The Research Council of Norway

University of Stavanger

Lattice real-time simulations with machine learned optimal kernels

on behalf of **Daniel Alvestad**
Faculty of Science and Technology
Department of Mathematics and Physics
University of Stavanger

with Alexander Rothkopf & Rasmus Larsen

D. A., R. Larsen, A.R., JHEP 08 (2021) 138 and JHEP 04 (2023) 057

as well as with Denes Sexty & Nina Lampl

D. A. , A. R., N. Lampl, D. Sexty (in preparation)

NPACT
Norwegian Particle, Astroparticle & Cosmology Theory network

The XLth International Symposium on Lattice Field Theory – August 3rd 2023 – virtual

Real-time quantum dynamics

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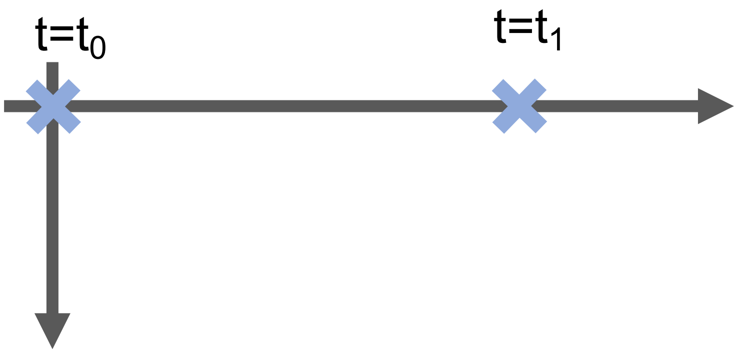
- The path integral at finite temperature on the Schwinger-Keldysh contour



Goal: evaluation of real-time observables

$$\langle O(t_0)O(t_1)\rangle = \mathrm{Tr}[\, \rho\, O(t_0)O(t_1)\,]$$

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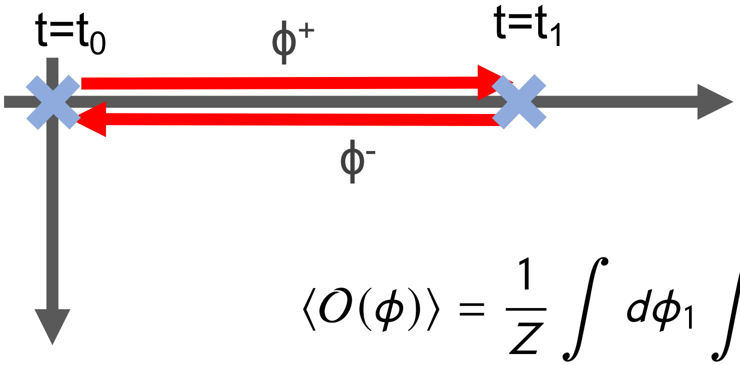

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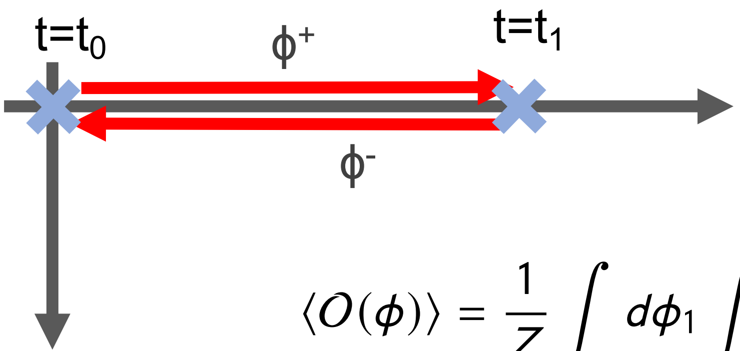

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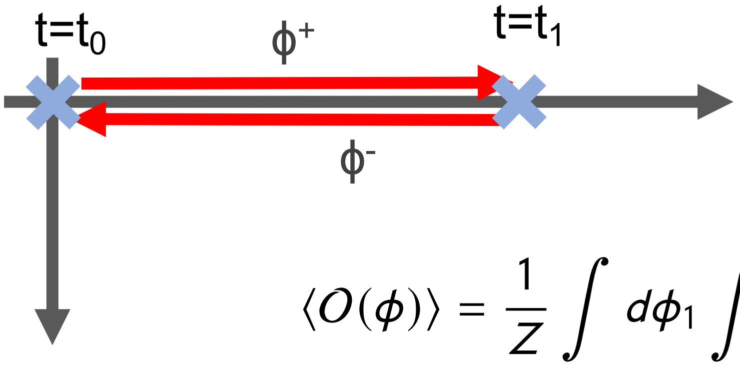

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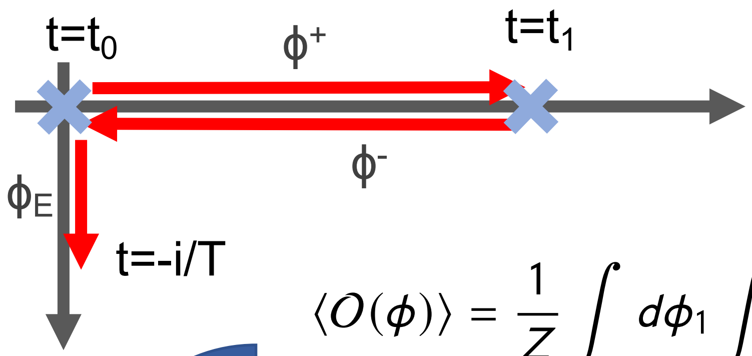

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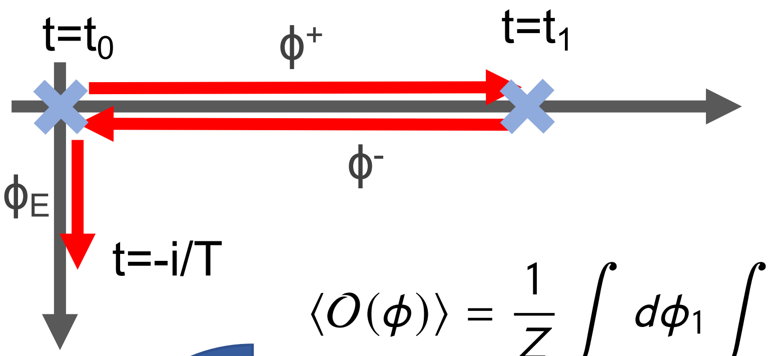

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Real-valued Feynman weight:
Monte-Carlo methods applicable

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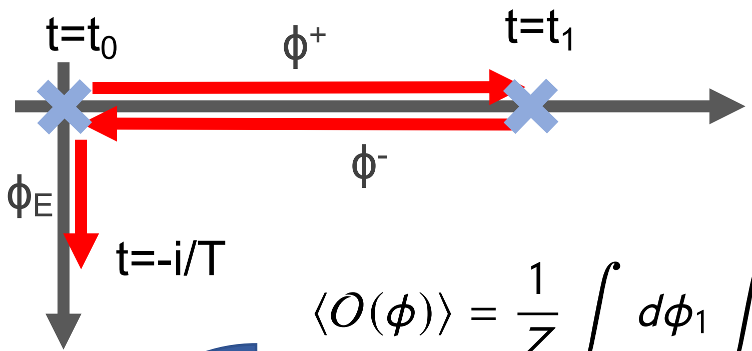

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Pure phase Feynman weight implies MC sign problem. One strategy: **Complex Langevin** see C. Berger et.al. Phys.Rept. 892 (2021)

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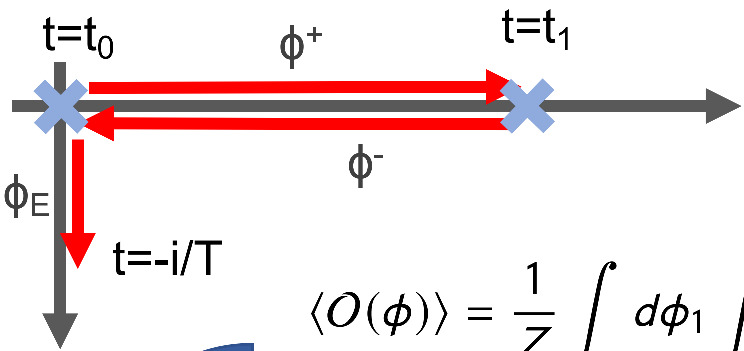

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- Sign problem is NP-hard: **no generic solution** strategy is likely to exist

Troyer, Wiese PRL 94 170201 (2004)

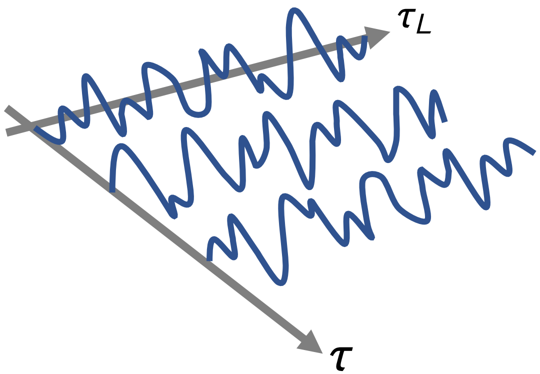
Stochastic Quantization

- Langevin evolution in fictitious additional time to reproduce quantum fluctuations

for an in-depth review: M. Namiki et.al. Stochastic Quantization (Springer) 1992

$$\frac{d\phi}{d\tau_L} = -\frac{\delta S_E[\phi]}{\delta\phi(x)} + \eta(x,\tau_L) \quad \text{with} \quad \langle\eta(x,\tau_L)\rangle = 0, \quad \langle\eta(x,\tau_L)\eta(x',\tau_L')\rangle = 2\delta(x-x')\delta(\tau_L-\tau_L')$$

Stochastic partial differential equation (SDE) with Gaussian noise



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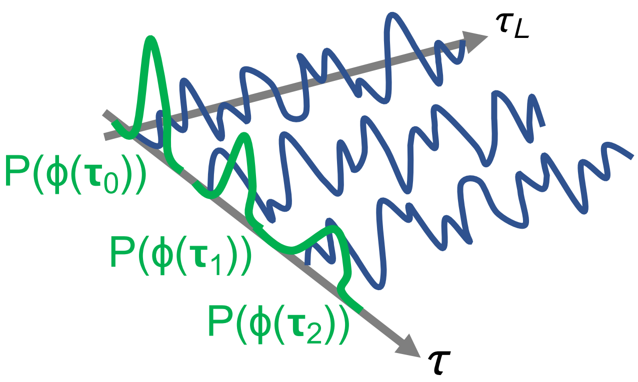

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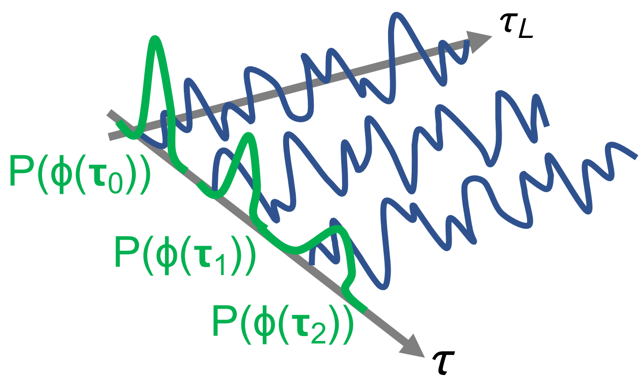

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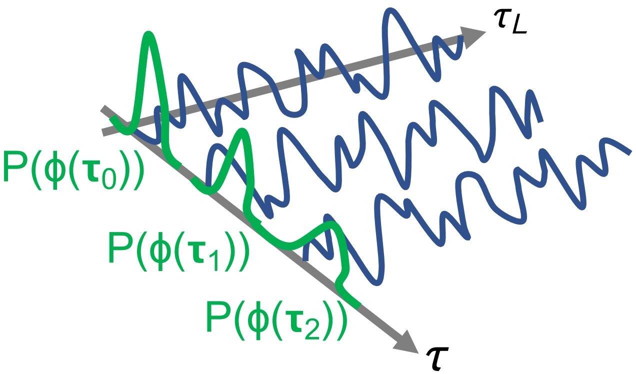

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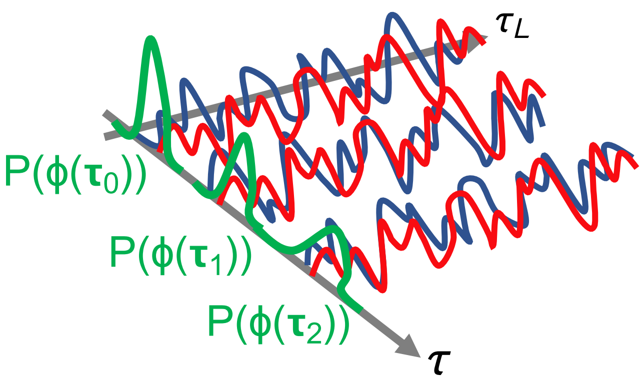

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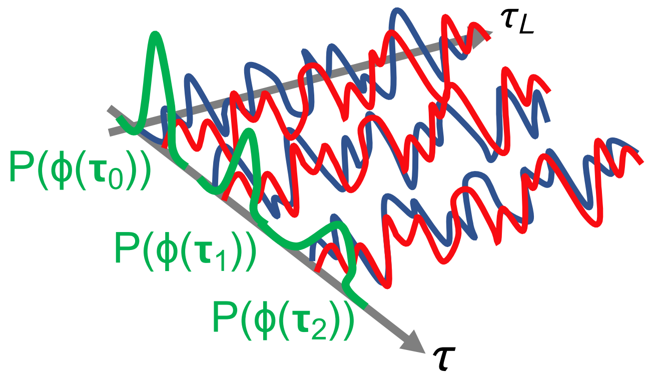

