Kernel controlled real-time Complex Langevin simulation

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Lattice 2022

The Research Council of Norway

NPACT Norwegian Particle, Astroparticle & Cosmology Theory network

Introduction

- Real-time simulation (sign-problem)

- Complex Langevin equation $\phi \to \phi^R + i\phi^I$
(Stochastic Differential equation)

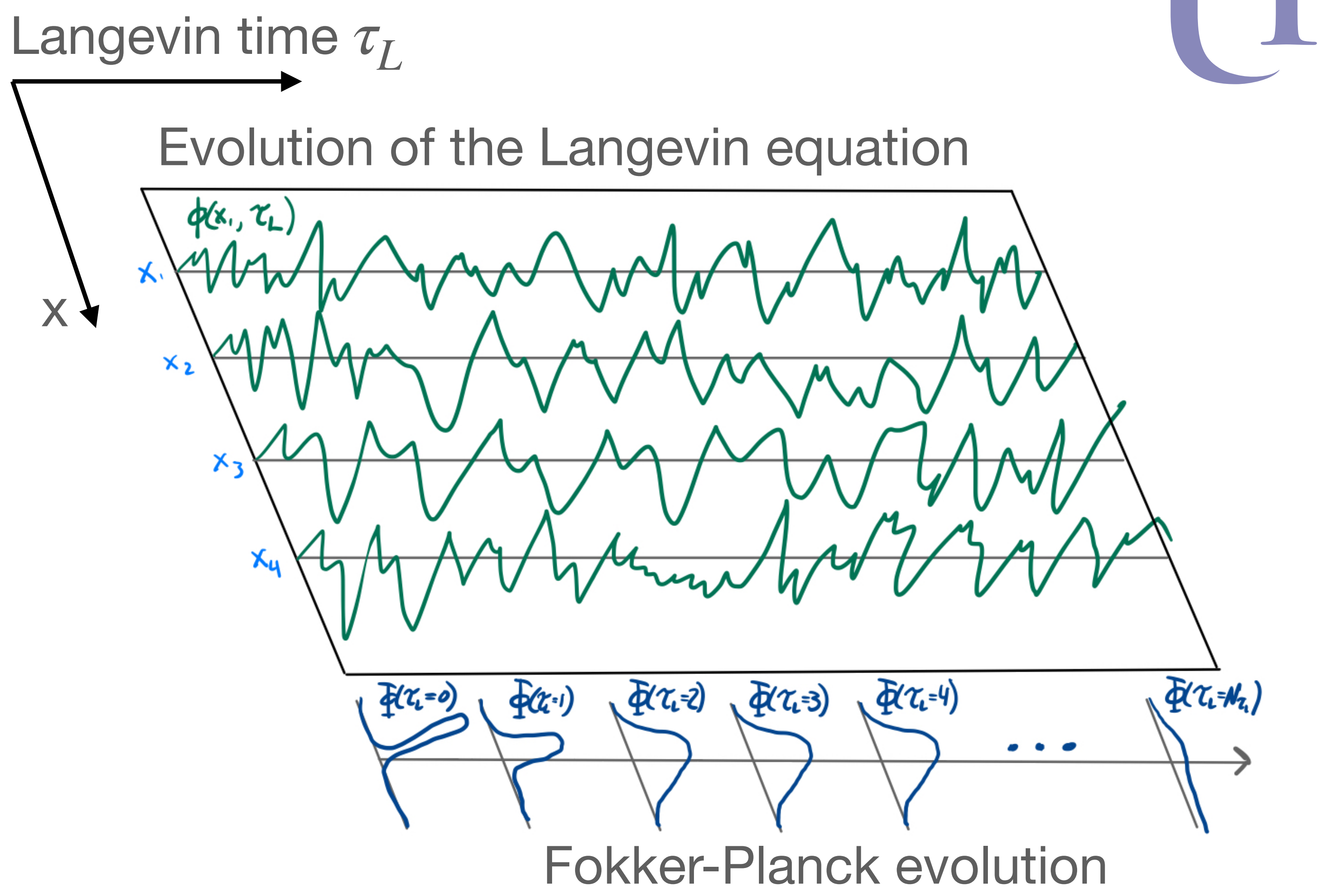
$$\frac{d\phi}{d\tau_L} = i\frac{\delta S[\phi]}{\delta \phi(x)} + \eta(x,\tau_L) \quad \text{with}$$

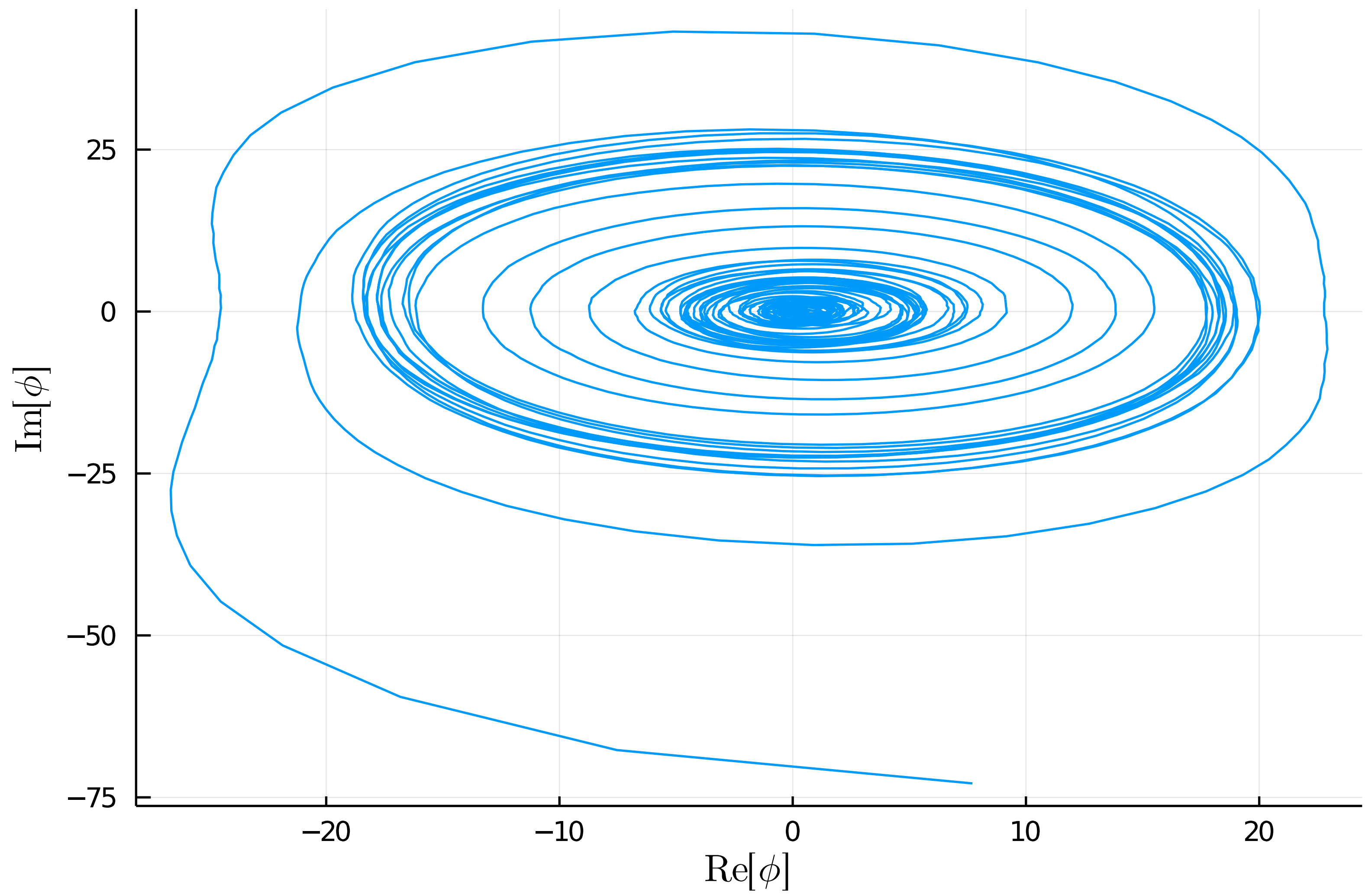
$$\langle \eta(x,\tau_L)\rangle = 0, \quad \langle \eta(x,\tau_L)\eta(x',\tau_L')\rangle = 2\delta(x-x')\delta(\tau_L-\tau_L')\,.$$

- Fokker-Planck equation

$$\frac{\partial}{\partial t}\Phi(x,t) = \sum_j \frac{\delta}{\delta\phi_j}\left[\frac{\delta}{\delta\phi_j} + \frac{\delta S[\phi]}{\delta\phi_j}\right]\Phi(x,t) = -H_{\mathrm{FP}}\Phi(x,t)$$

- Problems
  - Runaway solutions
  - Convergence to the wrong solution





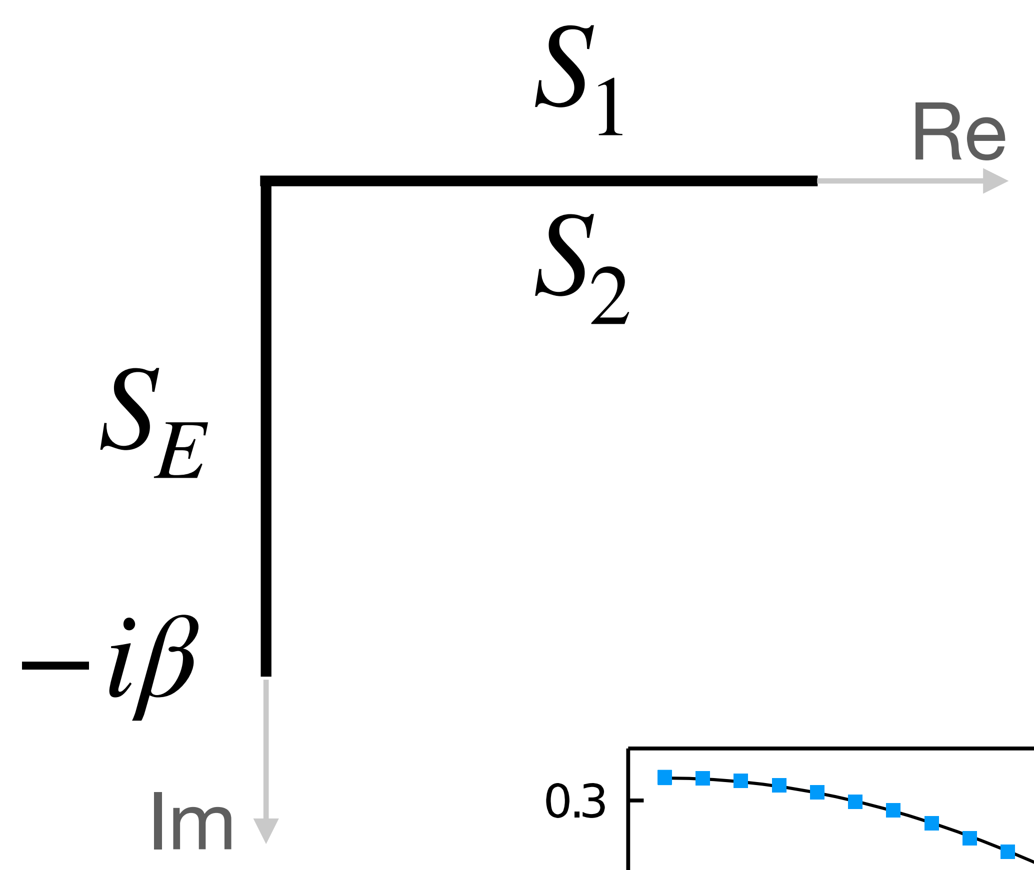
Problem of stability in real-time simulations

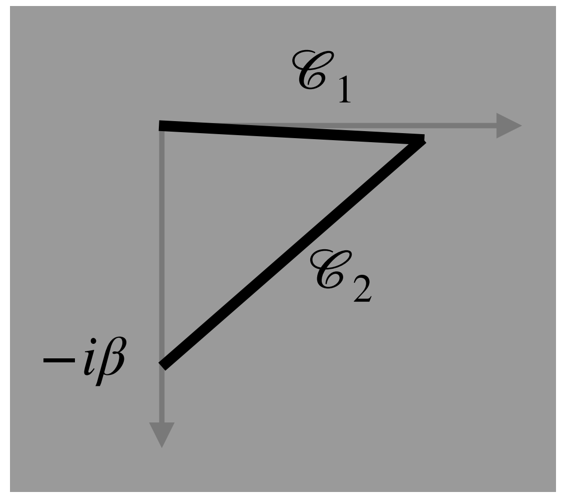
- Runaway solutions
- Adaptive step-size
- Regularisation via use of implicit scheme D.A, Larsen, Rothkopf (2021) arxiv: 2105.02735
  - General Euler-Maruyama scheme

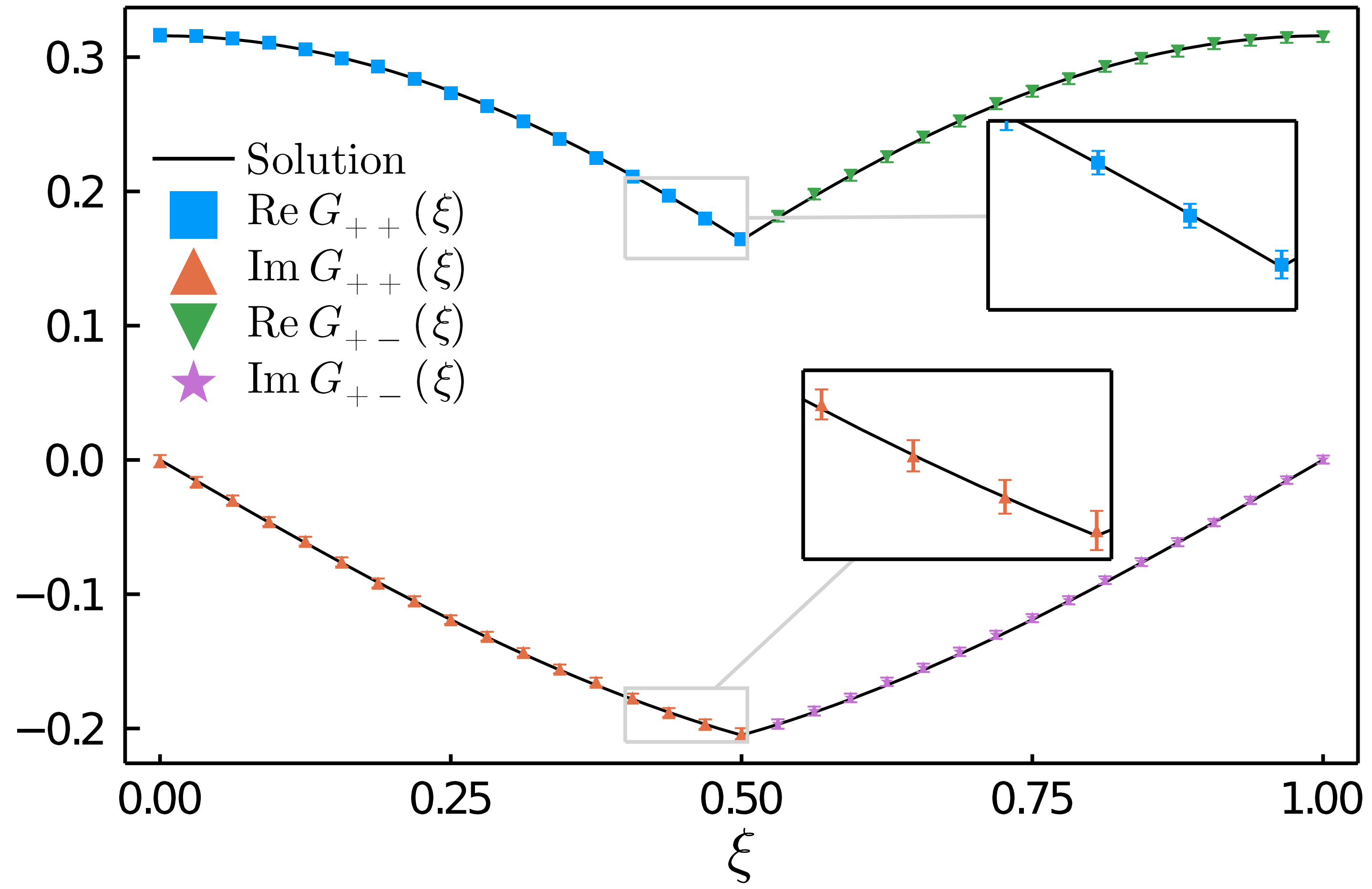
$$\phi_j^{\lambda+1} = \phi_j^{\lambda} + i\epsilon_j \left[\theta \frac{\partial S^{\lambda+1}}{\partial \phi_j} + (1-\theta) \frac{\partial S^{\lambda}}{\partial \phi_j} \right] + \sqrt{\epsilon_j}\eta_j^{\lambda}$$

- Strongly coupled quantum anharmonic oscillator with $\beta = 1,\, m = 1,\, \lambda = 24$ on a real-time contour

$$S = \int dx_0 \left\{ \frac{1}{2}\left(\frac{\partial \phi}{\partial x_0}\right)^2 - \frac{1}{2} m \phi^2 - \frac{\lambda}{4!}\phi^4 \right\}$$







Contour: $\beta = 1,\, x_0^{\max} = 0.5$

Solver: Euler-Mayruyama with $\theta = 0.6$

Simulations done with the DifferentialEquations.jl library in Julia

Problem of wrong convergence

- Boundary terms Scherzer, Seiler, Sexty, Stamatescu (2018+2019)
- Gauge Cooling Seiler, Sexty, Stamatescu (2013)
- Dynamical stabilisation Attanasio, Jäger (2019)
- Modification to CLE
  - Coordinate Transformations Aarts et. al. (2013)
  - Kernels Söderberg (1988), Okamoto et. al. (1989)

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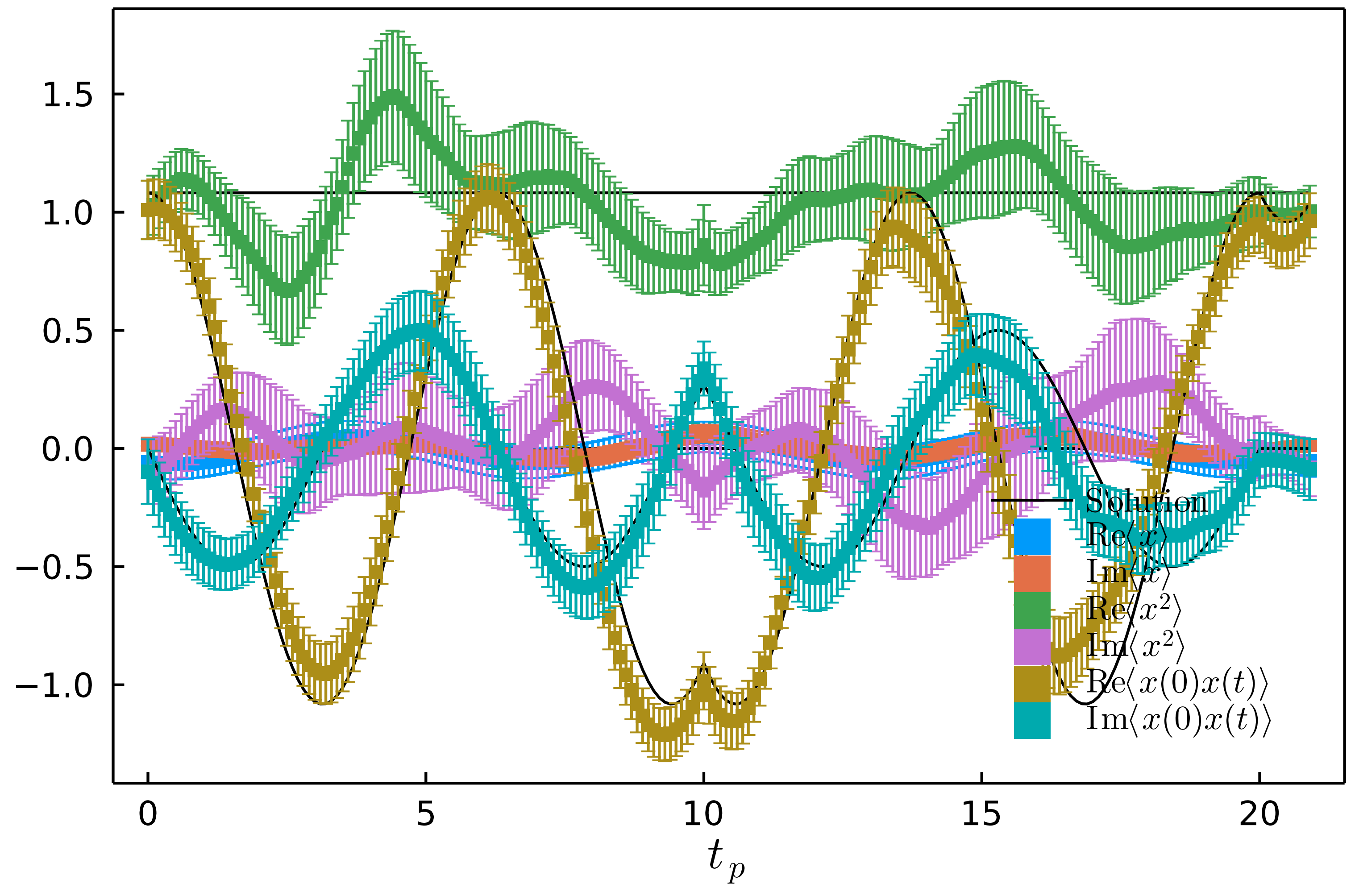
Kernelled complex Langevin

- Additional freedom in Fokker-Planck equation; regain same equilibrium distribution
- Kernelled Langevin $d\phi = \left(-K[\phi]\frac{\partial S[\phi]}{\partial \phi} + \frac{\partial K[\phi]}{\partial \phi}\right) d\tau_L + \sqrt{K[\phi]}dW$
- Free theory propagator: $S = \phi^\dagger M \phi, \quad K = -M^{-1}, \quad K\,\partial_\phi S[\phi] = -\phi,$
  $d\phi = -\phi + \sqrt{-M^{-1}}dW$

