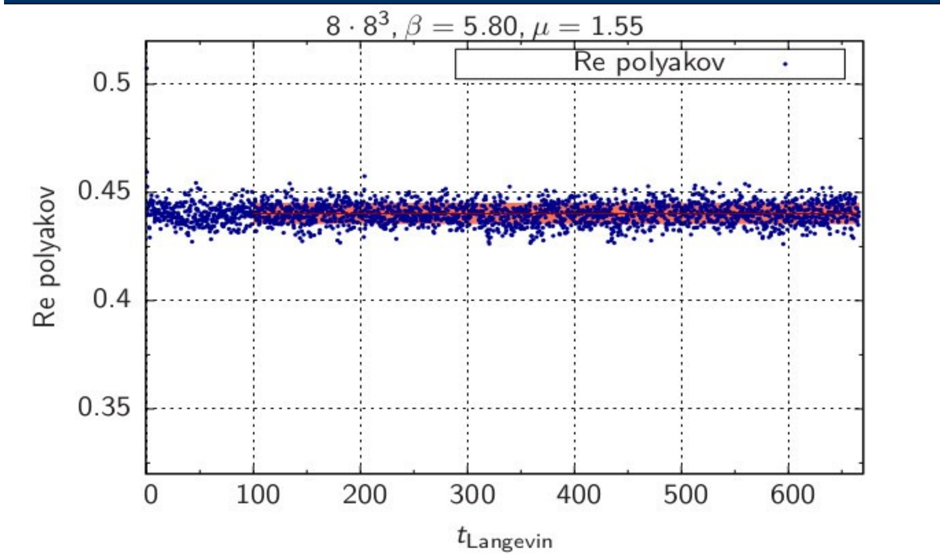
Large lattice:
phase transition clearly visible