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$$\langle O[\phi]\rangle \leftrightarrow \lim_{T\to\infty}\frac{1}{T}\int_0^T d\tau_L O[\phi_R(x,\tau_L) + i\phi_I(x,\tau_L)]$$

Two challenges for Complex Langevin

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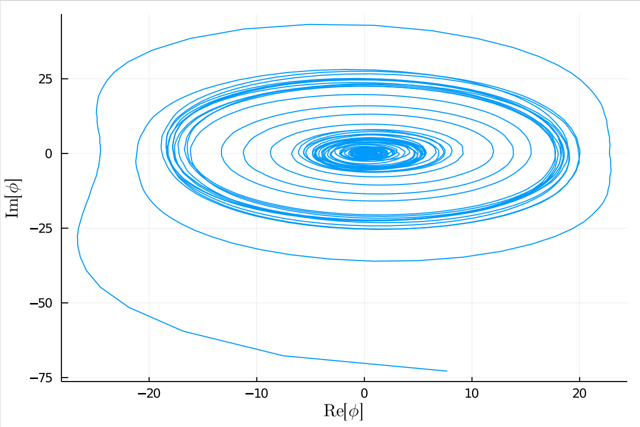
Divergent solutions (runaways)



In practice: use adaptive step size in attempt to keep solution finite

see e.g.: G. Aarts et.al. PLB 687(2-3), 154–159 (2010)

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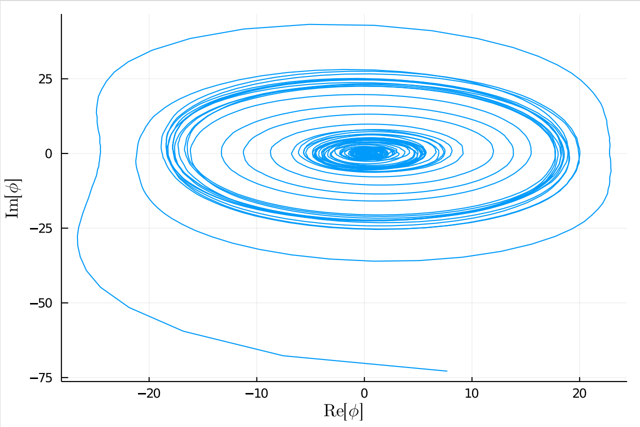

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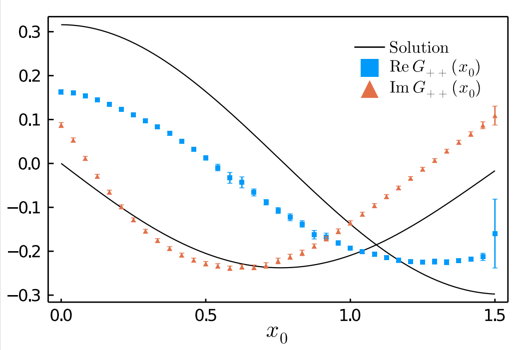
Convergence to incorrect solutions as real-time extent increases



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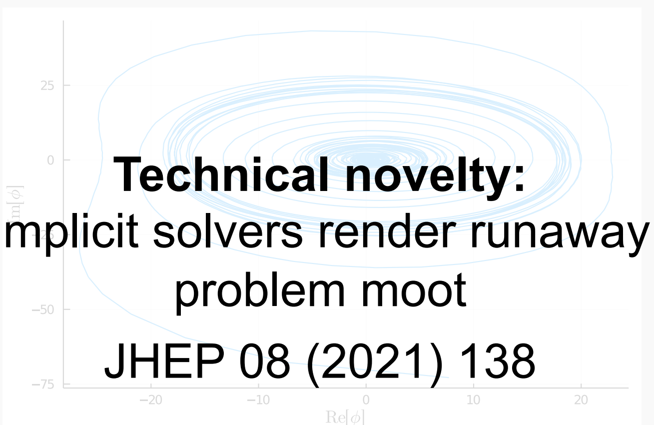

Technical novelty:
Implicit solvers render runaway problem moot
JHEP 08 (2021) 138

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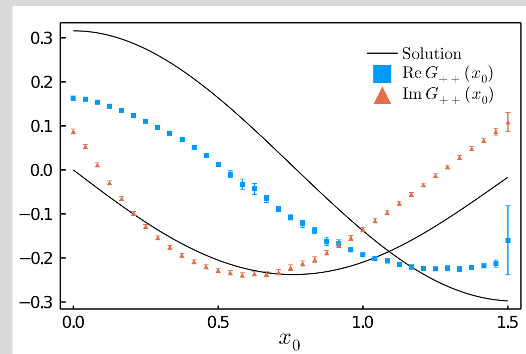

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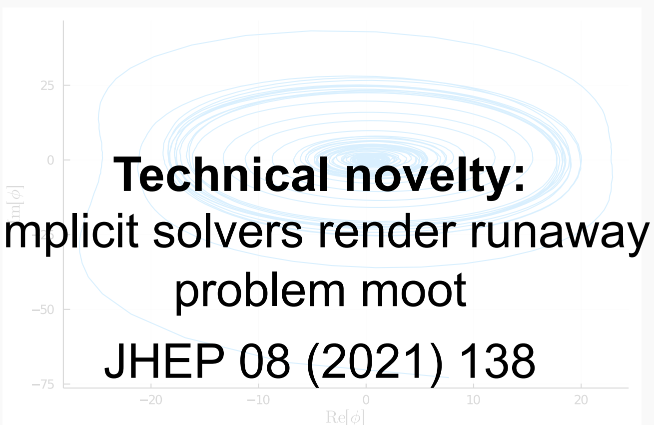

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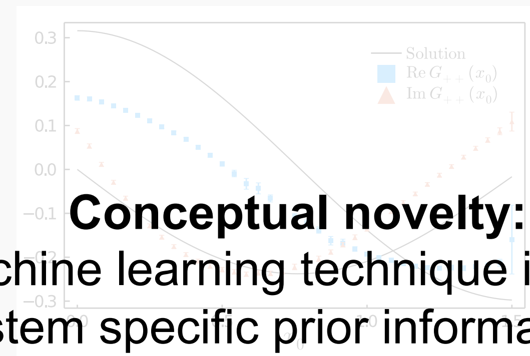

Conceptual novelty:
Machine learning technique infuses system specific prior information - loop-hole to beat the NP-hard sign problem
JHEP 04 (2023) 057

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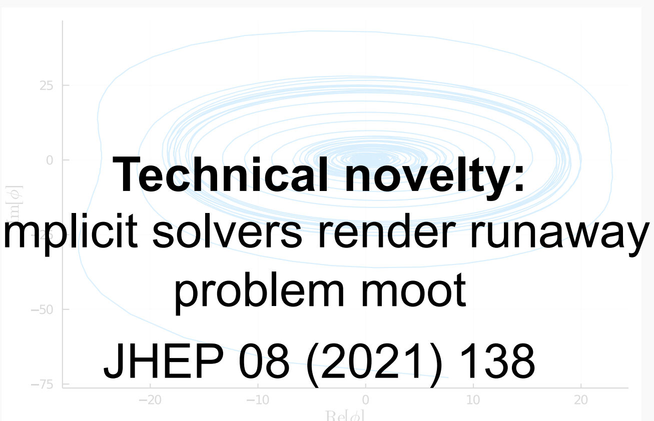

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provide stability needed to carry out ML optimization

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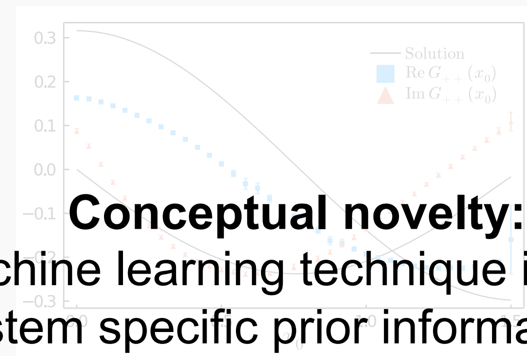
Convergence to incorrect solutions as real-time extent increases



Conceptual novelty:
Machine learning technique infuses system specific prior information - loop-hole to beat the NP-hard sign problem
JHEP 04 (2023) 057

Only a posteriori criterion available: tails in histogram of field d.o.f.

see e.g.: G. Aarts et.al. Eur. Phys. J. C71 (2011) 1756

Implicit solvers for Complex Langevin

University of Stavanger

- Numerical solution of stochastic dynamics in the literature: explicit forward Euler

$$\frac{d\phi}{d\tau_L} = i\frac{\delta S[\phi]}{\delta\phi(x)} + \eta(x,\tau_L)$$

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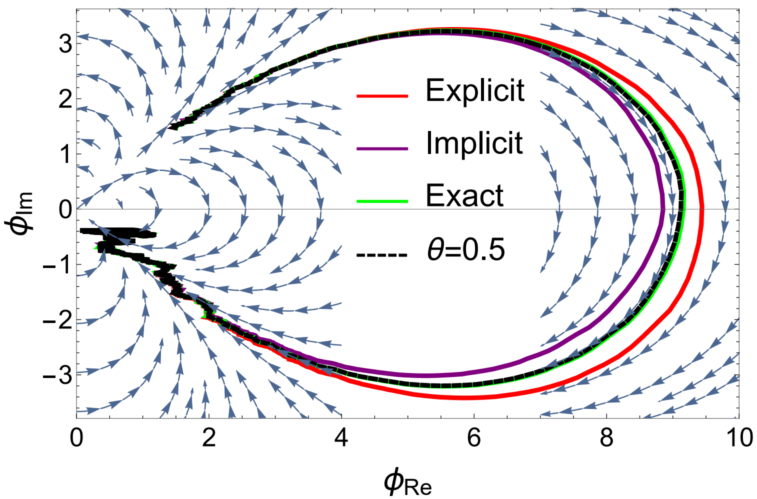

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general Euler-Maruyama scheme

Kloeden, P.E., Platen, E.: Numerical Solution of Stochastic Differential Equations, 1–50 (1992)

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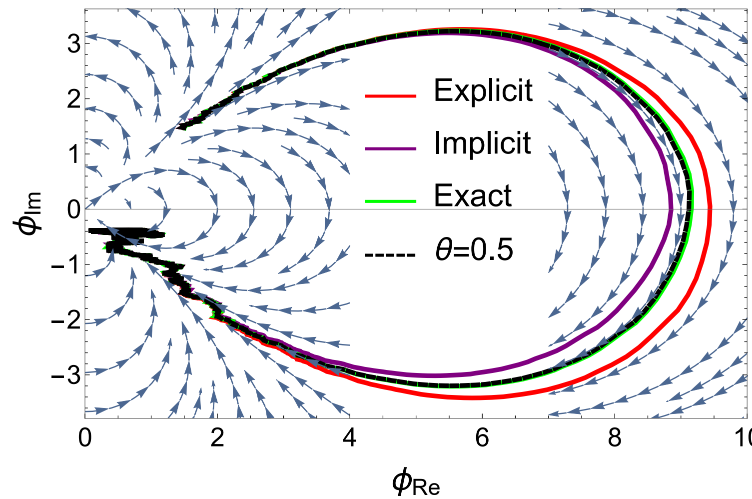

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- Inherent regularization allows for the first time to simulate on untilted SK contour

D. Alvestad, R. Larsen, A.R. JHEP 08 (2021) 138

$$S_\theta = \frac{1}{2}\phi\left(M + i\epsilon\theta M^2\right)\phi = S_{\text{explicit}} + \frac{i\epsilon}{2}\theta\sum_j S_j^2$$

CL at short real-times in 0+1d

- Direct simulations **anharmonic oscillator** on the canonical SK contour in **thermal equilibrium** possible m=1 λ=24 βm=m/T=1

D. Alvestad, R. Larsen, A.R. JHEP 08 (2021) 138

$$S = \frac{1}{2}\sum_j \left\{ \frac{(\phi_{j+1}-\phi_j)^2}{a_j} - a_j\left[V(\phi_{j+1})+V(\phi_j)\right] \right\} \qquad V(\phi_j) = \frac{\lambda}{4!}\phi_j^4$$

$$i\frac{\delta S[\phi]}{\delta \phi_j} = \frac{i}{\frac{1}{2}\left(|a_j|+|a_{j-1}|\right)}\left\{ \frac{\phi_j-\phi_{j-1}}{a_{j-1}} - \frac{\phi_{j+1}-\phi_j}{a_j} - \frac{1}{2}\left[a_{j-1}+a_j\right]\frac{\partial V(\phi_j)}{\partial \phi_j} \right\}$$

CL at short real-times in 0+1d

University of Stavanger

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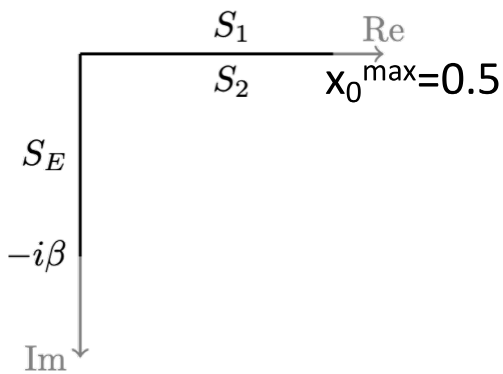
D. Alvestad, R. Larsen, A.R. JHEP 08 (2021) 138



