

Complex Langevin simulations for QCD-like models

Gert Aarts^a, Erhard Seiler^b, Denes Sexty^c and Ion-Olimpiu Stamatescu^c

^a Phys. Dept., Swansea University, UK, ^b M.P.I. f. Physik, Munich, Germany,
^c Inst. Theor. Physik, Univ. Heidelberg, Germany

Set up of the Complex Langevin Equation for simulations of problems with complex action.

Motivation and recalling LE

The Complex Langevin Equation (CLE) has the potential to simulate lattice models for which usual importance sampling fails (sign problem). In many cases, especially for QCD at non-zero density, the CLE in principle provides the (only) approximation free procedure.

While the Langevin equation (LE) for *real* problems is well defined and comparable with Monte Carlo (MC) simulations, its redefinition as CLE is, however, more involved. To develop the CLE to a reliable method is both a rewarding and a tough task. Our working program is:

- Define and study the properties of the CLE.
- Apply and discuss CLE for simple models.
- Perform CLE analysis of heavy dense lattice QCD.
- Perform the CLE analysis of full QCD at non-zero chemical potential (cf. talk by Denes Sexty).

The Langevin equation

The LE for a real field $\varphi(x)$ evolving in the process time t (here discretized, Itô calculus) is:

$$\delta\varphi(x;t) = K[\varphi(x;t)]\delta t + \eta(x;t)$$

$$\langle\eta(x;t)\rangle = 0, \quad \langle\eta(x;t)\eta(x,t_1)\rangle = 2\delta t\delta_{x,x_1}\delta_{t,t_1}$$

with the associated Fokker-Planck equation (FPE)

$$\partial_t P(\varphi,t) = \partial_\varphi(\partial_\varphi - K)P(\varphi,t).$$

If the drift $K = -\partial_\varphi S$ with S a positive definite action we then have asymptotically

$$t \rightarrow \infty, P(\varphi,t) \rightarrow P_{as}(\varphi) = \exp(-S)$$

Set up for the CLE

For a complex action the drift is also complex and this automatically provides an imaginary part for the field. This implies setting up the problem in the complexification of the original manifold

$$R^n \rightarrow C^n \text{ or } SU(n) \rightarrow SL(n,C).$$

The CLE then amounts to two related, real LE with independent noise terms - here for just one variable $x \rightarrow z = x + iy$ and with $K = -\partial_z S(z)$:

$$\delta z(t) = K(z)\delta t + \sqrt{N_R}\eta_R + i\sqrt{N_I}\eta_I$$

i.e. $\delta x(t) = \text{Re} K(z)\delta t + \sqrt{N_R}\eta_R(t)$
 $\delta y(t) = \text{Im} K(z)\delta t + \sqrt{N_I}\eta_I(t)$

$$\langle\eta_R\rangle = \langle\eta_I\rangle = 0, \quad \langle\eta_R\eta_I\rangle = 0$$

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

The probability distribution $P(x,y;t)$ realized in the process evolves according to a real FPE:

$$\partial_t P(x,y,t) = L^T P(x,y,t)$$

$$L = (N_R\partial_x + \text{Re}K(z))\partial_x + (N_I\partial_y + \text{Im}K(z))\partial_y$$

One can also define a complex distribution $\rho(x,t)$

$$\partial_t \rho(x,t) = L_0^T \rho(x,t), \quad L_0 = (\partial_x + K(x))\partial_x$$

with the asymptotic solution $\rho(x) = \exp(-S(x))$ and formally prove for *analytic* observables $O(z)$

$$\int O(x+iy)P(x,y,t)dx dy = \int O(x)\rho(x,t)dx.$$

The formal proof has, however, loopholes related to a too weak decay of $P(x,y,t)$ in y .

Problems and Tests for effective models.

Problems and models

Very many studies for CLE since the papers of Parisi and of Klauder (1983), many critical (a few quotations: Ambjorn, Hueffel, Gausterer, Karsch, Okano, Nakamura, Guralnik, ..).

Problems studied in our group:

- Real time simulations, non-equilibrium QFT.
- **Chemical potential** (Spin model, xy , QCD).
- θ -term.