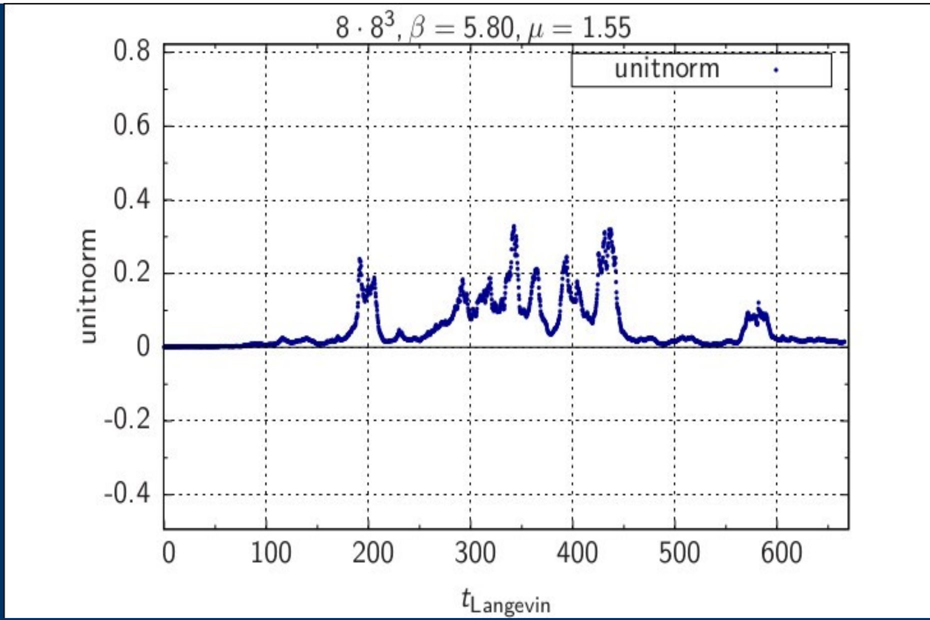
for $\beta > \beta_{min}$

Mapping the phase diagram

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







fixed $\beta = 5.8$ → $a \approx 0.15\,\text{fm}$

$\kappa = 0.12$

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

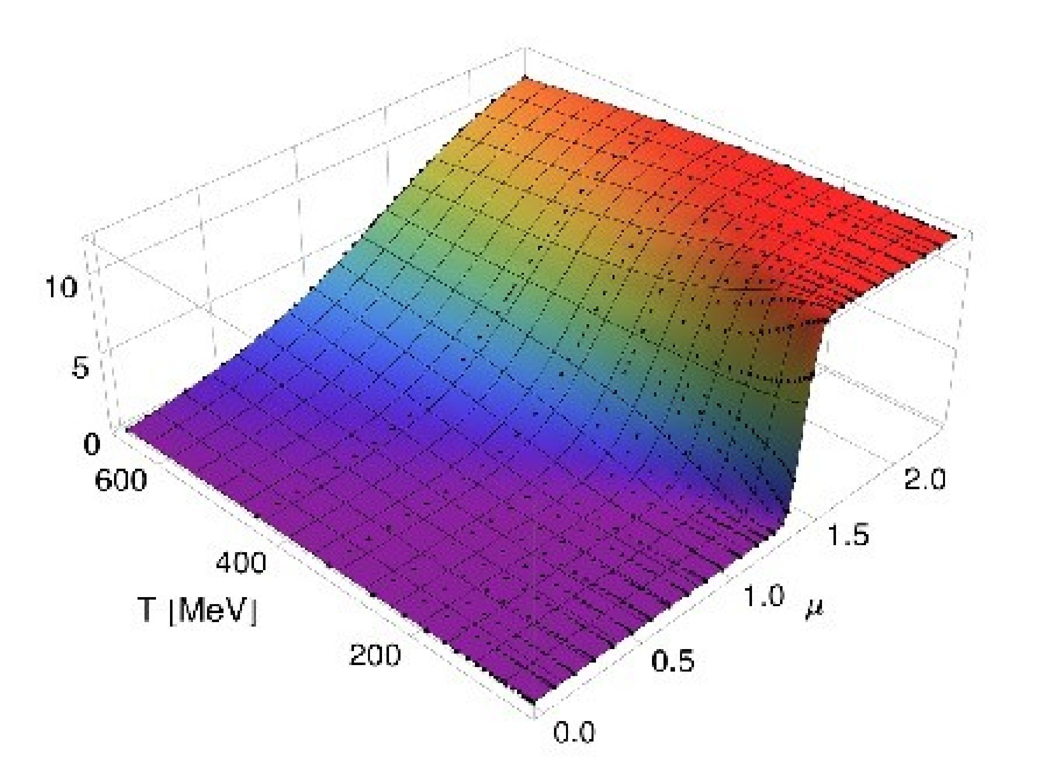
$N_t * 8^3$ lattice

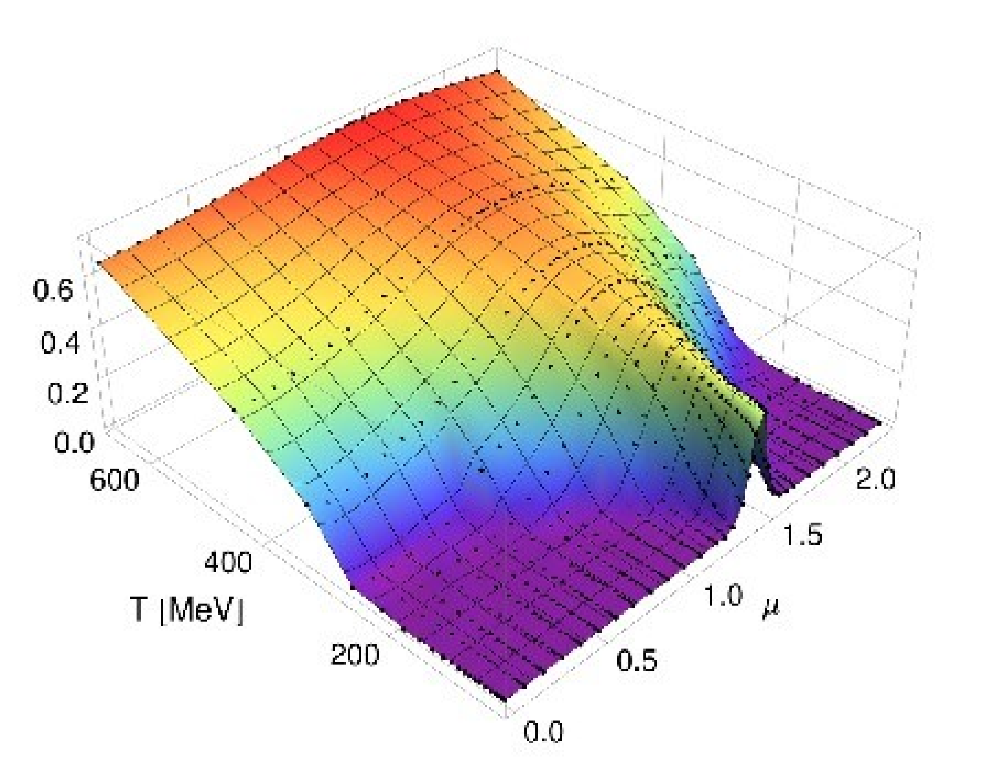
$N_t = 2..28$

Temperature scanning

Phase diagram in HDQCD

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



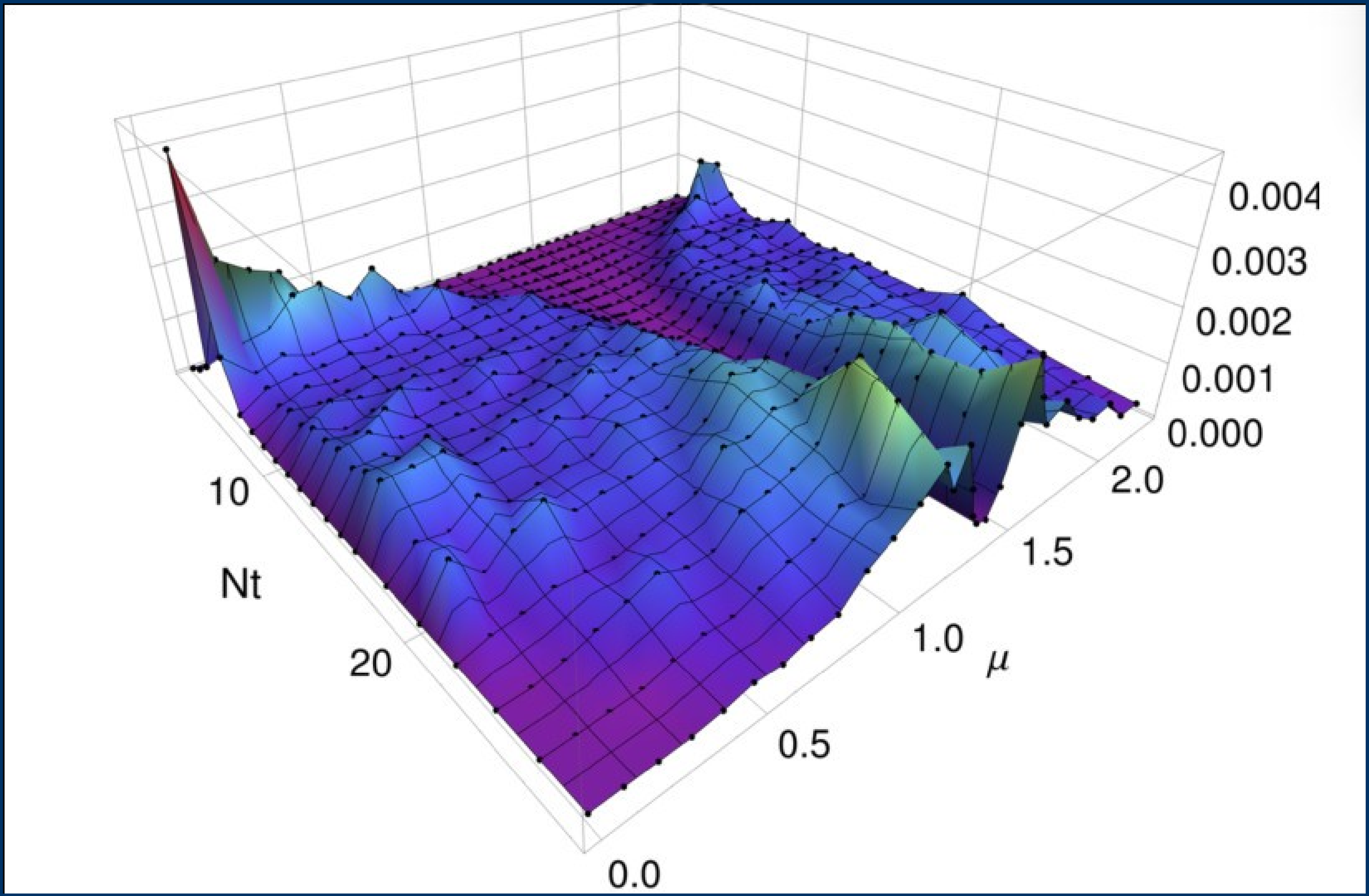


Onset in fermionic density
Silver blaze phenomenon

Polyakov loop
Transition to deconfined state

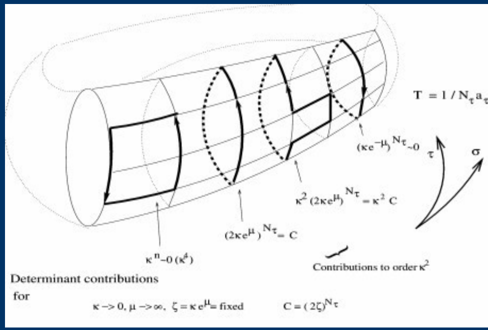
$\beta = 5.8 \quad \kappa = 0.12 \quad N_f = 2 \quad N_t = 2 \ldots 24$