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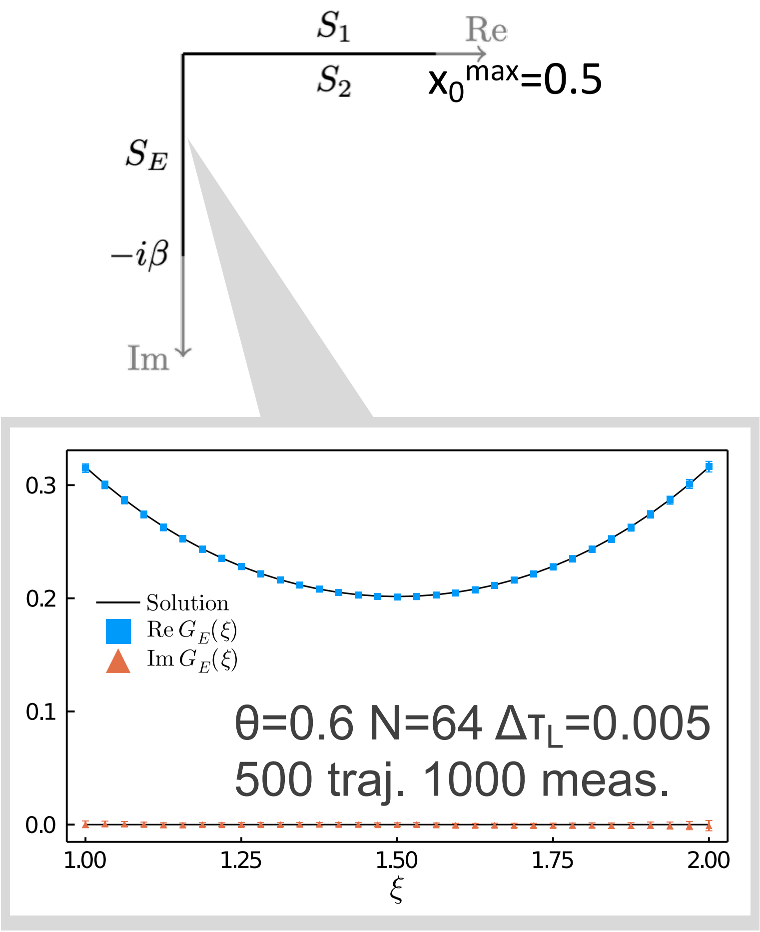

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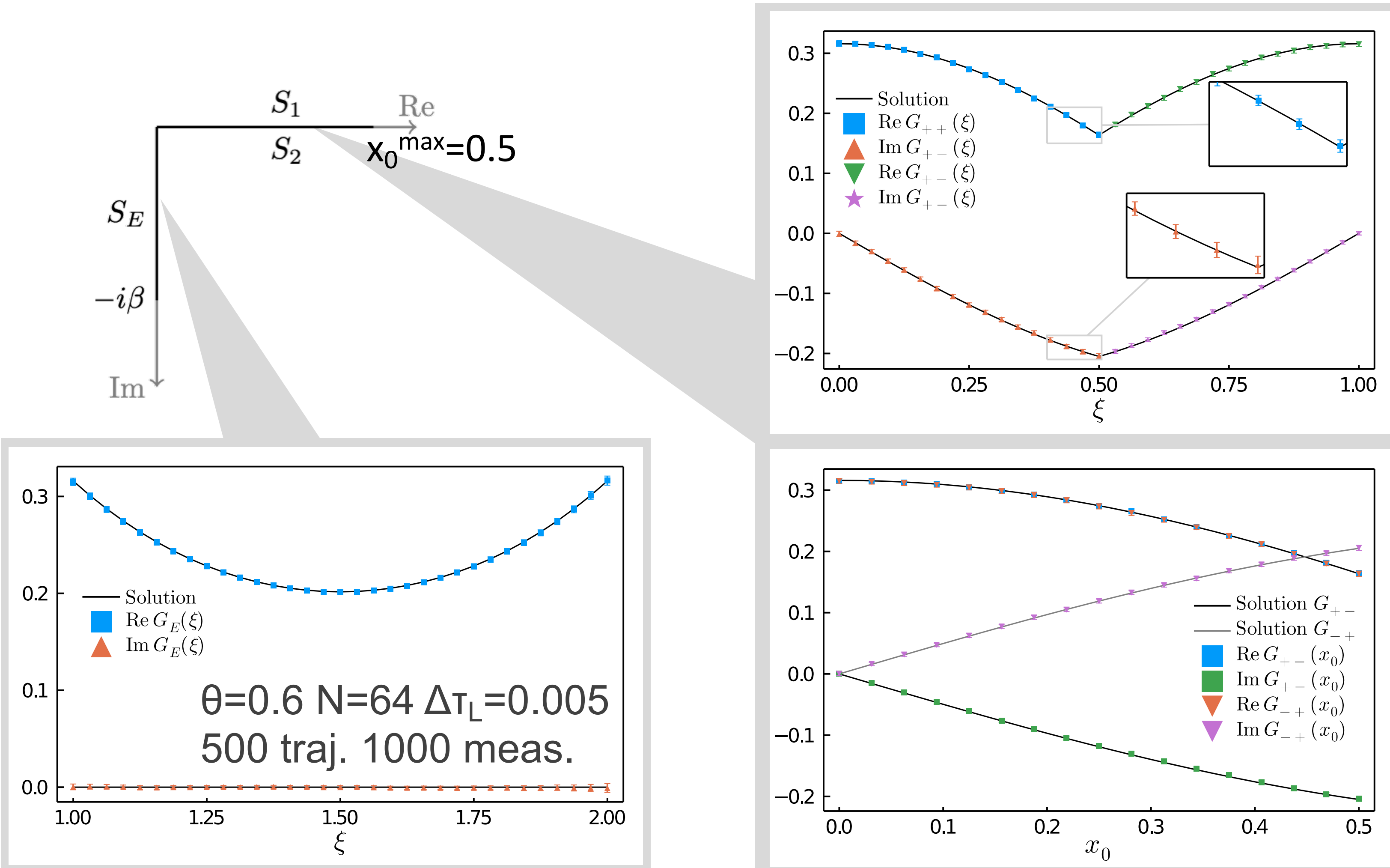
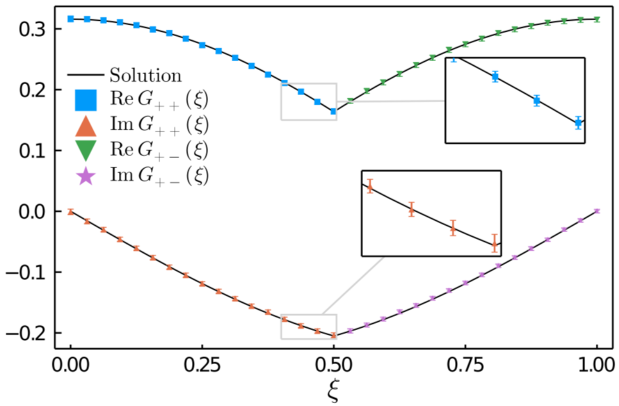
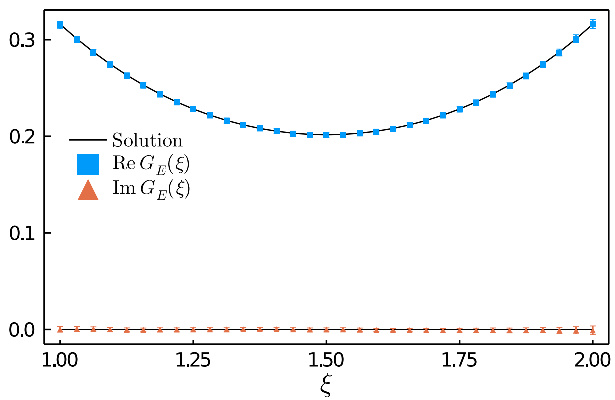


What happens at later real-time?

University of Stavanger





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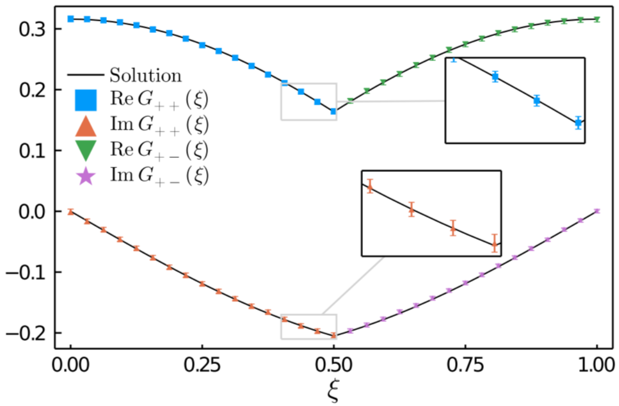

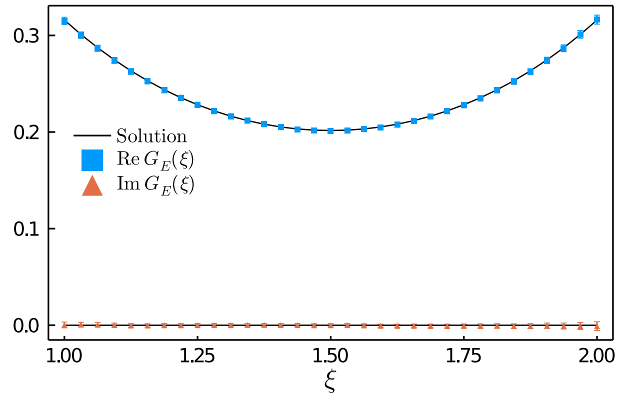

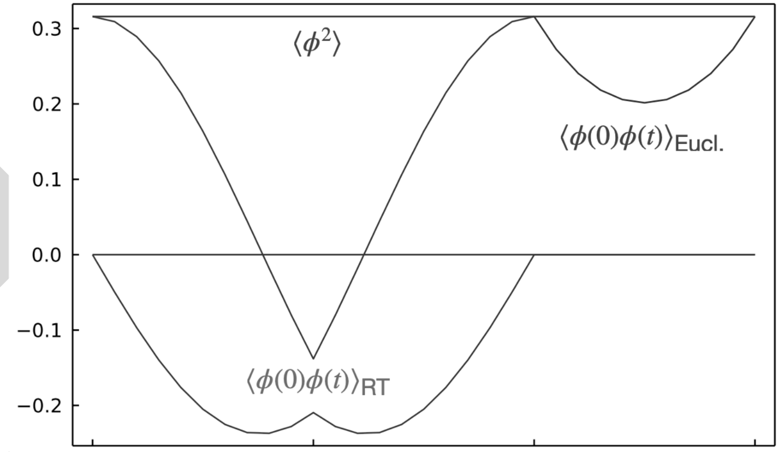

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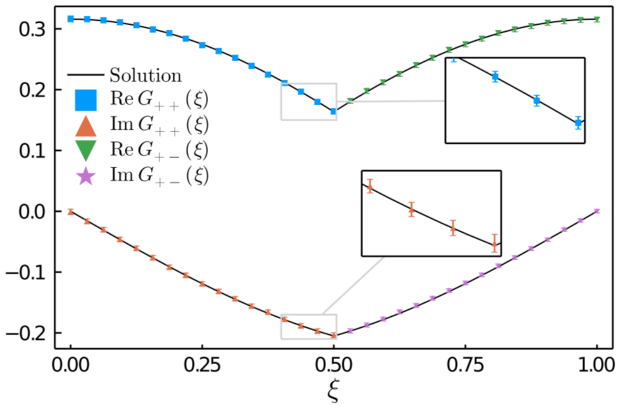

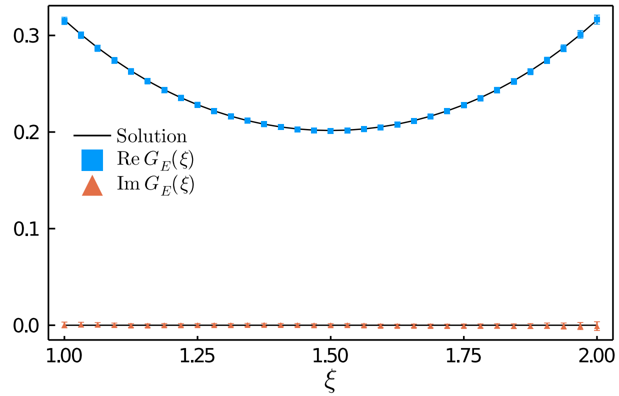

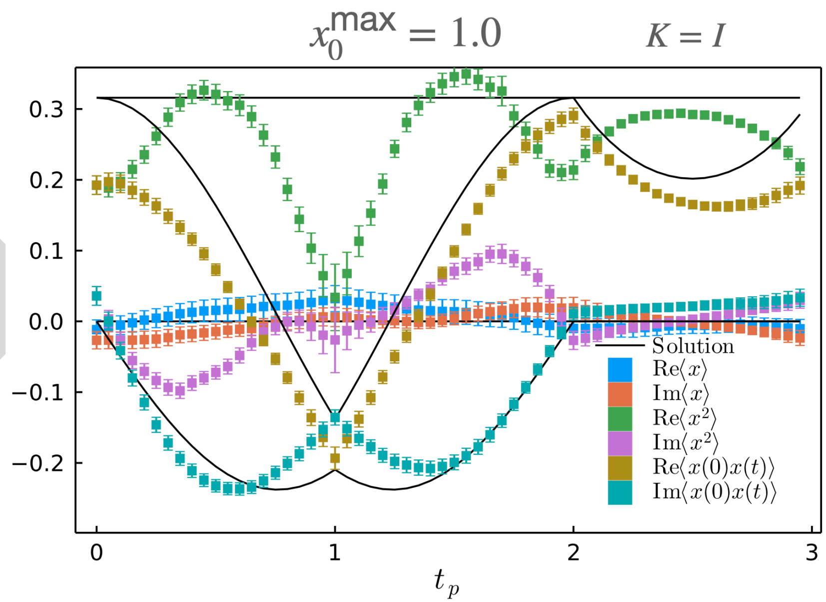

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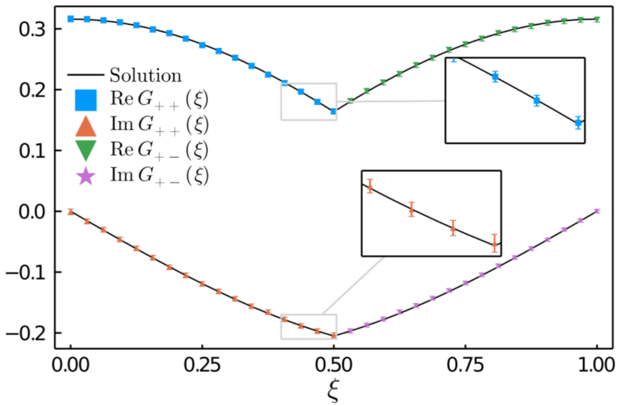

