Developing the Complex Langevin approach for finite density QCD

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, B. Jäger (Swansea) and J. Pawlowski (Heidelberg).

Creutz Fest 2014, BNL

History ...

1968 Bucharest , IBM

1980 Munich , Cray 1 (vectorization)
1 year after the Creutz, Jacobs, Rebbi and Creutz' seminal papers

today (graphic cards, clusters, Blue gene ...)

1. Introduction

Just recall: what is CLE and what is it good for.

Langevin Equation.

Stochastic process which can be used for numerical simulations.
Uses a classical drift derived from the action and random noise.

Real Langevin simulations are comparable with MC, step size dependence can be kept below statistical errors.

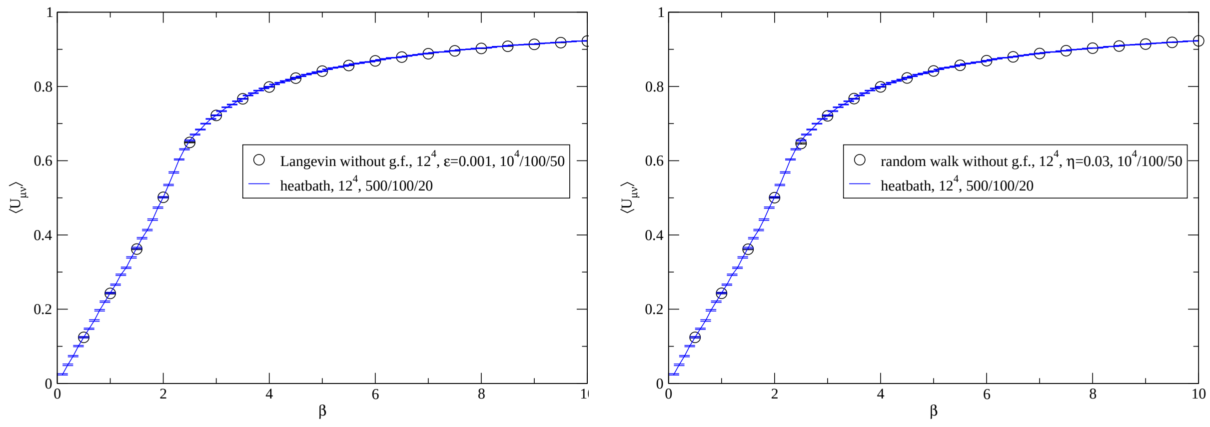


Figure 1: Plaquette averages by LE and RW compared with MC

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

CLE is the extension of the LE algorithm to the case of complex action.

This is possible *in principle* since the process does not rely on a probability interpretation of the Boltzmann factor.

Physical problems with complex action:

1. real time simulations, non-equilibrium QFT
2. **chemical potential**
3. $\theta-$ term ...

CLE provides in all these cases an approach - sometimes, the only one $\longrightarrow$ develop this approach to a reliable method (rewarding but hard). Start a new approach before having solved all problems of principle ..

J. Berges and IOS, PRL 2005; J. Berges, S. Borsanyi, D. Sexty, IOS, PRD 2007; J. Berges, D. Sexty, NPhB 2008; G. Aarts and I.O.S., 2009; L. Bongiovanni et al, Lattice 2014

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.(Wrong convergence was found in some special cases.)
New interest in connection with problems for which no other general solution is available

The present general work and our working programme :

1. Theoretical discussion [A, 3].

2. Study the various aspects of the problem on simple models used as effective models, and more involved soluble models: Random matrices, Thirring model [A, 1, 2, 4].

3. Extend the analysis to HDQCD [A, 5].

4. Study full QCD [A].

Our group [A, many papers since 2008, list in *Group Work*] 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, M. Neuman, O. Philipsen, JHEP 2012 ; J. Langelage, S. Lottini, O. Philipsen, 2014* [5], . . .

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

Complex action $\longrightarrow$ complex drift $\longrightarrow$ imaginary parts for the variables

$\longrightarrow$ Process defined on the complex extension of the original manifold:

$$R^n \longrightarrow C^n \;,\; SU(n) \longrightarrow SL(n, C), \; \ldots \; .$$

The CLE with complex drift $K(z) = -\nabla_z S$ for a complex variable

$$z(t) = x(t) + i\, y(t) \tag{1}$$

amounts to two related, real LE with independent noise terms

$$\delta z(t) \;=\; K(z,t)\, \delta t + \eta(t)\,, \quad \eta = \sqrt{N_R}\, \eta_R + \mathrm{i} \sqrt{N_I}\, \eta_I \tag{2}$$

$$\text{i.e. :} \qquad \delta x(t) = Re\, K(z,t)\, \delta t + \sqrt{N_R}\, \eta_R(t) \tag{3}$$

$$\delta y(t) = Im\, K(z,t)\, \delta t + \sqrt{N_I}\, \eta_I(t) \tag{4}$$

$$\langle \eta_R \rangle \;=\; \langle \eta_I \rangle = 0\,, \quad \langle \eta_R^2 \rangle = \langle \eta_I^2 \rangle = 2\, \delta t\,, \; \langle \eta_R \eta_I \rangle = 0\,, \quad N_R - N_I = 1$$

In the following $N_I = 0$.

The processe realizes asymptotically a positive definite $P(x, y)$.

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

$$\langle \mathcal{O} \rangle_P \equiv \frac{\int \mathcal{O}(x+iy)P(x,y)dxdy}{\int P(x,y)dxdy}, \quad \langle \mathcal{O} \rangle_\rho \equiv \frac{\int \mathcal{O}(x)\rho(x)dx}{\int \rho(x)dx}. \tag{5}$$

This is what we calculate This is what we want to get

Note: the formal proof of equivalence relies among others on
1) holomorphy of the drift and of the observables
2) sufficient fall off of $P(x, y)$ at large arguments.

Since we shall concentrate on gauge models models x will be compact.

There is evidence that in some cases CLE leads to wrong results.

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

"Problems of principle":

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

4. Non-holomorphy of the drift formally invalidates the equivalence proof and may lead to wrong convergence. E.g., poles of $K(z)$.

Solutions:

1.-3. To unprecise sampling and skirts – unsufficient fall off of $P(x,y)$:
$\longrightarrow$ constrain the distribution $P(x,y)$ by performing allowed changes of the process without affecting the expectation values - gauge cooling. Together with adaptive step size this practically eliminates run-aways and numerical imprecisions.