Polyakov loop susceptibility

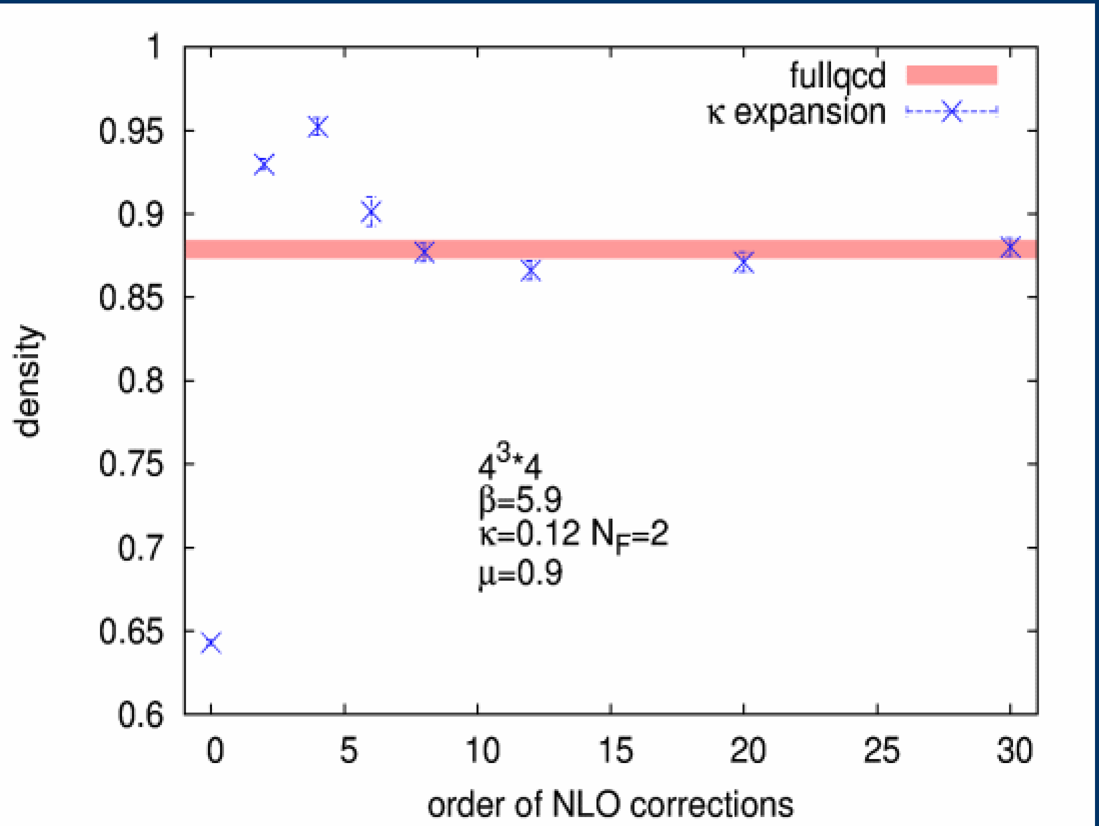


Hint of first order deconfinement and first order onset transition

κ_s Expansion



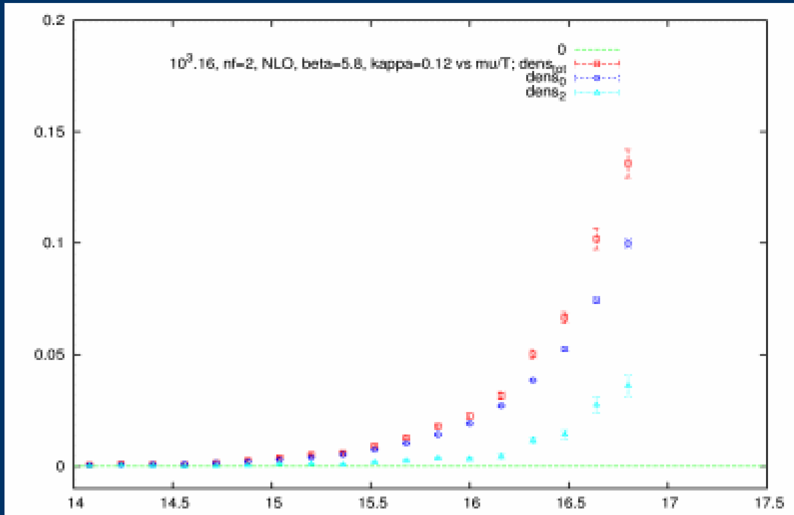
HDQCD $\kappa_s = 0$ → κ_s expansion → full QCD