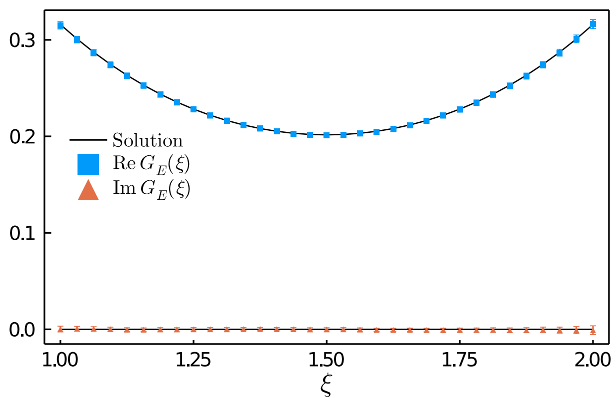

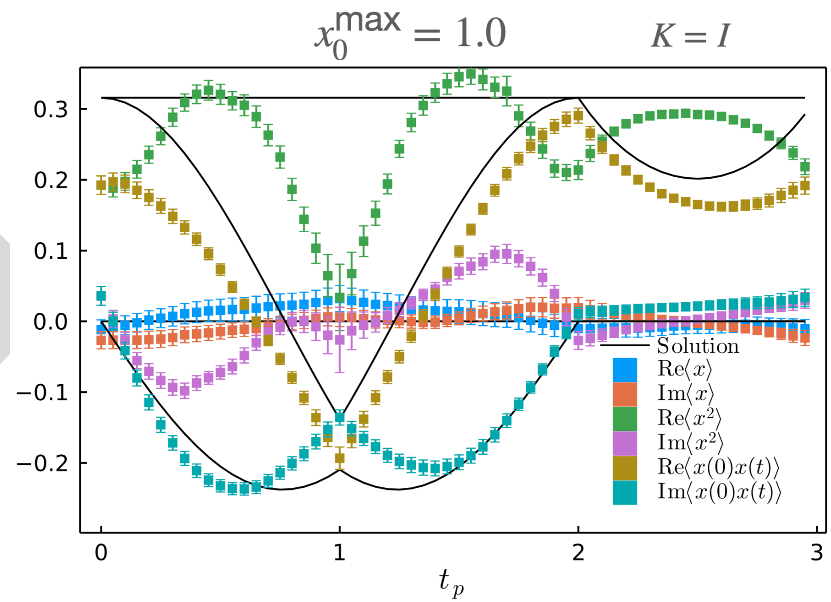

- Convergence to incorrect solution without apparent pathologies

Convergence in CL

$$\lim_{\tau_L \to \infty} \int d\phi_R d\phi_I \mathcal{O}(\phi_R + i\phi_I) P_{\text{CL}}[\phi_R, \phi_I, \tau_L] \stackrel{?}{=} \int d\phi \, \mathcal{O}(\phi) \, e^{iS}$$

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- Necessary, while not sufficient criterion for correct convergence: absence of **boundary terms**

developed in: G. Aarts et.al. Eur. Phys. J. C71 (2011) 1756
see also: D. Alvestad, R. Larsen, A.R. JHEP 04 (2023) 057

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    Seiler, Sexty, Stamatescu, PLB 04 62 (2013)
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- Our idea for NP-hard sign problem: incorporate **system specific prior information** without affecting the proof of convergence

Kernelled complex Langevin

University of Stavanger

- Simultaneous modification of drift and noise allows to alter FP spectrum

$$\frac{d\phi}{d\tau_L} = iK[\phi]\frac{\partial S}{\partial \phi} + \frac{\partial K[\phi]}{\partial \phi} + \sqrt{K[\phi]}\eta$$

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Okamoto, Okano, Schülke, Tanaka, PLB 324 684 (1989)

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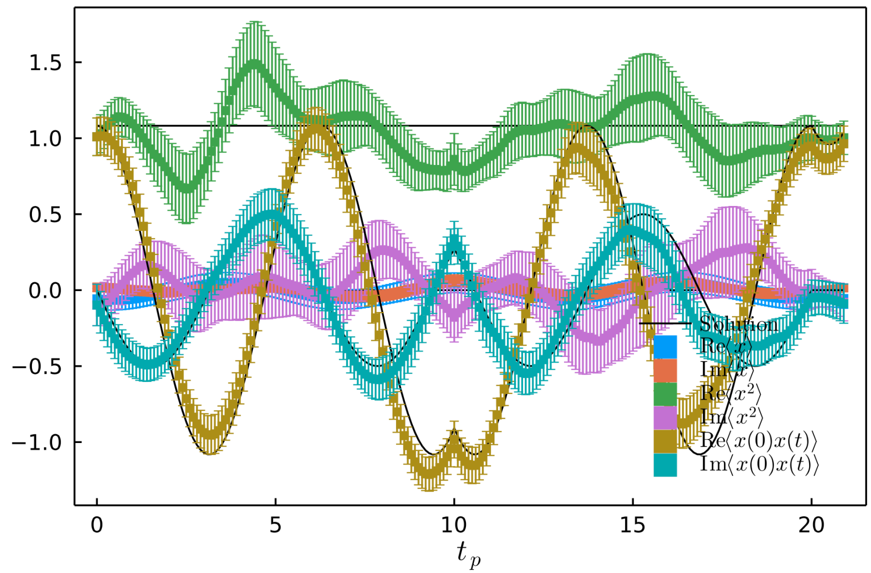

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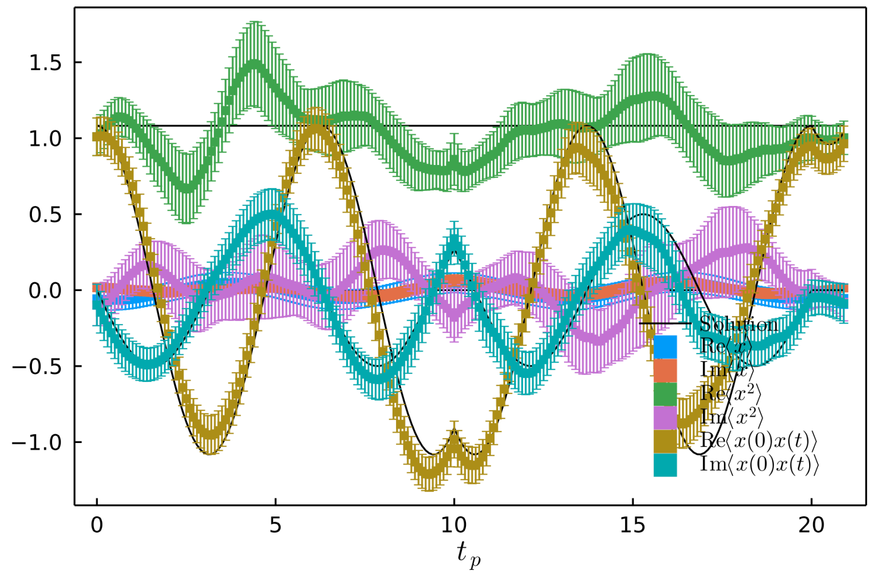

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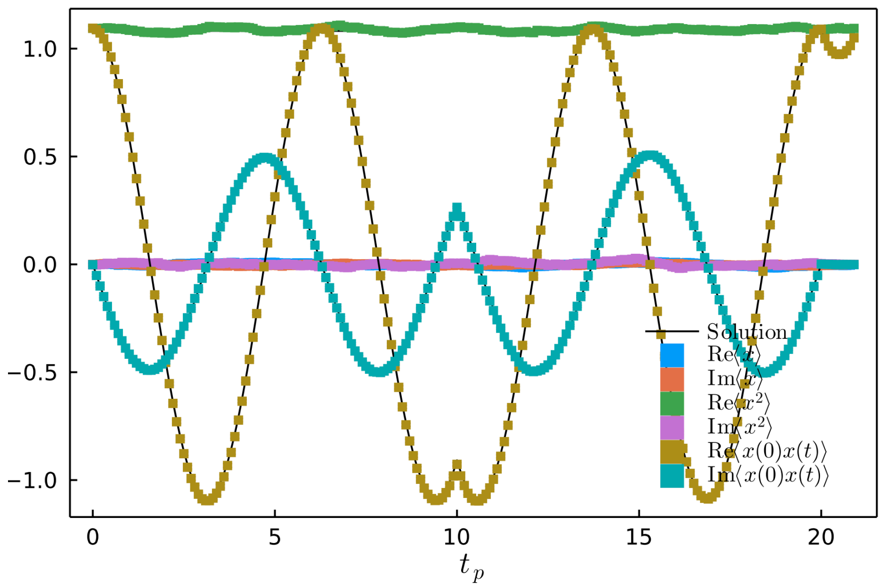

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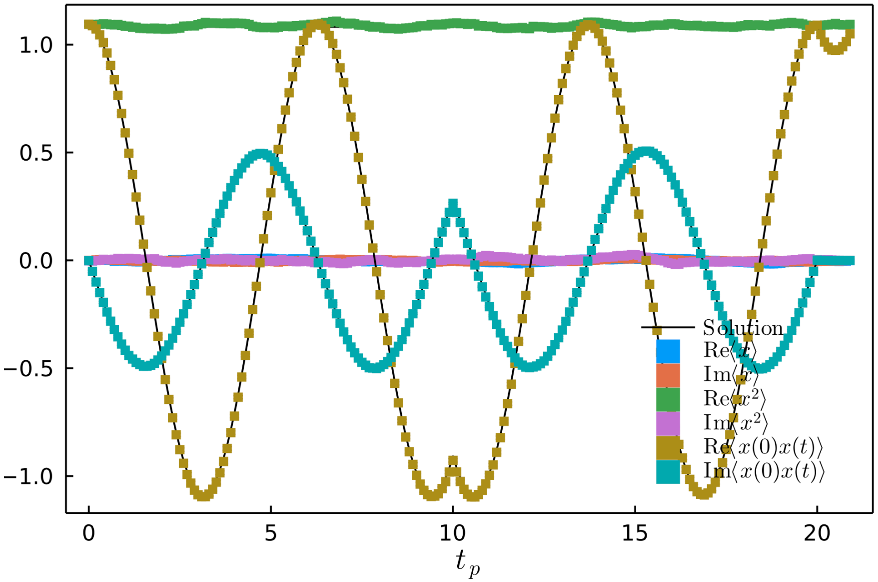


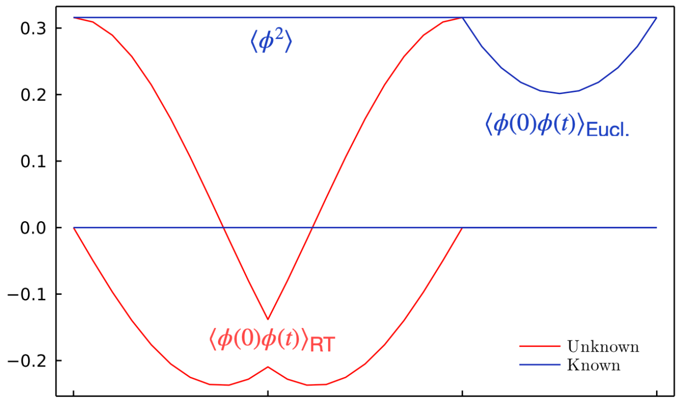
- Allows us to extend correct convergence to any real-time extent in free theory

Systematic learning of optimal kernels

University of Stavanger

- **Optimality via prior information**: Symmetries, Euclidean correlator, Boundary

D. Alvestad, R. Larsen, A.R. JHEP 04 (2023) 057



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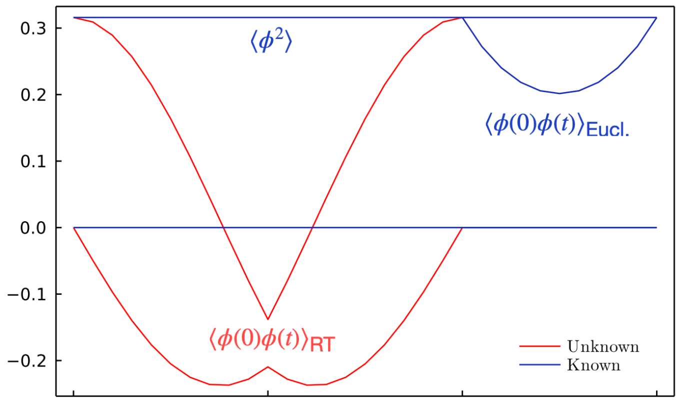
$$L^{\text{sym}} = \sum_t \left\{ \langle \phi_t \rangle^2 + \langle \phi_t^3 \rangle^2 + \left(\langle \phi_t^2 \rangle - \phi^2 \right) \right\}$$

$$L^{\text{bnd}} = \sum_i \sum_k \left\{ \langle L_c[\phi_i] \mathcal{O}_k \rangle_Y \right)^2$$

$$L^{\text{eucl}} = \sum_i \left\{ \left(\langle \phi_0 \phi_i \rangle - D_i^E \right)^2 \right\}$$



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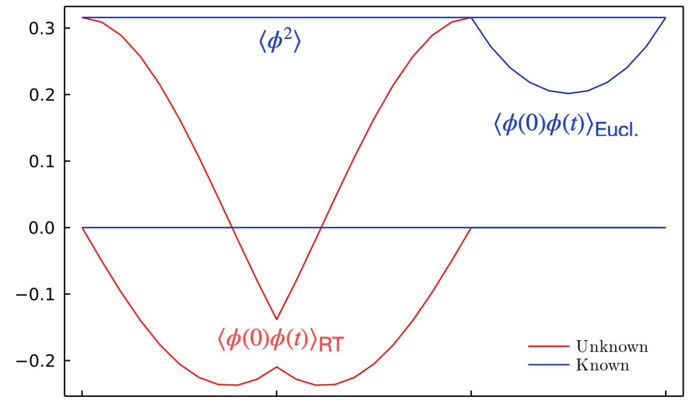

