Complex Langevin boundary terms in lattice models

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1. Complex Langevin
2. Boundary terms, calculated by surface or volume integrals
3. test in full QCD, 3d XY model
4. Correction using boundary terms

Importance Sampling and Sign Problem

We are interested in a system
Described with the partition sum:

$$Z = \int D\phi\, e^{-S} = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \sum_C W[C]$$

Usually: Markov Chain Monte Carlo $\ldots \rightarrow C_{i-1} \rightarrow C_i \rightarrow C_{i+1} \rightarrow \ldots$

Probability of visiting C $p(C) \sim W[C]$ $\langle X \rangle = \frac{1}{N} \sum_i X[C_i]$

This works if we have $W[C] \geq 0$ Otherwise we have a Sign problem

Workaround: Dual variables, Density of States,
Reweighting, Taylor expansion, Imaginary potentials, etc.

Using analyticity: Lefschetz Thimbles, Complex Langevin

Complex Langevin Equation

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:

$$\langle O \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T O(x(\tau))\, d\tau = \frac{\int e^{-S(x)} O(x)\, dx}{\int e^{-S(x)}\, dx}$$

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

<u>The field is complexified</u>

real scalar $\longrightarrow$ complex scalar

link variables: SU(N) $\longrightarrow$ SL(N,C)

compact $\quad$ non-compact

$$det(U) = 1, \quad U^{+} \neq U^{-1}$$

Analytically continued observables

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

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

Argument for correctness of CLE results

If there is fast decay $P(x,y) \rightarrow 0$ as $x,y \rightarrow \infty$

and a holomorphic action $S(x)$

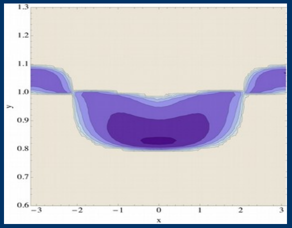
then CLE converges to the correct result

[Aarts, Seiler, Stamatescu (2009)
Aarts, James, Seiler, Stamatescu (2011)]

Loophole 1: 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
$\longrightarrow$ meromorphic drift



No problems if poles are not ‘touched’ by distribution

satisfied for: HDQCD, full QCD at high temperatures

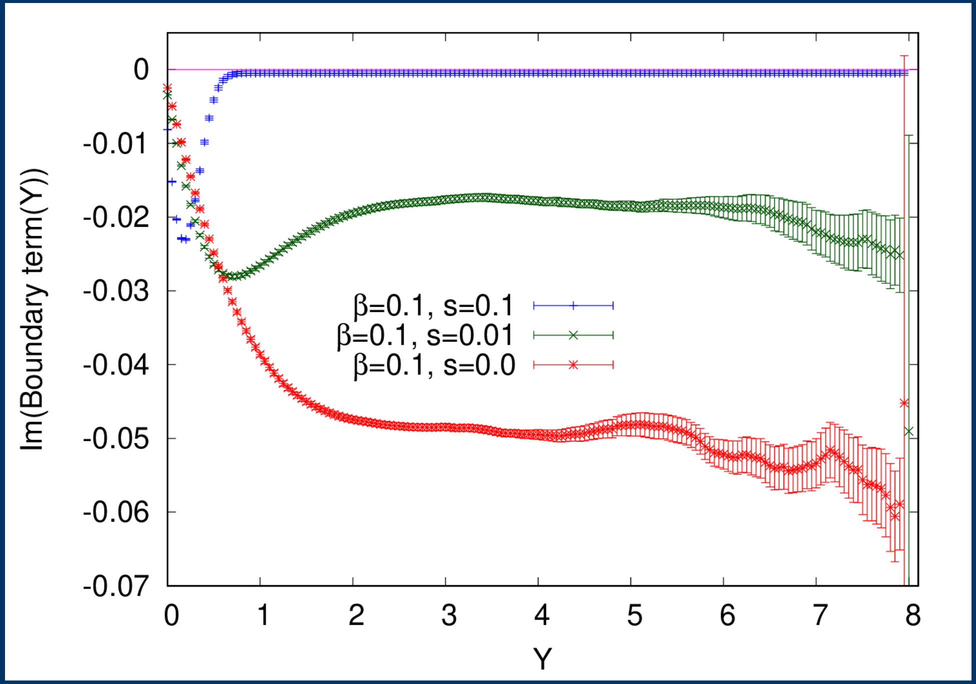
[Aarts, Seiler, Sexty, Stamatescu ‘17]

[See next talk by Erhard Seiler for boundary terms at poles]

Loophole 2: decay not fast enough

boundary terms can be nonzero
explicit calculation of boundary terms possible

[Scherzer, Seiler, Sexty, Stamatescu (2018)+(2019)]



Unambigous detection of boundary terms

given by plateau as 'cutoff' $Y \to \infty$

Observable cheap also for lattice systems

Measuring “corrected observable”

in case boundary term nonzero

Now the details...

