Real-time simulations using complex Langevin

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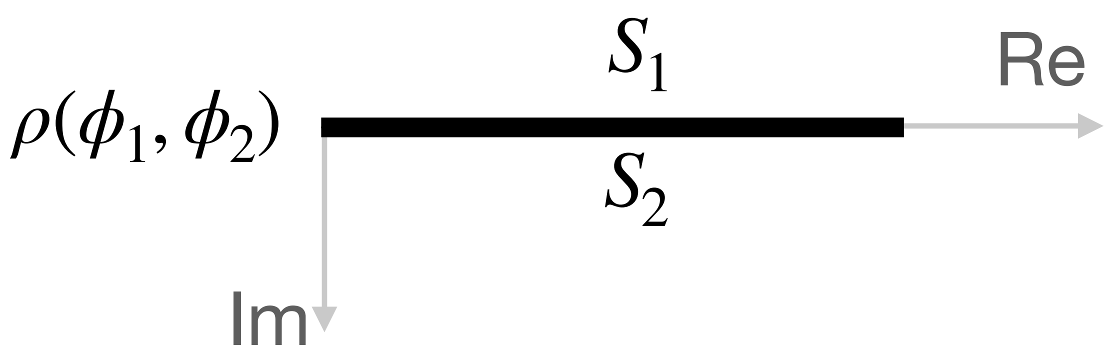
The Research Council of Norway

Norwegian Particle, Astroparticle & Cosmology Theory network

Real-time simulations and the sign problem

- Real-time simulations (Minkowski): $\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \ \mathcal{O}(x) e^{iS[\phi]}$
  - Schwinger-Keldysh contour
  - Thermal equilibrium
- Complex Feynman weight



$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi_1 \int D\phi_2 \rho(\phi_1, \phi_2) \int_{\phi_1}^{\phi_2} D\phi^+ D\phi^- \mathcal{O}(\phi) e^{iS[\phi^+] - iS[\phi^-]}$$

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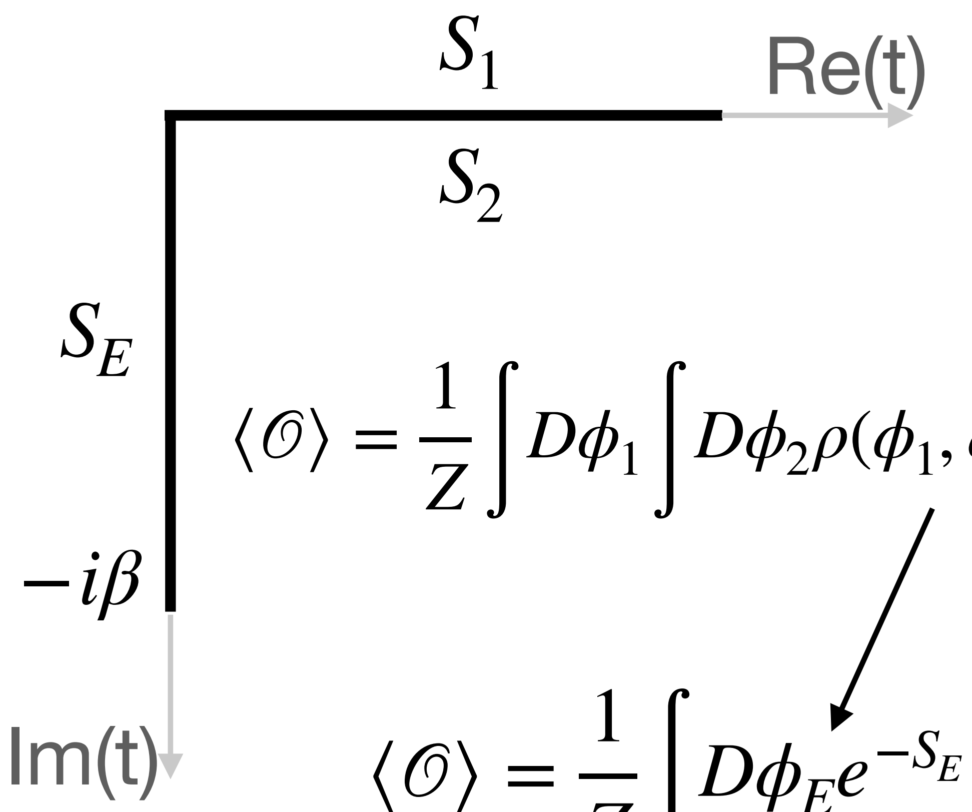

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$$\langle \mathcal{O} \rangle = \frac{1}{Z}\int D\phi_E e^{-S_E} \int D\phi^+ D\phi^- \mathcal{O}(\phi) e^{iS[\phi^+] - iS[\phi^-]}$$

$$iS[\phi^+] - iS[\phi^-] - S_E[\phi_E] \rightarrow iS[\phi]$$

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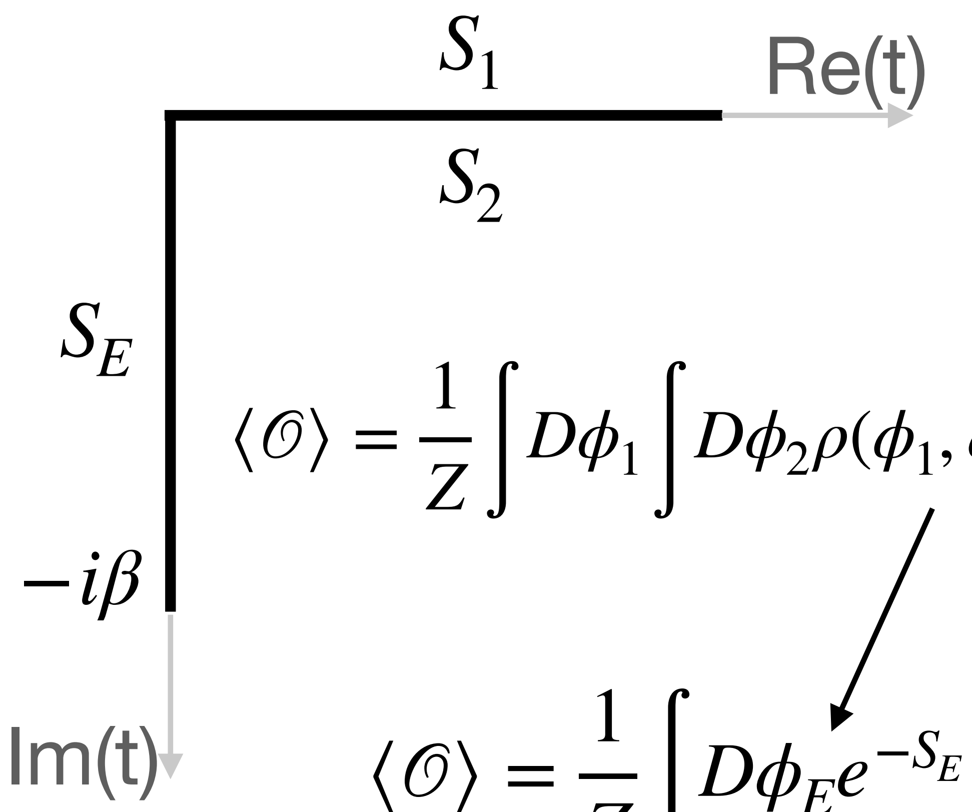

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$$iS[\phi^+] - iS[\phi^-] - S_E[\phi_E] \to iS[\phi]$$

Importance sampling not possible

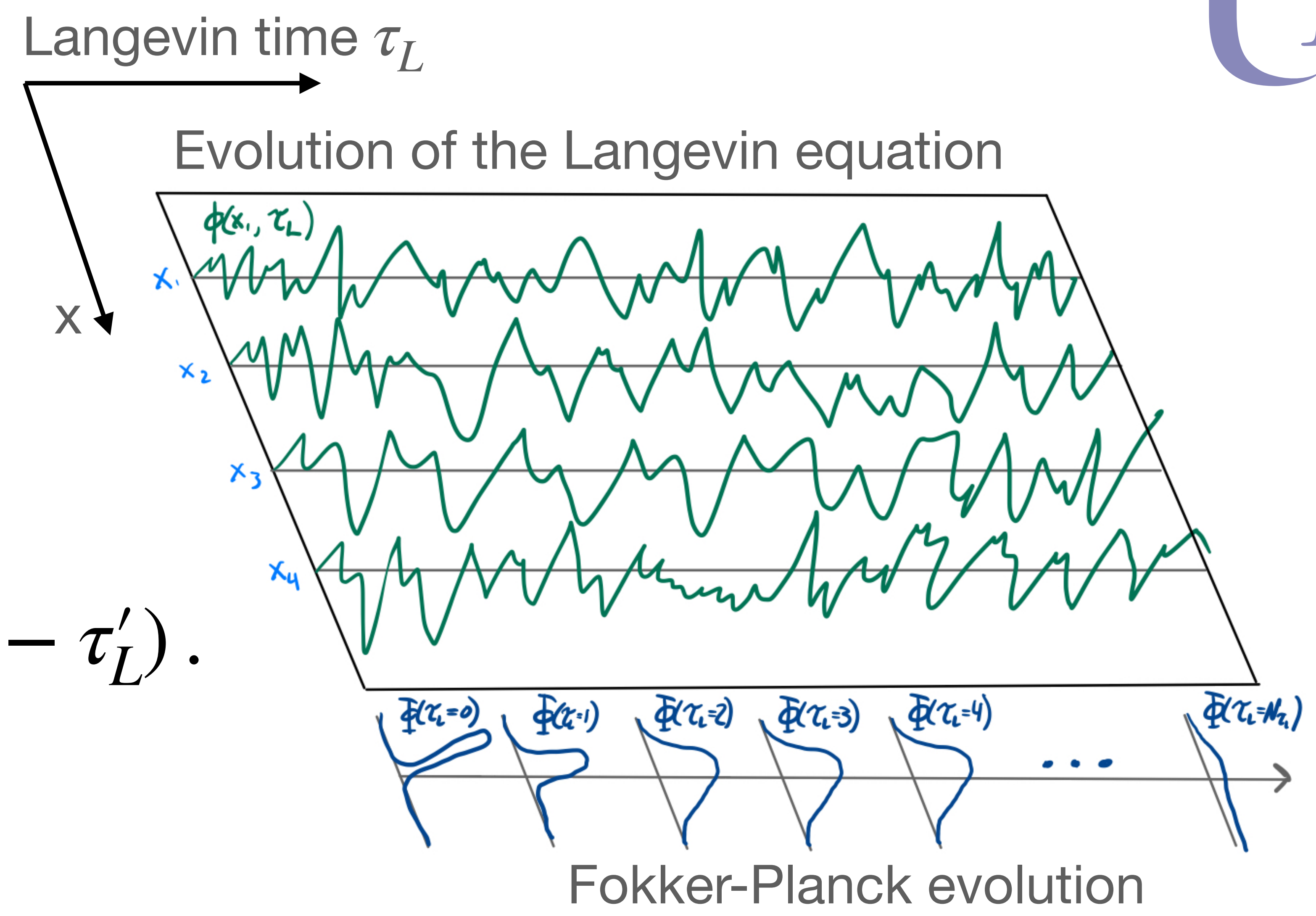
Complex Langevin, Lefschetz thimbles, Tensor networks,….

Langevin equation

- Langevin equation
  (Stochastic Differential equation)

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

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



- Fokker-Planck equation (Real)

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

- Equilibrium distribution of FP $\rightarrow e^{-S[\phi]}$

$$\langle \mathcal{O}\rangle = \underbrace{\lim_{\tau_L\to\infty}\int D\phi\;\Phi(\phi,\tau_L)\mathcal{O}(\phi)}_{\text{Fokker-Planck}} = \underbrace{\lim_{T\to\infty}\int_0^T d\tau_L\;\mathcal{O}(\phi(\tau_L))}_{\text{Langevin}}$$

Real-time complex Langevin

- Complexifying fields: $\phi \rightarrow \phi^R + i\phi^I$
- Scales linear with size of problem

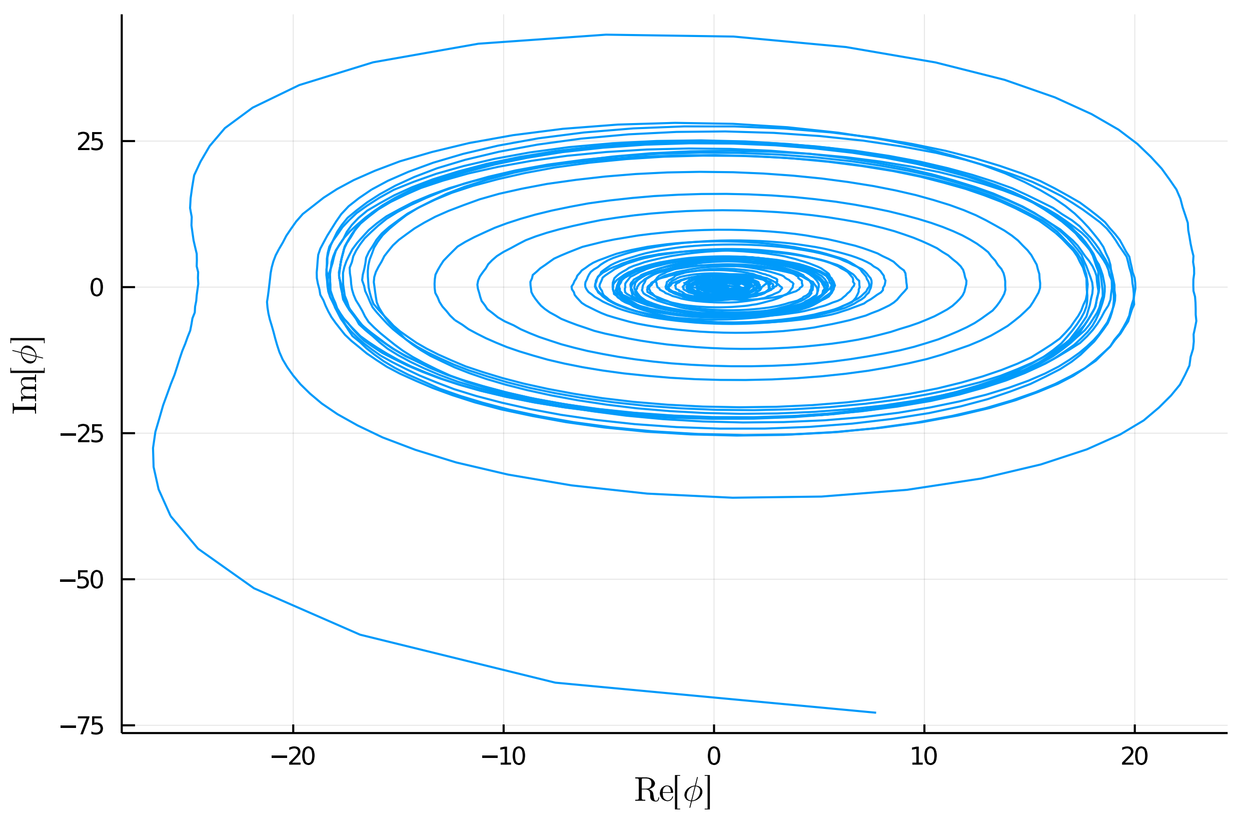
Complex Langevin equation

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

Stable solver

Get control of the numerics

Real-time complex Langevin = Stiff problem



Regulator

Regulate integral

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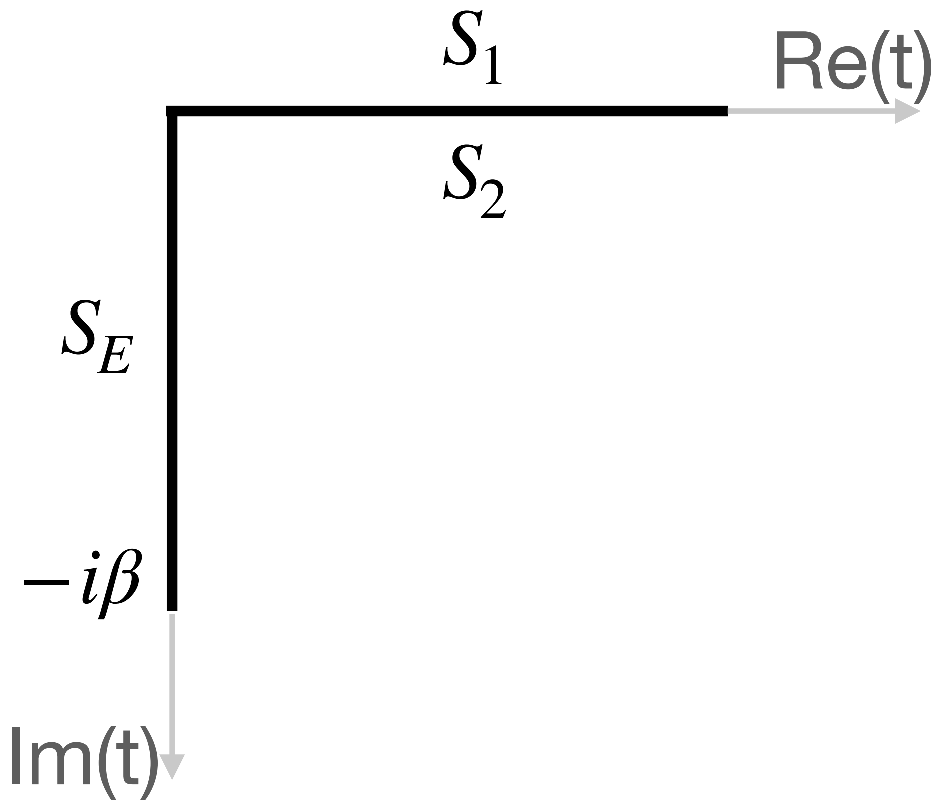
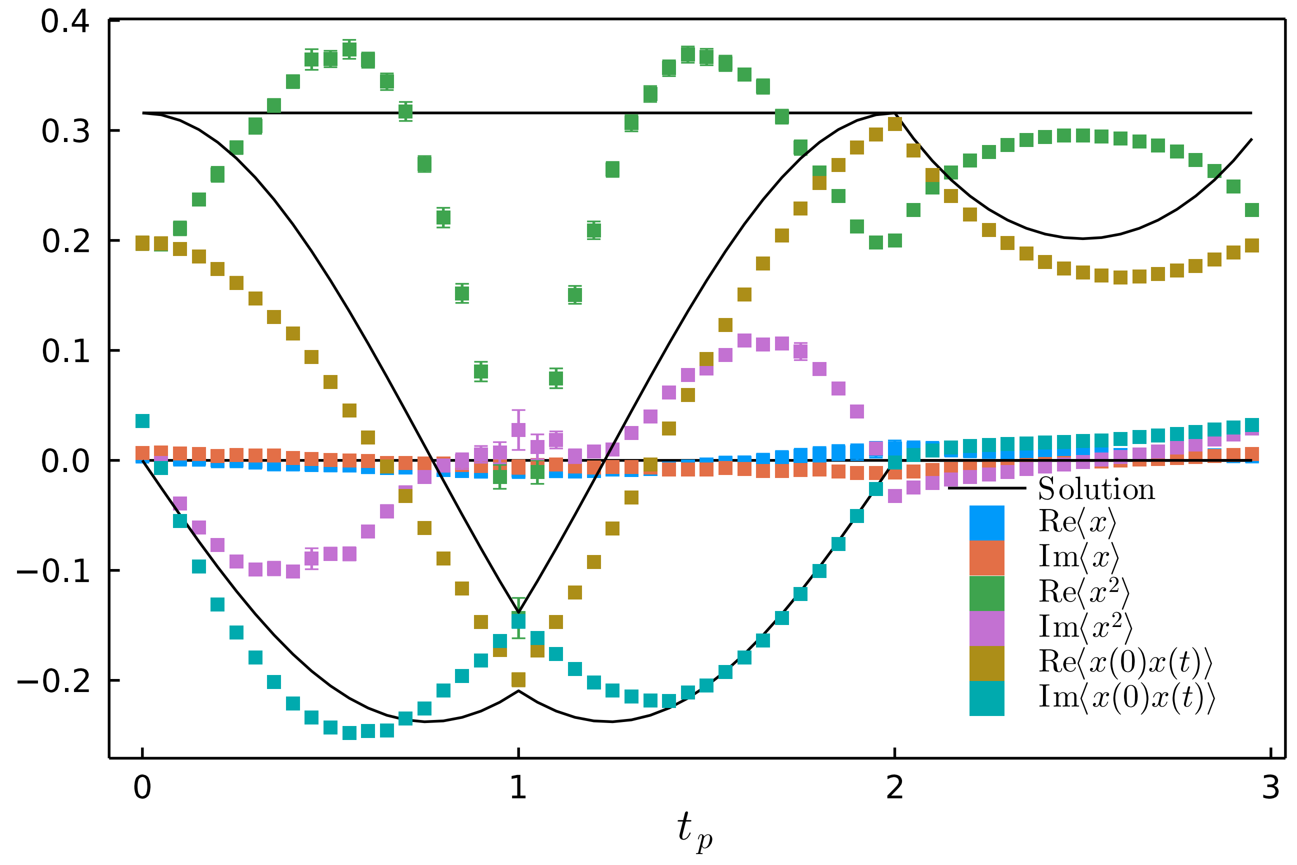


Convergence problem

Understand convergence problem of the complex Langevin



Real-time complex Langevin: Benchmark problem

- Strongly coupled quantum anharmonic oscillator with $m = 1, \lambda = 24, \beta = 1$ [Berges, Borsanyi, Sexty, Stamatescu (2007)]

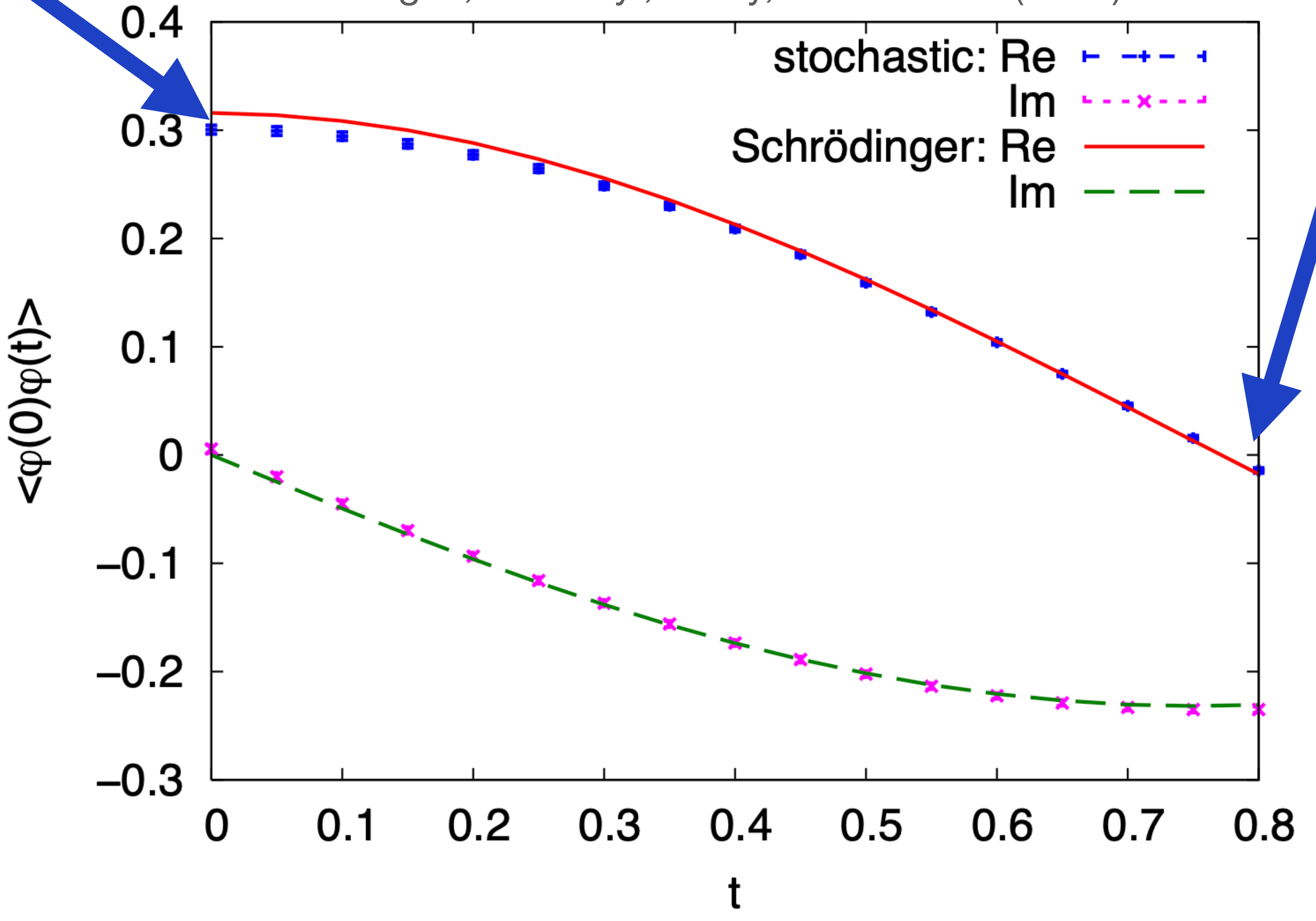
$$S = \int dx_0 \left\{ \frac{1}{2}\left(\frac{\partial \phi}{\partial x_0}\right)^2 - \frac{1}{2} m \phi^2 - \frac{\lambda}{4!}\phi^4 \right\}$$

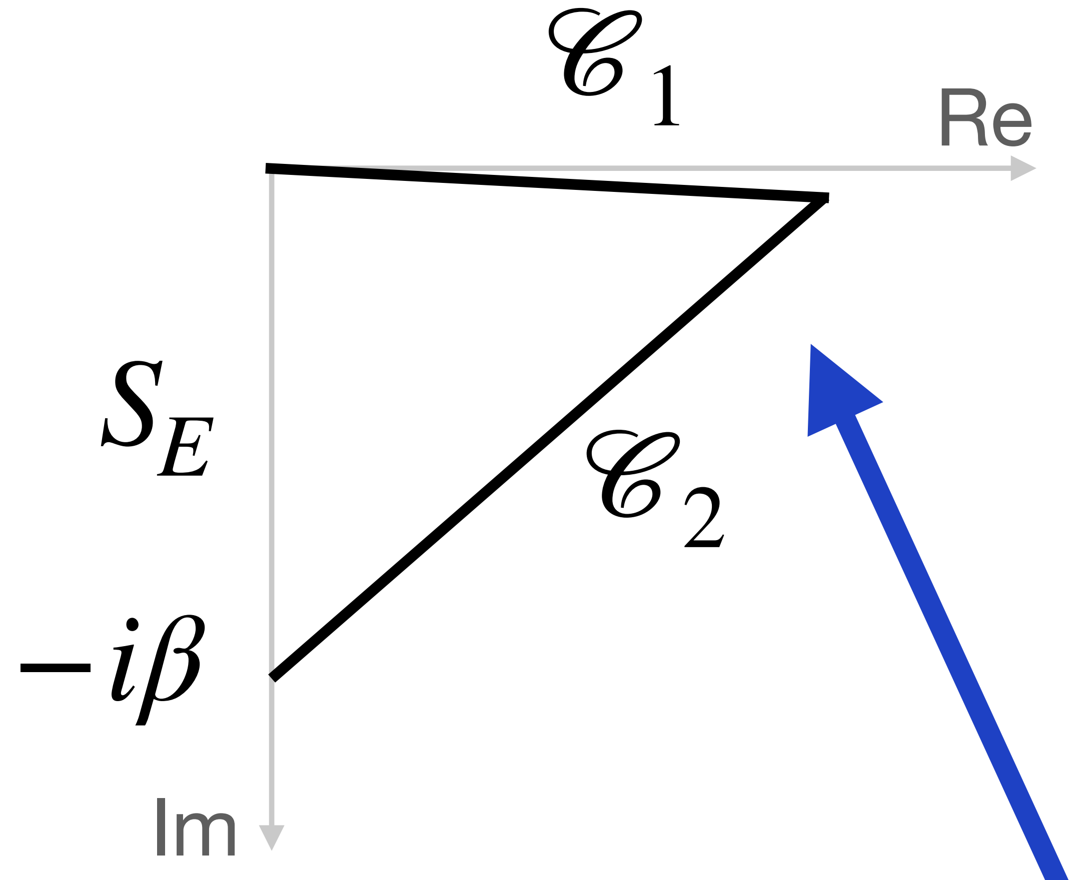
Extending the real-time contour

Deviation due to discretisation or CL?

