Approaching finite density QCD using Complex Langevin Simulation

I.-O. Stamatescu (Heidelberg)

Results in the frame of common work with:

G. Aarts (Swansea), E. Seiler (Munich) and D. Sexty (Heidelberg)

and further collaboration with

L. Bongiovanni and J. Pawlowski (Heidelberg).

SIGN 2014, Darmstadt

Two main topics: Set Up and Applications.
Summarize and give some further results to Denes Sexty's and Erhard Seiler's talks.

Items of the discussion

1. (Very) brief introduction
2. CLE: set up, proofs and problems
3. Tests in effective models
4. Gauge Cooling
5. Analysis of HDQCD
6. Discussion

1. Introduction

Langevin Equation.

Real Langevin simulations are comparable with MC, step size dependence is below statistical errors.

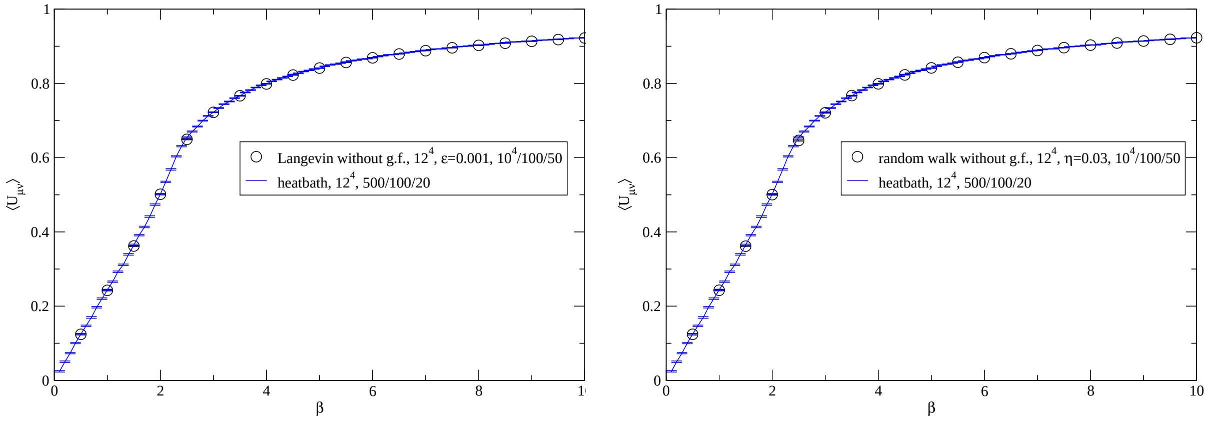


Figure 1: Plaquette averages by LE and RW compared with MC

General discussion and application to Gauge Theory: *G. Batrouni, G. Katz, A. Kronfeld, G. Lepage, B. Svetitsky, K. Wilson (1985)*

Extension to Complex Langevin is possible, since the process needs no probability interpretation of the measure.

Much work since the original papers of *Parisi* and of *Klauder (1983)*, both theoretical and aplicative, here only a few:

H. Hueffel, H. Rumpf, PLB 1984; F. Karsch, H. Wyld, PRL 1985; H. Gausterer, J. Klauder, PRD 1986; T. Matsui, A. Nakamura, 1986; J. Ambjorn, M. Flensburg, C. Peterson, NPhB 1986; J. Flower, S. Otto, S. Callahan, PRD 1986; M. Fukugita, Y. Oyanagi, A. Ukawa, PRD 1987; K. Okano, L. Schulke, B. Zheng PLB 1991; K. Fujimura, K. Okano, L. Schulke, K. Yamagishi, B. Zheng, NPhB 1994; ...

Interest went down when difficulties appeared.

New interest in connection with problems for which no other general solution is available: non-eqilibrium QFT, QCD at non-zero density, ...

The present general work and our working programme :

1. Theoretical discussion [A, 3].
2. Study the various aspects of the problem on simple, soluble models used as effective models, Random matrices, Thirring model [A, 1, 2, 4].
3. Extend the analysis to more complex models with non-trivial phase structure XY-model, $SU(3)$ spin model [A].
4. Extend the analysis to full QCD-approximations (HDQCD) [A, 5].
5. Study full QCD [A].

Our group [A, many papers since 2008] and *beyond: C. Pehlevan, G. Guralnik, NPhB 2009* [1]; *J. Pawlowski, C. Zielinski, PRD 2013* [2]; *A. Duncan, M. Niedermaier, Ann.Ph. 2013* [3]; *A. Mollgaard, K. Splittorff, 2013* [4]; *M. Fromm, J. Langelage, S. Lottini, O. Philipsen, JHEP 2012* [5] ...

2. CLE: the drunkard's complex walk ...

Complex action $\longrightarrow$ complex drift $K(z) = -\nabla_z S$, $\longrightarrow$ imaginary parts for the variables $\longrightarrow$ Process on the complex extension of the original manifold: $z(t) = x(t) + i\, y(t)\ ,\ x \in \mathcal{M}_r\ ,\ z \in \mathcal{M}_c$

The processe realizes a positive probability distribution $P(x, y)$.

Formal equivalence theorem: for analytic observables $O(x, y)$ the averages over the process reproduce the ensemble averages with the (complex!) distribution $\rho(x) = \exp(-S(x))$: $\langle \mathcal{O} \rangle_{P(t)} = \langle \mathcal{O} \rangle_{\rho(t)}$,

As with every numerical method the formal proof of equivalence relies on certain conditions to be fulfilled, here in particular:
1) holomorphy of the drift and of the observables,
2) sufficient fall off of $P(x, y)$ in the $y-$direction.

Cf Erhard Seiler's talk.

Notice: there are many processes $K(z)$ ($P(x, y)$) leading formally to the desired EV's. This can be used in controlling the method.

Possible sources of wrong evolution:

"Practical problems":

1. Accumulation of numerical errors. Typical effect: run-aways, divergence of some quantities. $K(z)$ becomes unbounded.

2. Unprecize sampling - in the presence of trajectories of $K(z)$ going far in the y direction.

"Problems of principle":

3. Unsufficient fall off of $P(x, y)$ in the y direction - can spoil the formal proof of equivalence.

4. Non-holomorphy of the drift. Can invalidate the formal proof of equivalence. Typical for us: poles of $K(z)$ (zeroes of $\rho(z)$).

We have approached these problems one after the other.

We defined *Consitency Conditions* and other signals of wrong evolution.

We found solutions to most of the problems what allowed us to start physical applications.

Solutions:

1. Run-aways: efficiently eliminated by adaptive step size.

2./3. Unprecize sampling and Skirts- unsufficient fall off of $P(x, y)$: constrain the distribution $P(x, y)$ by performing allowed changes of the process (without affecting the expectation values).

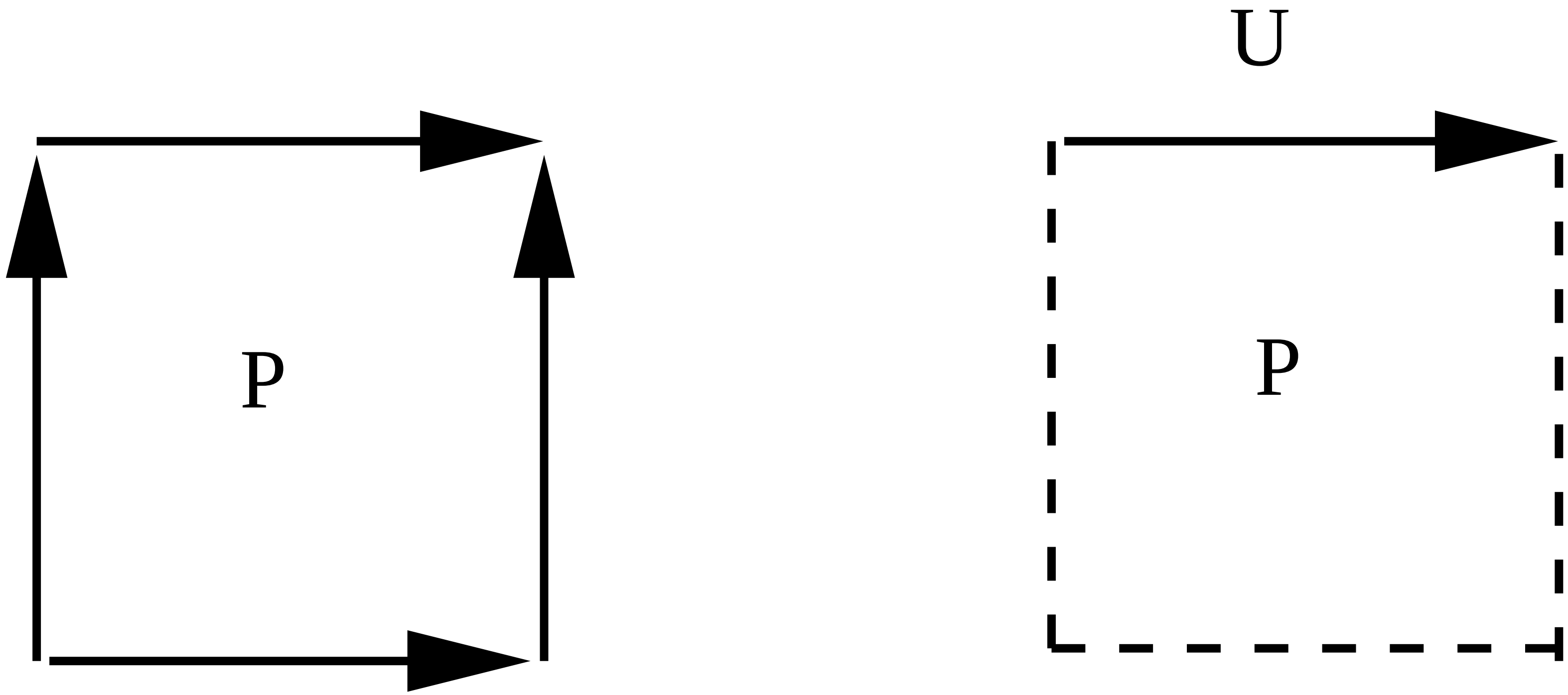
4. Meromorphic drift: In realistic cases (e.g., QCD) the poles do not seem to raise difficultiess, at least in the region of physical interest. However, we want to arrive at a systematic way to handle this problem, (at present: only partial results). *(cf E. Seiler's talk)*