Sketch of the proof

$P(x,y,t)$: probability density on the complex plane at Langevin time t

Real Fokker-Planck equation

$$\frac{\partial P}{\partial \tau}=\frac{\partial}{\partial x}\left(\frac{\partial P}{\partial x}-K_x P\right)-\frac{\partial}{\partial y}(K_y P) \quad \text{with} \quad K_i=-\partial_i S$$

Real action $\rightarrow$ $K_y=0$, positive eigenvalues of H_{FP}

$$P(x,y,\infty)=\delta(y)\exp(-S(x))$$

$\rho(x,t)$: complex measure evolving with the complex Fokker-Planck equation
(not associated to a stochastic process)

$$\partial_t \rho(x,t)=\partial_x(\partial_x-K_x)\rho(x,t)=L_c^T\rho(x,t)$$

Stationary solution: $\rho(x,\infty)=\exp(-S(x))$

CLE works, if

What we want		What we get with CLE
$\int dx\, \rho(x) O(x)$	$=$	$\int dx\, dy\, P(x,y) O(x+iy)$

$$\langle O(x)\rangle_{\rho(t)} = \langle O(x+iy)\rangle_{P(t)}$$

$$O(z,t) = e^{L_c t} O(z,0)$$

with $L_c = (\partial_z + K(z))\partial_z$

Interpolating function:

$$F(t,\tau) = \int P(x,y,t-\tau) O(x+iy,\tau)\, dx\, dy$$

$$F(t,0) = \langle O(x+iy)\rangle_{P(t)}$$

$$F(t,t) = \int P(x,y,0) O(x+iy,t)\, dx\, dy$$

$$= \int \rho(x,0)\delta(y) O(x+iy,t)\, dx\, dy$$

Choose to be
on real axis initially

$$= \int \rho(x,0) O(x,t)\, dx = \int \rho(x,t) O(x,0)\, dx = \langle O(x)\rangle_{\rho(t)}$$

$\partial_\tau F(t,\tau) = 0$ can be seen with partial integrations
using Cauchy-Riemann eqs. for $\partial_x O(x+iy,\tau)$

QED

Boundary term defined on a surface

$$\partial_\tau F_O(t,\tau) = B_O(Y,t,\tau) = \int K_y(x,Y) P(x,Y,t-\tau) O(x+iY,\tau)\, dx$$
$$- \int K_y(x,-Y) P(x,-Y,t-\tau) O(x-iY,\tau)\, dx$$

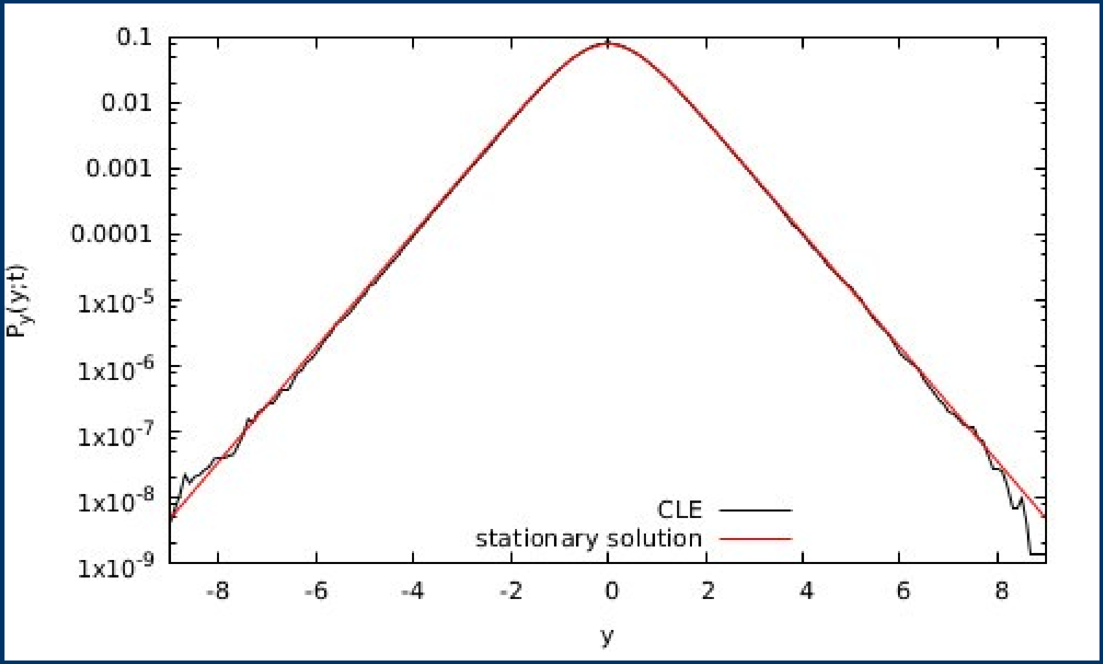
One plaquette model

$$S(\varphi)=i\beta\cos(\varphi) \qquad \langle e^{ikx}\rangle=(-i)^k\frac{J_k(\beta)}{J_0(\beta)}$$