We basically address here QCD with chemical potential, here to fix the concepts, the grand canonical ensemble (Wilson fermions):

$$Z = \int DU e^{-S}, \quad S = S_{\text{YM}} - \log \det W \quad (1)$$

$$W = 1 - \kappa \sum_{i=1}^3 \left(\Gamma_{+i} U_{x,i} T_i + \Gamma_{-i} U_{x,i}^{-1} T_{-i} \right) - \kappa \gamma \left(e^{\mu} \Gamma_{+4} U_{x,4} T_4 + e^{-\mu} \Gamma_{-4} U_{x,4}^{-1} T_{-4} \right)$$

T : lattice translations, $\Gamma_{\pm\mu} = 1 \pm \gamma_{\mu}$, $\kappa \sim 1/M$, γ bare anisotropy parameter. The temperature is introduced as $aT = \frac{\gamma}{N_c}$. We have $\det W(\mu) = [\det W(-\mu)]^*$ (complex).

CLE does not have an overlap problem such as the reweighting methods (RWM) and does not involve approximations like expansion methods (EM): The ensemble is generated at the actual values of the parameters without restriction in the latter.

CLE has, however, reliability problems which need to be understood and solved.

One link effective model

A paradigmatic effective model is one SU(3) link U . Diagonalizing U we obtain the reduced model

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

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

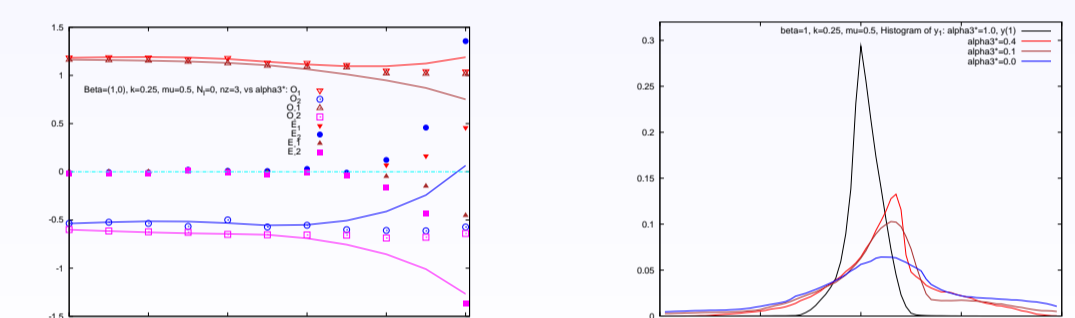
$$D = 1 + C \text{tr} U + C^2 \text{tr} U^{-1} + C^3, \quad C = 2\kappa e^{\mu}$$

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

(H : Haar measure, $w_1 + w_2 + w_3 = 0$, complex). The α 's simulate the staples of the neighbours.

As a general remark, observe that one first needs to complexify the variables (here in going from SU(3) to SL(3,C)). Notice also that ambiguities which may arrive by rewriting the complex determinants as part of the action drop out in deriving the corresponding drifts, which are just $\partial_w D/D + \partial_w \tilde{D}/\tilde{D}$. The analytic structure of the drift will show, among others, poles coming from the zero's of the determinants which will also influence the CLE flow. We observe that correct results obtain if the flow does not drift too far in the non-compact directions. This must be monitored and suggests possibilities to redesign the process to ensure reliability.

In this model, for α complex, far from 1 CLE departs from the exact results (solid lines). This correlates with wide skirts of the $\text{Im}w$ -distributions.



Many Links models and Gauge Cooling.

The Polyakov chain model

To see the effect of many variables we consider an exactly soluble Polyakov chain model:

$$-S = (\beta + 2\kappa e^{\mu})P + (\beta + 2\kappa e^{-\mu})P^{-1}$$

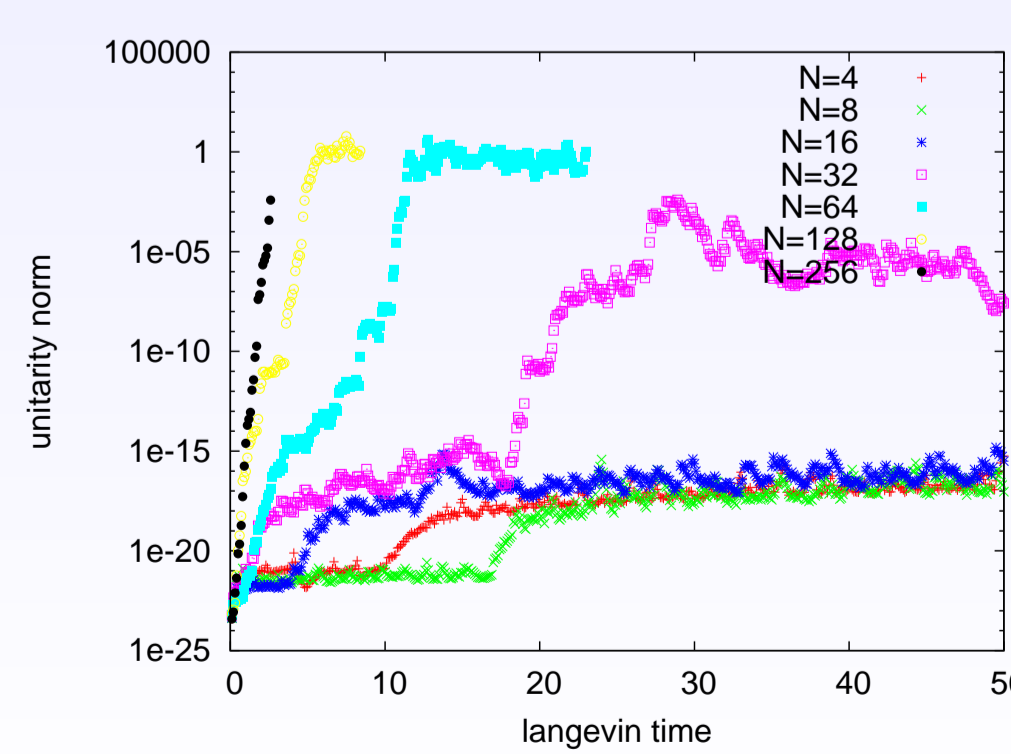
with $P = \text{Tr}(U_1 \cdots U_N)$, N up to 1024. The process runs in all $8N$ (complex) "angles" A_i^q of the links, with real noise ($\epsilon = \delta t$ discretization step):

$$\delta A_i^q = \epsilon K_i^q(U) + \sqrt{\epsilon} \eta, \quad U_i \rightarrow e^{i \sum_a \lambda_a \delta A_i^a} U_i$$

We observe wrong evolution setting in for large N even for the real case ($\mu = 0$) if we let the process evolve in the imaginary direction, although both drift and noise in this directions are 0! We can measure this effect by measuring the departure of the links from unitarity with the *unitarity norm*

$$U = \sum_{\text{links}} \left[\frac{1}{2} \text{Tr} (U U^\dagger + U^{-1} U^{-1\dagger}) - 3 \right]$$