3. Learning from tests in effective models

Skirts and numerical imprecisions

In the following we shall stick to SU(3) $\longrightarrow$ SL(3,C). aiming at QCD with chemical potential.

The one link SU(3) reduced model



Effective model for QCD: one link in the field of its neighbors.

$$-S = \frac{\beta}{2}\left(\mathrm{tr}UA + \mathrm{tr}A^{-1}U^{-1}\right) + \ln D + \ln \tilde{D} \quad (1)$$

$$D = 1 + C\mathrm{tr}U + C^2\mathrm{tr}U^{-1} + C^3, \quad C = 2\kappa \mathrm{e}^{\mu} \quad (2)$$

$$\tilde{D} = 1 + \tilde{C}\mathrm{tr}U^{-1} + \tilde{C}^2\mathrm{tr}U + \tilde{C}^3, \quad \tilde{C} = 2\kappa \mathrm{e}^{-\mu} \quad (3)$$

The matrices $A \in GL(3, C)$ simulate the staples, $D\tilde{D}$ the determinant.

After "Cartan" reduction:

$$-S = \frac{\beta}{2}\sum_{i=1}^{3}\left(\alpha_i e^{iw_i} + \alpha_i^{-1} e^{-iw_i}\right) + \ln D + \ln\tilde{D} + f\ln H \tag{4}$$

$$H = \sin^2\frac{w_2 - w_3}{2}\sin^2\frac{w_3 - w_1}{2}\sin^2\frac{w_1 - w_2}{2}, \;\; w_1 + w_2 + w_3 = 0$$

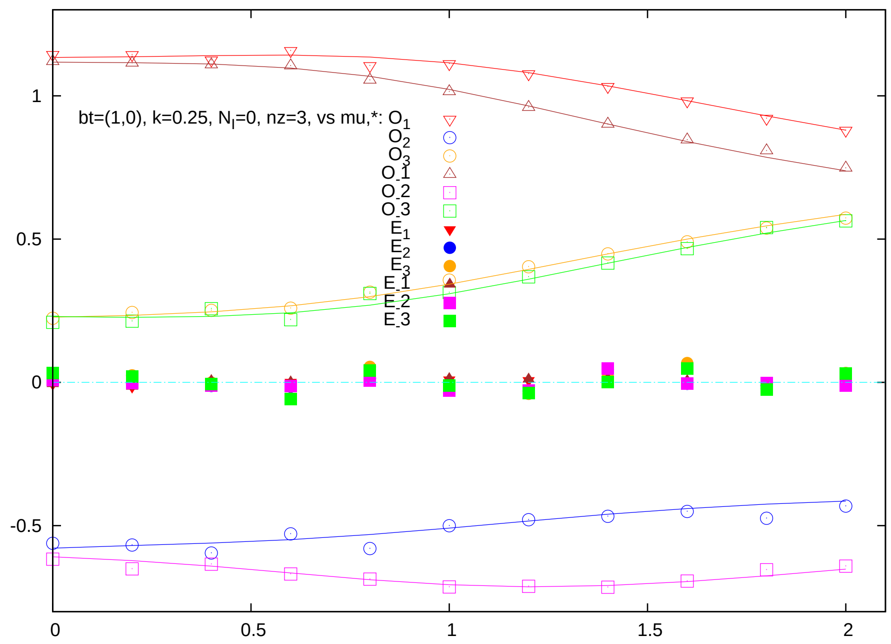
Effect of the neighbors: coded in the complex coefficients α.

Observables and CC conditions :

$$O_n = \mathrm{tr}(\hat{U}^n) = \mathrm{e}^{i\,nw_1} + \mathrm{e}^{i\,nw_2} + \mathrm{e}^{i\,nw_3} \tag{5}$$

$$E_n = \left(\nabla^2 + K\nabla\right) O_n, \;\; K = -\nabla S \tag{6}$$

The process runs in three or (equivalently) two angles, with correspondingly three (two) noise terms.



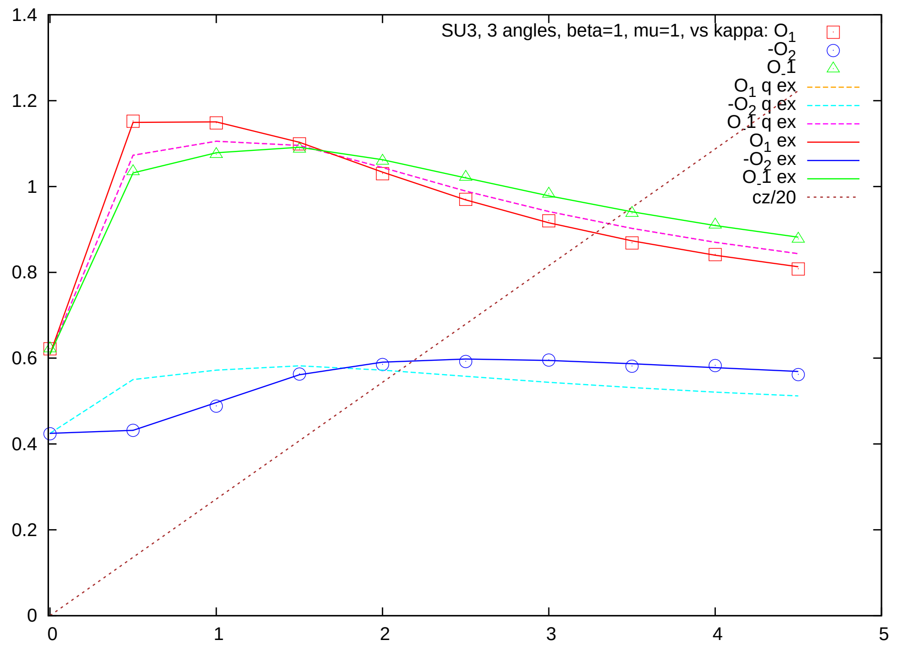
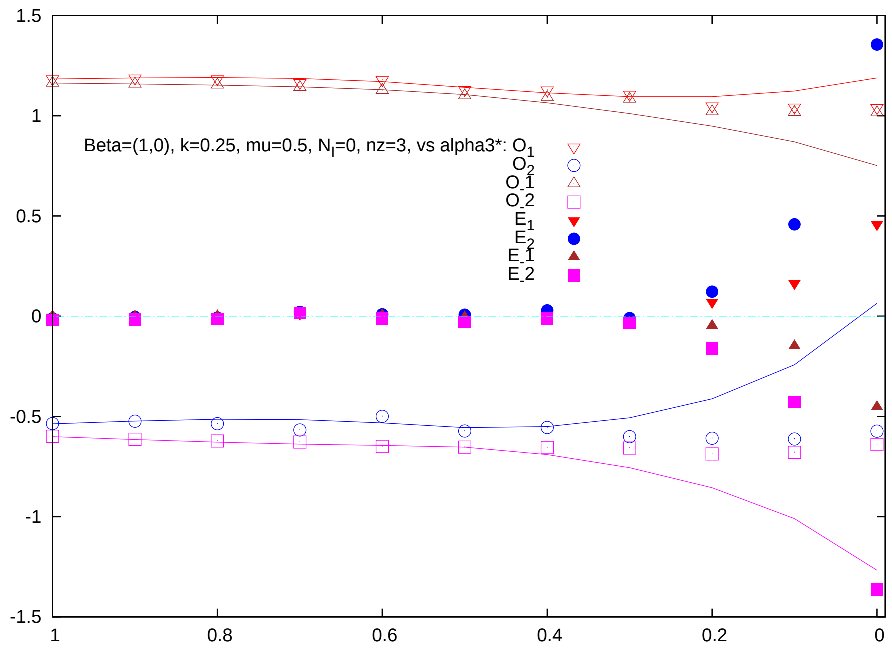


Figure 2: Effective model, $\alpha = 1$. *Left*: Dependence of the observables and CC's on μ. *Right* Dependence of the observables on κ. $O_n = \mathrm{Tr}U^n$.