Exact asymptotic solution of CLE [Salcedo, 2017]

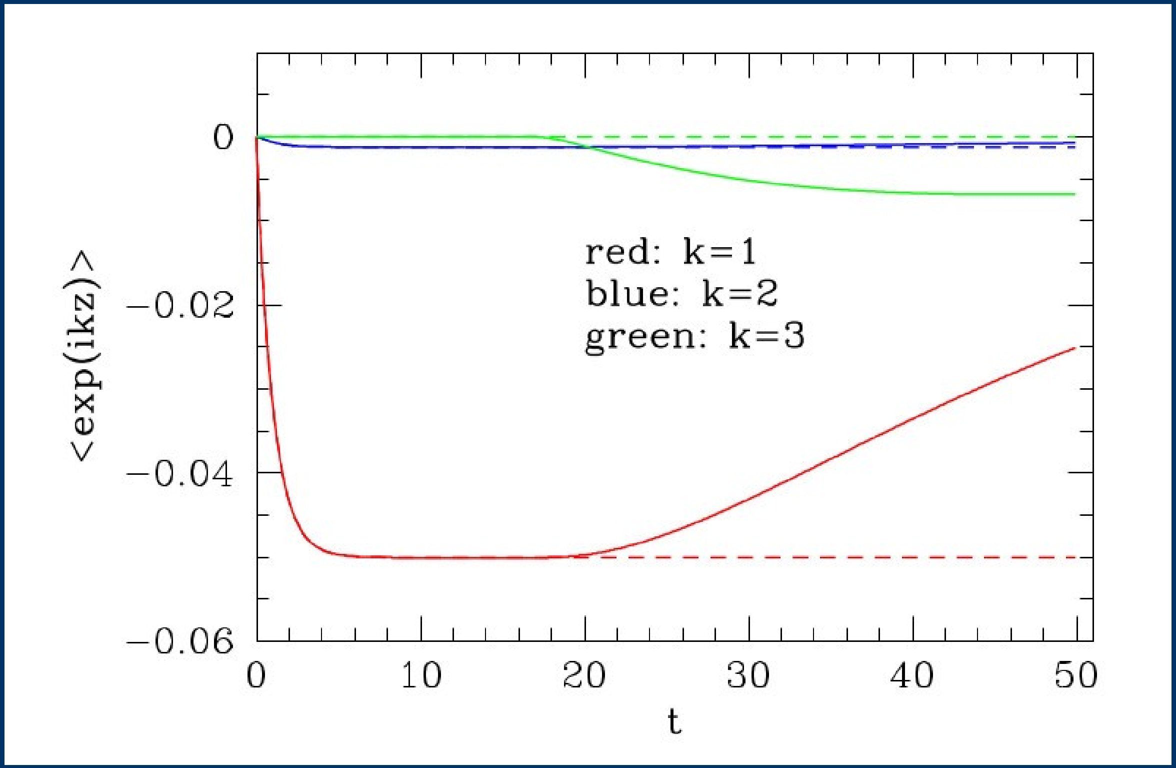
$$P_a(x,y)=\frac{1}{4\pi\cosh^2 y} \qquad \text{independent of } x \text{ and } \beta$$

$$\langle e^{ix}\rangle_{P_a}=0, \quad \langle e^{ikx}\rangle_{P_a} \text{ for } k\geq 2 \text{ is undefined or divergent}$$



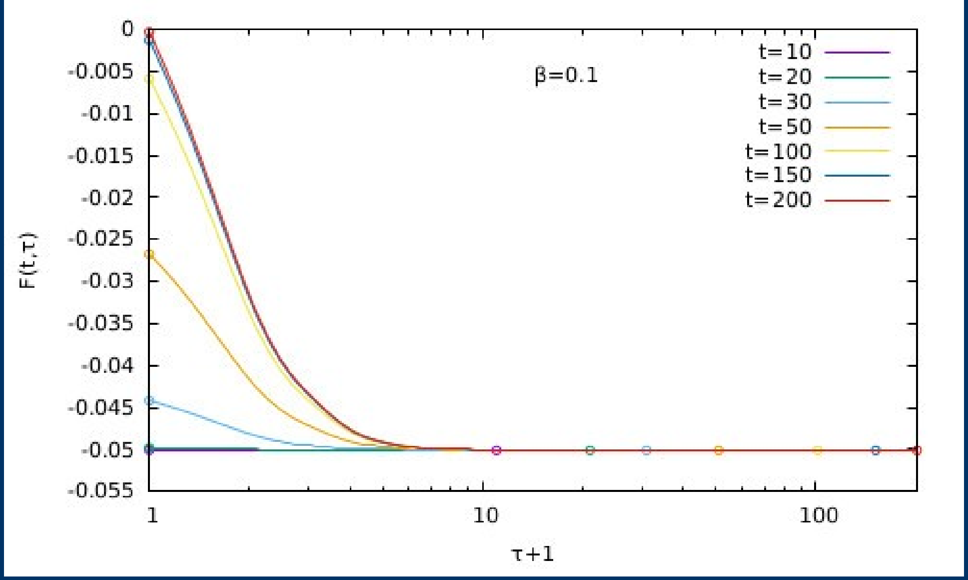
CLE reproduces this (incorrect) solution