Remove runaway solutions a-priori

Berges, Borsanyi, Sexty, Stamatescu (2007)





Remove forward and backward tilt

Stable solver and Regulator

Simple overview of SDE solver

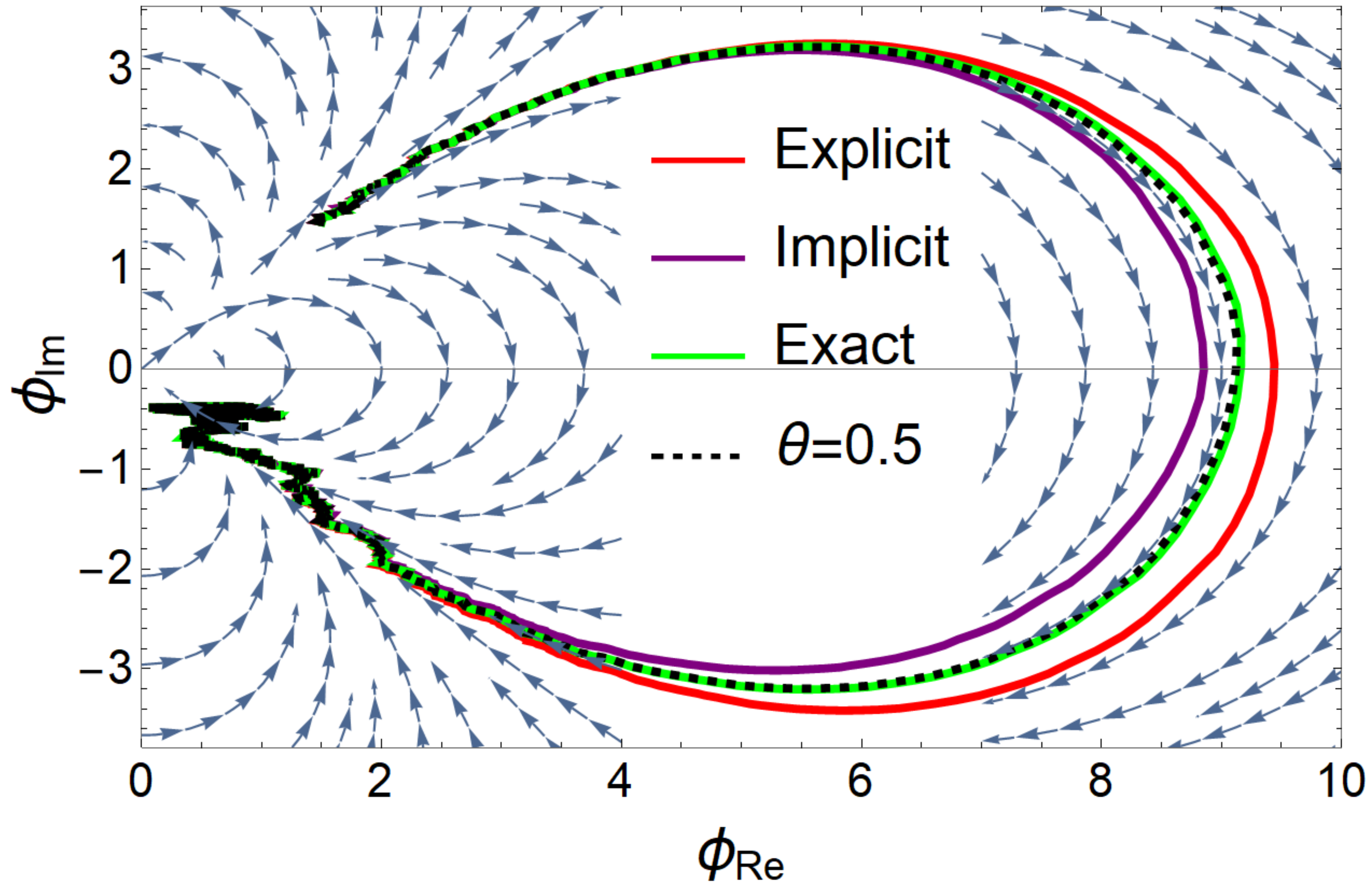
- General Euler-Maruyama Scheme:

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

CLE:

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

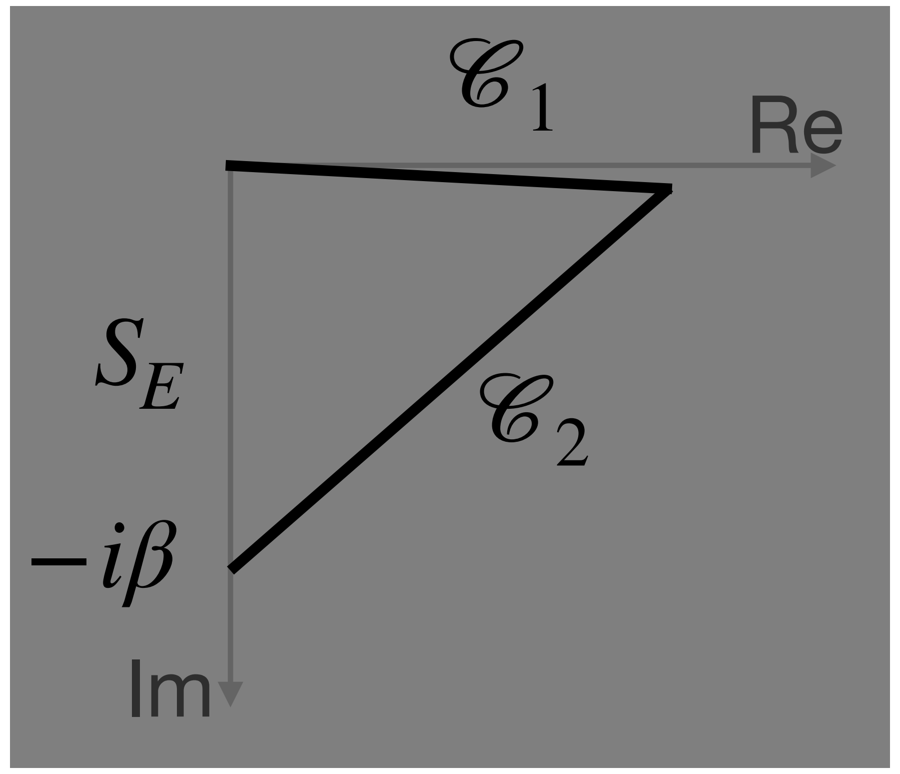
  - Explicit ($\theta = 0.0$): Overshooting
  - Implicit ($\theta = 1.0$): Undershooting
  - Semi-implicit ($\theta = 0.5$): Stable and close to the exact solution
  - For all $\theta \geq 0.5$ we get rid of runaways (Unconditionally stable)

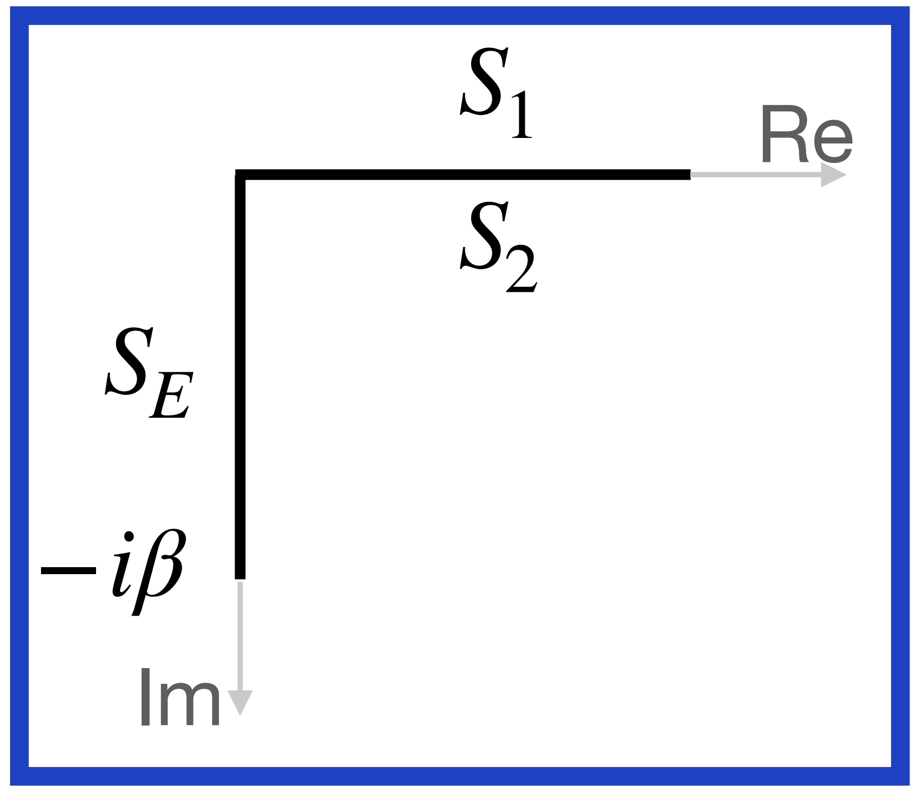


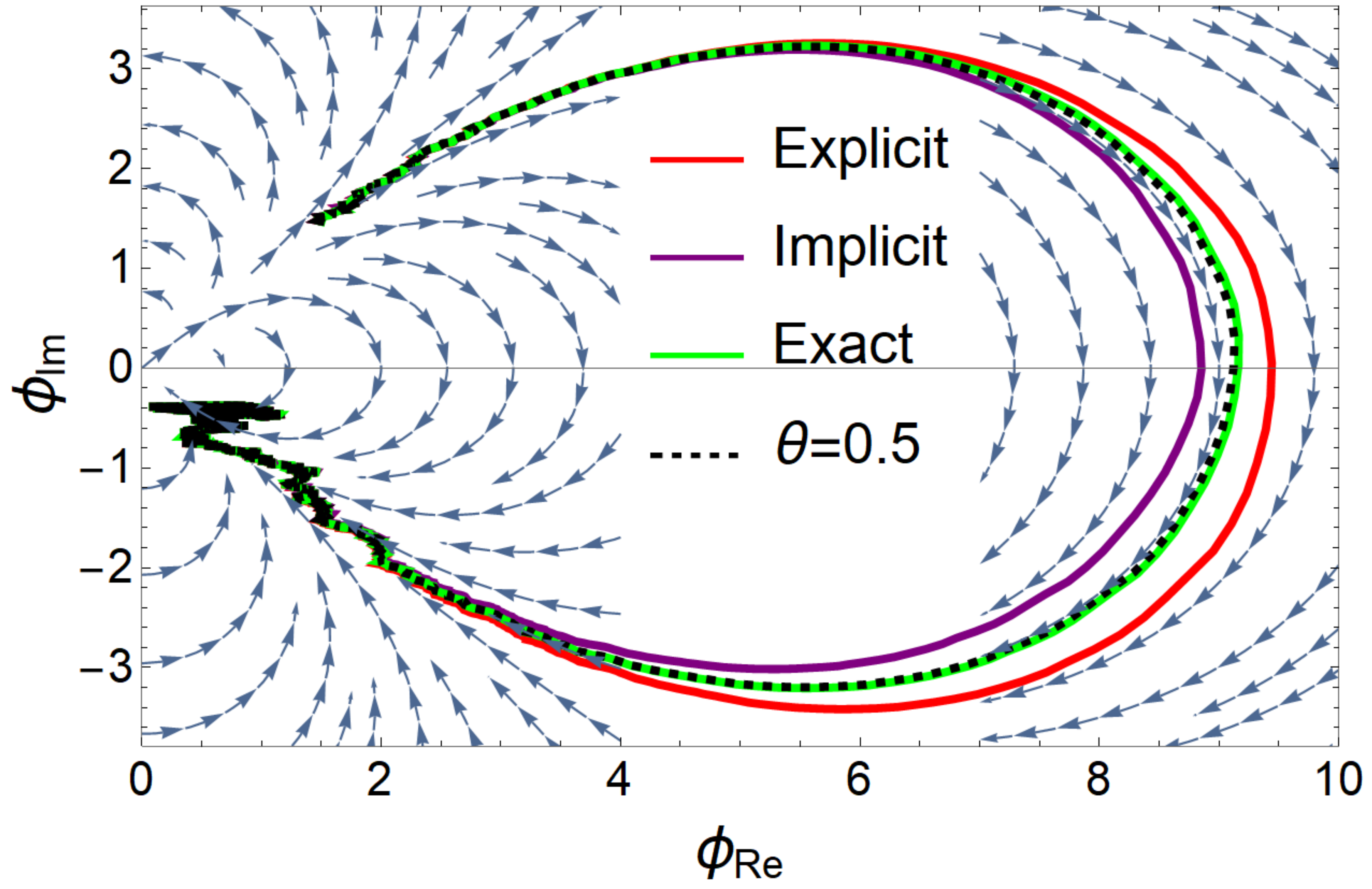
Simulations done with the DifferentialEquations.jl library in Julia

Regularisation of real-time contour

- Old way: Explicit scheme + tilting (Adaptive step-size)
- Implicit solver: No runaway solutions
- Regularisation; Infinitesimal damping term:
  $\bar{S} = S + iR(\phi, \epsilon)$
  - $R = \frac{1}{2}\epsilon\phi^2$
  - Tilted contour
  - Implicit scheme



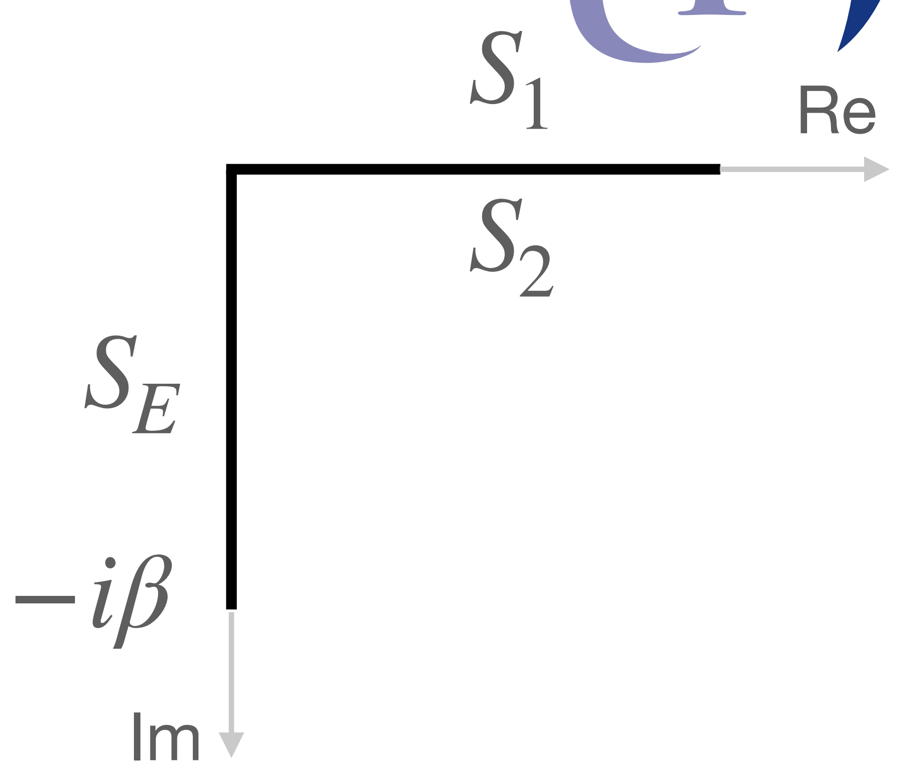


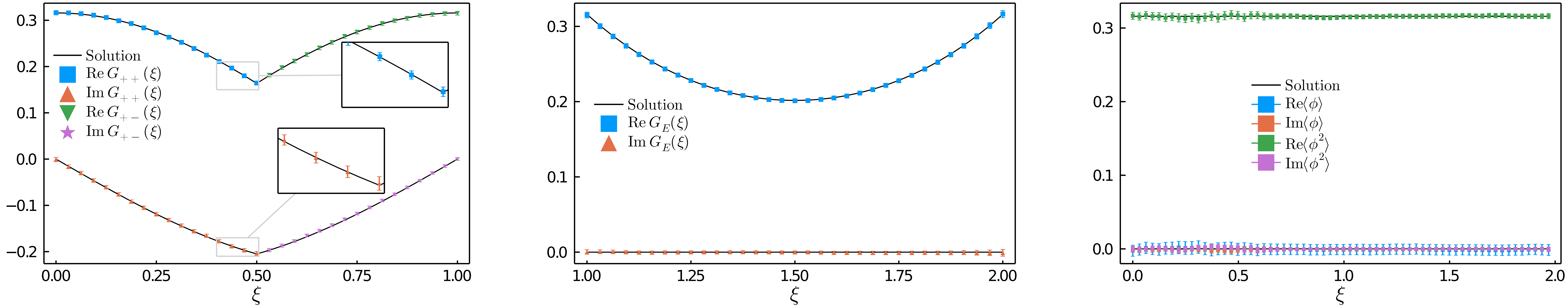


Dynamics in thermal equilibrium

- Strongly coupled quantum anharmonic oscillator with $m = 1$, $\lambda = 24$ (same as in Berges, Borsanyi, Sexty, Stamatescu, 2007)
- Regulator: $\theta = 0.6$, Contour: $\beta = 1.0$, $x_0^{\text{max}} = 0.5$
- $G_{++}(\xi) = \langle \phi(0)\phi(\xi) \rangle - \langle \phi(0) \rangle \langle \phi(\xi) \rangle$ for $\xi \leq 0.5$
- $G_E(\xi) = \langle \phi(0)\phi(\xi) \rangle - \langle \phi(0) \rangle \langle \phi(\xi) \rangle$ for $\xi \geq 1$

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



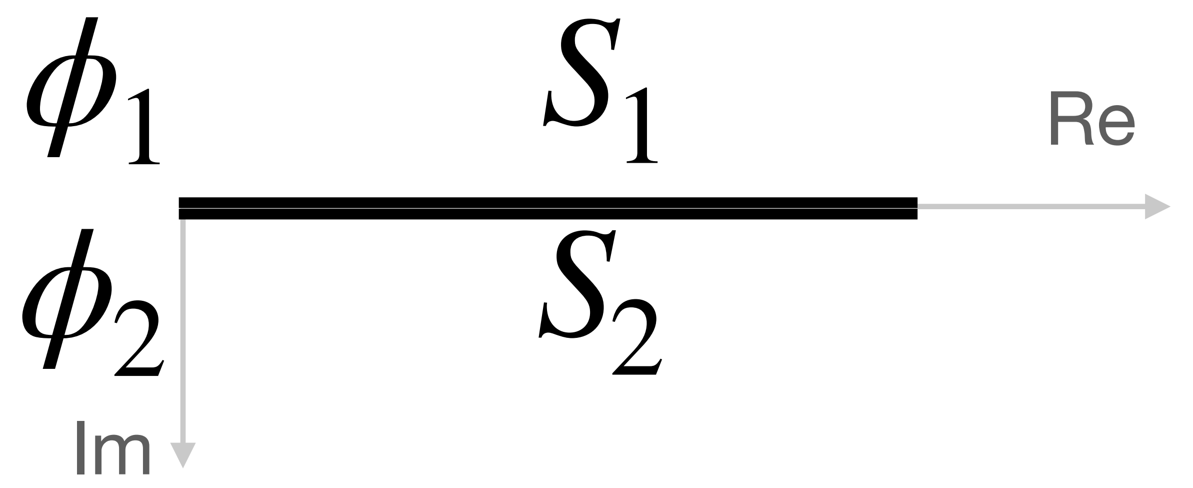


Non-Equilibrium dynamics

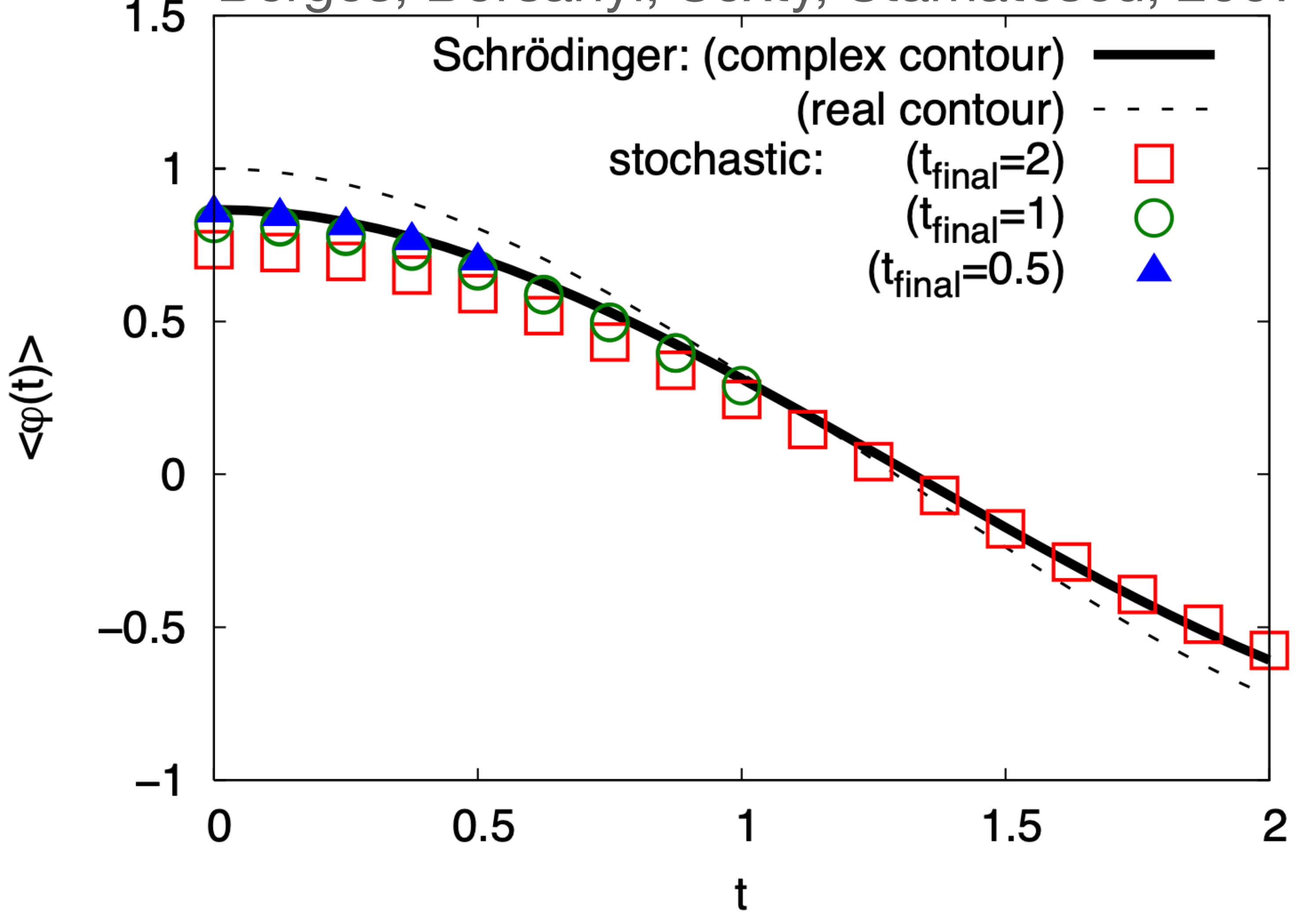
- Gaussian initial density matrix with
  $\langle \phi_0 \rangle = 1, \langle \dot{\phi}_0 \rangle = 0, \langle \phi_0 \phi_0 \rangle = 1, \langle \dot{\phi}_0 \dot{\phi}_0 \rangle = \frac{1}{4}$
  (Berges, Borsanyi, Sexty, Stamatescu, 2007)

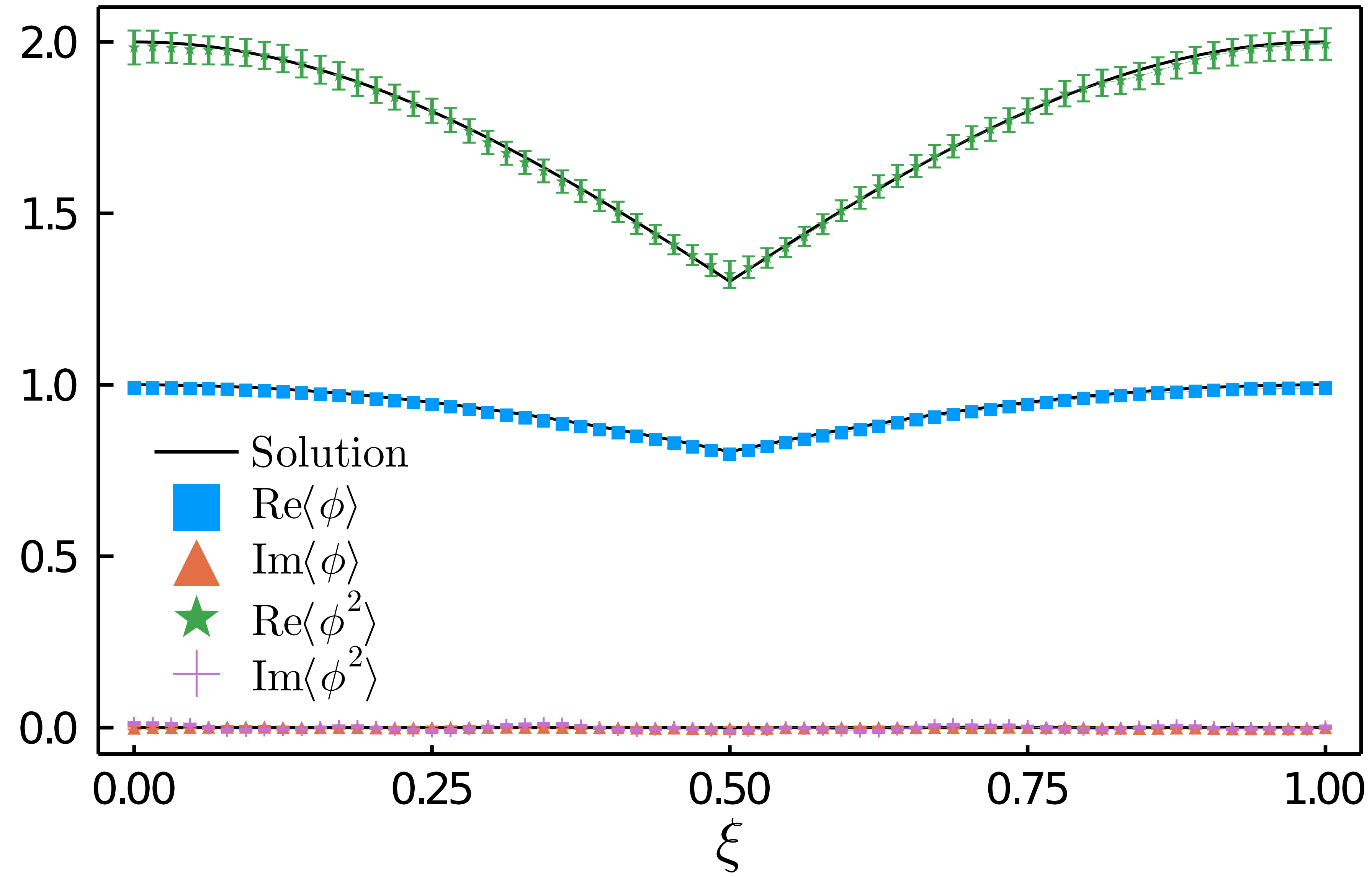
- Small coupling $\lambda = 1$ and regulator $\theta = 0.6$

- Full access to G_{+-} and $G_{-+}(x_0) = \langle \phi_2\, \phi(x_0) \rangle - \langle \phi_2 \rangle \langle \phi(x_0) \rangle$



Berges, Borsanyi, Sexty, Stamatescu, 2007





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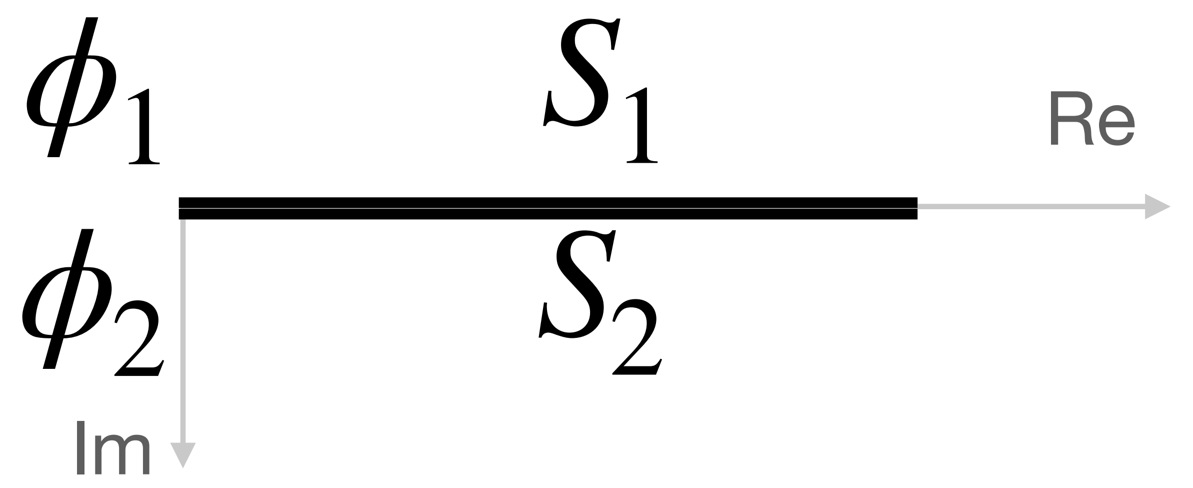