Free theory

No kernel



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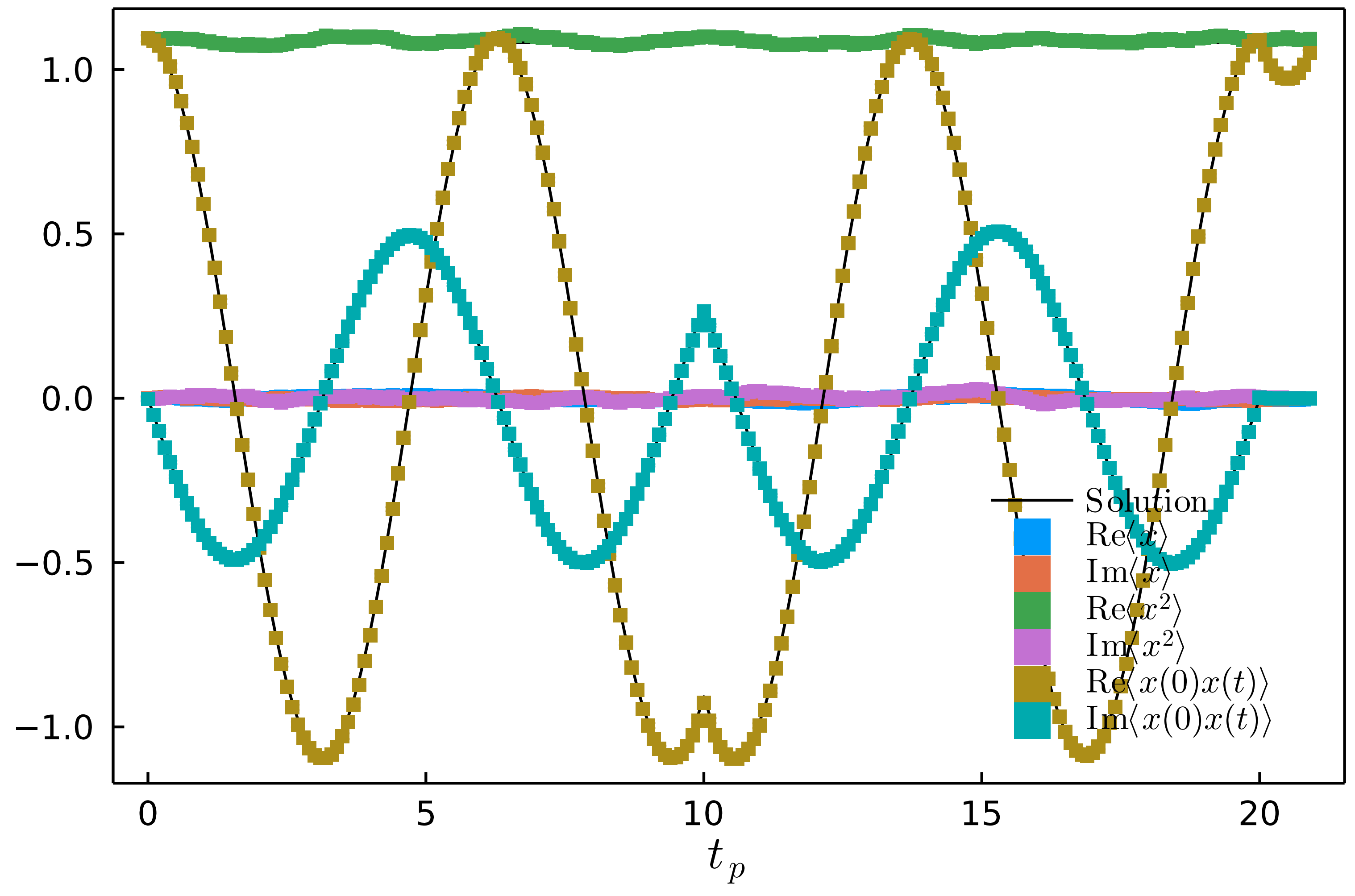
$K = M^{-1}$



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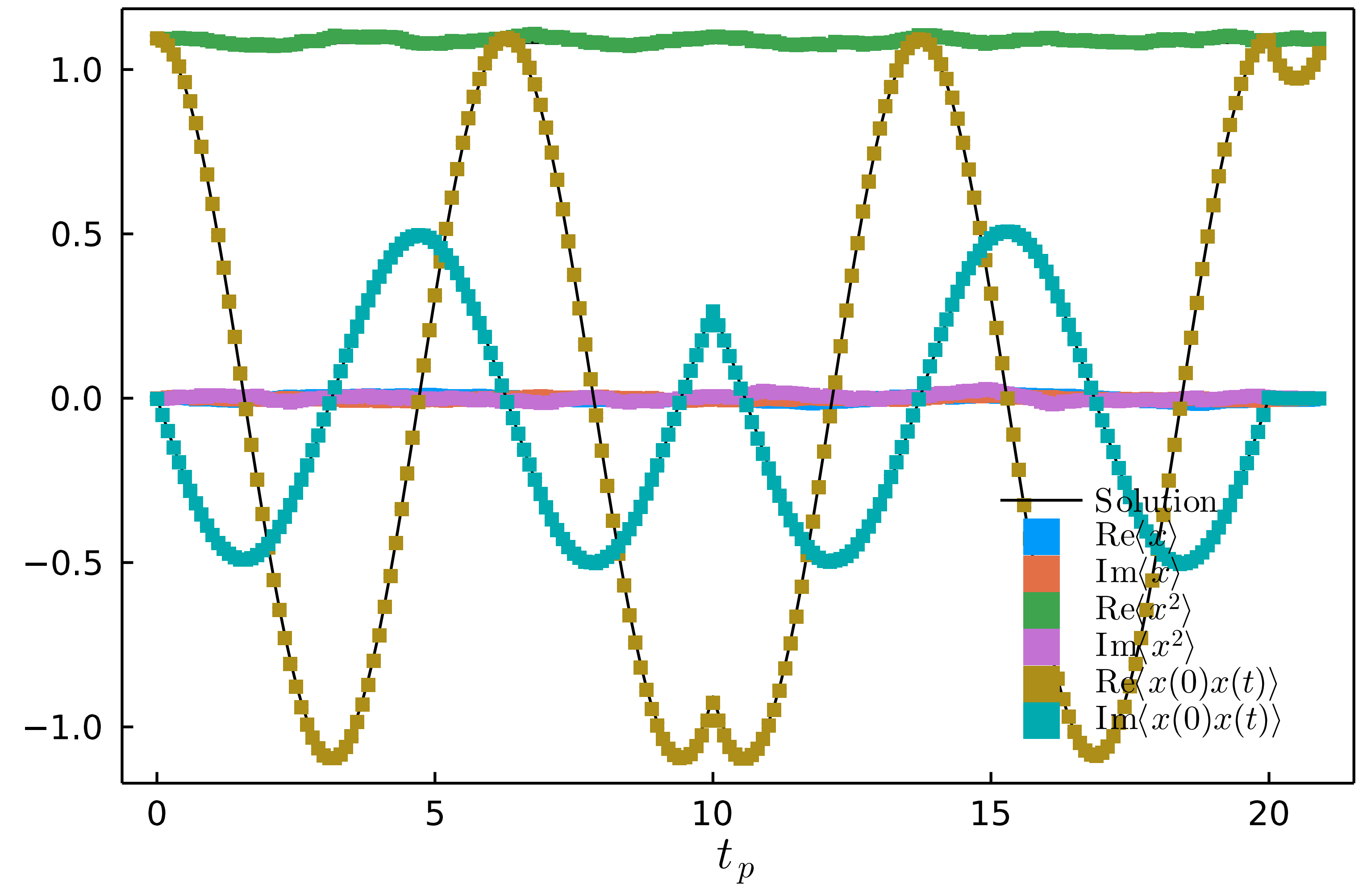
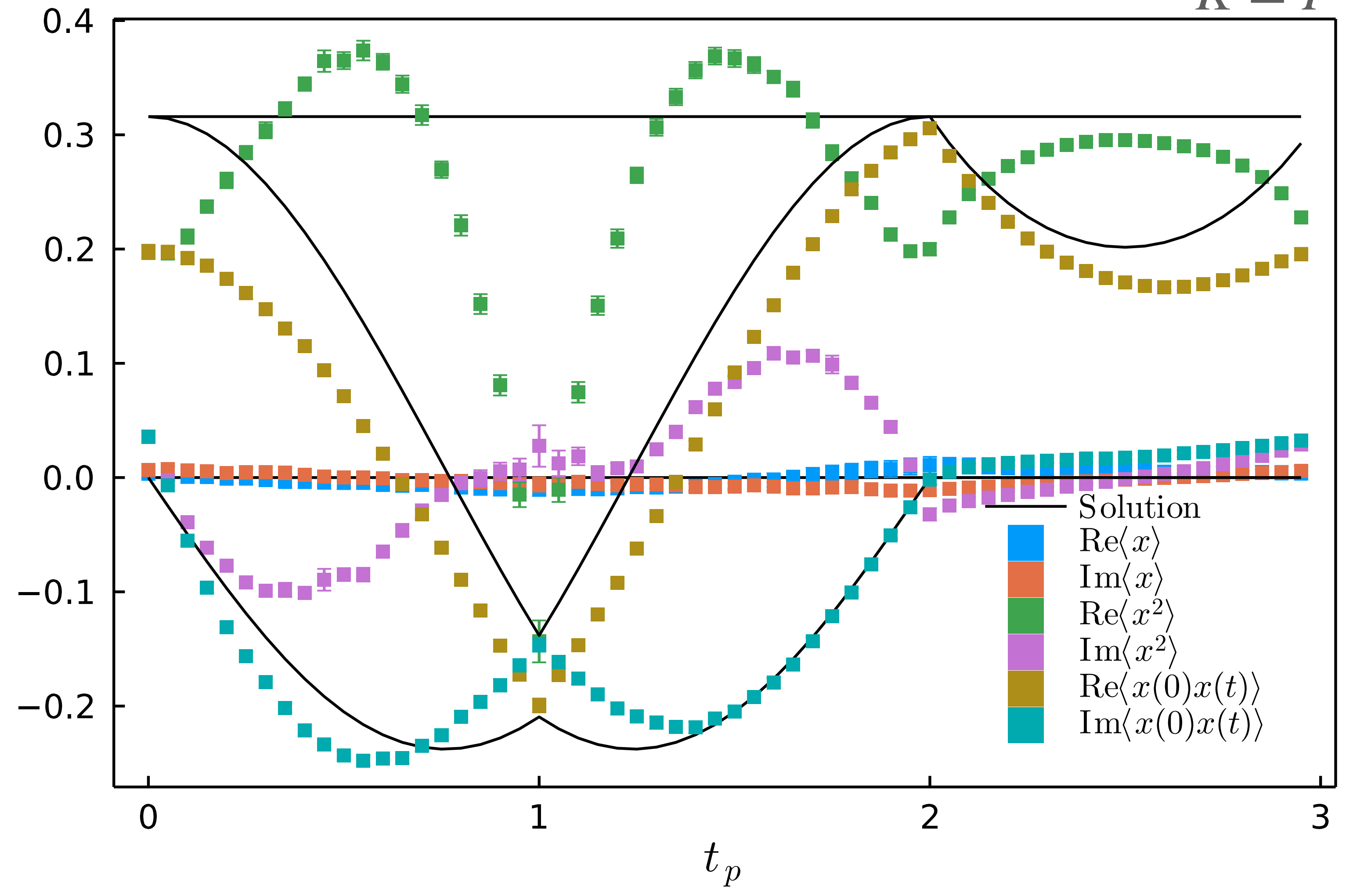


Interactive theory

$K = I$



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Systematic scheme to construct kernels

Free theory

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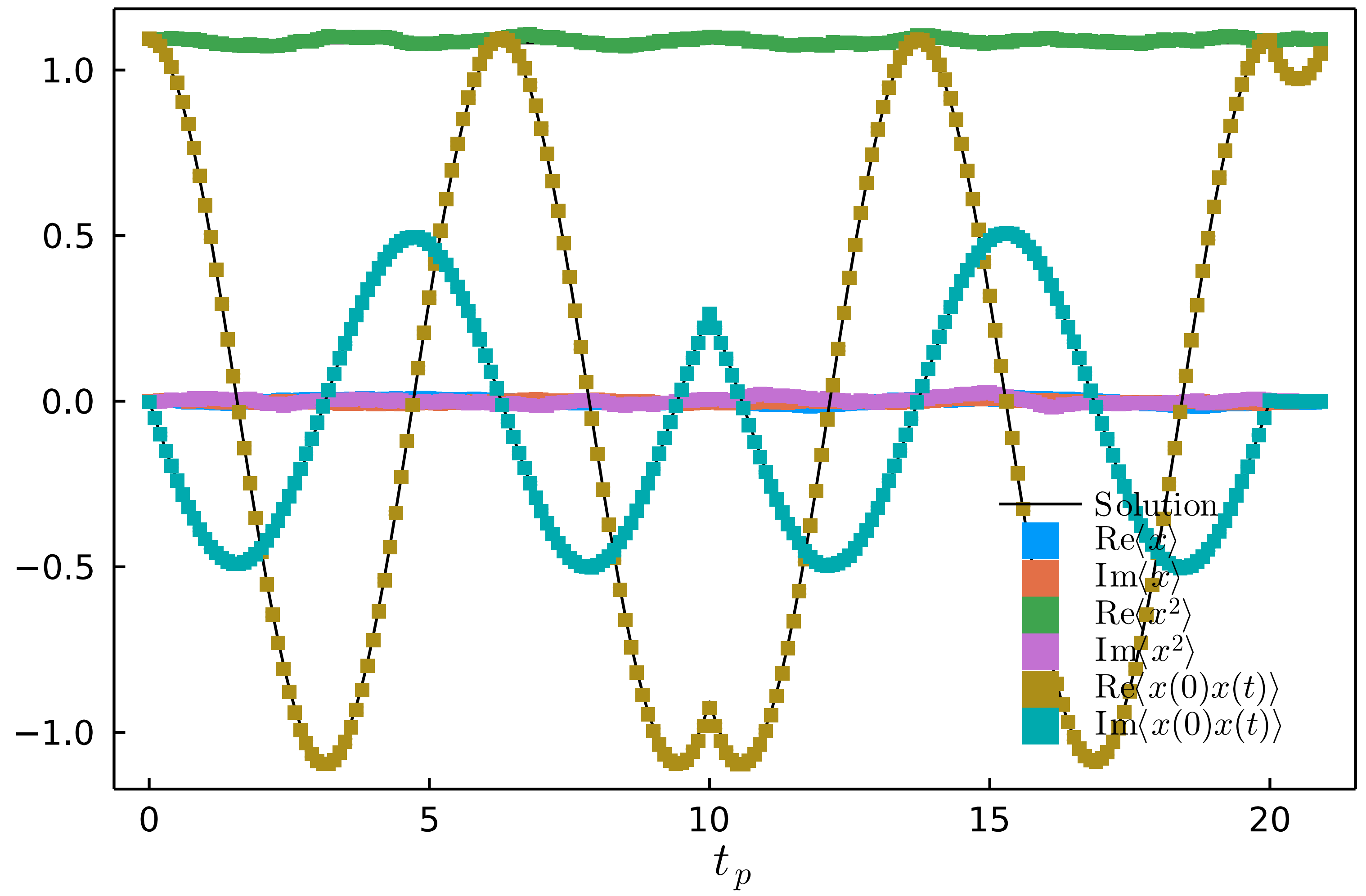
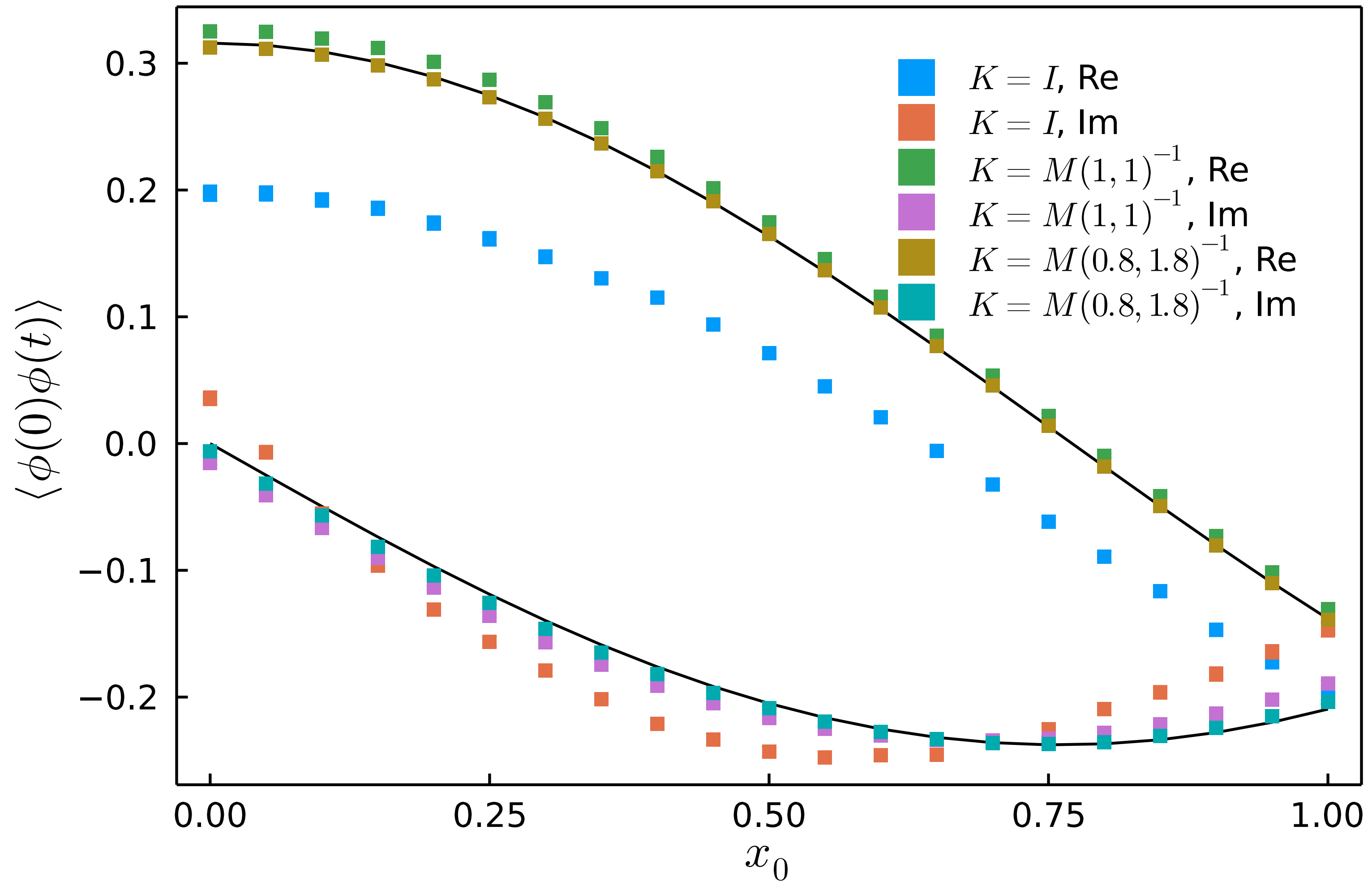
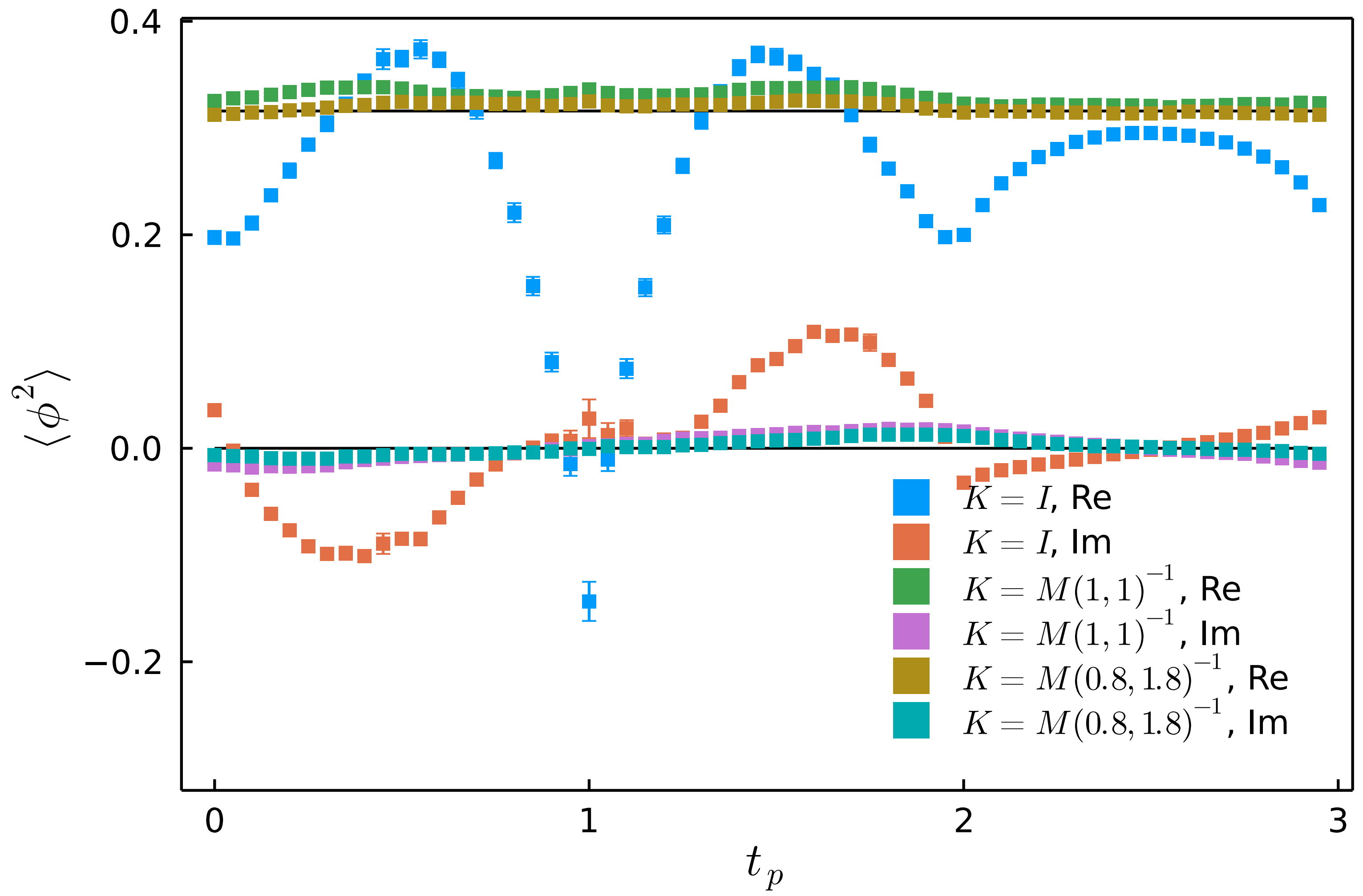