Langevin time evolution



For short times
plateau at the correct value

asymptotic result incorrect



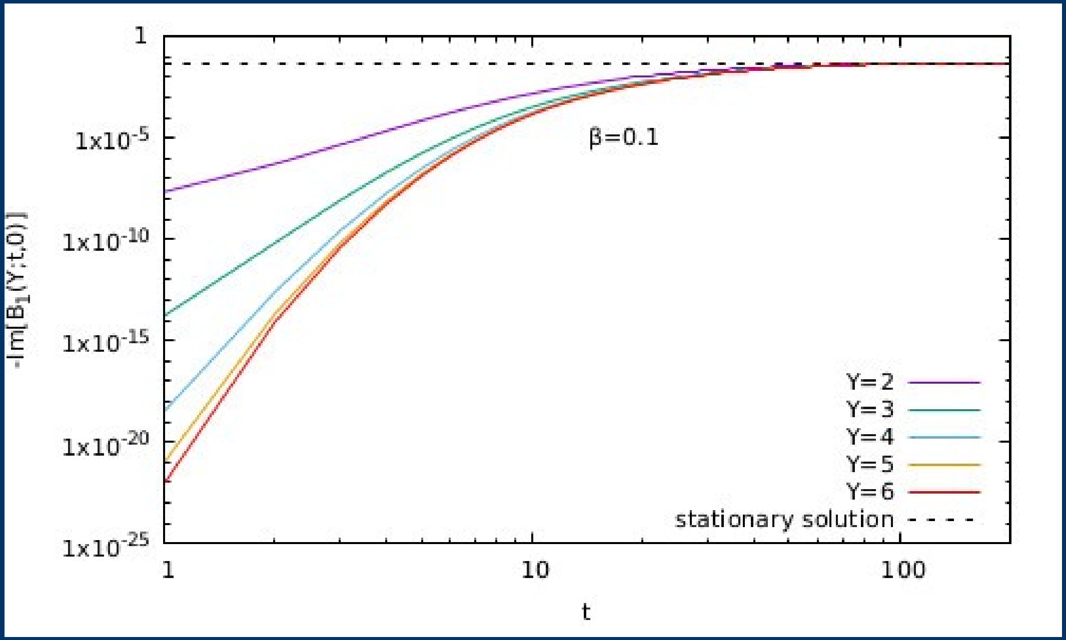
$F(t,0)-F(t,t)$ gets >0 above $t=20$

Largest slope at $\tau=0$

$$\partial_\tau F_{(t,\tau=0)}=B(t,0)$$

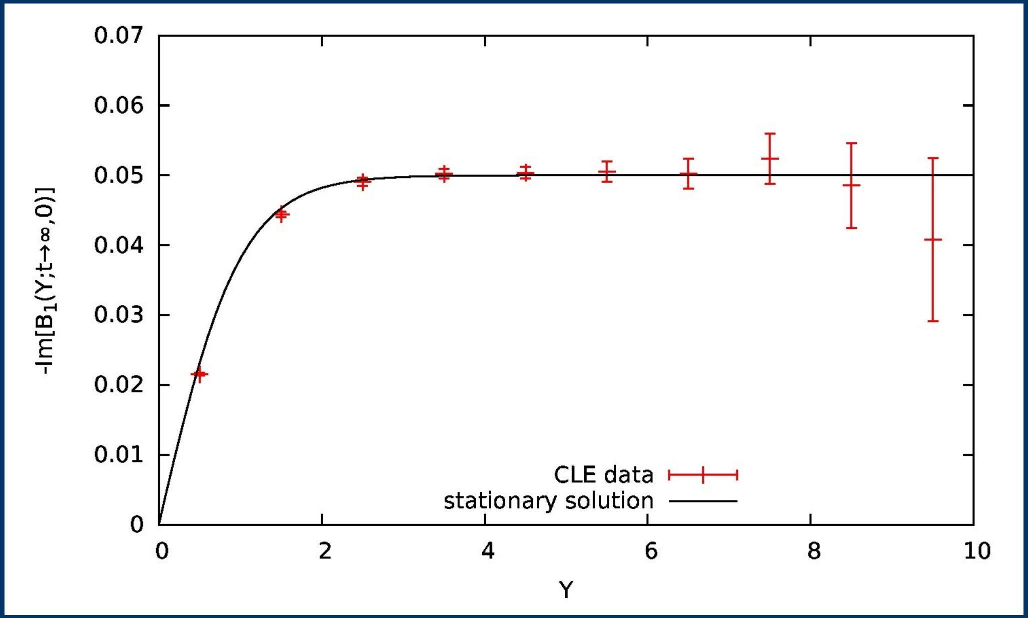
seems like a good proxy for
$F(t,0)-F(t,t)$