4. Concerning meromorphic drift: In realistic cases (e.g., QCD) the poles do not seem to raise difficulties, 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).

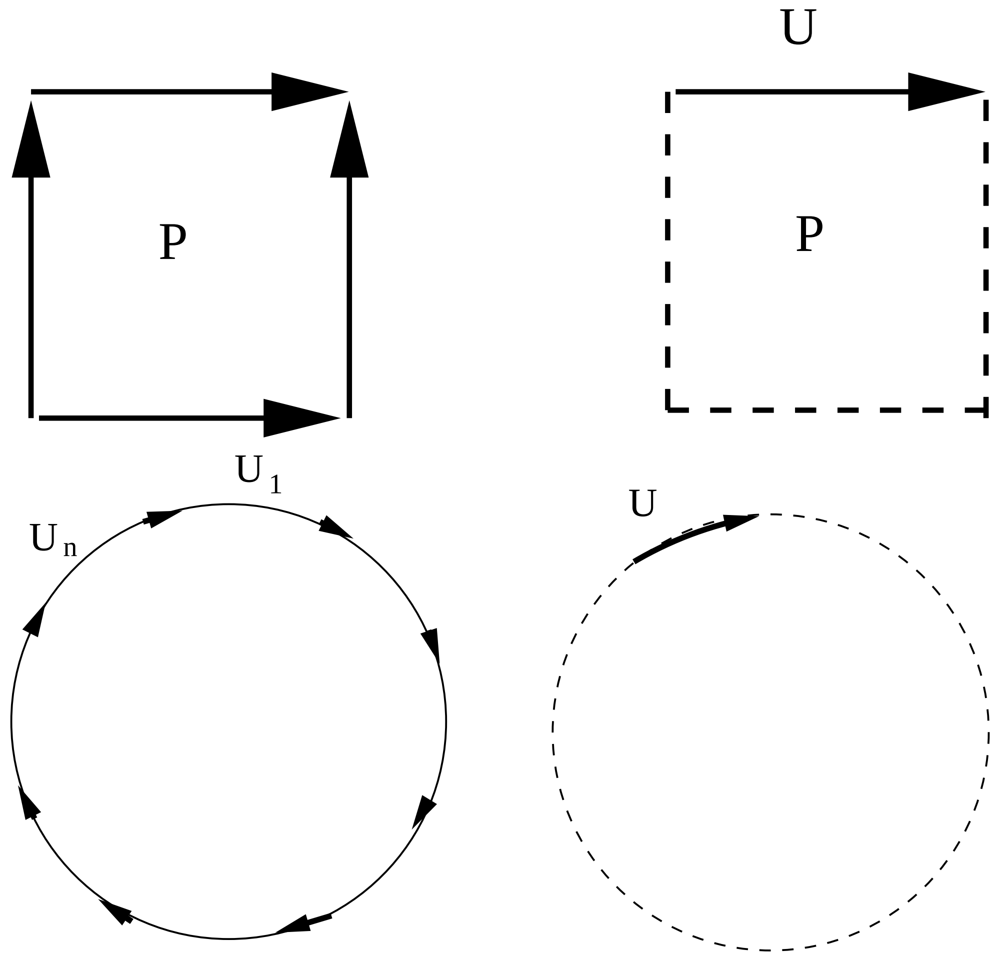
Notice: there are many processes $K(z)$ $(P(x,y))$ leading formally to the desired EV's. This can be used in controlling the method.

We want to develop the CLE method for QCD at non-zero chemical potential $\longrightarrow$ we shall stick to SU(3) $\longrightarrow$ SL(3,C):

- Illustration of the problems, solutions and approaches in simple models
- Design the method for QCD

3. Learning from simple models

The one link SU(3) reduced and the Polyakov chain model



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

$$-S \;=\; \frac{\beta}{2}\left(\mathrm{tr}UA+\mathrm{tr}A^{-1}U^{-1}\right)+\ln D+\ln\tilde{D} \tag{6}$$

$$D=1+3C\,P+3C^2\,P'+C^3 \;=\; (1+C^3)(1+a\,P+b\,P') \tag{7}$$
$$\tilde{D}=1+3\tilde{C}\,P'+3\tilde{C}^2\,P+\tilde{C}^3 \;=\; (1+\tilde{C}^3)(1+\tilde{a}\,P'+\tilde{b}\,P) \tag{8}$$

$$C \;=\; 2\kappa\mathrm{e}^{\mu},\quad \tilde{C}=2\kappa\mathrm{e}^{-\mu},\quad P=\frac{1}{3}\mathrm{tr}U,\quad P'=\frac{1}{3}\mathrm{tr}U^{-1} \tag{9}$$

The matrices $A\in GL(3,C)$ simulate the staples. After "Cartan" reduction (H: reduced Haar measure):

$$-S \;=\; \frac{\beta}{2}\sum_{i=1}^{3}\left(\alpha_i e^{iw_i}+\alpha_i^{-1}e^{-iw_i}\right)+\ln D+\ln\tilde{D}+\ln H \tag{10}$$
$$O_n \;=\; \mathrm{tr}(\hat{U}^n)=\mathrm{e}^{i\,nw_1}+\mathrm{e}^{i\,nw_2}+\mathrm{e}^{i\,nw_3} \tag{11}$$