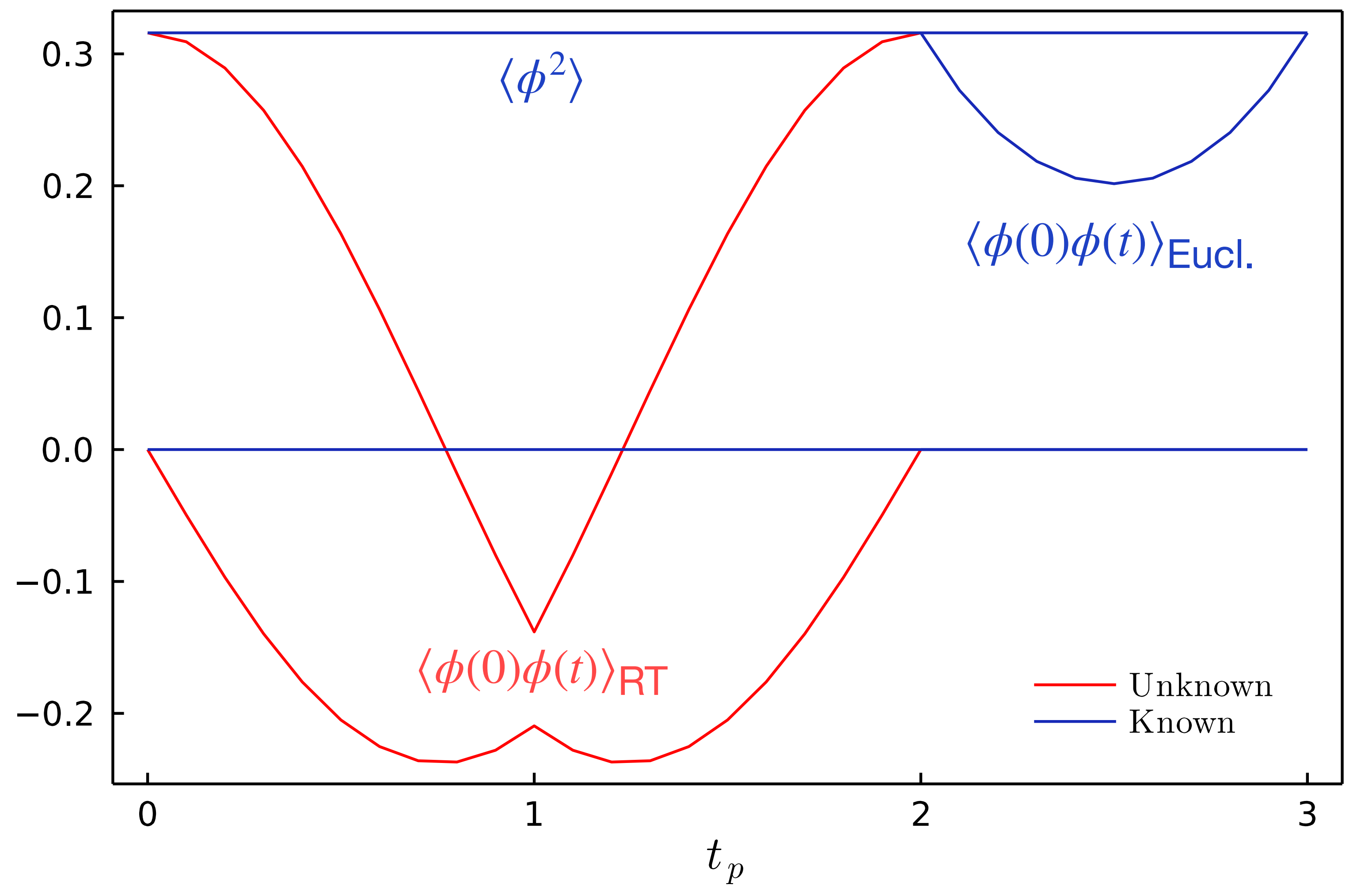
Interactive theory





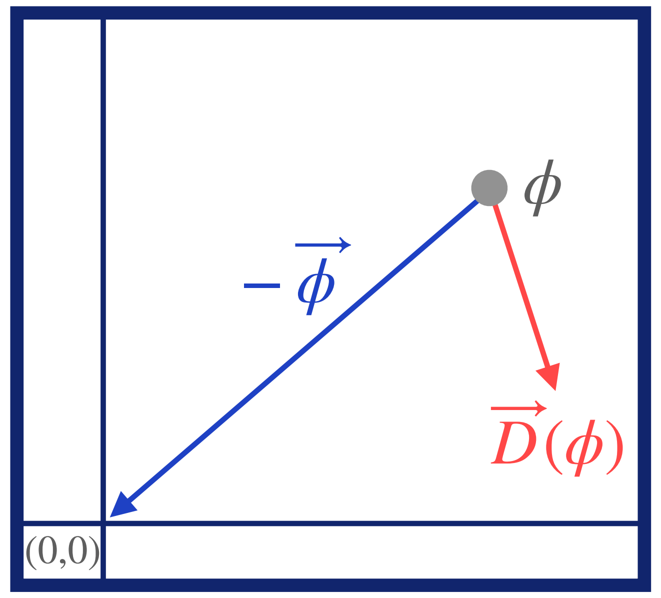
Construct kernel

- Can we find a kernel by using prior knowledge about the Complex Langevin and the model
- Known information
  - L^{Sym}: Symmetries of the model, ex. $\langle \phi^n \rangle =$ const. (known from Euclidean simulation)
  - $L^{\text{Eucl.}}$: Euclidean part of real-time contour
  - L^{BT}: There should be no boundary terms
- Minimising using the above loss functions require the derivative $\dfrac{d\phi}{dK}$ which includes propagating through the whole simulation.
  - Possible due to auto-differentiation and sensitivity analysis
  - Currently too expensive due to highly stiff problem (real-time)



Local loss function

- Boundary terms accumulate with too slow falloff in the distribution.
- Minimising the drift out from origin ($D = K\dfrac{\delta S}{\delta \phi}$)



$$L_D = \frac{1}{N}\sum_i^N \left| D(\phi_i)\cdot(-\phi_i) - |D(\phi_i)|\,|\phi_i| \right|^2$$

- Evaluate the gradient $\nabla_K L_D(\{\phi\})$ using auto-differentiation
- Use L^{Sym}, L^{Eucl}, L^{BT} to test result from minimising L_D
- Minimising L_D same as minimising boundary terms: L^{BT}
- Holomorphic: Correctness criterion

Updating the kernel

Make configuration using $K_0 = I$: $\{\phi_i^0\}$

$$d\phi = K_0\, \partial_\phi S[\phi] + \sqrt{K_0} dW$$

Update kernel based on gradient of the loss function $\nabla_K L_D\left(\{\phi^0\}\right)$

Loop N times (index k)

Make configuration using K_k: $\{\phi_i^k\}$

$$d\phi = K_k\, \partial_\phi S[\phi] + \sqrt{K_k} dW$$

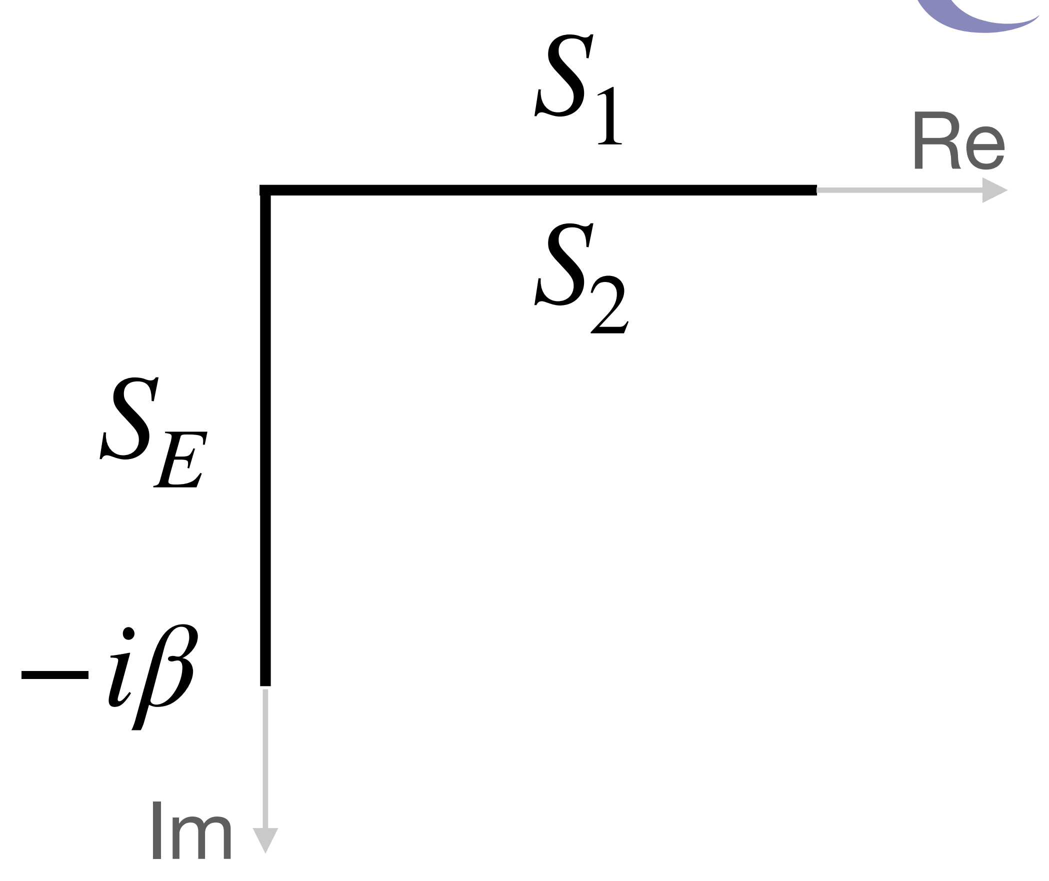
Update kernel based on gradient of the loss function $\nabla_K L_D\left(\{\phi^k\}\right)$

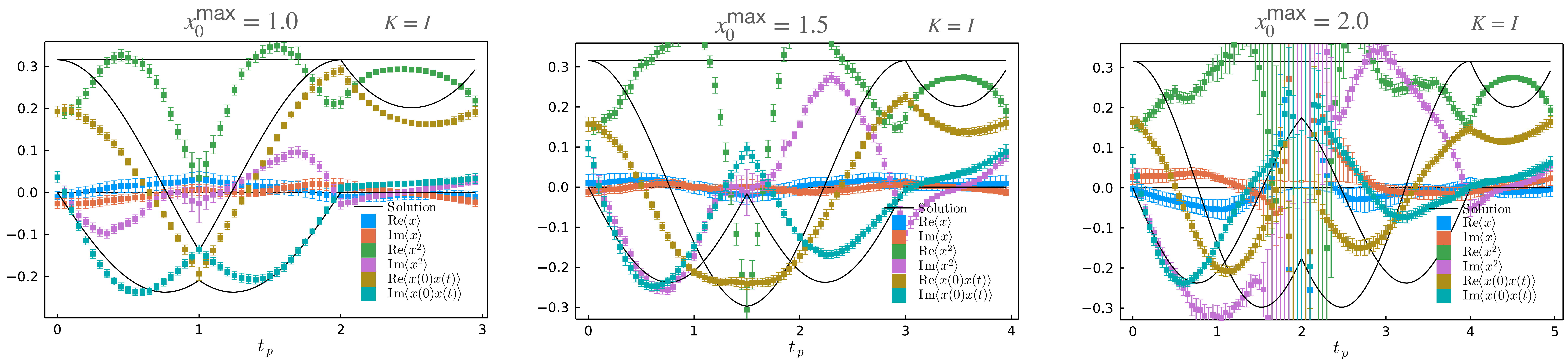
Measure L^{Sym}, L^{Eucl}, L^{BT}

Pick out the iteration with the smallest L^{Sym}, L^{Eucl}, L^{BT}

Real-time interactive theory results

- Strongly coupled quantum AHO with $m = 1$, $\lambda = 24$, $\beta = 1$ on a real-time contour
- Form of the kernel $K = e^{A+iB}$ where A and B are real matrices
- Optimisation using L_D, selecting iteration with best $L^{\text{Sym}} + L^{\text{Eucl.}}$
- Critical points away from the origin: $\frac{dS[\phi]}{d\phi} = 0$





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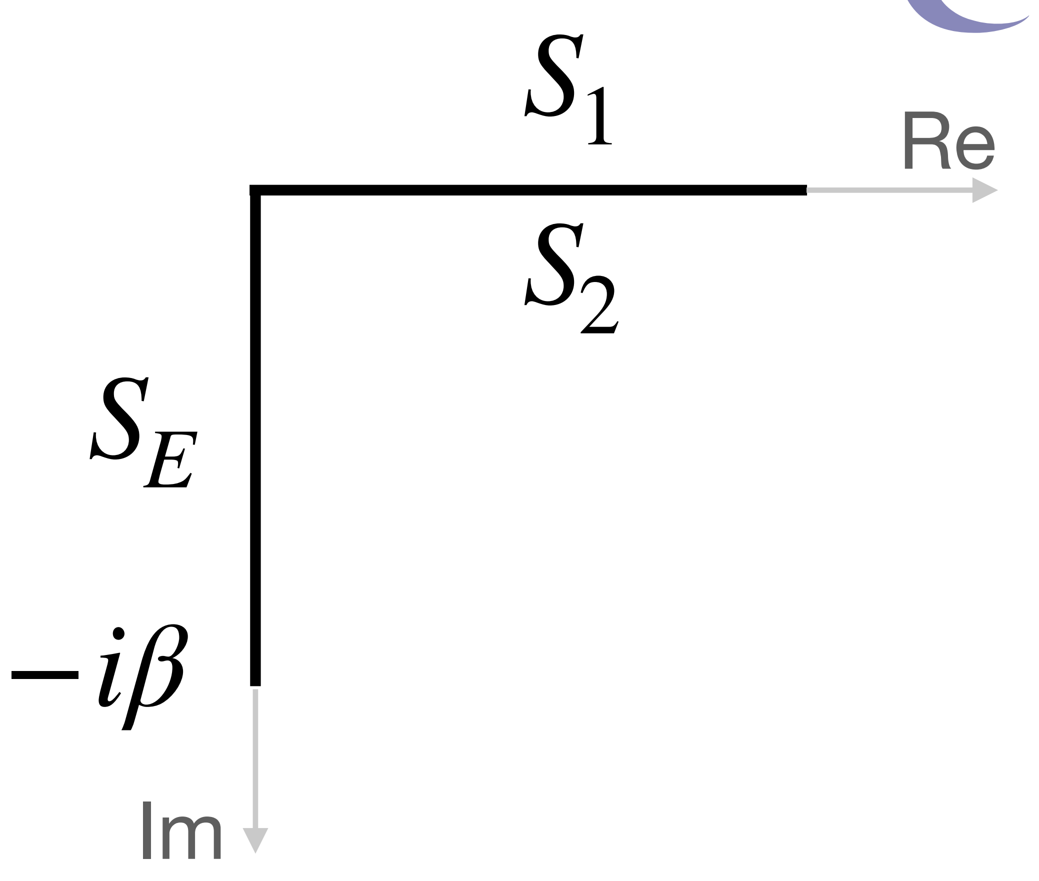

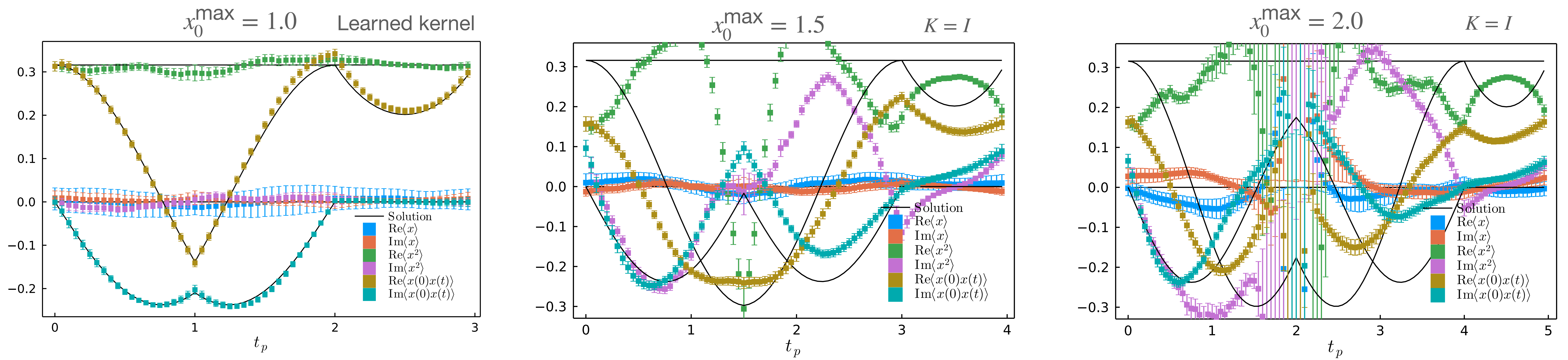

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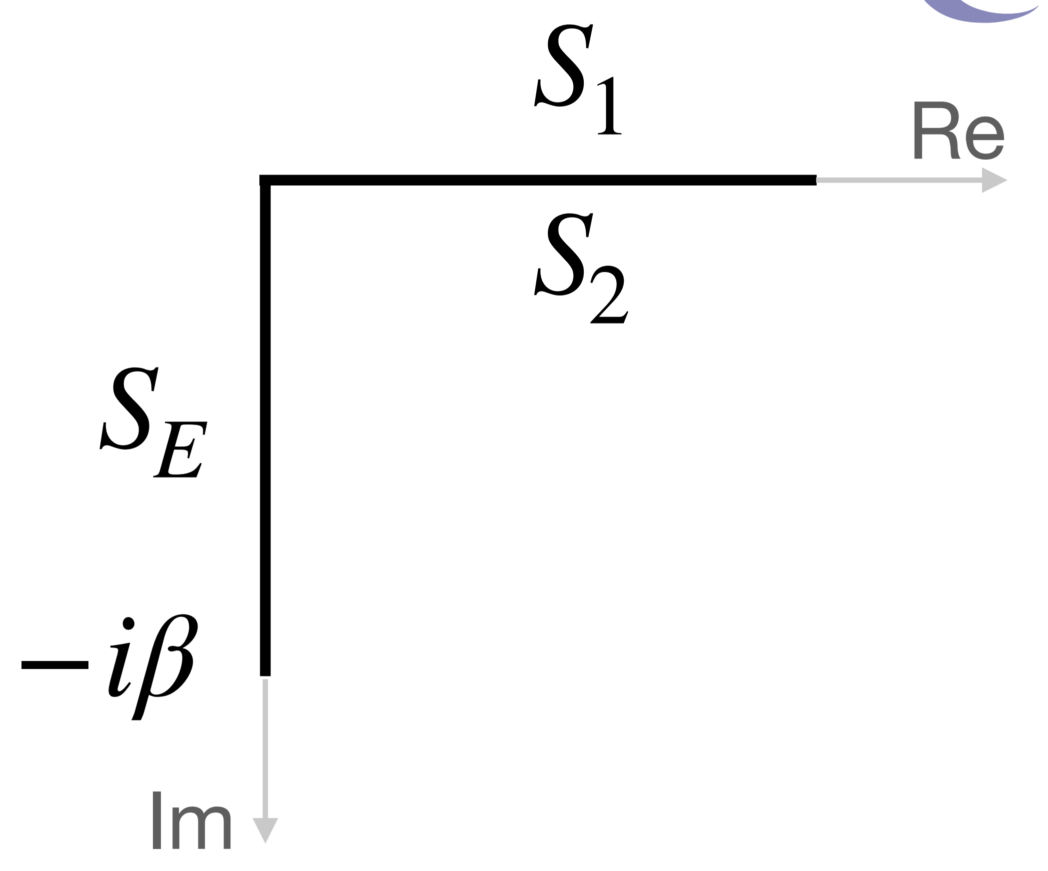