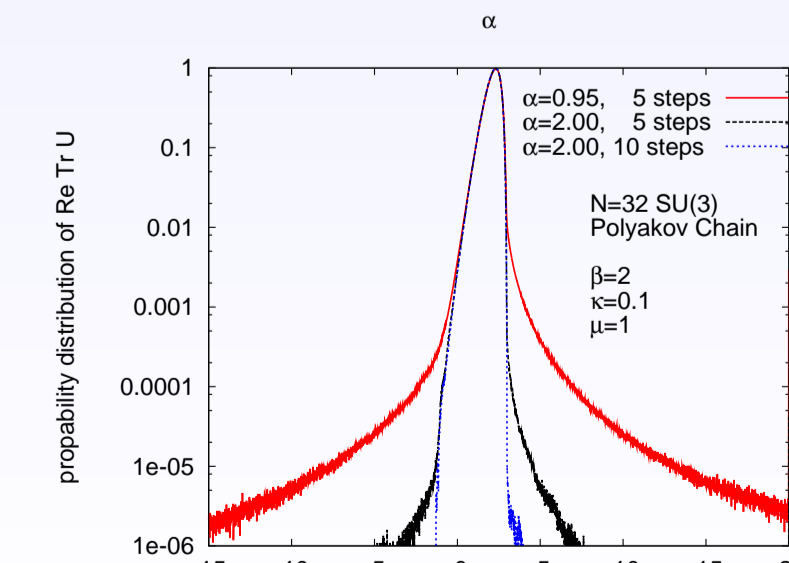
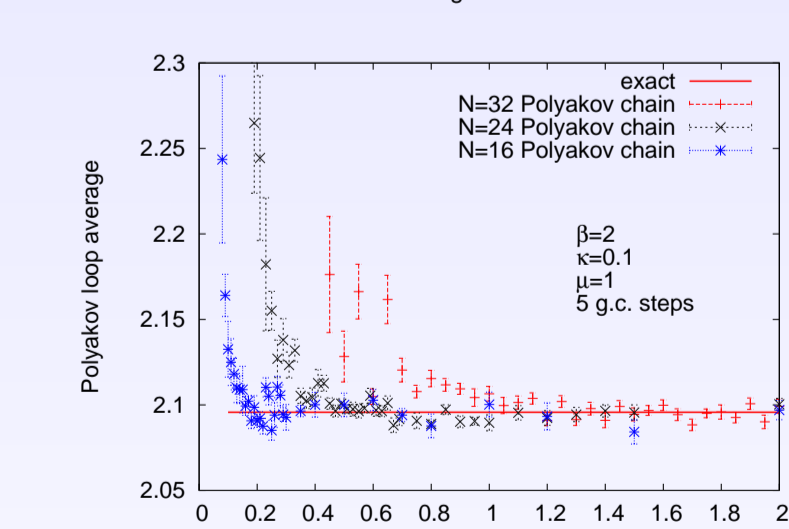
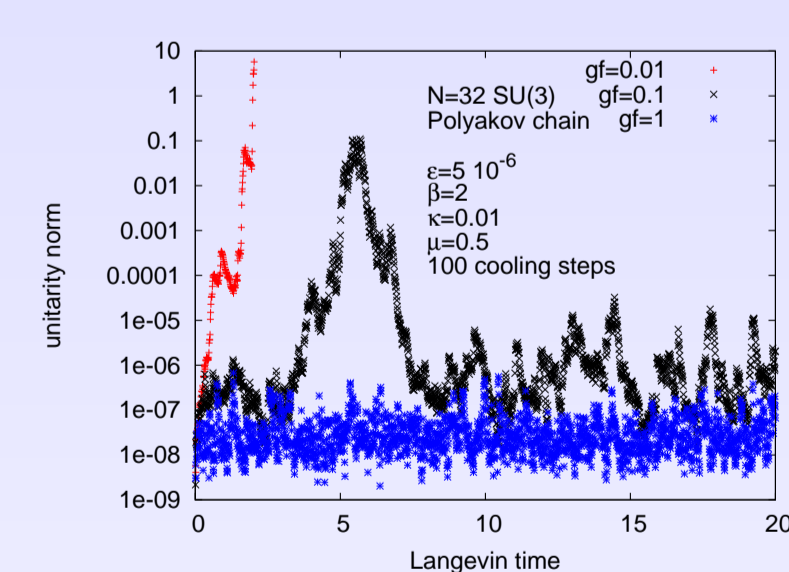
The above effect suggests that numerical imprecisions may trigger unstable modes preventing correct sampling. For simpler models fixing the gauge helped (Berges and Sexty, 2008).



Gauge cooling

Using the gauge symmetry of the problem we define a general *gauge cooling* procedure to bring the system as near as permitted to the unitary manifold. This proceeds by successive gauge transformations

$R_k = e^{i\alpha \epsilon dU}$, $U_k \rightarrow R_k U_k$, $U_{k-1} \rightarrow U_{k-1} R_k^{-1}$ with α : the strength of the *gauge force*, ϵ : step size. For $\mu > 0$ U should not be 0 but stabilize. This we see after enough cooling (large α and/or many cooling steps). Then also the results are correct and the non-compact distributions narrow.