Skirts and numerical imprecisions in the 1-link model

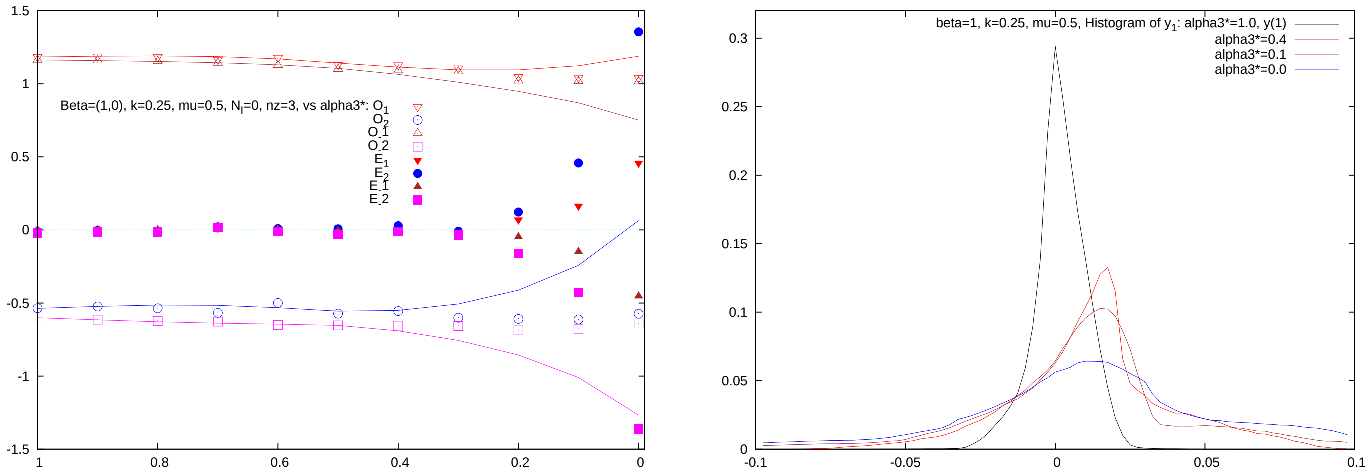


Figure 2: Effective model. *Left*: Dependence of the observables on Re α_3. *Right*: Histograms of the equilibrium measure for different Re α_3. Discrepant results correlate with wide skirts of the distributions.

For *gauge theories* skirts and wrong evolution are correlated with *uncontrolled departure* from the unitary manifold.

Gauge cooling

For a correctly evolving process a "unitarity norm" should *converge* to some (generally non-zero) value.

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

$$UN \equiv \sum_{links} \left[\frac{1}{2} tr \left(U\, U^{\dagger} + U^{-1}\, U^{-1\,\dagger} \right) - 3 \right] \tag{12}$$

This succeeds by successive gauge transformations of the links

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

- dS_G: the gradient of the UN
- α: the strength of the *gauge force*, ϵ: step size.

Gauge cooling for the Polyakov chain model

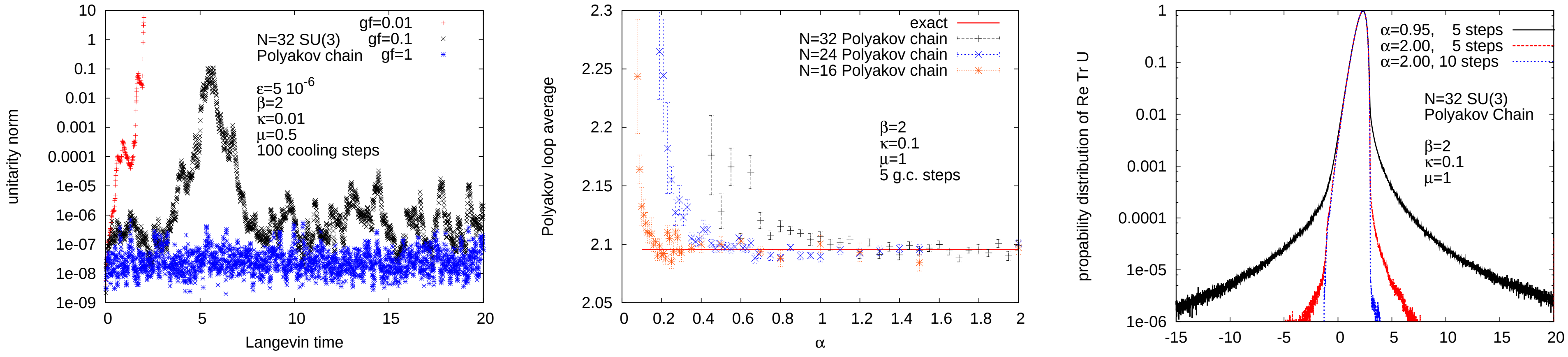


Figure 3: Polyakov chain, from left to right: evolution of the *UN* for various amount of cooling, observables' dependence on cooling, and distributions for various amount of cooling.

Gauge Cooling is a general method for gauge theories. It does not change gauge invariant quantities but *"repairs"* the process, that is, the sampling of the observables. Can be implemented as drift. Not to be confused with usual cooling or Wilson flow which change the action.

Expansion of the drift for the 1-link model

The fermionic part of the CLE drift $\sim \partial D/D + \partial\tilde{D}/\tilde{D}$. We can expand D^{-1} (and similarly: $\tilde{D}^{-1}$), dropping a constant factor and introducing a shift λ to increase the radius of convergence if necessary

$$D^{-1} = \frac{1}{1+Q} = (\lambda+1)\sum_{n=0}^{\infty}\left(\frac{\lambda-Q}{\lambda+1}\right)^n, \quad Q = a\,P + b\,P' \quad (13)$$

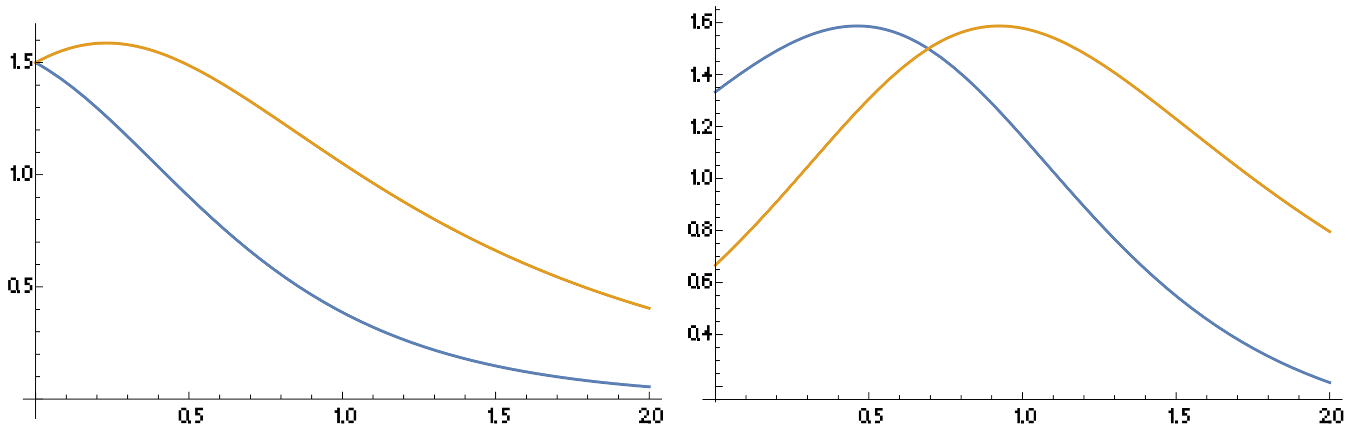


Figure 4: The coefficients $a = 3\,C/(1+C^3)$, $b = 3\,C^2/(1+C^3)$ for $\kappa = 0.5$ (left plot) and $\kappa = 0.25$ (right plot) vs μ.