- Autodifferentiation techniques to compute $\dfrac{\partial L^{\mathrm{tot}}}{\partial K_{ij}}$ (derivative of stochastic process)
[note: deterministic dynamics chaotic]

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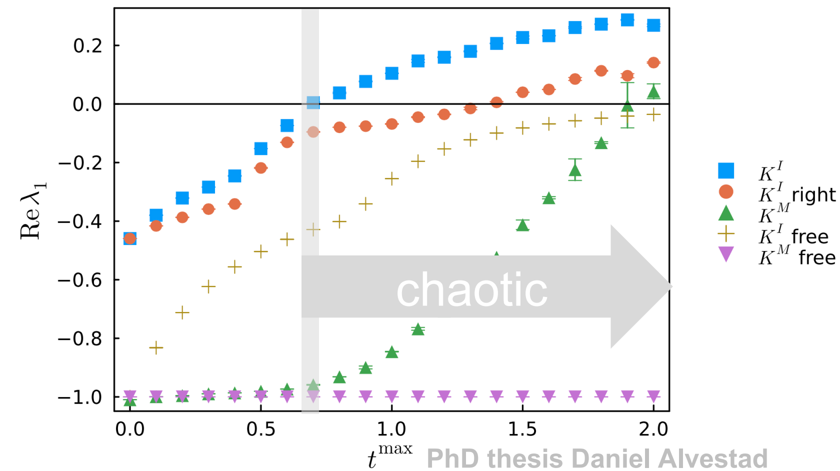
CL Lyapunov exponents



PhD thesis Daniel Alvestad

- Autodifferentiation techniques to compute $\dfrac{\partial L^{\rm tot}}{\partial K_{ij}}$ (derivative of stochastic process) [note: deterministic dynamics chaotic]

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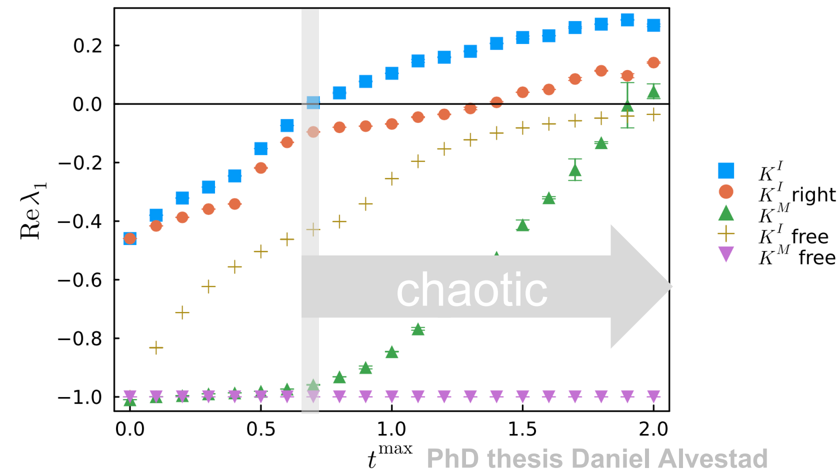

PhD thesis Daniel Alvestad

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- In principle possible, in practice slow: cheaper optimization functional instead

$$L^{\rm low\ cost} = \frac{1}{N_t} \sum_{i=1}^{N_t} \left| K \frac{\partial S}{\partial \phi}_t (-\phi_t) - \left| K \frac{\partial S}{\partial \phi}_t \right| |\phi_t| \right|^2$$

minimizes drift away from the origin (c.f. dynamic stabilization but holomorphic)

D. Alvestad, R. Larsen, A.R. JHEP 04 (2023) 057

$$L^{\rm low\ cost} = \frac{1}{N_t} \sum_{i=1}^{N_t} {\rm Im}[\phi]^2$$

inspired by study of novel boundary criterion for detection of incorrect convergence

N. Lampl and D. Sexty (in preparation)

Performance in 0+1d (AHO)

University of Stavanger

- Using a constant kernel $K = exp[A + iB]$ with A,B real matrices
- Optimize via low cost functional & check success via symmetries & Euclidean corr.

D. Alvestad, R. Larsen, A.R. JHEP 04 (2023) 057

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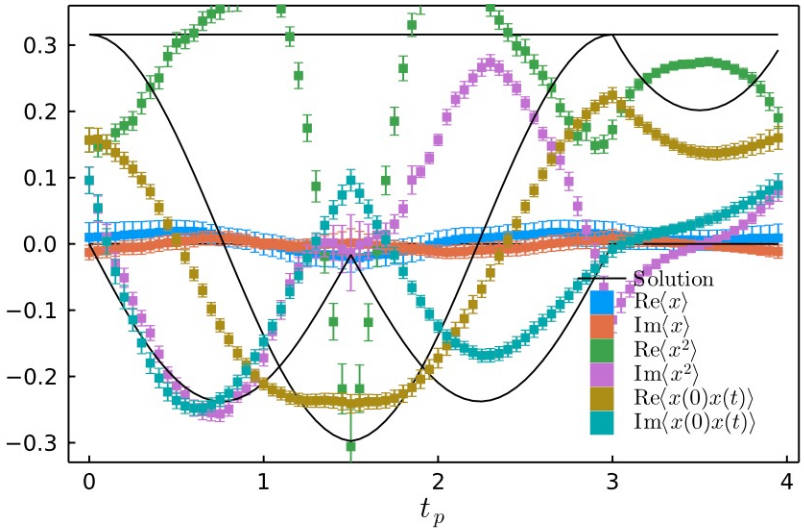

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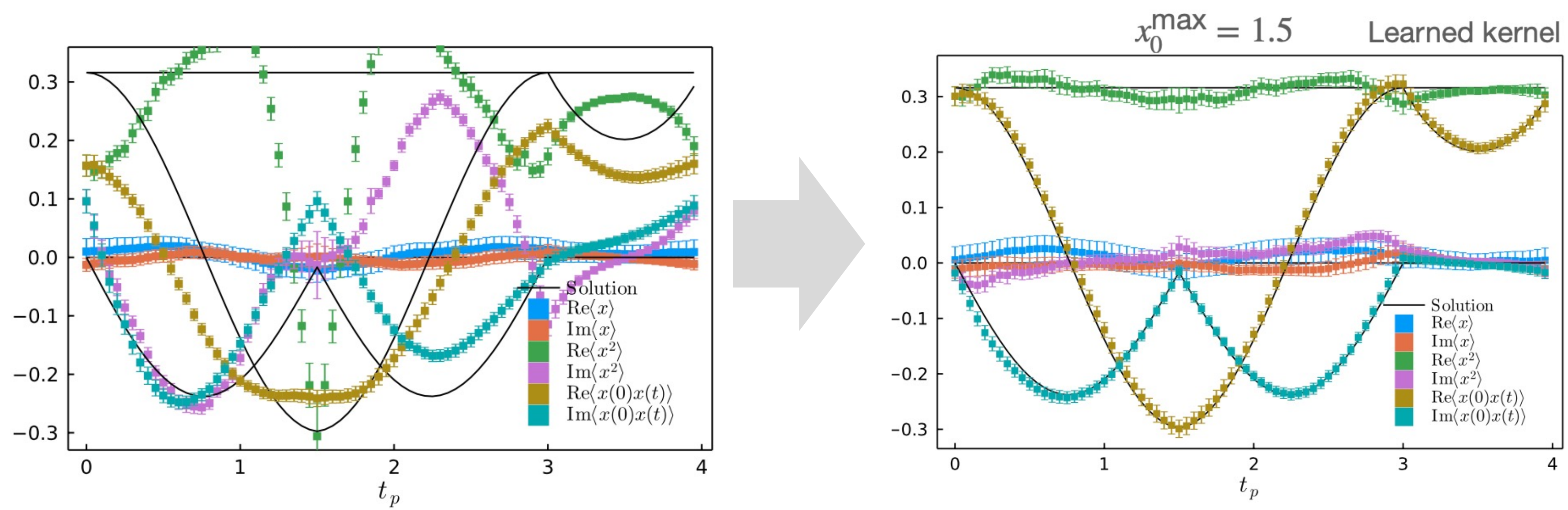

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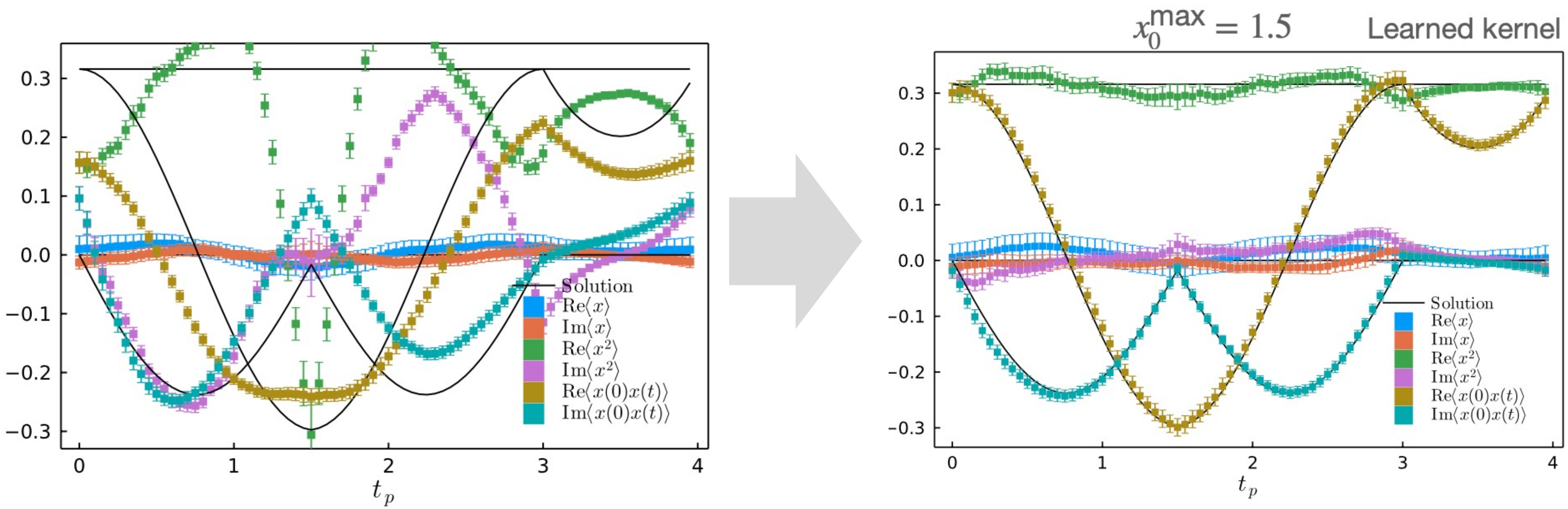
D. Alvestad, R. Larsen, A.R. JHEP 04 (2023) 057



- Achieve correct convergence up to **3x time extent** previously reported in literature

Recent results in 1+1d field theory

University of Stavanger

$$S[\phi] \equiv \sum_{t,n} a_t a \left[\frac{(\phi_{t+1,n} - \phi_{t,n})^2}{2a_t^2} + \frac{1}{2}\left(\frac{(\phi_{t+1,n+1} - \phi_{t+1,n})^2}{2a^2} + \frac{(\phi_{t,n+1} - \phi_{t,n})^2}{2a^2} \right) + \frac{1}{2}m^2 \frac{\phi_{t,n}^2 + \phi_{t+1,n}^2}{2} + \frac{\lambda}{4!} \frac{\phi_{t+1,n}^4 + \phi_{t,n}^4}{2} \right]$$

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- Found that for 1+1d low-cost functional proposed by Graz group offers even better performance. N. Lampl and D. Sexty (in preparation)

$$L^{\text{low cost}} = \frac{1}{N_t} \sum_{i=1}^{N_t} \text{Im}\left[\phi\right]^2$$

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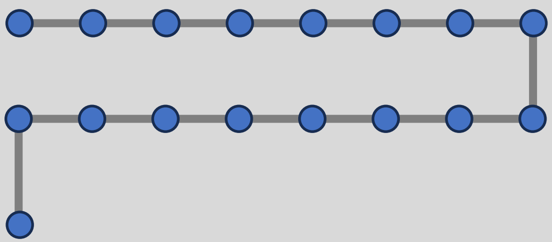

N_t=8 N_τ=2 a=0.2

m=1 λ=1 βm=m/T=0.4 N_x=8

A. Alexandru et.al. PRD 95 (2017) 11, 114501

- based on contour deformations
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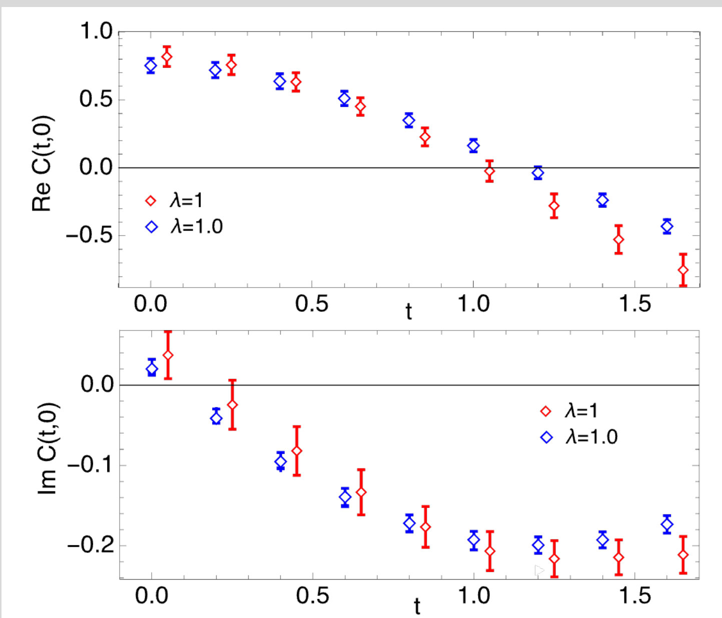

