Real time simulations of scalar fields with kernelled complex Langevin equation

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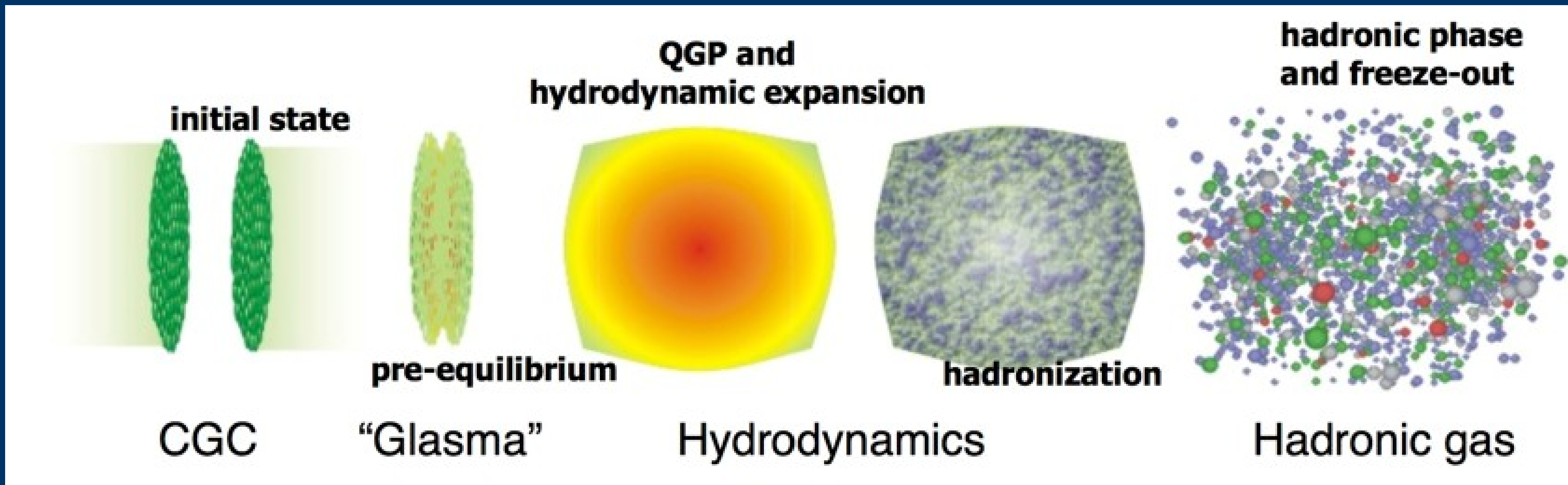
1. Introduction to Sign-problem of real-time physics and Complex Langevin
2. Kernels in the CLE – How to get rid of boundary terms
3. realtime scalars in 0+1 and 1+1 dimensions

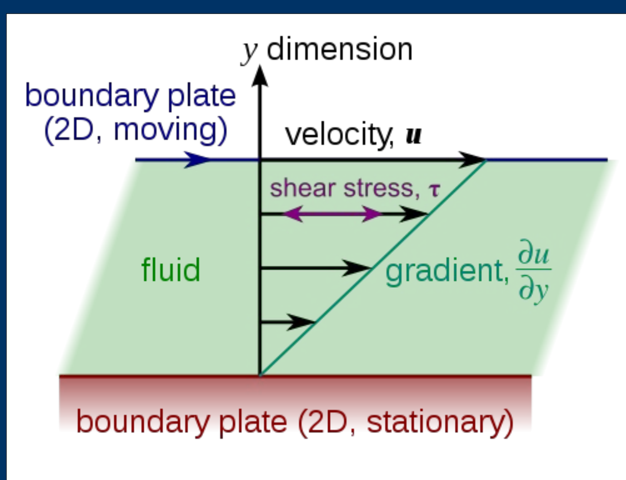
Heavy-Ion collisions



How does the Glasma equilibrate?
Non-equilibrium Quantum Field theory

$$|\Psi(t=0)\rangle \rightarrow |\Psi(t)\rangle$$

For hydrodynamics one needs equilibrium values of:
Equation of State ← "easy" to calculate
Transport coefficients: e.g. viscosity



Hard problem
Real-time correlator

$$\eta = \frac{1}{TV} \int_0^\infty dt \langle \sigma_{xy}(0) \sigma_{xy}(t) \rangle$$

Why is real-time QFT so hard?
→ Sign Problem

Path integral formulation of Quantum Mechanics

Quantum Mechanics with $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})$

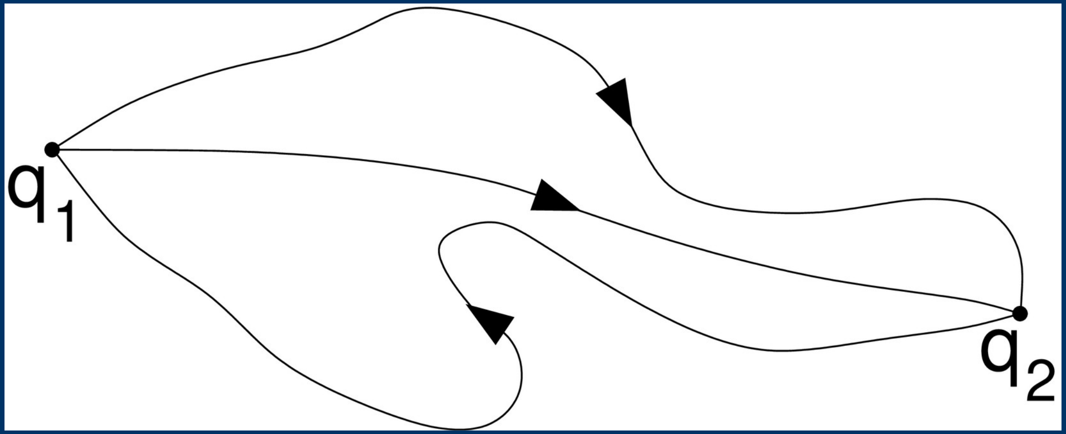
Time evolution given by Schrödinger eq. $i\,\partial_t \Psi(x,t) = \hat{H}\,\Psi(x,t)$ $\qquad |\Psi(x,t)\rangle = e^{-it\hat{H}} |\Psi(x,0)\rangle$

Equivalent formulation

Transition amplitude: $\langle q_2 | e^{-it\hat{H}} | q_1 \rangle = \int_{q_1}^{q_2} Dq\, e^{iS[q(t)]}$

Path integral: $\int_{q_1}^{q_2} Dq =$ normalized sum for all functions $q(t_1 \leqslant t \leqslant t_2)$

with correct bound. cond. $q(t_1) = q_1 \;\; q(t_2) = q_2$



Numerically advantegous

$q(t)$ instead of $\Psi(x,t)$

Thermodynamics

Imaginary time: $t \to -i\tau \qquad 0 < \tau < -i\beta$ $\qquad e^{-it\hat{H}} \to e^{-\beta\hat{H}}$

$$\langle q_1 | e^{-\beta\hat{H}} | q_2 \rangle = \int_{q_1}^{q_2} Dq\, e^{-S_E[q(t)]} \qquad S_E[q(t)] = \int_{t=0}^{t=\beta} dt \left(\frac{1}{2} m \dot{q}(t)^2 + V(q(t)) \right)$$

Langevin Equation (aka. stochastic quantisation)

Given an action $S(x)$

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

Gaussian noise

$$\langle \eta(\tau) \rangle = 0$$
$$\langle \eta(\tau)\eta(\tau') \rangle = \delta(\tau - \tau')$$

