Real-time simulations using complex Langevin

Daniel Alvestad, University of Stavanger
Collaborators: Rasmus Larsen and Alexander Rothkopf

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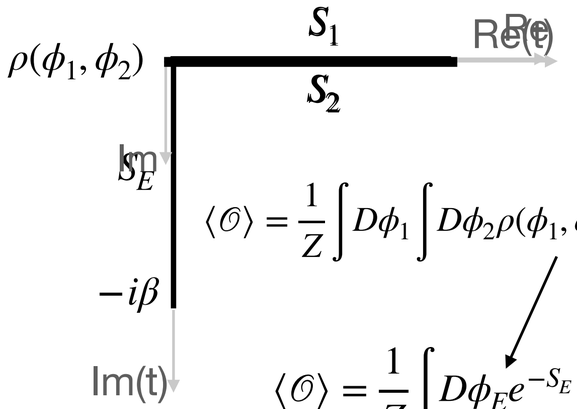
Norwegian Particle, Astroparticle & Cosmology Theory network

Real-time simulations

- Real-time simulations (Minkowski):

$$\langle \mathcal{O} \rangle = Tr[\rho \mathcal{O}] = \frac{1}{Z} \int D\phi \; \mathcal{O}(x) e^{iS[\phi]}$$

  - Schwinger-Keldysh contour
  - Non-equilibrium
  - Thermal equilibrium



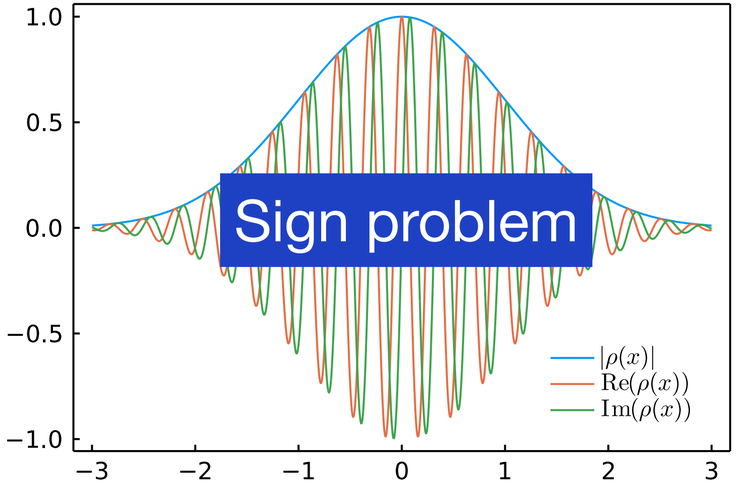
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi_1 \int D\phi_2 \rho(\phi_1, \phi_2) \int_{\phi_1}^{\phi_2} D\phi^+ D\phi^- \mathcal{O}(\phi) e^{iS[\phi^+] - iS[\phi^-]}$$

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

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

- Toy model: $\rho(x) = e^{-\frac{1}{2}x^2 + i\lambda x}$
  - Measure: $\langle \mathcal{O} \rangle = \frac{1}{Z} \int dx \; \mathcal{O}(x) \rho(x)$

Importance sampling not possible



Complex Langevin, Lefschetz thimbles, flowed manifolds,….

Langevin equation

- Langevin equation
  (Stochastic Differential equation)

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

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

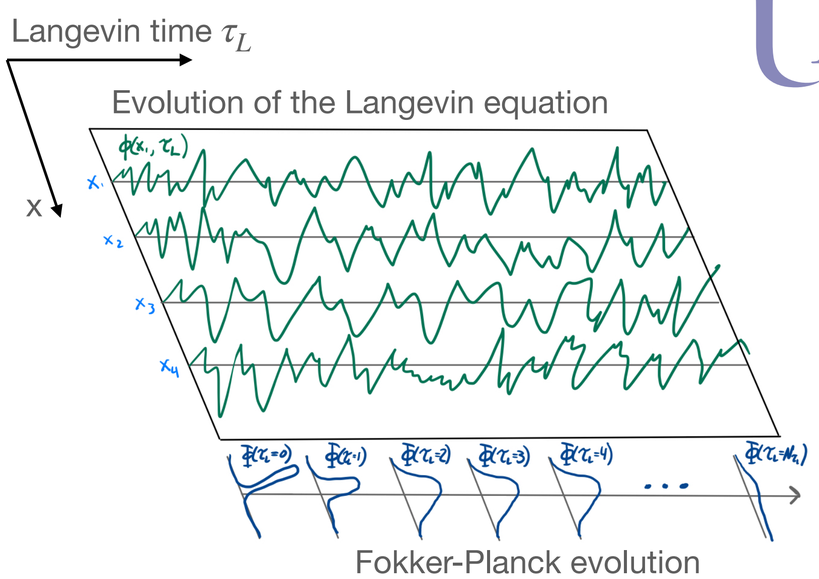
- Fokker-Planck equation (Real)