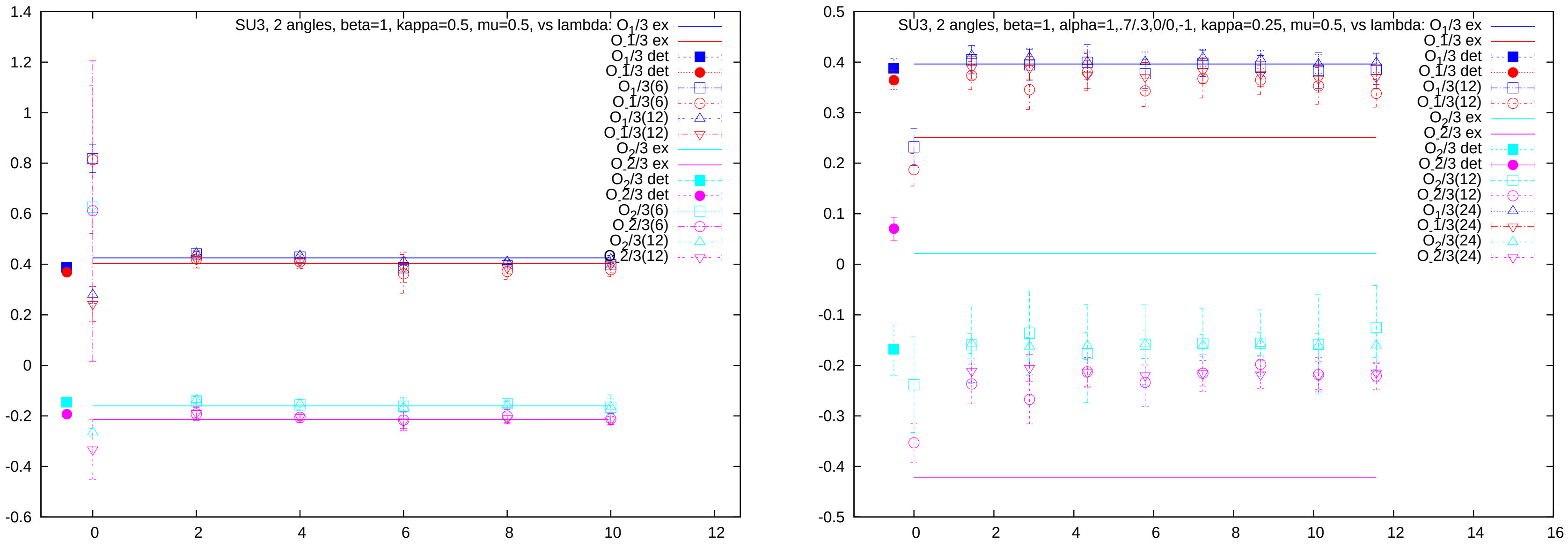


Figure 5: Expansion to order 6, 12 or 24 in absence (*left*) and presence (*right*) of skirts. Full symbols use the full determinant. $a = .9$, $b = 1.5$.

Conclusion: In absence of skirts both expansion and exact determinant work well, indicating negligeable effects from complex poles.

NB: Since the expanded drift is holomorphic, the effect of poles is to define the convergence region. This relates convergence to lack of effects from poles. This correlation can be spoiled by skirts.

4. Lattice QCD with chemical potential

Staggered and Wilson fermions

Gauge cooling, adpative step size

QCD grand canonical partition function, Wilson fermions:

$$Z = \int DU\, \mathrm{e}^{-S}, \qquad S = S_{YM} - \log \det M \tag{14}$$

$$\begin{aligned} M &= 1 - 2\kappa_s \sum_{i=1}^{3} \left(\Gamma_{+i} U_{x,i} T_i + \Gamma_{-i} U^{\dagger}_{x,i} T_{-i} \right) \\ &\quad -2\kappa_t \left(\mathrm{e}^{\mu} \Gamma_{+4} U_{x,4} T_4 + \mathrm{e}^{-\mu} \Gamma_{-4} U^{\dagger}_{x,4} T_{-4} \right) \end{aligned} \tag{15}$$

T: lattice translations, $\Gamma_{\pm\mu} = \frac{1}{2}(1 \pm \gamma_\mu)$, $\kappa_s = \kappa_t = \kappa$ (hopping parameter) $\sim 1/M$.

For both Wilson and staggered fermions the fermionic part of the drift implies inverting the big matrix M:

$$K_f \simeq \mathrm{tr} \left(M^{-1} D_{n\,\mu\,a} M \right) \tag{16}$$

HDQCD as first approximation

In the limit $\kappa \to 0, \quad \mu \to \infty, \quad \zeta = \kappa\, e^{\mu}\ :\ fixed$
only the Polyakov loops survive and the determinant factorizes in a product of determinants of the 1-link form:

$$\det M^0 = \prod_{\vec{x}} (1 + a\, P_{\vec{x}} + b\, P'_{\vec{x}}).$$

This can be used as the basis for a systematic analytic expansion of which the above limit is the LO.

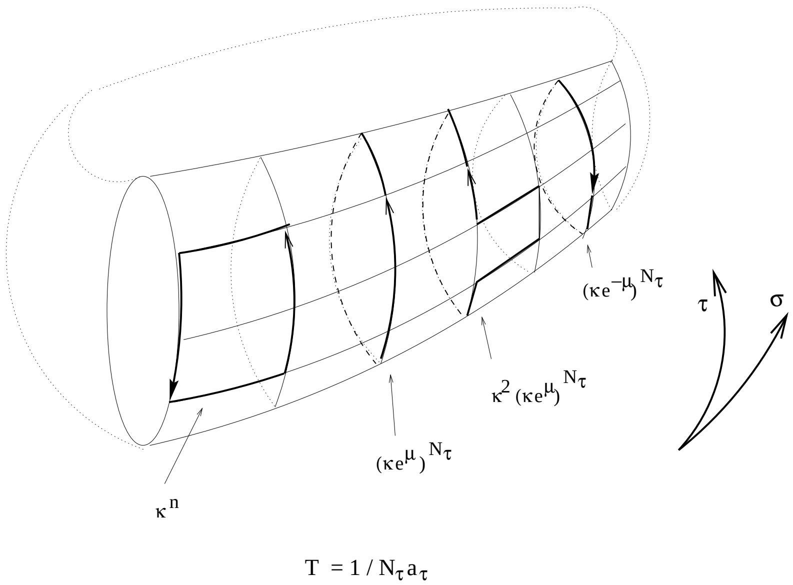


Figure 6: HDQCD and next order in the loop expansion.