Random walk in configuration space

Averages are calculated along the trajectories:

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

Numerically,
results are extrapolated to $\Delta\tau \to 0$

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
$\langle \eta(\tau) \rangle = 0$
$\langle \eta(\tau)\eta(\tau') \rangle = \delta(\tau - \tau')$

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

<u>The field is complexified</u>

real scalar → complex scalar

link variables: SU(N) → SL(N,C)
compact → non-compact

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

Analytically continued observables are calculated along the trajectories:

$$\langle O \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T O(x(\tau) + iy(\tau)) d\tau$$

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

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

Gaussian Example

$$S[x]=\sigma x^2+i\lambda x$$

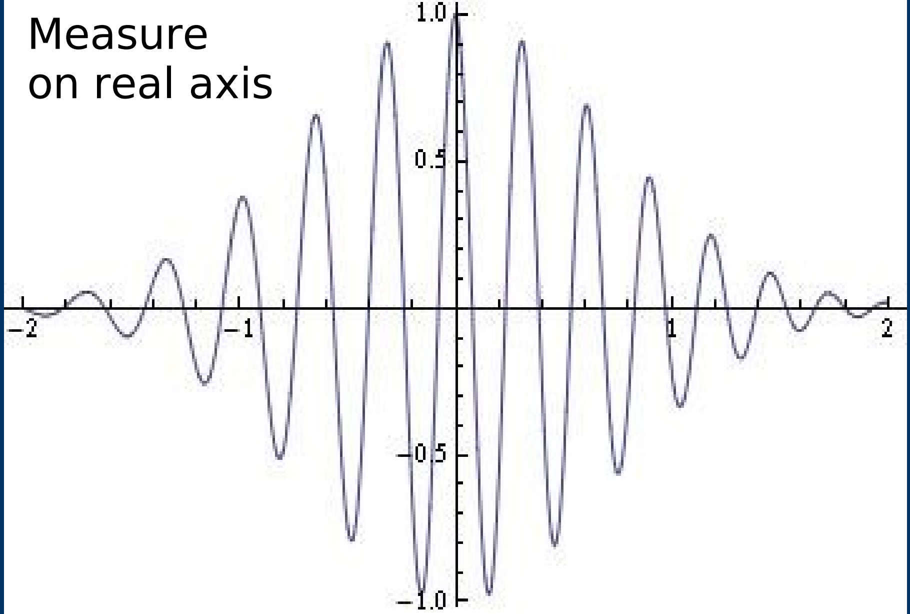
CLE

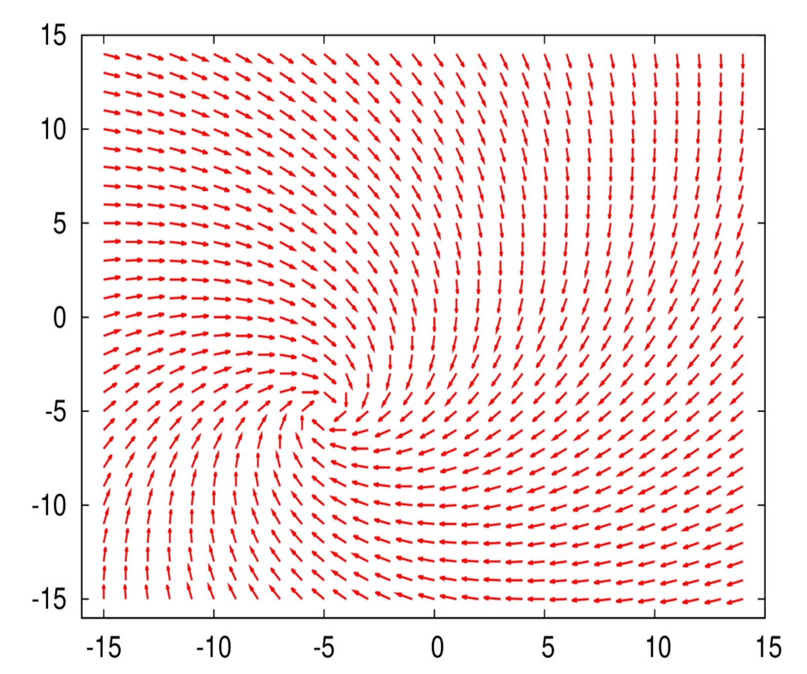
$$\frac{d}{d\tau}(x+iy)=-2\sigma(x+iy)-i\lambda+\eta$$

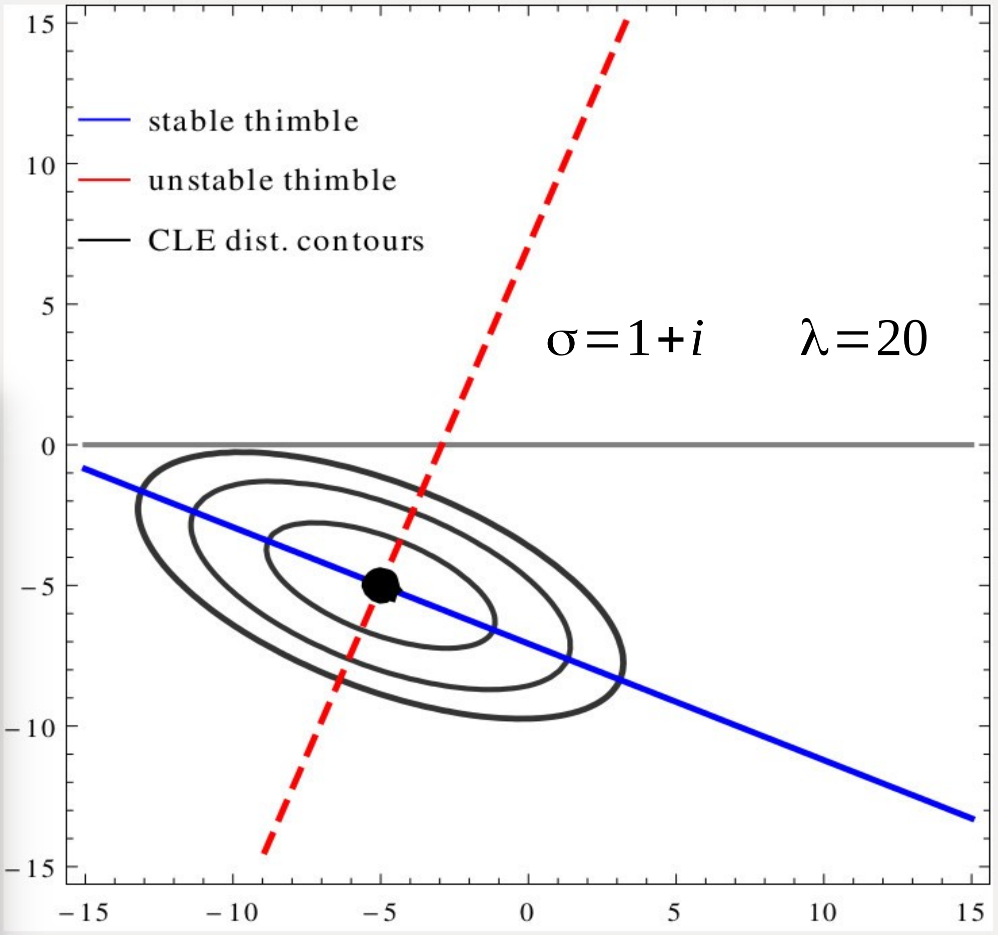
$$P(x,y)=e^{-a(x-x_0)^2-b(y-y_0)^2-c(x-x_0)(y-y_0)}$$