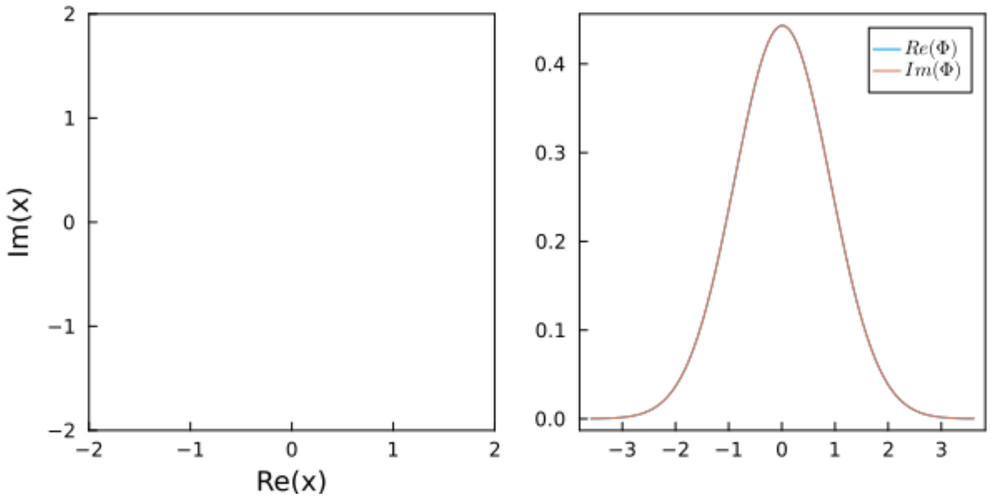
$$\frac{\partial}{\partial t}\Phi(x,t) = \sum_j \frac{\partial}{\partial \phi_j}\left[\frac{\partial}{\partial \phi_j} + \frac{\partial S[\phi]}{\partial \phi_j}\right]\Phi(x,t) = L_0^T\Phi(x,t)$$

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

Fokker-Planck Langevin

$$\langle \mathcal{O}\rangle = \lim_{\tau_L\to\infty}\int D\phi\ \Phi(\phi,\tau_L)\mathcal{O}(\phi) = \lim_{T\to\infty}\frac{1}{T}\int_0^T d\tau_L\ \mathcal{O}(\phi(\tau_L))$$





Real-time complex Langevin

- Complexifying fields: $\phi \to \phi^R + i\phi^I$
- Scaling of complex Langevin

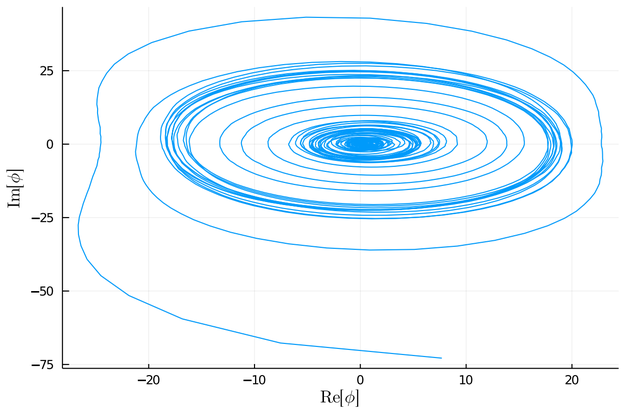
Complex Langevin equation

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

Stable solver

Get control of the numerics

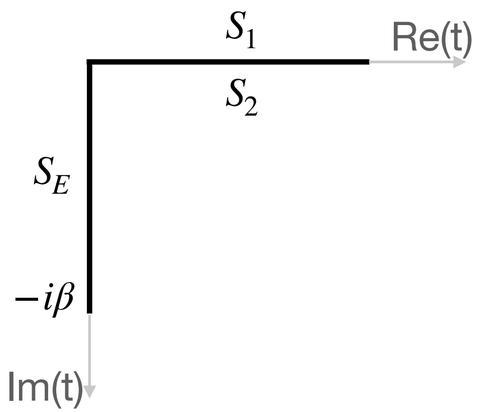
Real-time complex Langevin = Stiff problem