Boundary term



Boundary term

Calculated using Fokker-Planck discretised on a 2d grid



Using Complex Langevin only

Plateau clearly visible
At high cutoff statistics is worse

Need to measure on some surface
inconvenient in many dimensions

Boundary terms as a volume integral

[Scherzer, Seiler, Sexty, Stamatescu (2018+2019)]

Calculating an observable defined on a compact boundary in many dimensions can be inconvenient

$$\partial_\tau F_O(Y,t,\tau=0) = B_O(Y,t,\tau=0) =$$

$$\int_{-Y}^{Y} P(x,y,t) L_c O(x+iy) - \int_{-Y}^{Y} (L^T P) O(x+iy,0)$$

Observable with a cutoff
easy to do in many dimensions

Vanishes as process equilibrates

$L_c O(x+iy)$ consistency conditions $\approx$ Schwinger-Dyson eqs.

Order of limits crucial

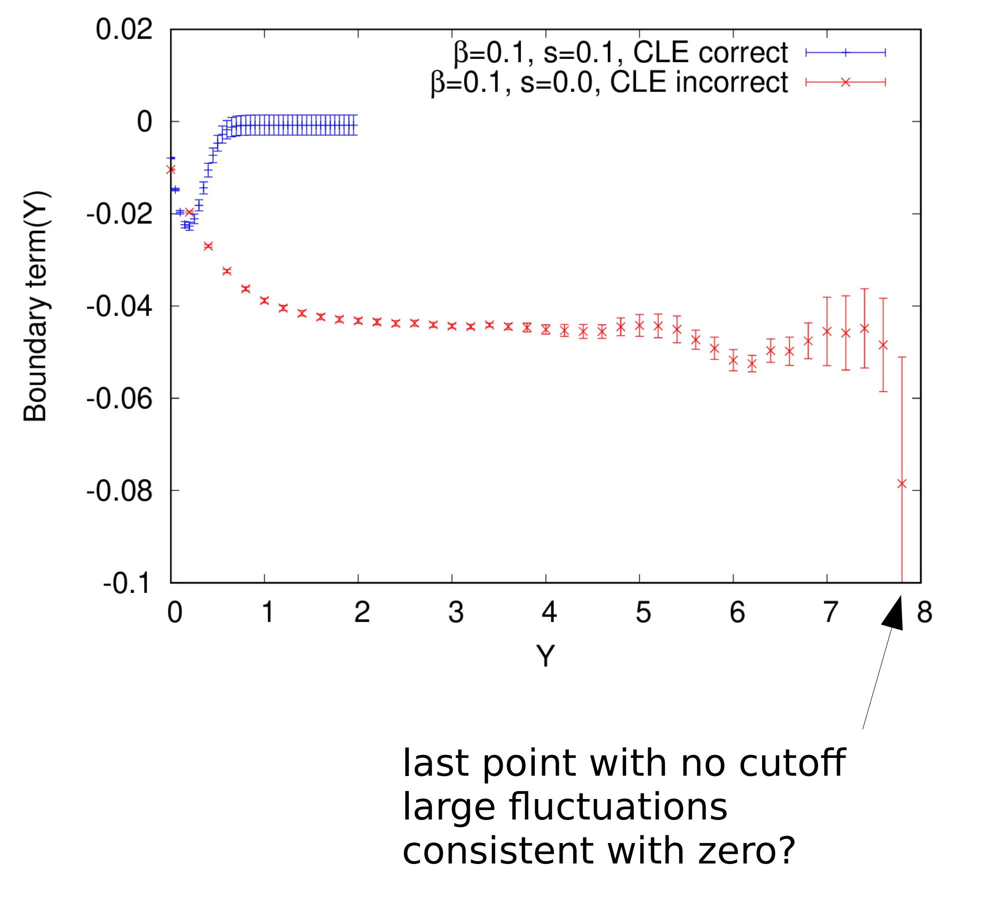
$$\lim_{t\to\infty} \lim_{Y\to\infty} \int_{-Y}^{Y} P(x,y,t) L_c O(x+iy) \text{ can be undefined}$$