Gaussian distribution around critical point

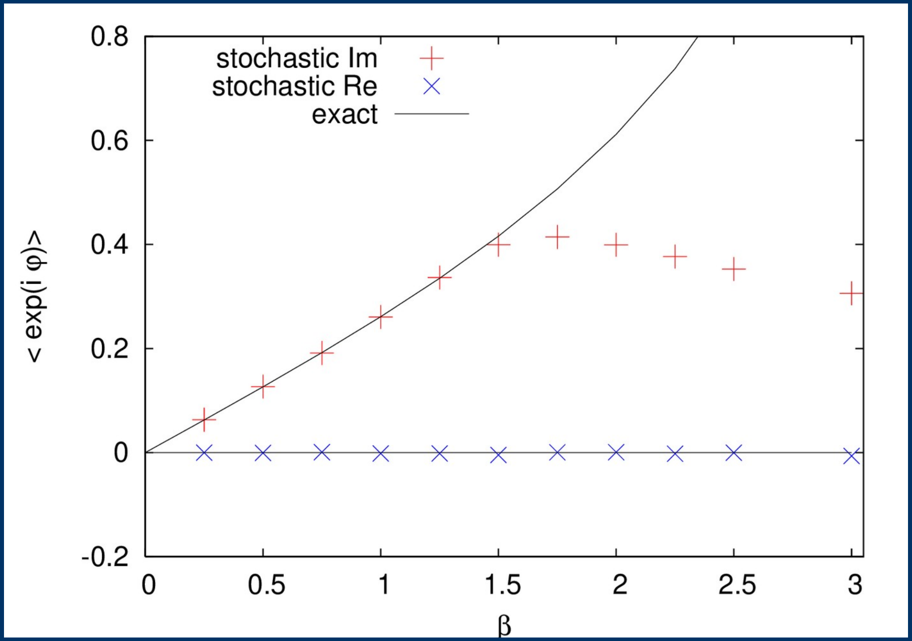
$$\left.\frac{\partial S(z)}{\partial z}\right|_{z_0}=0$$







For nontrivial models CLE may or may not give a correct answer



$$S(\varphi)=i\beta\cos\varphi+i\varphi$$

Do we know if it’s correct?

Reasons for incorrect results: slowly decaying distributions (Boundary terms)
different cycles contributing [See talk of Michael Mandl]
non-holomorphic actions

Diagnostic observables: boundary terms
certain non-holomorphic observables, histograms

What can we do if it’s incorrect?

Change variables
Use a kernel (see below)
Use a “regularization” [See talk of Michael Hansen]

Quantum oscillator

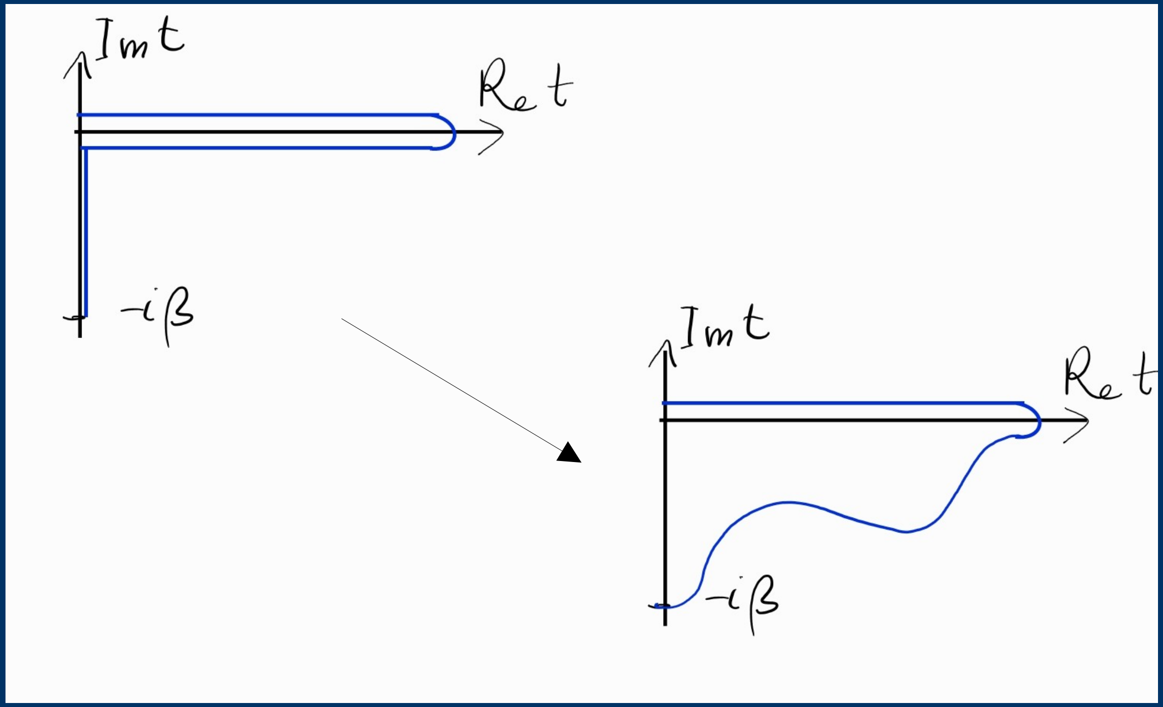
$$S=\int dt\,\frac{1}{2}\left(\frac{d\phi}{dt}\right)^2-\frac{1}{2}m^2\phi^2-\frac{\lambda}{4}\phi^4$$

Path integral $\int D\phi\, e^{iS}$

Suppose we are interested in $\langle e^{-\beta\hat{H}}\hat{\phi}(t)\hat{\phi}(0)\rangle=\mathrm{Tr}\left(e^{-\beta\hat{H}}e^{it\hat{H}}\hat{\phi}e^{-it\hat{H}}\hat{\phi}\right)$

This is time ordered if we take a complex time contour

Schwinger-Keldysh contour



$$e^{-\beta\hat{H}}e^{it\hat{H}}=e^{\int_t^{-i\beta}dt\,\hat{H}}$$

We can shift the contour into the complex plane

Discretisation

given t_n on a complex time-plane

$$\Delta t_n = t_{n+1} - t_n$$

$$S = \sum \Delta t_n \left(\frac{1}{2} \left(\frac{\phi_{n+1} - \phi_n}{\Delta t_n} \right)^2 - \frac{1}{2} m^2 \phi_n^2 - \frac{\lambda}{4} \phi_n^4 \right)$$

Thermal average

$$\mathrm{Tr}\left(e^{-\beta \hat{H}} e^{it\hat{H}} \hat{\phi} e^{-it\hat{H}} \hat{\phi} \right)$$

Path starts at $t=0$
Path ends at $t=-i\beta$
Periodical boundary conditions

Non-equilibrium time evolution

[Berges, Borsányi, Sexty, Stamatescu (2006)]

Using some initial density matrix ρ

$$\mathrm{Tr}\left(\rho e^{it\hat{H}} \hat{\phi} e^{-it\hat{H}} \hat{\phi} \right)$$

Fields no longer periodic
at $t=0$: two separate integrals for ϕ_i and ϕ_f

Especially easy in CLE with gaussian initial density matrix

Real-time two point function of quantum oscillator

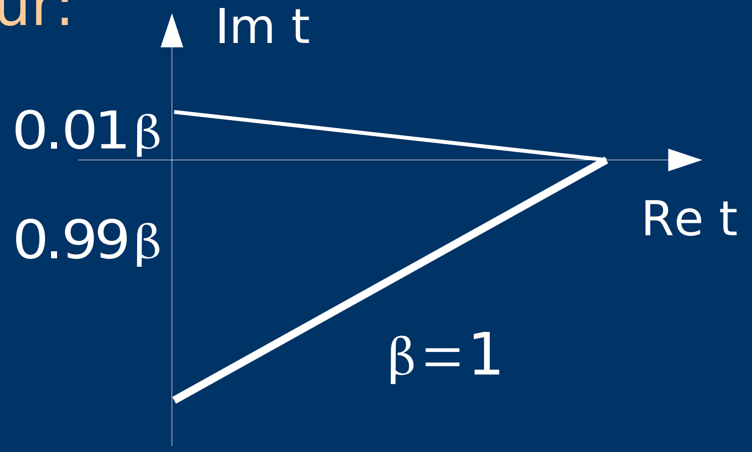
Thermal equilibrium:
periodic boundary cond.