Regulator

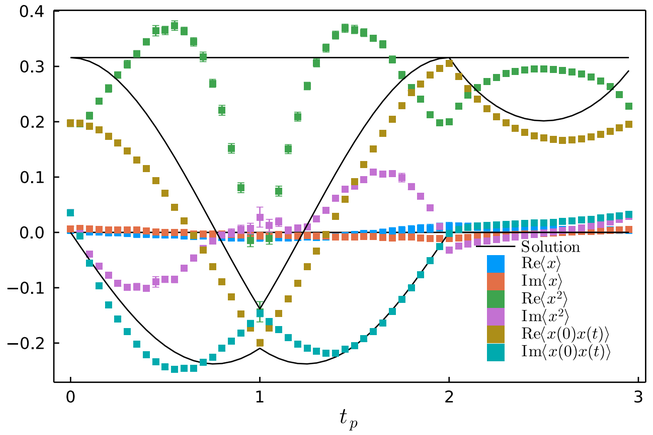
Regulate integral

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



Convergence problem

Understand convergence problem of the complex Langevin



Regularising real-time contour

Regularisation of real-time contour

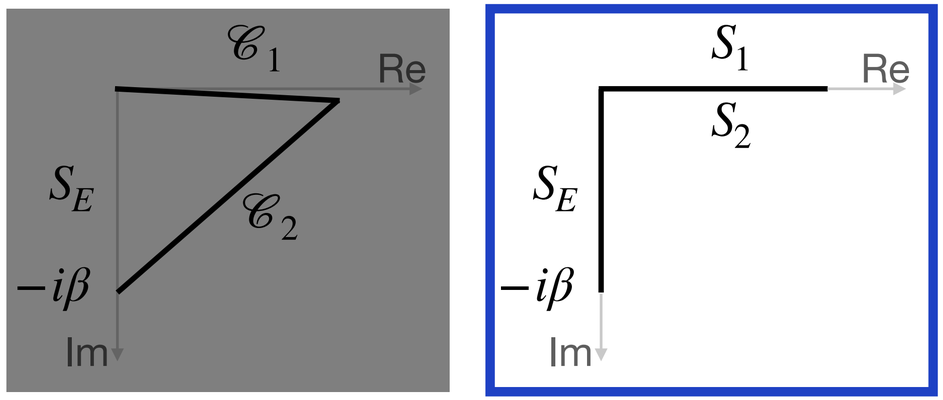
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \; \mathcal{O}(x) e^{iS[\phi]}$$

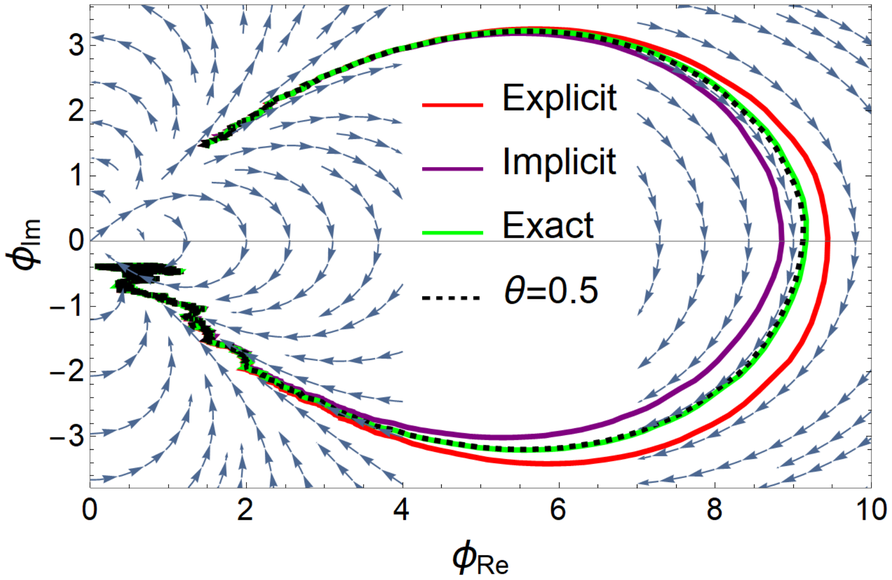
- Infinitesimal damping term:

$$\bar{S} = S + iR(\phi, \epsilon), \quad R = \frac{1}{2}\epsilon\phi^2$$

  - Tilting of the real-time contour
  - Problem with two limits $\Delta\tau \to 0, \quad \epsilon \to 0$
- Implicit solver
  - No runaway solutions
  - Regulator due to undershooting
- Kernel (Discussing this later)