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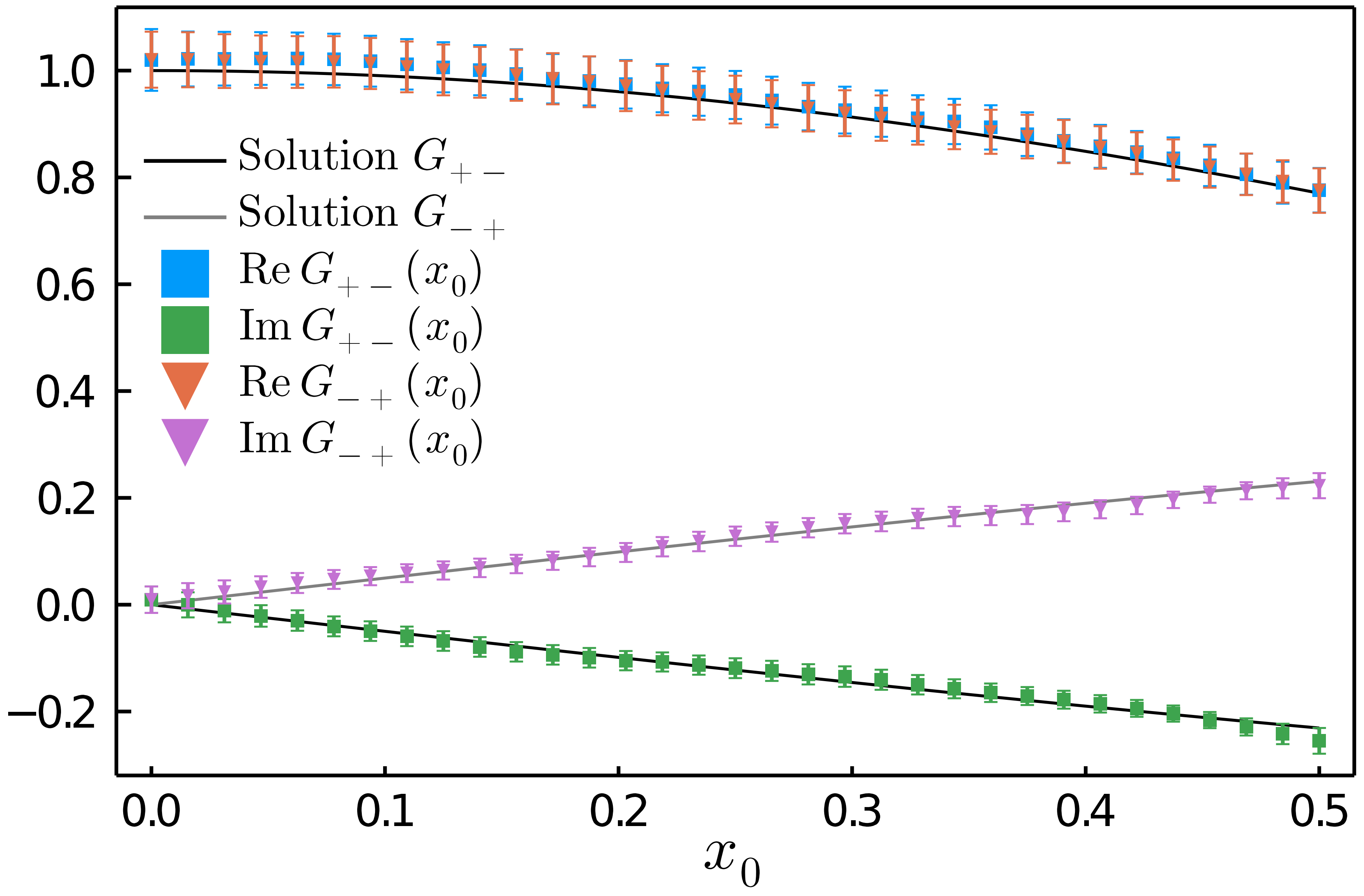
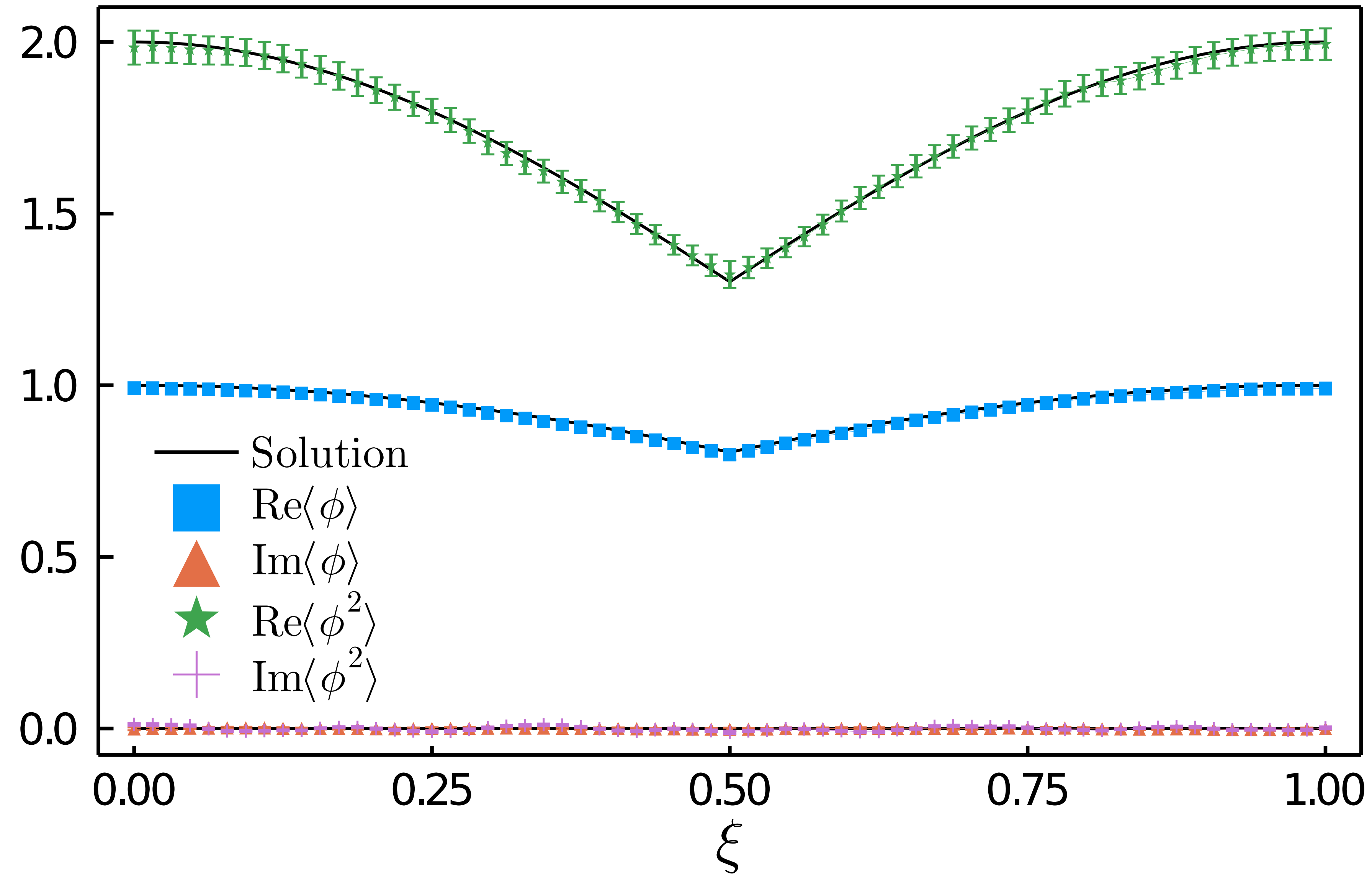




Real-time complex Langevin

Complex Langevin equation

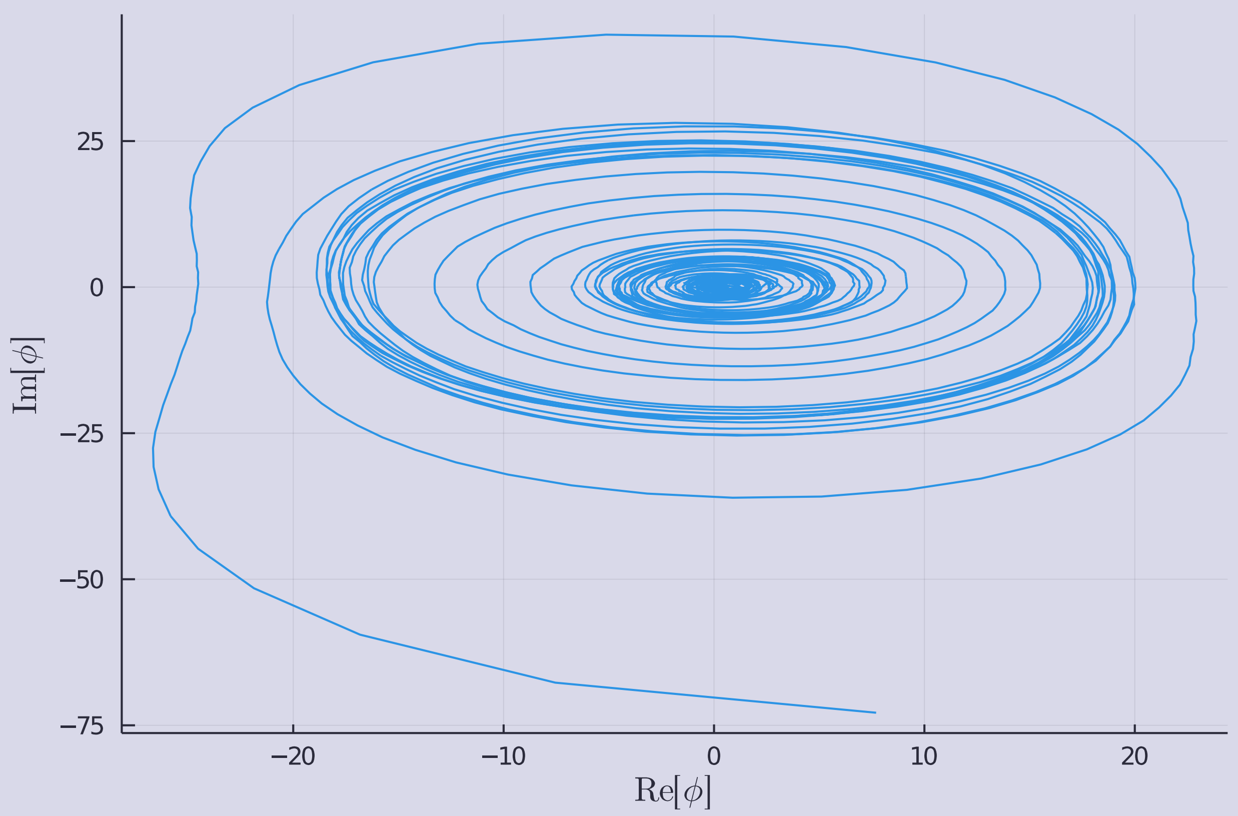
$$\boxed{\frac{d\phi}{d\tau_L} = i\frac{\delta S[\phi]}{\delta \phi(x)} + \eta(x, \tau_L)}$$

Numerics now under control

Stable solver

Get control of the numerics

Real-time complex Langevin = Stiff problem



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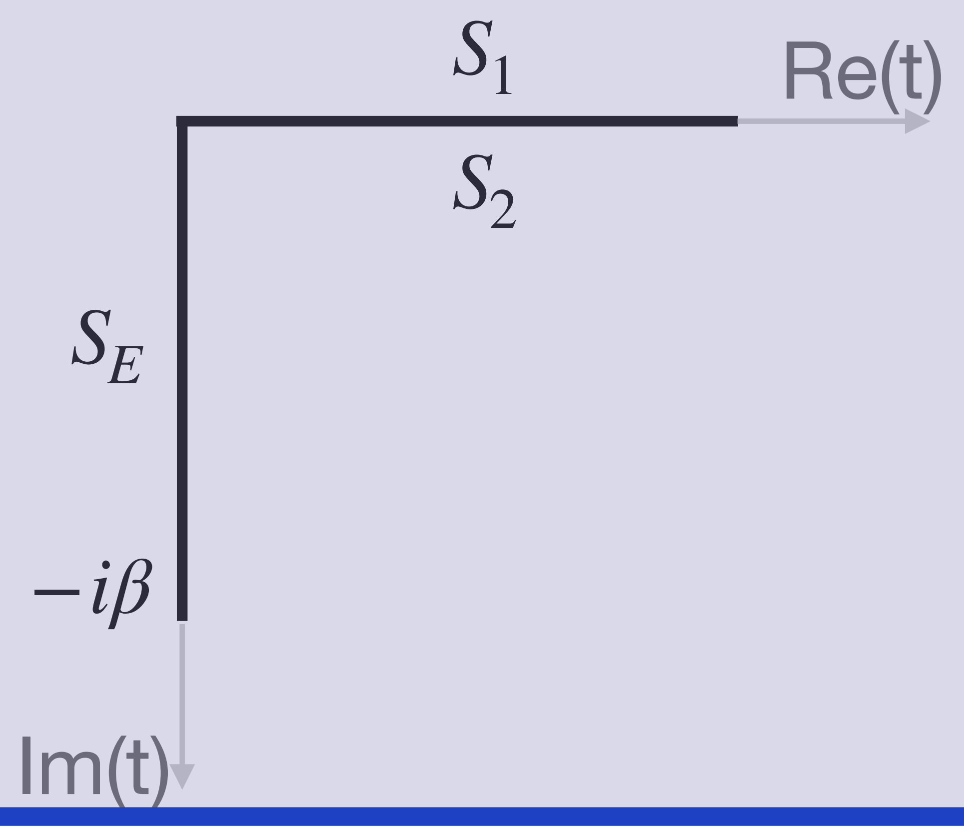

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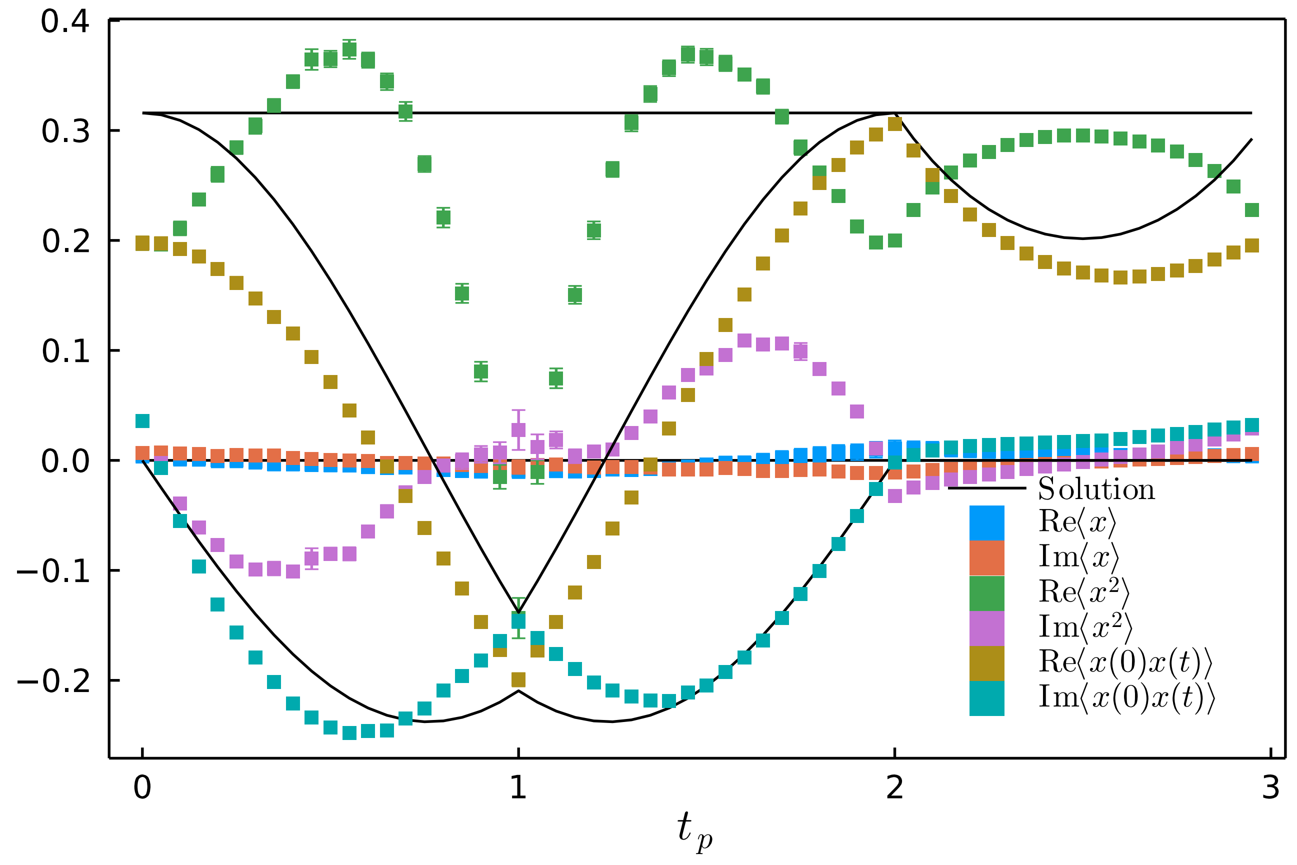
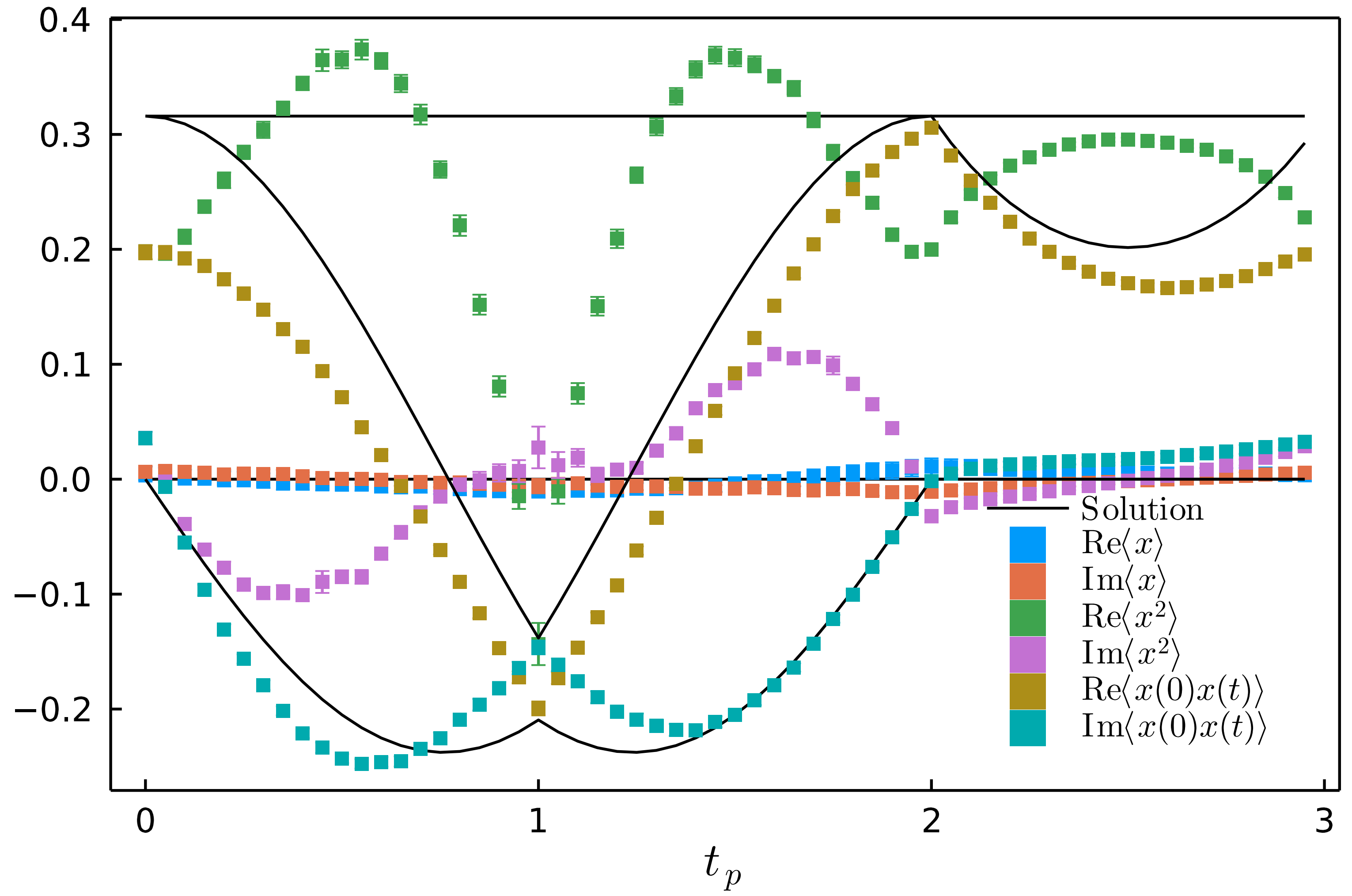


Convergence to the wrong solution problem

Problem of wrong convergence

- Taking $\Delta\tau \to 0$ (Langevin time-step) not solution
- Eigenvalues of Fokker-Planck equation
  - Fokker-Planck equilibrium distribution not e^{iS}



- Fixing the problem
  - Boundary terms, Gauge Cooling, Dynamical stabilisation

$$-D^a_{x,\nu}S[U] \to -D^a_{x,\nu}S[U] + i\alpha_{DS}M^a_x$$

  - Modification to CLE
    - Coordinate Transformations
    - Kernels

Kernelled complex Langevin

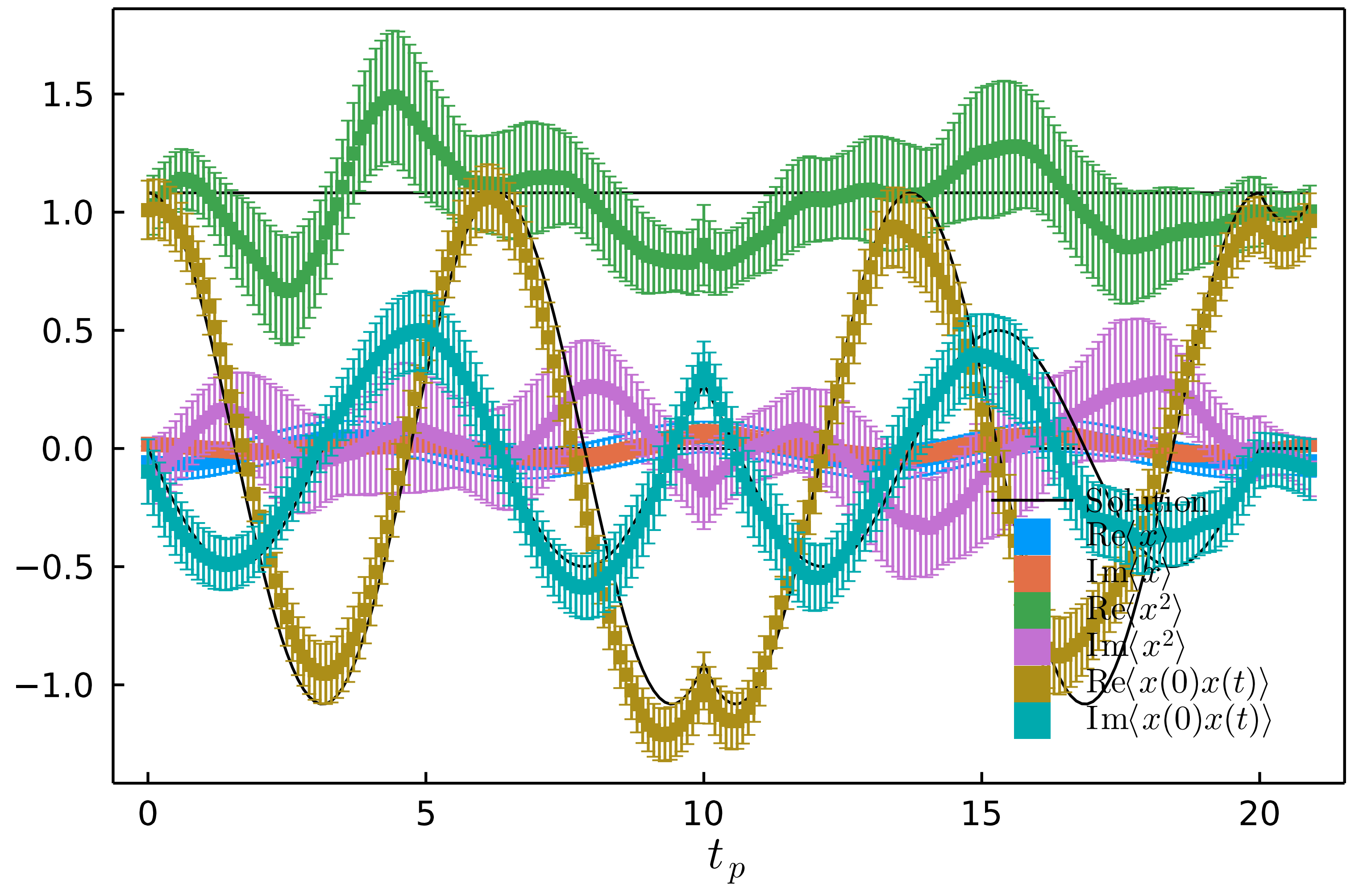
- Additional freedom in Fokker-Planck equation; regain same equilibrium distribution
- Kerneled Langevin $$d\phi = \left(-K[\phi]\frac{\partial S[\phi]}{\partial \phi} + \frac{\partial K[\phi]}{\partial \phi} \right) d\tau_L + \sqrt{K[\phi]}dW$$
- Free theory propagator:

$$i\frac{\partial S}{\partial \phi} = iM\phi, \quad K = iM^{-1}, \quad K\, i\frac{\partial S}{\partial \phi} = -\phi$$

$$d\phi = -\phi + \sqrt{iM^{-1}}dW$$

Free theory

No kernel



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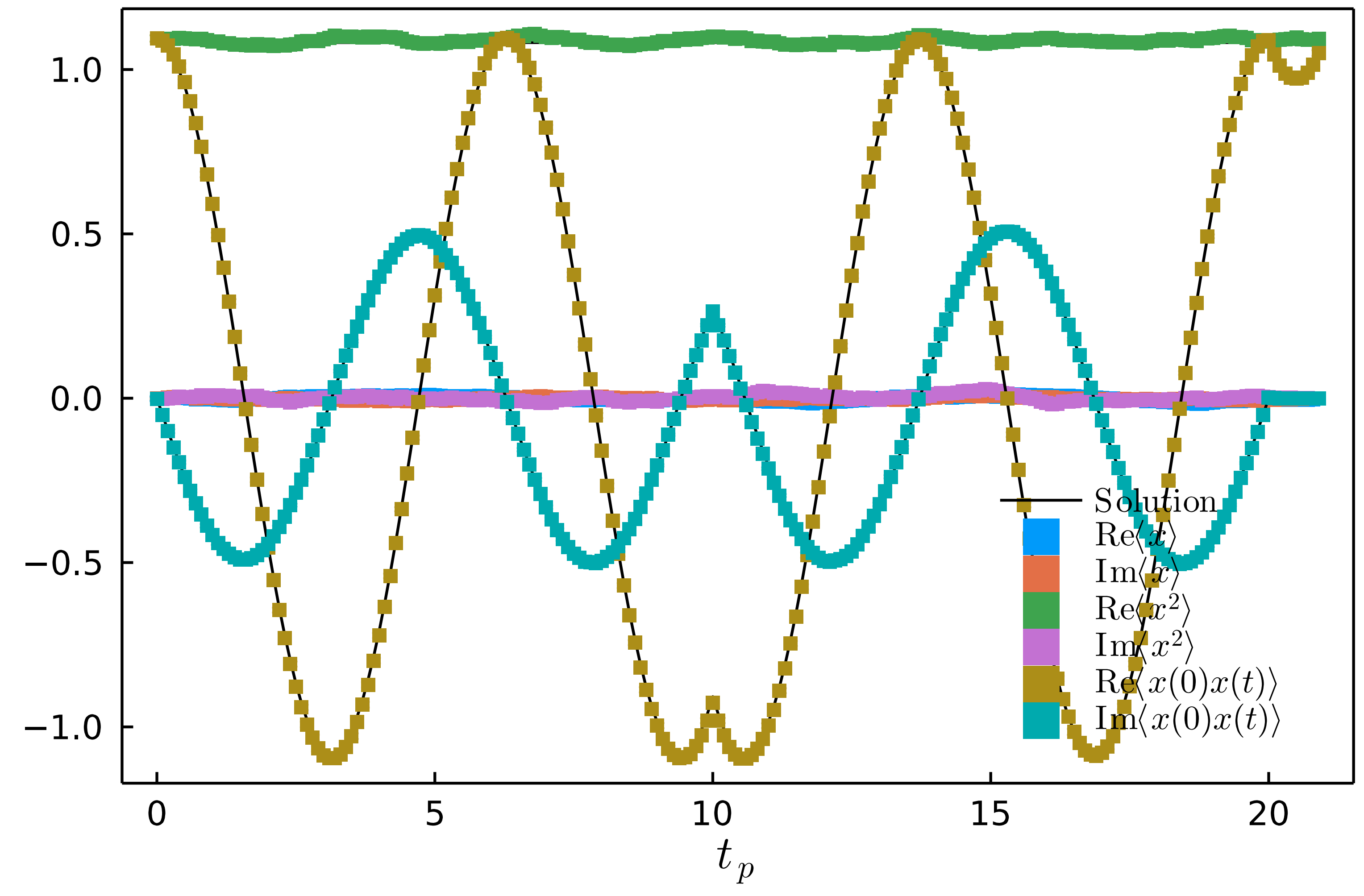