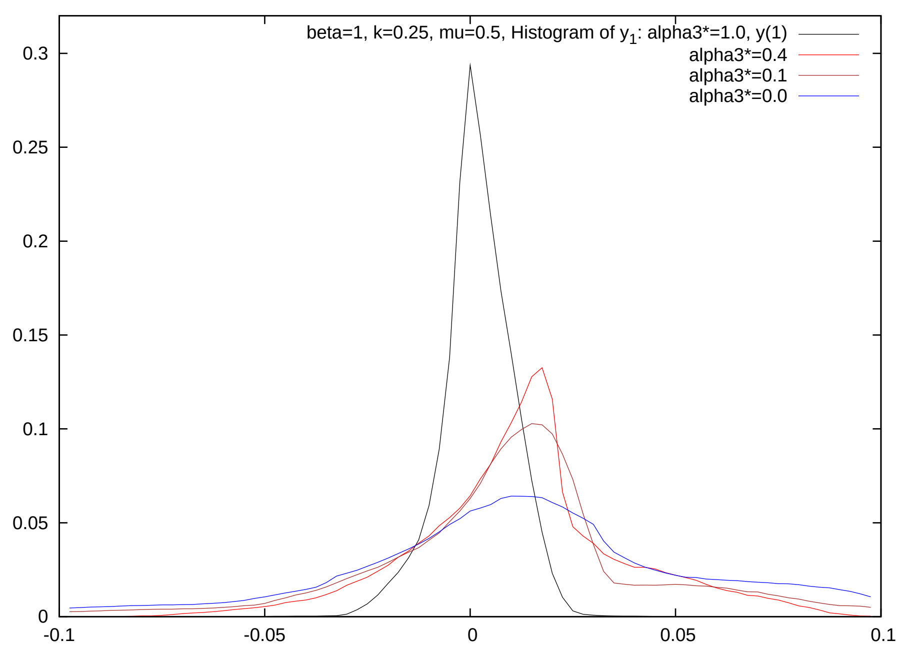
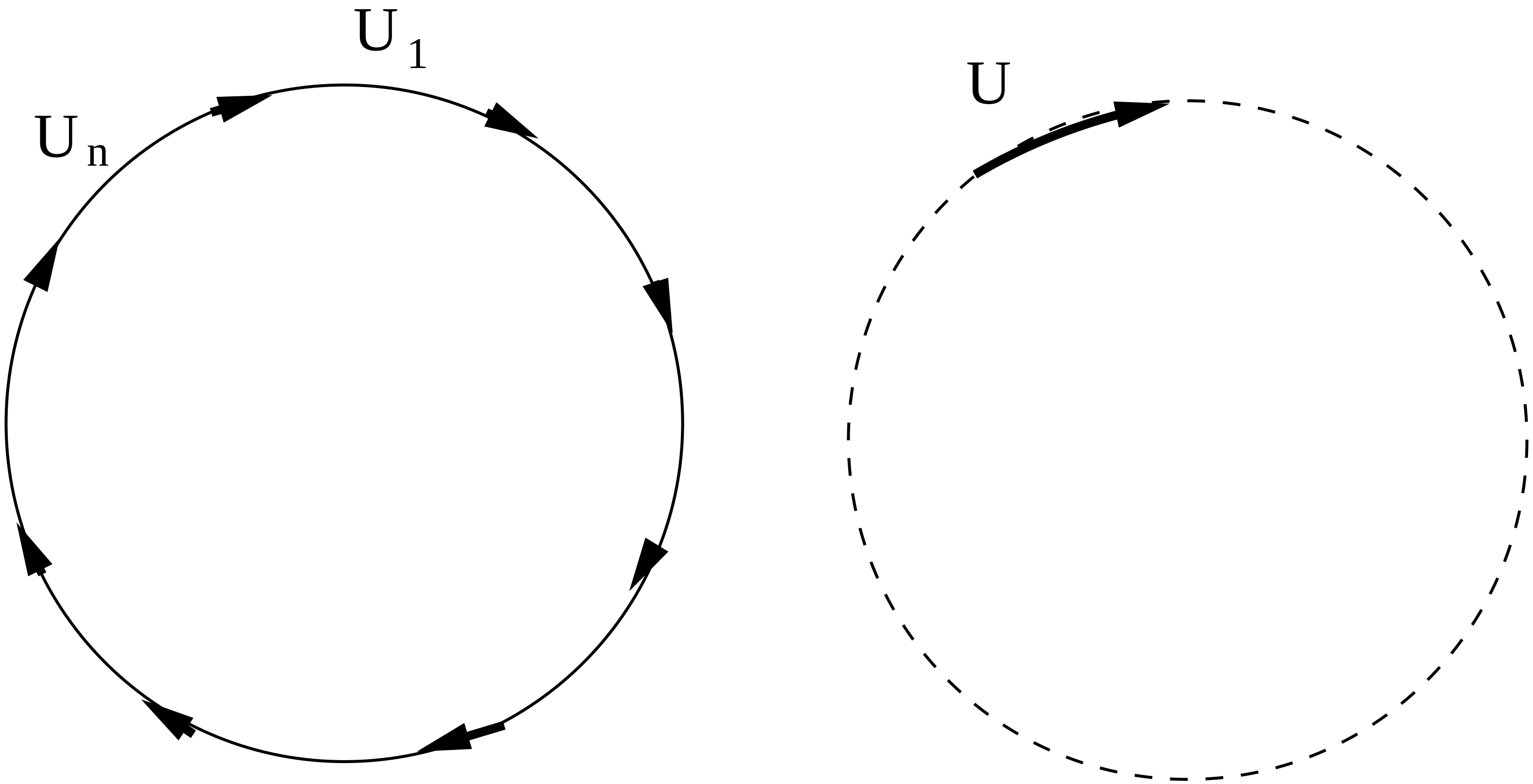


Figure 3: Effective model. *Left*: Dependence of the observables and CC's on Re α_3 (Im α_3 increases correspondingly, $\alpha_{1,2}$ kept fixed at some arbitrary complex values). The violation of the CC's signalizes discrepant results. *Right*: Im w-histograms of the equilibrium measure for different Re α_3. Discrepant results corrrelate with wide skirts.

The Polyakov chain



Many variables (as in lattice theory): closed Polyakov line with n links.

The model is soluble (gauge transformation to 1 link model), but the process is done in n links.

Action :

$$-S = (\beta + 2\,\kappa \mathrm{e}^{\mu})\, Tr\,(U_1 \cdots U_n) + (\beta + 2\,\kappa \mathrm{e}^{-\mu})^*\, Tr\left(U_n^{-1} \cdots U_1^{-1}\right)$$

The process runs in all $8\,n$ (complex) angles, with real noise:

$$\Delta A^a_{i,\mu} = \epsilon K^a_{i,\mu}(U) + \sqrt{\epsilon}\,\eta\ , \quad U_{i,\mu} \longrightarrow \mathrm{e}^{i\,\sum_a \lambda_a\,\Delta A^a_{i,\mu}}\,U_{i,\mu} \tag{7}$$

We observe wrong evolution setting in for large n even for values of the parameters for which at $n = 1$ everything works fine! This effect correlates with wide skirts of the y-distributions.

We learn from these exercises that:

- Wide skirts of the distributions (far diffusing scatter plots) lead to wrong results.

- These effects apparently come from
  - incorrect sampling and accumulation of numerical errors
  - violation of the equivalence proof by boundary terms.

- For *gauge theories* a clear signal of wrong evolution is *uncontrolled departure* from the unitary manifold.

- This suggests using *gauge symmetry* to redesign the process such that it stays as near as possible to the unitary manifold.

4. Gauge cooling

For a correctly evolving process a "unitarity norm" such as $trU\,U^\dagger - 3$ should *converge* to some (generally non-zero) value.

Since the clear symptom of incorrect evolution is the *divergence of the unitarity norm (UN)* we introduce a gauge cooling to minimize the unitarity norm

$$UN \equiv \sum_{links} \left[\frac{1}{2} tr\left(U\,U^\dagger + U^{-1}\,U^{-1\,\dagger} \right) - 3 \right] \tag{8}$$

This succeeds by successive gauge transformations of the links

$$R_k \;=\; e^{-\alpha\,\epsilon\,dS_G}\;,\; U_k \longrightarrow R_k\,U_k\,,\; U_{k-1} \longrightarrow U_{k-1} R_k^{-1} \tag{9}$$

$$dS_G : \text{the gradient of the UN}$$

$$\alpha : \text{the strength of the gaugeforce},\; \epsilon : \text{step size.}$$

Cf. also Denes Sexty's talk.

