Complex Langevin and Boundary Terms

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common work with

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1. CL Setup
2. Formal argument
3. Uncovering the boundary terms
4. Analysis of a simple model
5. Conclusions, outlook, etc

1. CLE Setup

Complex action $\longrightarrow$ complex drift $\longrightarrow$ imaginary parts for the variables $\longrightarrow$ Process defined on the complex extension $\mathcal{M}_c$ of the original manifold $\mathcal{M}_r$: $\quad \mathbb{R}^n \longrightarrow \mathbb{C}^n$, $SU(n) \longrightarrow SL(n,\mathbb{C})$, ...

CLE for a complex variable $z = x + \mathrm{i}\, y$, complex drift $K(z)$:

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

$\longrightarrow$ two related, real LE with independent noise terms

$$\delta x(t) = K_x(z,t)\,\delta t + \sqrt{N_R}\,\eta_R(t), \quad K_x(z) = \mathrm{Re}K(z)$$
$$\delta y(t) = K_y(z,t)\,\delta t + \sqrt{N_I}\,\eta_I(t), \quad K_y(z) = \mathrm{Im}K(z) \tag{1}$$

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

Associated Random Walk (RW) process:

$$\delta x(t) = \begin{array}{lll} 0 & \text{with pbb.} & 1-q, \\ \pm\omega_x & \text{with pbb.} & \frac{1}{2}q\,(1 \pm \tanh(\frac{1}{2}\,\omega_x K_x/\sqrt{N_R})), \quad \omega_x = \sqrt{2\delta t/q} \end{array}$$

$$\delta y(t) = \begin{array}{lll} 0 & \text{with pbb.} & 1-q, \\ \pm\omega_y & \text{with pbb.} & \frac{1}{2}q\,(1 \pm \tanh(\frac{1}{2}\,\omega_y K_y/\sqrt{N_I})), \quad \omega_y = \sqrt{2\delta t/q}. \end{array}$$

Directly derived from a master equation, only needs *transition pbb's*.

Can be useful for encompassing non-ergodicity, also in r̂eal models.

The parameters q, N_I can be chosen adequately; typically $N_I = 0$ for CL and $0 \leq q \leq 1, N_I \geq 0$ for random walk.

To the processes corresponds a Fokker-Plank equation (FPE)

$$\partial_t P(x,y;t) = L^T P(x,y;t), \quad L = (\nabla_x + K_x)\,\nabla_x + K_y \nabla_y.$$

The CL realises a positive definite $P(x,y;t)$ on $\mathcal{M}_c$ obeying an FPE:

$$\partial_t P(x,y;t) = L^T P(x,y;t)\,, \quad L = (\nabla_x + K_x)\,\nabla_x + K_y \nabla_y$$

with EV's of the observables $\langle \mathcal{O} \rangle_{P(t)} \propto \int dx\, dy\, P(x,y;t)\, O(x + i\, y)$.
This is the *real* evolution.

Parallels the evolution of the complex measure $\rho(x,t)$ on the original manifold $\mathcal{M}_r$ (no associated process !)

$$\partial_t \rho(x;t) = L_\rho^T \rho(x;t), \quad L_\rho = (\nabla_x + K)\,\nabla_x\,, \quad \rho(x;\infty) \propto \exp\left[-S(x)\right]$$

with EV's of the observables $\langle \mathcal{O} \rangle_{\rho(t)} \propto \int dx\, \rho(x;t)\, O(x)$.
This is the *correct* evolution.

Task : prove $\langle \mathcal{O} \rangle_{P(\infty)} = \langle \mathcal{O} \rangle_{\rho(\infty)}$

We have traced back the failing of the CL simulation to three sources:

a. Non-holomorphicity of the action.

b. Large contributions in the non-compact directions.

c. Non-ergodicity.

Thereby non-ergodicity is a known problem in any stochastic simulation, in some cases is even milder in CL.

Non-holomorphicity is theoretically reducible to convergence questions or additional boundaries. (Remarks in the Discussion.)

Large non-compact contributions have various effects, also numerical. Here we are concerned with a problem of principle: boundary terms from the "integration" over the non-compact variables.
This appears as particulary important - and subtle.