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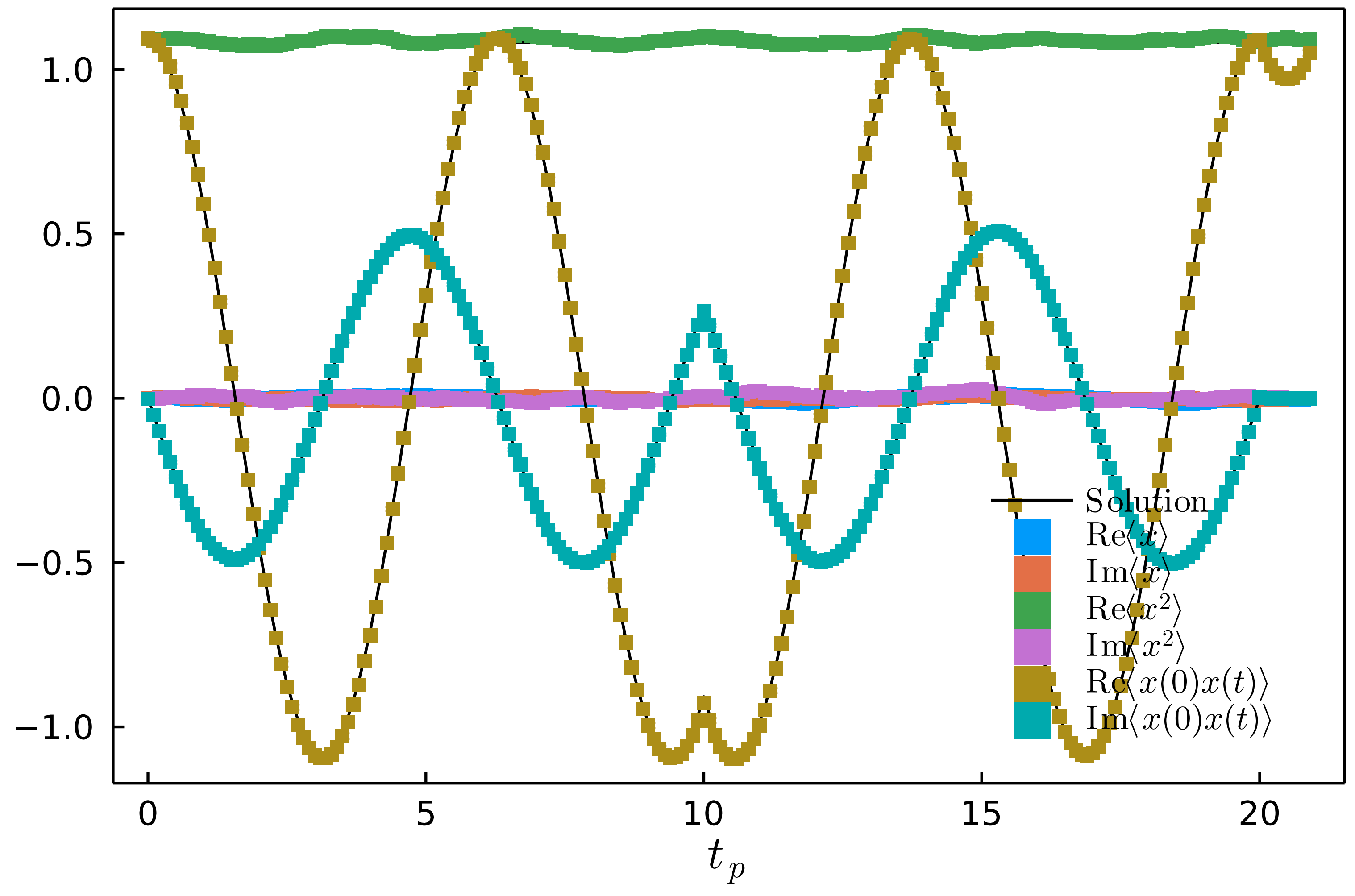
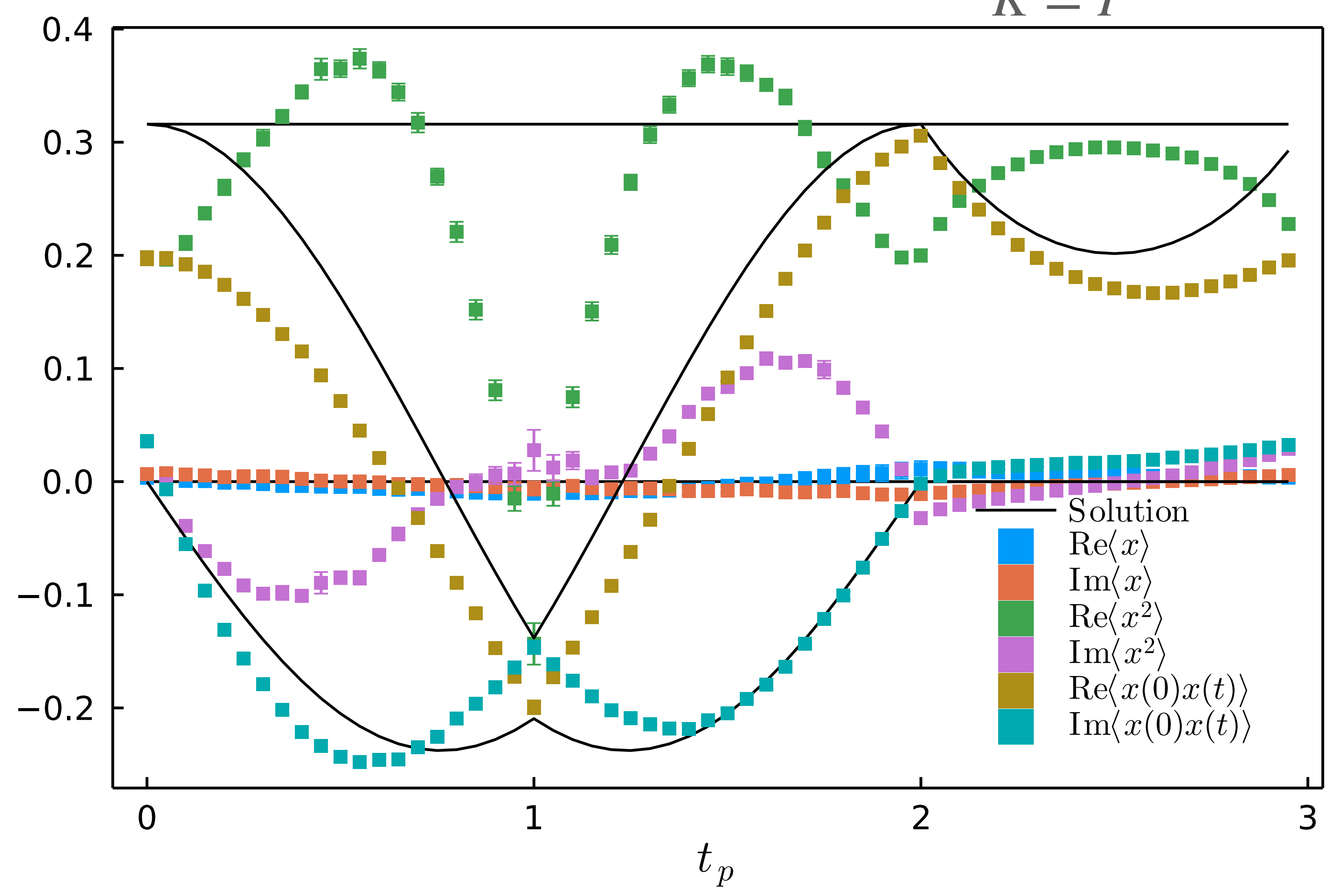


Interactive theory $K = I$



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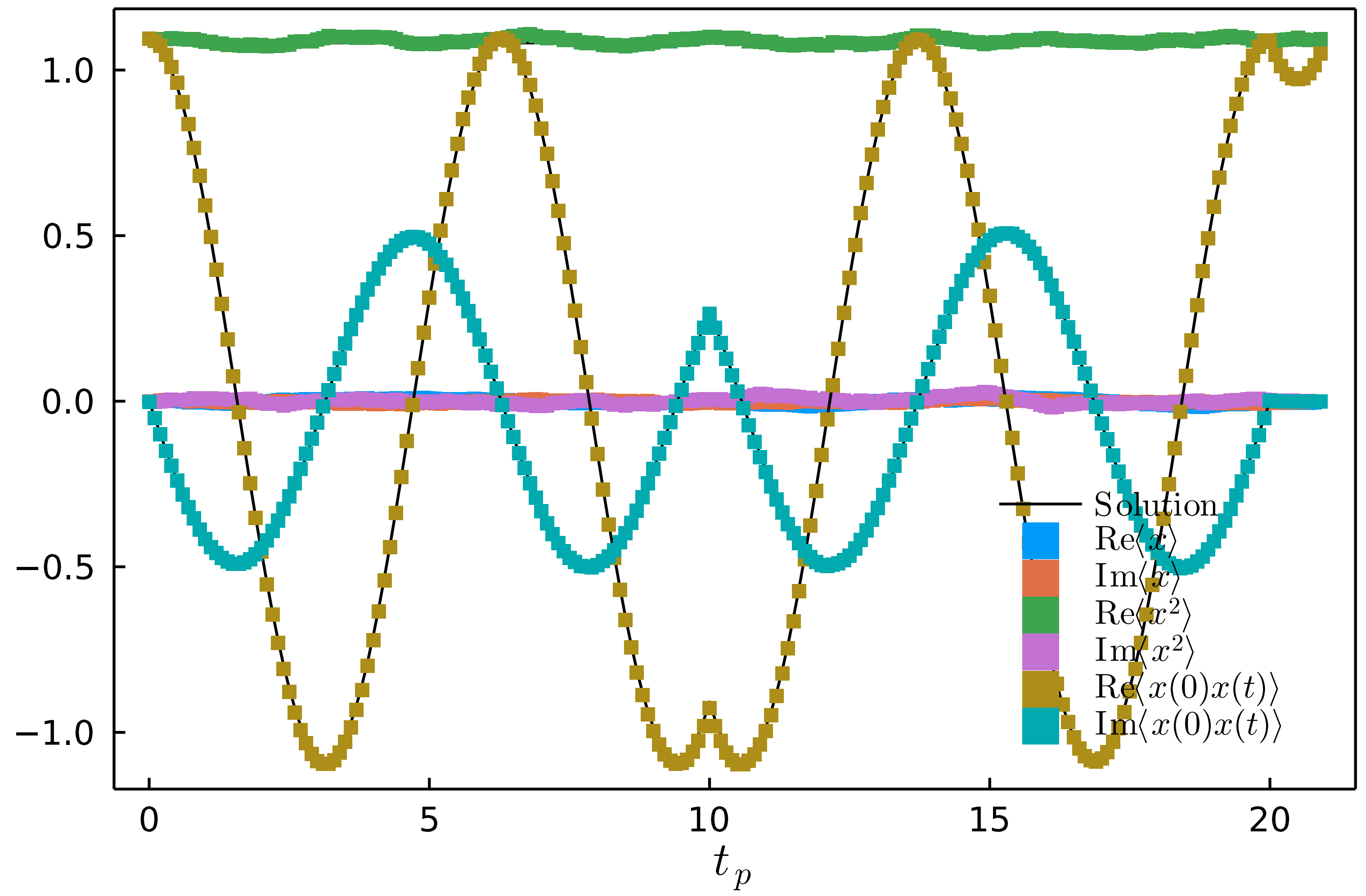

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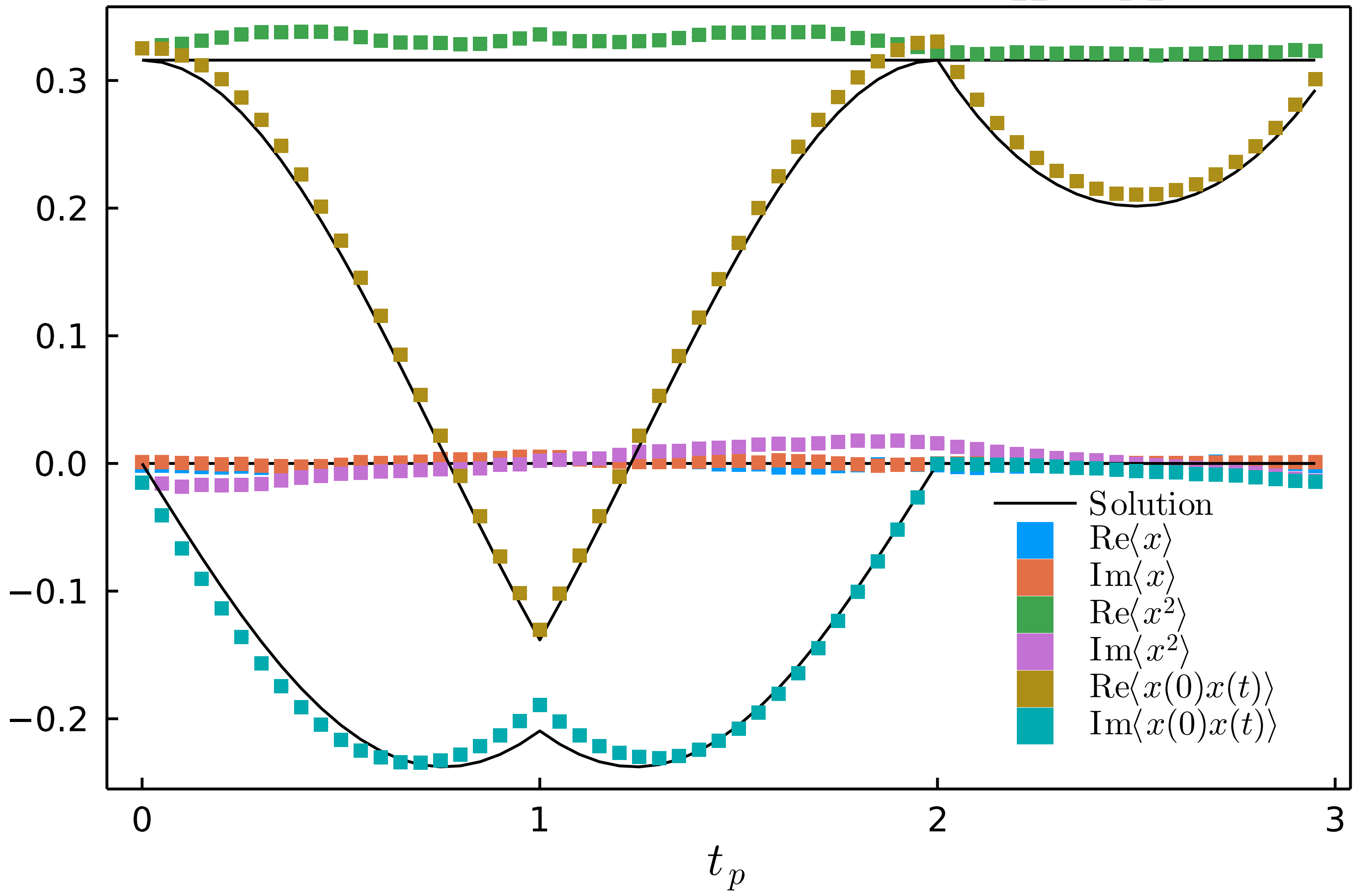

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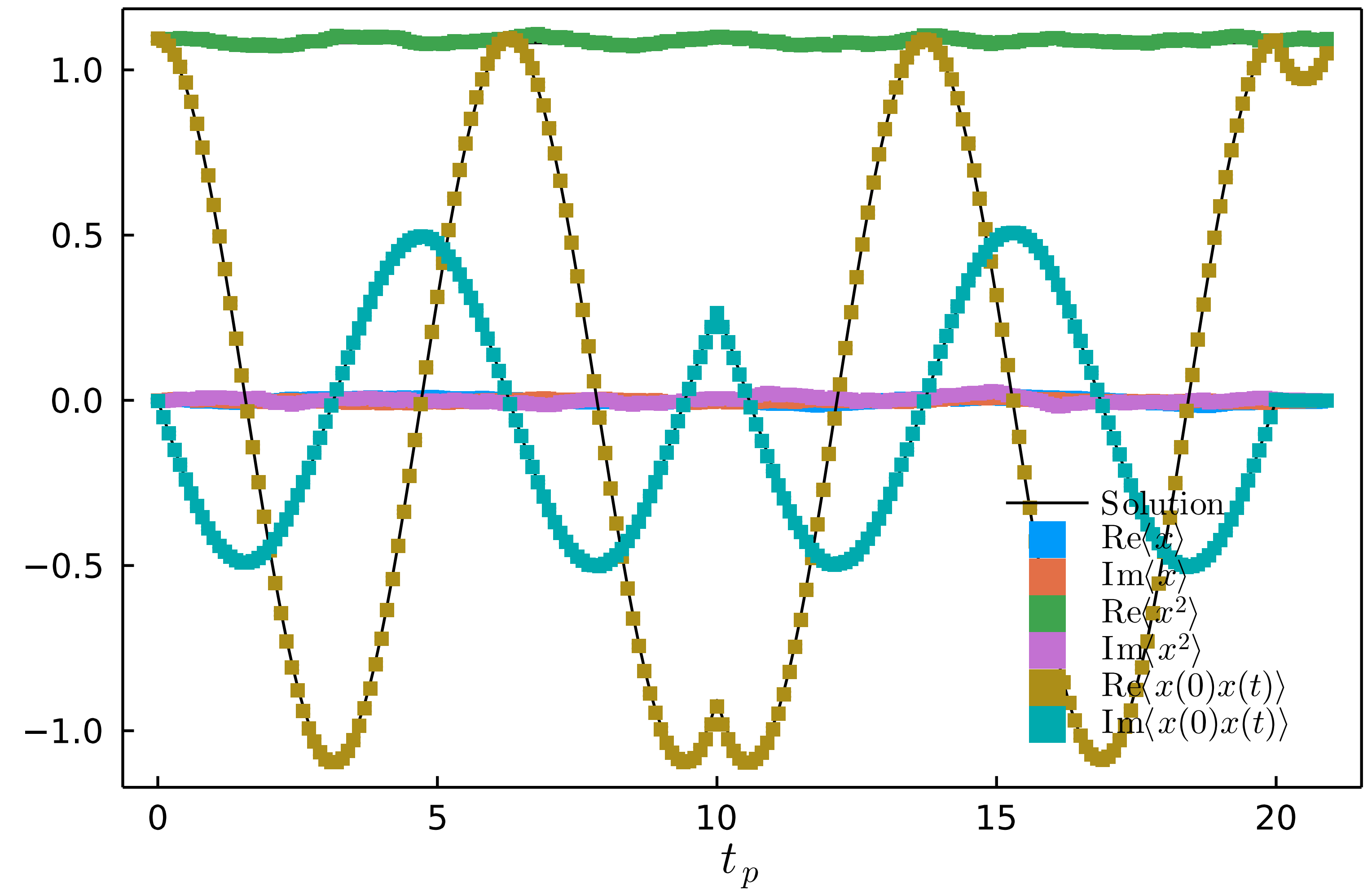
Systematic scheme to construct kernels

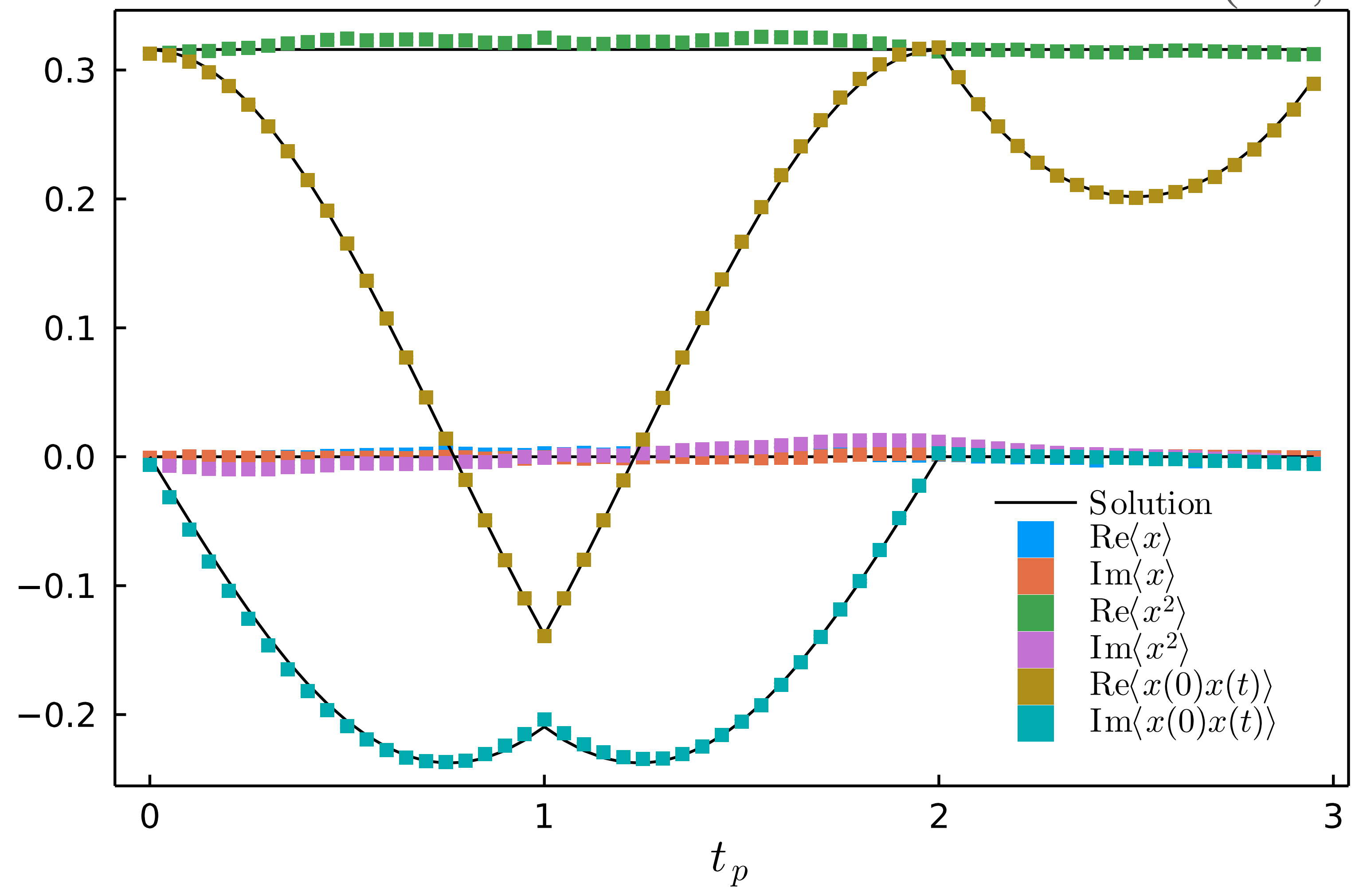
Free theory

$K = M^{-1}$



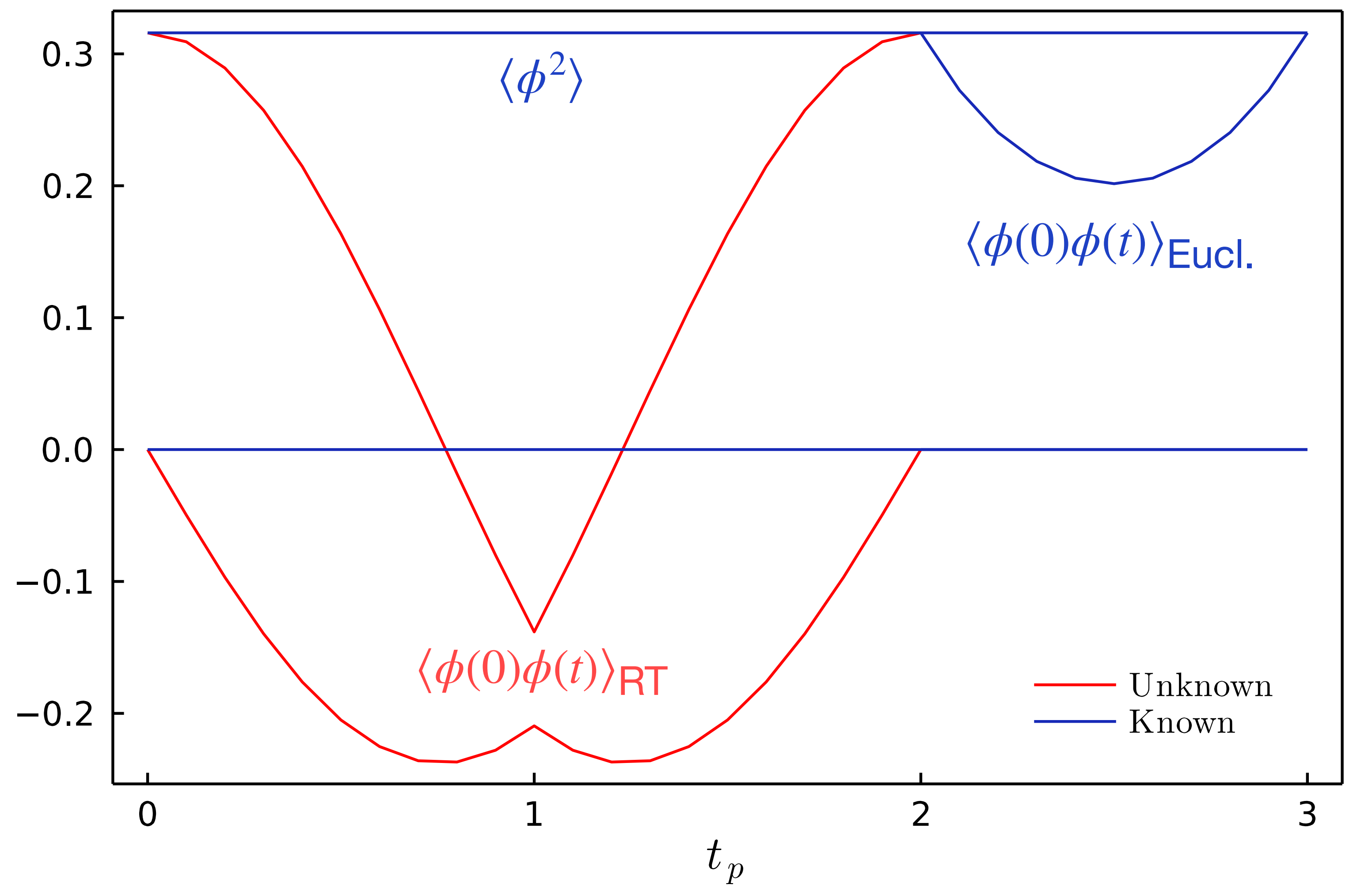
Interactive theory

$K = M^{-1}(0.8,1.8)$



Construct kernel

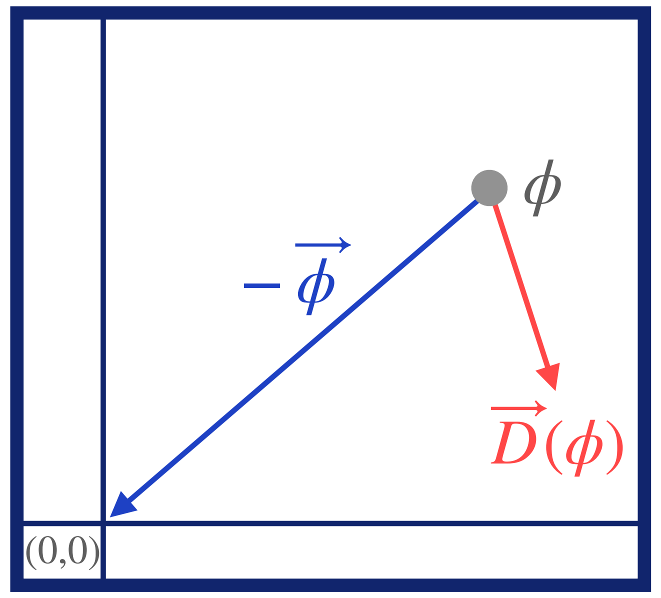
- Can we find a kernel by using prior knowledge about the Complex Langevin and the model
- Known information
  - L^{Sym}: Symmetries of the model, ex. $\langle \phi^n \rangle = $ const. (known from Euclidean simulation)
  - L^{Eucl}: Euclidean part of real-time contour
  - L^{BT}: There should be no boundary terms
- Minimising using the above loss functions require the derivative $\frac{d\phi}{dK}$ 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 ($D = K\dfrac{\delta S}{\delta \phi}$)