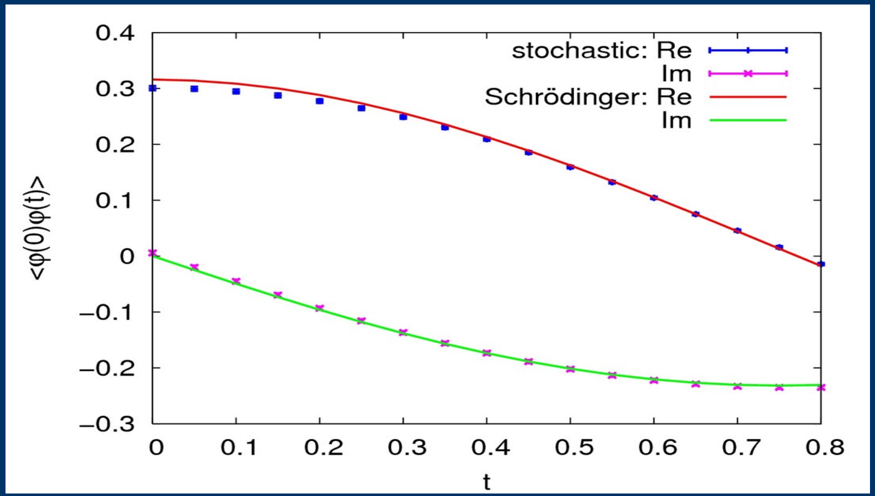
[Berges, Borsanyi, Sexty, Stamatescu (2006)]

Imaginary extent gives $\beta = \frac{1}{T}$

short real-time extent

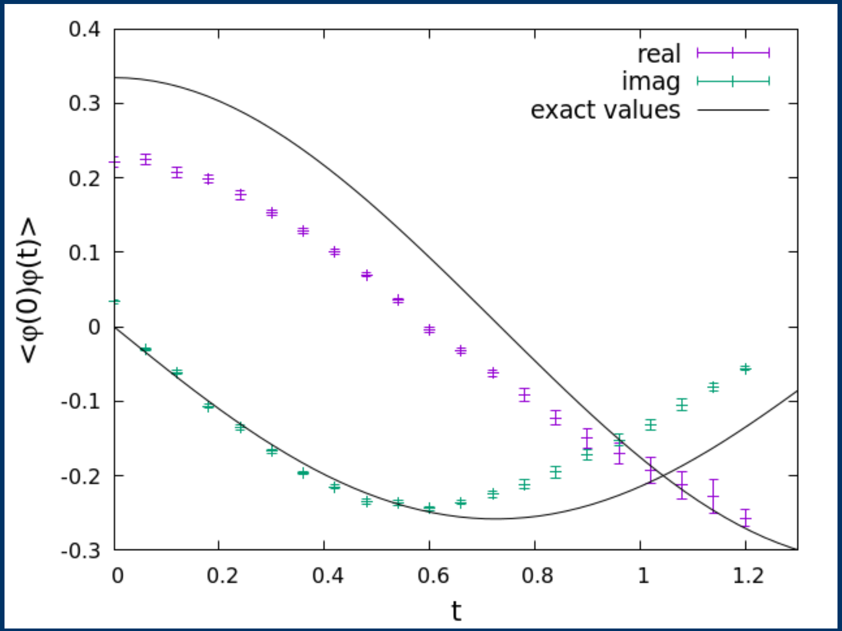
Asymmetric contour:





large real-time extent

Boundary terms appear



Kernels in the Langevin equation

Introducing a Kernel [Soderberg (1987), Okamoto et. al. (1988)]

$$\dot{z} = -\frac{\partial S}{\partial z} + \eta \quad \rightarrow \quad \dot{z} = -K(z)\frac{\partial S}{\partial z} + \frac{\partial K(z)}{\partial z} + \sqrt{K(z)}\eta$$

For real action,
equilibrium distribution unchanged.

Fokker-Planck equation:

$$\partial_\tau P = \partial_x K(x)(\partial_x + S')P$$

Kernel = field dependent diffusion const.

For complex action
Complexified distribution might change,
boundary terms may or may not appear/disappear
results are still a linear combination of integration cycles for zero boundary

Many variables – matrix Kernel

$$\frac{d\phi_i}{d\tau} = -H_{ij}(\phi)H^T_{jk}(\phi)\frac{\partial S}{\partial \phi_k} + \partial_k(H_{ij}(\phi)H^T_{jk}(\phi)) + H_{ij}(\phi)\eta_j$$

Can one use a Kernel to decrease boundary terms in the CLE?

[see also: Michael Mandl's talk]

Yes! search for a kernel using stochastic gradient descent
Loss function: Size of the distribution in imaginary directions

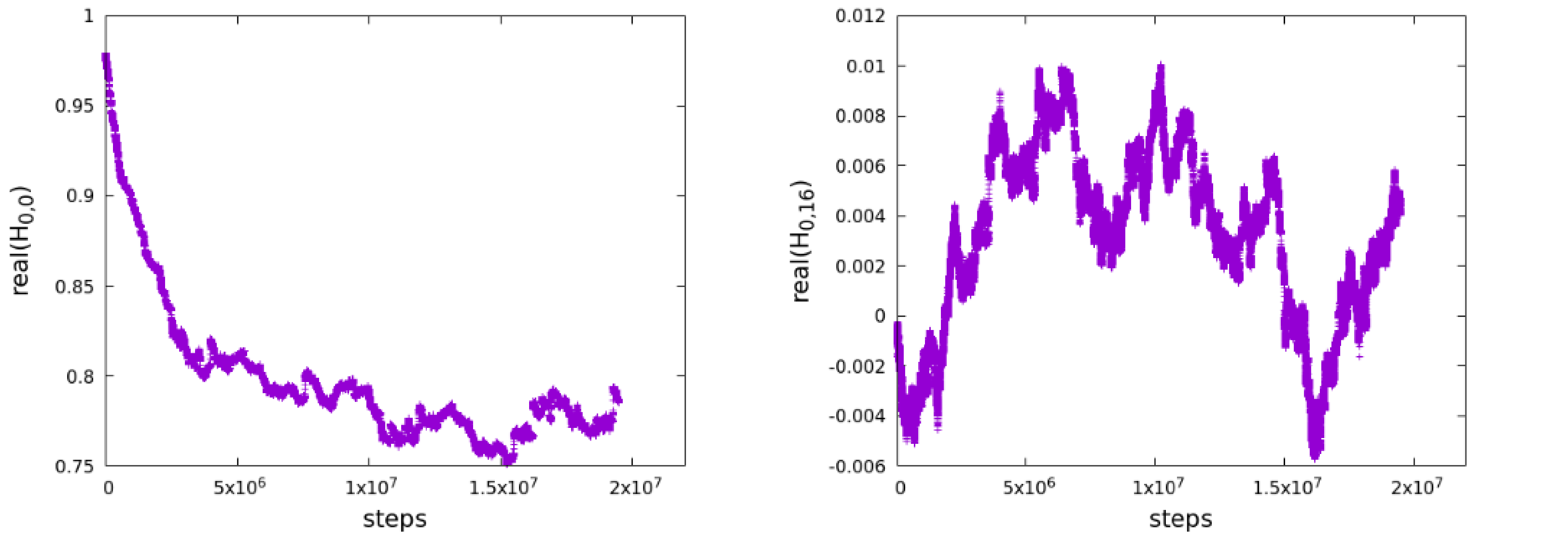
[Rothkopf, Larsen, Alvestad(2023); Lampl, Sexty (2024)]