2. Formal argument

Formal equivalence theorem:

for analytic observables $O(x, y)$ the averages over the process reproduce asymptotically the correct averages:

$$\langle \mathcal{O} \rangle_P = \langle \mathcal{O} \rangle_\rho \tag{2}$$

[Aarts, Seiler, Stamatescu, 2010]

Outline of the equivalence proof for holomorphic drift.

Consider

$$\langle \mathcal{O} \rangle_{P(t)} \equiv \frac{\int \mathcal{O}(x+iy) P(x,y;t) dx dy}{\int P(x,y;t) dx dy}, \quad \langle \mathcal{O} \rangle_{\rho(t)} \equiv \frac{\int \mathcal{O}(x) \rho(x;t) dx}{\int \rho(x;t) dx}.$$

Define interpolation function $(\tau \leq t)$

$$F_{\mathcal{O}}(t,\tau) \equiv \int P(x,y;t-\tau) \mathcal{O}(x+iy;\tau) dx dy, \tag{3}$$

$$F_{\mathcal{O}}(t,0) = \langle \mathcal{O} \rangle_{P(t)}, \qquad F_{\mathcal{O}}(t,t) = \langle \mathcal{O} \rangle_{\rho(t)}. \tag{4}$$

with "correctly evolved" $\mathcal{O}(t) = \mathrm{e}^{tL_\rho} \mathcal{O}(0)$ and matched initial conditions $P(x,y;0) = \rho(x;0)\, \delta(y)$ for *real* and *correct* evolutions.

The first equality in (4) is obvious, the second one follows from integration by parts in x which is typically compact.

Proof and loophole.

Equality $\langle \mathcal{O} \rangle_{P(t)} = \langle \mathcal{O} \rangle_{\rho(t)}$ is ensured if $F_{\mathcal{O}}(t,\tau)$ is independent of τ:

$$\frac{\partial}{\partial \tau} F_{\mathcal{O}}(t,\tau) = -\int \left(L^T P(x,y;t-\tau)\right) \mathcal{O}(x+iy;\tau) dx dy + \int P(x,y;t-\tau) L \mathcal{O}(x+iy;\tau) dx dy. \tag{5}$$

Using integration by parts $\longrightarrow$ RHS $=$0.

This assumes neglecting boundary terms from the y-integration.

Loophole: Non-zero boundary terms from slow decay of P L O!

3. Uncovering the boundary terms

Here: boundary terms arriving from the behaviour at large y – large noncompact directions.
(x typically compact $\longrightarrow$ neglect x boundary contributions.

For an observable $\mathcal{O}$ we have

$$\frac{\partial}{\partial \tau} F_{\mathcal{O}}(t,\tau) \equiv B_{\mathcal{O}}(t,\tau) = \int \left(\partial_y K_y P(x,y;t-\tau)\right) \mathcal{O}(x+iy;\tau) dx dy$$

to be interpreted as the limit $Y \to \infty$ of the integral for $|y| \leq Y$.

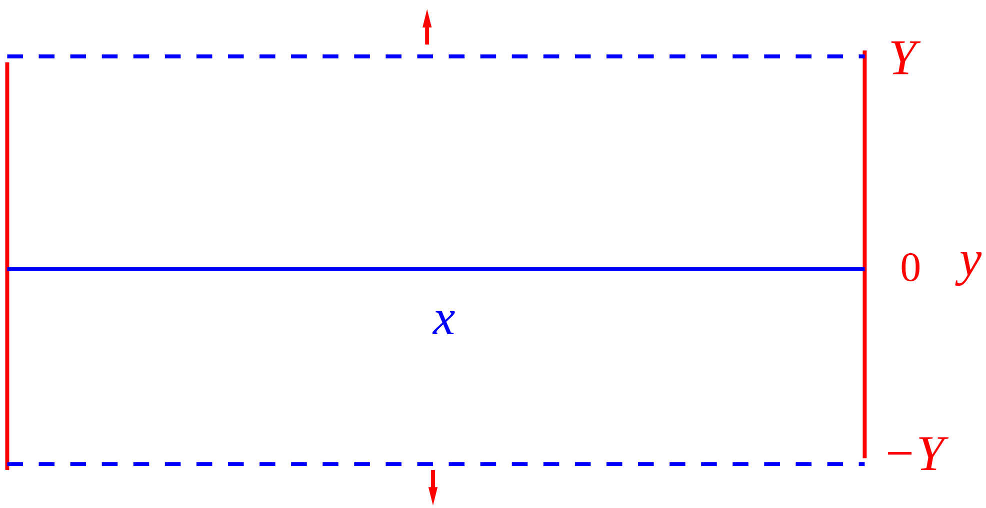
[Scherzer, Seiler, Sexty, Stamatescu 2018]