Tests in HDQCD

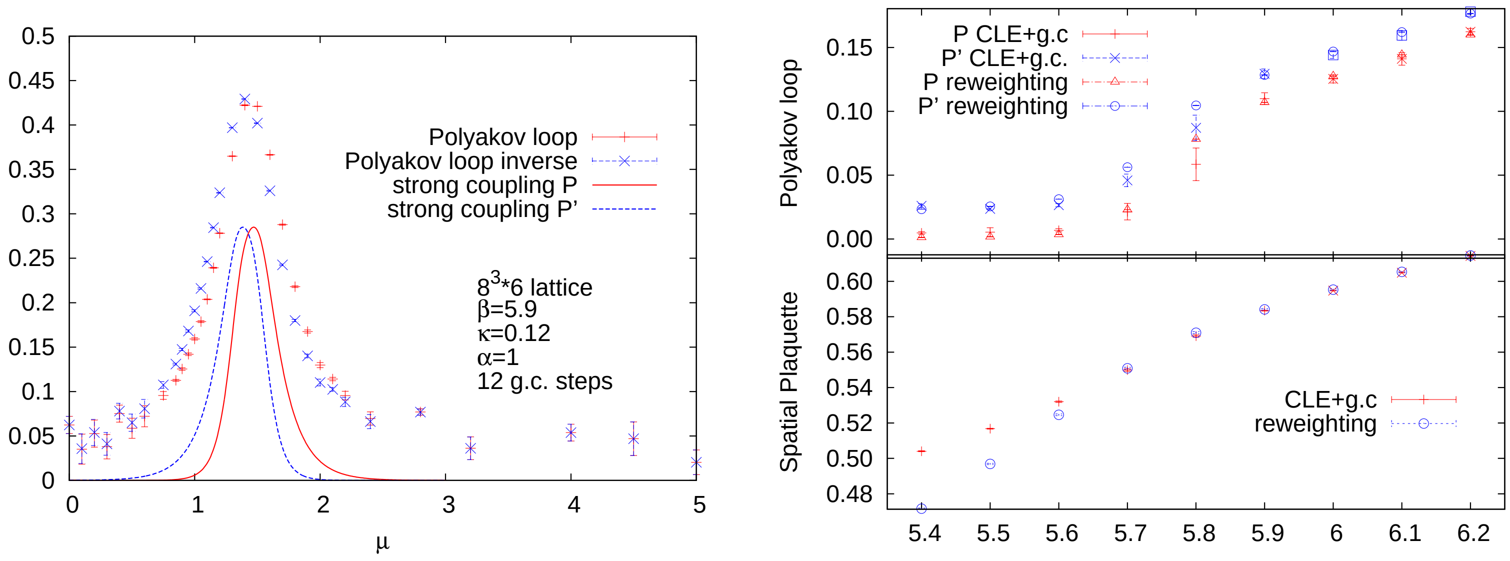


Figure 7: HDQCD. *left*: CLE results, P, P' vs μ at $\beta = 5.9$ on a $8^3 \times 6$ lattice; solid lines: analytic strong coupling result. *right*: CLE and RW results vs β at $\mu = 0.85$, 6^4 lattice.

The comparison with RW data suggests that CLE may have problems below $\beta = 5.7$ (rough configurations). This threshold turns out to depend only mildly on μ and on the lattice size.

HDQCD has been used to investigate the phase diagram.