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



- 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: $\{\phi_i^k\}$

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

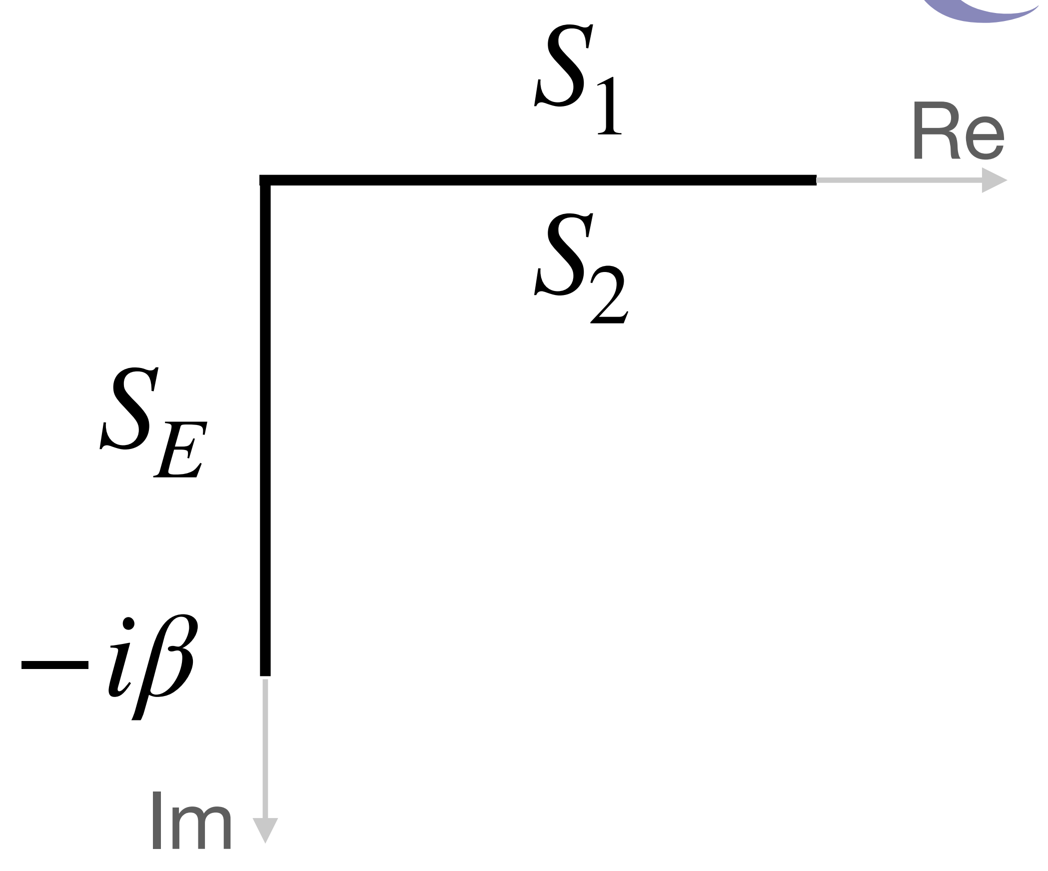
Update kernel based on gradient of the loss function $\nabla_K L_D\left(\{\phi^k\}\right)$

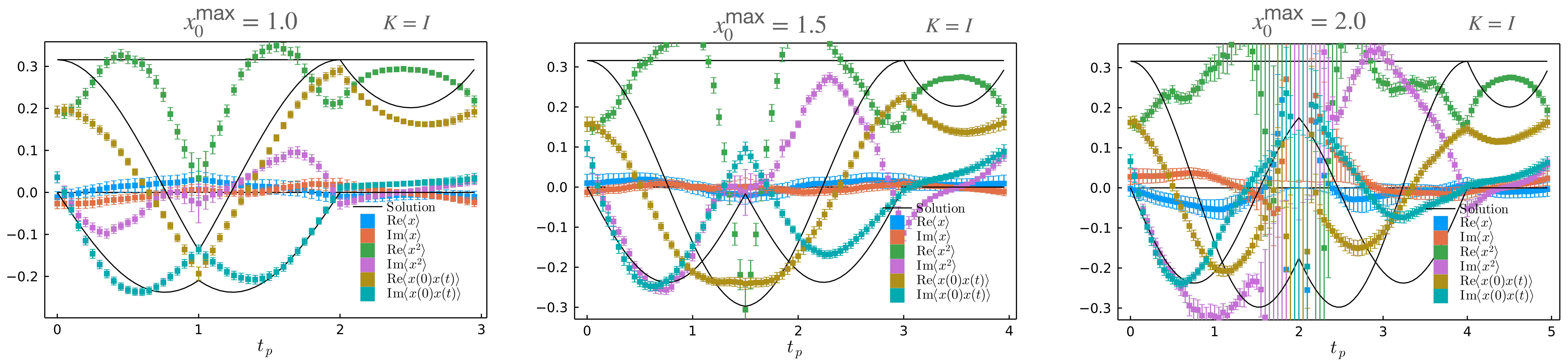
Measure L^{Sym}, L^{Eucl}, L^{BT}

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: $\dfrac{dS[\phi]}{d\phi} = 0$





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
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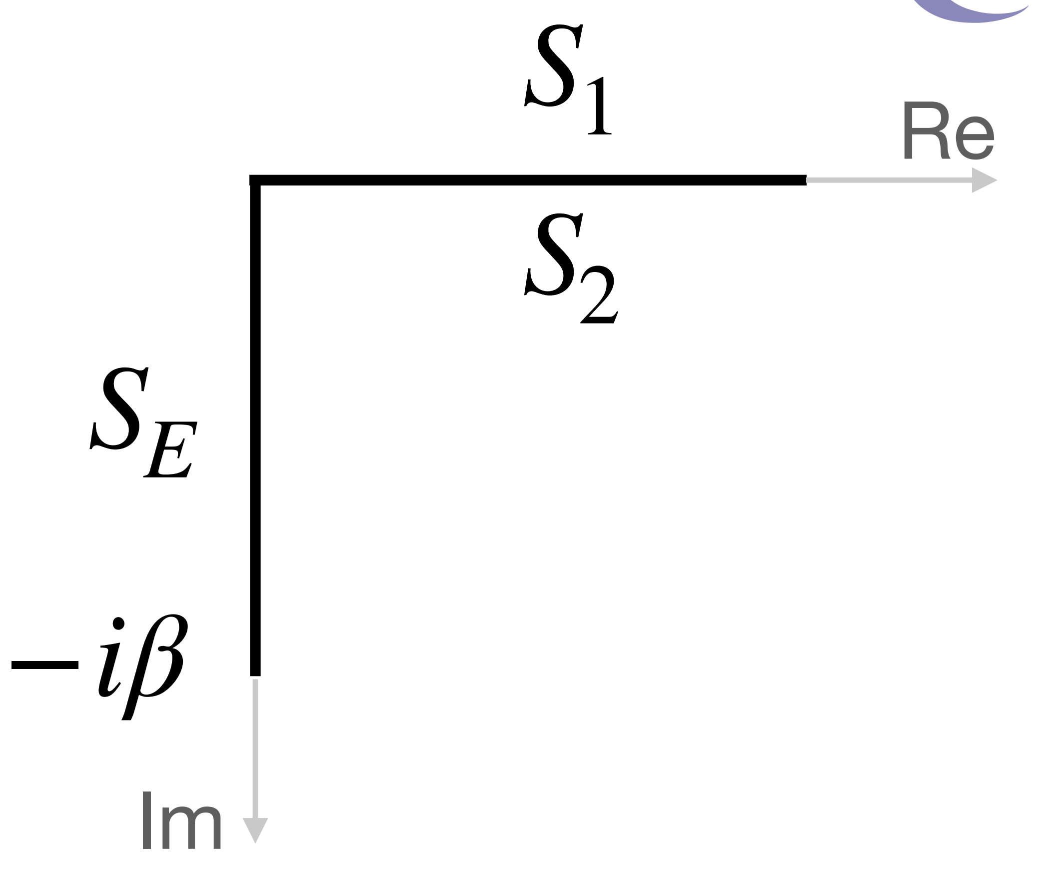

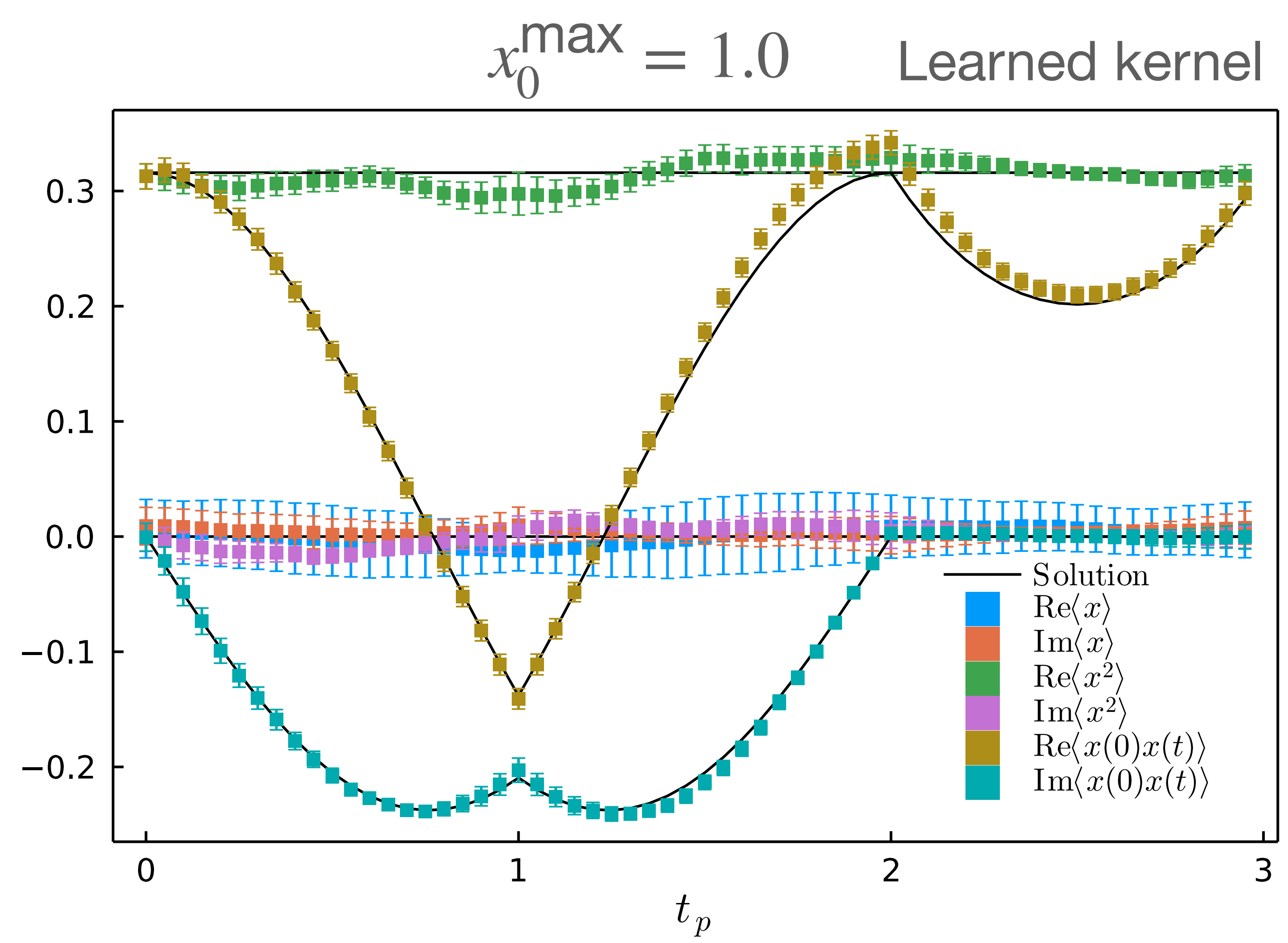

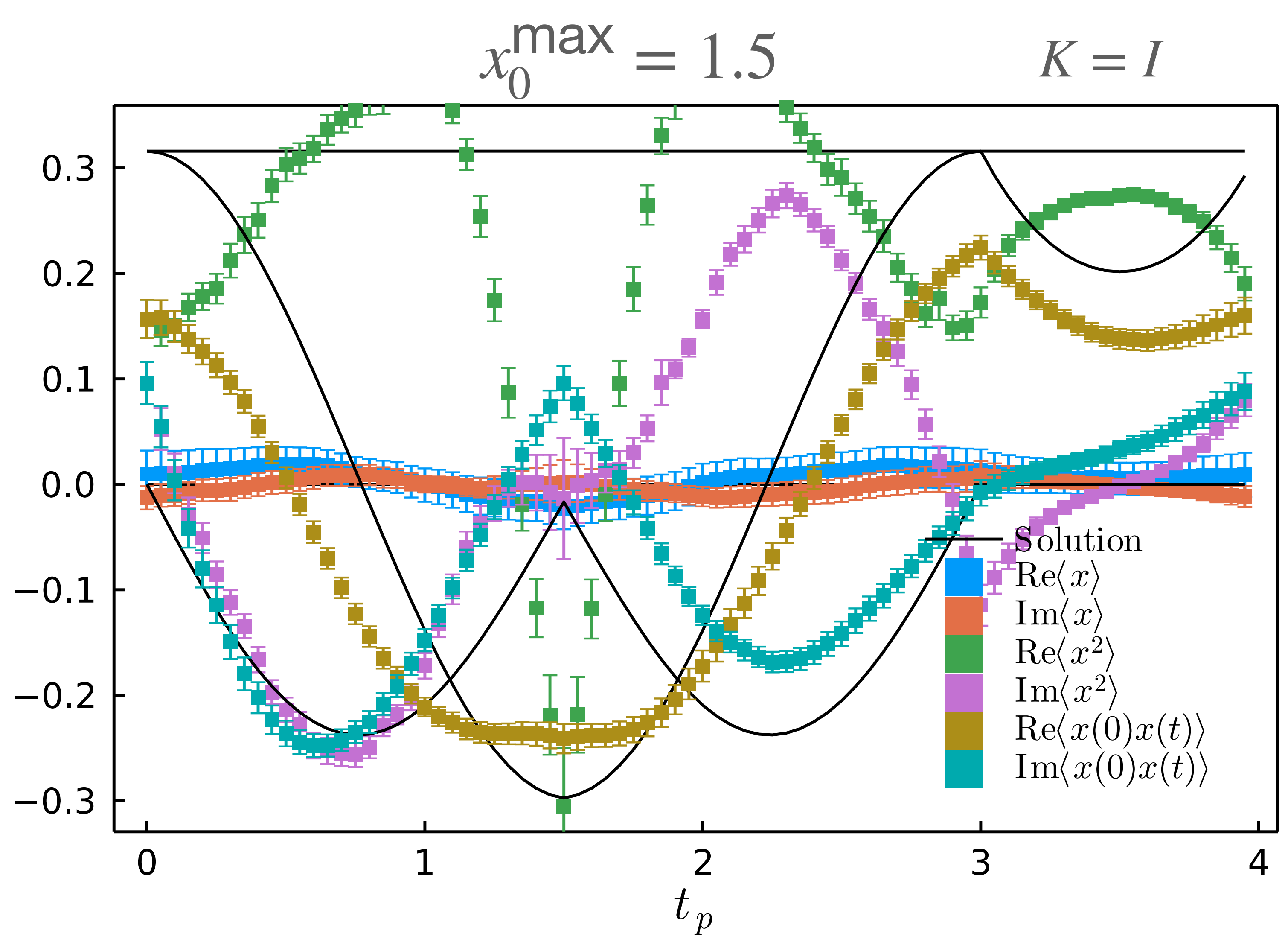

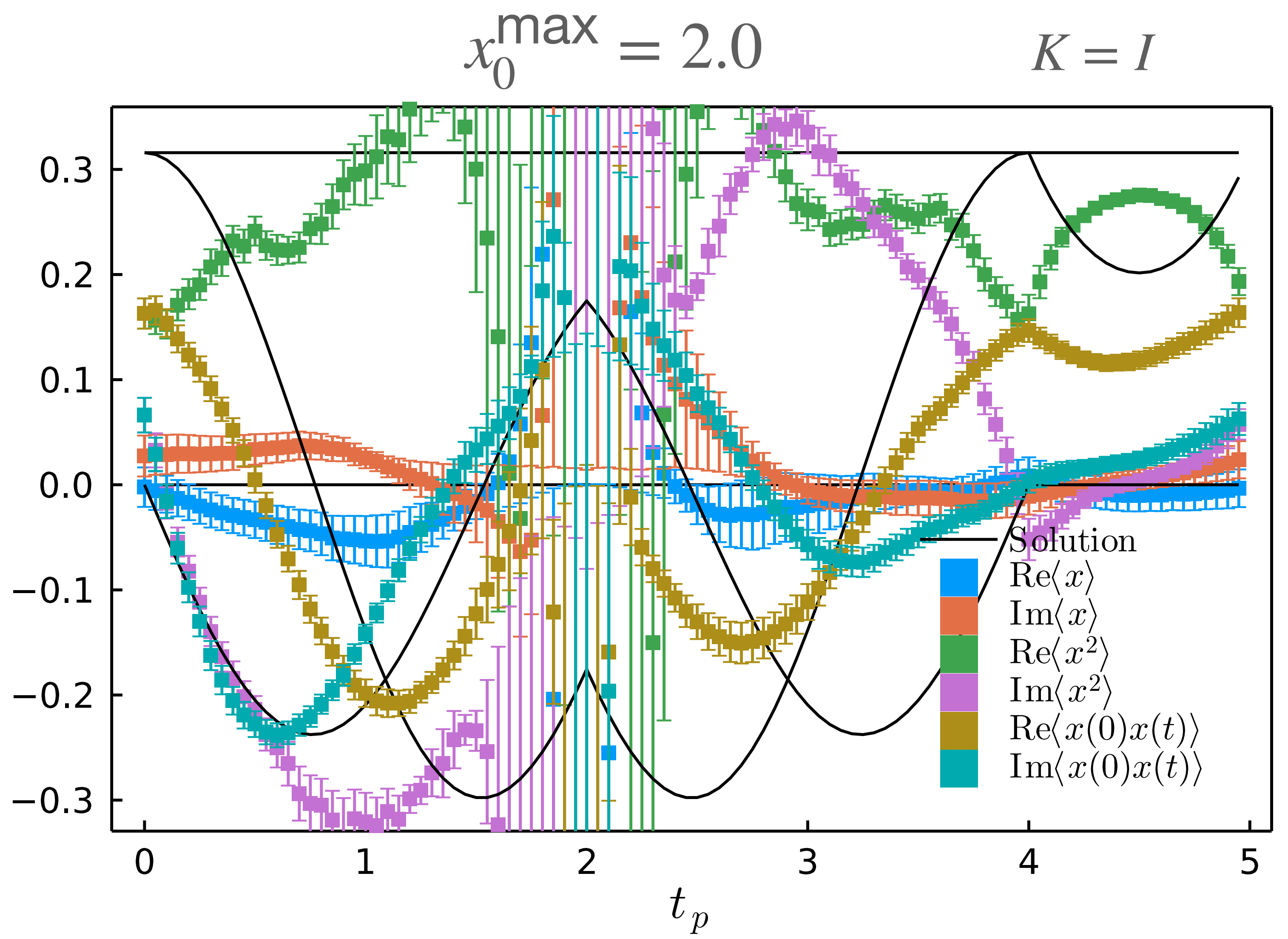

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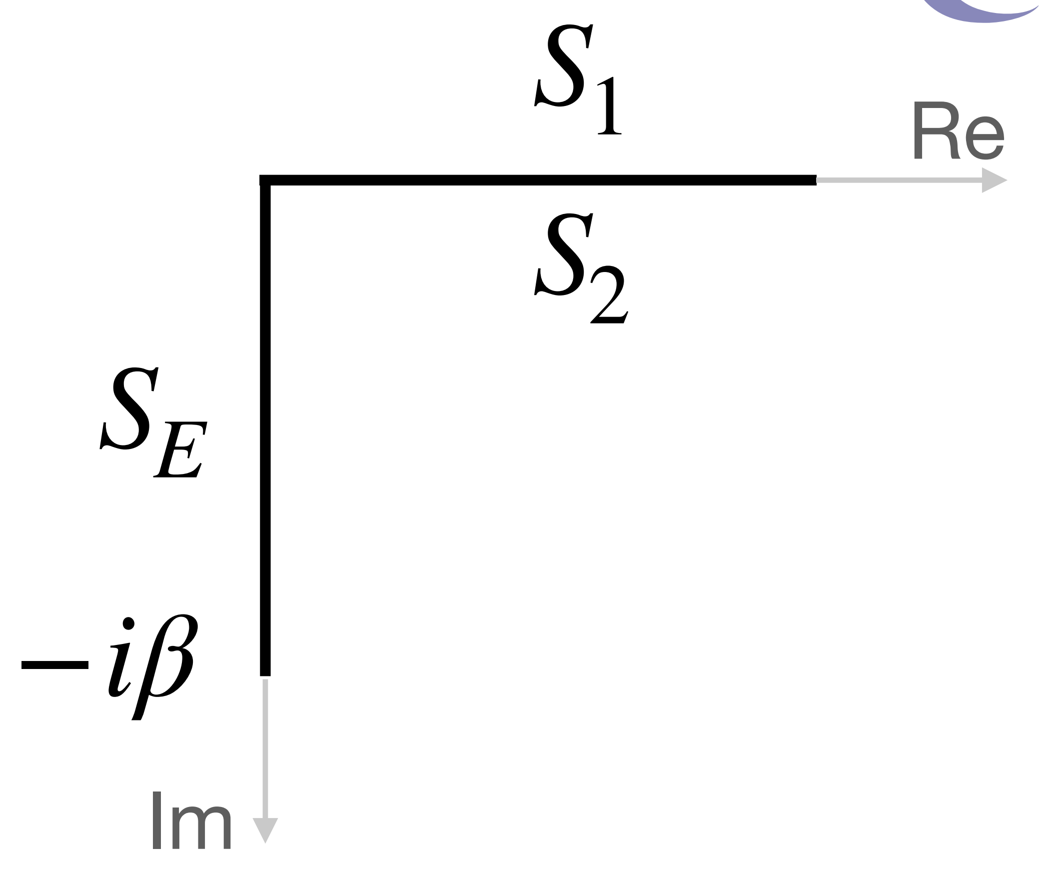