Integration by parts at finite Y $\longrightarrow$

$$B_{\mathcal{O}}(Y;t,\tau) = \int [K_y(x,Y)P(x,Y;t-\tau)\mathcal{O}(x+iY;\tau) \\ - K_y(x,-Y)P(x,-Y;t-\tau)\mathcal{O}(x-iY;\tau)]dx$$

making concrete the boundary contribution. Finally take

$$B_{\mathcal{O}}(t,\tau) = \lim_{Y\to\infty} B_{\mathcal{O}}(Y;t,\tau)$$



Observe careful limit procedures!

4. Analysis of a simple model

Measure, observables and “correct” EV’s:

$$\rho = \frac{1}{Z(\beta)} \exp\left[-i\beta \cos(x)\right], \tag{6}$$

$$\mathcal{O}_k = \exp(i\,k\,x), \tag{7}$$

$$\langle \mathcal{O}_k \rangle_\rho = (-i)^k \frac{J_k(\beta)}{J_0(\beta)} \neq 0\,. \tag{8}$$

No ergodicity or holomorphicity problems!

[Stamatescu; Berges and Sexty, 2008]

CLE and FPE

Complexification: $x \longrightarrow z = x + i\,y$

CL process:

$$\delta x(t) = K_x(z,t)\,\delta t + \eta_R(t)\,, \quad K_x = \mathrm{Re}\,\frac{\rho'}{\rho} = -\beta\cos(x)\sinh(y)$$

$$\delta y(t) = K_y(z,t)\,\delta t\,, \quad K_y = \mathrm{Im}\,\frac{\rho'}{\rho} = \beta\sin(x)\cosh(y)$$

Real evolution of observables and probability (CLE and FPE-PDE):

$$\partial_t \mathcal{O}_k(z;t) = L\mathcal{O}_k(z;t), \qquad \partial_t P(x,y;t) = L^T P(x,y;t)$$

$$L = [\partial_x + K_x]\,\partial_x + K_y\partial_y$$

[Scherzer, Seiler, Sexty, Stamatescu 2018]

CL produces incorrect results!

The FPE has an exact, analytic, asymptotic solution! *[Salcedo, 2017]*

$$P(x,y) = \frac{1}{4\pi\cosh^2(y)} \longrightarrow \langle \mathcal{O}_1 \rangle_P = 0 \neq \langle \mathcal{O}_1 \rangle_\rho \qquad (9)$$

and $\langle \mathcal{O}_k \rangle_P$ undefined for $|k| = 2$, divergent for $|k| \geq 2$, all $\neq \langle \mathcal{O}_k \rangle_\rho$.