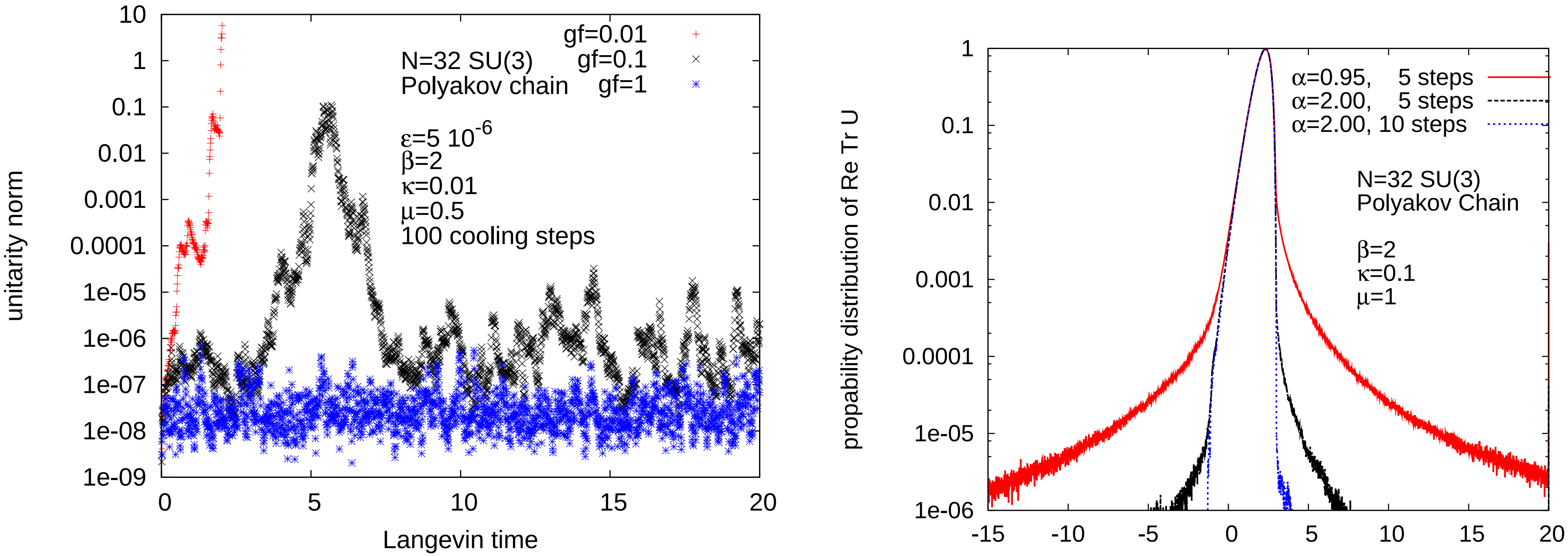


Figure 4: Polyakov chain, $n = 32$. Evolution of the *UN* (*left*), and $y-$ distributions (*right*) for various coolings ($gf \equiv \alpha$). Divergent *UN* correlates with wide skirts in the distributions.

Notice:

- Gauge Cooling is a general method for $SL(n, C)$ gauge theories.
- It *modifies* the CLE process. It can be realized as gauge transformations interspersed with the CLE process **or** as additional drift in the process *along* the gauge orbits - akin with stochastic gauge fixing.
- It does not change the observables but *"repairs"* the process, that is, the sampling of the observables.
- It must not be confused with usual cooling, since it does not change gauge independent quantities, in particular the action.

5. Lattice QCD with chemical potential, HD approximation, Wilson fermions

Hopping parameter expansion (loop expansion)

Smit, Kawamoto (1982), IOS (1982):

$$\begin{aligned} \mathrm{Det}\, W &= \exp(\mathrm{Tr} \ln W) \\ &= \exp\left[-\sum_{l=1}^{\infty} \sum_{\{\mathcal{C}_l\}} \sum_{s=1}^{\infty} \frac{\left(\kappa_\lambda^l g_{\mathcal{C}_l}\right)^s}{s} \mathrm{Tr}_{\mathrm{D,C}} \mathcal{L}_{\mathcal{C}_l}^s \right] \\ &= \prod_{l=1}^{\infty} \prod_{\{\mathcal{C}_l\}} \mathrm{Det}_{\,\mathrm{D,C}} \left(1 - (\kappa_\lambda)^l g_{\mathcal{C}_l} \mathcal{L}_{\mathcal{C}_l}\right) \end{aligned} \tag{10}$$

with $\mathcal{C}_l$ a closed, non-self-repeating path, λ the links on $\mathcal{C}_l$ and

$$\mathcal{L}_{\mathcal{C}_l} = \left(\prod_{\lambda \in \mathcal{C}_l} \Gamma_\lambda U_\lambda \right)^s, \; g_{\mathcal{C}_l} = \left(\epsilon\, \mathrm{e}^{\pm N_\tau \mu_f}\right)^r \tag{11}$$

with non-trivial $g_{\mathcal{C}_l}$ for loops winding r times in the ± 4 direction with periodic(antiperiodic) b.c. ($\epsilon = +1(-1)$) and $\kappa_\lambda = \kappa$ or $\kappa\,\gamma$.

The lattice HDM-QCD model *I. Bender, T. Hashimoto, F. Karsch, V. Linke, A. Nakamura, M. Plewnia, IOS, W. Wetzel*, 1991:

In the limit $\kappa \to 0,\ \mu \to \infty,\ \ \zeta = \kappa\, \mathrm{e}^{\mu}\ : \mathit{fixed}$ only Polyakov loops survive in the loop expansion and the determinant factorizes.

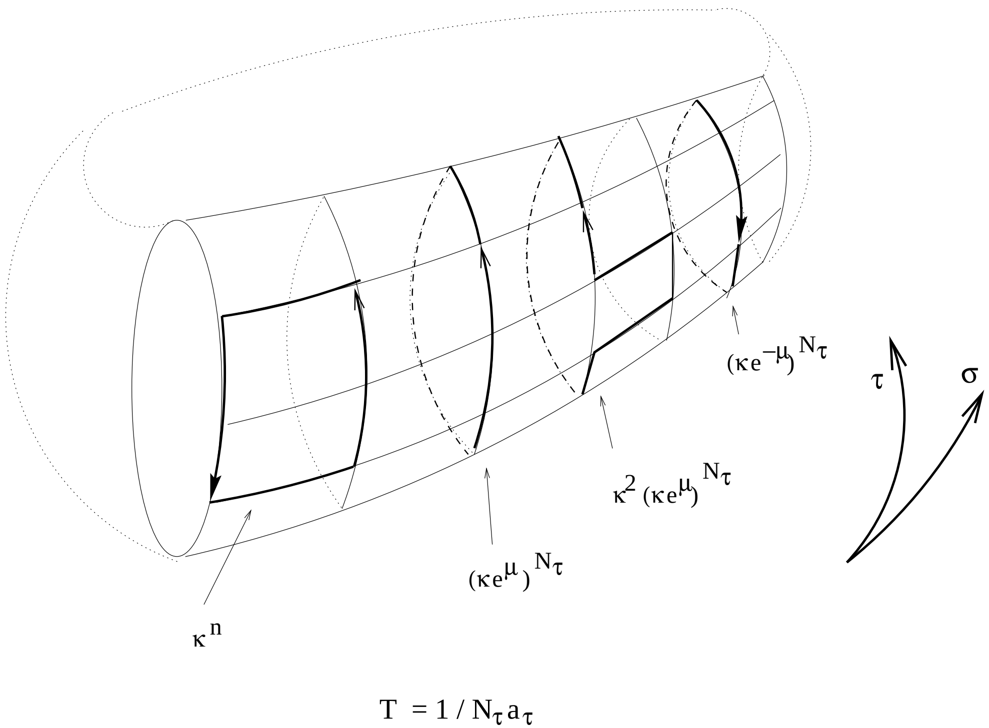


Figure 5: The HDM - QCD model: 0-th and 2-nd order. κ^2 , κ^4 orders: straightforward (beware combinatorics).