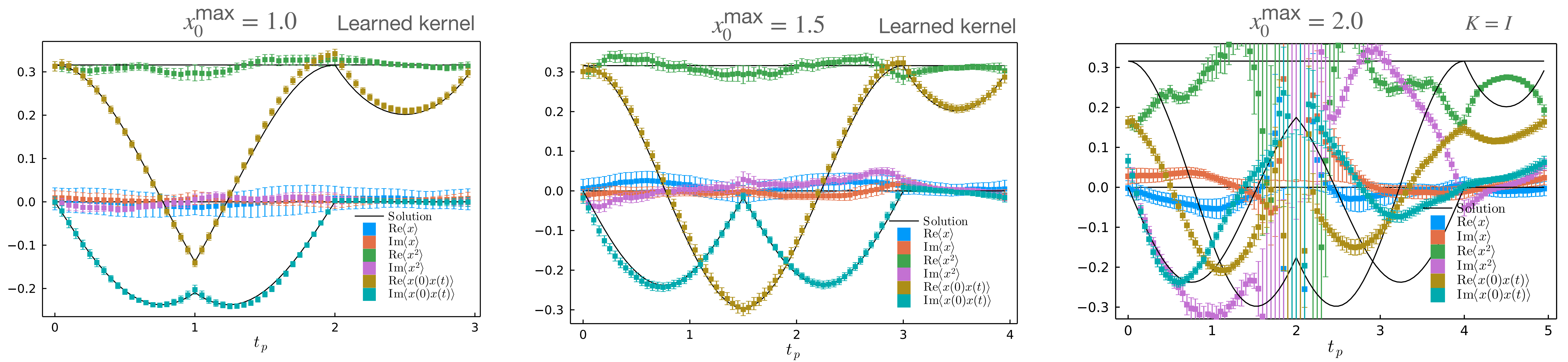

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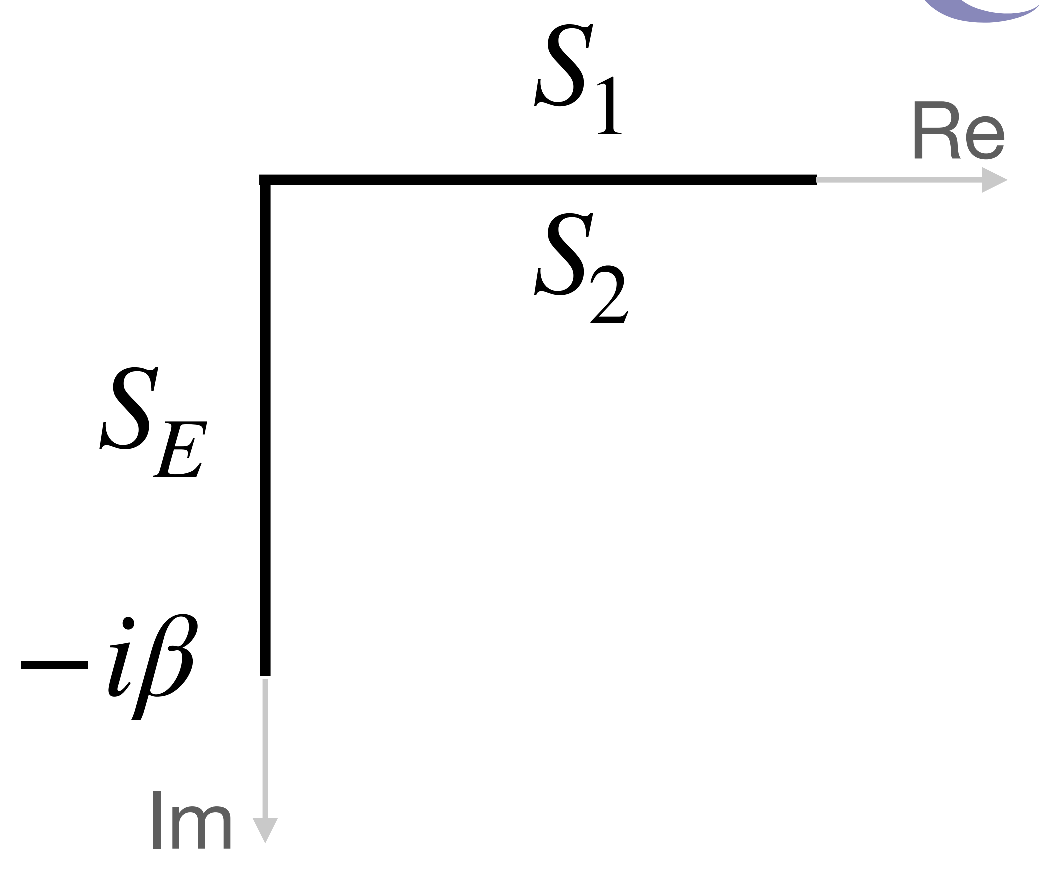
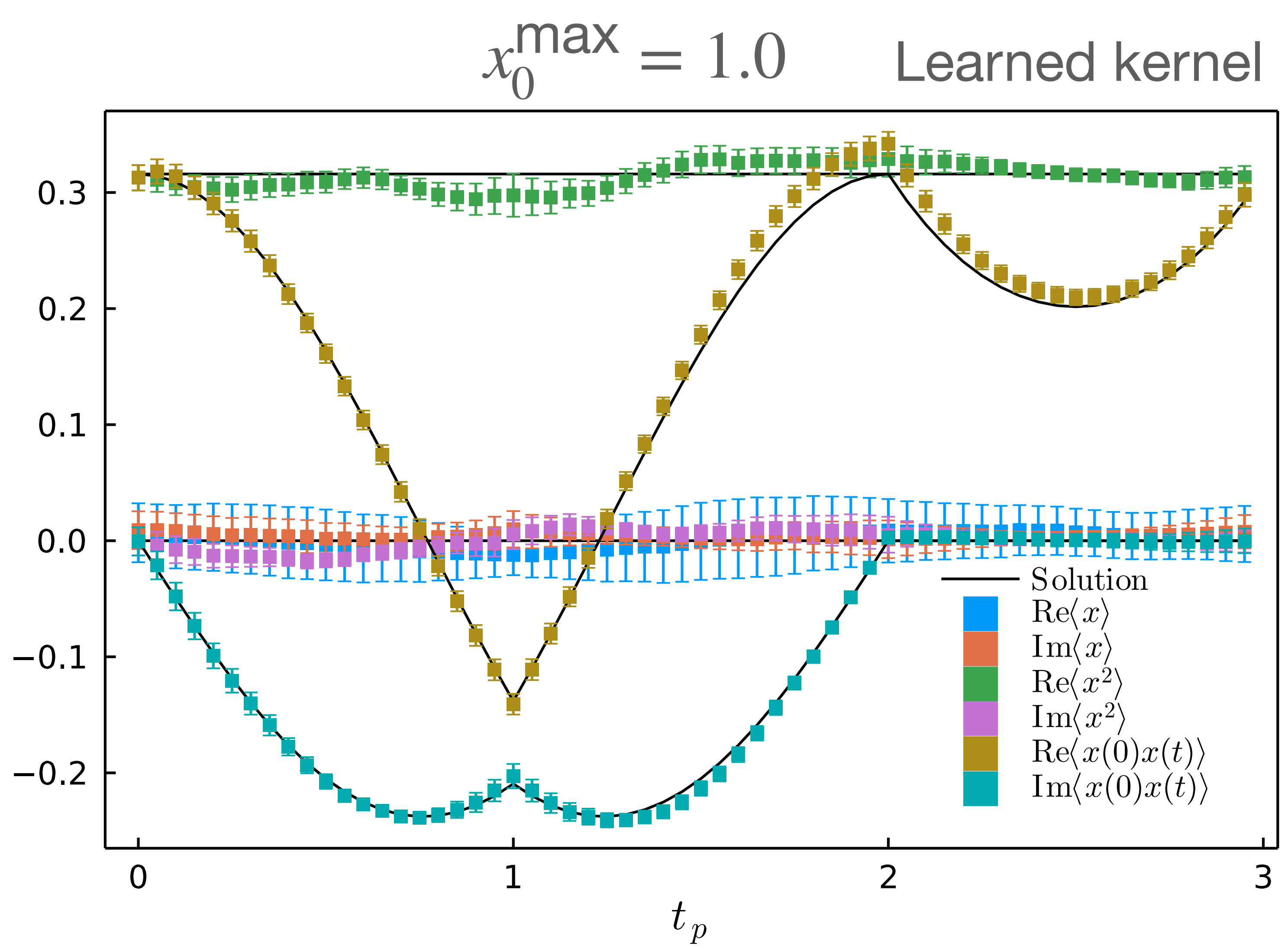
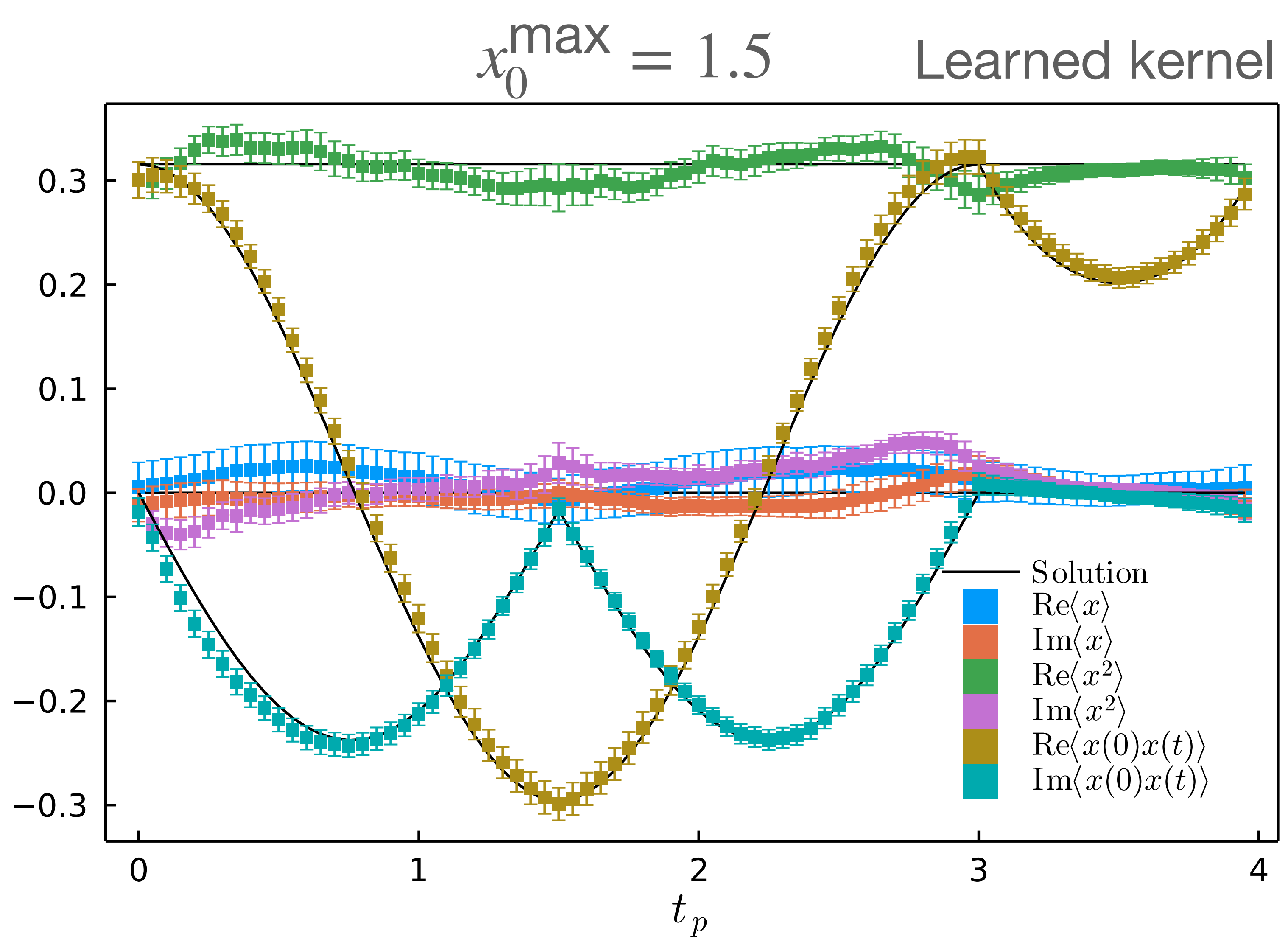
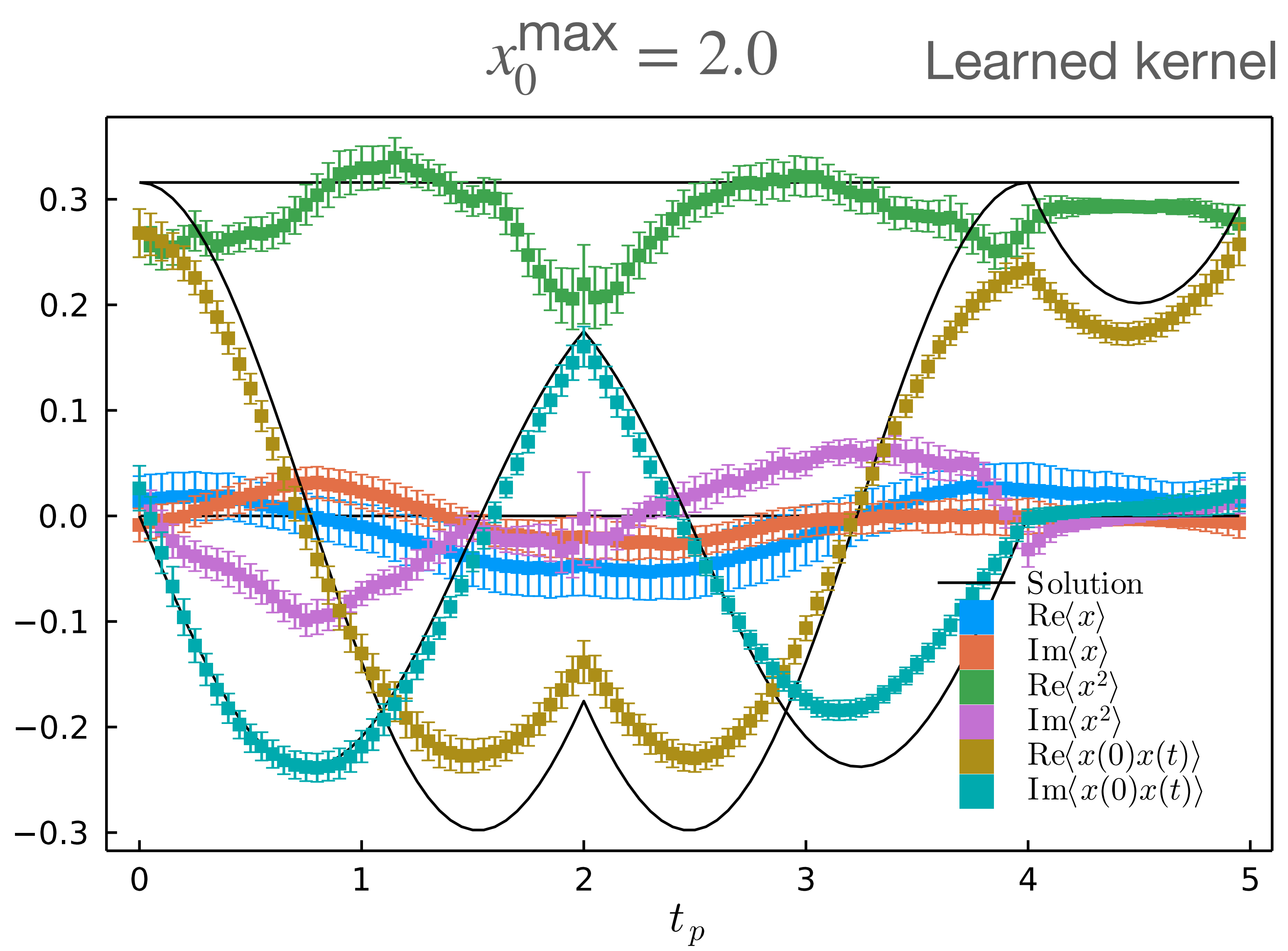




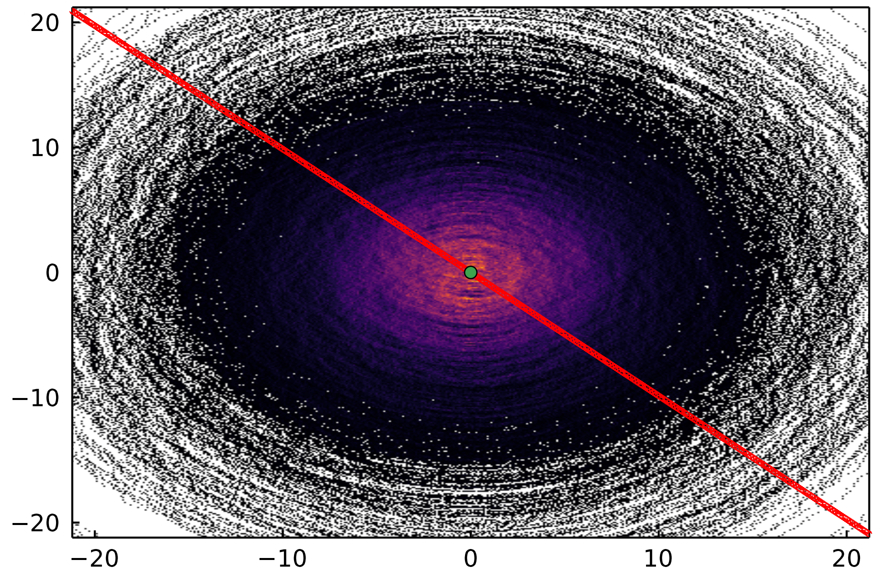




Connection with thimbles

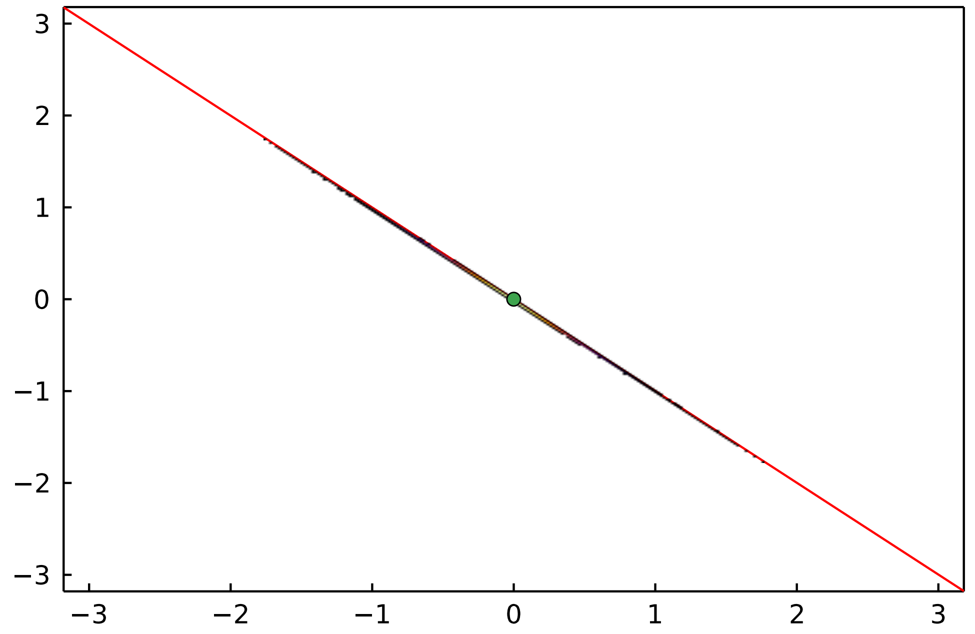
- Lefschetz thimbles: $\dfrac{d\phi}{d\tau} = \overline{\dfrac{dS[\phi]}{d\phi}}$
- Simplest model: $S = \dfrac{1}{2}ix^2$

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



Optimising L_D=0

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



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

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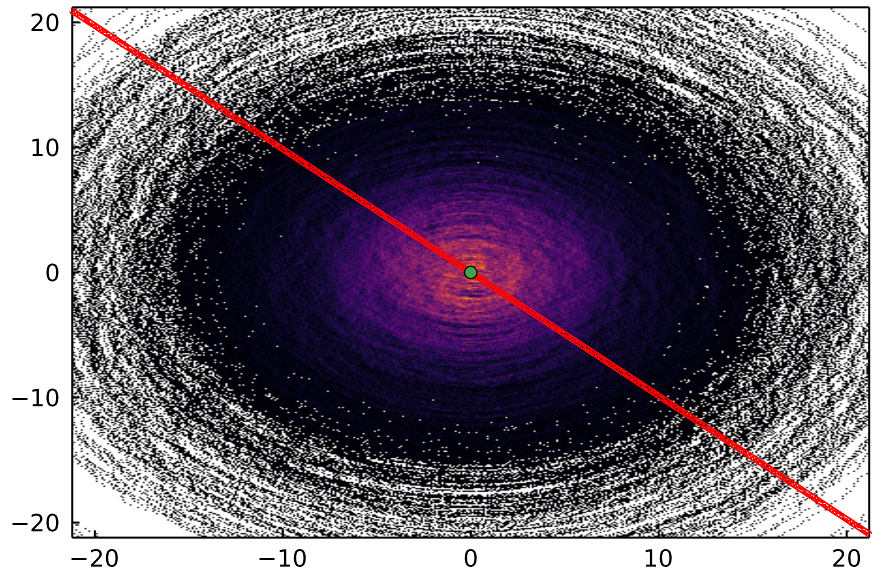

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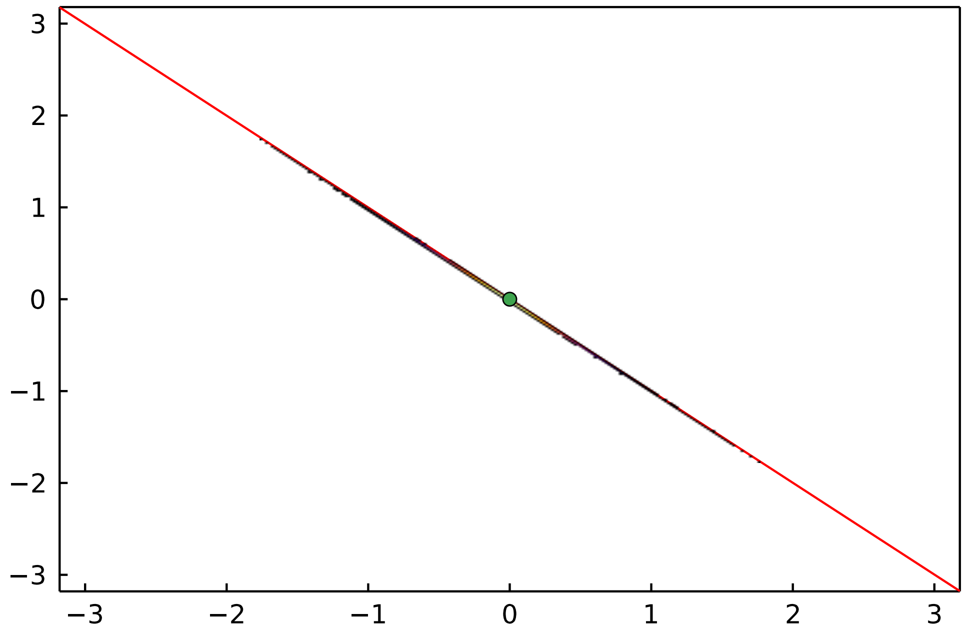

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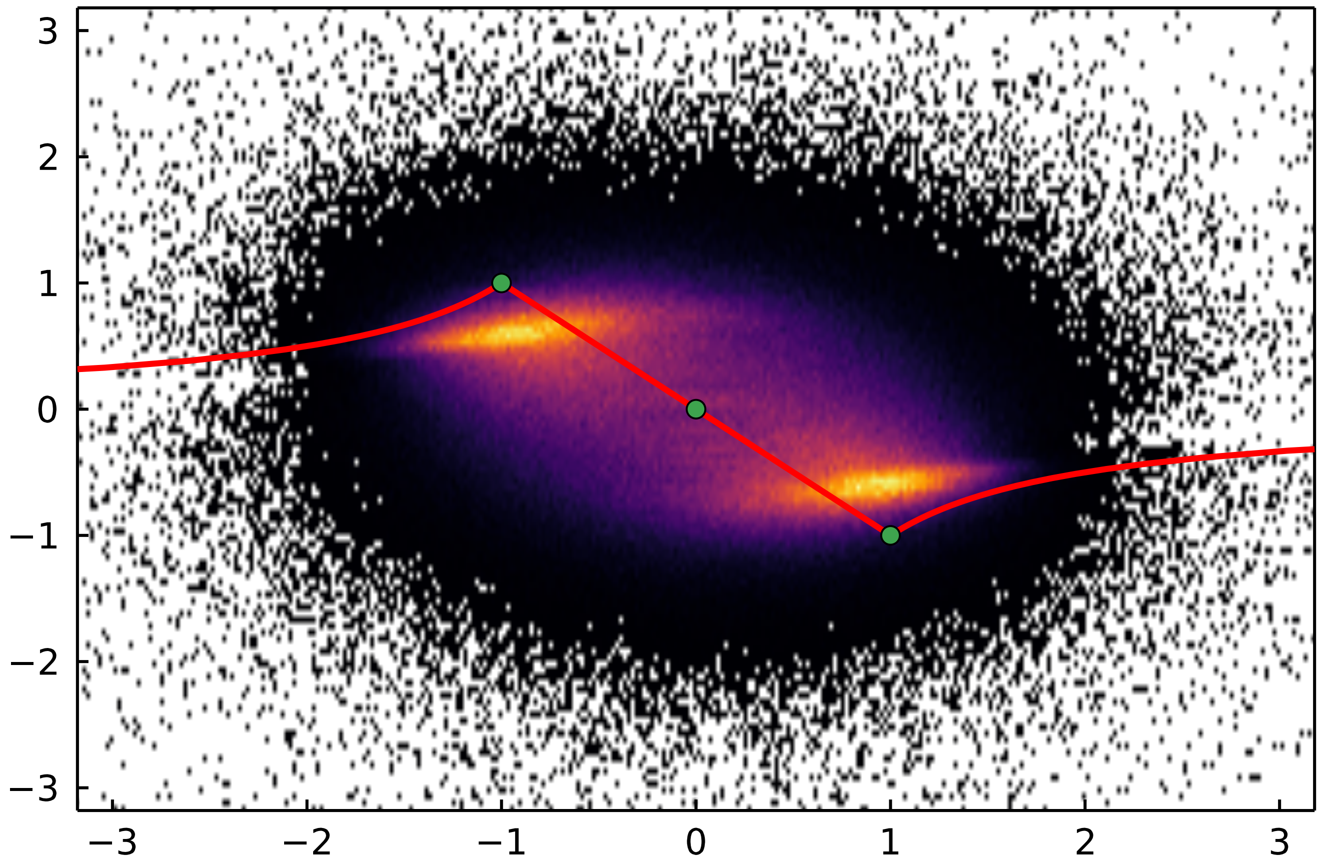
- Models with more than one critical point $S = 2i\phi^2 + \dfrac{1}{2}\phi^4$



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

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

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

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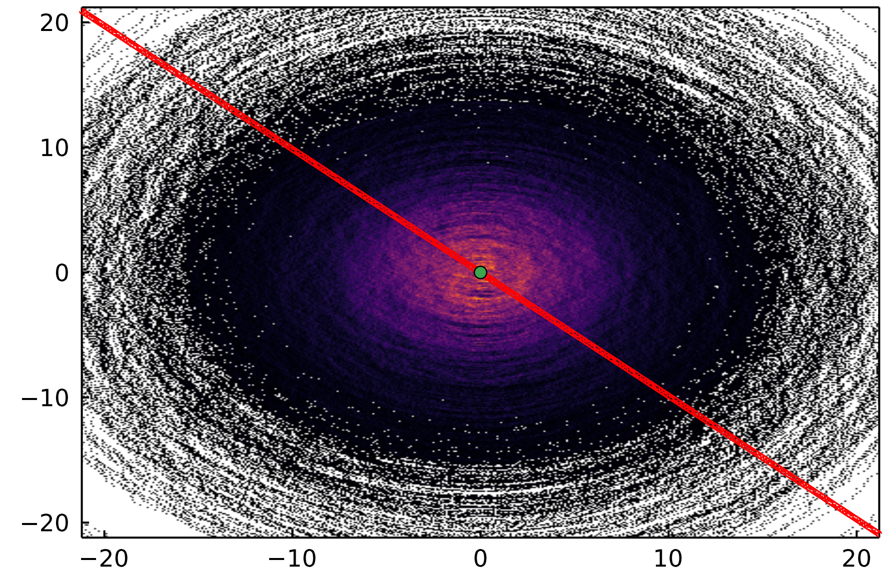

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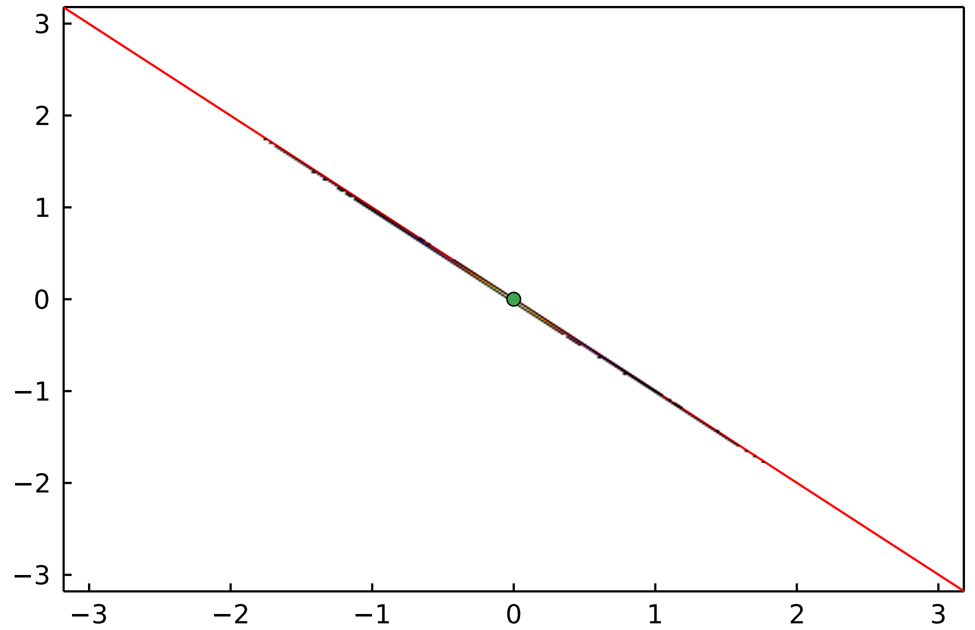

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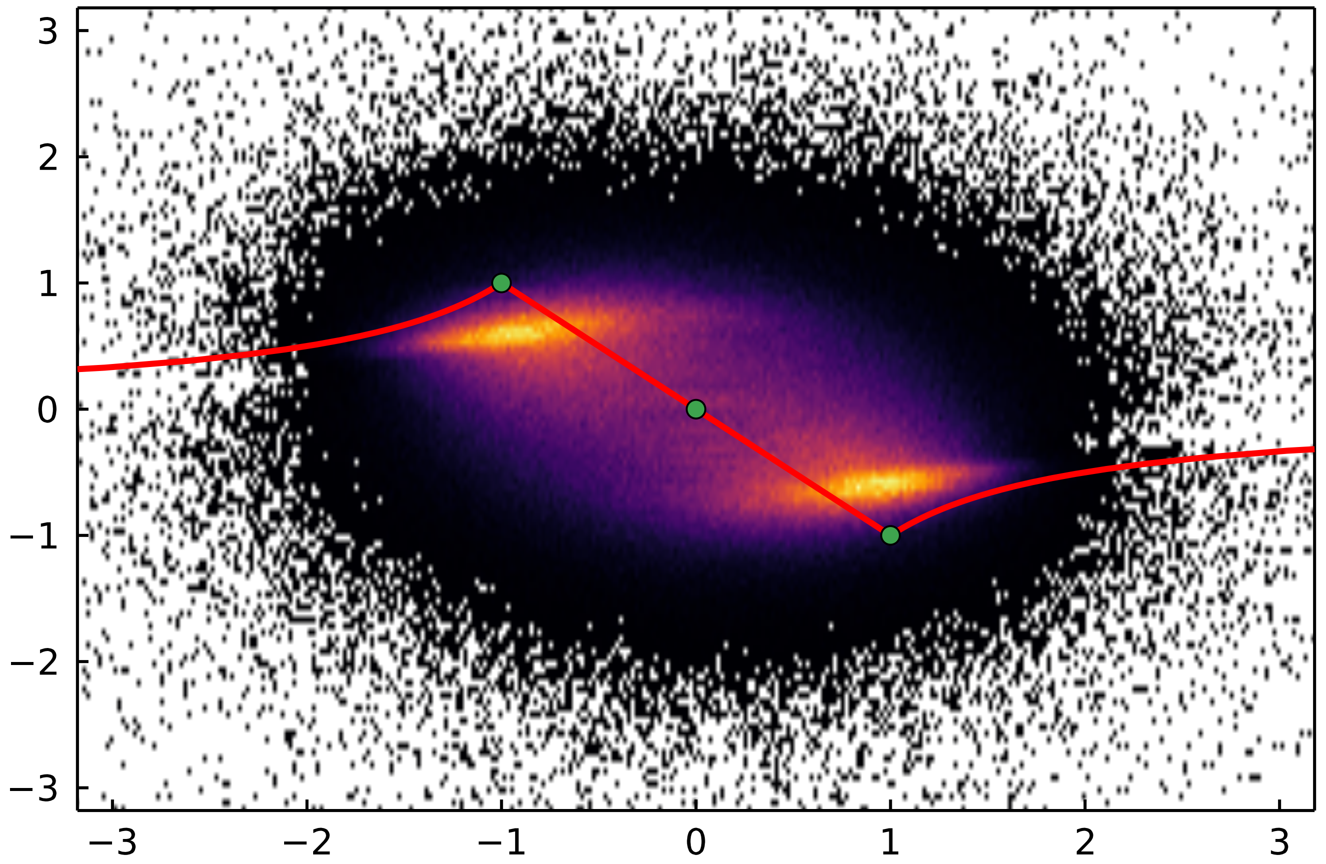

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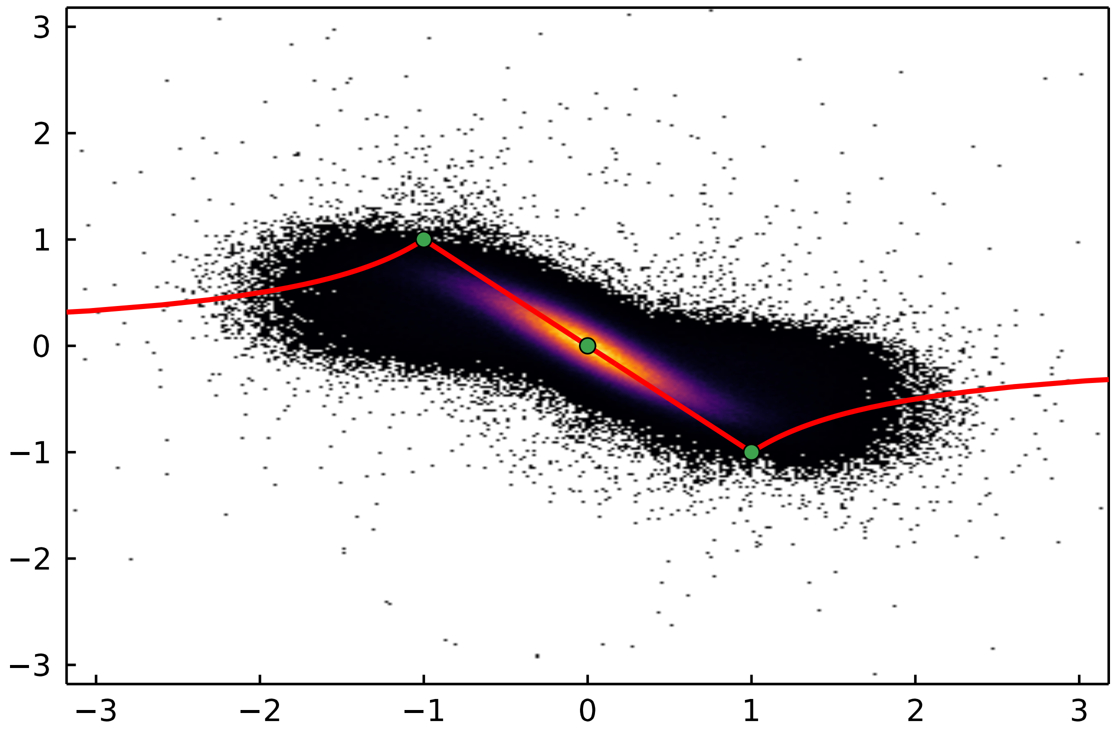
Optimising L_D for a constant kernel $K = e^{i\theta}$