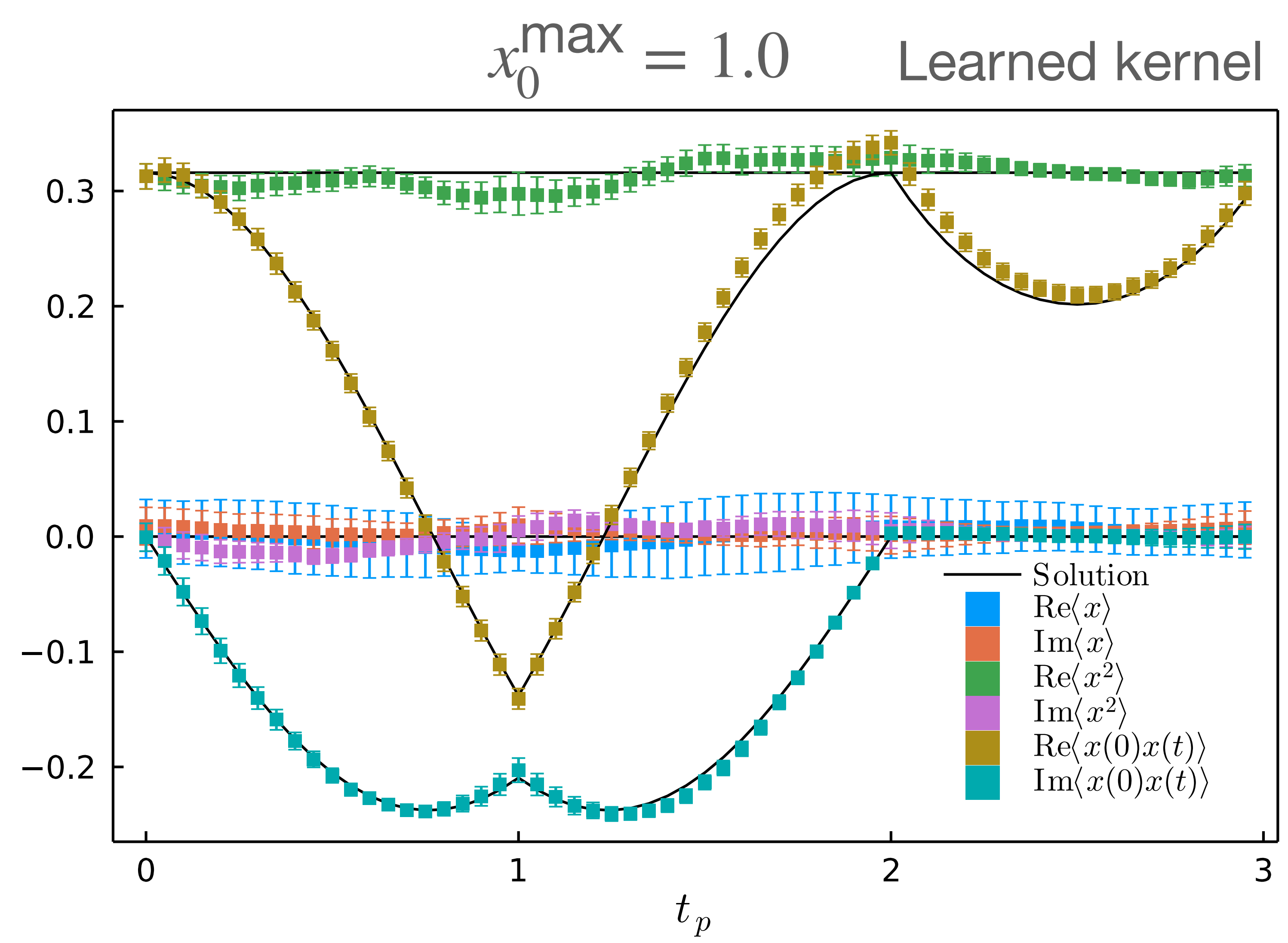

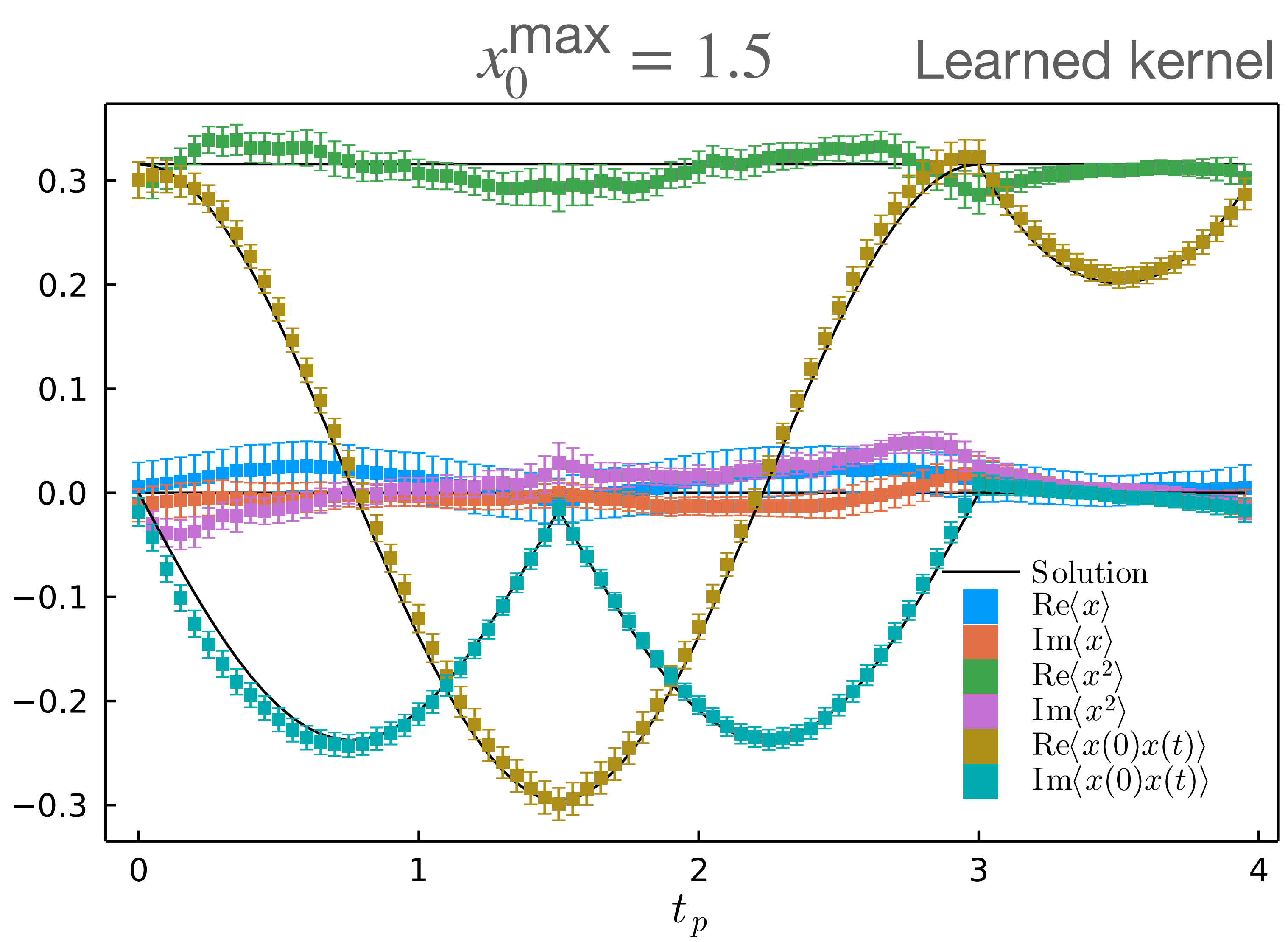

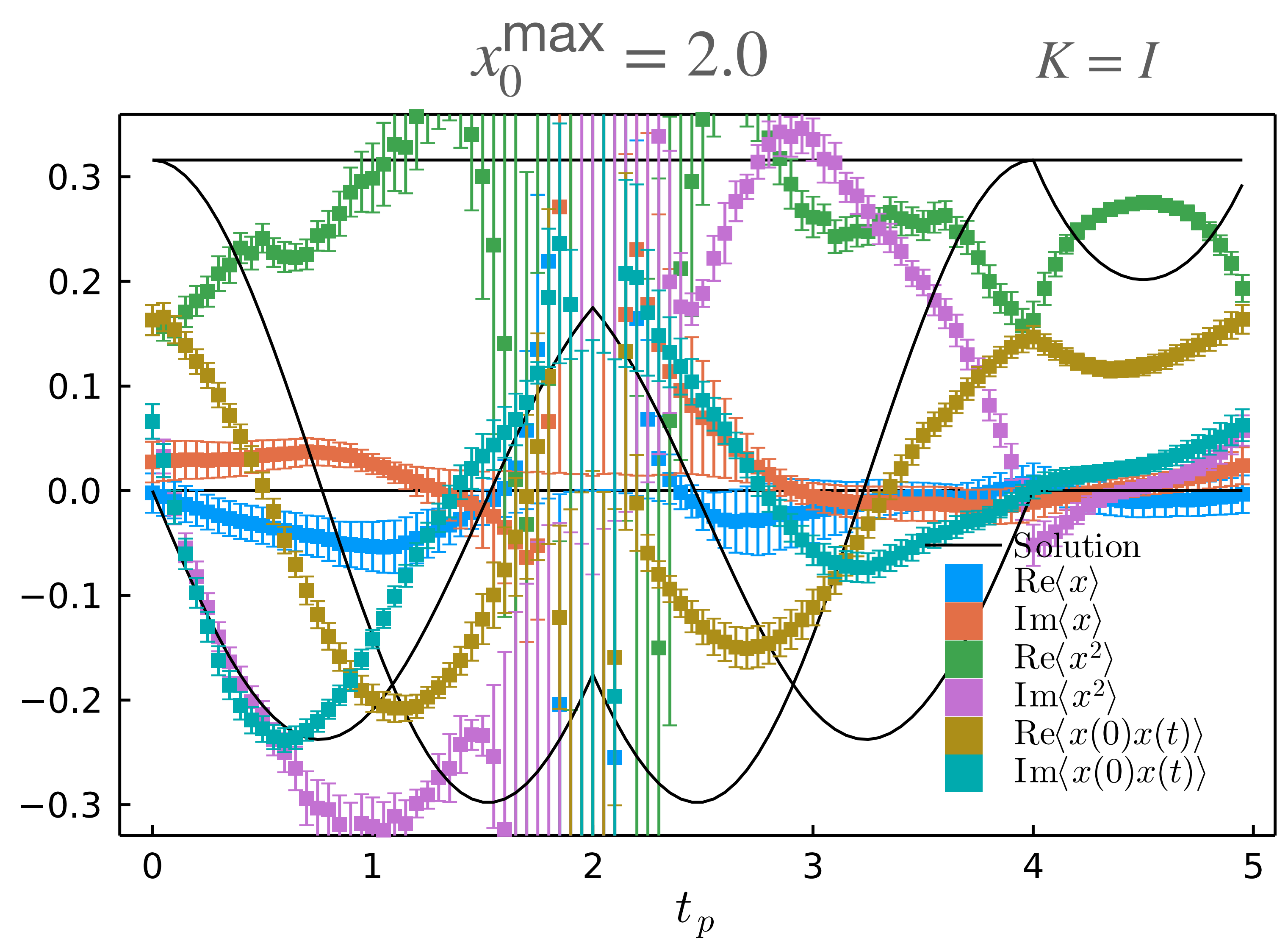

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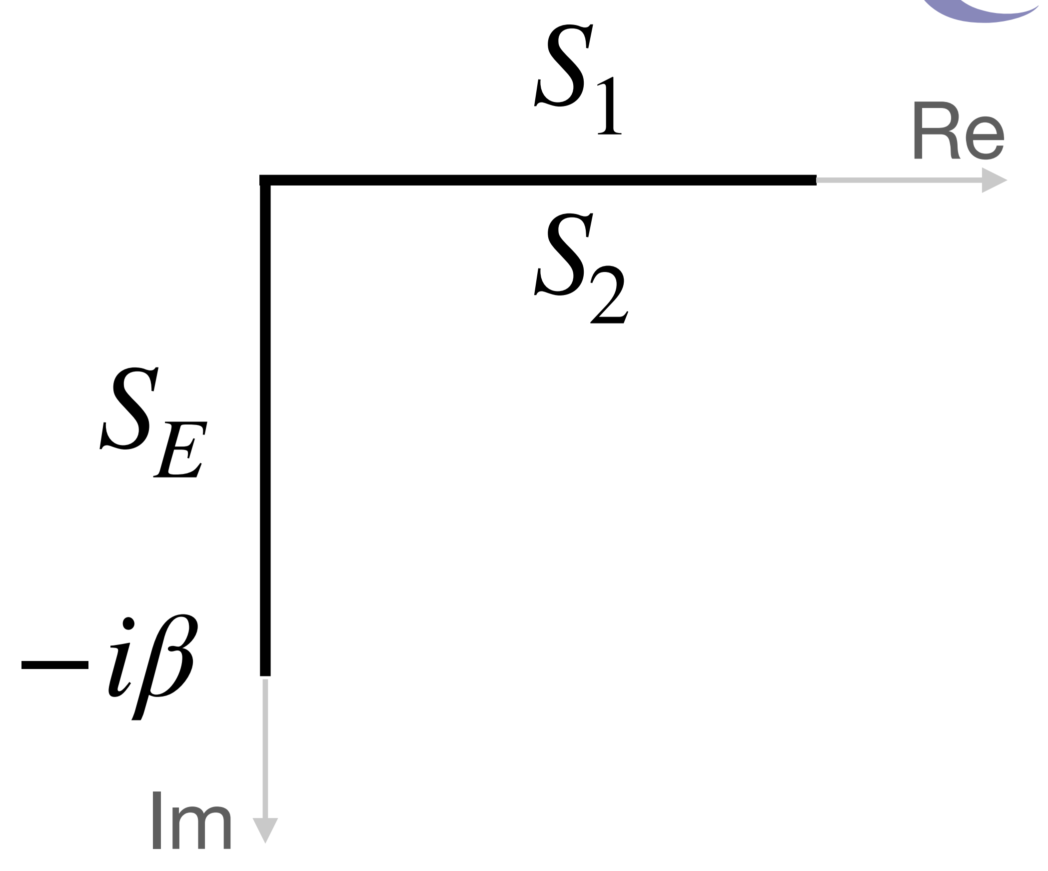
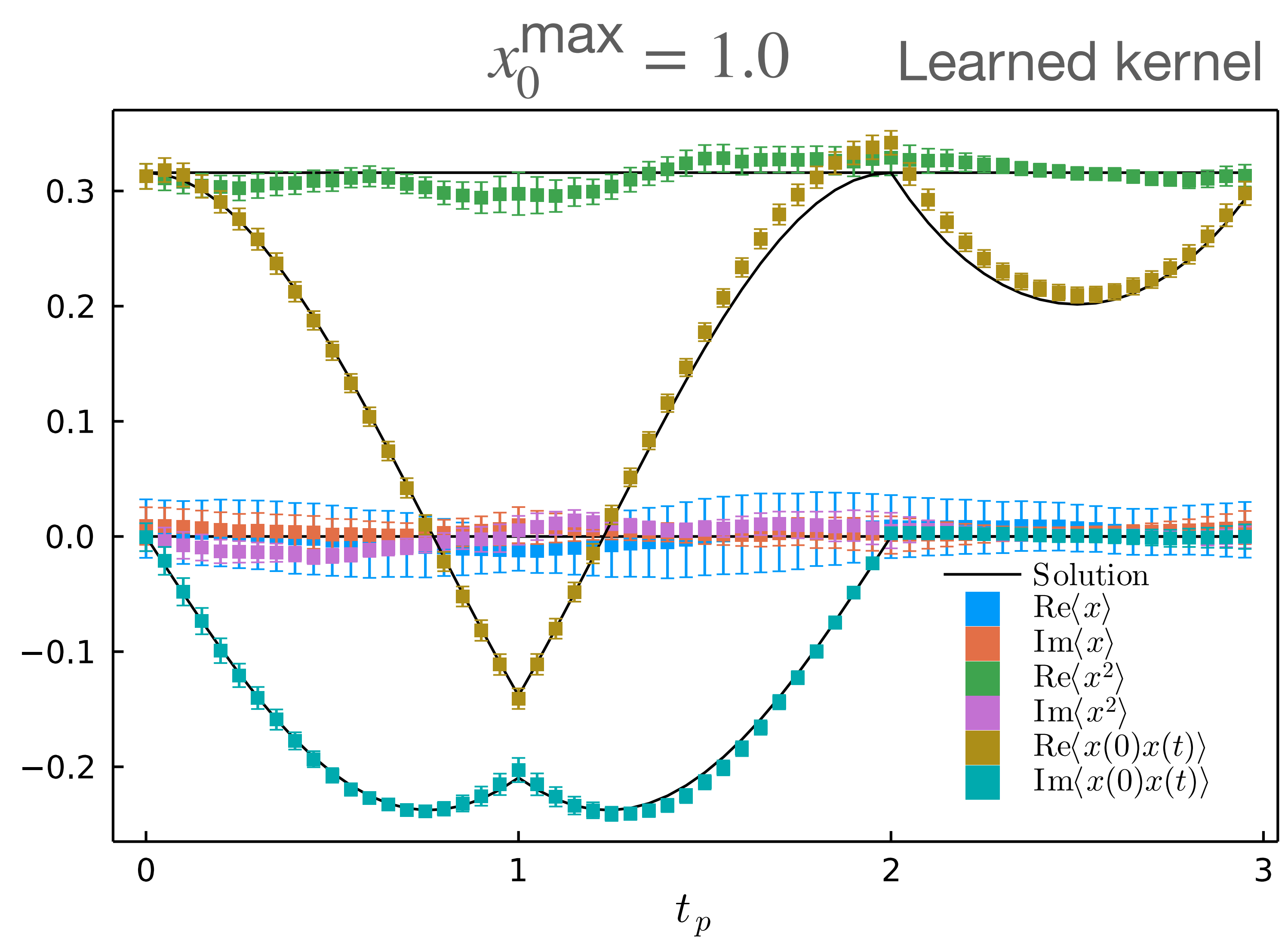
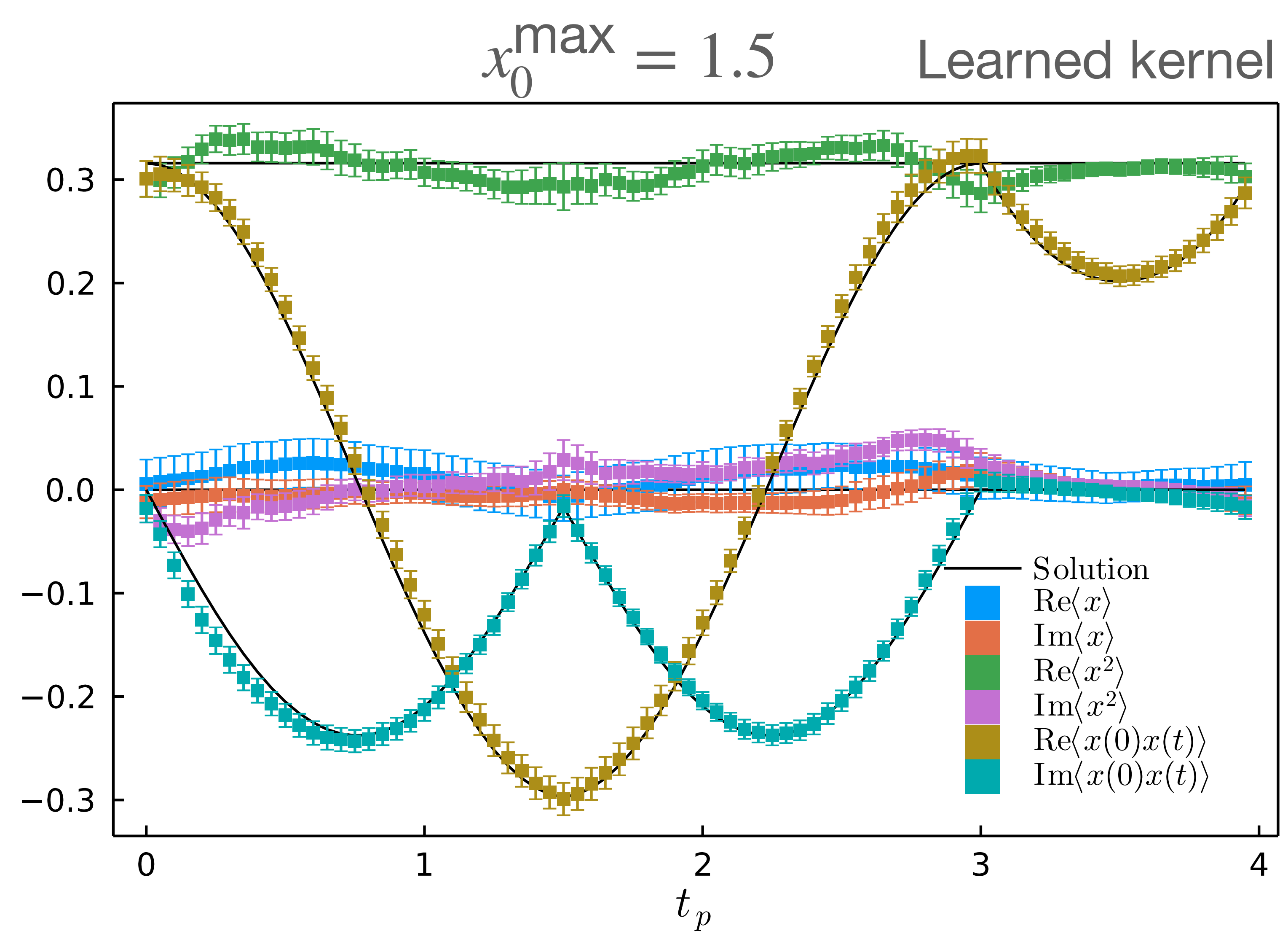
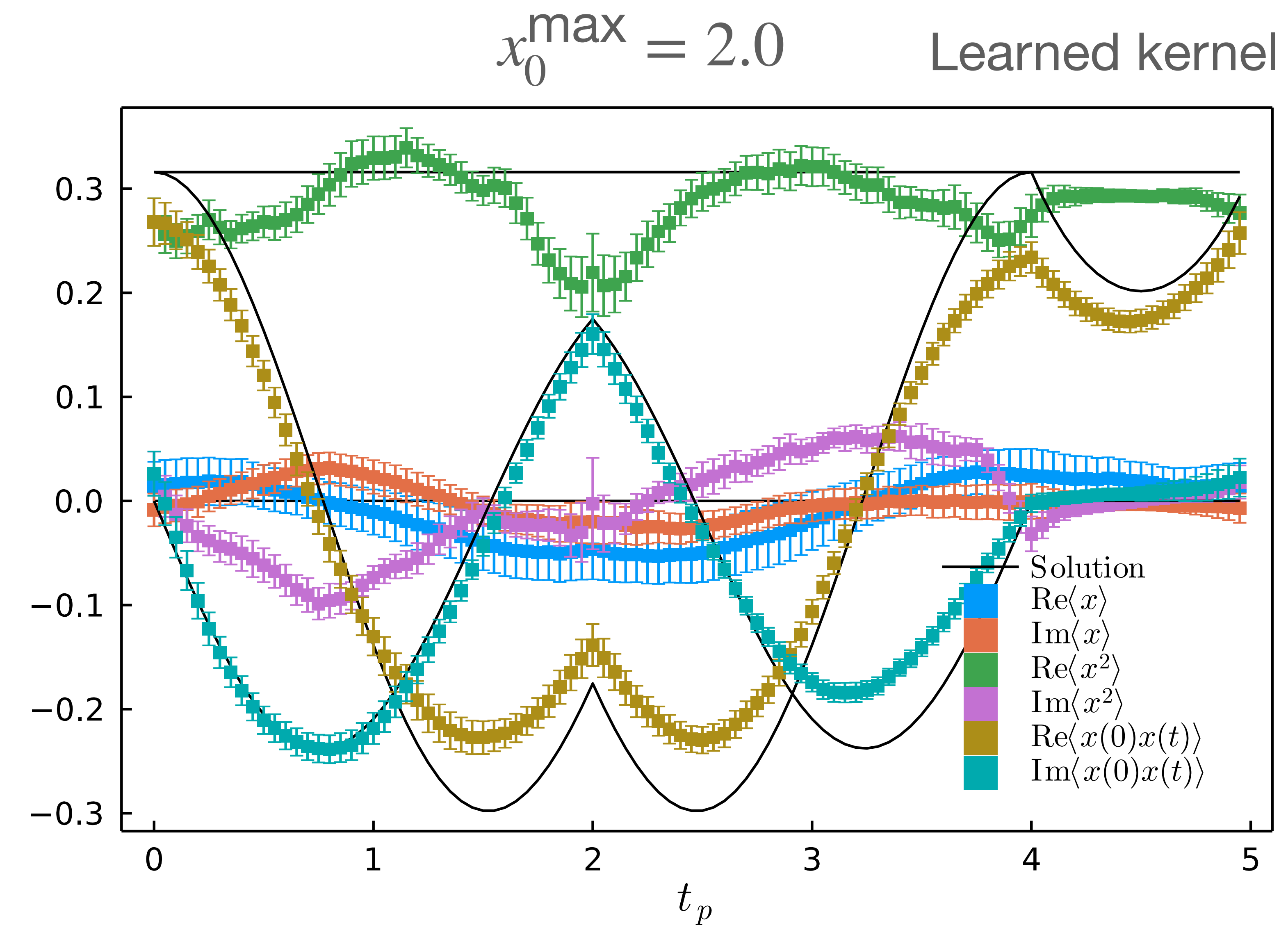