D.A, Larsen, Rothkopf (2021)
arxiv: 2105.02735

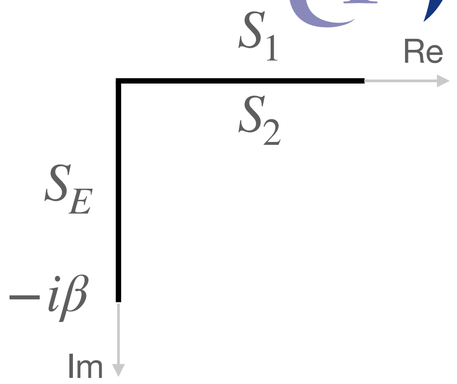




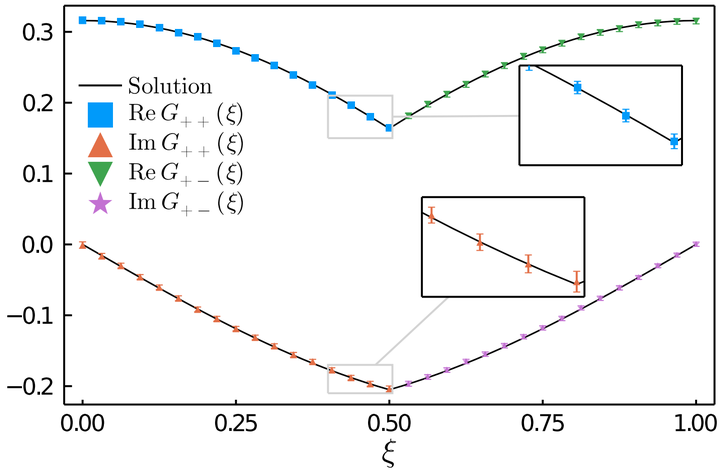
Dynamics in thermal equilibrium

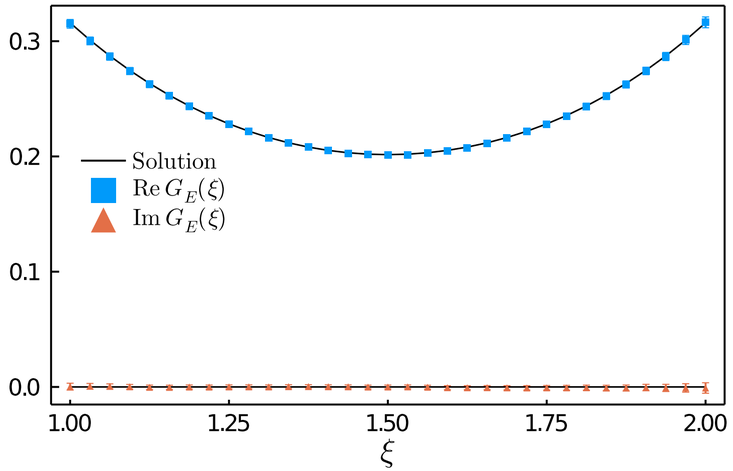
- Strongly coupled quantum anharmonic oscillator with $m = 1$, $\lambda = 24$ (same as in Berges, Borsanyi, Sexty, Stamatescu, 2007)

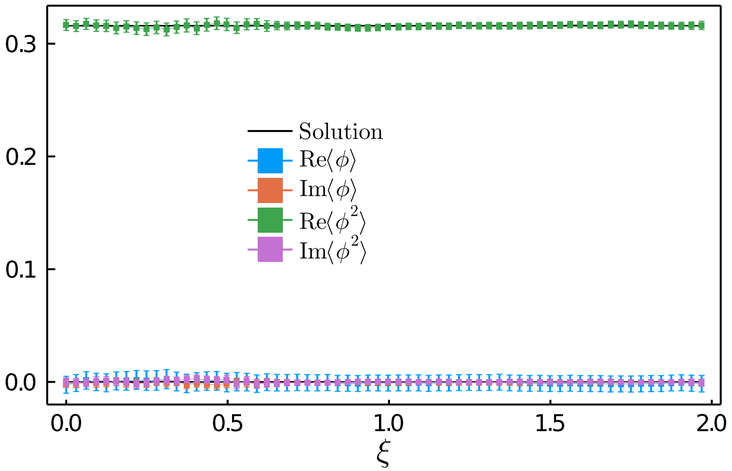
$$S = \int dx_0 \left\{ \frac{1}{2}\left(\frac{\partial \phi}{\partial x_0}\right)^2 - \frac{1}{2} m\phi^2 - \frac{\lambda}{4!}\phi^4 \right\}$$