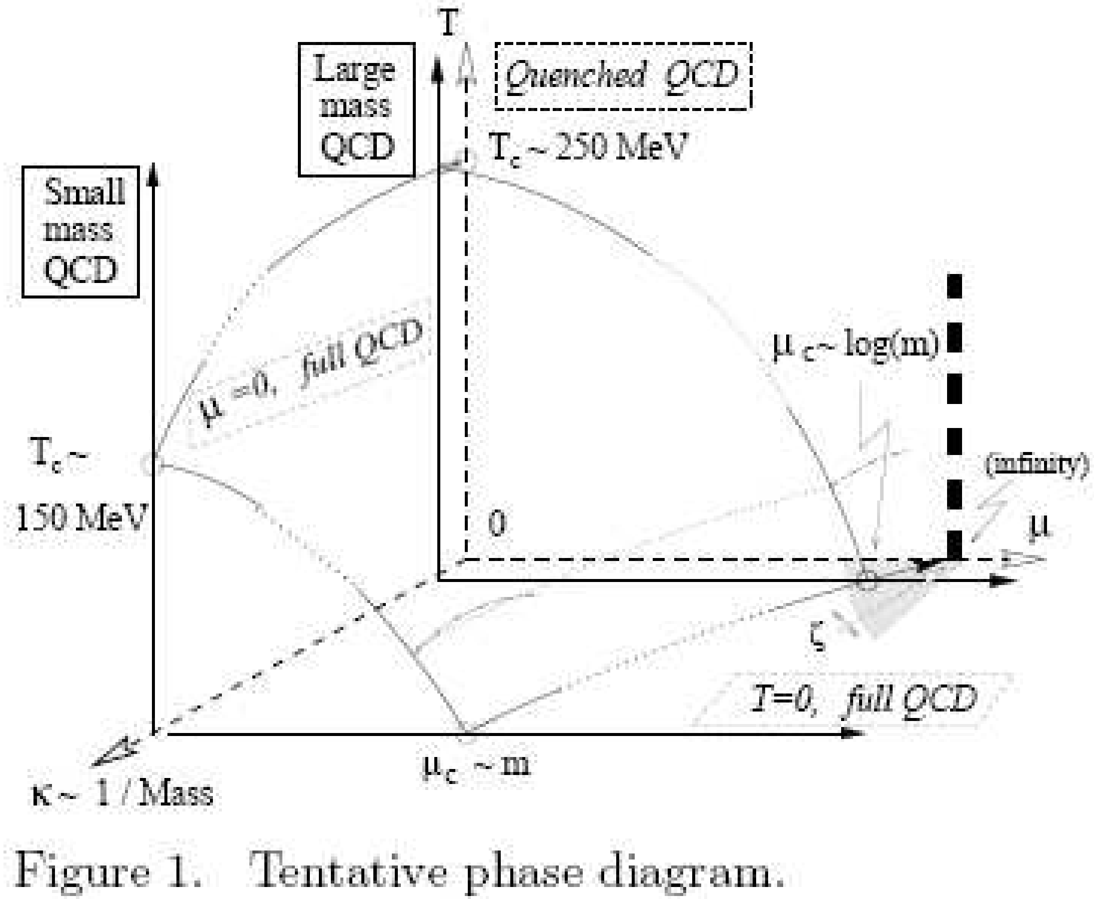


Figure 6: HDM-QCD: Tentative phase structure.

Recent applications:

HDM-QCD:

- Fixed charge ("quenched finite density QCD"), *J. Engels, O. Kaczmarek, F. Karsch, E. Laermann NPhProc 1999*
- Explicite formulae, colour condensate (full Y-M action, phase reweighting) *R. Hofmann and IOS, NPhProc 2004*
- Phase diagram, quark prop., (full Y-M action, ph. RW; compare MF and order β s.c.) *R. De Pietri, A. Feo, E. Seiler, IOS, PRD 2007*

HD-QCD (symmetrized HDM, *G. Aarts and I0S, JHEP 2008*) :

- Strong coupling expansion, reweighting and CLE *P. de Forcrand, M. Fromm, PRL 2010, M. Fromm, J. Langelage, S. Lottini, M. Neuman, O. Philipsen, PRL 2012*
- CLE, full Y-M action *E. Seiler, D. Sexty, IOS, PLB 2013*

Further: Gluons and light quarks on heavy dense background, Upper corner of Columbia plot, Dense mattter, Neutron stars, ..

HDM-QCD: reweighting results

RW, *De Pietri et al* (phase reweighting, temporal gauge).

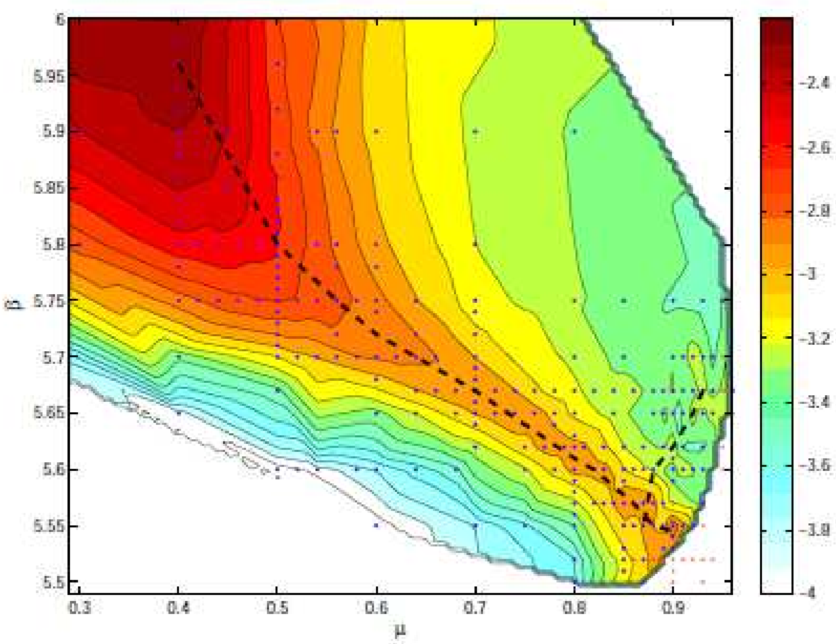


FIG. 15: Landscape of the Polyakov loop susceptibility. The color scale (left) is based on $\log_{10}(\chi_P)$

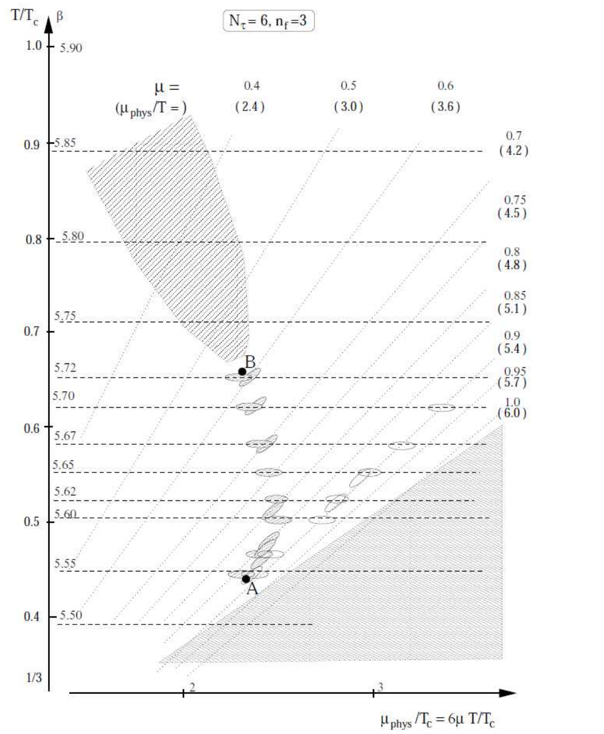


FIG. 17: Phase diagram in the β (or T/T_c) - μ_{phys}/T_c QCD plane. The dotted straight lines correspond to constant μ, the dashed ones to constant β. The blobs, shadowing and other features are explained in the text.

Figure 7: HDM-QCD, 3 flavours, order κ^2: Polyakov loop susceptibility and phase structure.

HDQCD: CLE and RW results

HDQCD ("symmetrized" HDM), Wilson fermions, full Y-M action. Order $(\kappa N_t)^2$ and higher corrections: decorated Polyakov loops.

$$S = \frac{\beta}{6} S_{YM}(\{U\}) + \ln\det \mathbf{M}(\mu) \tag{12}$$

$$\det \mathbf{M}(\mu) \equiv \prod_x \mathrm{Det}\,(\mathbf{1} + C\mathcal{P}_x)^2 \,\mathrm{Det}\left(\mathbf{1} + C'\mathcal{P}_x^{-1}\right)^2 \tag{13}$$

$$\mathrm{Det}\,(\mathbf{1} + C\mathcal{P}_x)^2 = (1 + C^3 + 3CP_x + 3C^2P'_x)^2 \tag{14}$$

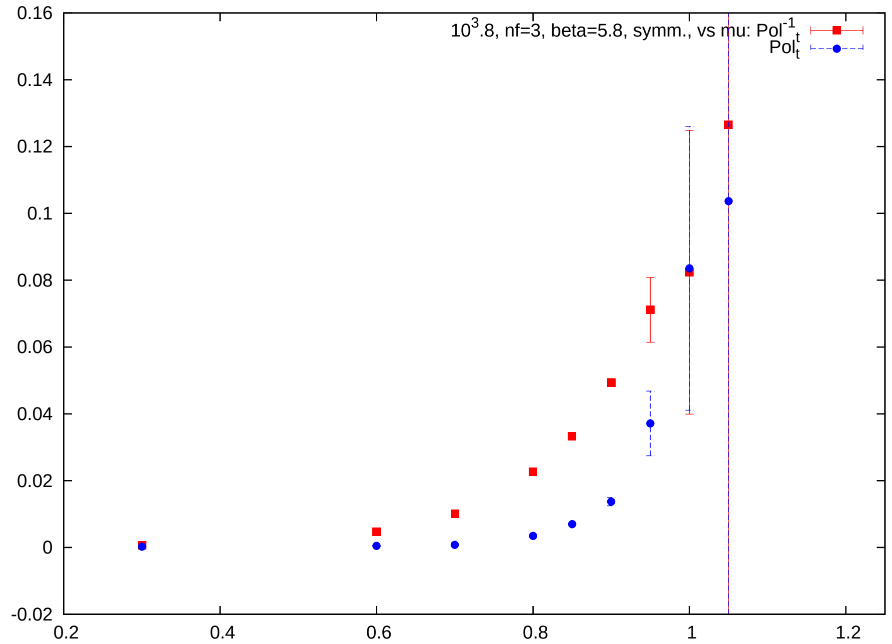
$$C = [2\kappa \exp(\mu))]^{N_t}\ ,\ C' = [2\kappa \exp(-\mu)]^{N_t} \tag{15}$$

$$\mathcal{P}_x = \prod_{\tau=0}^{N_\tau - 1} U_{x+r\hat{0},0}\ ,\ P_x = \frac{1}{3}\mathrm{tr}\,\mathcal{P}_x; \quad P'_x = \frac{1}{3}\mathrm{tr}\,\mathcal{P}_x^{-1}\,. \tag{16}$$

We measure also plaquettes, density and the average phase factor

$$\langle n \rangle = \frac{1}{V}\frac{\partial \ln Z}{\partial \mu}, \quad \langle e^{2i\phi}\rangle \equiv \left\langle \frac{\det \mathbf{M}(\mu)}{\det \mathbf{M}(-\mu)} \right\rangle \tag{17}$$

RW for HDQCD.