The LC (and numerical FPE) reproduce these (incorrect!) results

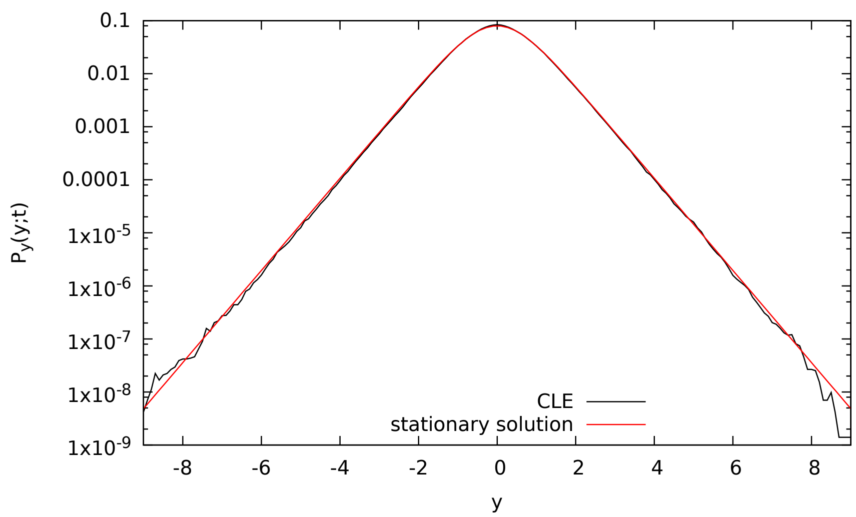


Figure 1: Analytic FPE solution and CL asymptotic histogram

A more detailed look: non-trivial LC/FPE evolution

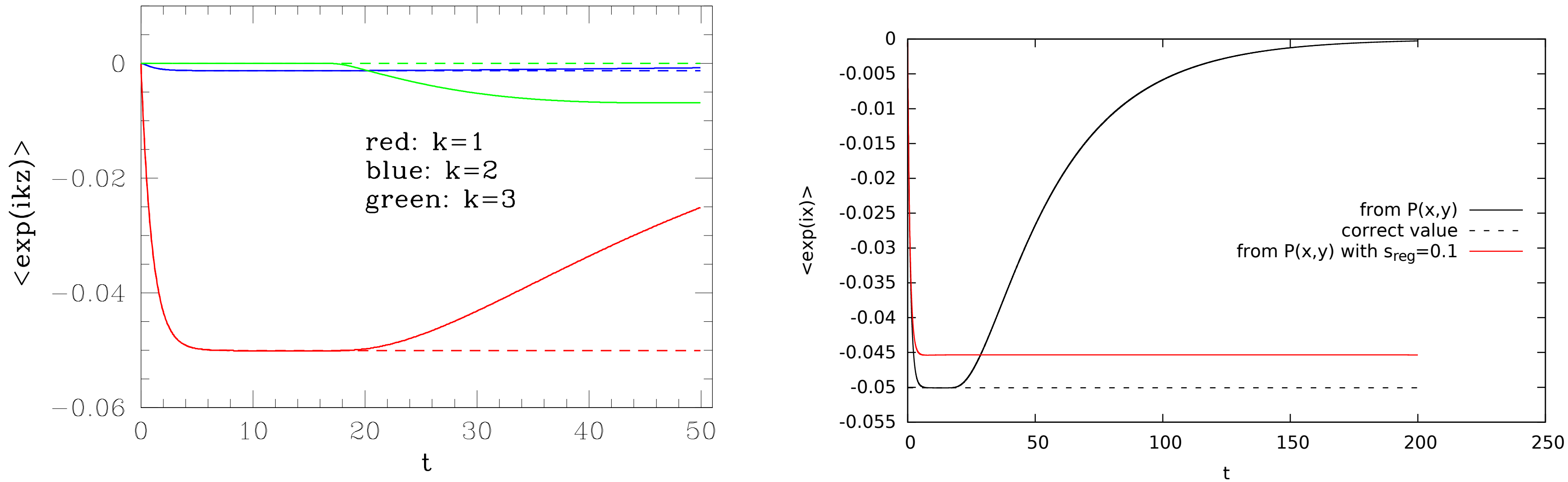


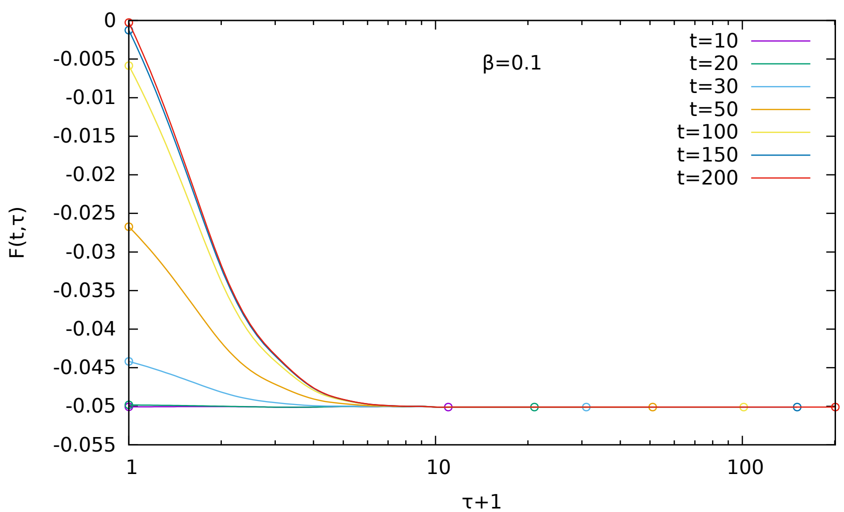
Figure 2: FPE evolution of the $\mathcal{O}_k$ at $\beta = 0.1$. (Red line in right hand side plot comes from a modified model, see ch. 4.)