Two minimas

Fokker-Planck eigenvalues

Converges to correct solution

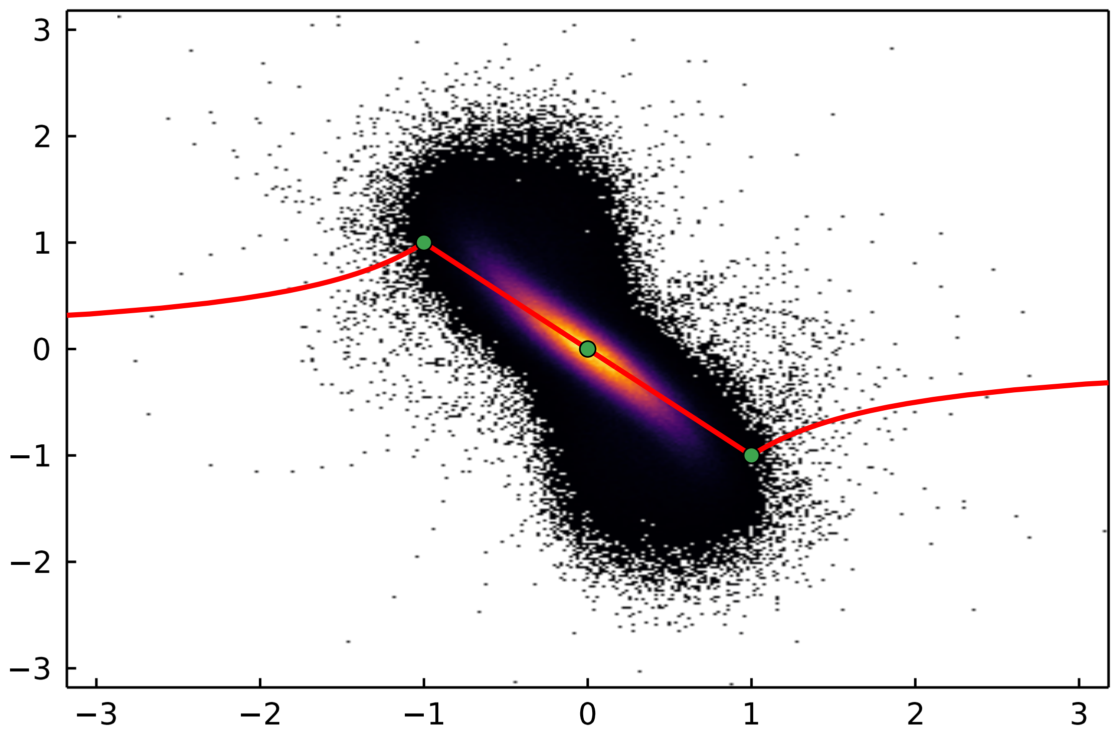


$K_N \frac{dS[\phi]}{d\phi} = e^{-i\frac{\pi}{3}}(4i\phi + 2\phi^3)$

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

And

Converges to wrong solution



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

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

Boundary terms and kernels

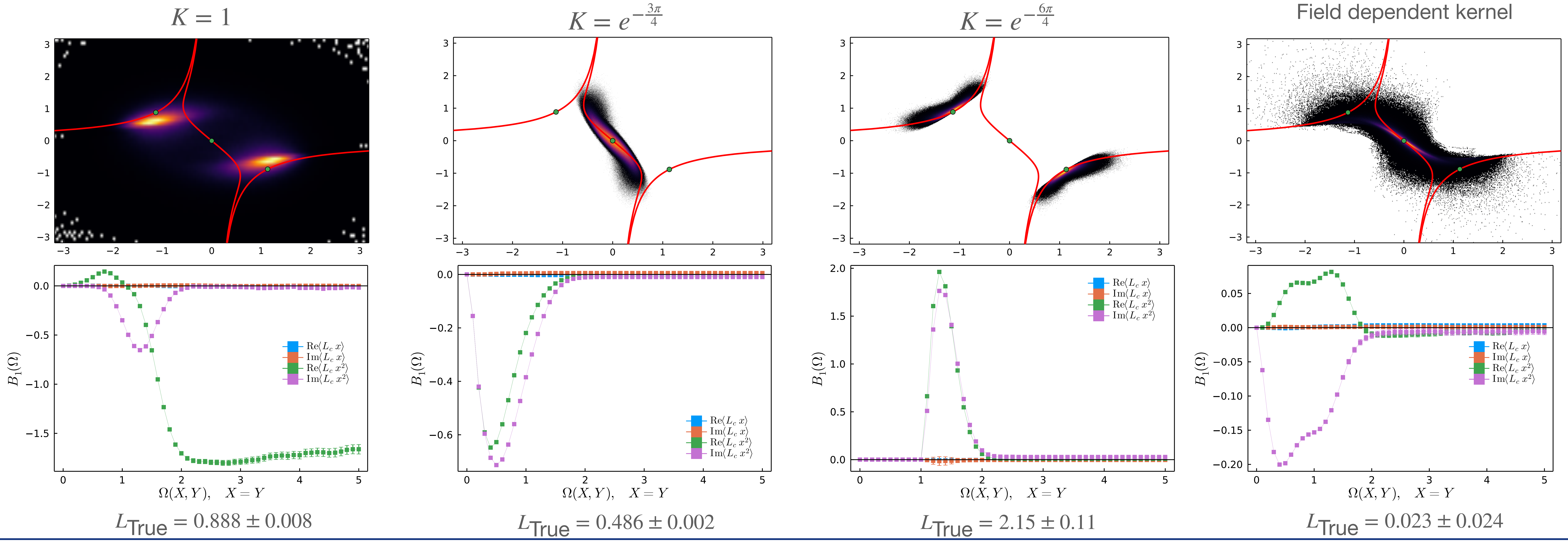
$$S = \frac{1}{2}\sigma x^2 + \frac{\lambda}{4!}x^4$$

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

- 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?



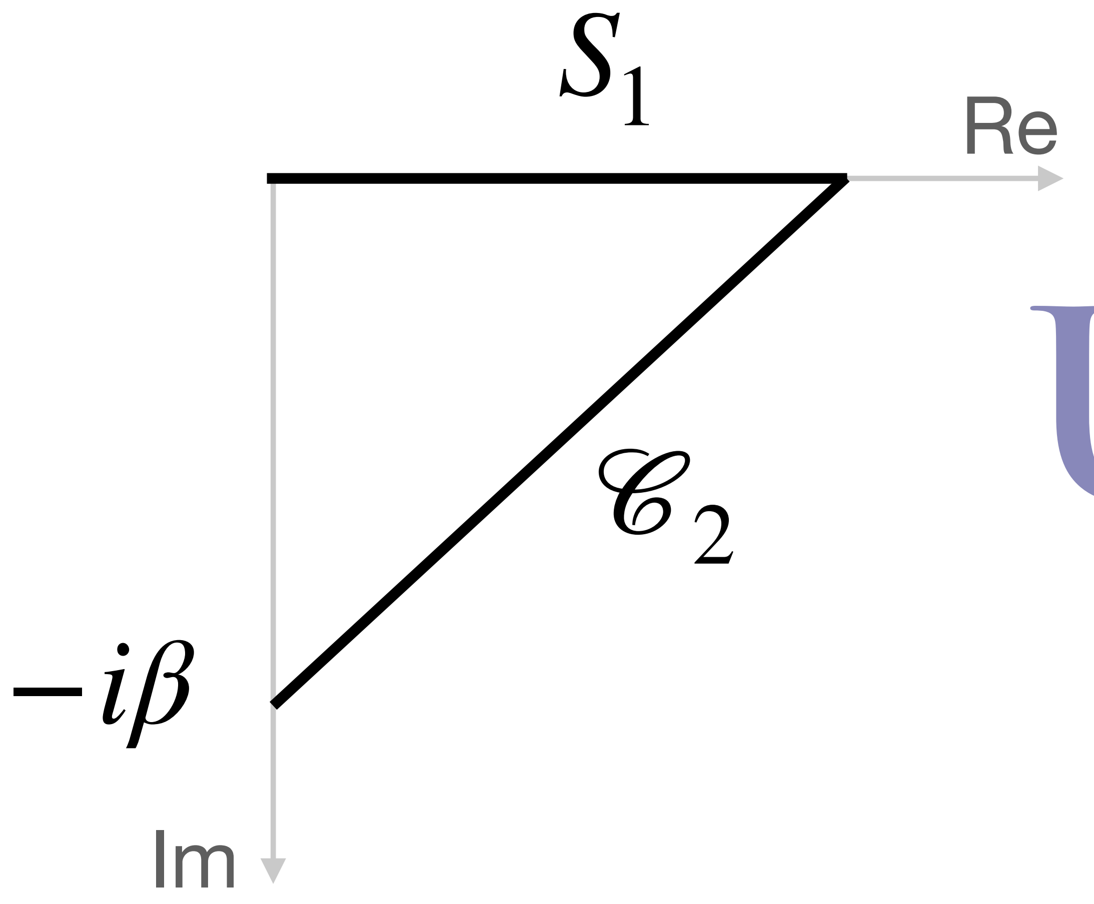
Summary and outlook

- Implicit scheme; Stabilise and regularise real-time CL

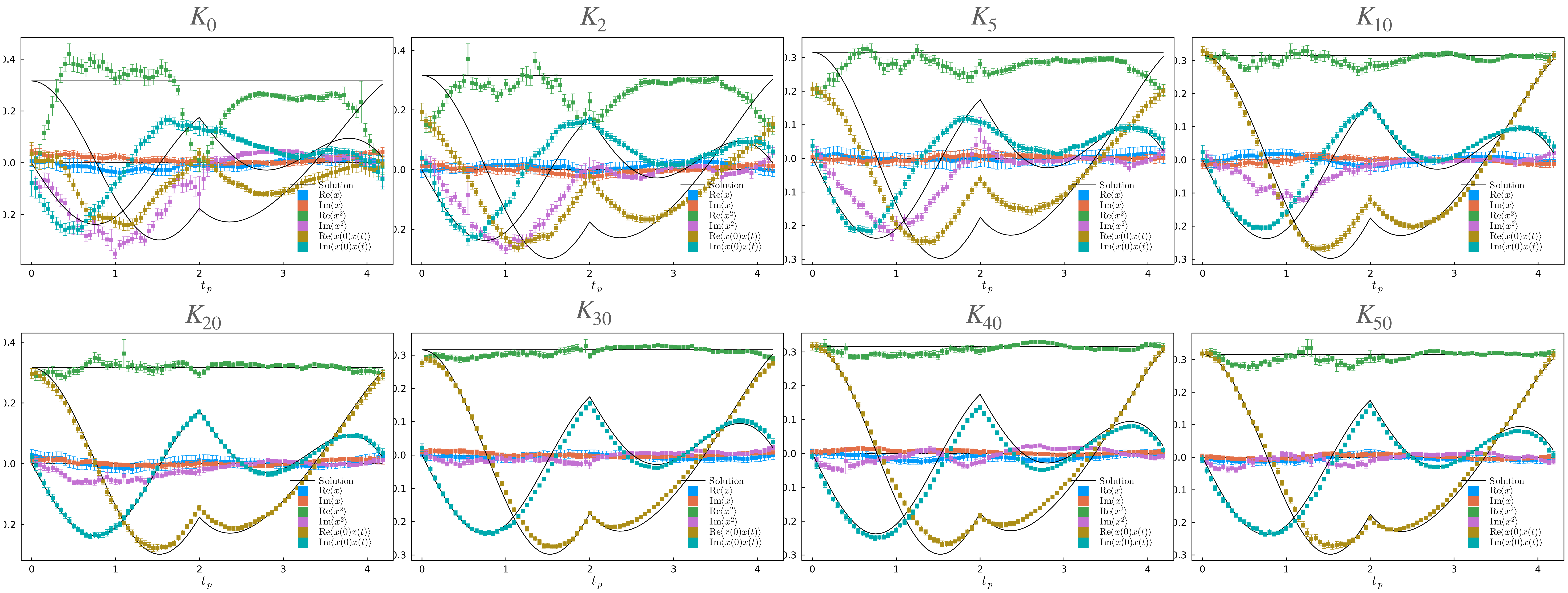
- Goal: extending real-time convergence CL
- Kernel controlled complex Langevin
  - No convergence problem for free scalar theory
  - Learning kernel in thermal ϕ^4 theory

- 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

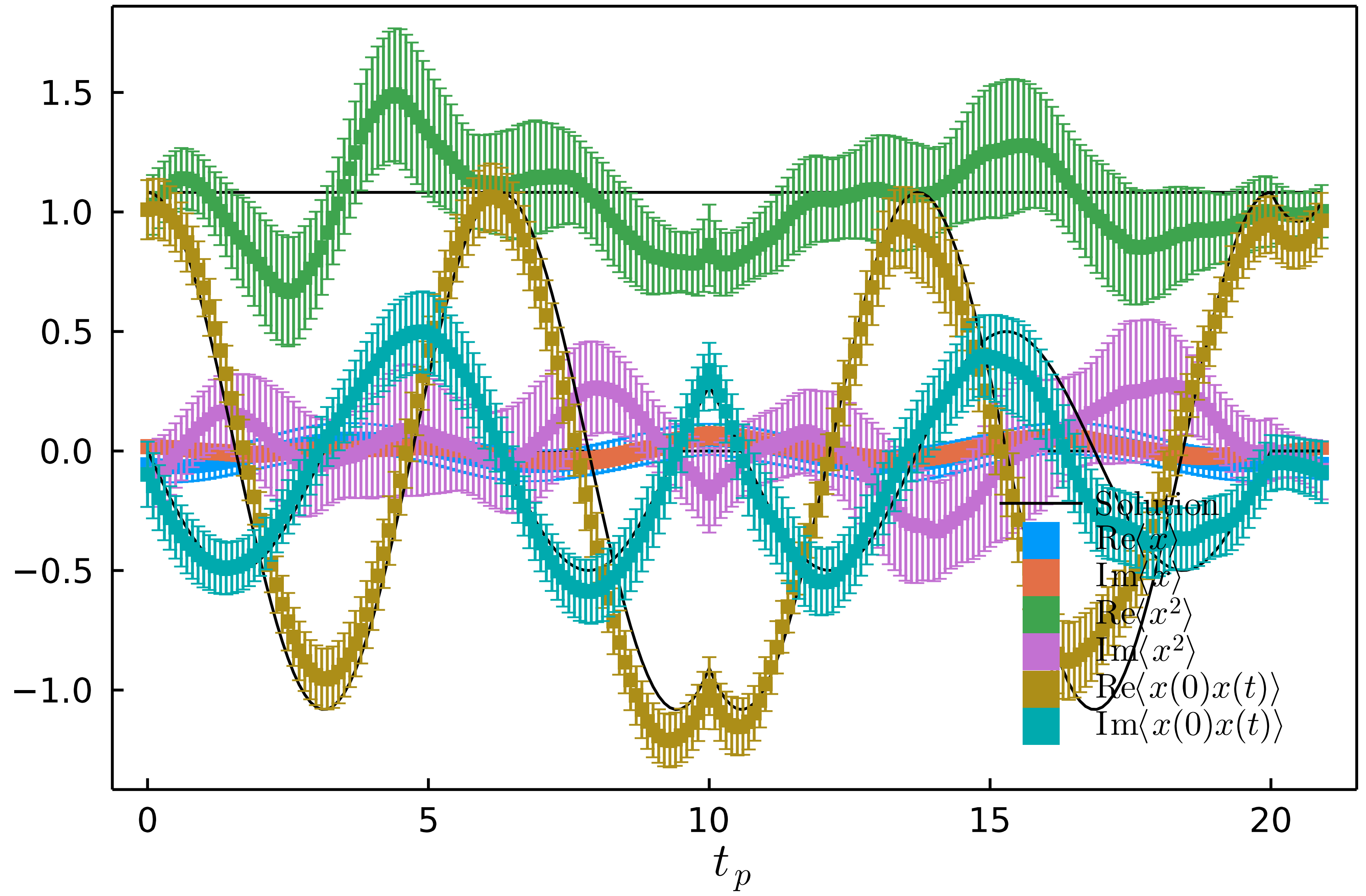


- Follow real axis up to $x_0^{\text{max}} = 2.0$
- Using $\beta = 1.0$, $m = 1$, $\lambda = 24$
- Form of the kernel $K = e^{A+iB}$



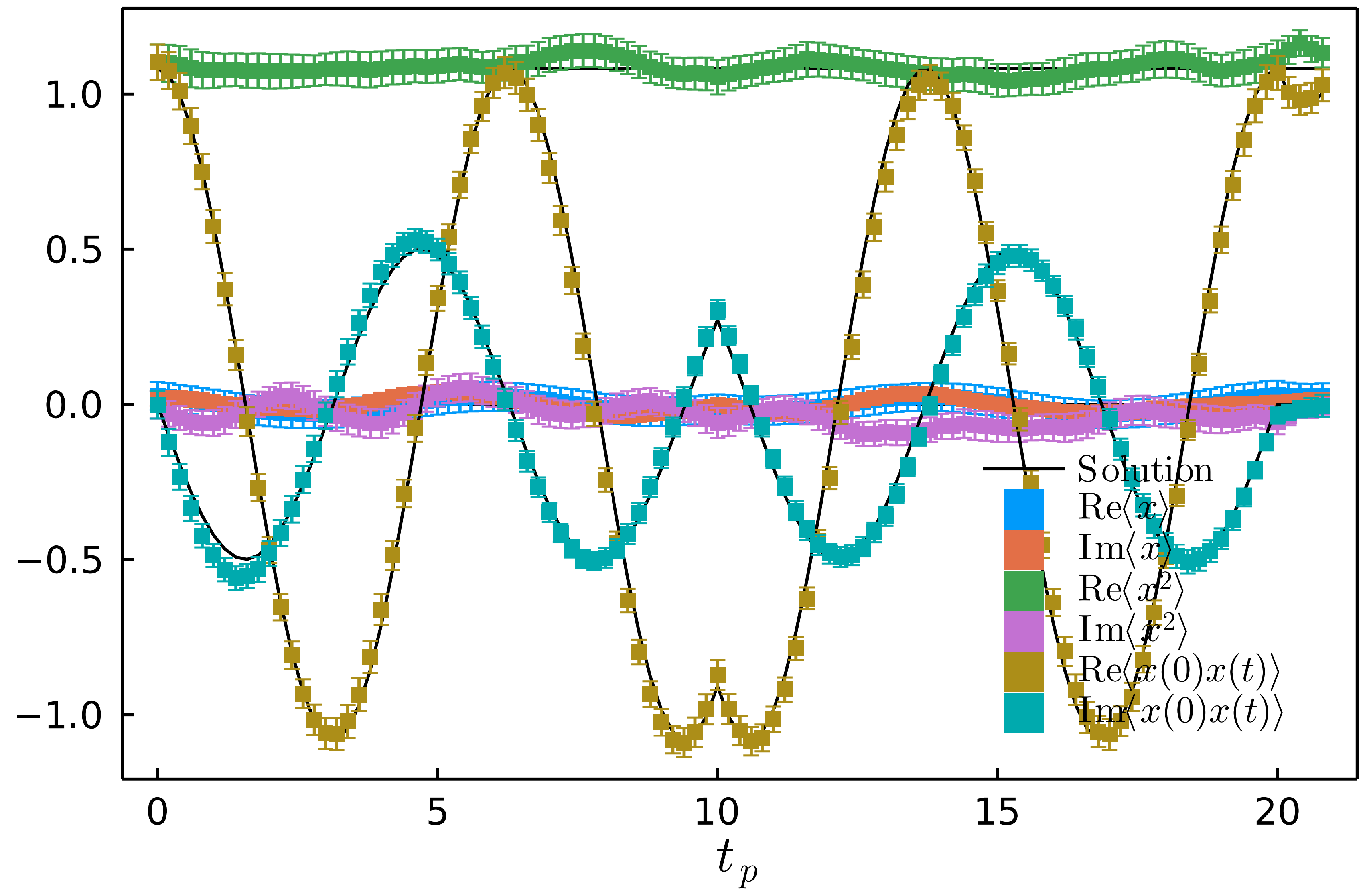
Learning free theory kernel

- 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

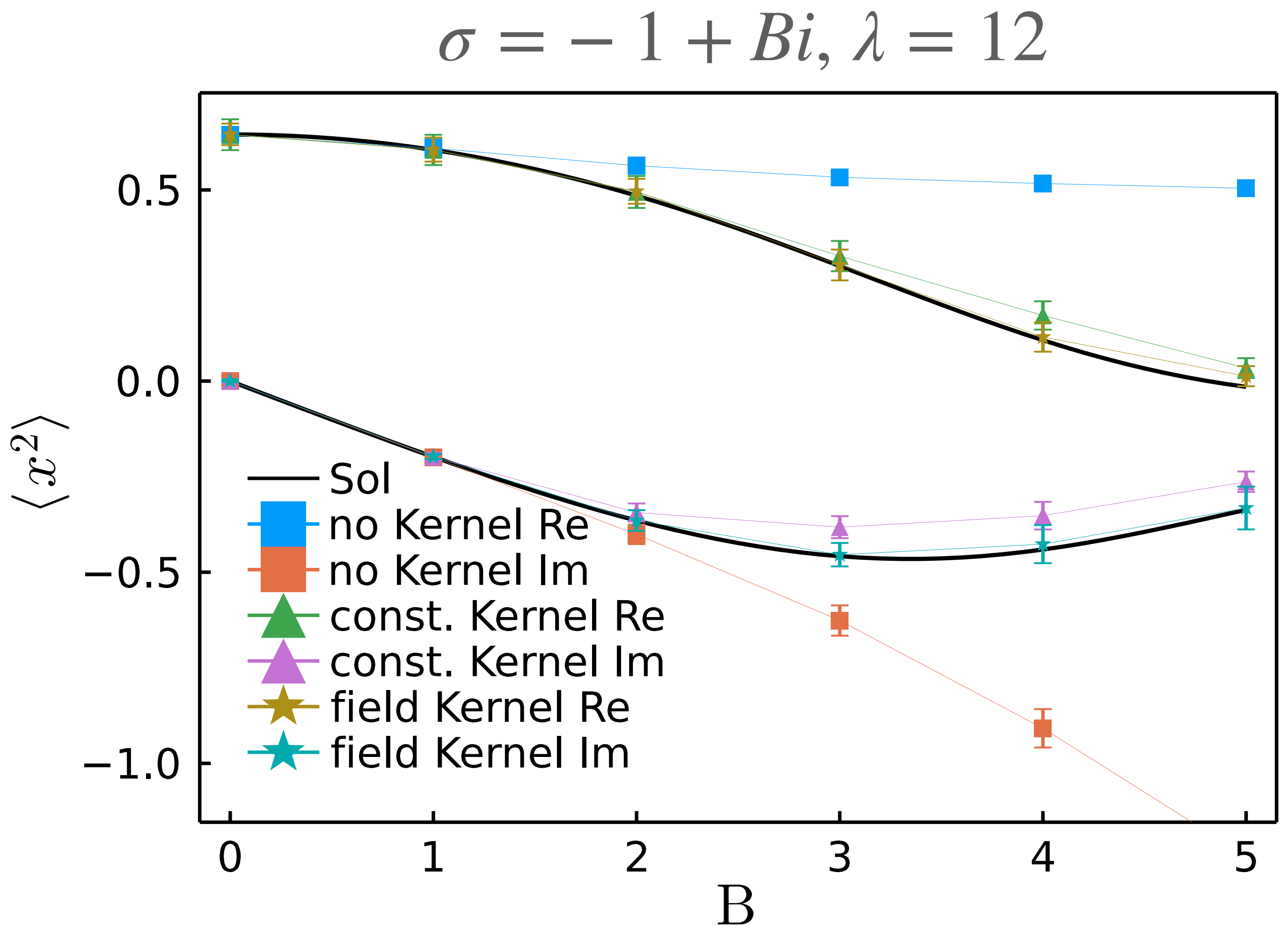
$$S = \frac{1}{2}\sigma x^2 + \frac{\lambda}{4!}x^4$$

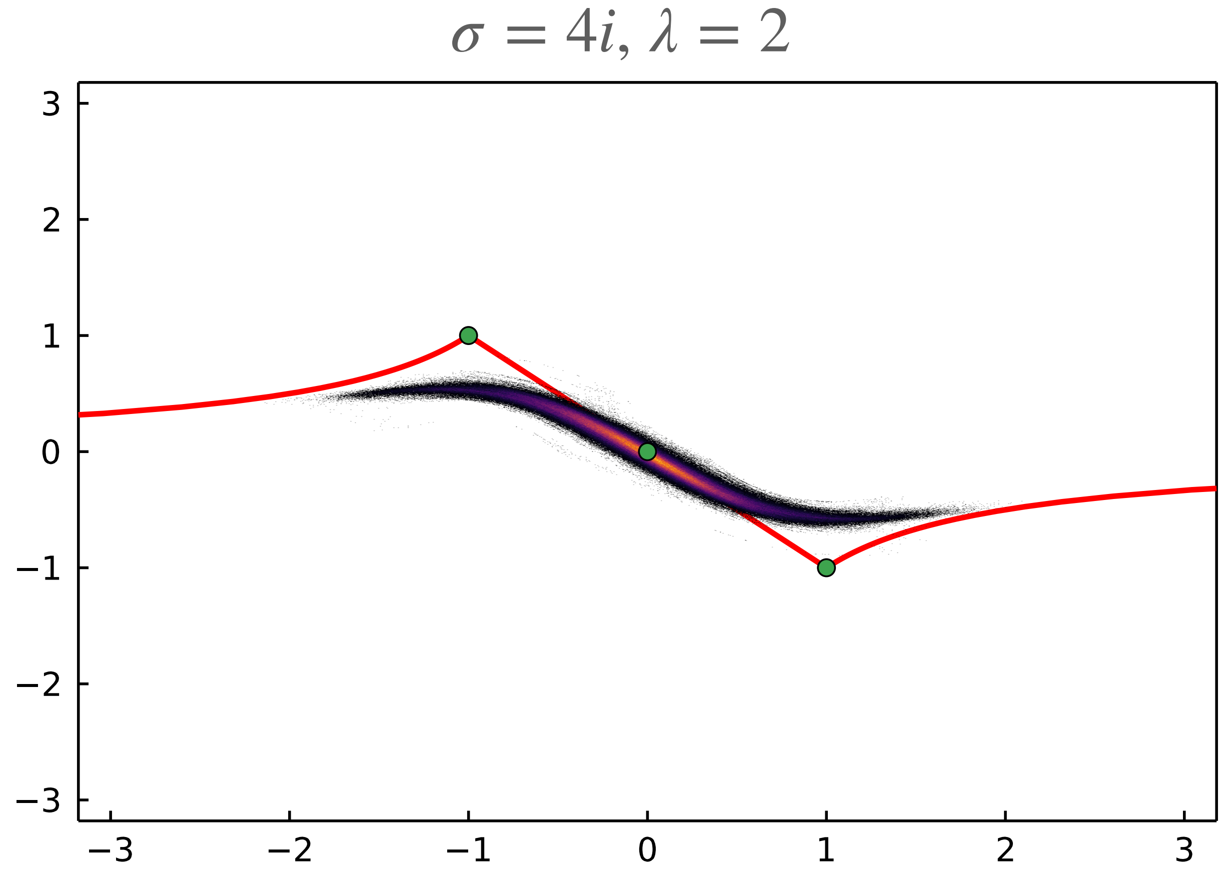
- Need to add extra derivative term

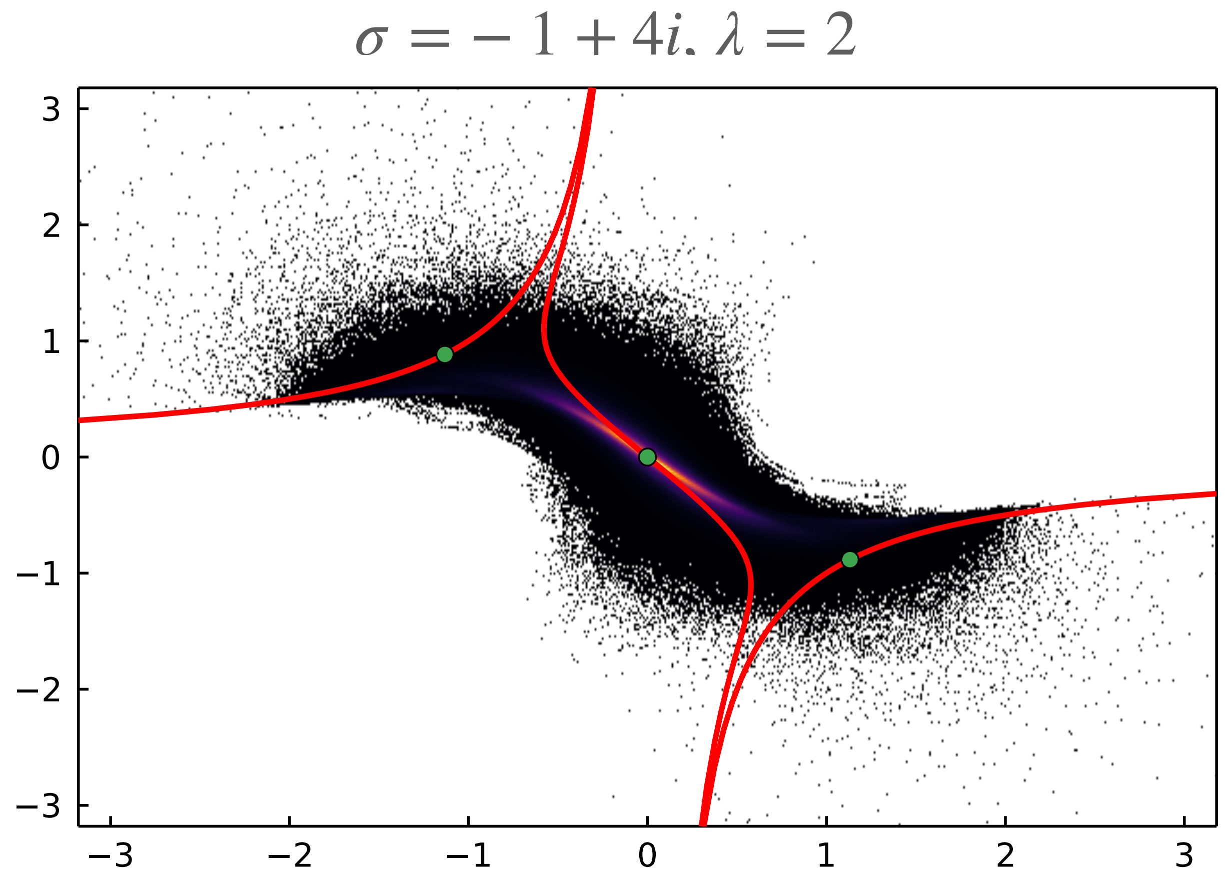
$$\frac{d\phi}{d\tau_0} = K[\phi]\frac{\delta S[\phi]}{\delta\phi} + \frac{\partial K[\phi]}{\partial\phi} + \sqrt{K[\phi]}\xi$$