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

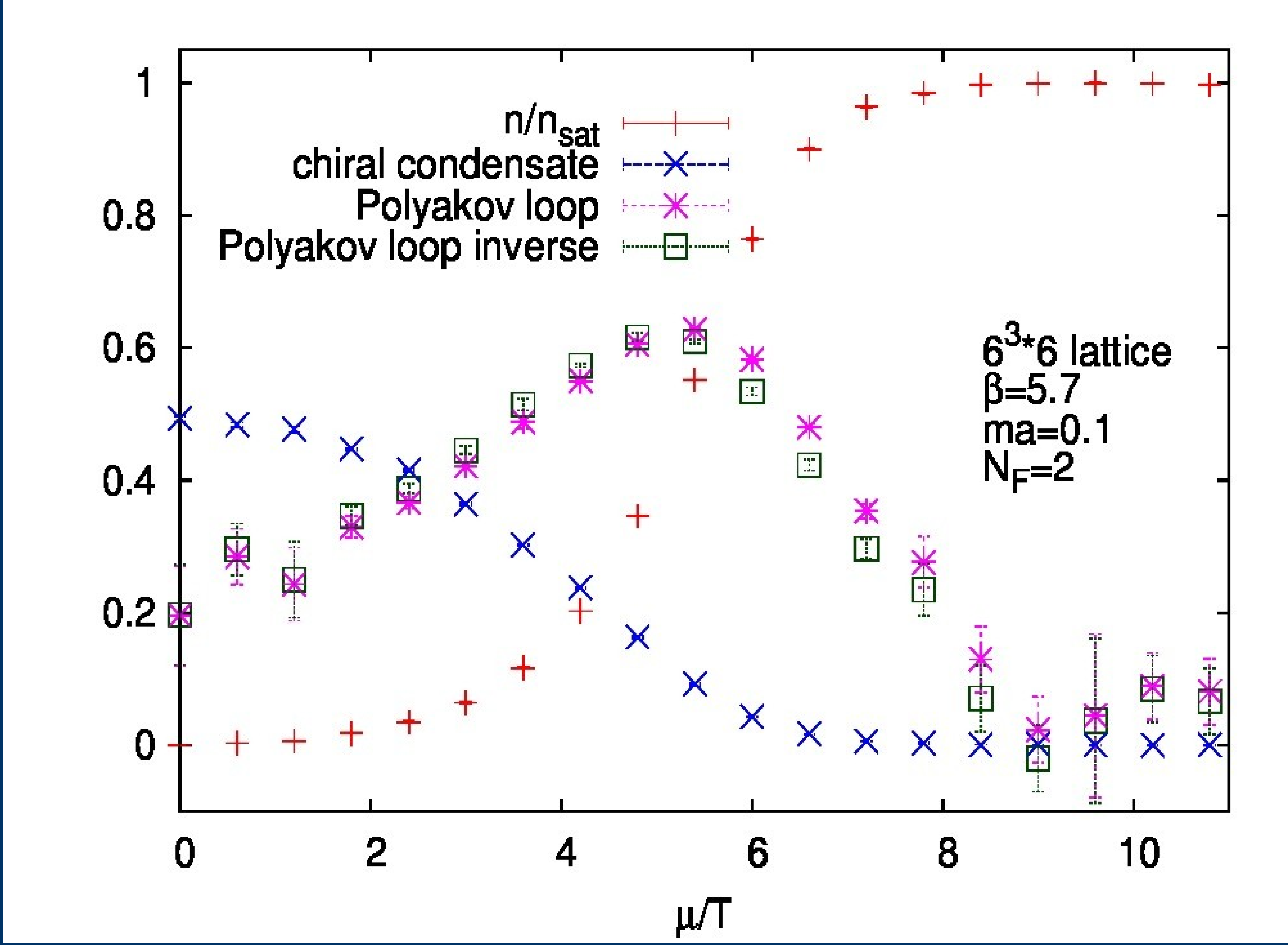
$$K^F_{ax\nu}=\frac{N_F}{4}D_{ax\nu}\ln\det M=\frac{N_F}{4}\mathrm{Tr}\left(M^{-1}M'_{\nu a}(x,y,z)\right)$$