Gradient descent

$$\phi_i' = -H_{ij} H^T_{jk} \frac{\partial S}{\partial \phi_k} \Delta\tau + H_{ij} \eta_j \sqrt{2 \Delta \tau}$$

1. collect average for $\frac{\partial \sum (\mathrm{Im}\, \phi_i')^2}{\partial H_{ij}} = \partial_{H_{ij}} \mathrm{Loss}$ during CL simulation with current H

2. update H $H_{ij} \rightarrow H_{ij} - \partial_{H_{ij}} \mathrm{Loss}$



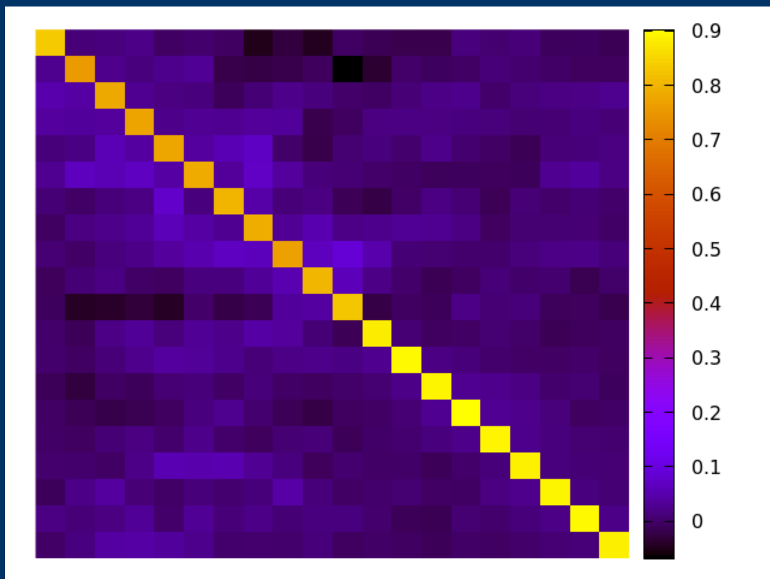
(a) Convergence of the real part of the matrix element $H_{0,0}$

(b) Convergence of the real part of the matrix element $H_{0,16}$

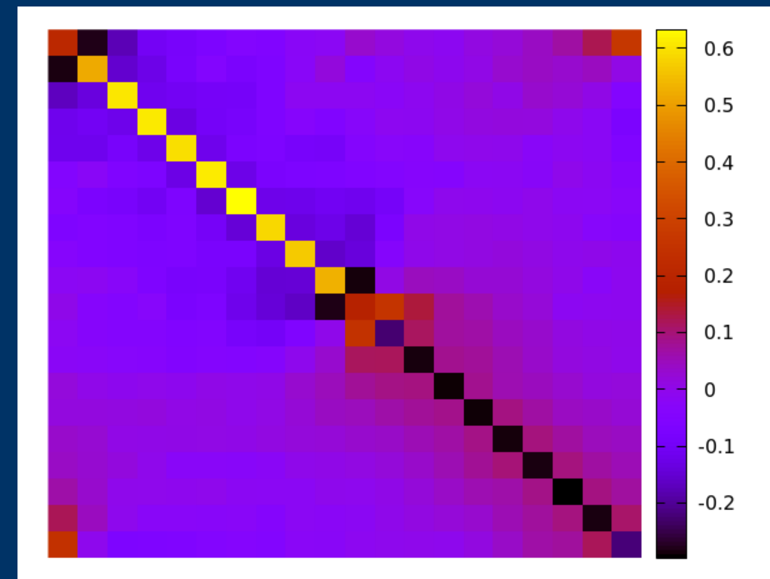
First step: Field independent matrix kernel

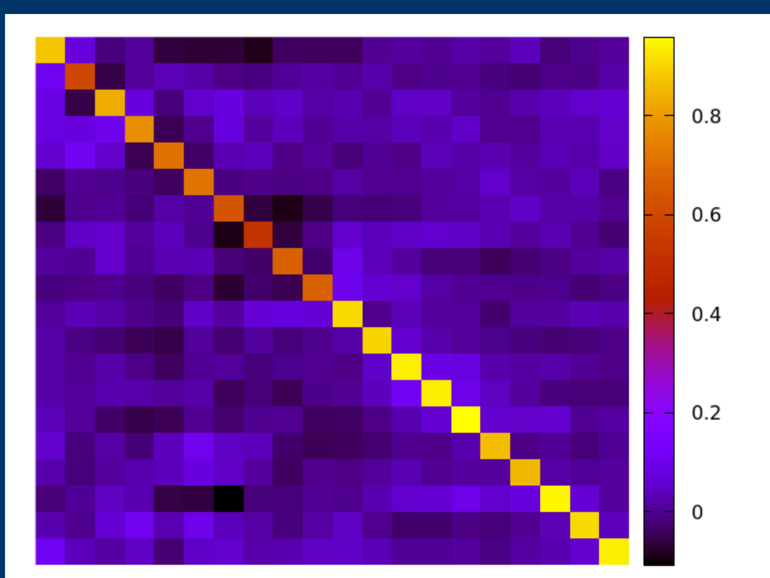
[Lampl, Sexty (2024)]