- 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 $\xi \geq 1$



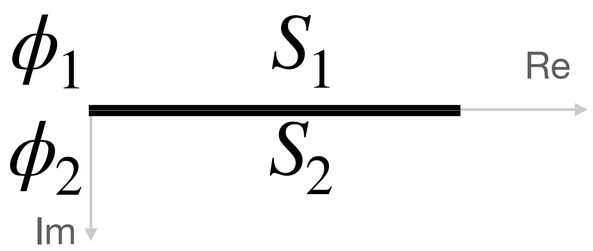


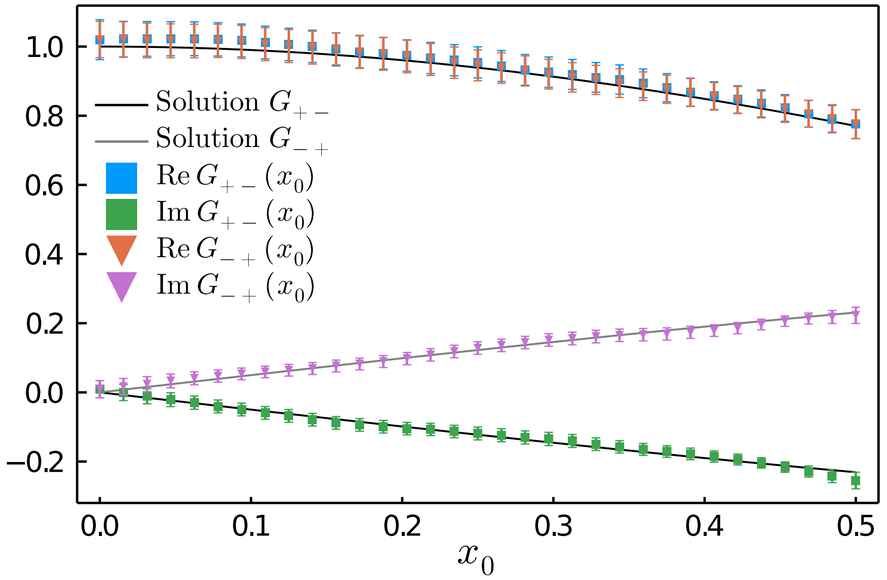


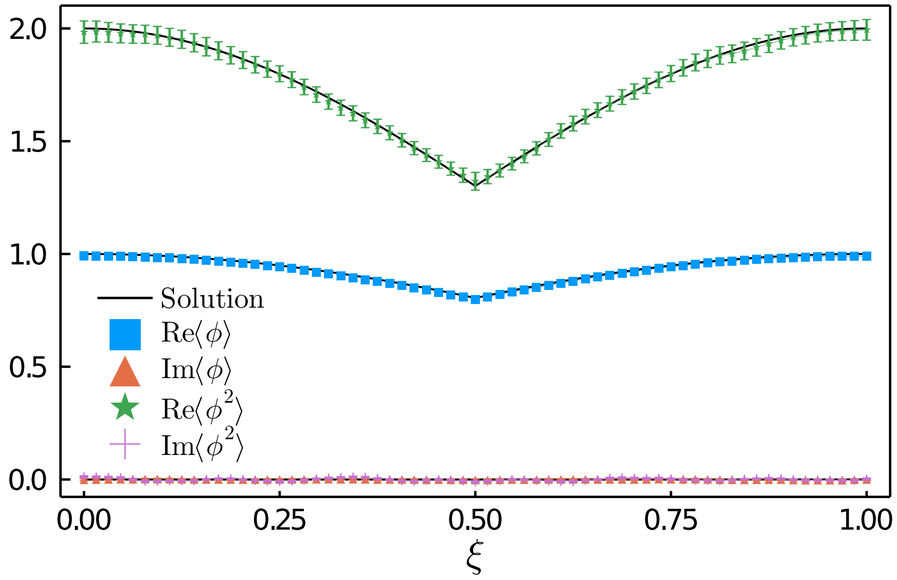
Simulations done with the DifferentialEquations.jl library in Julia