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



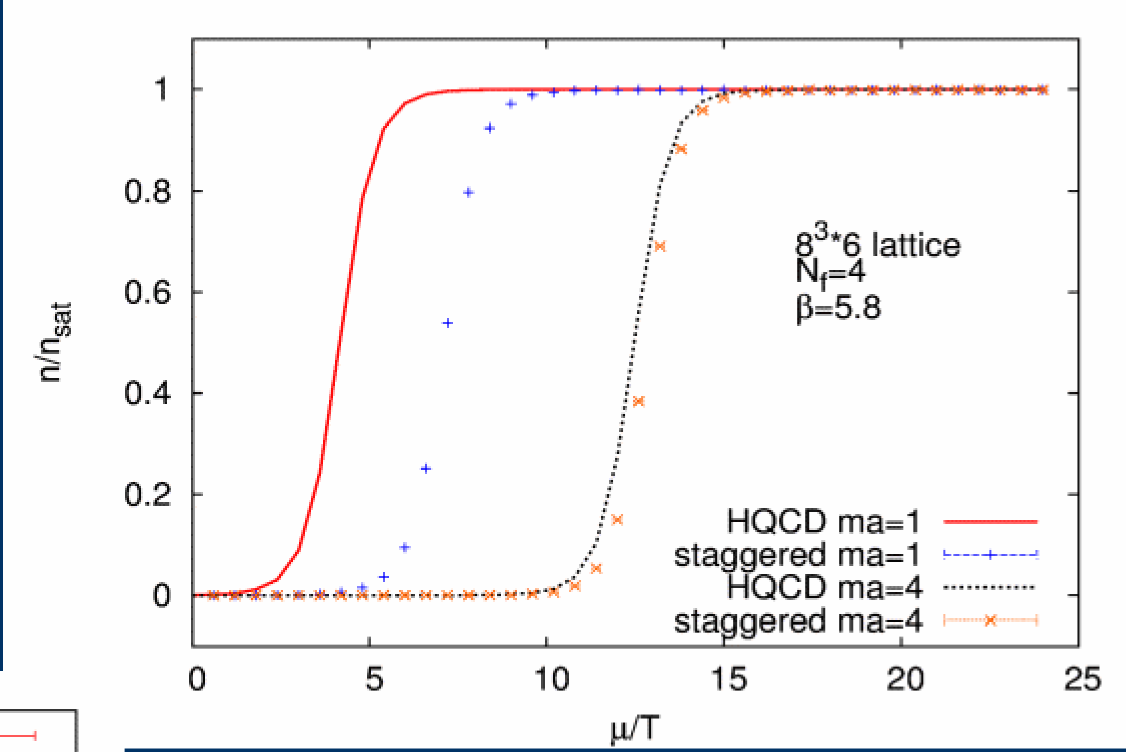
High temperature $T > T_c$

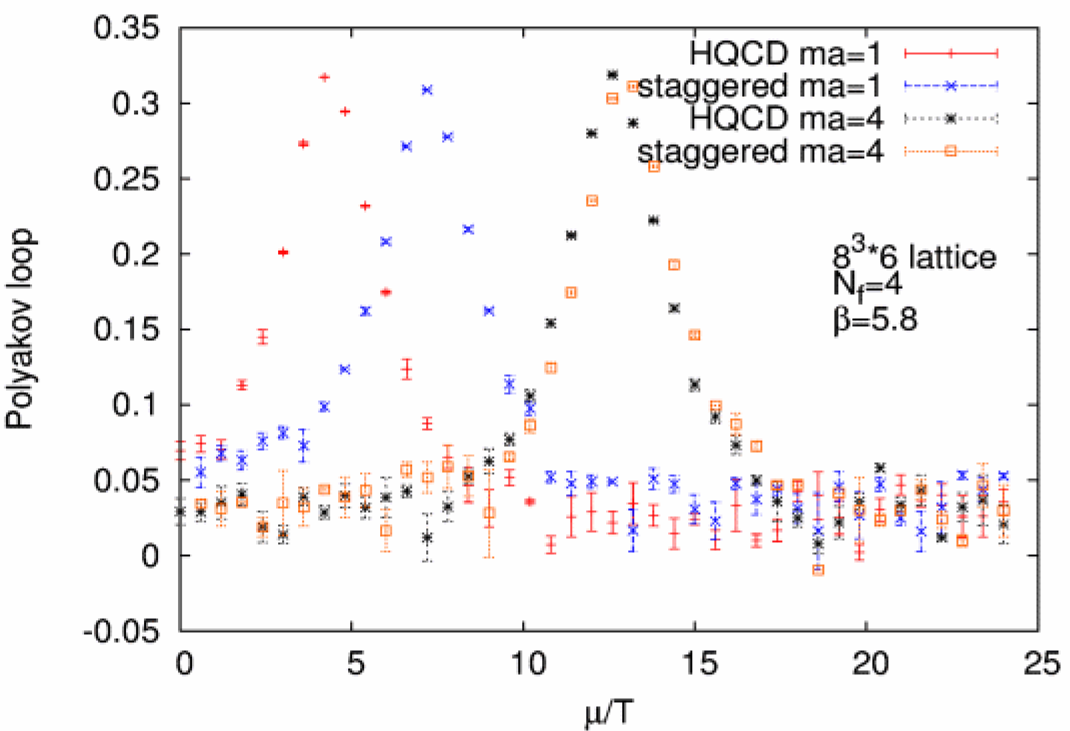
In saturation Z_3 symmetric pure gauge theory is recovered