CLE: full QCD and comparison with HDQCD

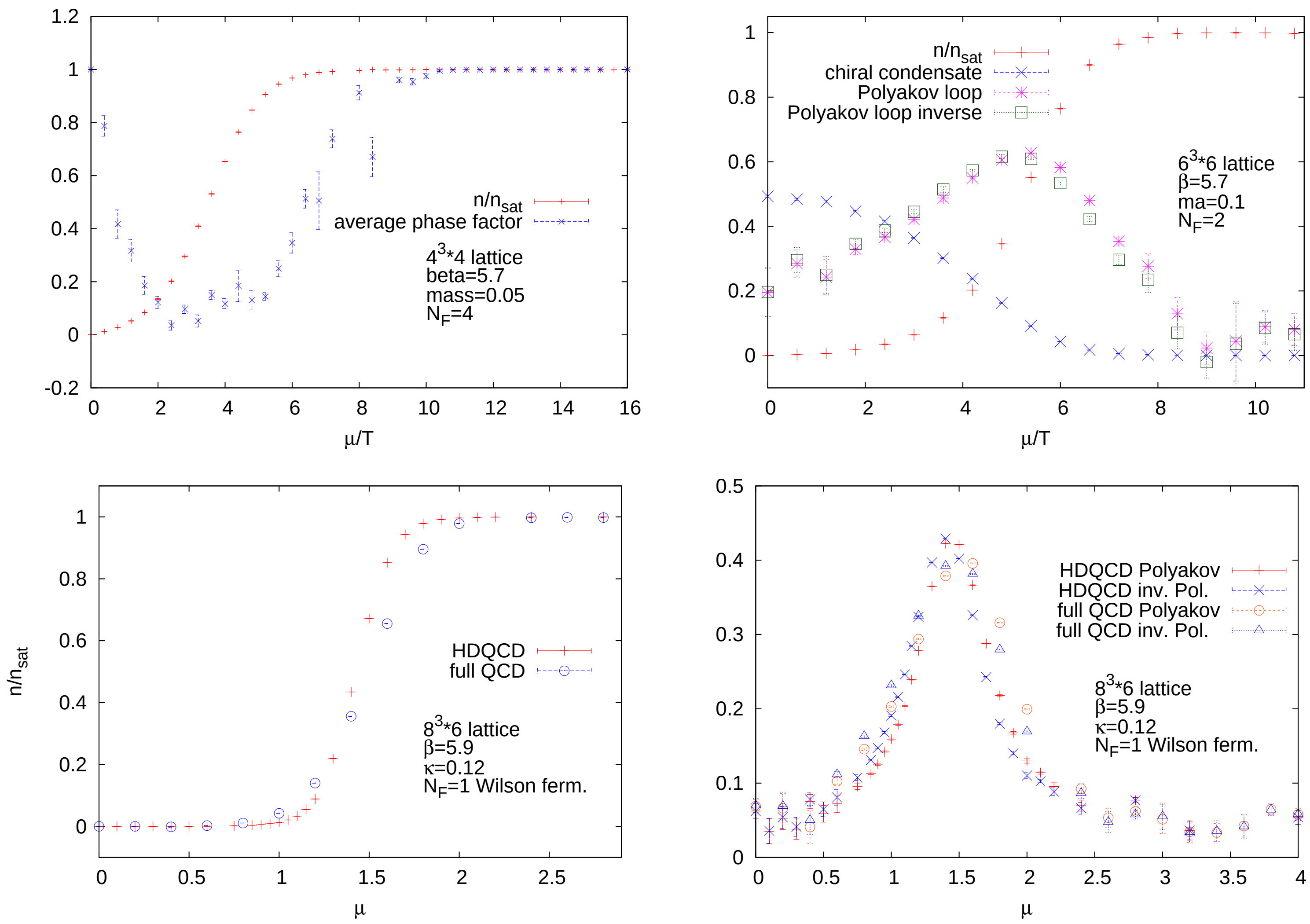


Figure 8: *Upper plots*: QCD with staggered fermions. *Lower plots*: QCD with Wilson fermions *and* comparison with HDQCD.

5. Systematic expansion to all orders in κ

Since already HDQCD has a certain qualitative agreement with the full theory it is tempting to write down a systematic expansion.

We separate temporal and spatial hoppings

$$M \;=\; 1 - \kappa Q \;=\; 1 - R - \kappa_s S, \qquad R = \kappa_t Q_t, \qquad S = Q_s$$

and write 2 expansions for the determinant and the drift, where we also make use of the orthogonality of the $\Gamma_{\pm\mu}$.

The $\kappa-$ expansion:

$$\det M = \mathrm{exp}\left\{-\sum_n \frac{\kappa^n}{n} Q^n\right\}, \qquad K_{x\nu a} = -\sum_{n=1}^{\infty} \kappa^n \mathrm{tr}\left(Q^{n-1} D_{x\nu a} Q\right).$$

is fast but less well behaved since it will include terms $\sim \kappa \mathrm{e}^{\mu}$, moreover it will not show μ dependence before the order N_t. The drift is holomorphic.

The κ_s- expansion:

$$\det M = \det M^0 \text{exp}\left\{-\sum_n \frac{\kappa_s^n}{n}\left(\frac{S}{1-R}\right)^n\right\} \tag{17}$$

$$K_{xia} = K^0_{xia} - \sum_{n=1}^{\infty} \kappa_s^n \text{tr}\left(\frac{1}{1-R}(D_{xia}S)\left[\frac{1}{1-R}S\right]^{n-1}\right), \tag{18}$$

$$K_{x4a} = K^0_{x4a} - \sum_{n=1}^{\infty} \kappa_s^n \text{tr}\left(\frac{1}{1-R}(D_{x4a}R)\left[\frac{1}{1-R}S\right]^{n}\right), \tag{19}$$

($\det M^0$, K^0 given by the *analytic* LO expressions) *is less fast but better behaved. The drift may have (controllable) singularities at the zeroes of* $\det M^0$. *A nested expansion (with $\Lambda =$ adequately chosen and respecting commutations) will make the drift holomorphic:*

$$(1-R)^{-1} = (\Lambda+1)^{-1}\sum_n\left(\frac{\Lambda-R}{\Lambda+1}\right)^n \tag{20}$$

Tests of the expansions

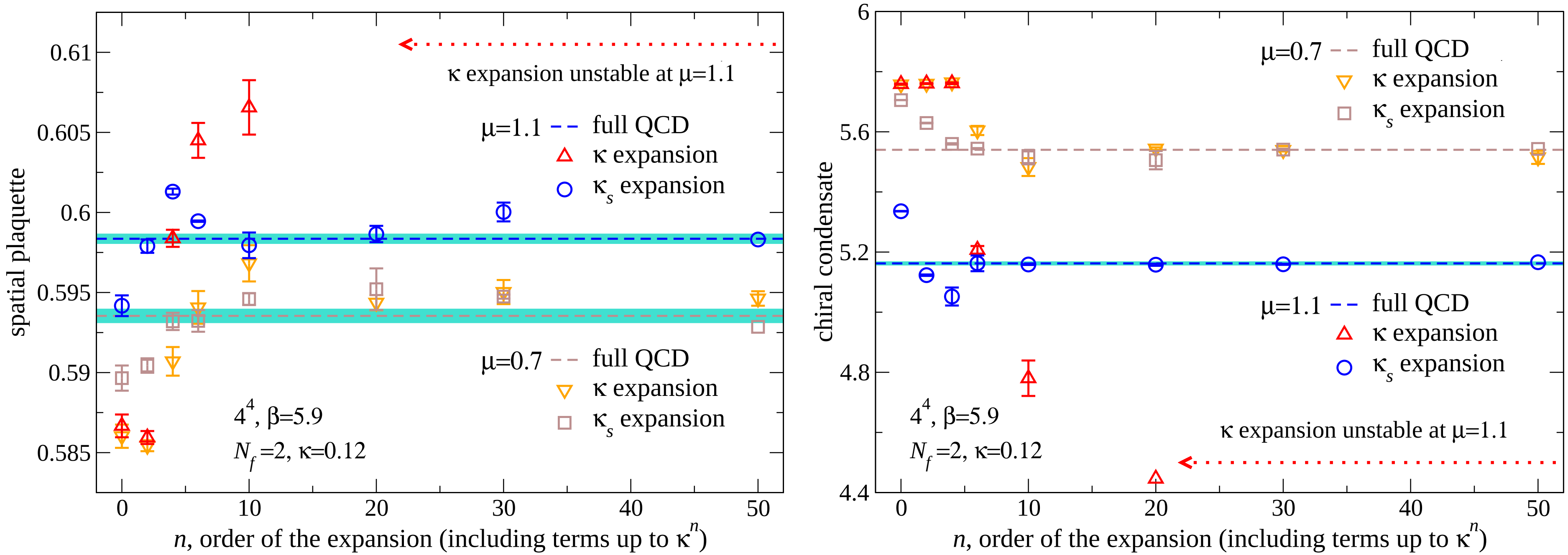


Figure 9: QCD, Wilson fermions, $\kappa = 0.12$, full and expansions vs $\kappa-$order. The $\kappa-$expansion does not converge at large μ.