Notice: Plateau for intermediary t at the correct value!

The interpolation function

$$F_{\mathcal{O}}(t,\tau) \equiv \int P(x,y;t-\tau)\mathcal{O}(x+iy;\tau)dxdy, \qquad (10)$$

$$F_{\mathcal{O}}(t,0) = \langle\mathcal{O}\rangle_{P(t)}, \qquad F_{\mathcal{O}}(t,t) = \langle\mathcal{O}\rangle_{\rho(t)}. \qquad (11)$$



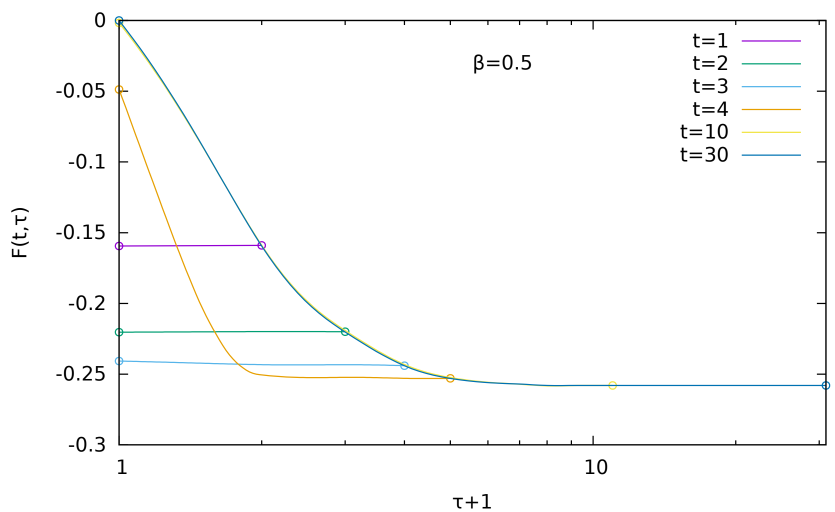


Figure 3: $F_1(t,\tau)$ vs τ at $\beta = 0.1$ and $\beta = 0.5$, various t.

Notice: Slope approximately maximal ($\longrightarrow$ maximal B_1) at $\tau = 0$!

Boundary terms

Boundary term for O_1, $B_1 = \partial_\tau F_1(t,\tau)$, at $\tau = 0$:

$$B_1(Y;t,0) = \beta \int \sin(x)\cosh(Y) \mathrm{e}^{i\,x}[P(x,Y;t)\mathrm{e}^{-Y} - P(x,-Y;t)\mathrm{e}^{Y}]dx$$