Comparison of HDQCD in LO and full QCD

Similar behaviour at intermediate masses

Quantative agreement at high masses

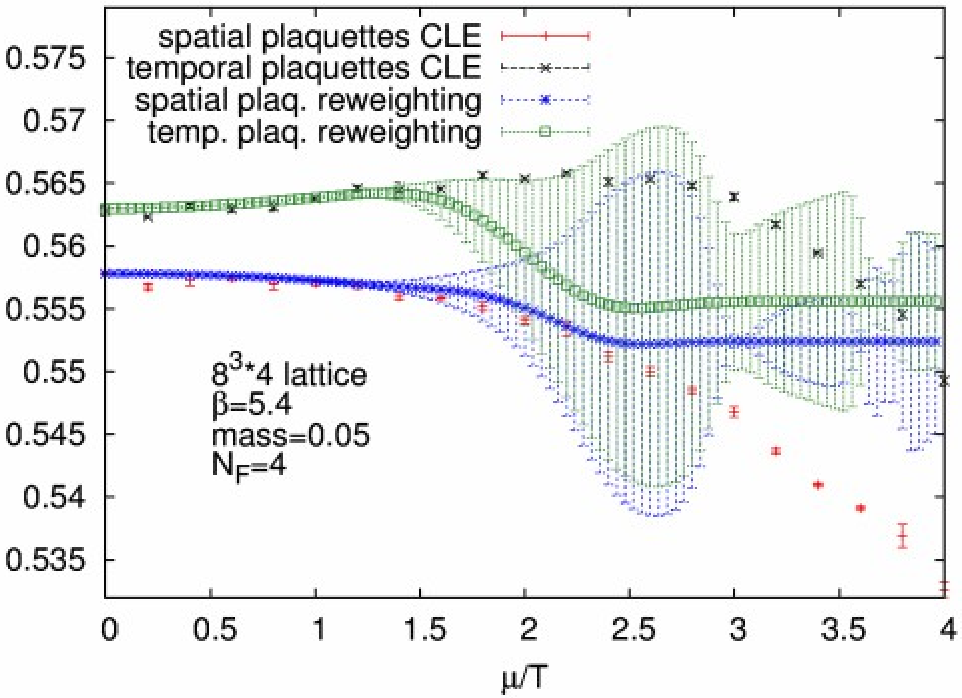


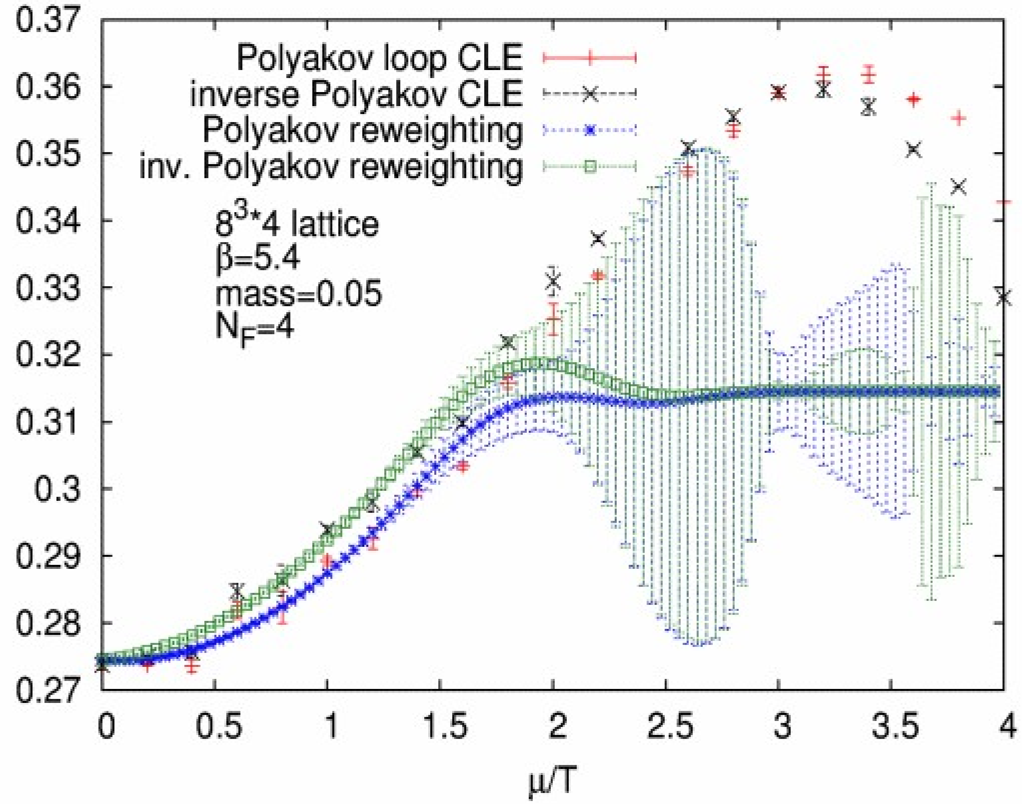


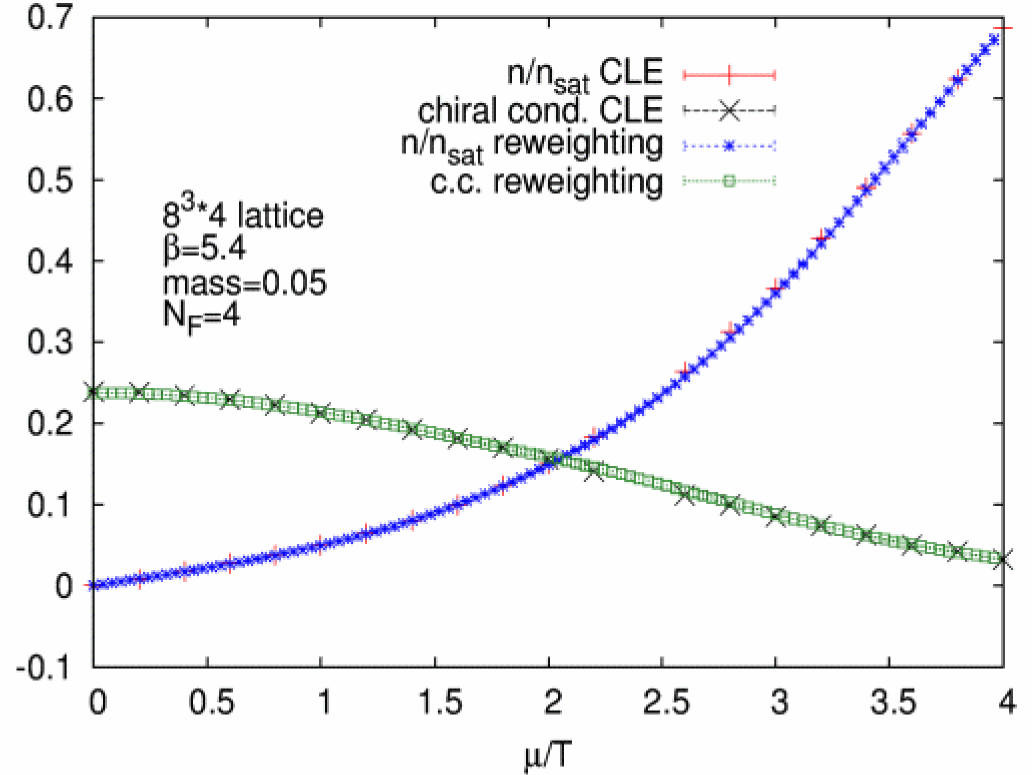
Comparison with reweighting for full QCD