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







Real-time complex Langevin

Complex Langevin equation

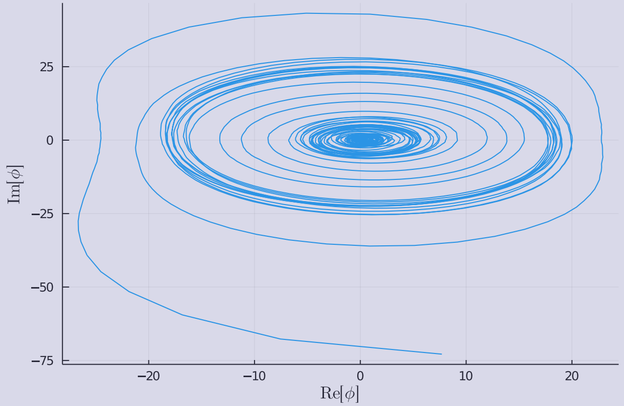
$$\frac{d\phi}{d\tau_L} = i\frac{\delta S[\phi]}{\delta\phi(x)} + \eta(x,\tau_L)$$

Numerics now under control

Stable solver

Get control of the numerics

Real-time complex Langevin = Stiff problem



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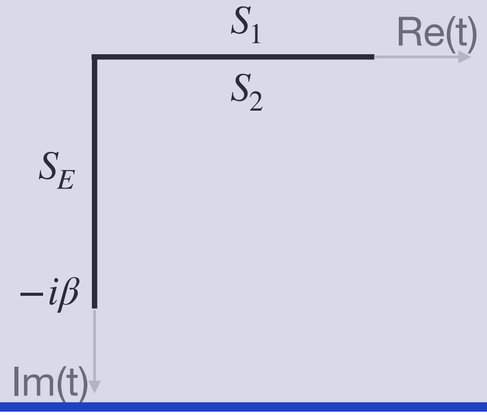

Convergence problem

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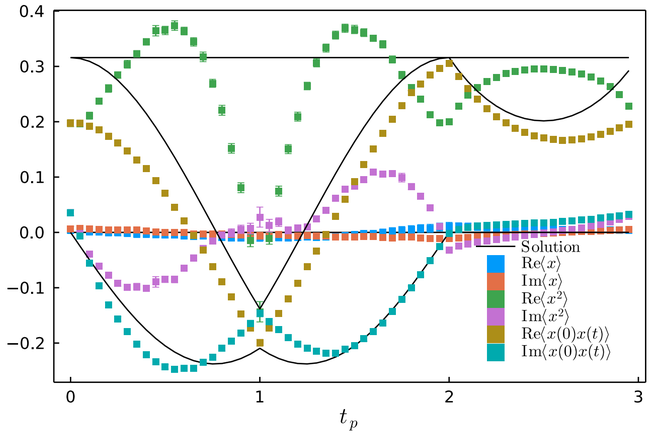


Kernel controlled complex Langevin

Kernel controlled Langevin equation

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

$$\frac{\partial}{\partial t}\Phi(x,t) = \sum_j \frac{\partial}{\partial \phi_j}\left[\frac{\partial}{\partial \phi_j} + \frac{\partial S[\phi]}{\partial \phi_j}\right]\Phi(x,t) = L_0^T\Phi(x,t)$$

- Freedom in Fokker-Planck equation (Real)

$$\frac{\partial}{\partial t}\Phi(x,t) = \sum_{j,l} \frac{\partial}{\partial \phi_j} K_{jl}[\phi]\left[\frac{\partial}{\partial \phi_l} + \frac{\partial S[\phi]}{\partial \phi_l}\right]\Phi(x,t) = L_0^T\Phi(x,t)$$