real part | imaginary part

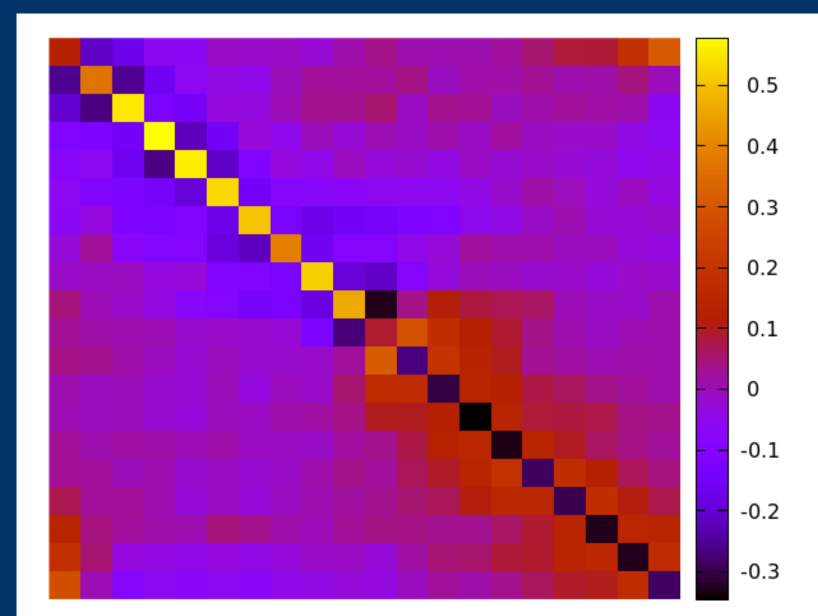


Real-time extent
$t = 1.2$





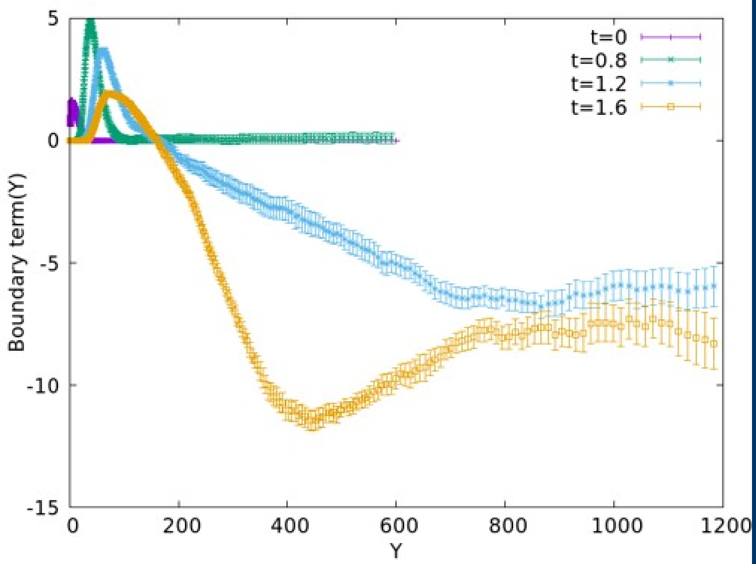
$t = 2.0$



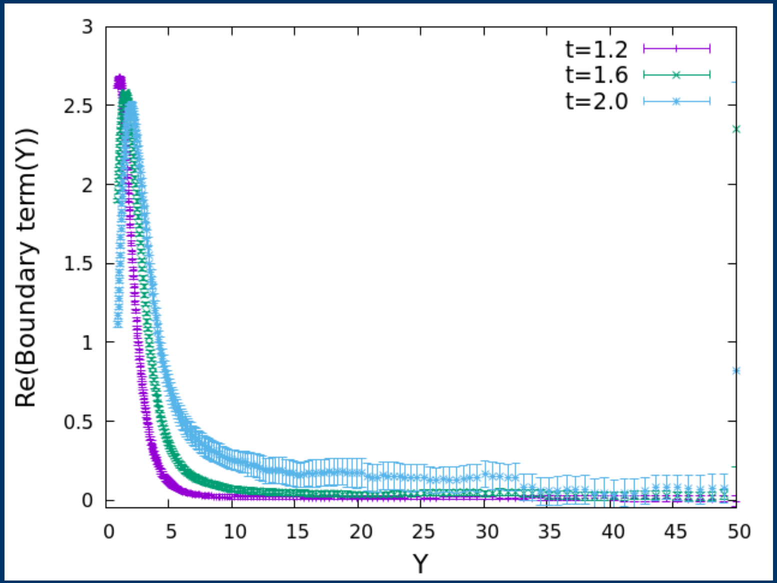
Boundary terms

Boundary terms of $\phi(t)^2$

Without Kernel:



With optimized kernel:

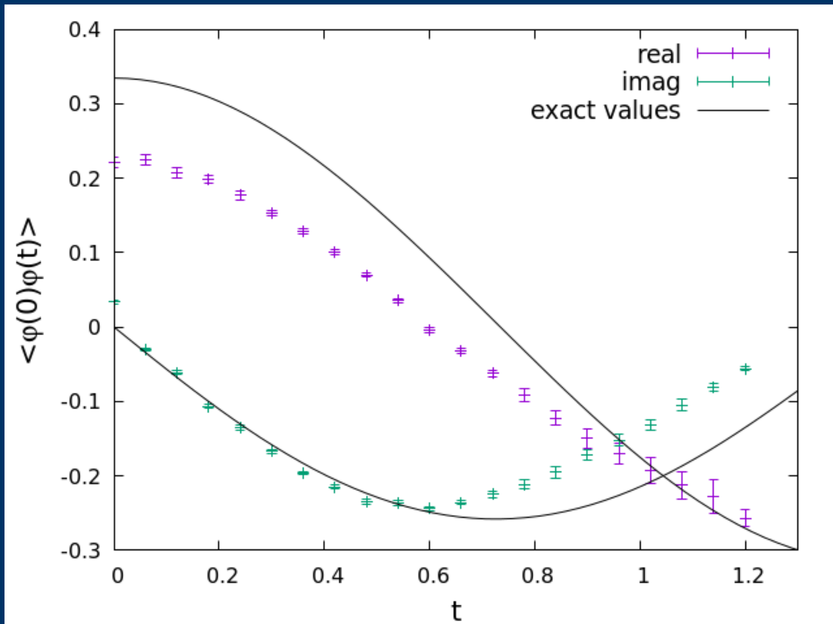


Actually, for an anharmonic quantum oscillator it's also easy to calculate exact results (e.g. diagonalize Hamiltonian)