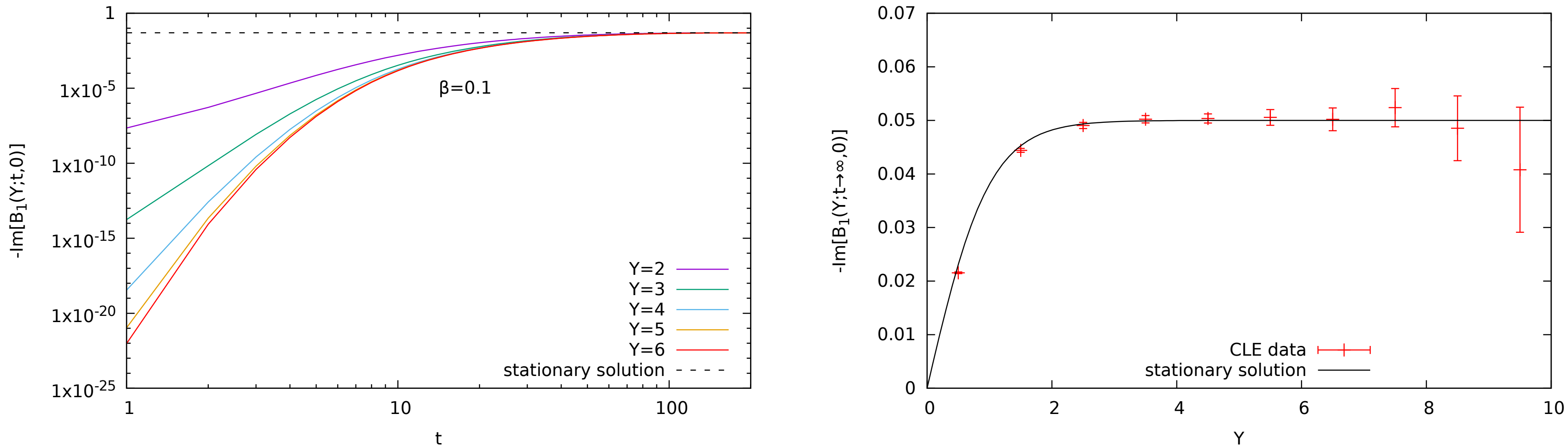


Figure 4: B_1 at $\beta = 0.1$: FPE vs t, various Y and CL vs Y at large t.

Notice: B_1 saturates at non-zero values for large Y.

Boundary terms and CL evolution

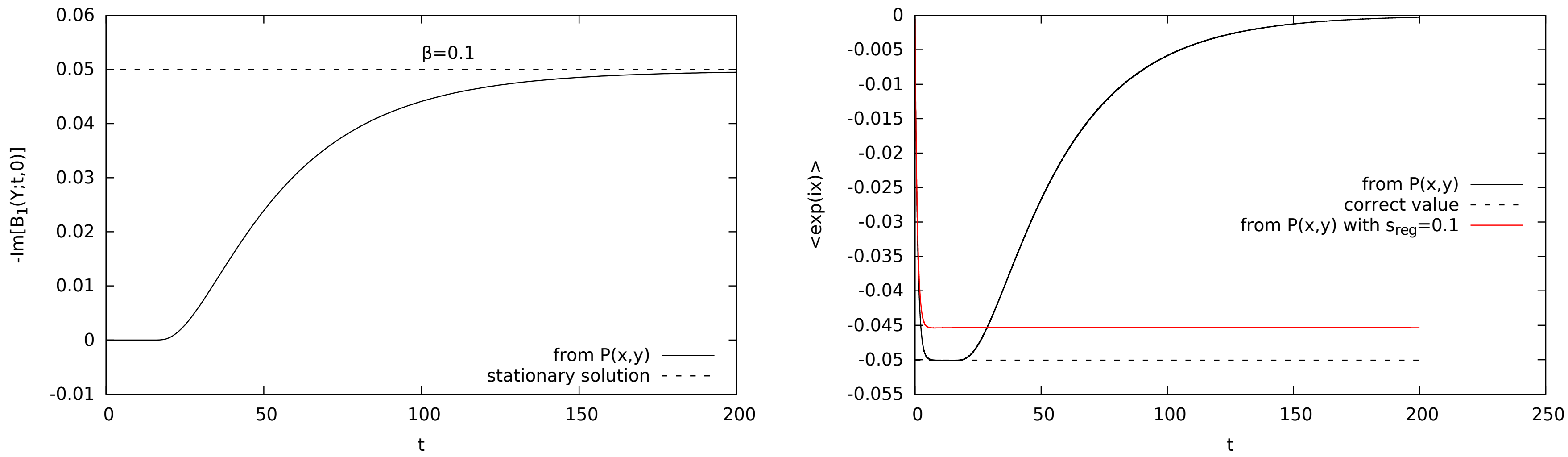


Figure 5: $\beta = 0.1$, evolution of B_1 and of $\mathcal{O}_1$.

Notice clear correlation between the behaviour of $\mathcal{O}_1$ and of B_1 !

We hence demonstrated that incorrect results are due to boundary terms building up in the Langevin evolution *[Aarts et al, 2011]*.