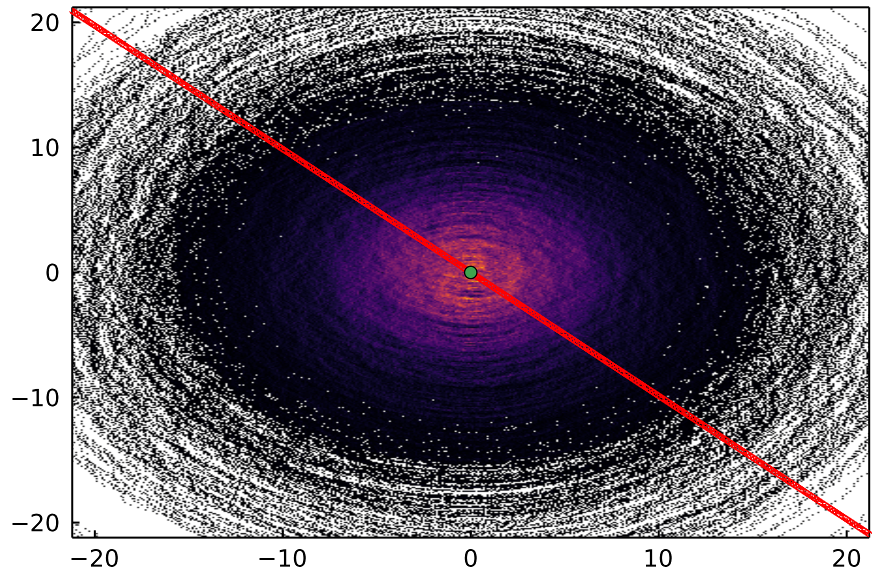




Connection with thimbles

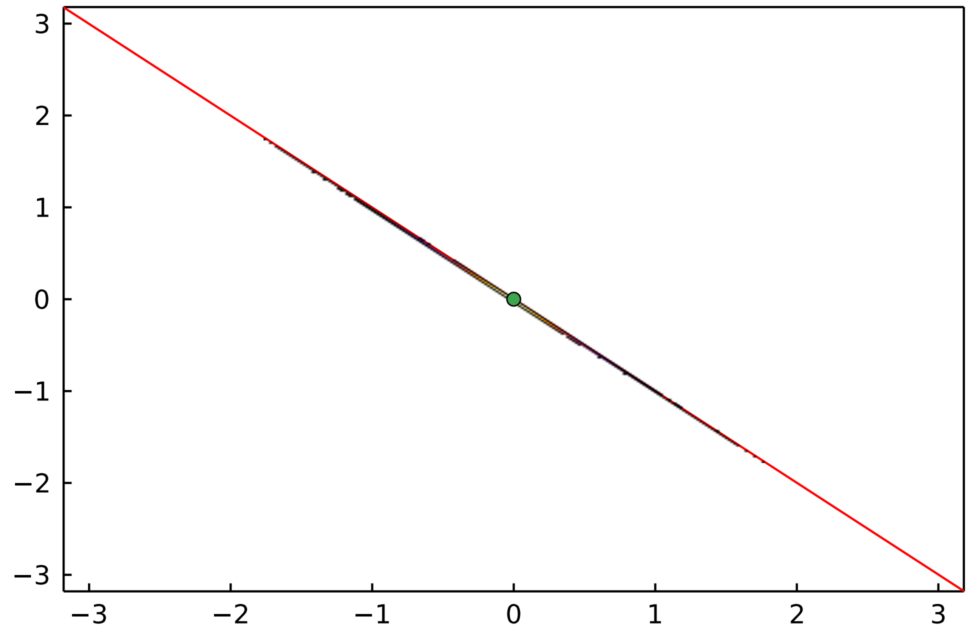
- Lefschetz thimbles: $\frac{d\phi}{d\tau} = \overline{\frac{dS[\phi]}{d\phi}}$
- Simplest model: $S = \frac{1}{2}ix^2$

$K_0 \frac{dS[\phi]}{d\phi} = i\phi$



Optimising L_D=0

$K_N \frac{dS[\phi]}{d\phi} = \frac{-1}{i} i\phi = -\phi$



Noise coefficient $\sqrt{K} = \sqrt{\frac{-1}{i}}$ same as slope of thimble

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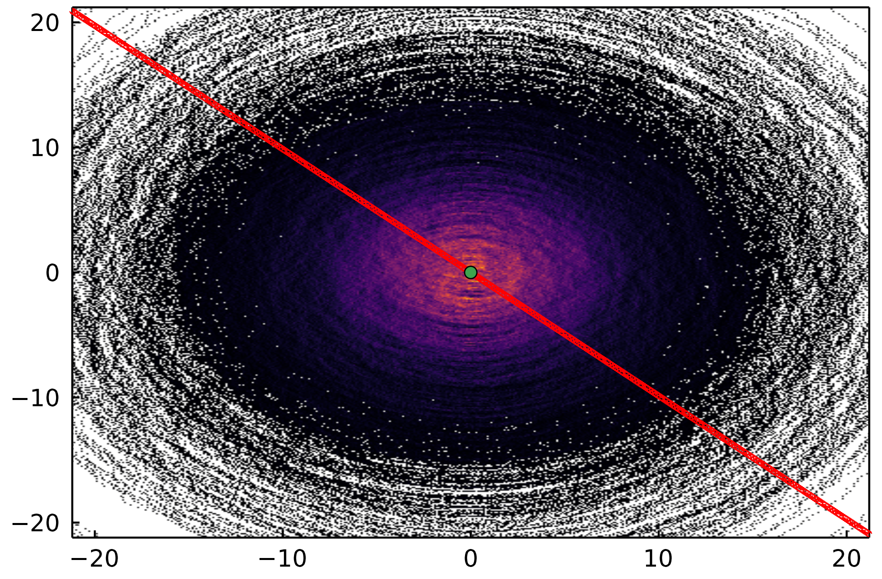

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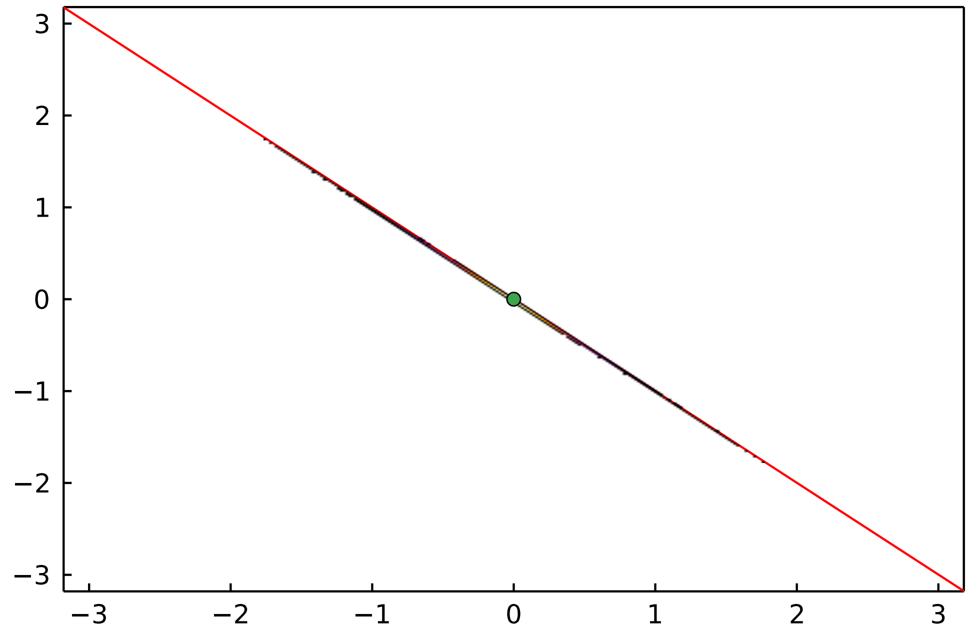

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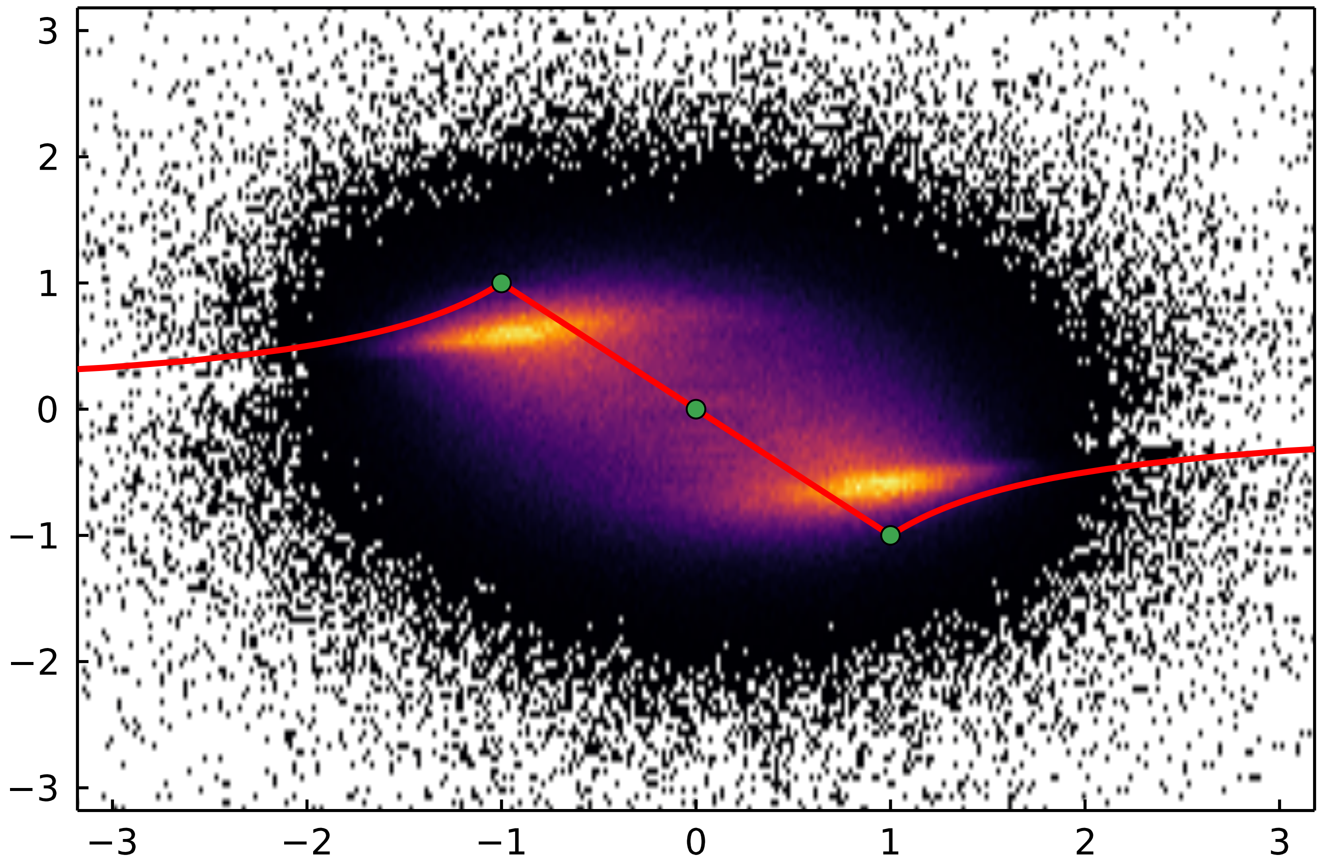
- Models with more than one critical point $S = 2i\phi^2 + \dfrac{1}{2}\phi^4$



$K_0 \dfrac{dS[\phi]}{d\phi} = 4i\phi + 2\phi^3$

$L_{\text{True}} = 0.218 \pm 0.004$

$L_{\text{True}} = |\langle x \rangle - \langle x \rangle_{\text{True}}| + |\langle x^2 \rangle - \langle x^2 \rangle_{\text{True}}|$

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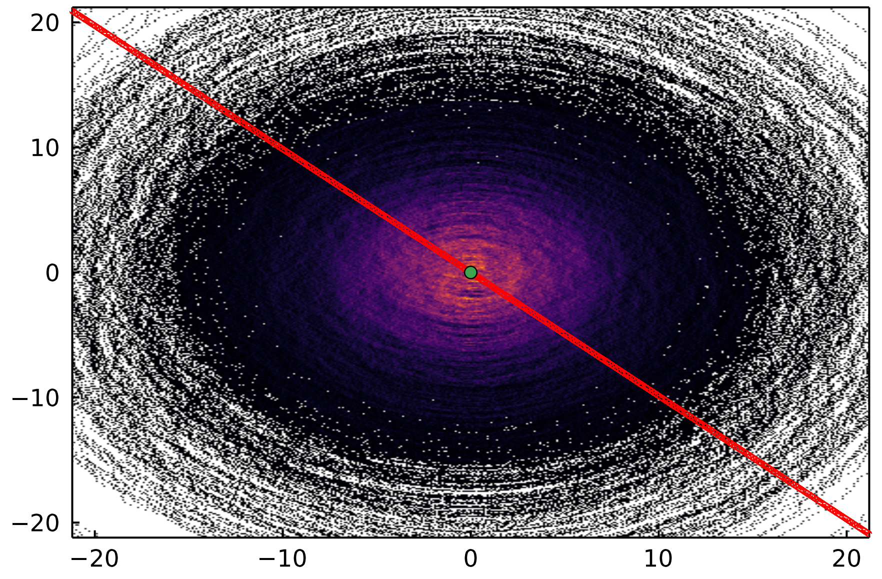

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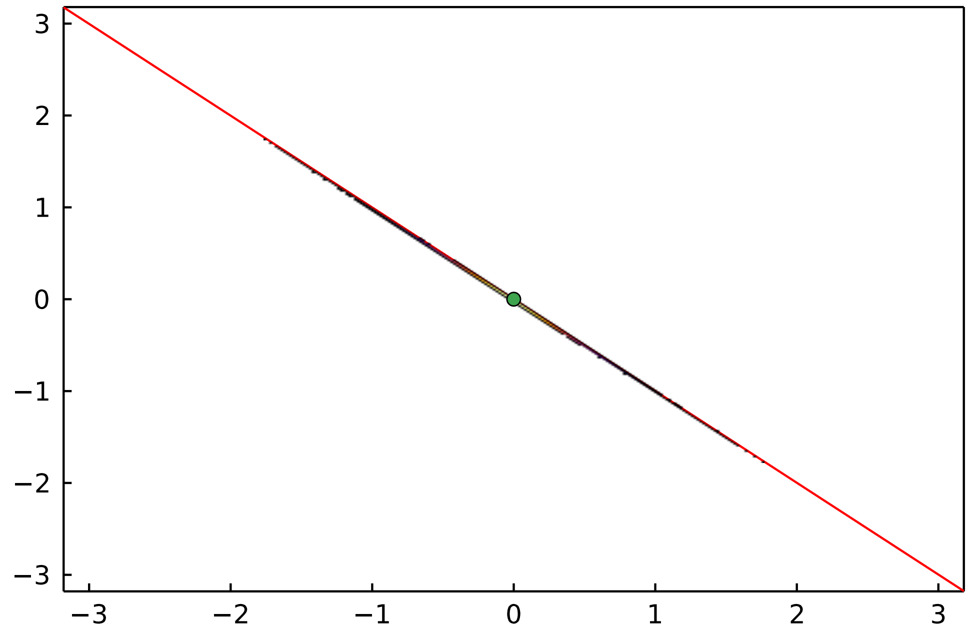

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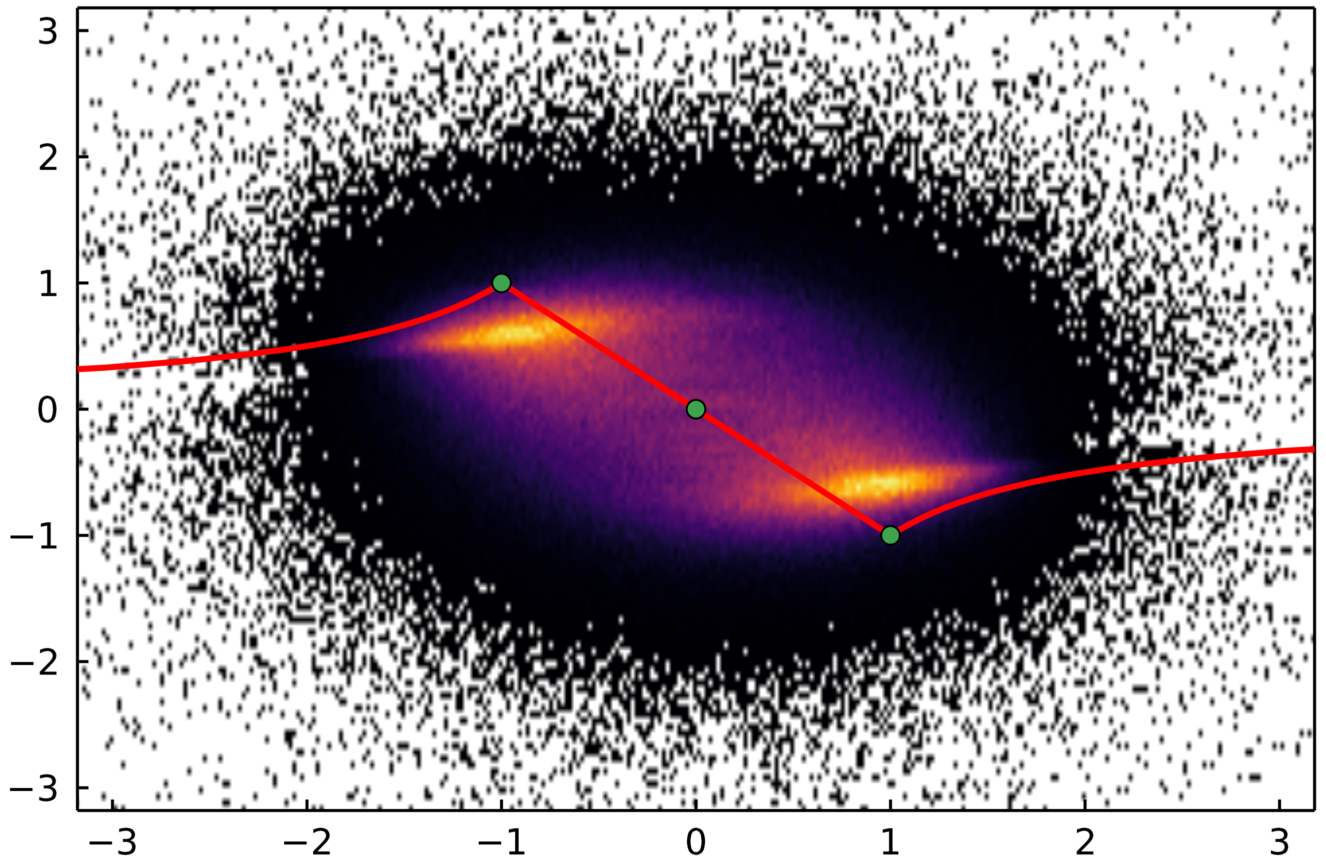

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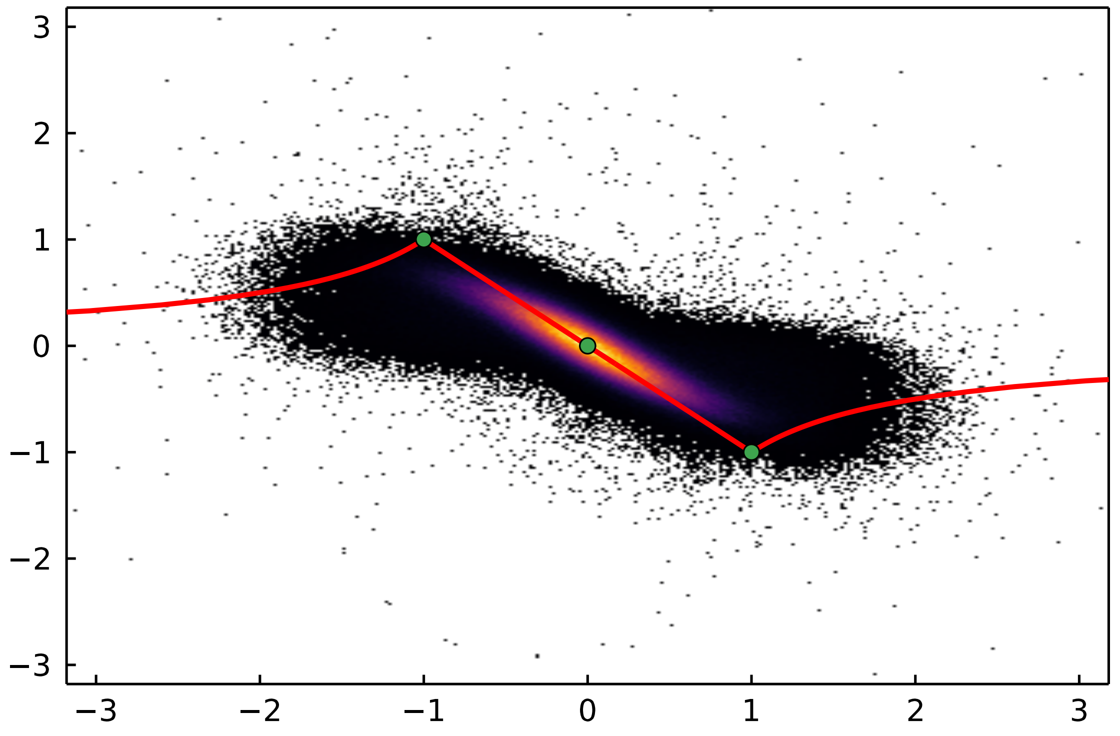
Optimising L_D for a constant kernel $K = e^{i\theta}$