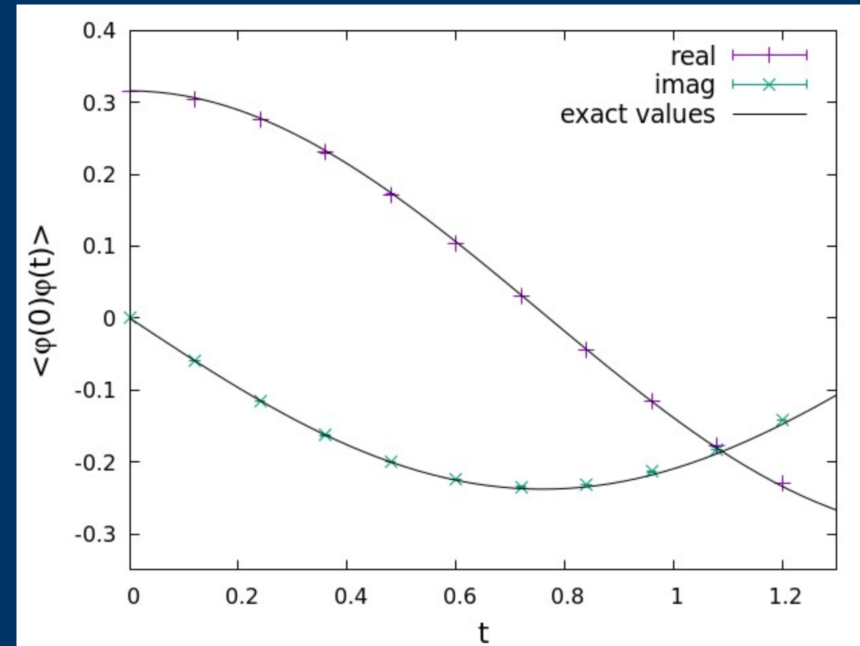
→ Compare to exact

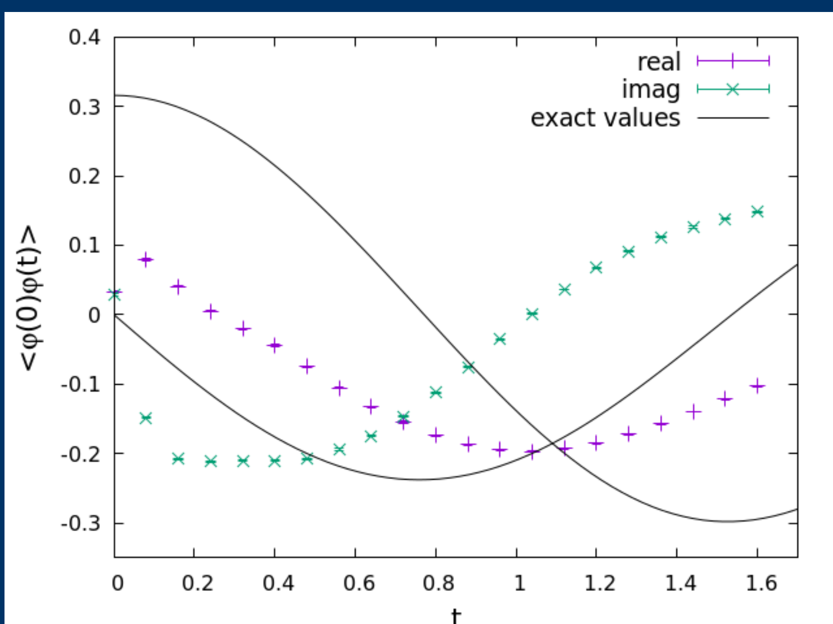
Without kernel

With learned kernel

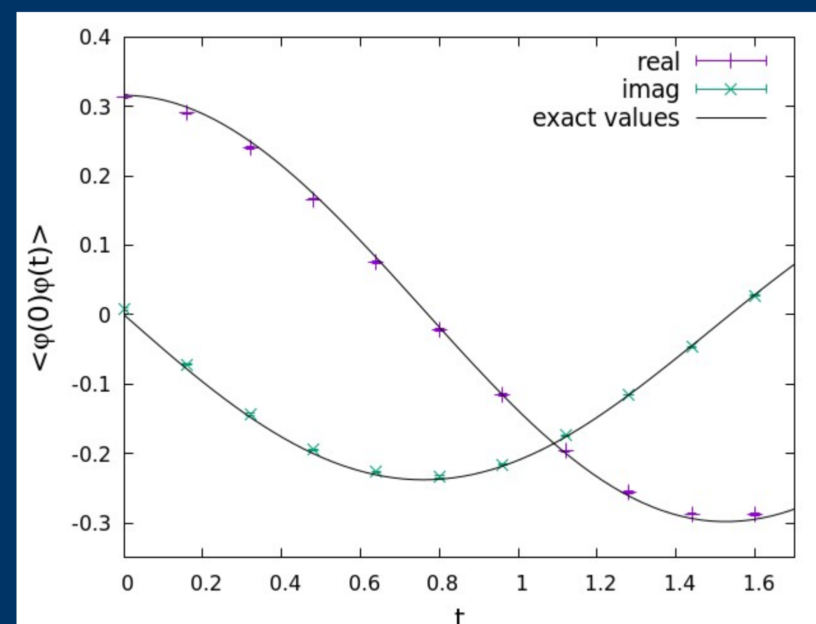


$t = 1.2$





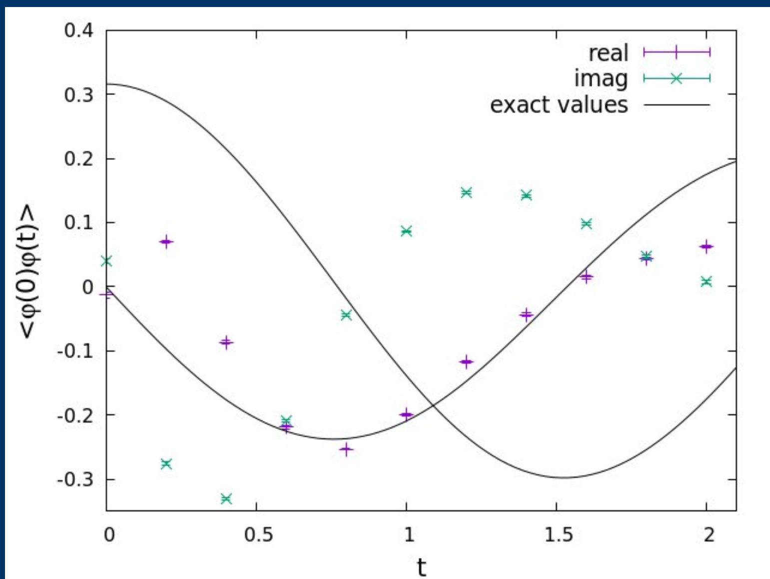
$t = 1.6$



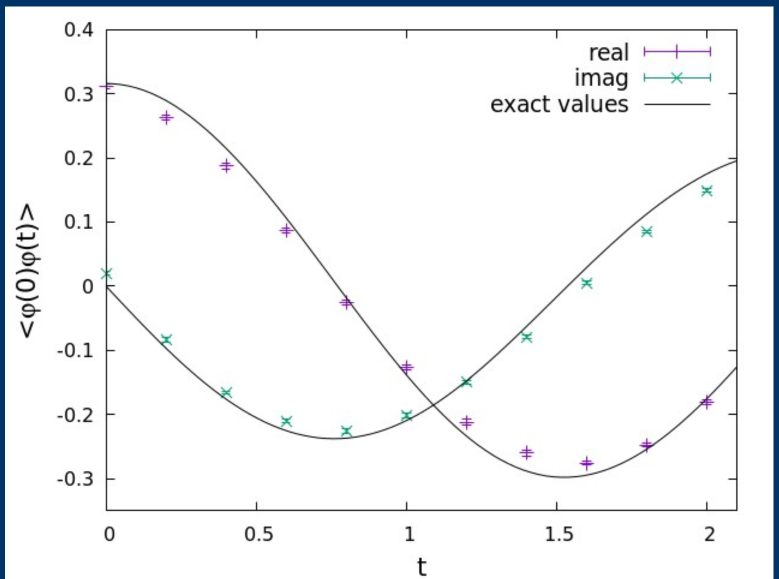
Increasing real time extent, boundary terms appear again