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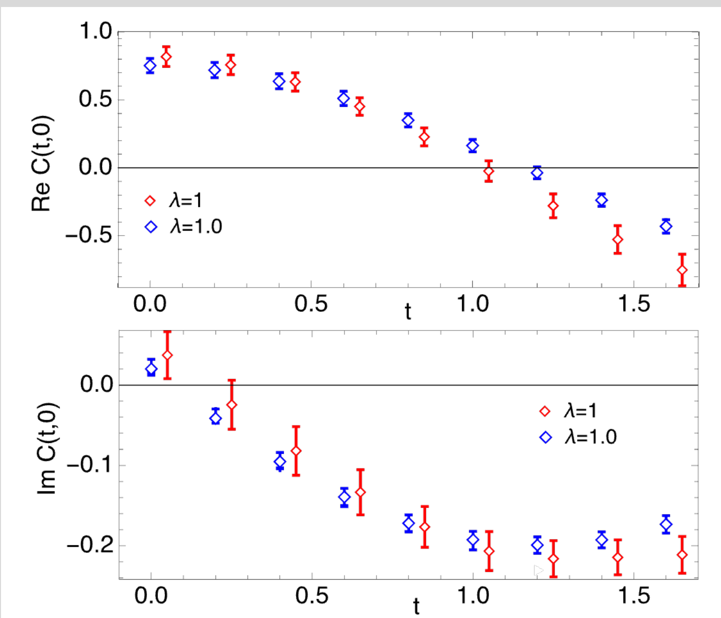

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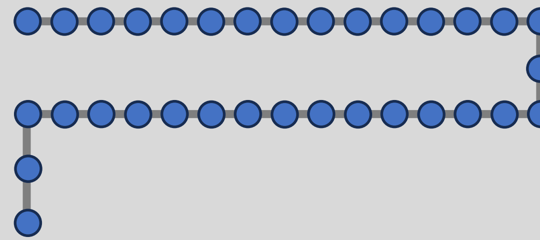
Optimal learned CL kernels



N_t=16 N_τ=4 a_t=0.1 a_s=0.2

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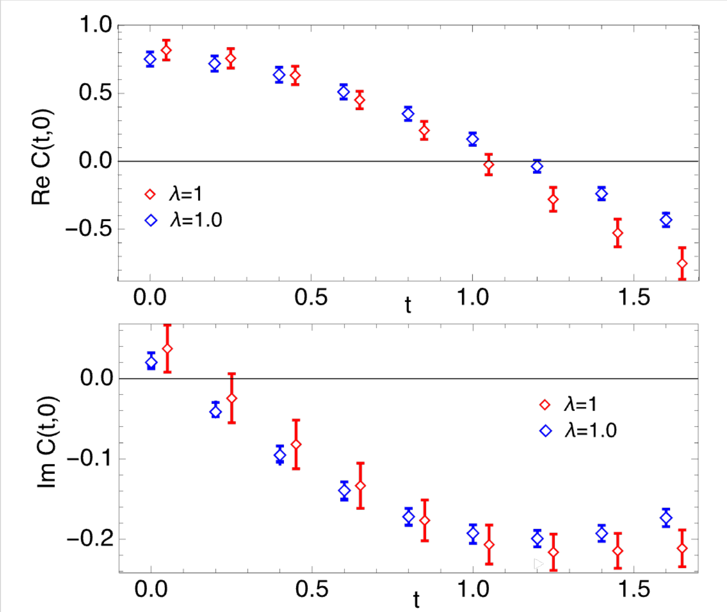

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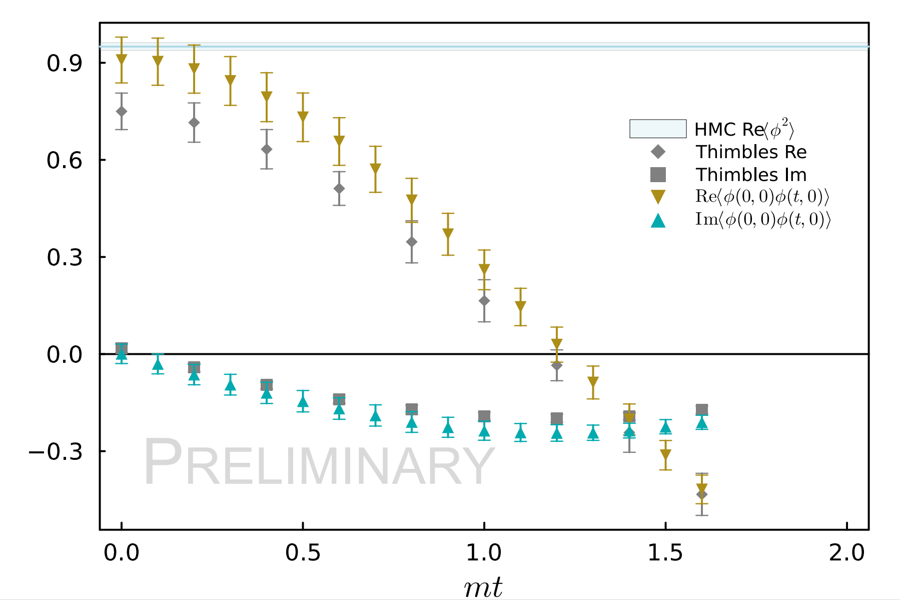

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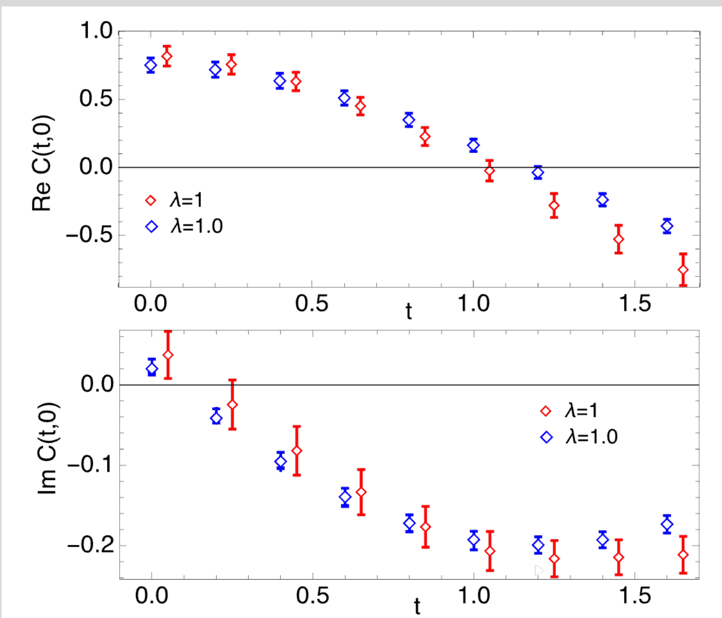

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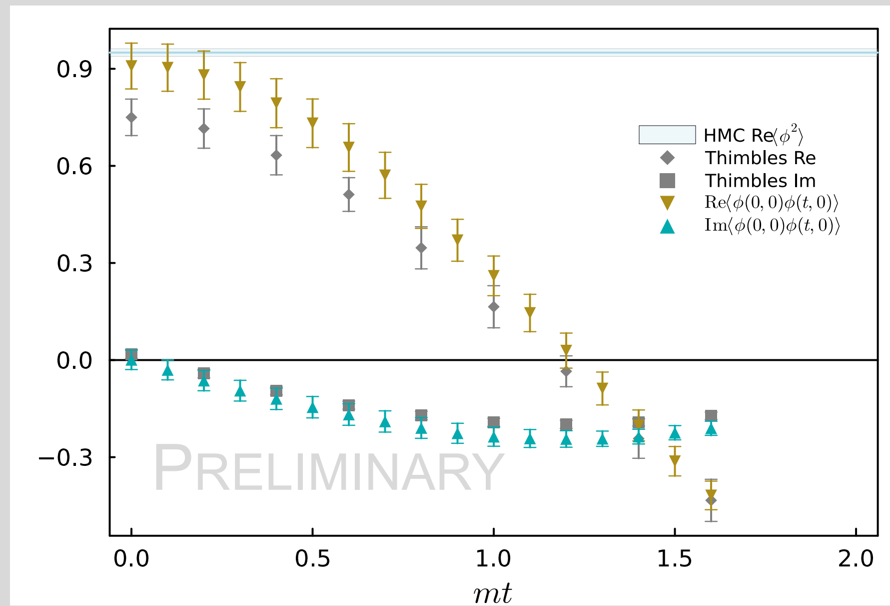

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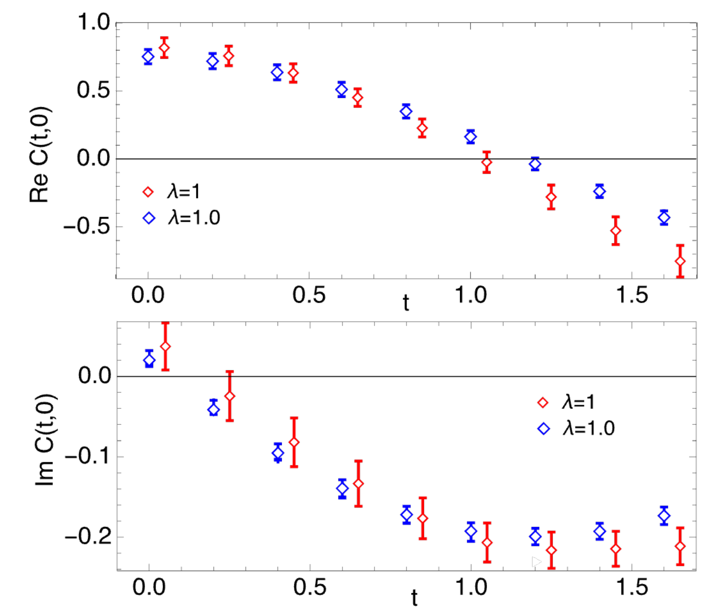

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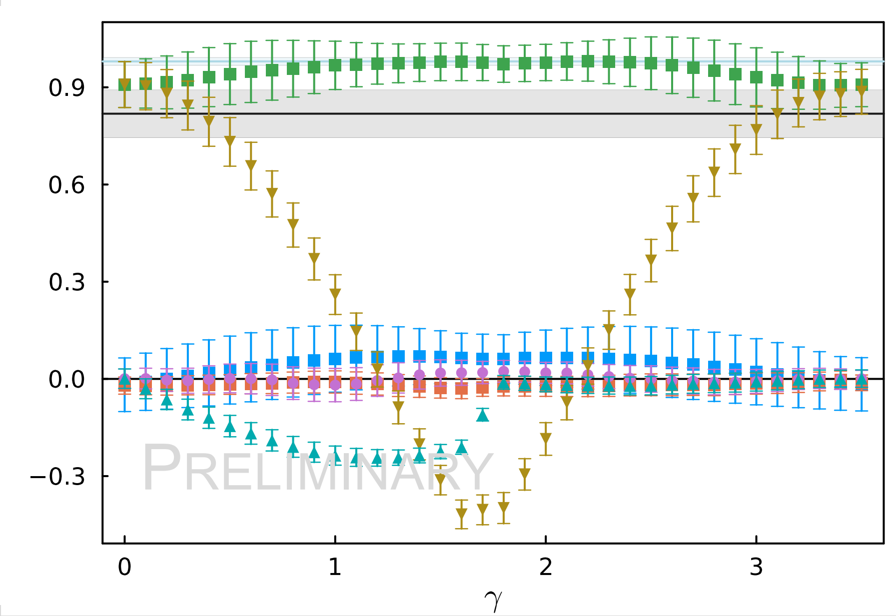

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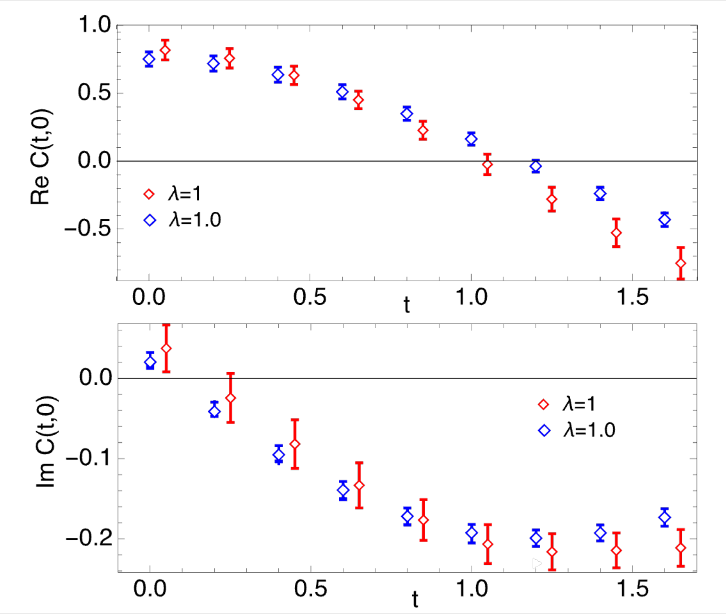