Can they be eliminated?

Eliminating the boundary terms by regularization

Damping factor:

$$\rho(x) \longrightarrow \rho(x) e^{-\frac{s}{2} x^2} \tag{12}$$

(see also *[Loheac and Drut, 2017]*). This changes the dynamics.

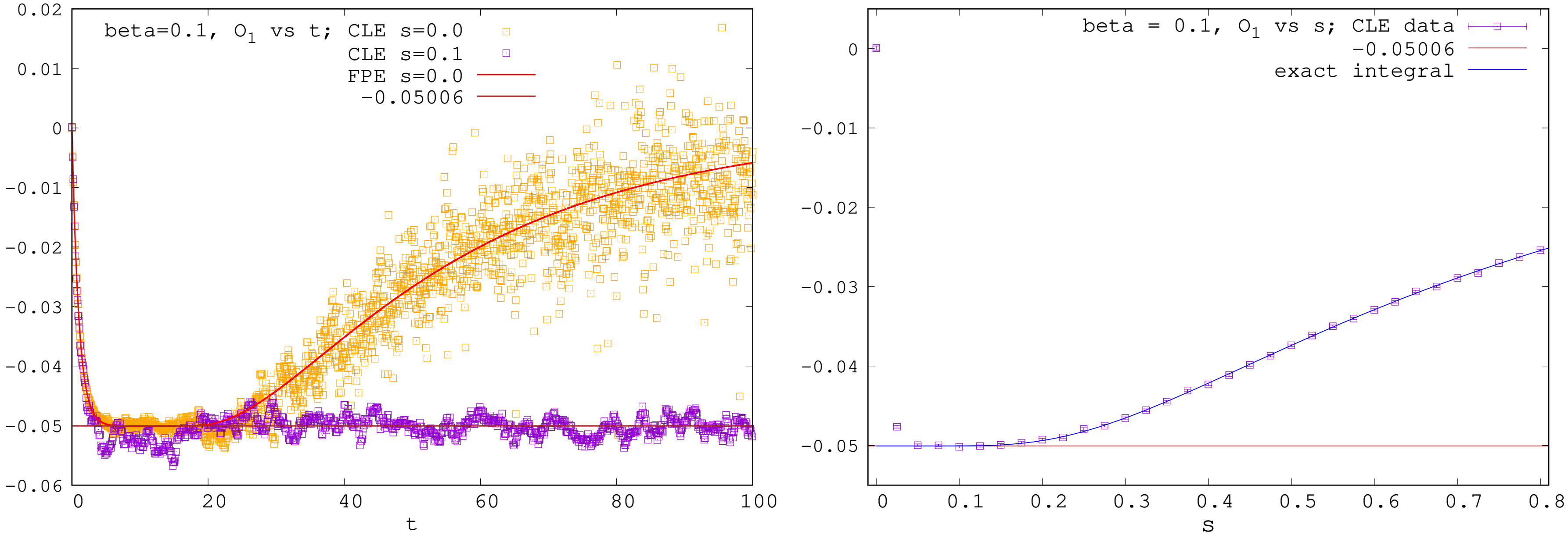


Figure 6: $\beta = 0.1$, $\mathcal{O}_1$ vs t at $s = 0.1$ and vs s at large t.

Here the regularized model has no boundary terms for $\forall s$, correct and real evolutions agree. $\exists s$ extending the original (correct) plateau to ∞.

Extrapolation?