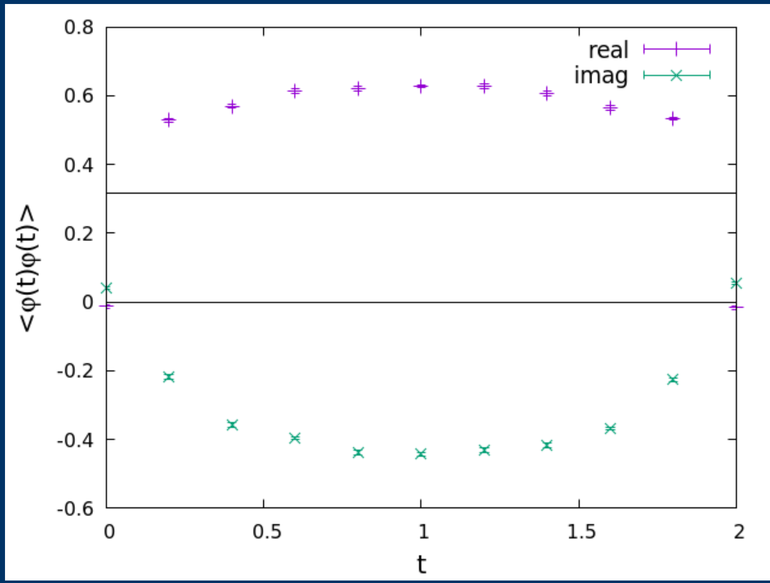
Without kernel

With learned kernel

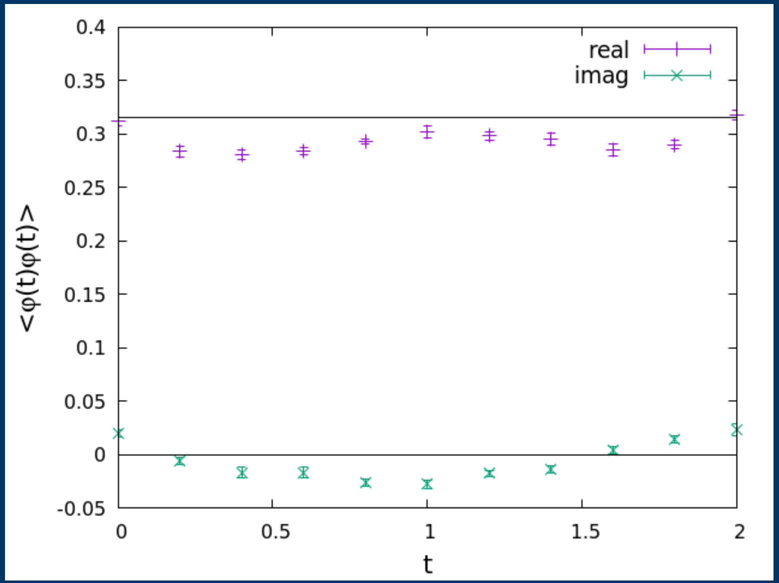


$t = 2.0$



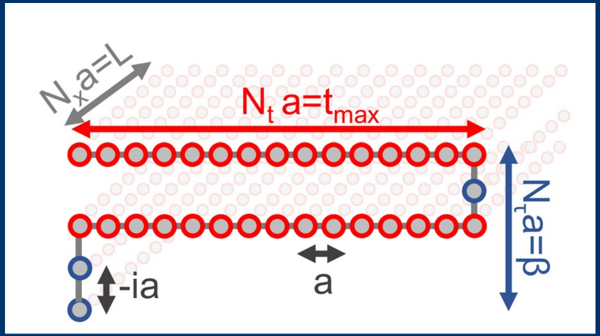


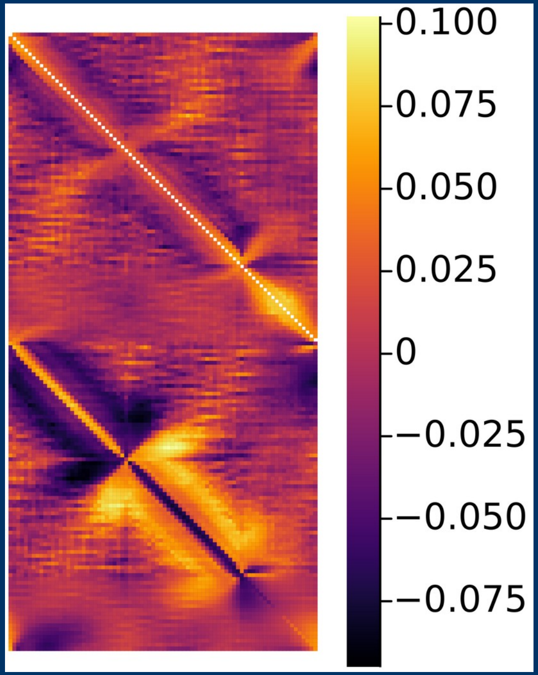
$t = 2.0$



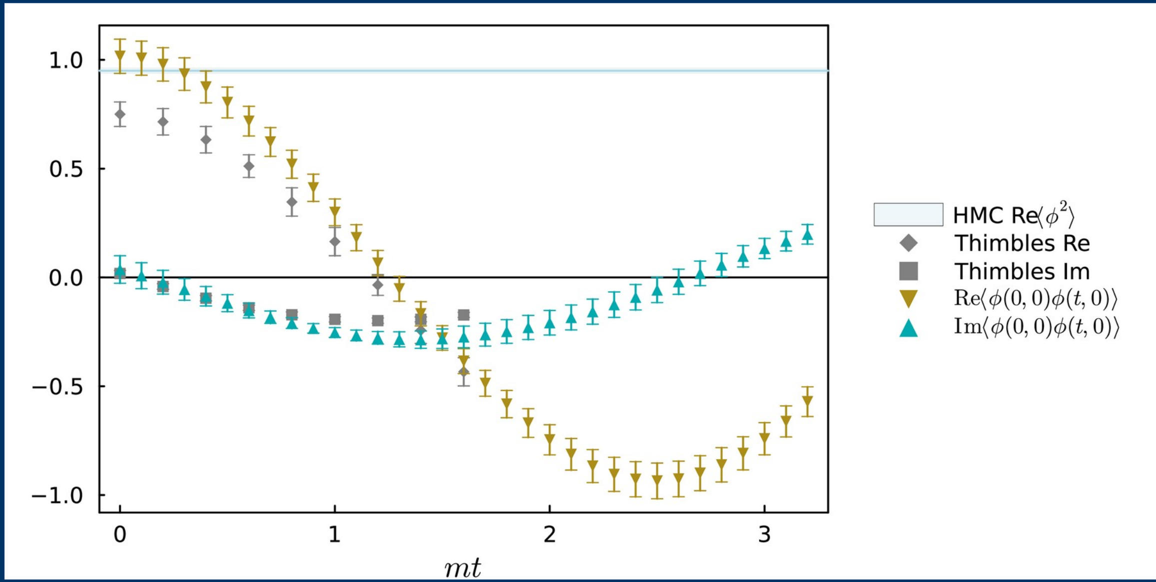
Scalar fields in 1+1 dimension [Alvestad, Rothkopf, Sexty (2024)]

Dense constant Kernel
on the Schwinger-Keldysh contour





two point function: $\langle \phi(0)\phi(t)\rangle$



Thimble result till t=1.6
[Alexandru et. al. (2022)]

CLE till t=3.2 (at least)

$N_x=16\quad N_t=32\quad N_\tau=4$

Summary

Real-time QFT Severe Sign problem

Studying quantum oscillator and scalar field theory
Discretised on a Schwinger-Keldysh-like temporal contour

Breakdown of CLE at large time-extents due to boundary terms
kernels change breakdown time
optimal kernel through machine learning

For 1+1d scalars CLE with optimal kernel
Reaches furthest from ab initio methods at hand

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

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

Measuring boundary terms

$$\int_{-Y}^{Y} P(x,y,t)\, L_c O(x+iy) = \int P(x,y,t)\, L_c O(x+iy)\, \theta(Y-y)$$

$$L_c = \sum \partial_i^2 + K_i \partial_i$$

Many variables: define cutoff to extend SU(N) manifold
to compact submanifold of SL(N,C)

$$\text{e.g.} \quad \operatorname{Im} z\,; \quad \max_i Tr\left(U_i^{+} U_i - 1\right)^2$$

Measure “unitarity norm” and observable

→ Analyze for any cutoff

Trick for second term:

$$\sum K_i \partial_i O = \frac{1}{\epsilon}\left[O(z(\tau+\epsilon, \eta=0)) - O(z(\tau))\right]$$

Measure observable after doing a noiseless update step with stepsize ϵ