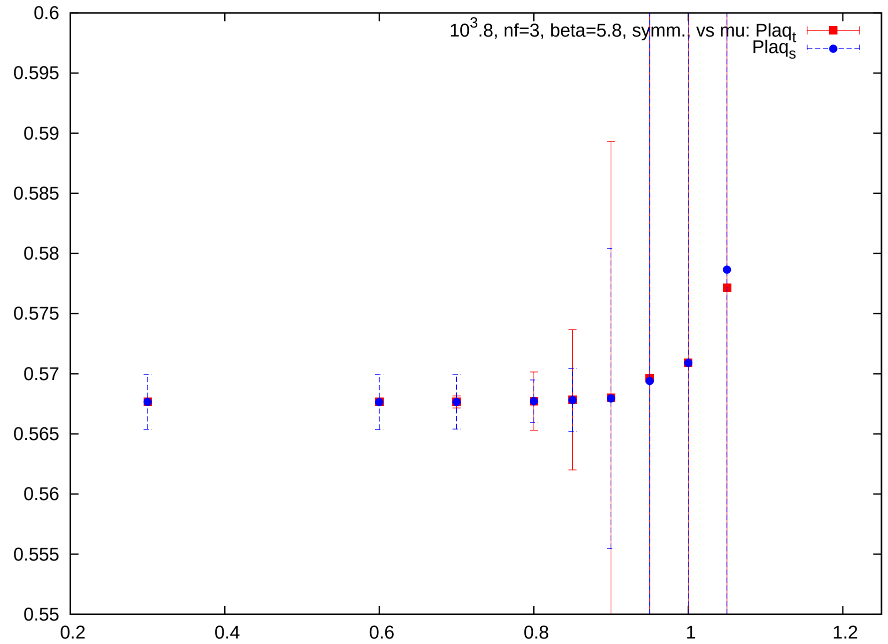


Figure 8: HD-QCD, 3 flavours: Polyakov loops and Plaquettes $(10^3 8, \beta = 5.8,$ reweighting).

CLE for HDQCD using cooling.

We observe the same behaviour as in the Polyakov chain model. The effect of cooling is dramatic.

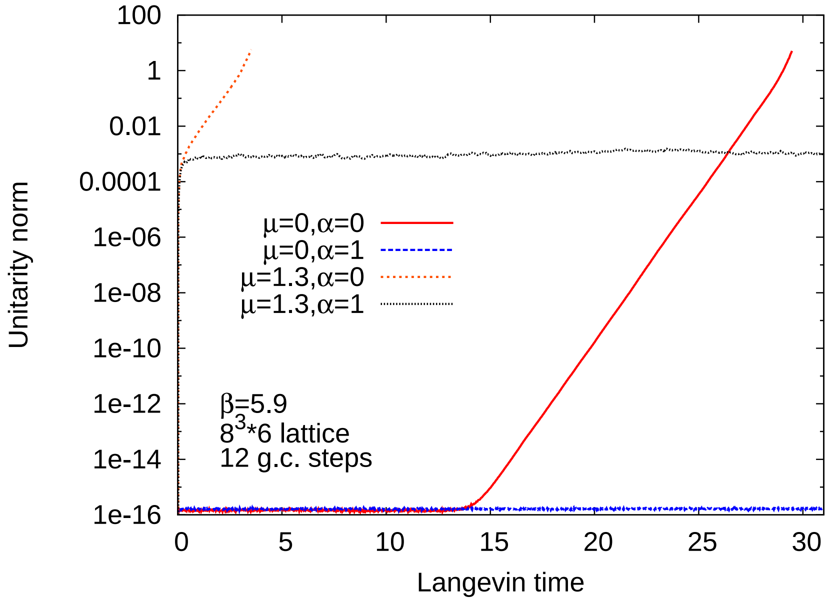
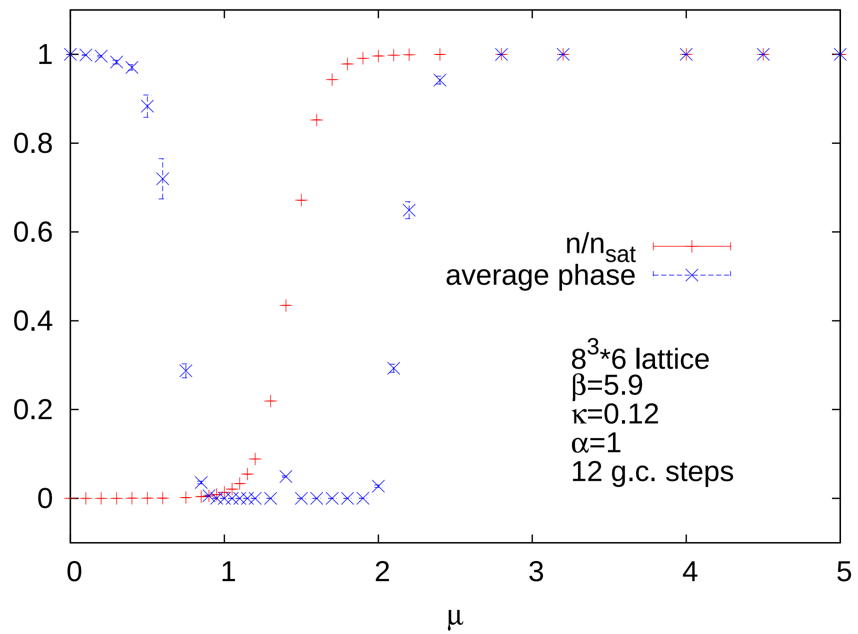


Figure 9: HDQCD: evolution of the unitarity norm with and without g.c. for $\beta = 5.9$, $8^3 \times 6$ lattice.



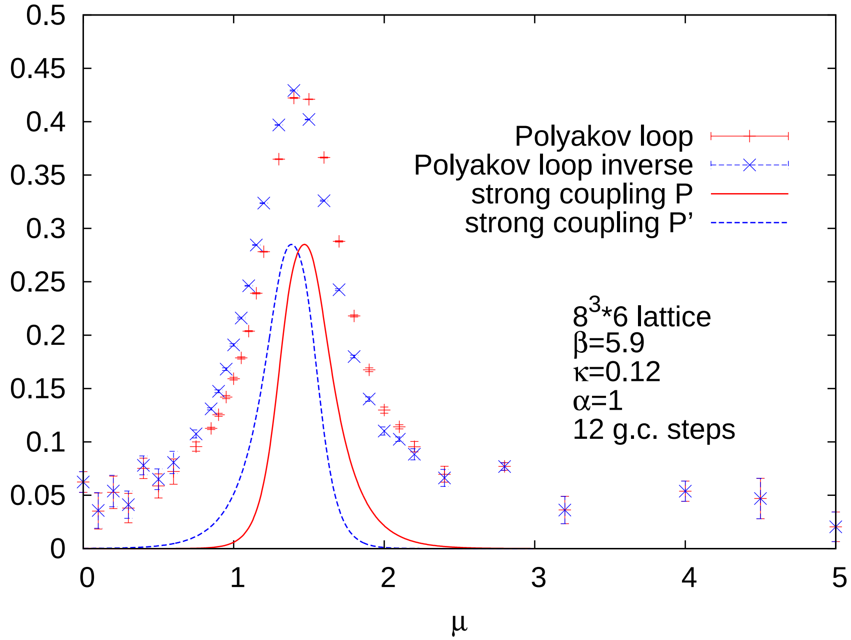


Figure 10: HDQCD. *Left*: Baryon density and average phase for $\beta = 5.9$, $8^3 \times 6$ lattice. *Right*: $\langle \mathcal{P} \rangle$, $\langle \mathcal{P}' \rangle$ vs. μ at $\beta = 5.9$ on a $8^3 \times 6$ lattice; solid lines: analytic strong coupling result.

HDQCD: comparison CLE with RW.