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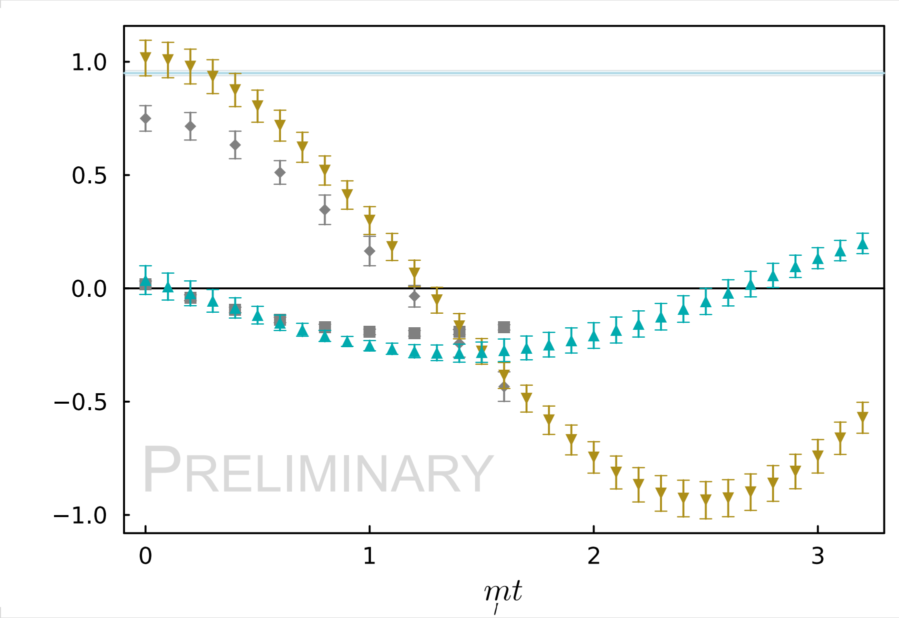

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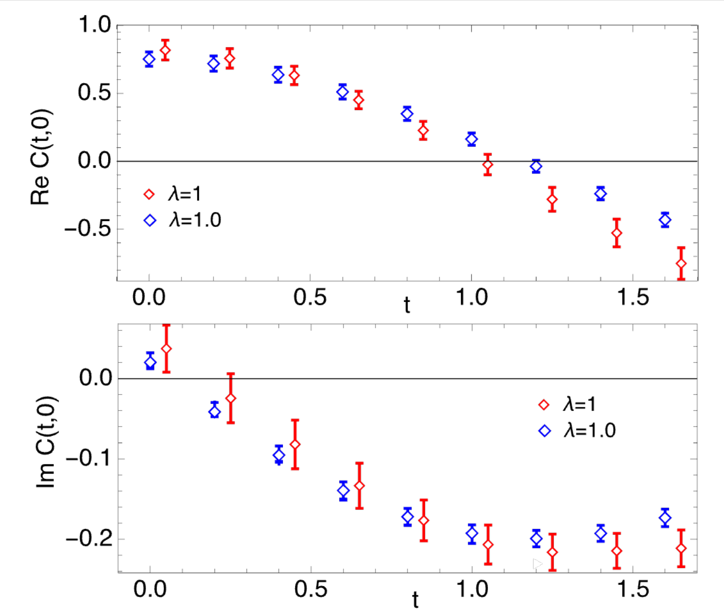

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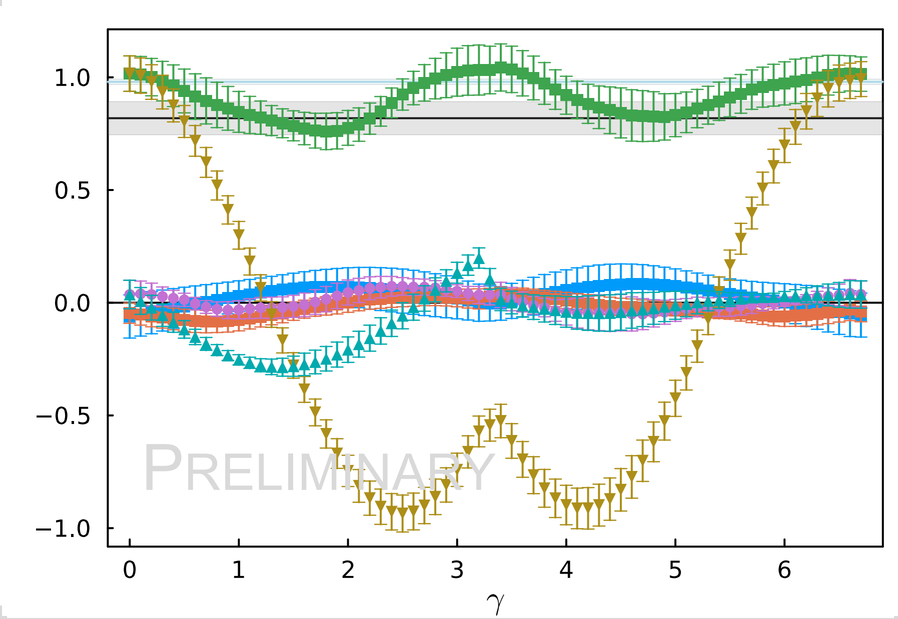

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University of Stavanger

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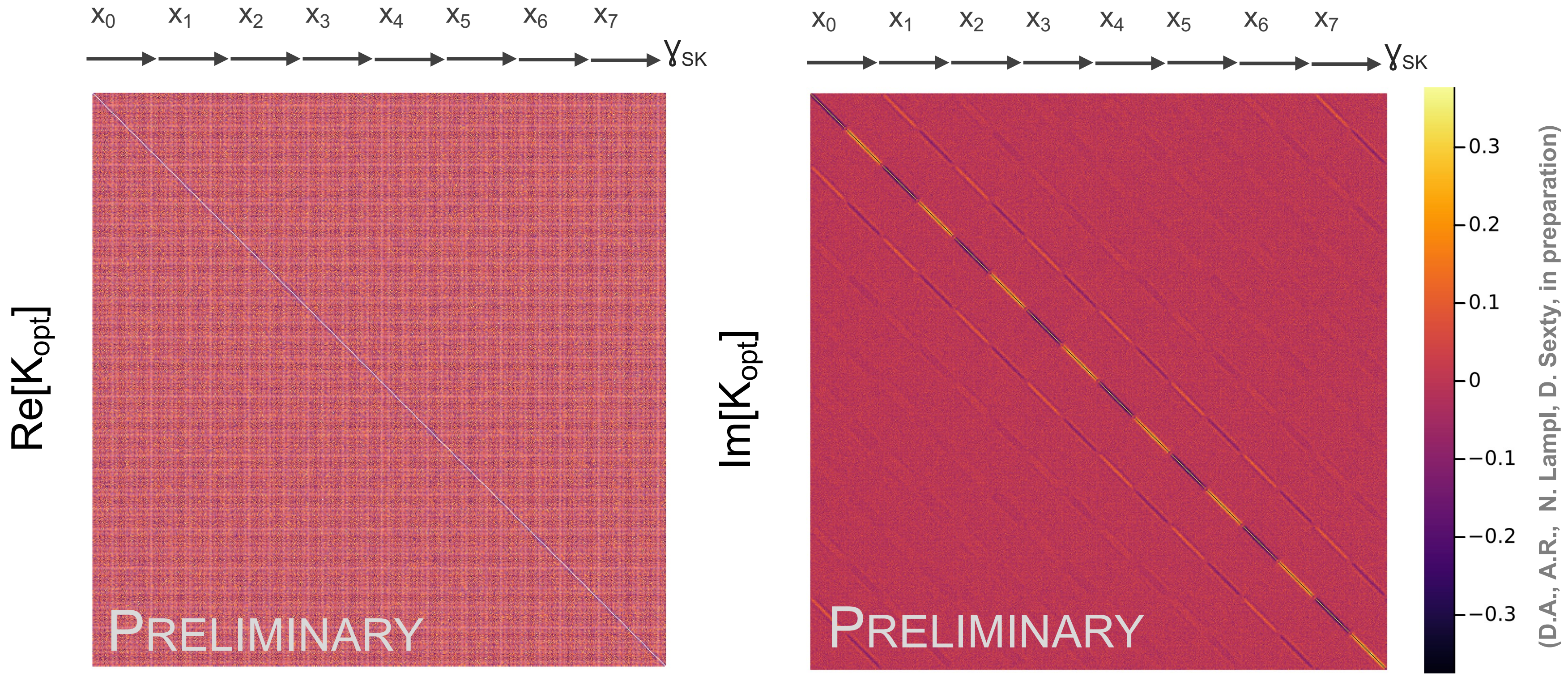
  Im[K] banded structure in spatial dimension with diminishing amplitude



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University of Stavanger

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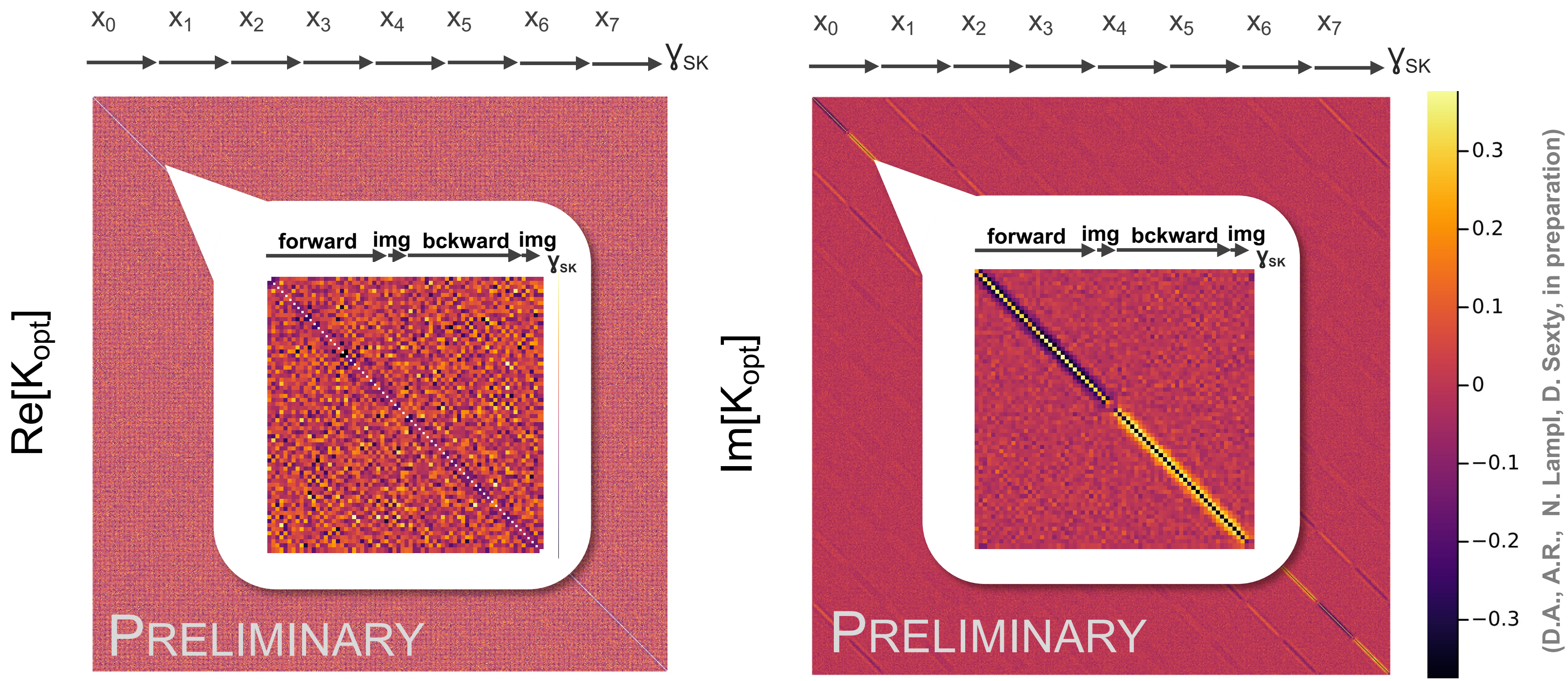

- Derivative-like pattern in **Im[K] mixing neighboring d.o.f.** on the SK contour

Conclusion & Outlook

University of Stavanger

- Overcoming **NP-hard sign problem** central to progress in theoretical physics
- **Complex Langevin** one possible path forward, but hampered by two major challenges: **instabilities** and **convergence to incorrect** solutions
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- Optimal **kernels in QM**: 3x extended range of validity of real-time CL
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- Next step: **2+1d simulations**, cost effective optimization strategies for **field dependent kernels** (adjoint sensitivity analysis, shadowing method (NILSS), etc.)