Reweighting from ensemble at

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



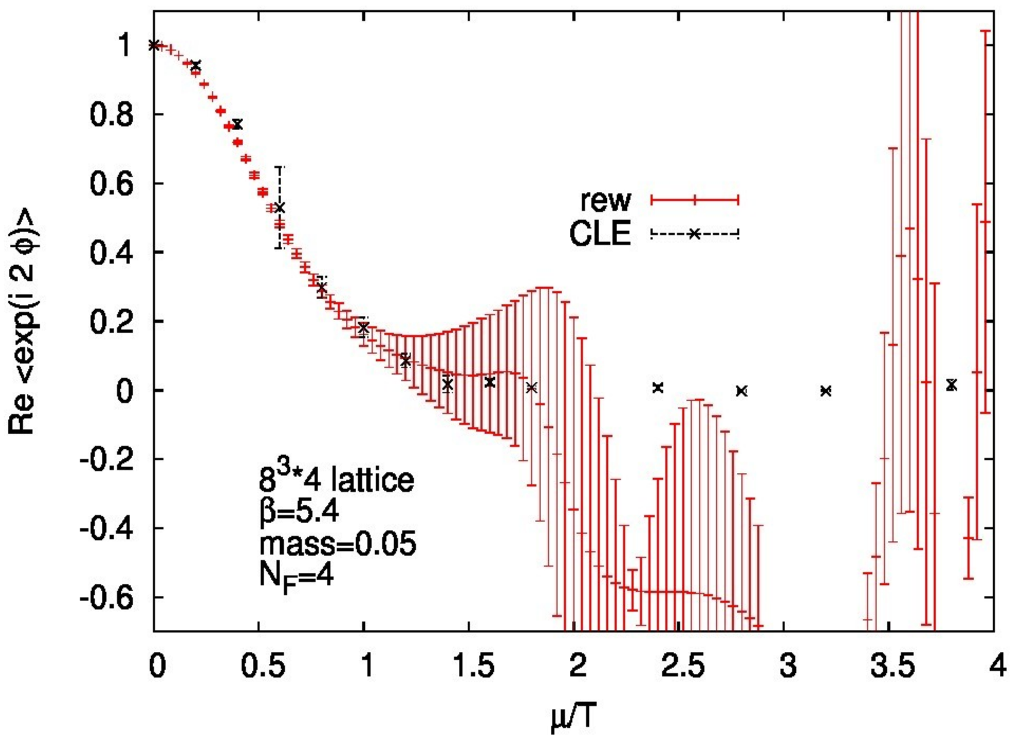


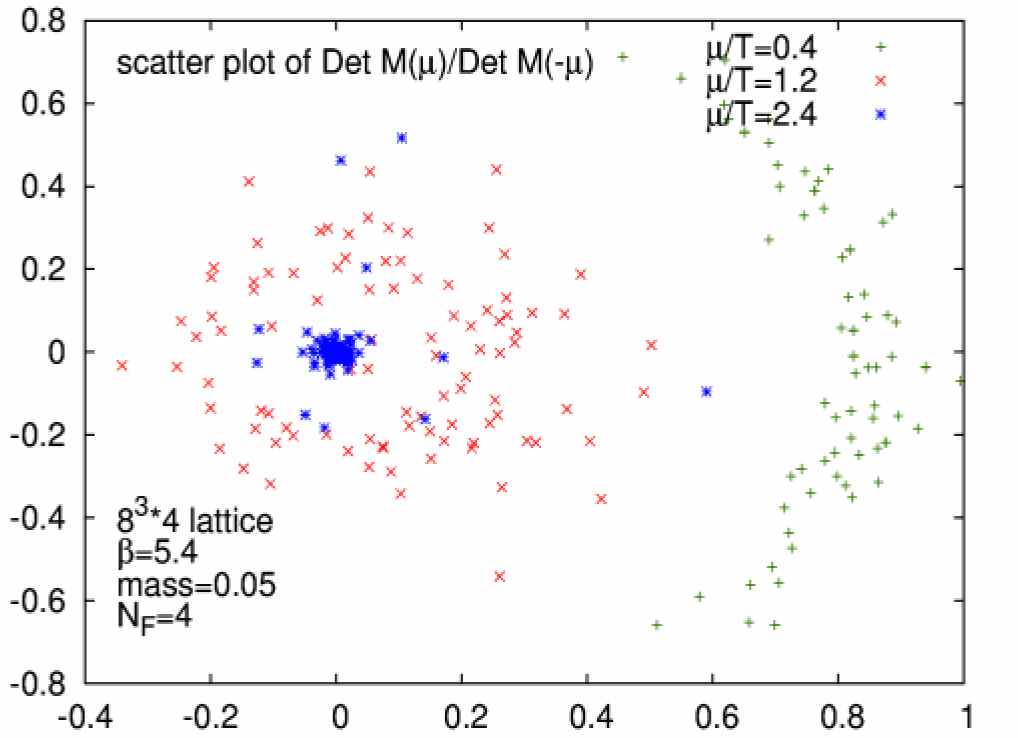


[Fodor, Katz, Sexty (in prep.)]