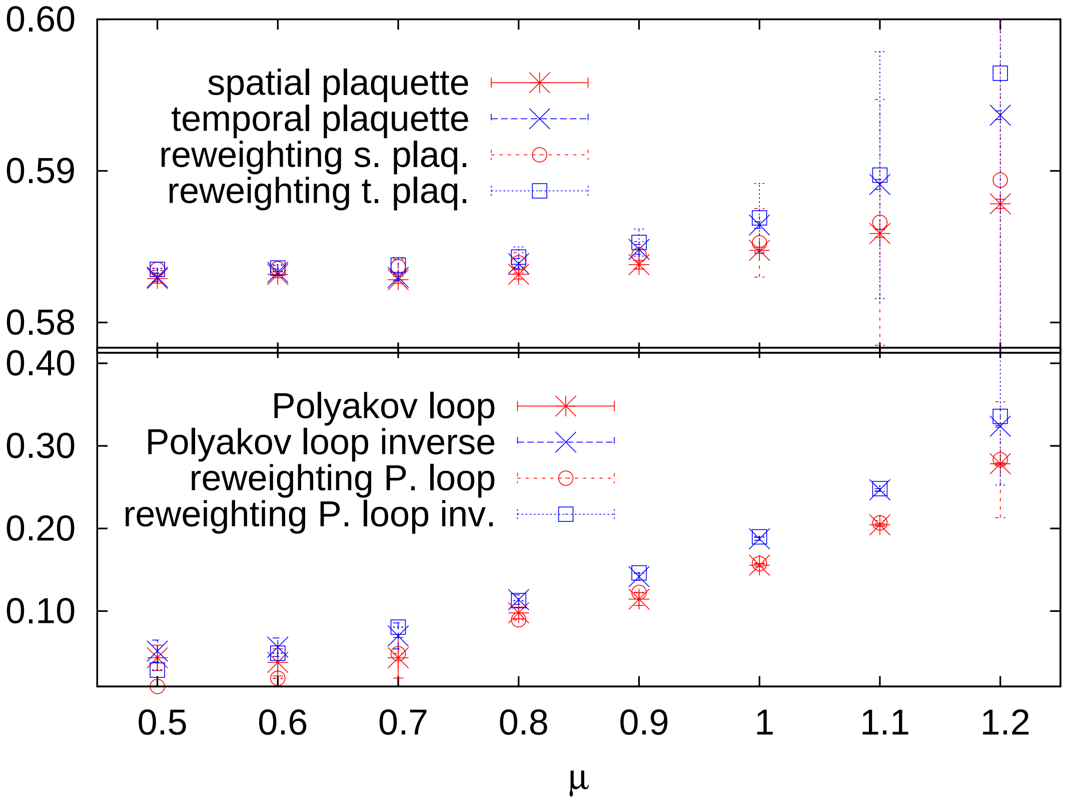


Figure 11: HDQCD: $\langle P \rangle$, $\langle P' \rangle$ and plaquettes for CLE *and* RW (6^4 lattice, $\alpha = 1$, 12 g.c. steps, adaptive step size) at $\beta = 5.9$ vs μ. Large errors only affect RW at large μ.

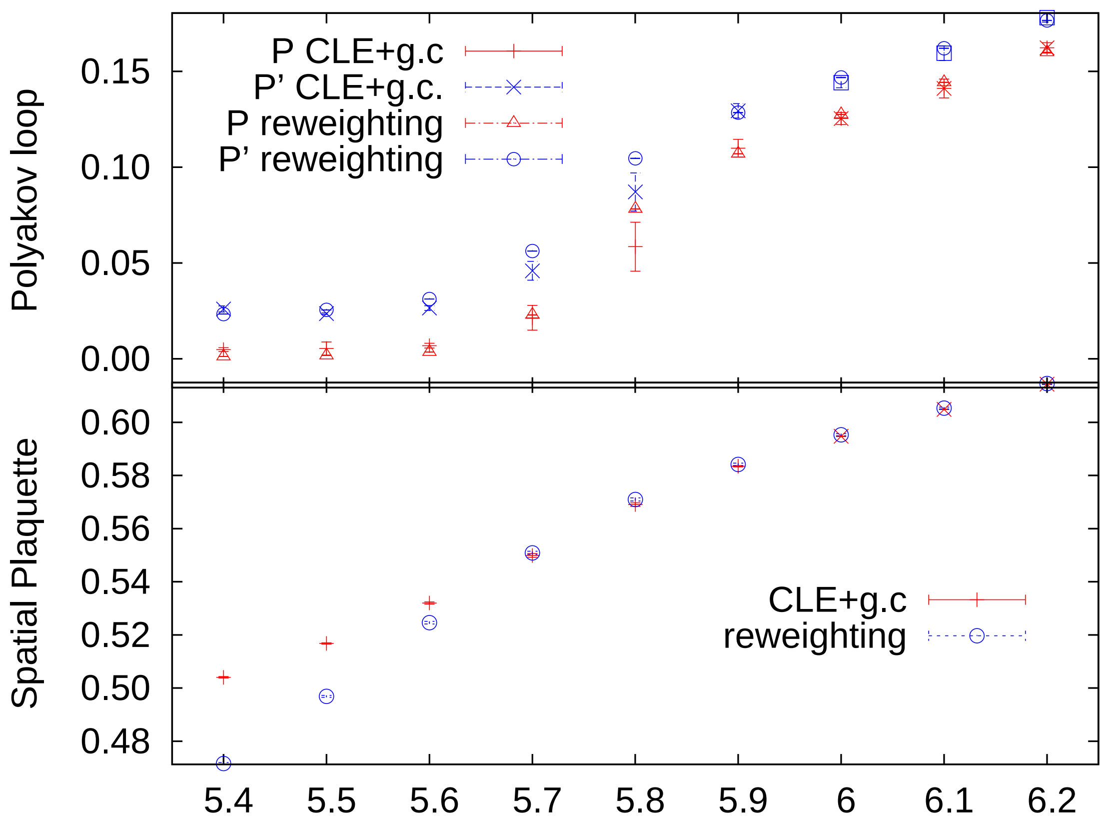


Figure 12: HDQCD: $\langle P \rangle$, $\langle P' \rangle$ and plaquettes for CLE *and* RW (6^4 lattice, $\alpha = 1$, 12 g.c. steps, adaptive step size) at $\mu = 0.85$ vs β).

Good agreement, only discrepancy in the plaquettes below $\beta \sim 5.6$.

The *deterioration threshold at* $\beta \sim 5.6$ appear to be independent on the lattice size and only weakly dependent on μ, and thus stay well below the phase transition on large lattices. A continuum limit would thus be safe both in the deconfined and in the confined phase.

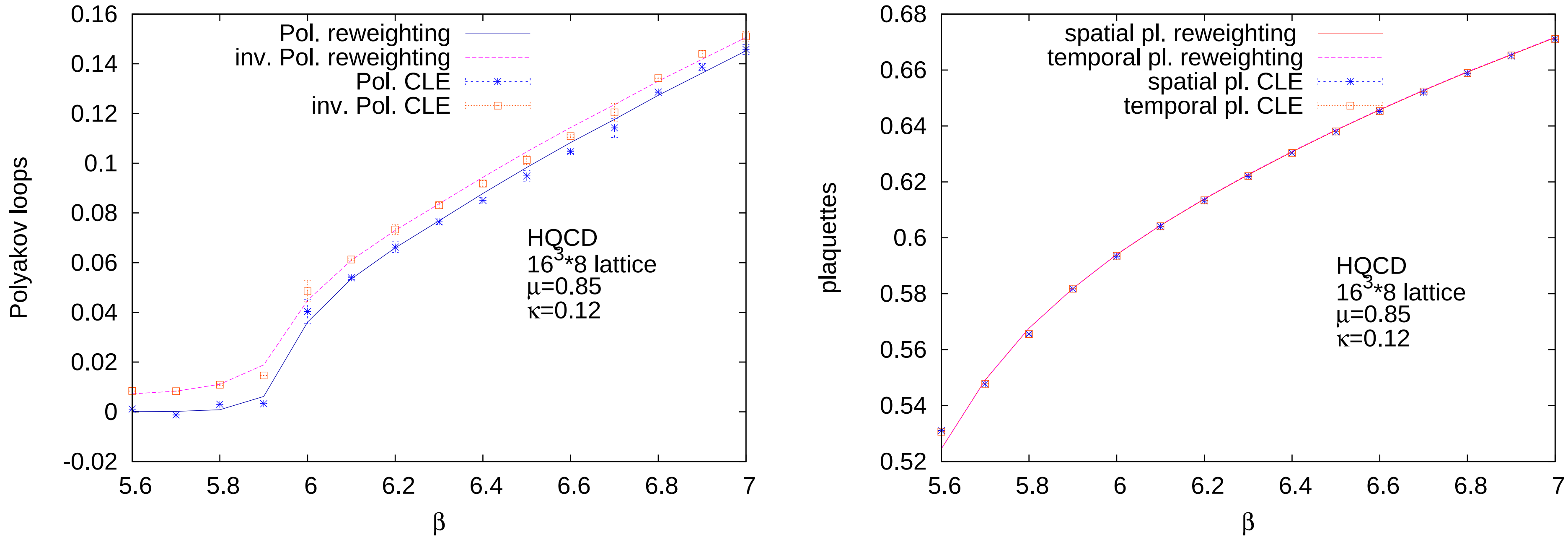


Figure 13: HDQCD: CLE and RW on $16^3.8$ lattices, Polyakov loops (*left*) and plaquettes (*right*).