Two minimas

Fokker-Planck eigenvalues

Converges to correct solution

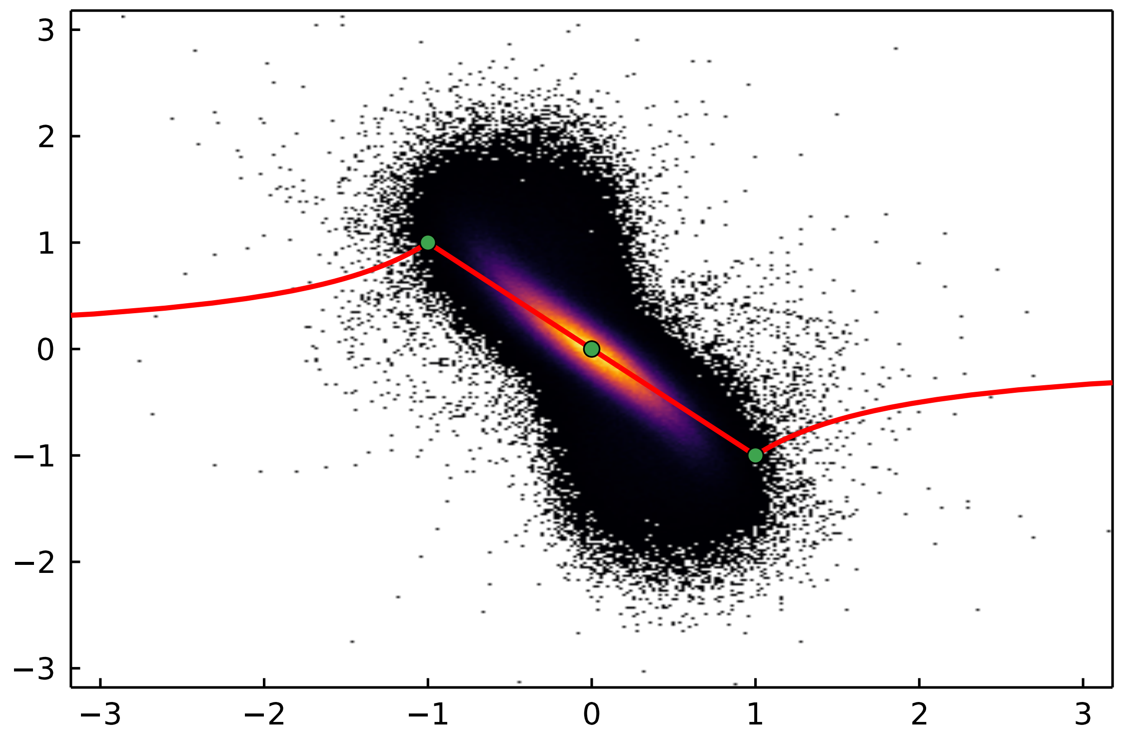


$K_N \dfrac{dS[\phi]}{d\phi} = e^{-i\frac{\pi}{3}}(4i\phi + 2\phi^3)$

$L_{\text{True}} = 0.0057 \pm 0.0061$

And

Converges to wrong solution



$K_N \dfrac{dS[\phi]}{d\phi} = e^{-i\frac{2\pi}{3}}(4i\phi + 2\phi^3)$

$L_{\text{True}} = 0.3086 \pm 0.0059$

Boundary terms and kernels

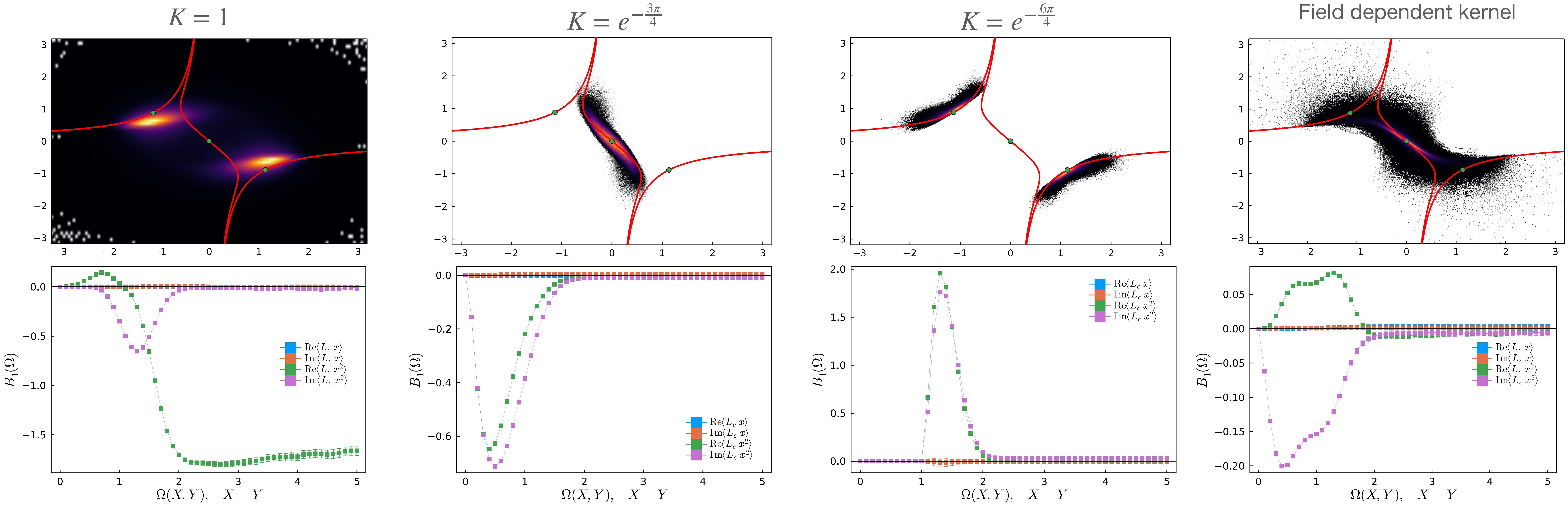
$$S = \frac{1}{2}\sigma x^2 + \frac{\lambda}{4!}x^4$$

$$\sigma = -1 + 4i, \lambda = 2$$

- Minimising L_D minimise the boundary terms:
  - $B_1(Y) = \left\langle L_c \mathcal{O}(x+iy) \right\rangle = \left\langle (\nabla_x + \nabla S) K \nabla_x \mathcal{O}(x+iy) \right\rangle_Y$

$L_{\text{True}} = |\langle x \rangle - \langle x \rangle_{\text{True}}| + |\langle x^2 \rangle - \langle x^2 \rangle|$

- No boundary terms $\neq$ true solution when using a kernel?

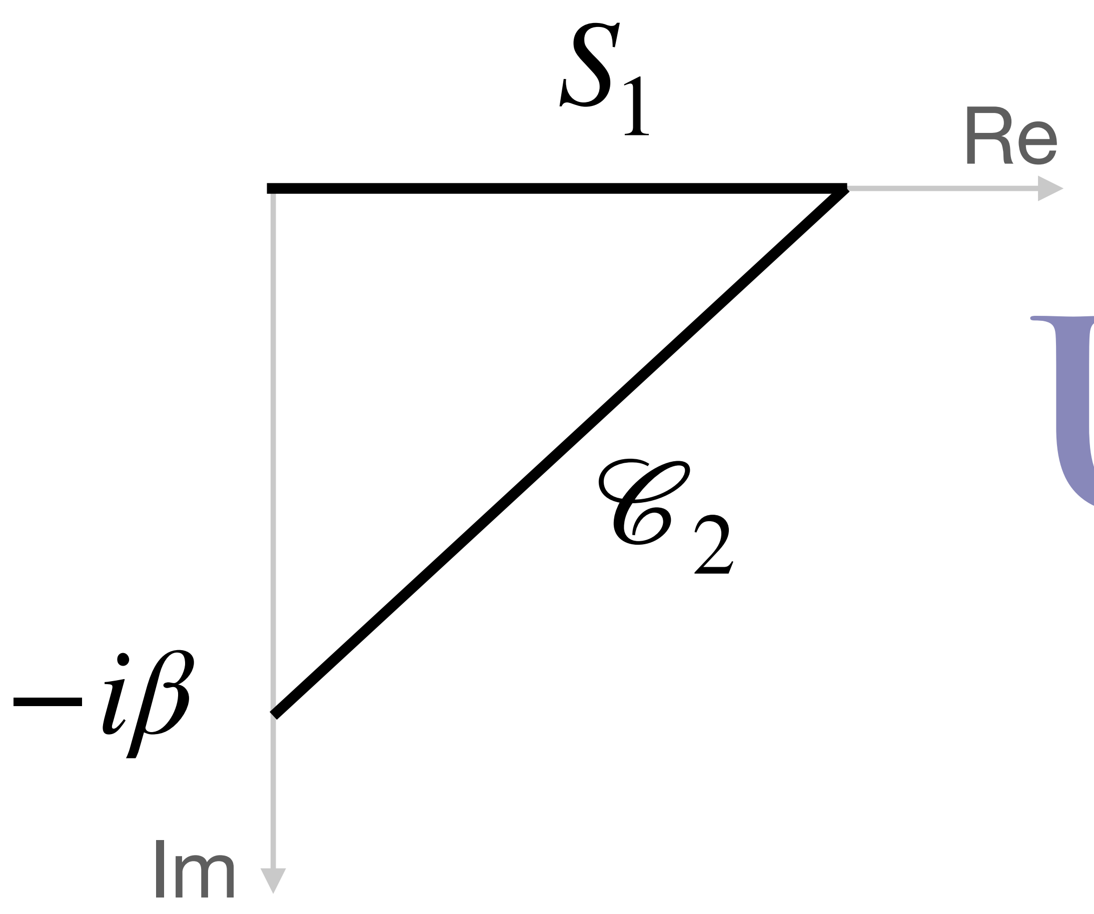


$L_{\text{True}} = 0.888 \pm 0.008$ | $L_{\text{True}} = 0.486 \pm 0.002$ | $L_{\text{True}} = 2.15 \pm 0.11$ | $L_{\text{True}} = 0.023 \pm 0.024$

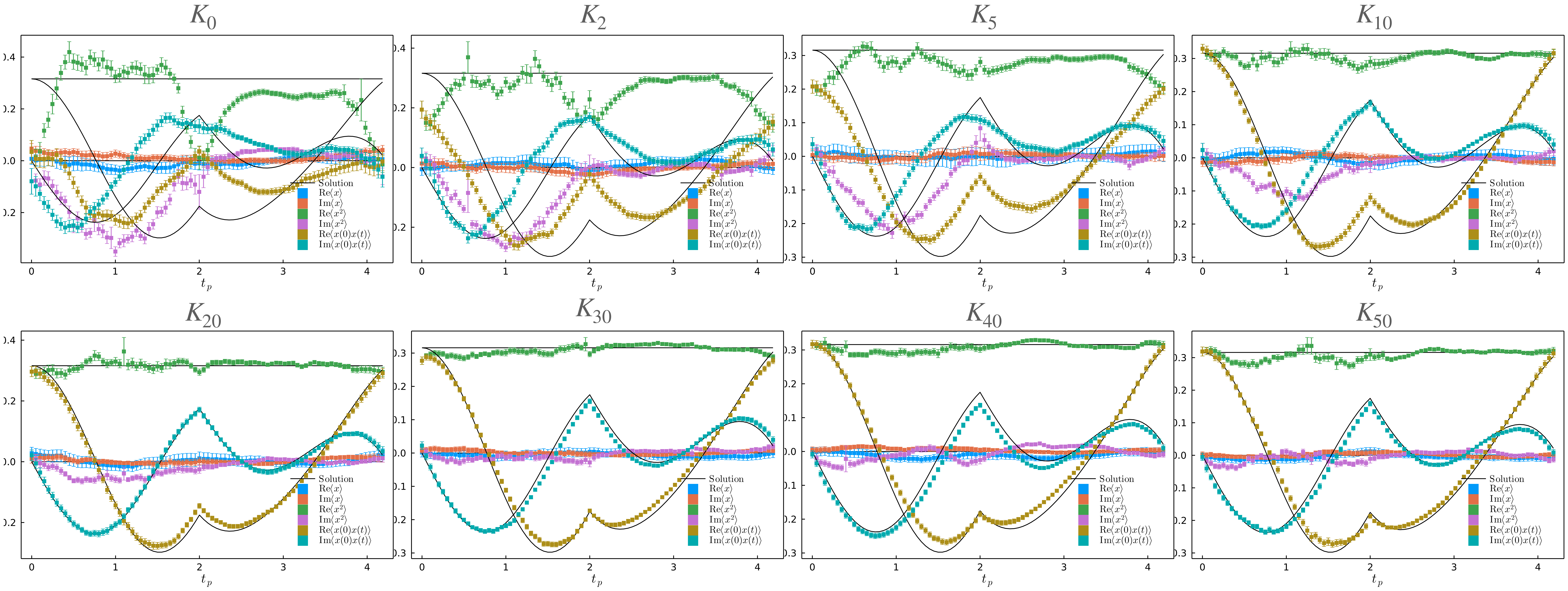
Summary and outlook

- Goal: extending real-time convergence CL
- Kernel controlled complex Langevin
  - No convergence problem for free scalar theory
  - Learning kernel in thermal ϕ^4 theory
- Kernel as appropriately parameterised function
  - Field dependent kernel
  - Generalise to any real-time
- Improved loss function including more than one of the critical points

Tilted contour

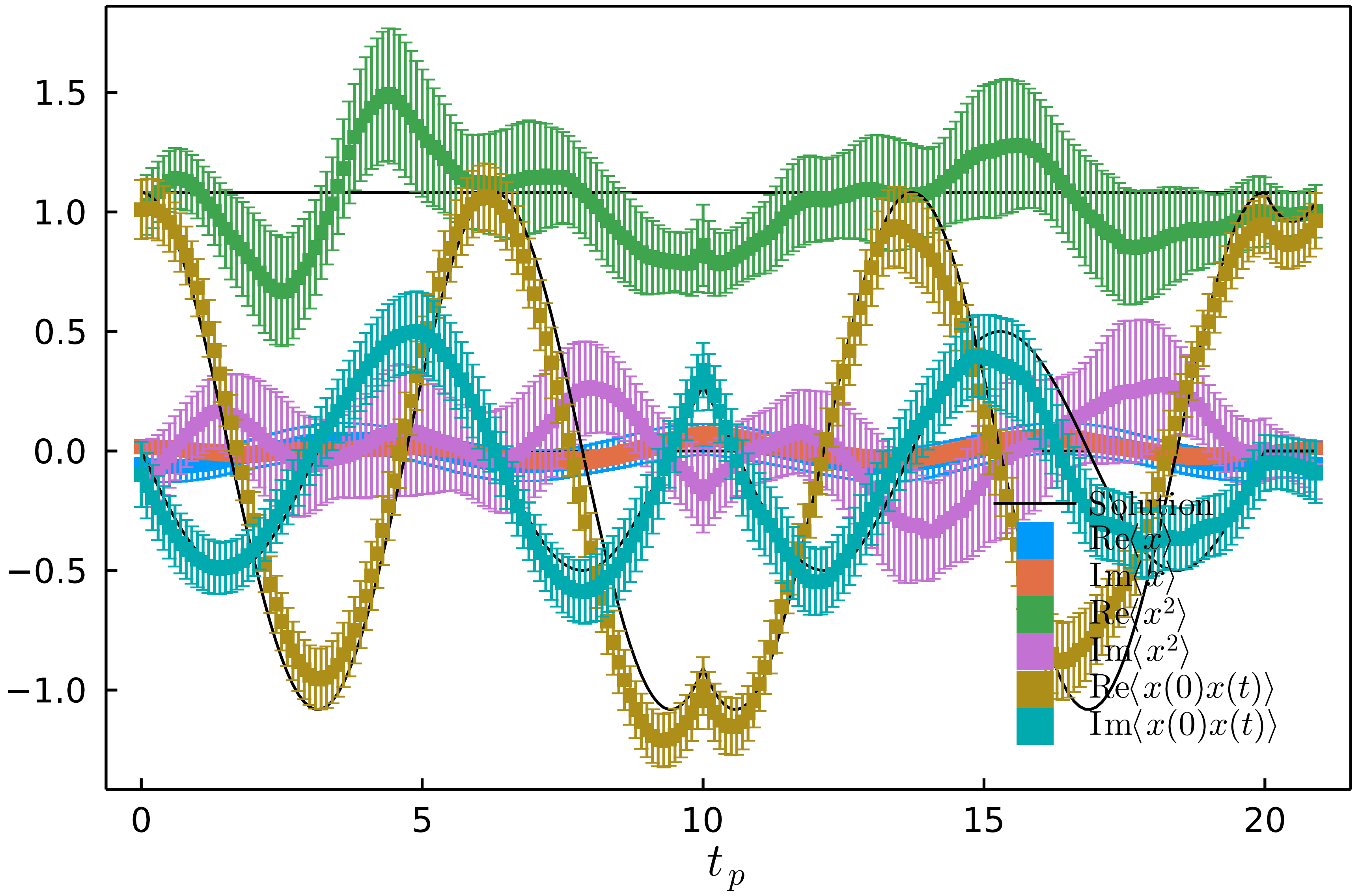


- Follow real axis up to $x_0^{\mathrm{max}} = 2.0$
- Using $\beta = 1.0$, $m = 1$, $\lambda = 24$
- Form of the kernel $K = e^{A+iB}$



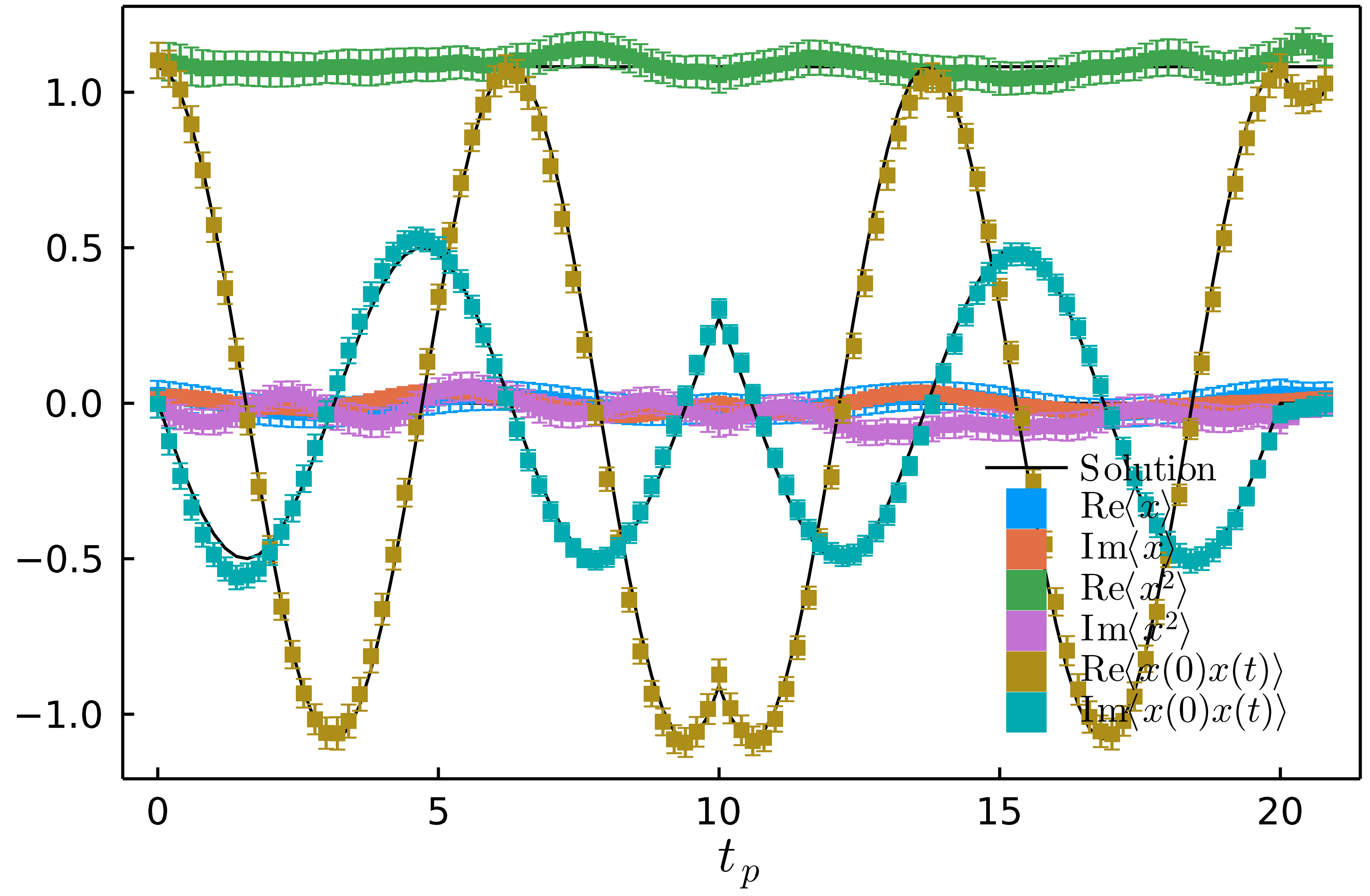
Learning free theory kernel

- Able to find kernel when only one critical point at the origin
- Kernel form $K = e^{A+iB}$