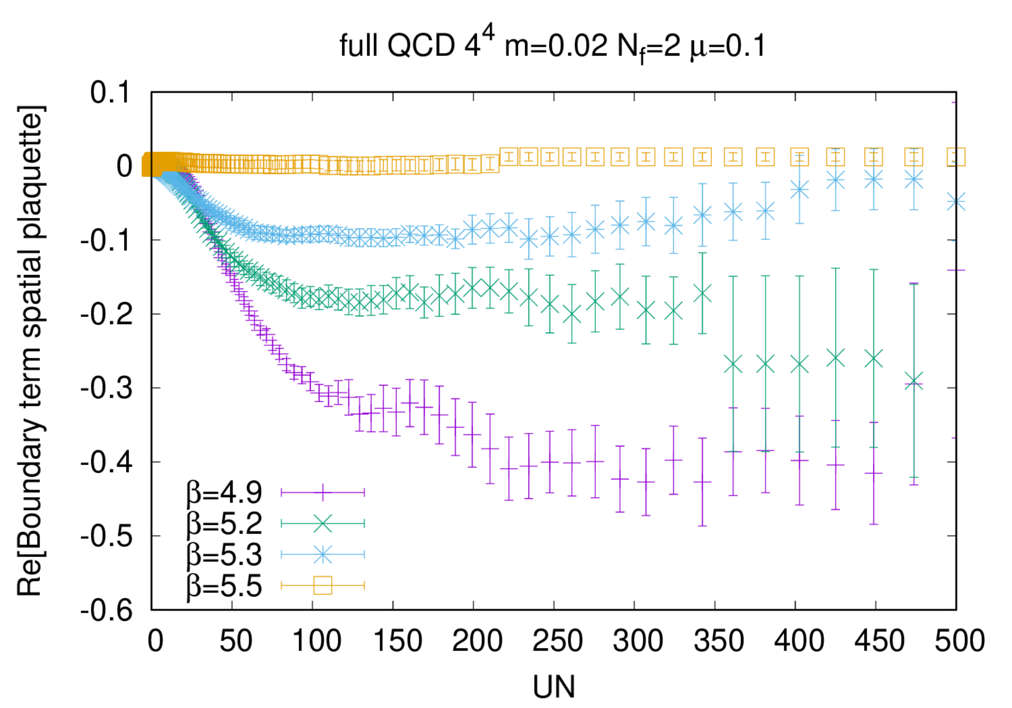
One plaquette model

$$S(x) = i\beta\cos(x) + \frac{s}{2}x^2$$

Full QCD

Boundary term for spatial plaquettes

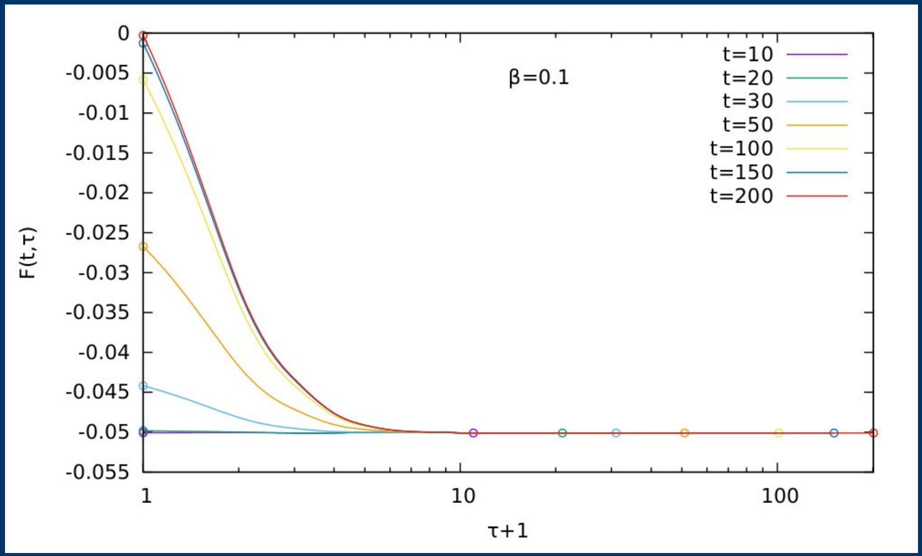




Unambigous detection of boundary terms

Observable cheap also for lattice systems

Correcting CLE using boundary terms



Interpolation function

$$F(t,\tau)=\sum A_n \exp(-\omega_n \tau)$$

Ansatz

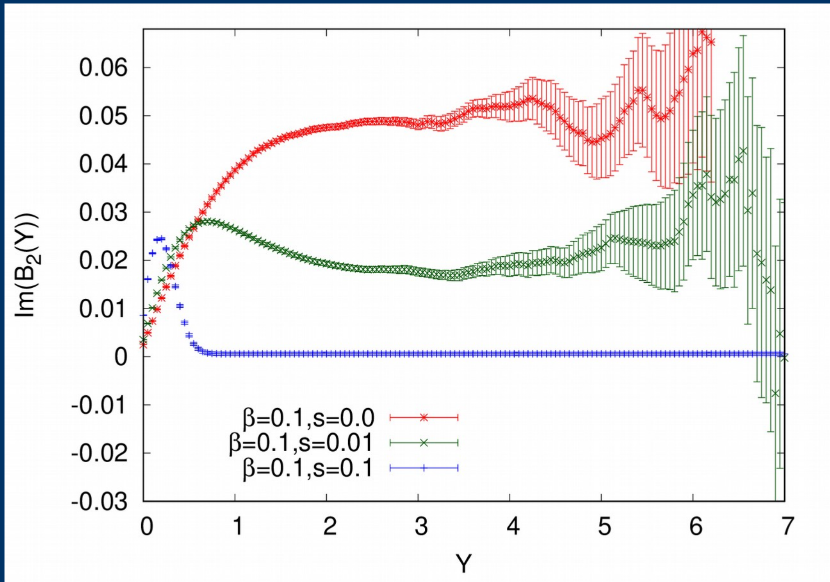
$$F(t,\tau)=A_0+A_1 \exp(-\omega_1 \tau)$$

Higher order boundary terms

$$\frac{\partial^n F(t,\tau)}{\partial \tau^n}=B_n=\langle L_c^n O\rangle$$

Systematic error of CLE

$$F(t,0)-F(t,t)=B_1^2/B_2$$



Test in U(1) toy model