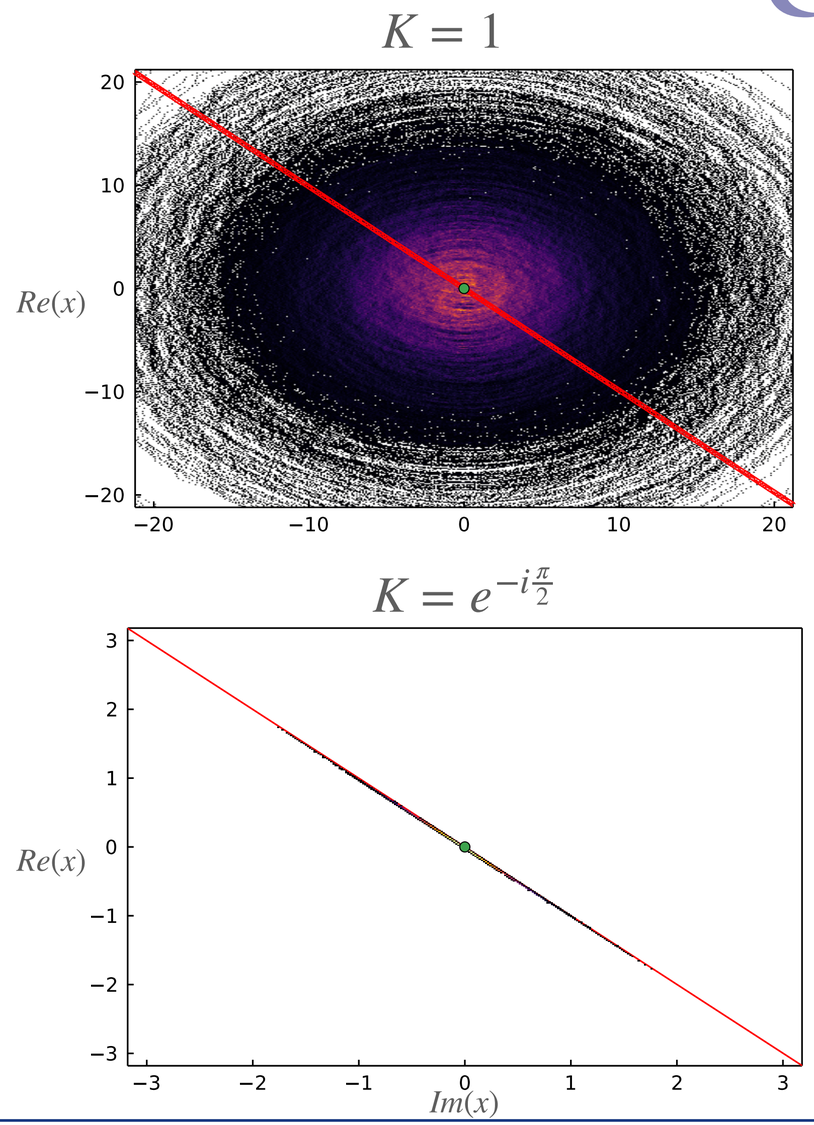
- Field independent kernelled Langevin equation

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

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

One-degree-of-freedom model

- Simple model $S = \frac{1}{2} i x^2, \quad \dot{x} = -K\, ix + \sqrt{K}\eta$
  - Optimal kernel for same model: $K = e^{-i\frac{\pi}{2}}$
  - CL with K: $\dot{x} = -x + e^{-i\frac{\pi}{4}}\eta$
- Thimble $\frac{d\tilde{x}}{d\tau} = \overline{\frac{dS}{d\tilde{x}}}$
- Solution $\tilde{x}(x, \tau) = x(\cosh\tau - i\sinh\tau)$
  - For $\tau \to \infty$ we have $\tilde{x}(x) = xe^{-i\frac{\pi}{4}} = x\sqrt{K}$
- Complex Langevin samples on the thimble
    - Kernel as a regulator