Optimising L_D using constant kernel

30 iterations



Field dependent kernel

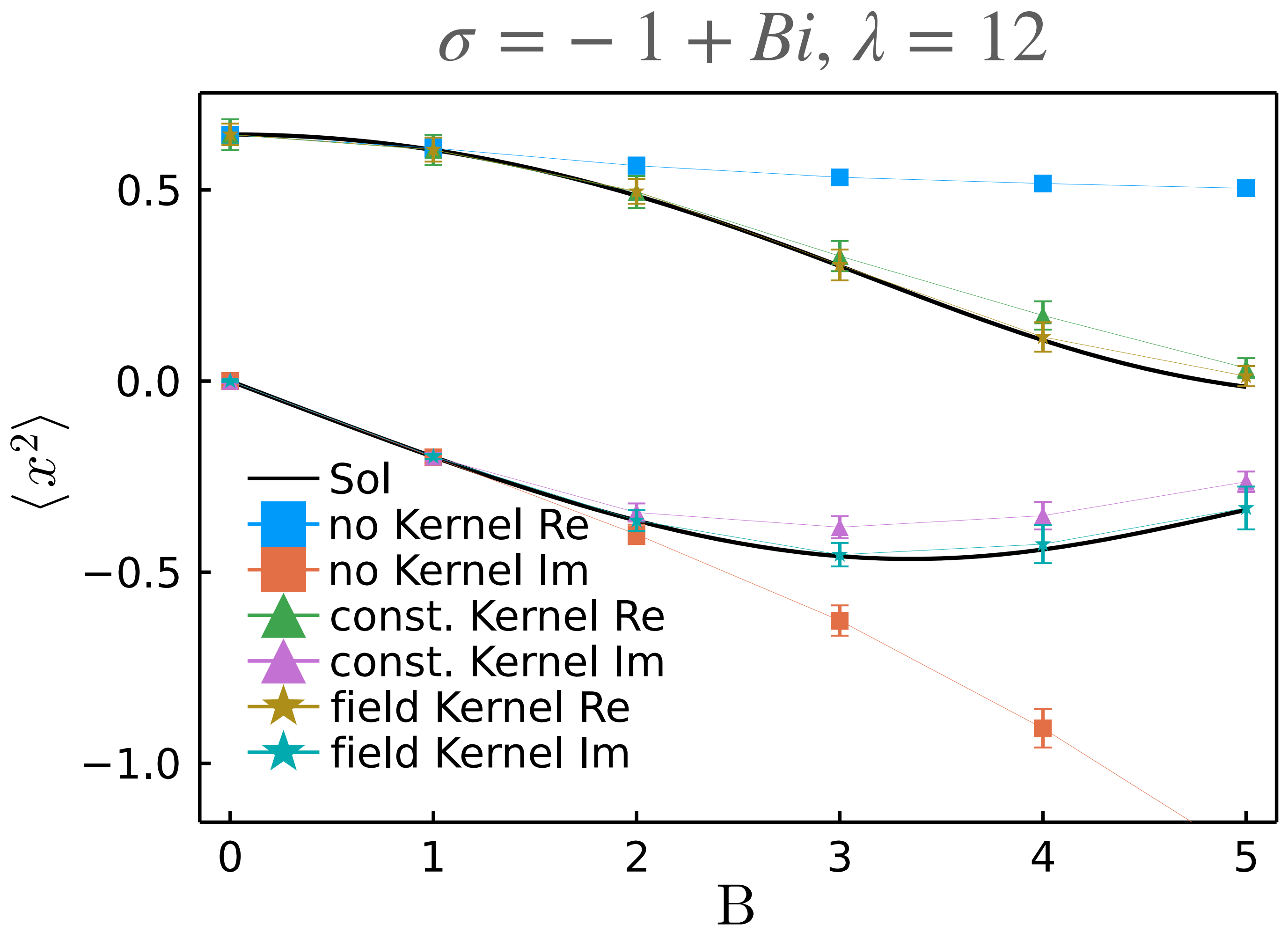
$$S = \frac{1}{2}\sigma x^2 + \frac{\lambda}{4!}x^4$$

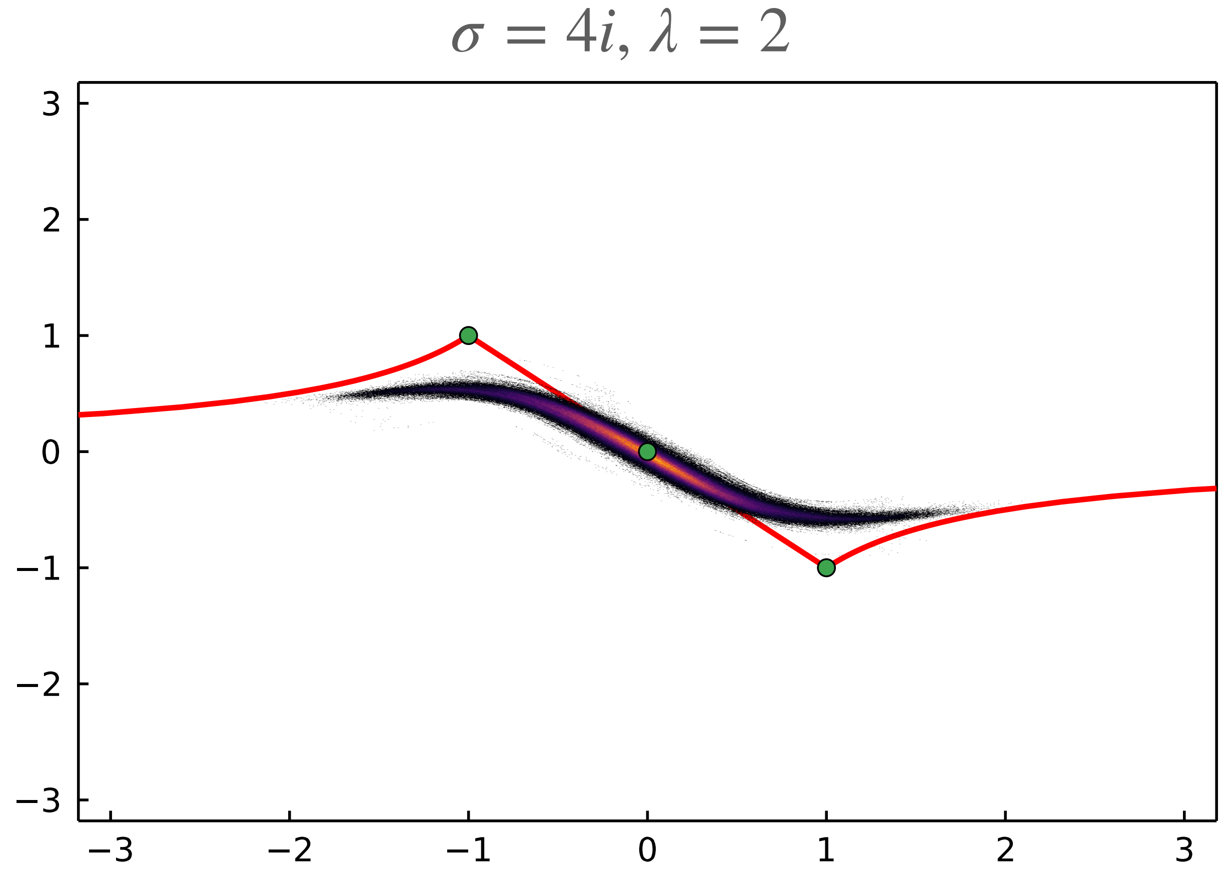
- Need to add extra derivative term

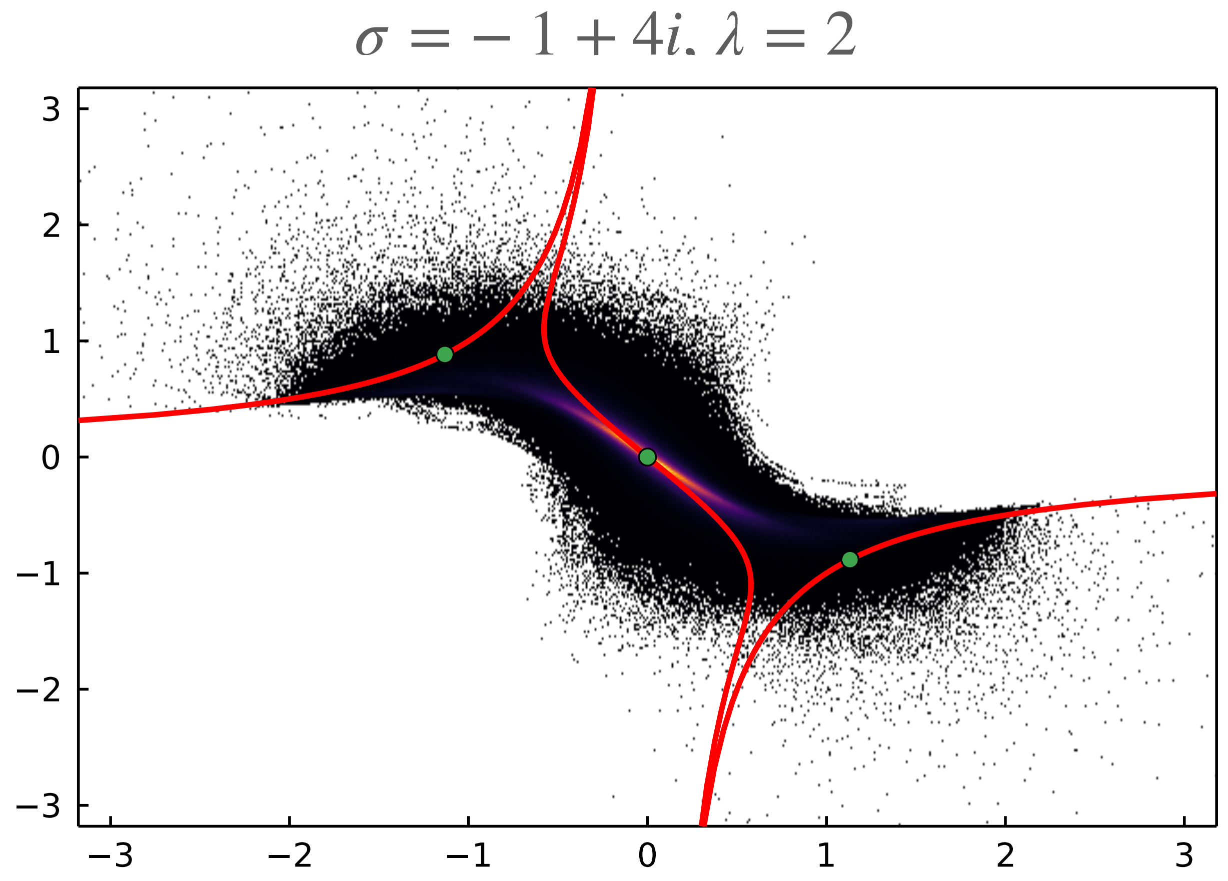
$$\frac{d\phi}{d\tau_0} = K[\phi]\frac{\delta S[\phi]}{\delta\phi} + \frac{\partial K[\phi]}{\partial\phi} + \sqrt{K[\phi]}\xi$$

$$K = \frac{1}{|\sigma|}f(x^2)e^{-i\theta_\sigma} + \frac{1}{|\lambda|}(1 - f(x^2))e^{-i\theta_\lambda}$$

$$f(x^2) = e^{-x^2(-\sigma/\lambda)}$$

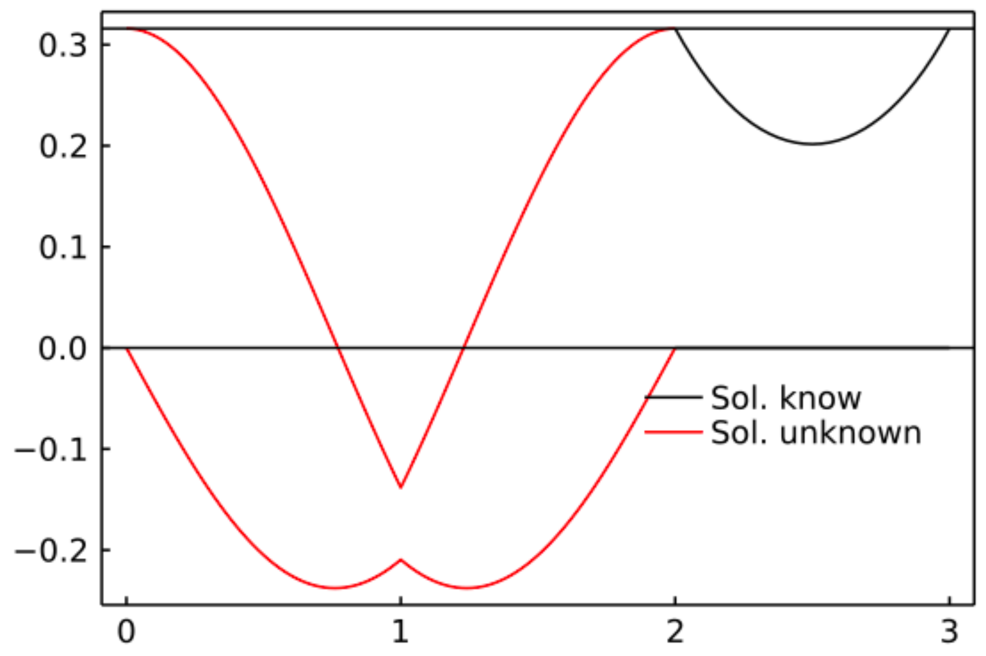


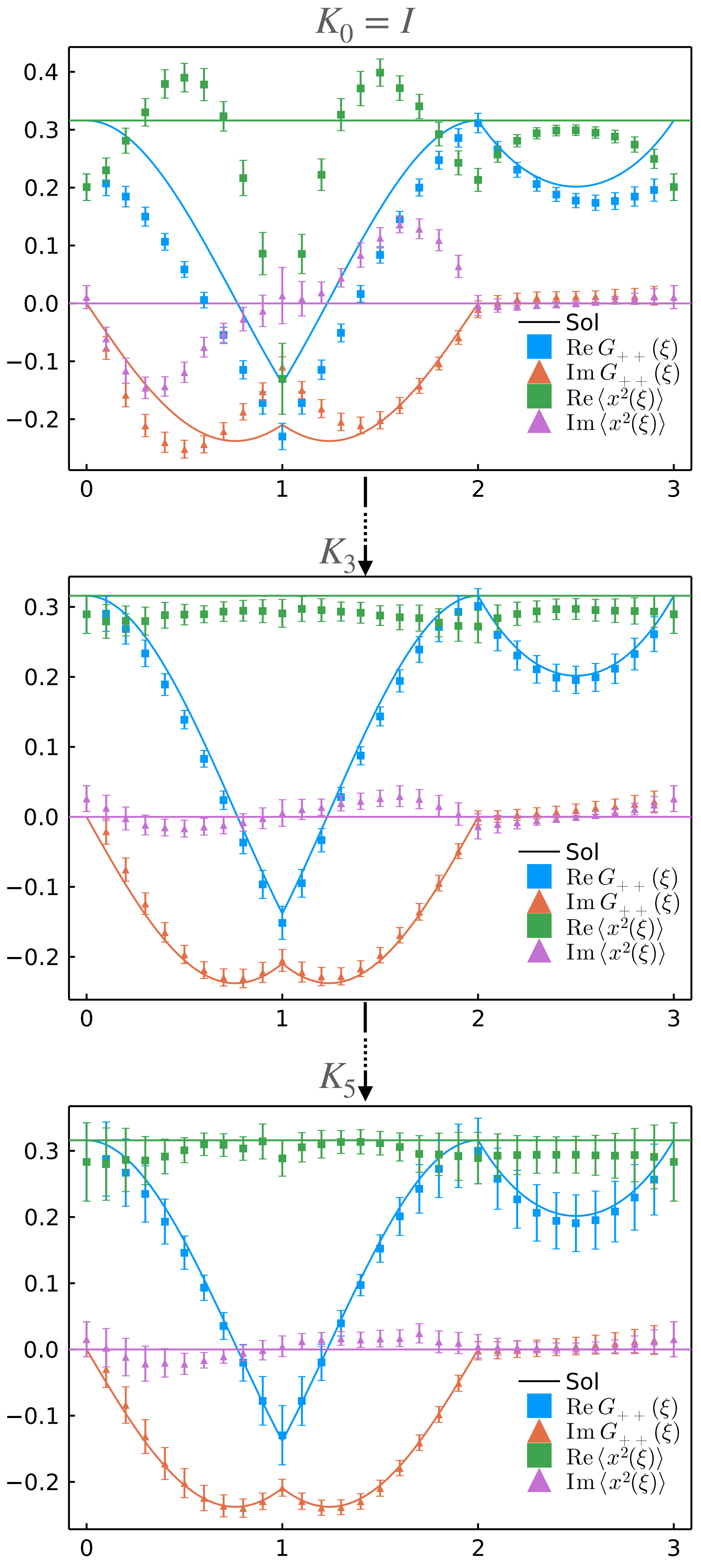




Construct kernel

- Can we find a kernel by using prior knowledge about the Complex Langevin and the model
- In thermal ϕ^4 we know:
    - $\langle x \rangle = 0$ and $\langle x^2 \rangle = \text{Re}\langle x^2 \rangle = \text{const.}$
    - Euclidean correlation $G(\xi)$ for $\xi \geq 2$
- Minimize $L(K) = \sum_i ||O_i - \langle O_i(K) \rangle||^2$
- Matrix kernel, starting out with $K_0 = I$
- Update K_n based on $\nabla L(K_n)$
- Contour: $\beta = 1.0$, $x_0^{\text{max}} = 1.0$
- Field dependent kernel