$$S(x)=i\beta\cos(x)+\frac{s}{2}x^2$$

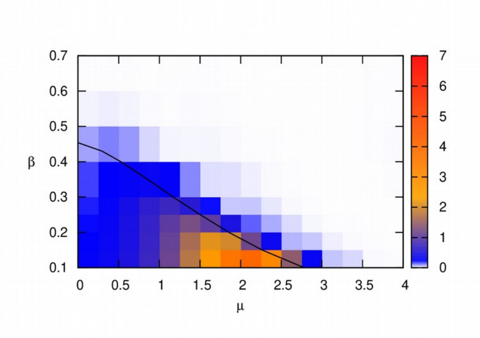
Measuring B_1, B_2 allows correction of results when CLE fails

β, s	B_1	B_2	B_1^2/B_2	CL error	CL	correct	corrected CL
0.1, 0	-0.04859(45)	0.0493(11)	0.04786(79)	0.04891(45)	-0.00115(45)	-0.05006	-0.04901(62)
0.1, 0.01	-0.01795(49)	0.01801(80)	0.01789(60)	0.01689(50)	-0.03318(50)	-0.05006	-0.05106(40)
0.1, 0.1	-0.00048(30)	0.00057(35)	0.00039(28)	0.00049(31)	-0.04957(31)	-0.05006	-0.04997(6)
0.5, 0	-0.2474(11)	0.237(11)	0.258(11)	0.25818(23)	0.00003(23)	−0.25815	-0.258(11)
0.5, 0.3	−0.05309(86)	0.0552(51)	0.0507(41)	0.04183(70)	-0.19658(70)	−0.23841	−0.2473(37)