Sign problem

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

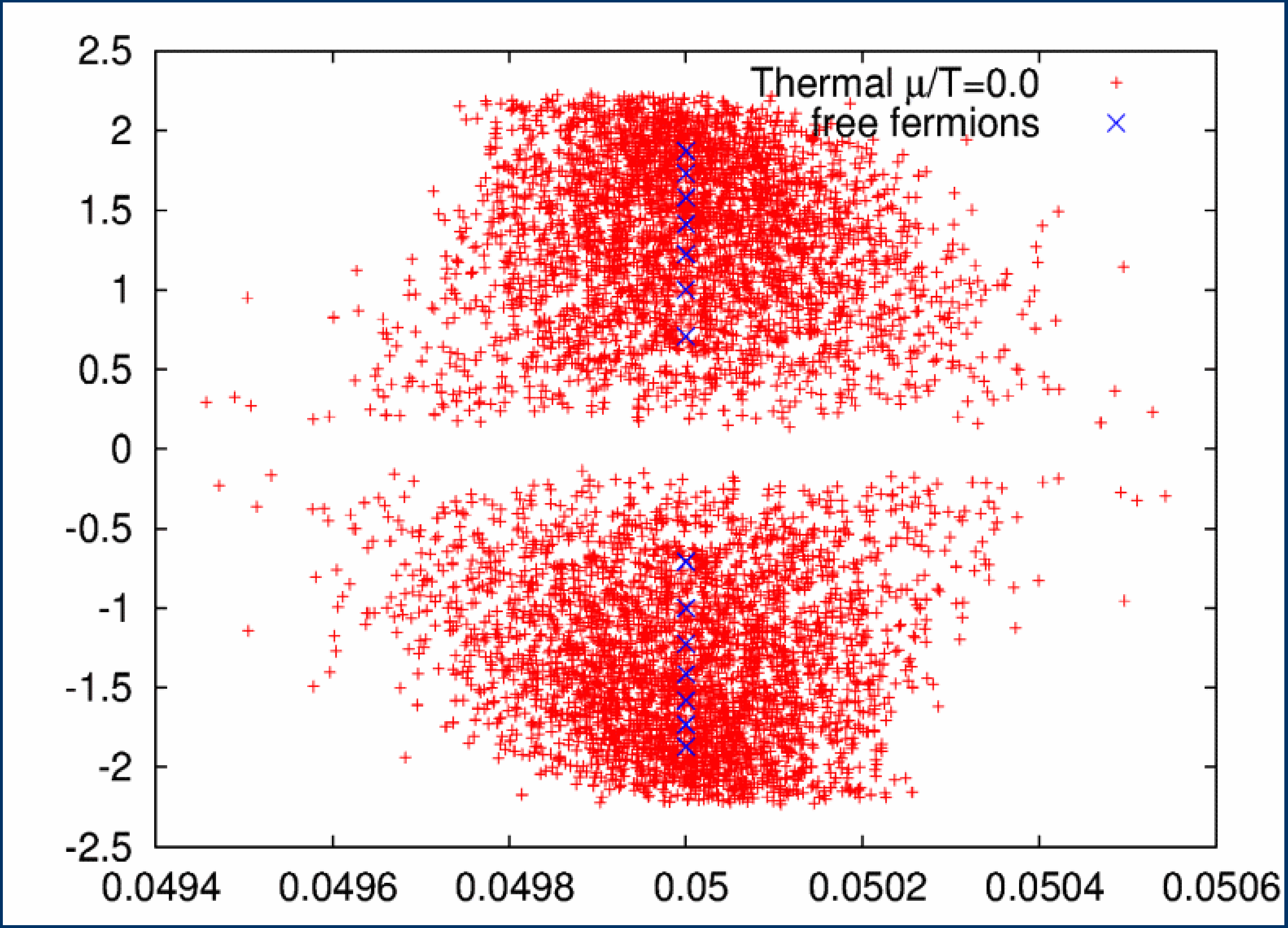




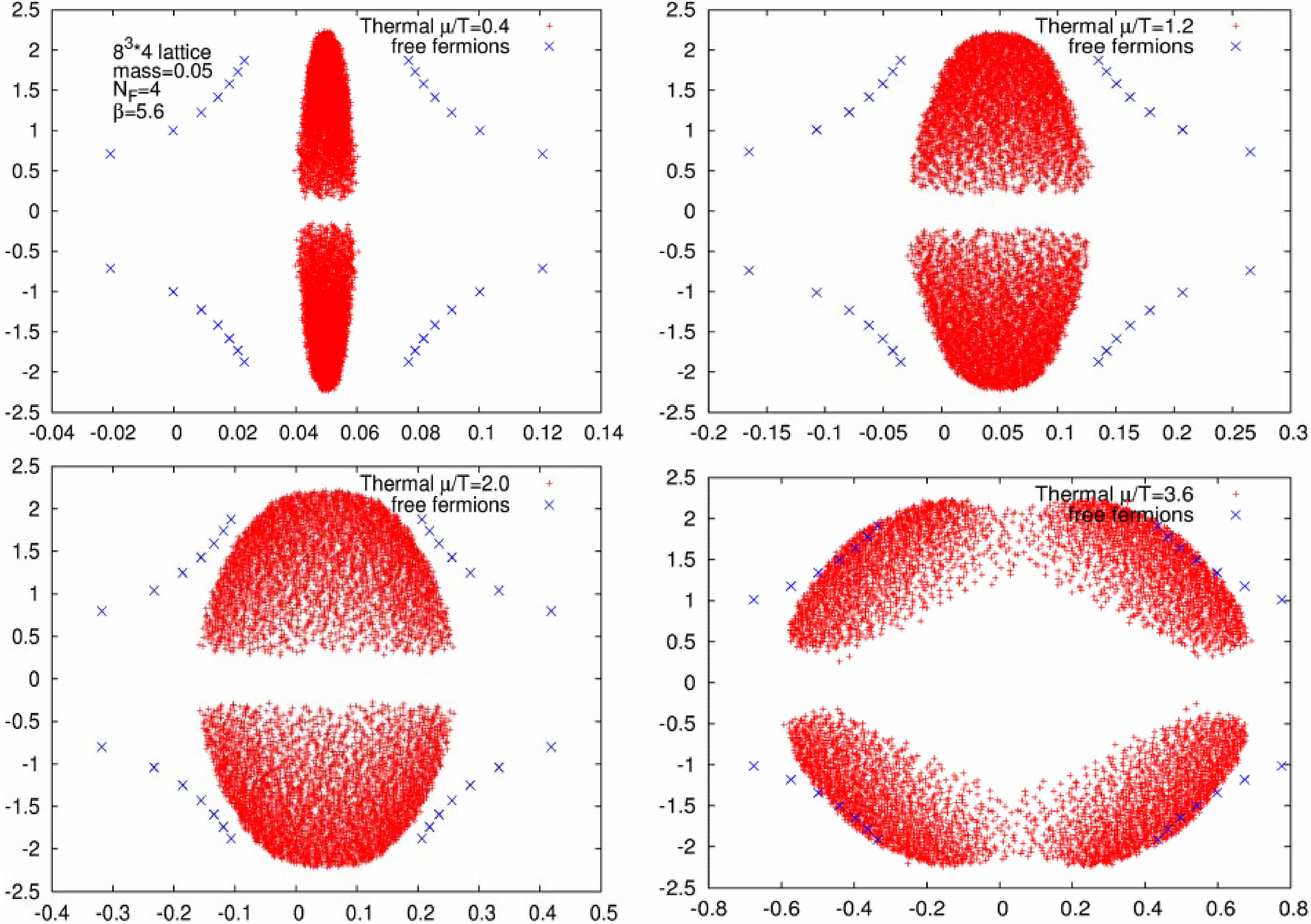
$$\langle \exp(2 i \varphi) \rangle = \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle$$

Spectrum of the Dirac Operator $N_F = 4$ staggered

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



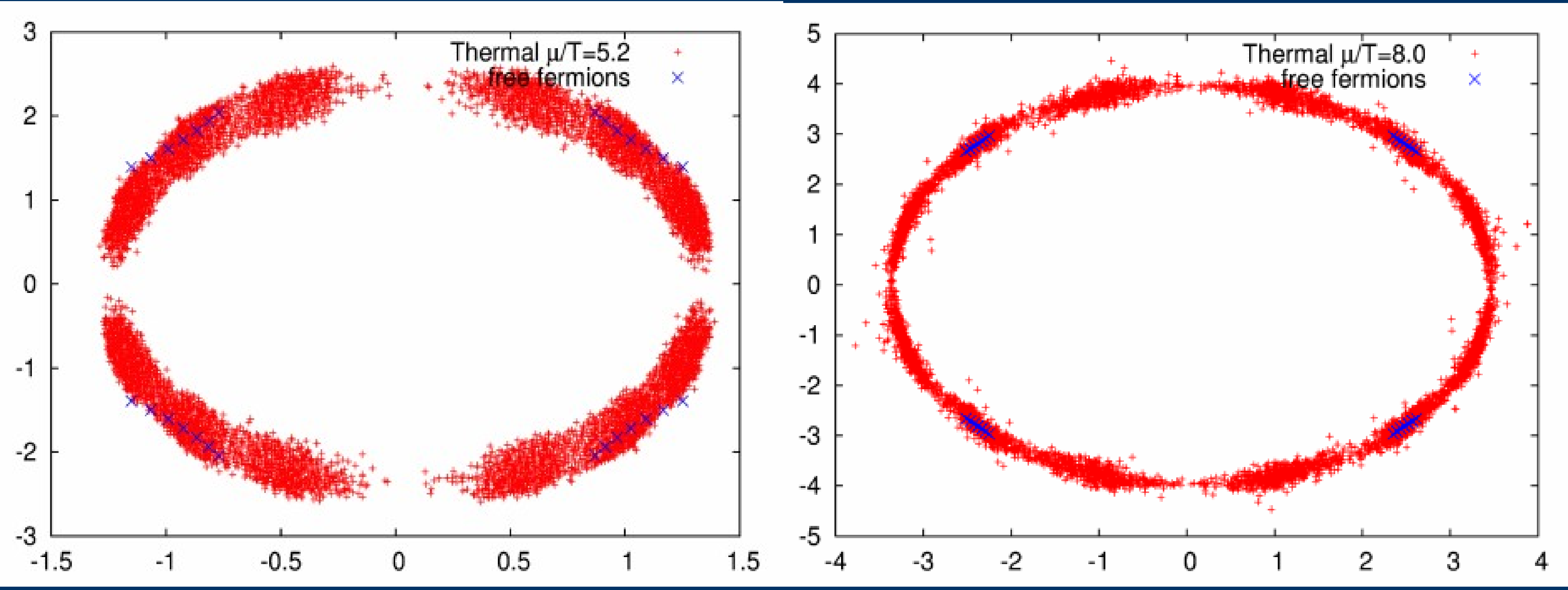
Spectrum of the Dirac Operator $N_F = 4$ staggered



Spectrum of the Dirac Operator

Large chemical potential, towards saturation

Fermions become "heavy"



Conclusions

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

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