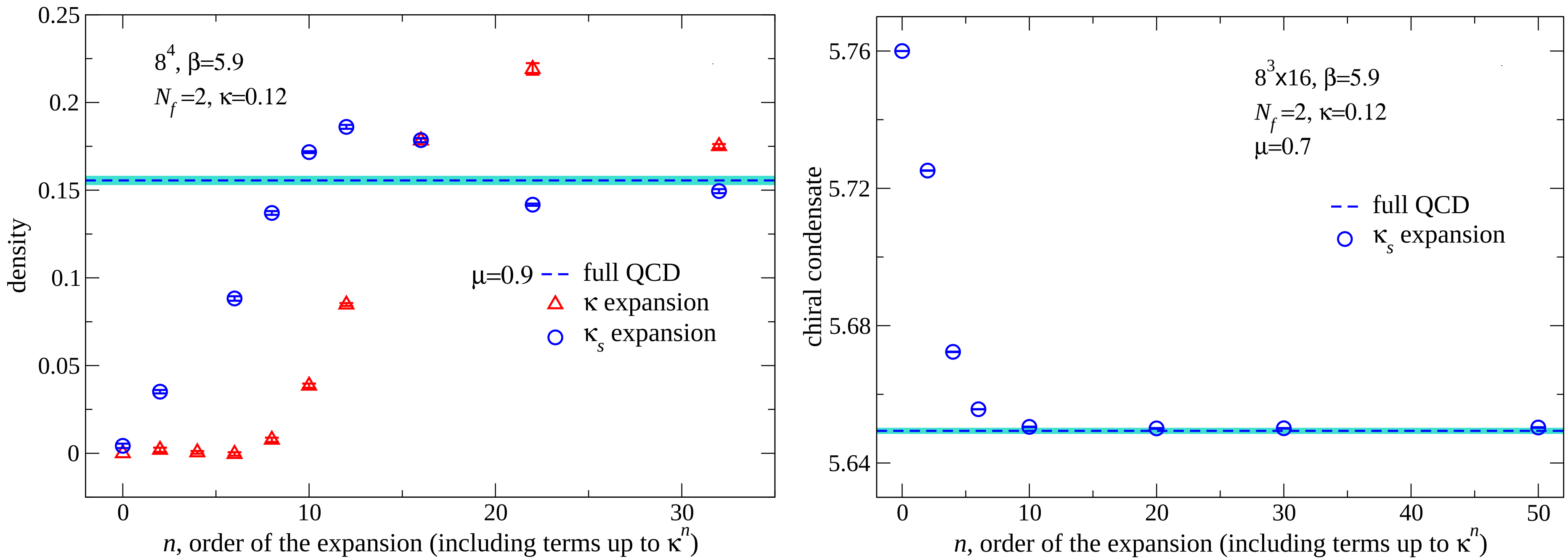


Figure 10: QCD, Wilson fermions, $\kappa = 0.12$, larger lattices, full and expansions vs $\kappa-$order. Increasing the lattice size does not affect the results.

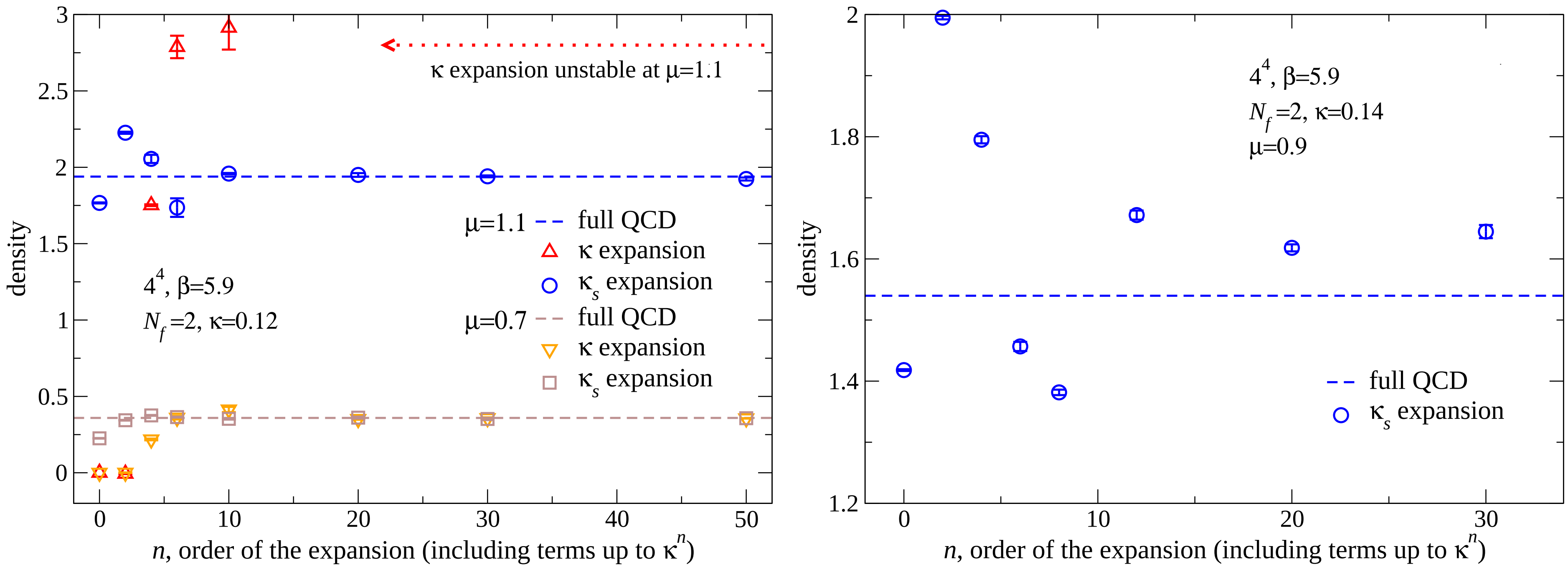


Figure 11: QCD, Wilson fermions, $\kappa = 0.12$ an 0.14, full and expansions vs $\kappa-$order. Increasing κ may lead to lack of convergence.