CLE: HDQCD, comparison with Full QCD

The comparison is done for 1 flavour, Wilson fermions, $8^3.6$ lattice.

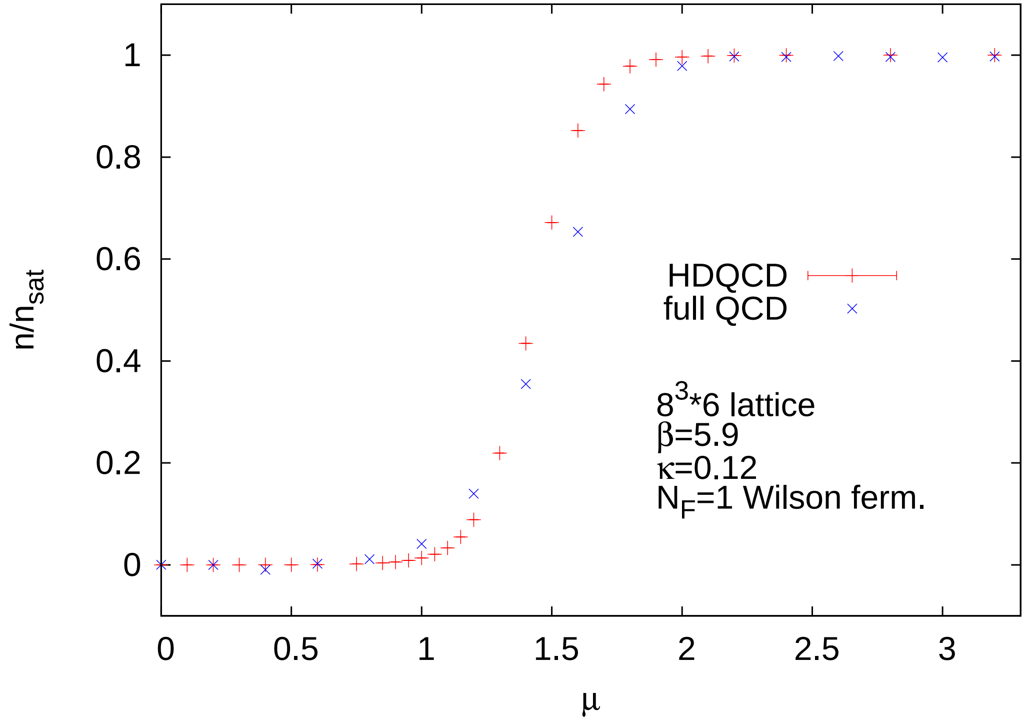
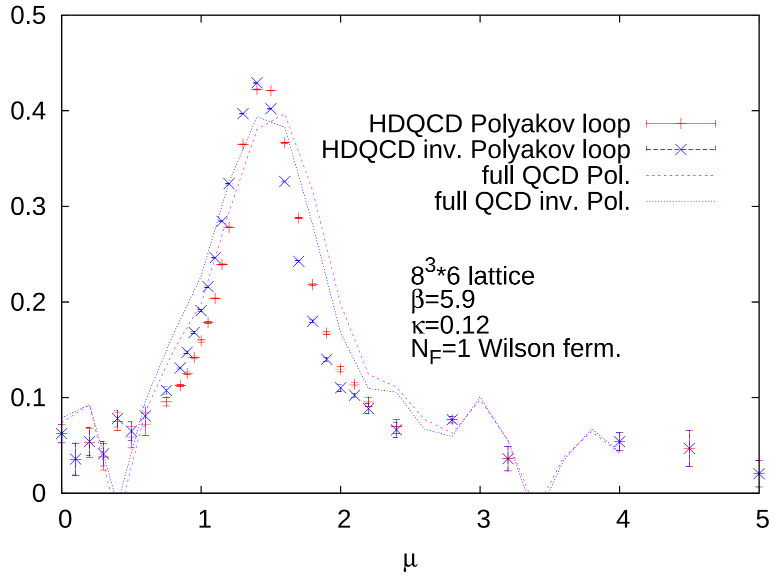


Figure 14: Comparison HDQCD and full QCD, CLE, Wilson fermions, $\kappa = 0.12$: baryonic density (normalized to saturation) vs μ.

HDQCD and full QCD: similar behaviour already at intermediary mass!



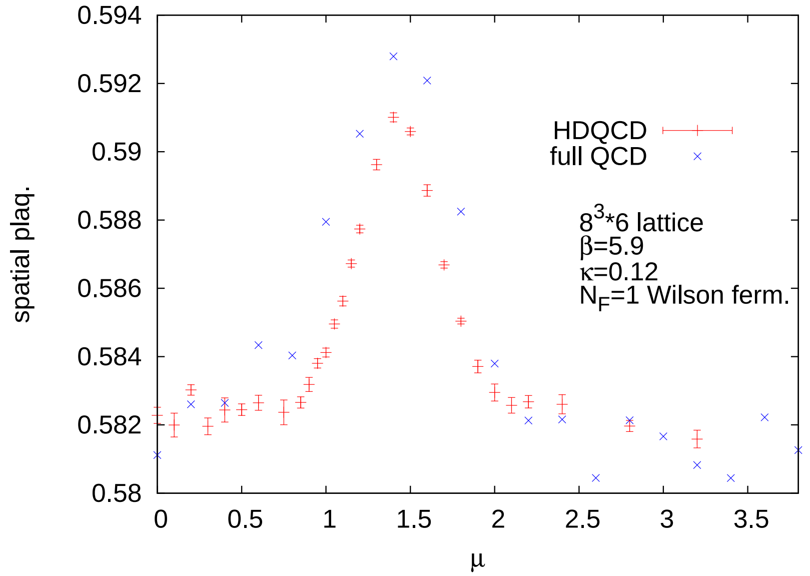


Figure 15: Comparison HDQCD and full QCD, CLE, Wilson fermions, $\kappa = 0.12$: Polyakov loops (*left*) and plaquettes (*right*) vs μ.

HDQCD reproduces the features of full QCD at semi-quantitative level. It may be used therefore for answering physical questions, at least at intermediary masses. Low temperatures may be reached (in work).

6. Summary

Insights, problems and solutions:

- Some problems seem to originate from a combination of the particularities of the drift flow and of numerical imprecisions.
- We could relate these problems to the behaviour of $P(x, y)$ in the imaginary direction and solve them for gauge theories (gauge cooling), fulfilling thereby one of the equivalence proof conditions.
- A remaining possible source of trouble can affect non-holomorphic drift. In realistic cases this does not seem to have significant effects. But we want to reach a systematic understanding.
- CLE with gauge cooling allowed us to analyze a QCD-model with direct physical applications, HDQCD, and especially full QCD aiming at physical results in the whole region of interest.

- CLE has the chance to become a versatile, general method for solving the problem of complex action (QCD with chemical potential, non-equilibrium QFT and real time evolution, etc).
- The method does not suffer of cancellations and of the overlap problem.
- The method works in a parameter range unreachable by any other method.
- The volume dependence for CLE is comparable with MC (and differs essentially from that of RW).
- The HD-QCD model reproduces many features of full QCD and may be very useful to describe physics for intermediary quark mass, all way to high density and down to low temperature. It is well amenable to CLE analysis.

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Some publications in our group, various combinations:

- Lattice simulations of real-time quantum fields, J. Berges, Sz. Borsanyi, D. Sexty, I.-O. S.
- Stochastic quantization at finite chemical potential, G. Aarts, I.-O. S.
- The Complex Langevin method: When can it be trusted? G. Aarts, E. Seiler, I.-O. S.
- Complex Langevin: Etiology and Diagnostics of its Main Problems, G. Aarts, F. A. James, E. Seiler, I.-O. S.
- Complex Langevin dynamics: criteria for correctness, G. Aarts, F. A. James, E. Seiler, I.-O. S.
- Complex Langevin dynamics in the SU(3) spin model at nonzero chemical potential revisited, G. Aarts, F. A. James

- Stability of complex Langevin dynamics in effective models G. Aarts, F. A. James, J.. Pawlowski, E. Seiler, D. Sexty, I.-O. S.
- Gauge cooling in complex Langevin for QCD with heavy quarks, E. Seiler, D. Sexty, I.-O. S.
- Controlling complex Langevin dynamics at finite density, G. Aarts, L. Bongiovanni, E. Seiler, D. Sexty, I.-O. S.
- Adaptive gauge cooling for complex Langevin dynamics, G. Aarts, L. Bongiovanni, E. Seiler, D. Sexty, I.-O. S.
- Localised distributions and criteria for correctness in complex Langevin dynamics, G. Aarts, P. Giudice, E. Seiler - Simulating full QCD at nonzero density using complex Langevin equation D. Sexty