Backup slides

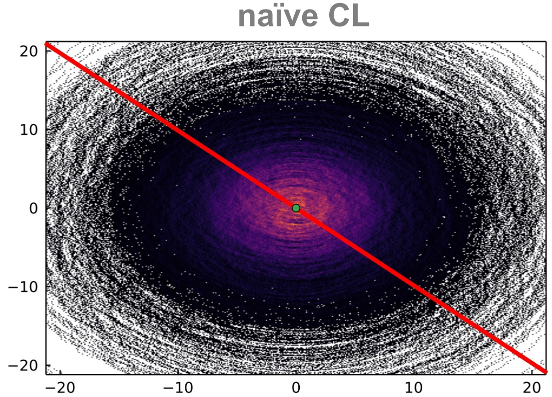
Limits to our current strategy

University of Stavanger

- Constant kernel works well in theories with single critical point at the origin

simple Gaussian model $S = \frac{1}{2} i x^2$

Lefschetz thimbles $\frac{d\phi}{d\tau} = \overline{\frac{dS}{d\phi}}$



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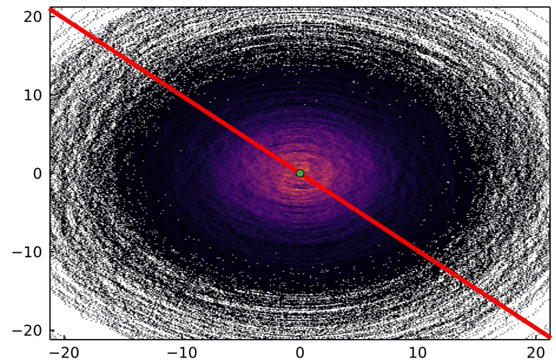
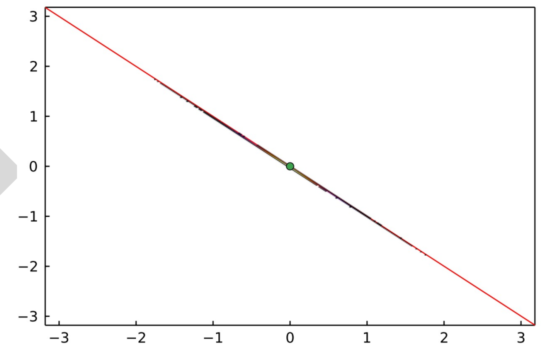


learned kernelled CL



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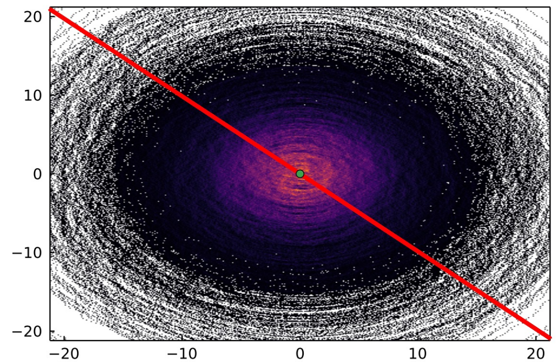

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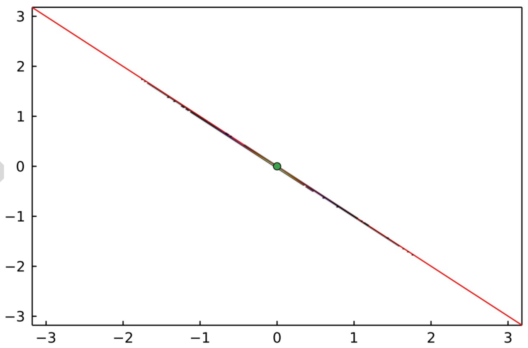

- Multiple critical points may require a field dependent kernel: $S = 2ix^2 + (1/2)x^4$

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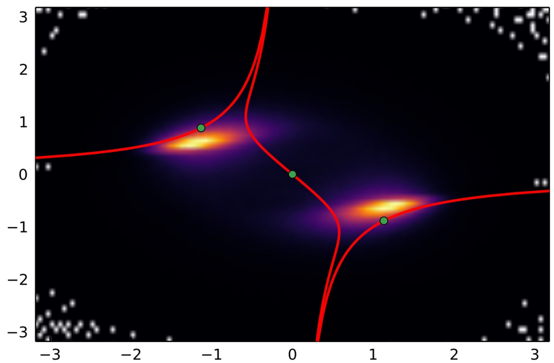

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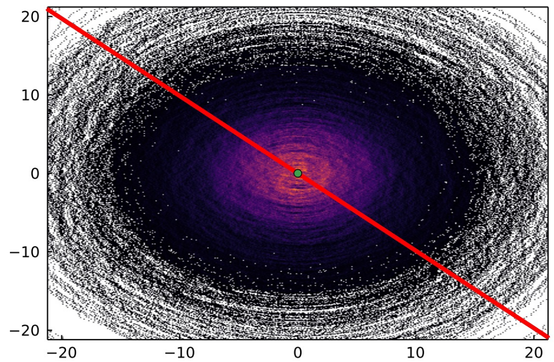

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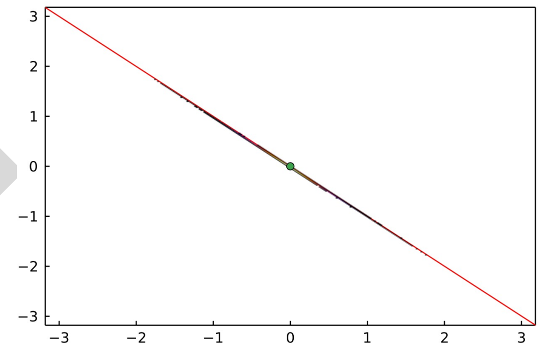

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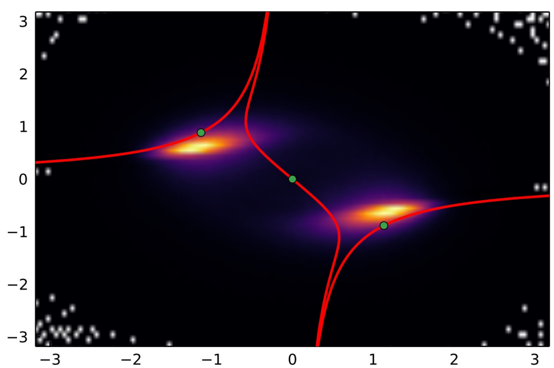

L^{tot}=0.888

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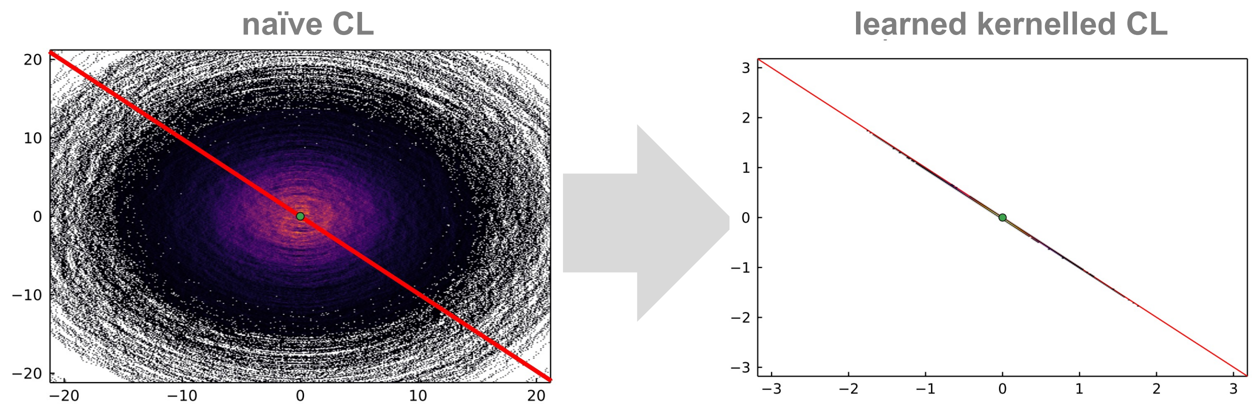

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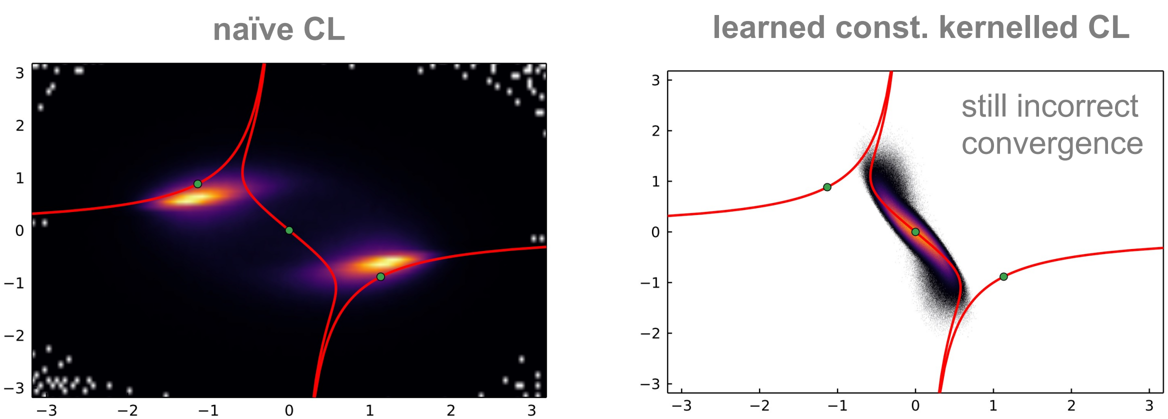

L^{tot}=0.888 L^{tot}=0.486

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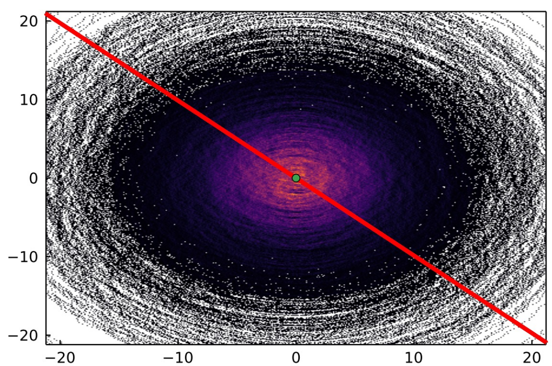

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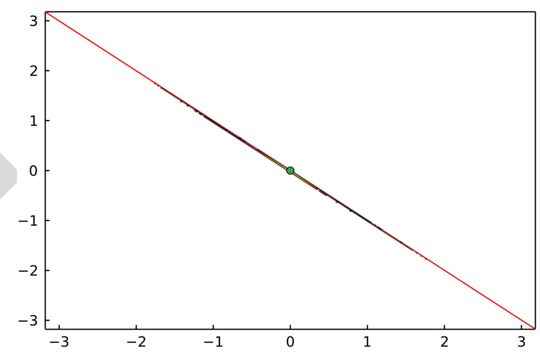

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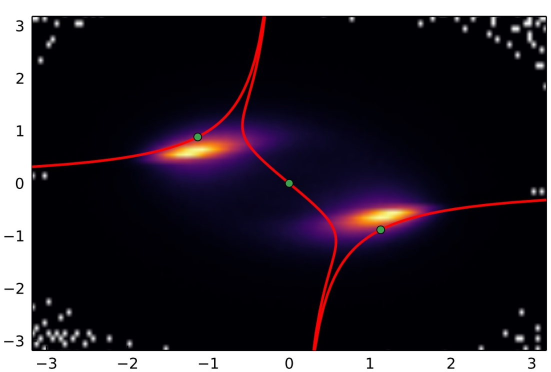

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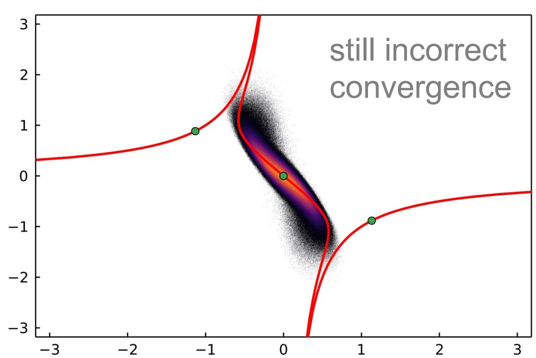

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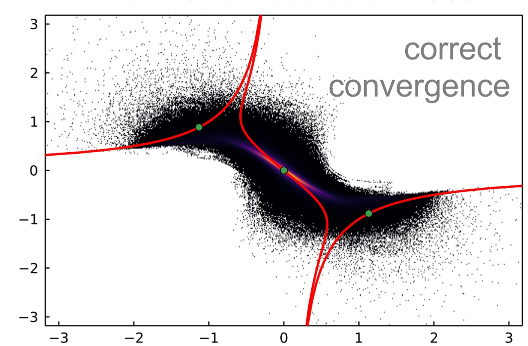
field dependent kernel from Okamoto et.al. 1989



L^{tot}=0.023

Two convergence criteria

University of Stavanger

- Non-unique optima from the low-cost functional: allow to avoid boundary terms
- Correct convergence iff **in addition** Fokker-Planck EV in lower half plane

see D. Alvestad, R. Larsen, A.RJHEP 04 (2023) 057 and PhD thesis D. Alvestad

$$S = \frac{1}{2}\sigma x^2 + \frac{\lambda}{4}x^4 \qquad \sigma = 4i,\ \lambda = 2$$

→

$$K = e^{i\theta}$$

single number, optimum found by scan of $L_{lowcost}$

Two convergence criteria

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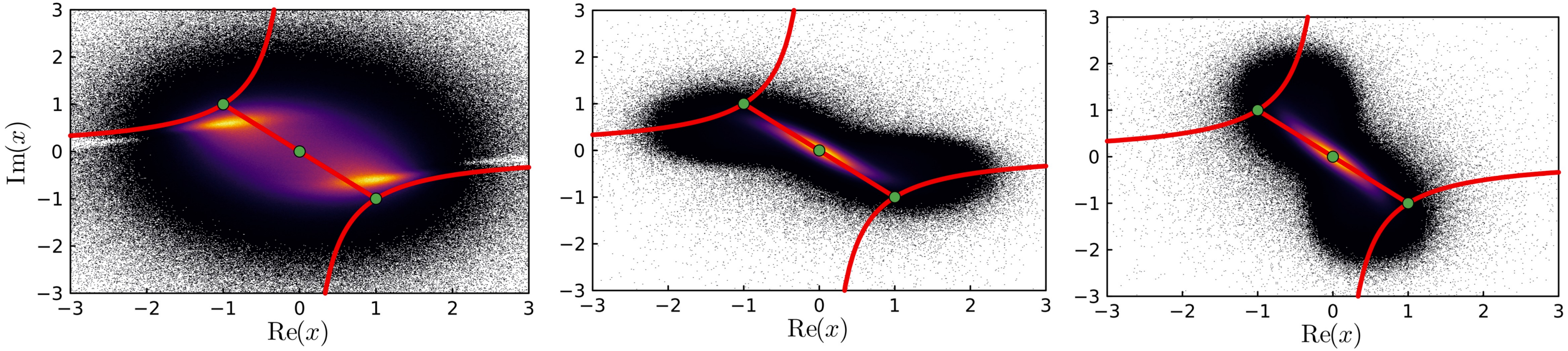

K=1

K=exp[-iπ/3]
correct convergence

K=exp[-i2π/3]
incorrect convergence

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single number, optimum found by scan of L_{lowcost}