Conclusion:

- The κ_s-expansion converges well onto the full QCD at not too small quark mass.

- It provides a good approximation at reasonable orders where it is still very much cheaper than full QCD (no inversion of large matrices!).

- The expanded and the full drifts have very different analytic structure. The good agreement of the results can be considered as a test of correctness and suggests that poles in the full drift are not relevant in the investigated region.

- Increasing the lattice size (decreasing the temperature) does not seem to affect the quality of the results, while decreasing the mass may be difficult.

6. Overview and outlook

We seem to succeed developing the CLE method to approach QCD at non-zero chemical potential in a large physical region of parameters.

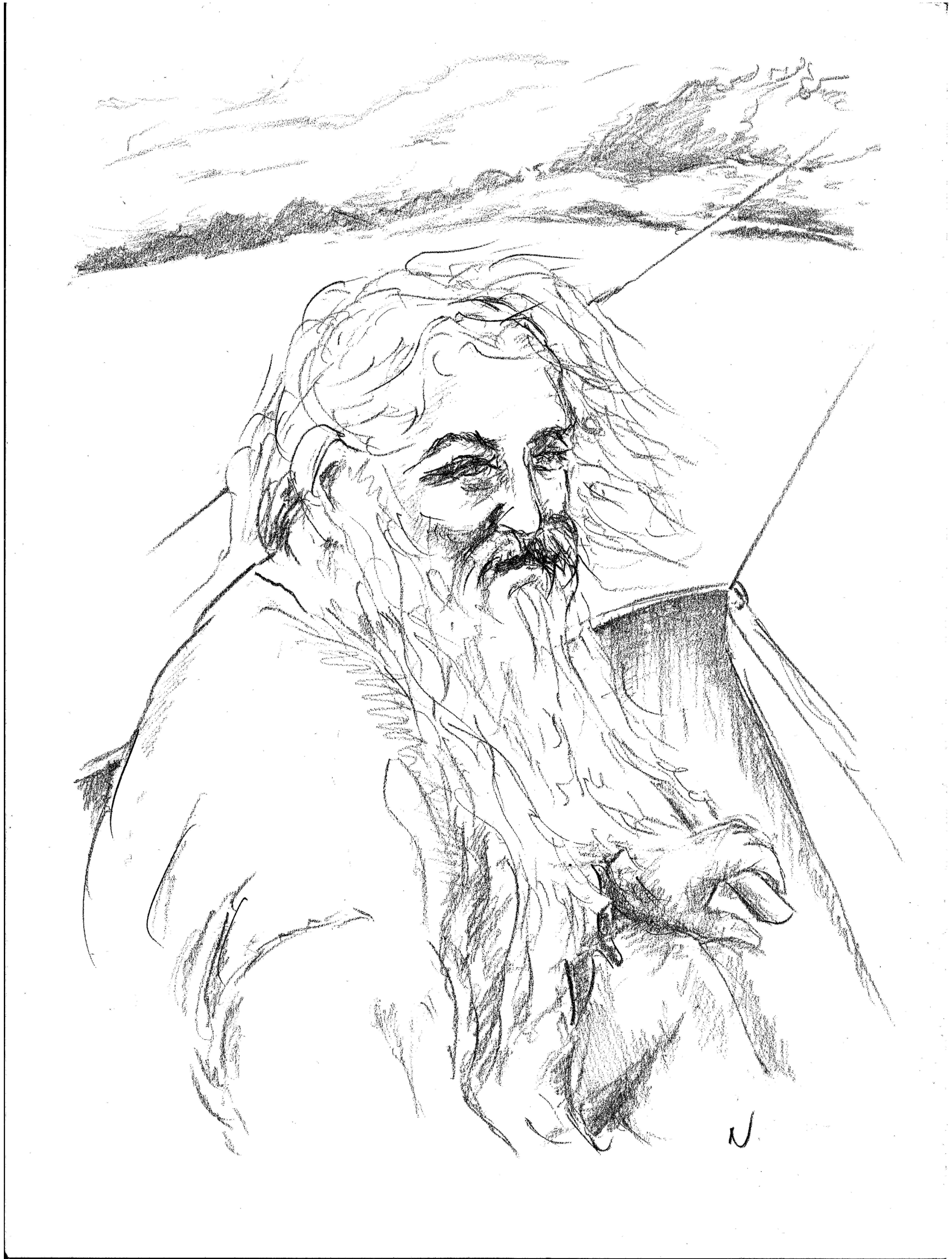
The gauge cooling method, technical improvements such as adaptive step size and criteria concerning the realized distribution, such as absence of skirts provide good means to control the CLE algorithm.

A systematic hopping parameter expansion appears quite efficient, both in practical and in theoretical sense:

- it provides fast algorithms, especially welcome on large lattices;

- it provides a test for the effects of non-holomorphy (or their absence) which as a theoretical problem for itself is still pending.

We are bound to start now more systematic investigations, also aiming at physical results.



Some publications

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
- Phase space of HDQCD using complex Langevin equation G. Aarts, B. Jaeger, E. Seiler, D. Sexty
- Some remarks on Lefschetz thimbles and CL dynamics G. Aarts, L. Bongiovanni, E. Seiler, D. Sexty
- Study of $\theta-$ vacua using CLE G. Aarts, L. Bongiovanni, E. Seiler, D. Sexty

Some directly relevant, recent publications

- J. Langelage, S. Lottini, O. Philipsen, arXiv:1403.4162.
- J. M. Pawlowski and C. Zielinski, Phys. Rev. D **87**, 094509 (2013), [arXiv:1302.2249 [hep-lat]]; Phys. Rev. D **87**, 094503 (2013) [arXiv:1302.1622 [hep-lat]].
- A. Duncan and M. Niedermaier, Annals Phys. **329**, 93 (2013).
- A. Mollgaard and K. Splittorff, arXiv:1309.4335 [hep-lat].
- M. Fromm, J. Langelage, S. Lottini, M. Neuman and O. Philipsen, arXiv:1207.3005 [hep-lat].
- P. de Forcrand and M. Fromm, Phys. Rev. Lett. **104** (2010) 112005 [arXiv:0907.1915 [hep-lat]].
- C. Pehlevan and G. Guralnik, Nucl. Phys. B **811** (2009) 519 [arXiv:0710.3756]