Heavy dense QCD

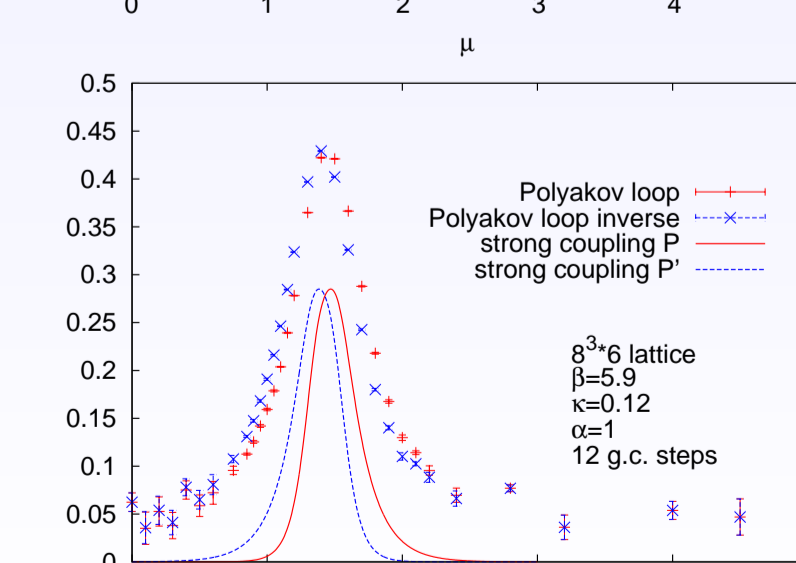
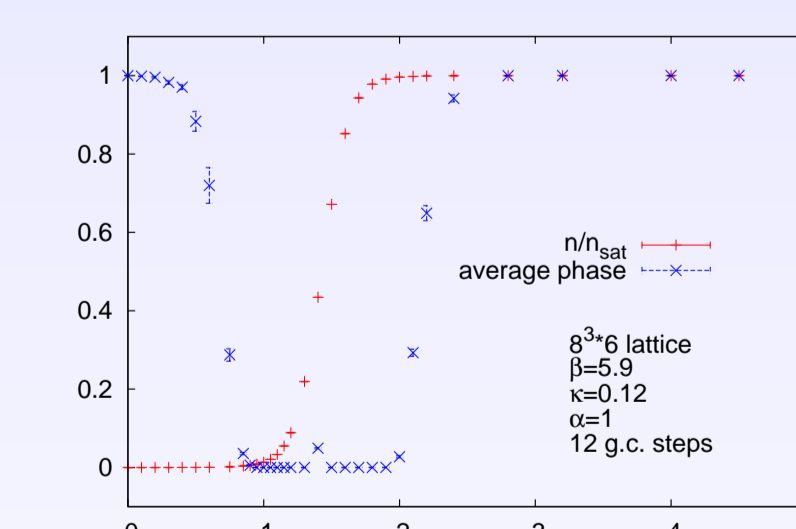
The heavy dense model (HQCD)

HQCD obtains in the hopping parameter expansion of the fermionic determinant in the double limit

$$\kappa \rightarrow 0, \quad \mu \rightarrow \infty, \quad \zeta = \kappa e^{\mu} : \text{fixed}$$

(Bender et al 1992). In this limit only the Polyakov loops survive and the determinant factorizes. This can be used, e.g. in refined RWM simulations (cf. De Pietri et al, 2007, where also the relevant formulae and the next corrections are given). The model represents a systematic approximation of QCD but also a model by itself, away from this limit (Aarts and Stamatescu, 2008).

We observe the same effects as for the Polyakov chain. The following results are obtained with sufficient cooling. We measure plaquettes, Polyakov loops P and P^{-1} , baryon density and the average phase: $\langle \exp(2i\phi) \rangle \equiv \langle \det \mathbf{M}(\mu) \det \mathbf{M}(-\mu)^{-1} \rangle$.



HQCD: comparison CLE and RWM

Both plaquettes and Polyakov loops agree extremely well for all values of μ in the deconfined region ($\beta = 5.9$, 6^4 lattice - the large errors belong to RWM). At fixed $\mu = 0.85$, 6^4 the agreement persists except for $\beta < 5.6$, indicating possible difficulties of the CLE. This effect seems, however, to be β and not scale dependent, for large lattices we can reach deep into the confining region (compare the 10^4 lattice, where the transition is expected at $\beta \simeq 5.9$). The excellent agreement between these two completely different methods validates both.

For a general review see Aarts et al, 2012.