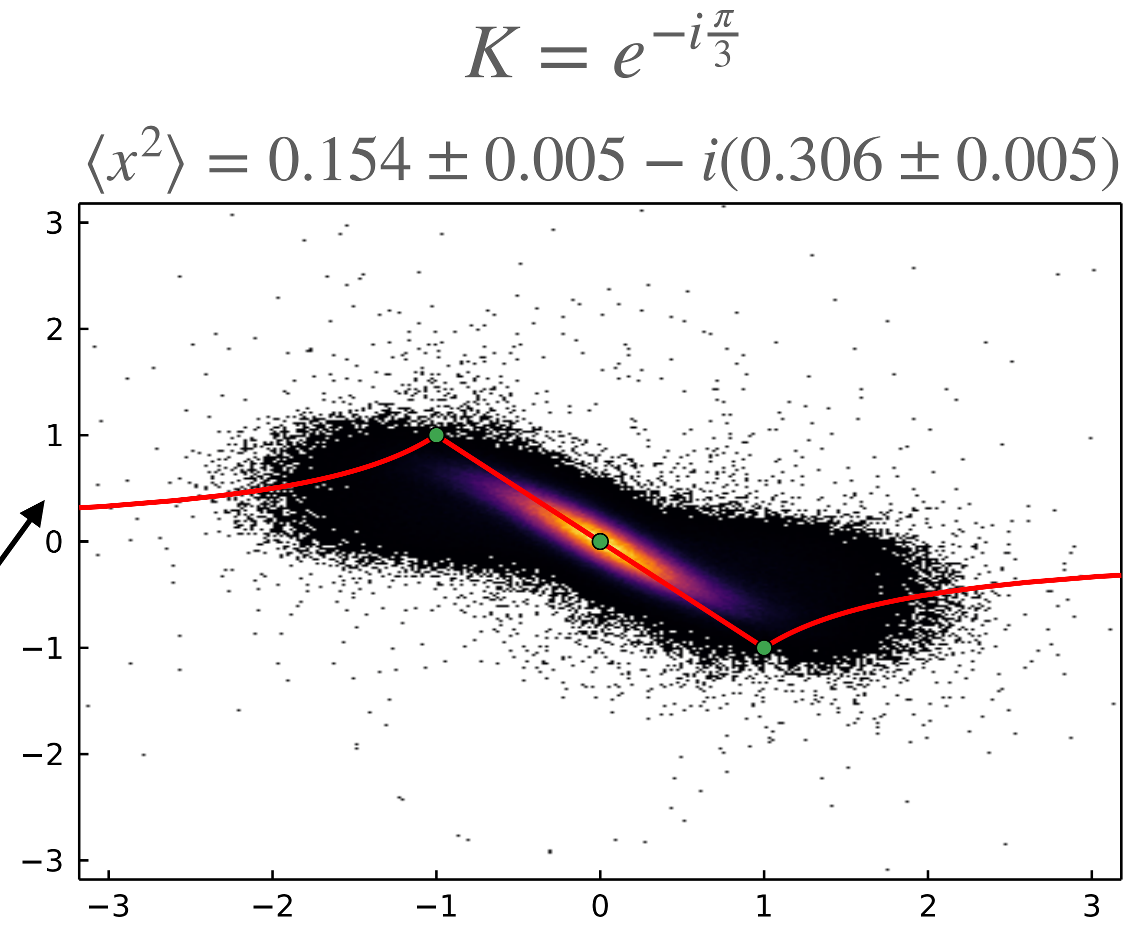


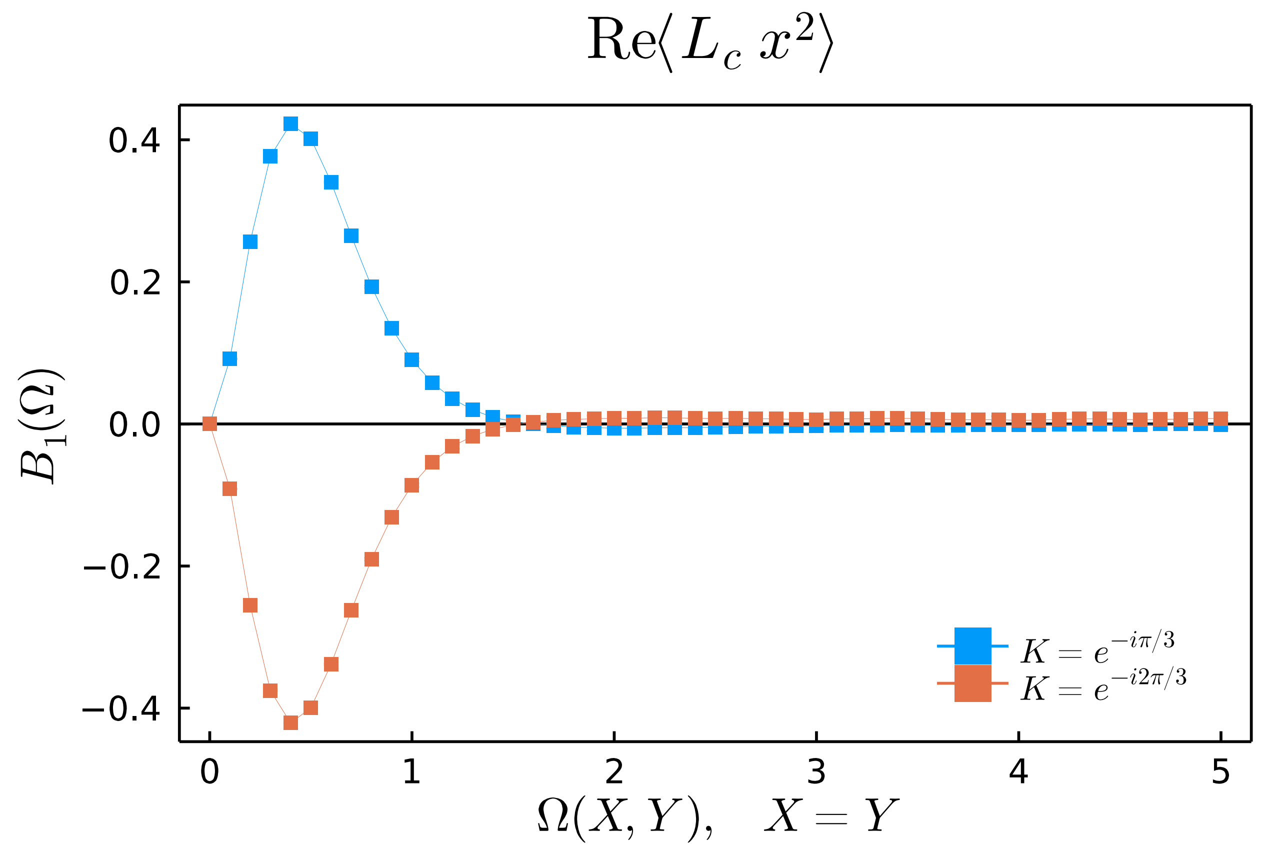
More info about simple model results

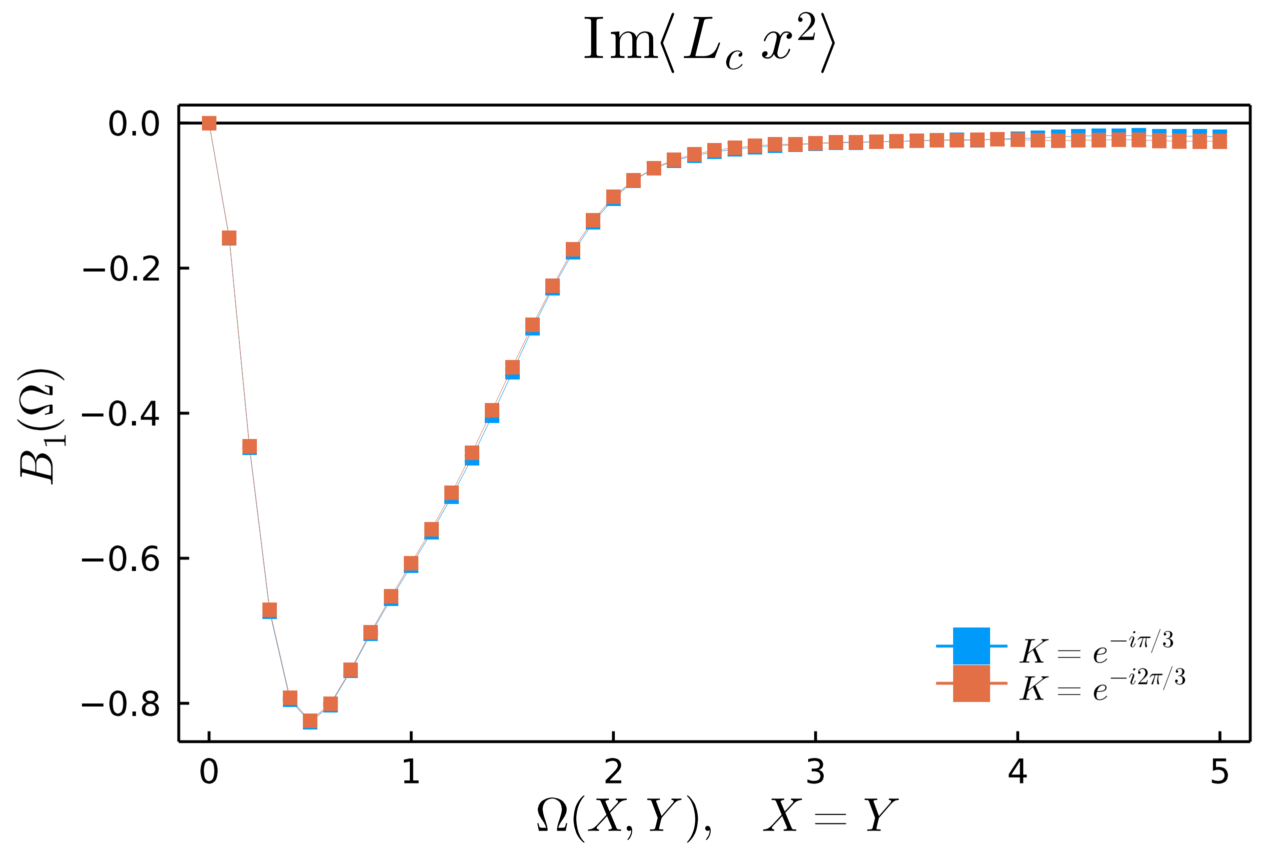
$$S = \frac{1}{2}\sigma x^2 + \frac{\lambda}{4!}x^4$$

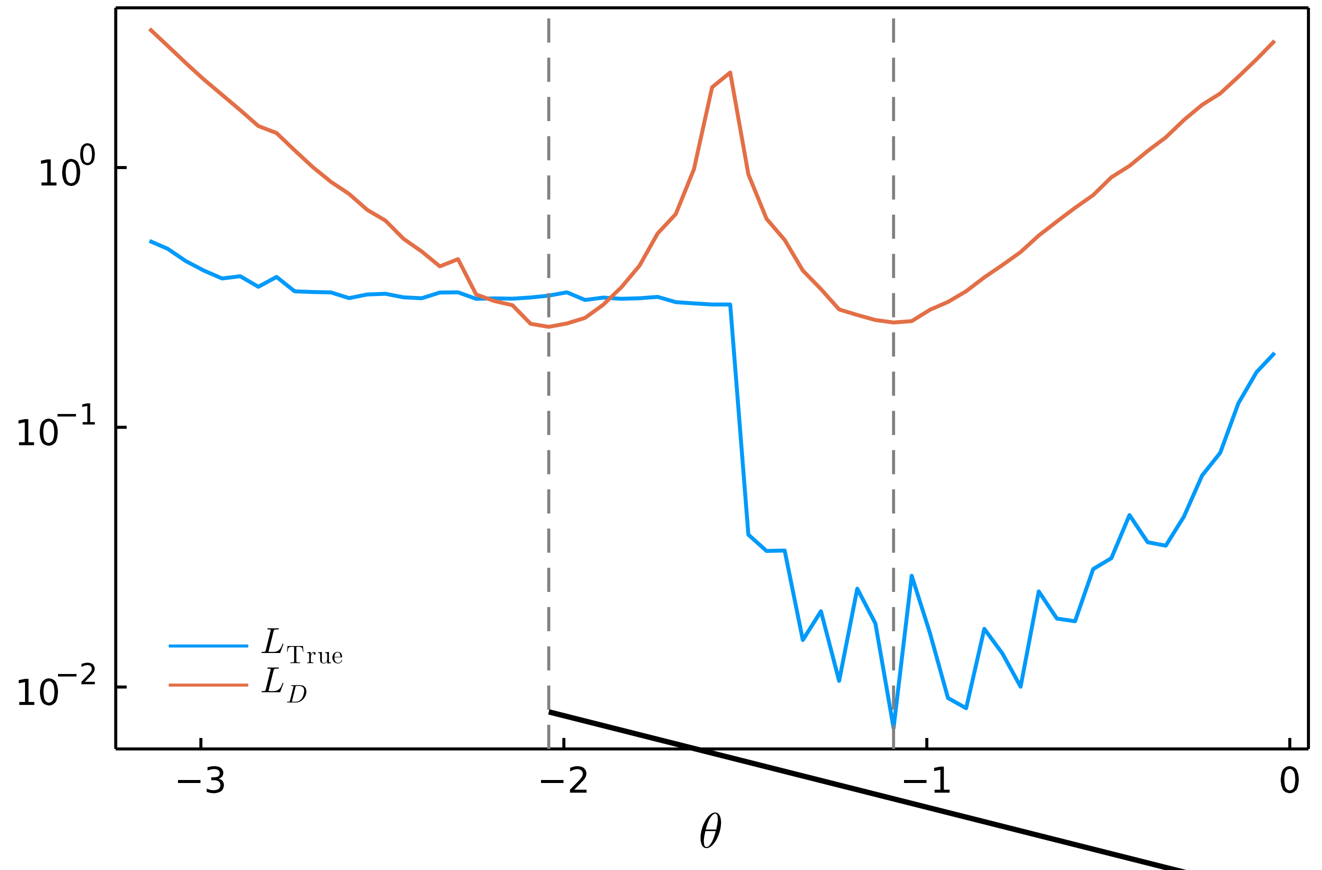
$\sigma = 4i,\ \lambda = 2$

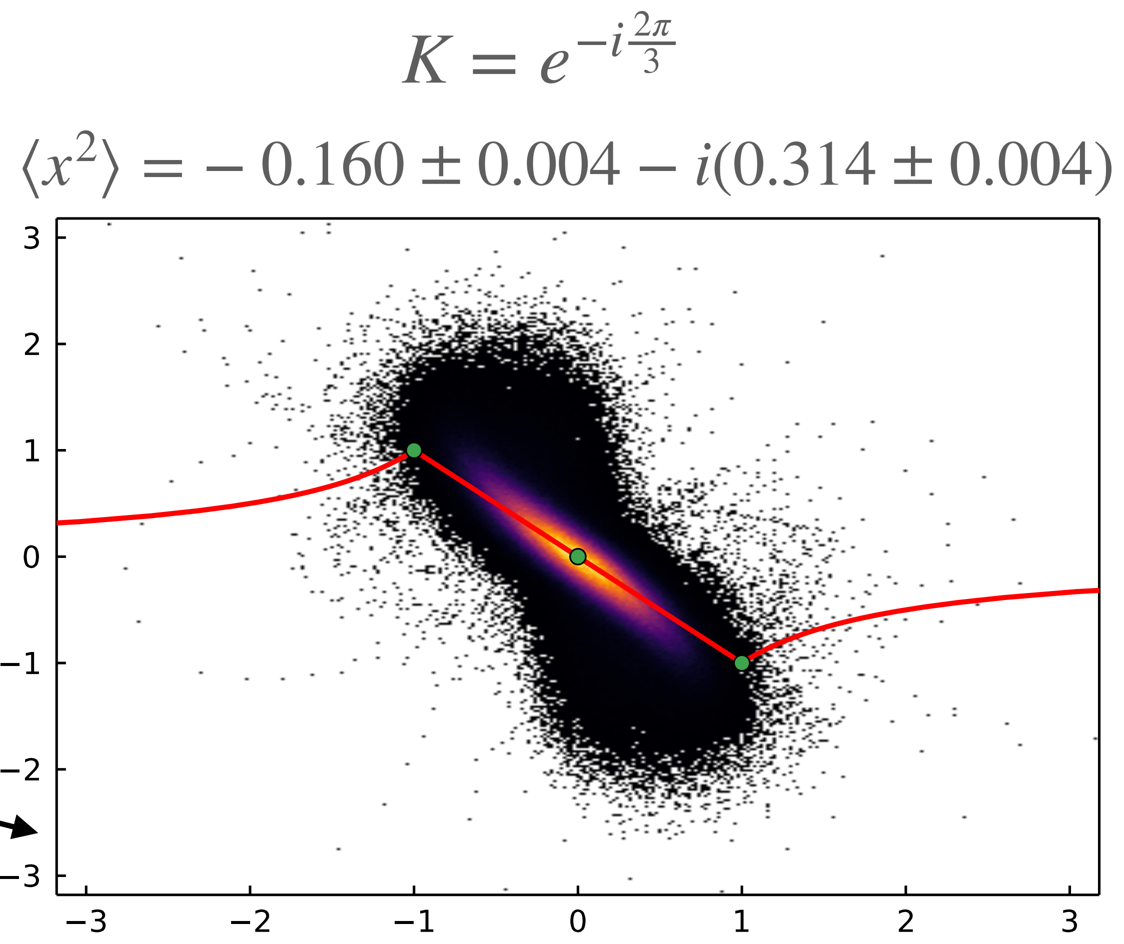
$\langle x^2 \rangle_{\text{true}} = 0.150077 - i0.307646$



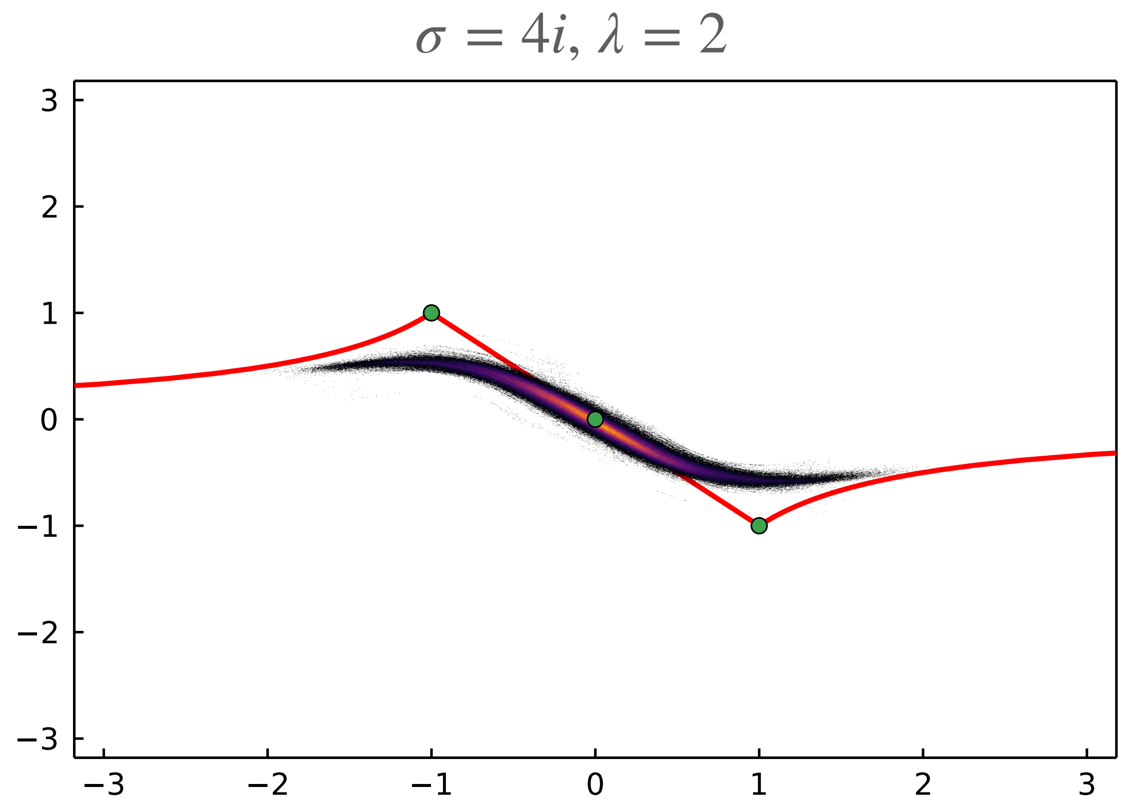


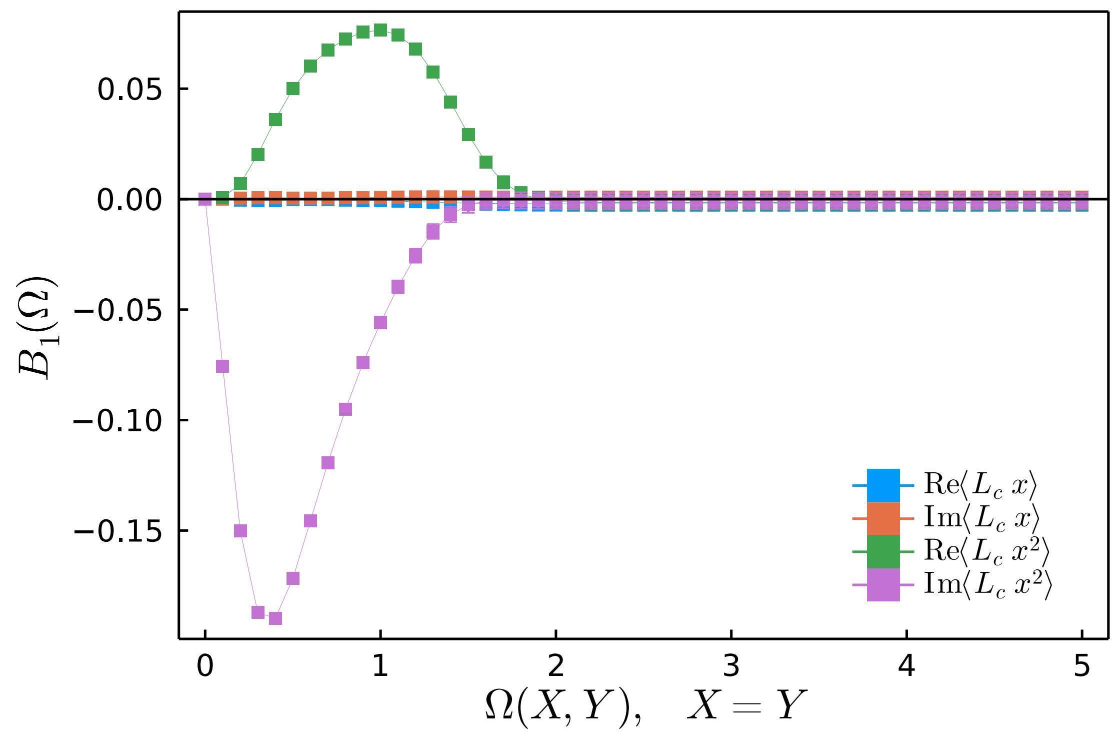






Field dependent





Simple overview of SDE solver (Solution to runaway problem)

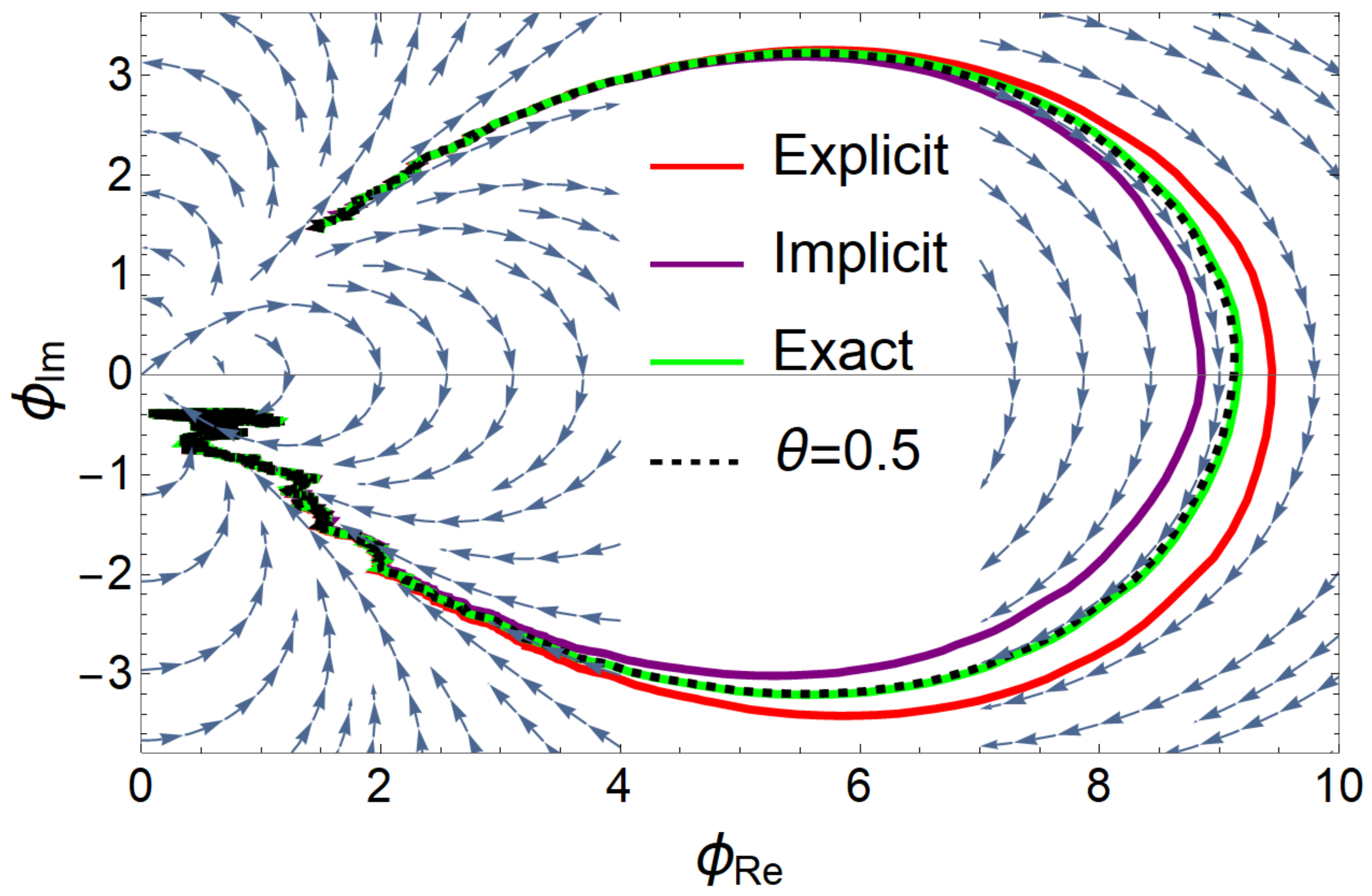
- General Euler-Maruyama Scheme:

$$\phi_j^{\lambda+1} = \phi_j^{\lambda} + i\epsilon_j \left[\theta \frac{\partial S^{\lambda+1}}{\partial \phi_j} + (1-\theta) \frac{\partial S^{\lambda}}{\partial \phi_j} \right] + \sqrt{\epsilon_j}\eta_j^{\lambda}$$

CLE:

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

  - Explicit ($\theta = 0.0$): Overshooting
  - Implicit ($\theta = 1.0$): Undershooting
  - Semi-implicit ($\theta = 0.5$): Stable and close to the exact solution
  - For all $\theta \geq 0.5$ we get rid of runaways (Unconditionally stable)



Simulations done with the DifferentialEquations.jl library in Julia