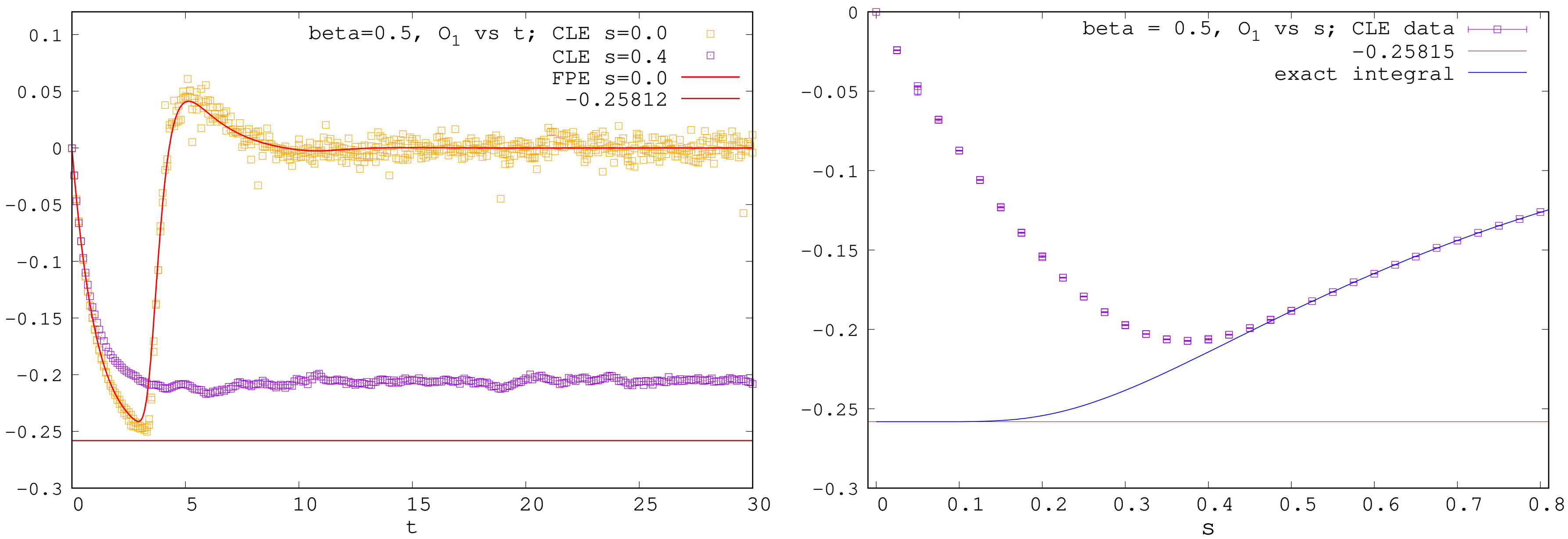


Figure 7: Regularization at $\beta = 0.5$, $\mathcal{O}_1$ vs t, $s = 0.4$ and vs s, large t.

Here the original model has no plateau. The regularized model has boundary terms for $s \leq 0.45$, CL is stabilized but at no s at the correct original value. Extrapolation to $s = 0$: suggestive but unprecise.

Other regularizations possible, e.g. damp only y, red line in Figs. 2, 5.

5. Conclusions

Summary and outlook

We have demonstrated explicitely that for holomorphic action incorrect LC evolution comes from boundary terms in the non-compact integration.

These terms are related to slow decay of the product $P\,K\,O$ and their uncovering implies a subtle limiting procedure.

On the basis of this study we conjecture that these terms can be estimated on-line in a CLE simulation and therefore may provide a criterium for correctness also for realistic lattice simulations.

Relation to the unitarity norm in gauge theories

A signal for the appearence of boundary terms can also be uncontrolled increase in some measure of non-compactness, e.g. the unitarity norm.

In this case the process samples dominant contributions at increasing distances from the compact subspace which would then generate boundary terms.

Conversely, as long as the unitarity norm stays small no significant boundary terms can appear.

An explicit estimation of the boundary term in corelation to the unitarity norm is feasible on-line and could substantiate this conjecture.

Further comments: what we did not touch here

Non-holomorphicity spoils the formal equivalence argument and was shown in models to lead to incorrect results (*[Mollgaard und Splittorff, 2013, Bloch, Glasaen, Verbarschot, Zafeiropoulos, 2018]*). The problem of zeroes in the measure was analyzed in detail for models as well as for QCD and the effects discussed in *[Aarts, Seiler, Sexty, Stamatescu 2017]*, see also *[Splittorff 2015]*, ...

Improvement of the CLE process besides using symmetries (such as gauge cooling) can be attempted by controllable changes of the dynamics but may require careful extrapolation (see *[Attanasio, Jaeger 2018], Nagata, Nishimura, Shimasaki 2016]*)

Also talks by *D. Sexty, F. Attanasio, M. Scherzer, B. Jäger, ...*