Test in 3d XY model

B_2 is very noisy, hard to measure

Step in the right direction



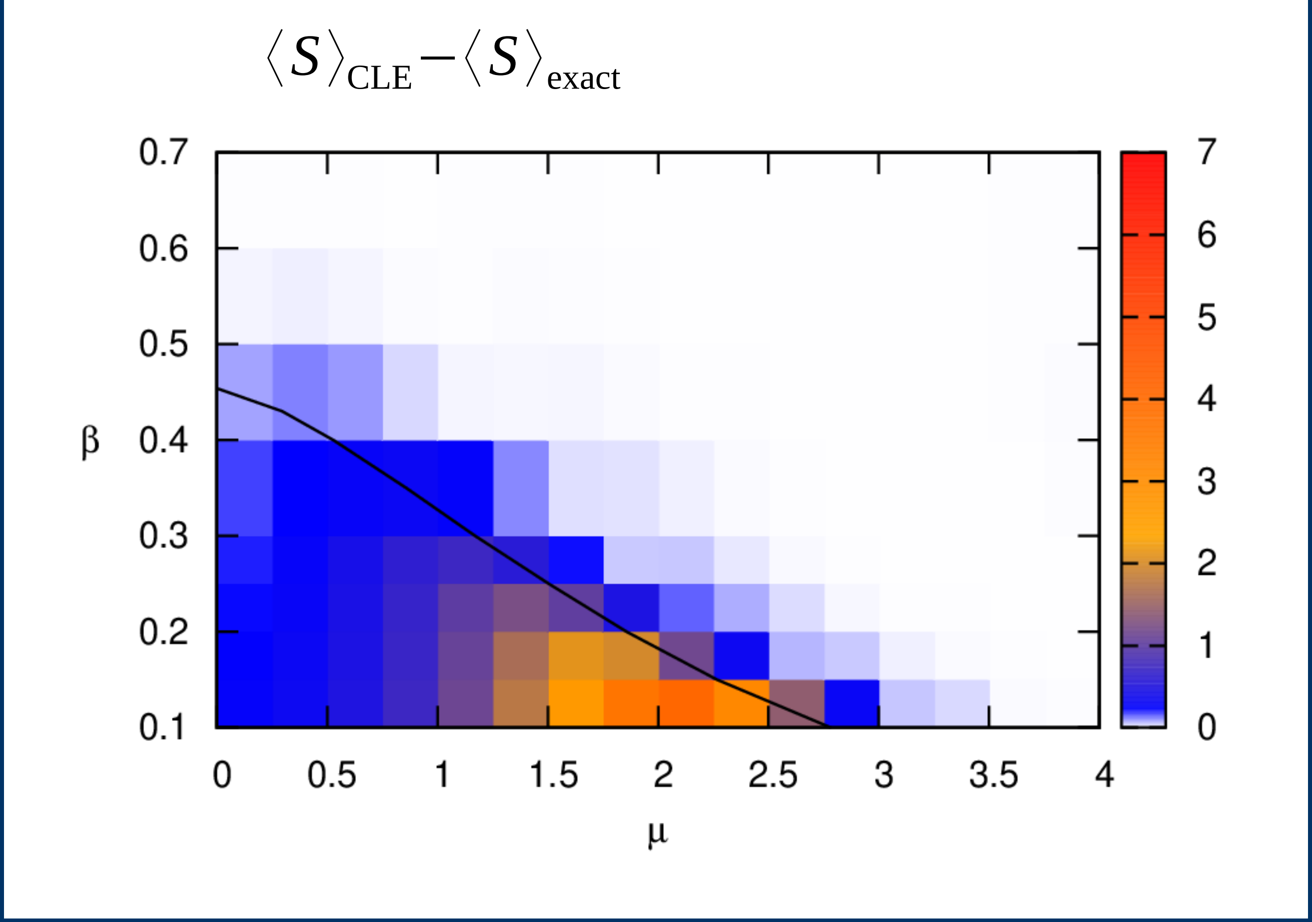
$\mathcal{O}$	β, μ^2	B_1	B_2	B_1^2/B_2	CL error	CL	worldline	corrected CL
S	$0.2, 10^{-6}$	0.02567(21)	−0.0730(47)	−0.00902(46)	−0.013029(65)	−0.075316(65)	−0.062288(17)	−0.06630(53)
	0.2,0.1	0.03309(25)	−0.0903(79)	−0.01213(89)	−0.0169974(91)	−0.0792922(91)	−0.062295(18)	−0.06716(90)
	0.2,0.2	0.03941(28)	−0.109(13)	−0.0142(17)	−0.0205408(80)	−0.0828399(80)	−0.062299(11)	−0.0686(17)
	$0.7, 10^{-6}$	$1.440(15) 10^{-4}$	$-7.33(17) 10^{-4}$	$-2.834(46) 10^{-5}$	$-1.23(33) 10^{-4}$	−1.482311(33)	−1.48219(35)	−1.482283(34)
	0.7,0.1	0.004783(50)	−0.0082(23)	−0.00278(69)	−0.002791(31)	−1.526766(31)	−1.52398(35)	−1.52399(72)
	0.7,0.2	0.006013(38)	−0.00873(96)	−0.00414(45)	−0.002488(29)	−1.568899(29)	−1.56641(20)	−1.56476(48)

XY model in d=3

$$S=-\beta\sum_x\sum_{\nu=1}^{3}\cos\left(\phi_x-\phi_{x+\nu}-i\mu\delta_{\nu 0}\right)$$

Can be solved exactly using dual variables (worldlines)

CLE fails in one of the phases



[plot from: Aarts and James (2010)]

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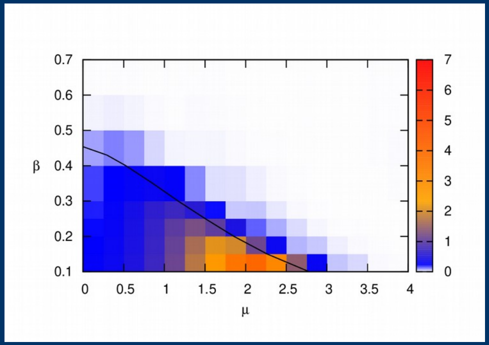
Step in the right direction



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Summary

CLE has potential problems with boundary terms and poles

Monitoring of the process is required:
measuring Boundary terms

lattice models with cheap observable

Correction with higher order boundary terms

Extra slides

HDQCD boundary terms