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

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

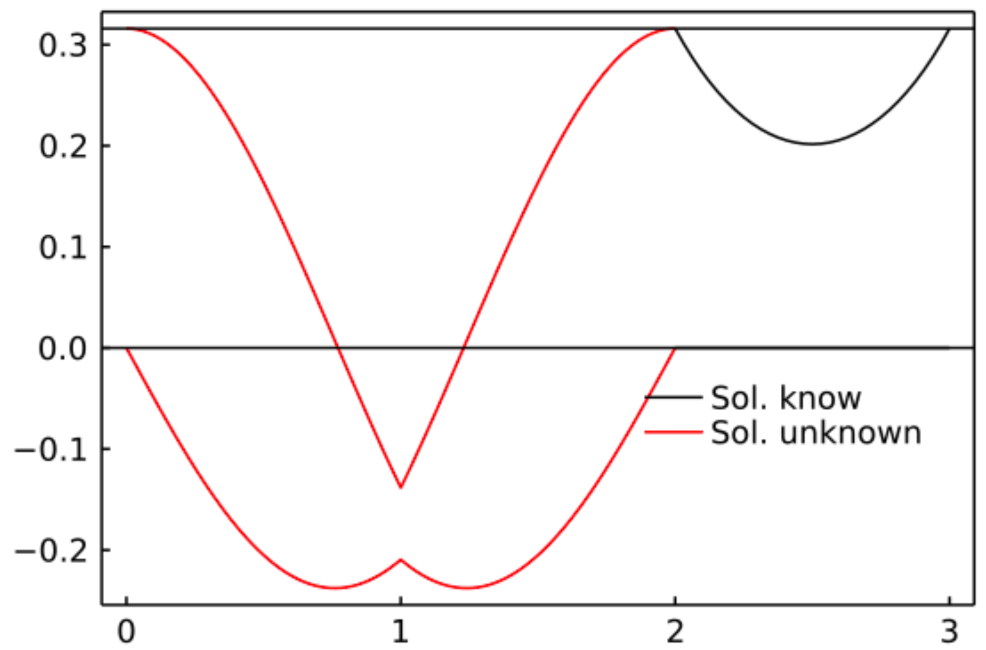


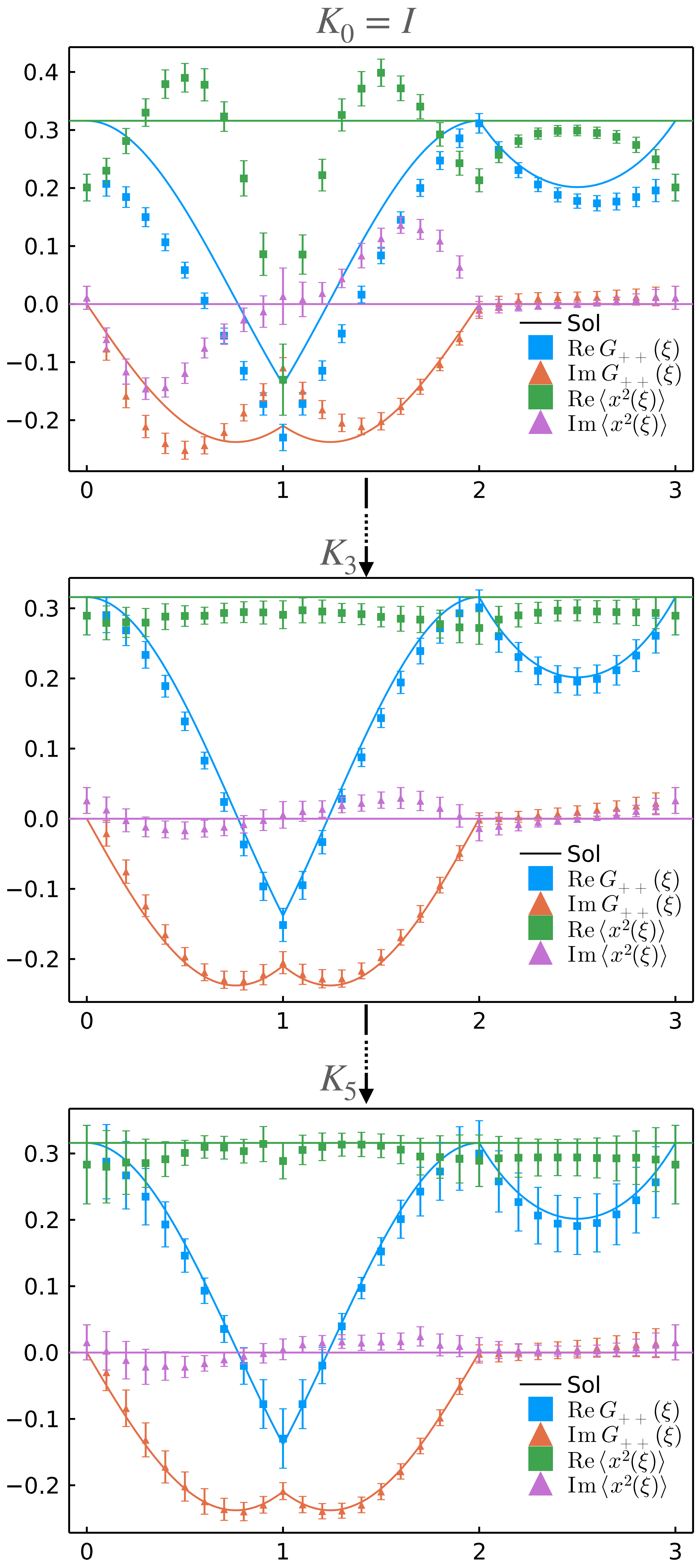




Construct kernel

- 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 $\langle x^2 \rangle = \mathrm{Re}\langle x^2 \rangle = \text{const.}$
  - 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: $\beta = 1.0$, $x_0^{\text{max}} = 1.0$





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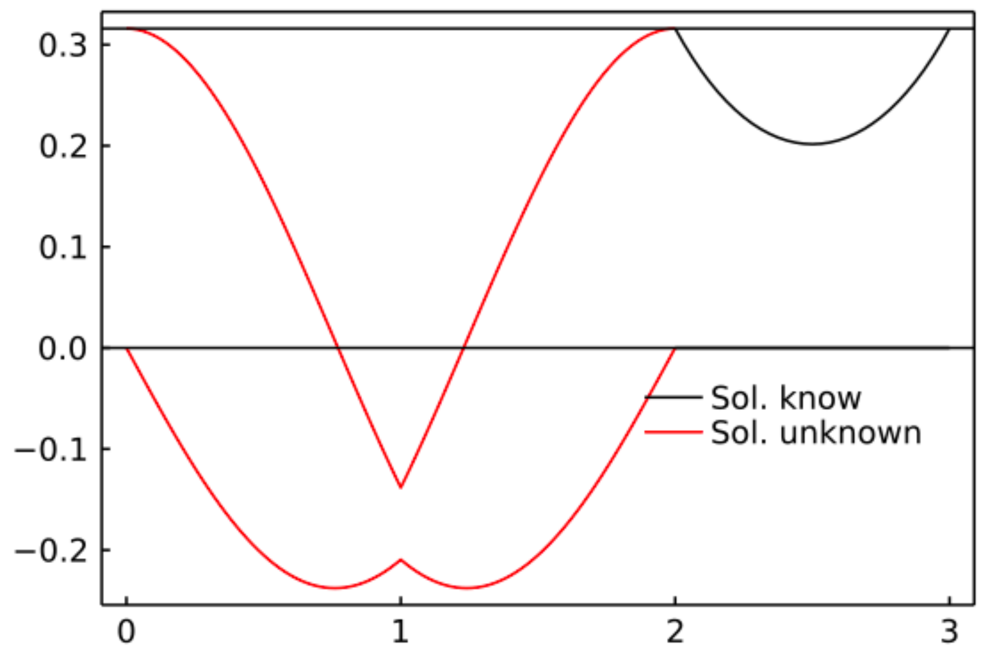
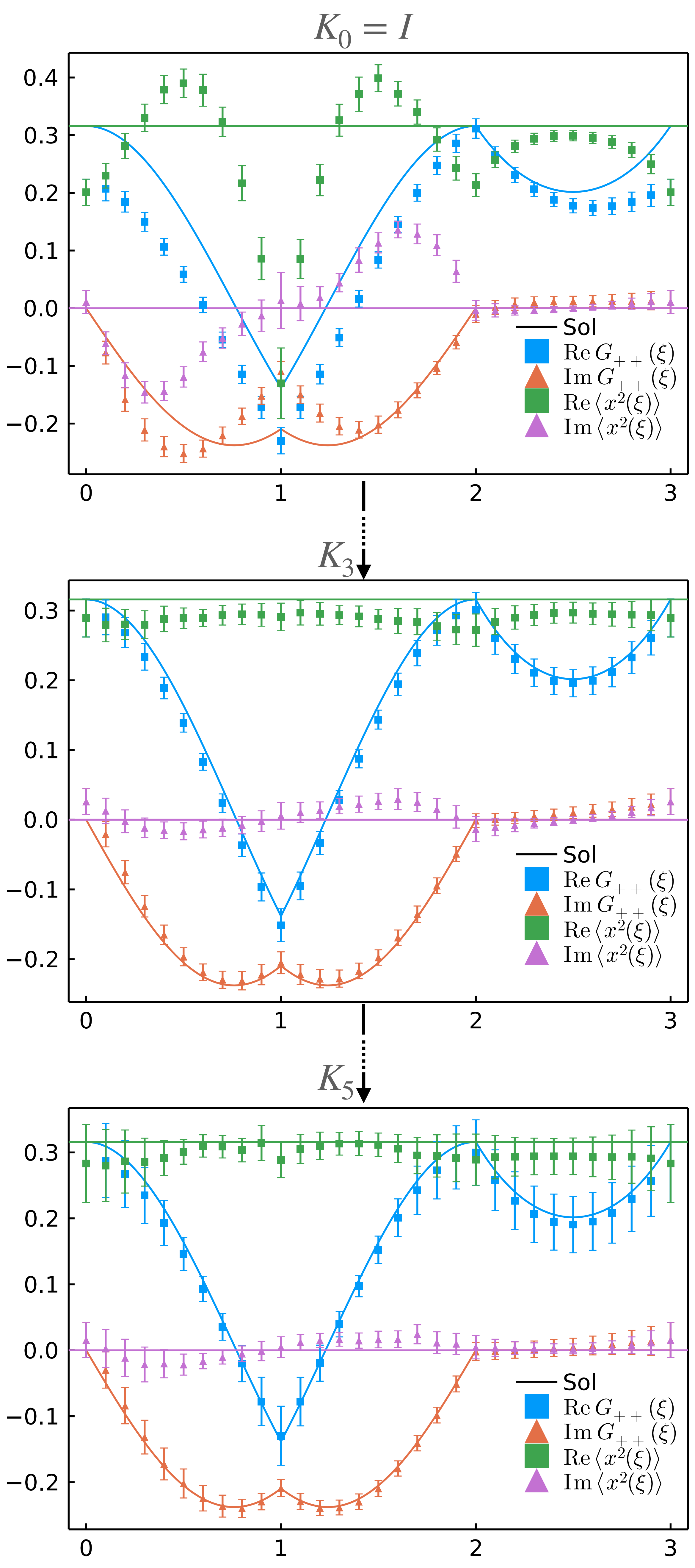
- Field dependent kernel



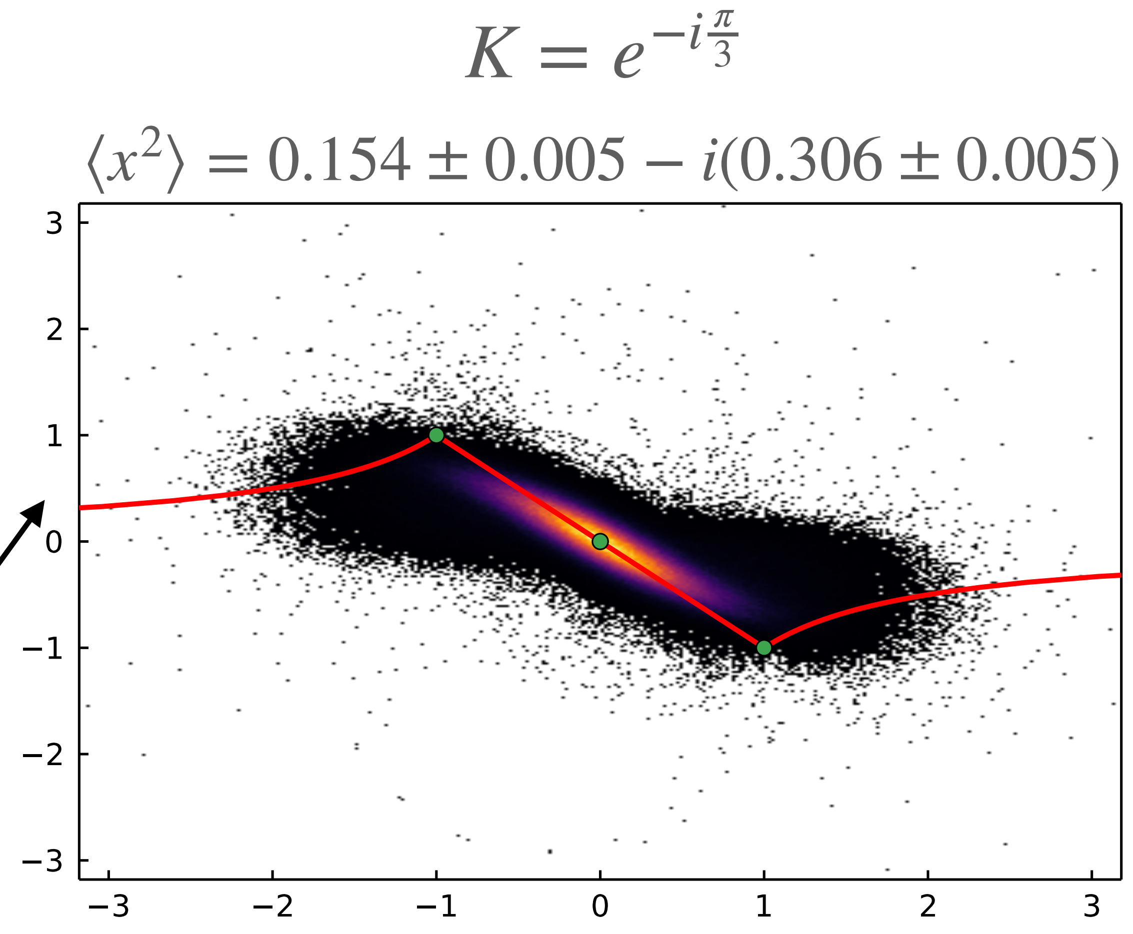


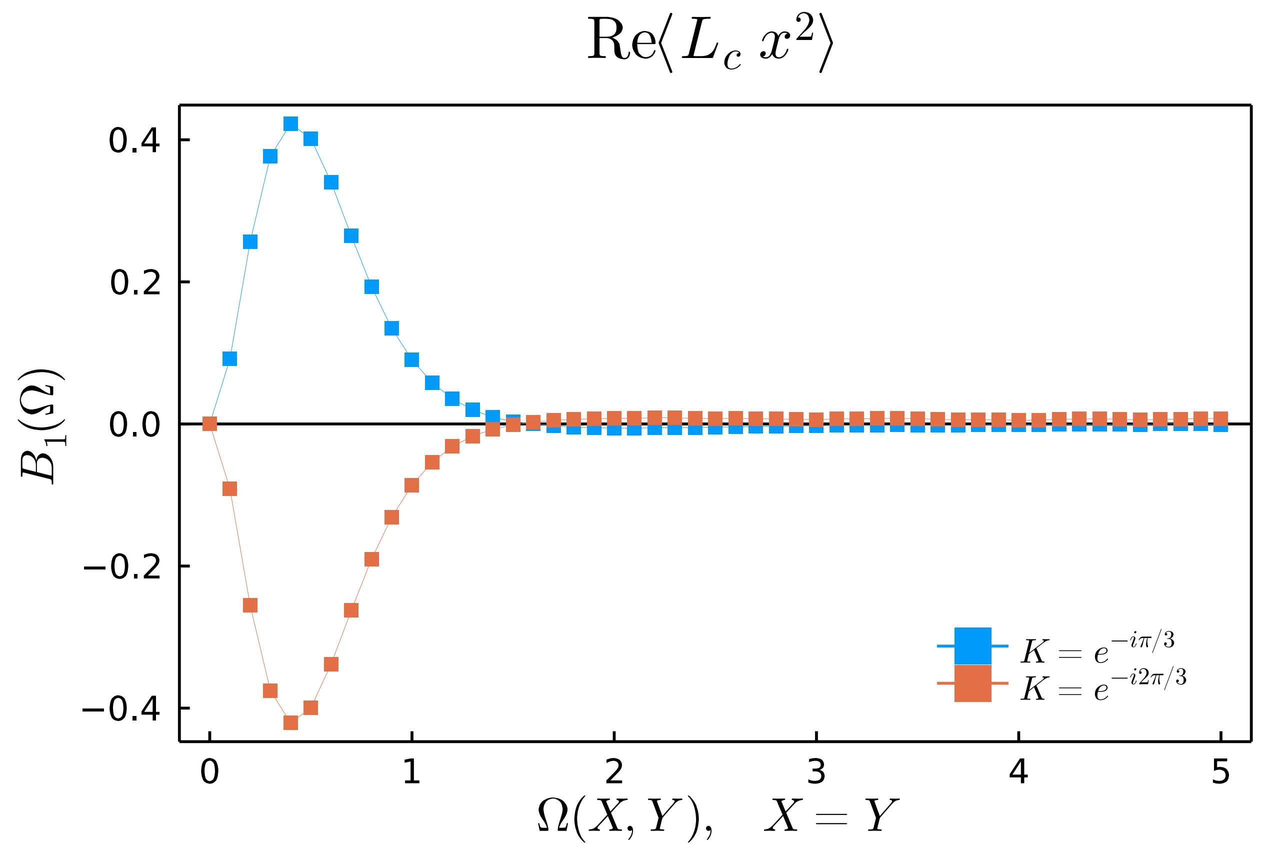
More info about simple model results

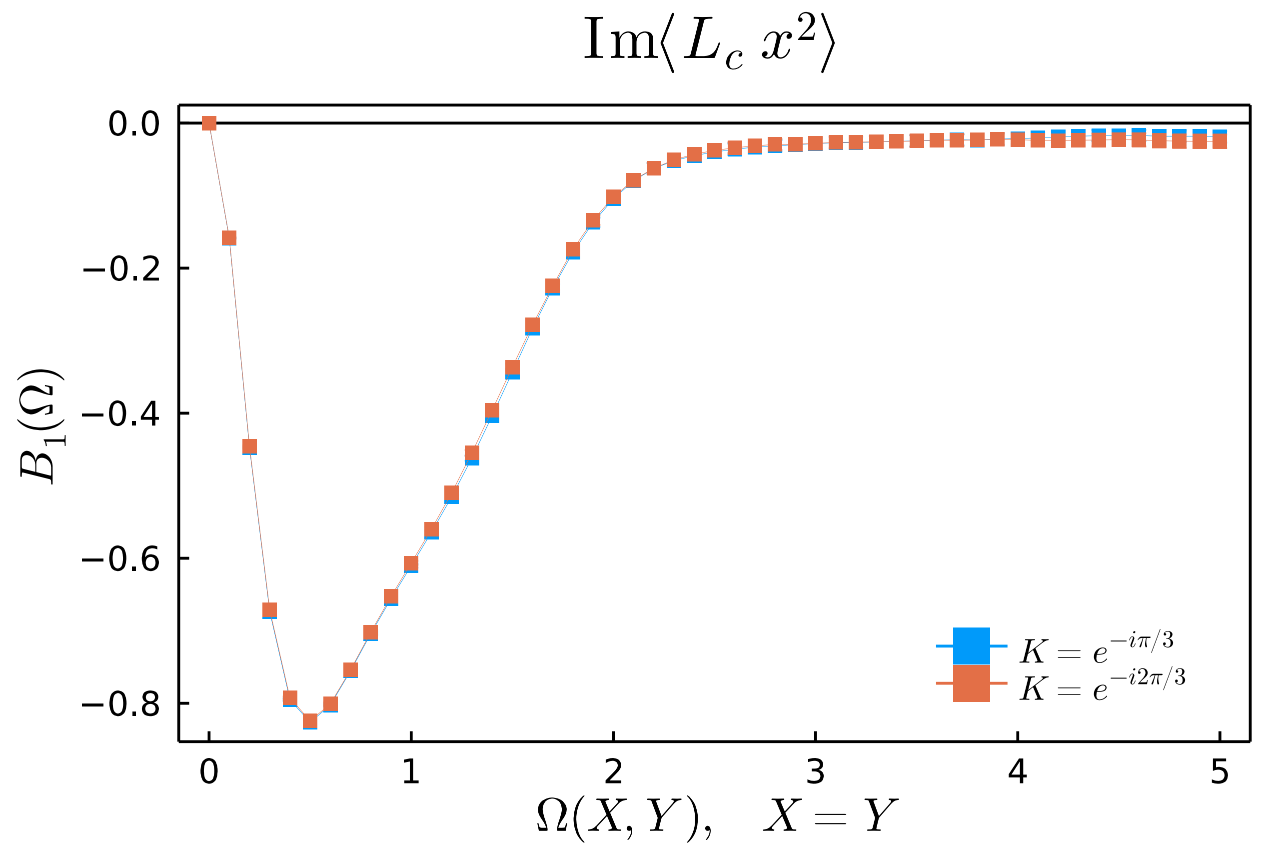
$$S = \frac{1}{2}\sigma x^2 + \frac{\lambda}{4!}x^4$$

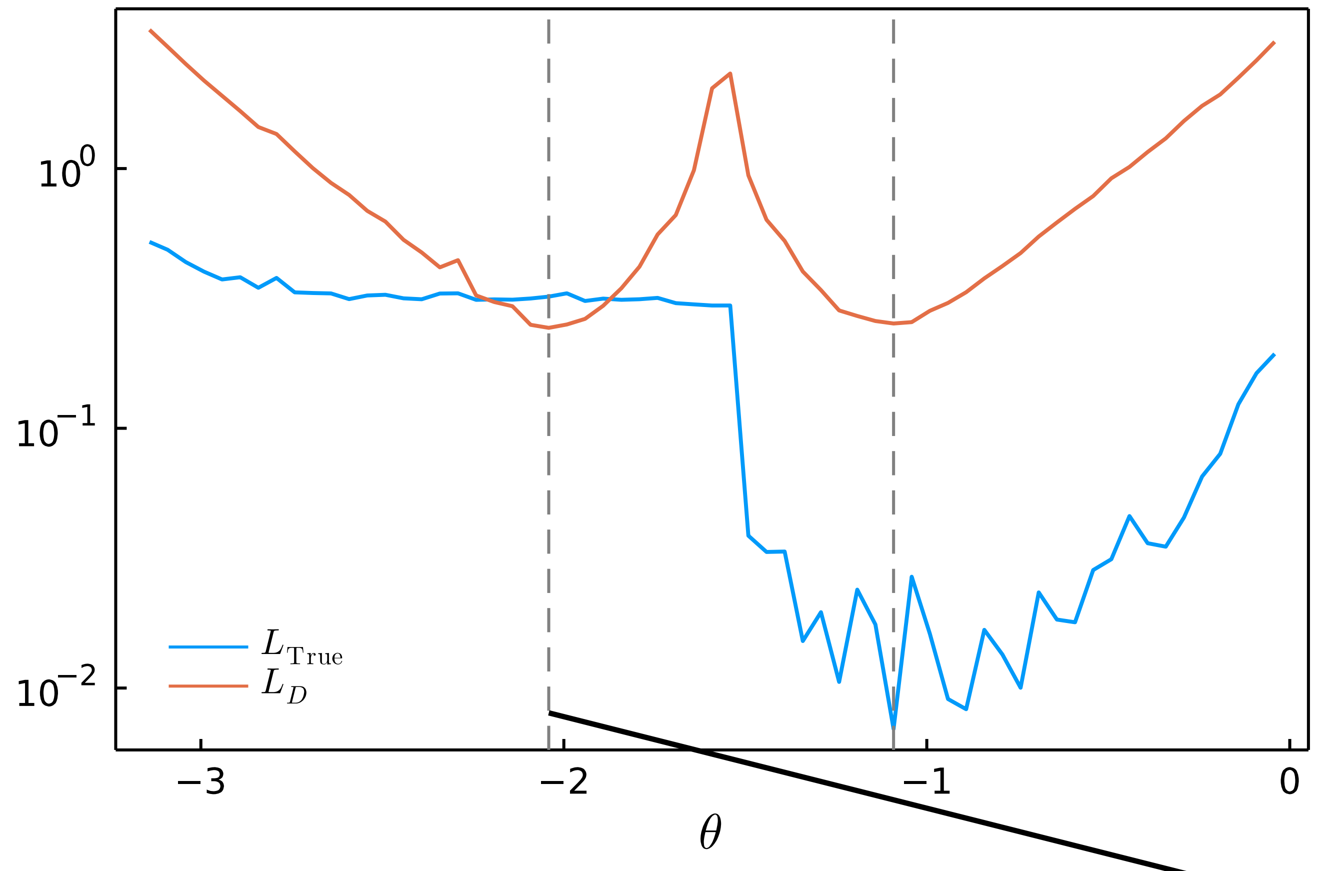
$\sigma = 4i,\ \lambda = 2$

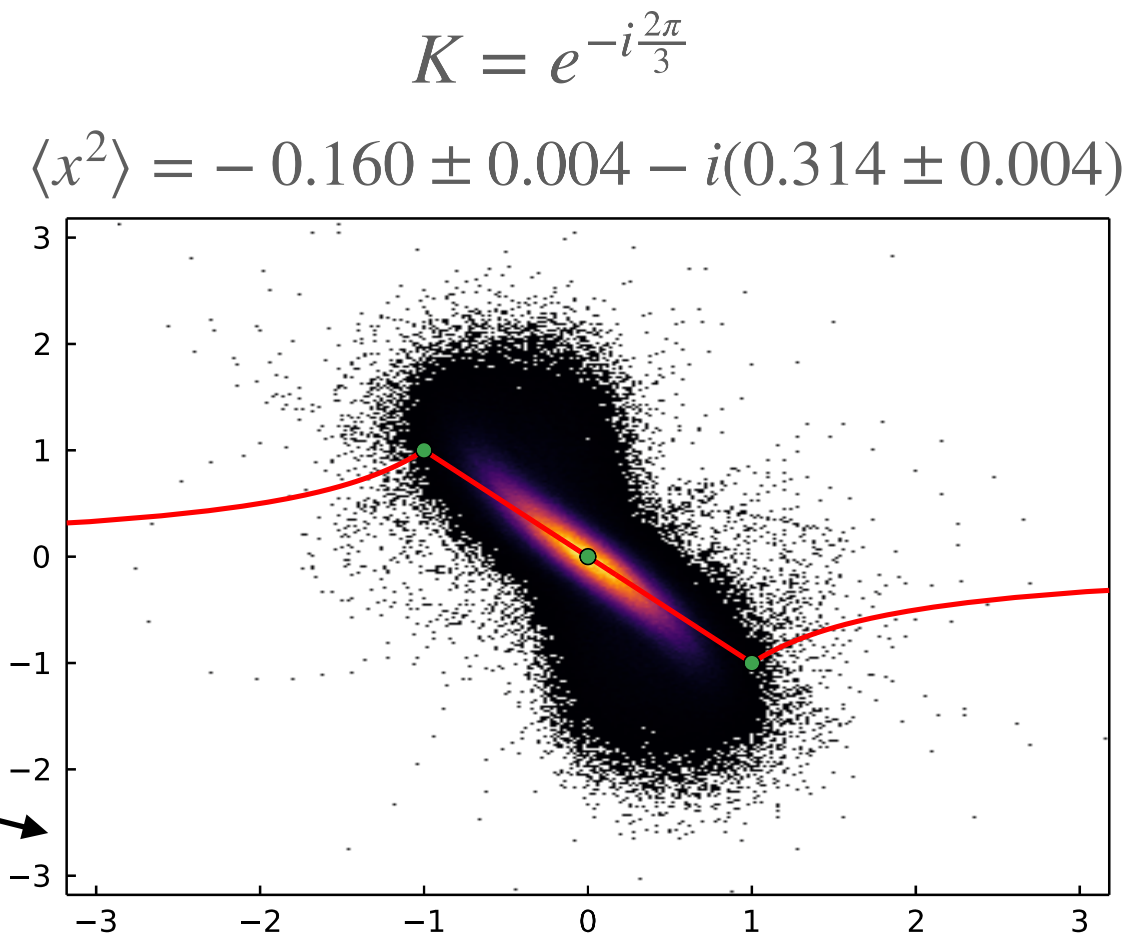
$\langle x^2 \rangle_{\text{true}} = 0.150077 - i0.307646$











Field dependent