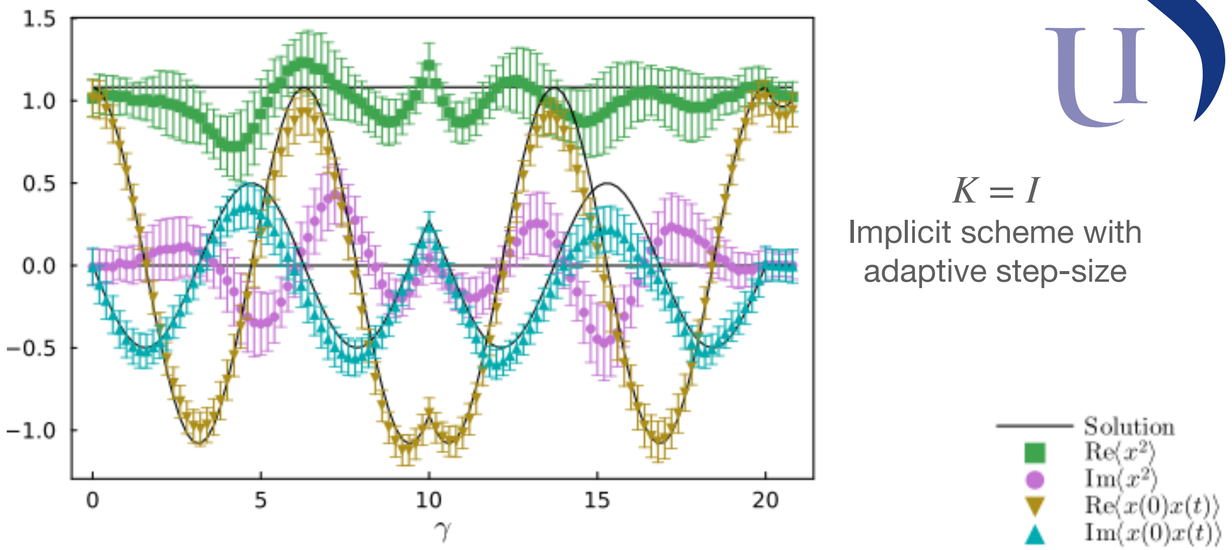
Free theory

$$\frac{\partial S}{\partial \phi} = iM\phi, \quad V = \frac{1}{2}m\phi^2, \quad m = 1$$

- Use propagator as kernel: $K = iM^{-1}$

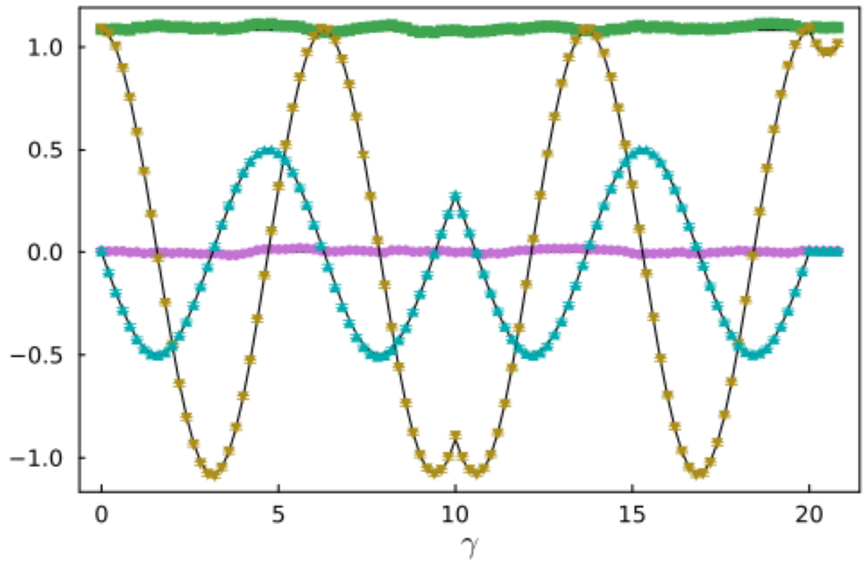
$$\dot{\phi} = Ki\frac{\partial S}{\partial \phi} + \sqrt{K}\eta = -\phi + \sqrt{K}\eta$$

No need for adaptive step-size or implicit scheme



$K = I$
Implicit scheme with adaptive step-size

$K = iM^{-1}$
Explicit scheme with fixed step-size



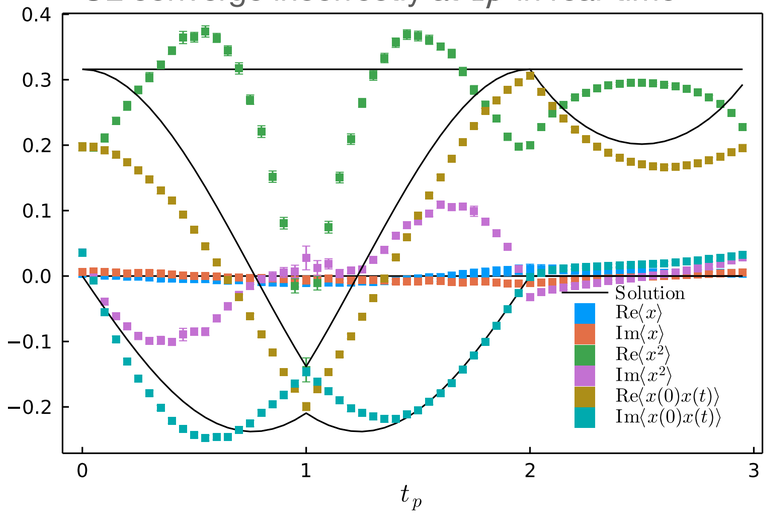
Problem of convergence to the wrong solution

Problem of wrong convergence

- Taking $\Delta\tau \to 0$ (Langevin time-step) not solution
- Correctness criterion: Boundary terms

  Aarts, James, Seiler, Stamatescu (2011)
- Real-time problems:
  - Fokker-Planck equilibrium distribution not e^{iS}?

CL converge incorrectly at 1β in real-time



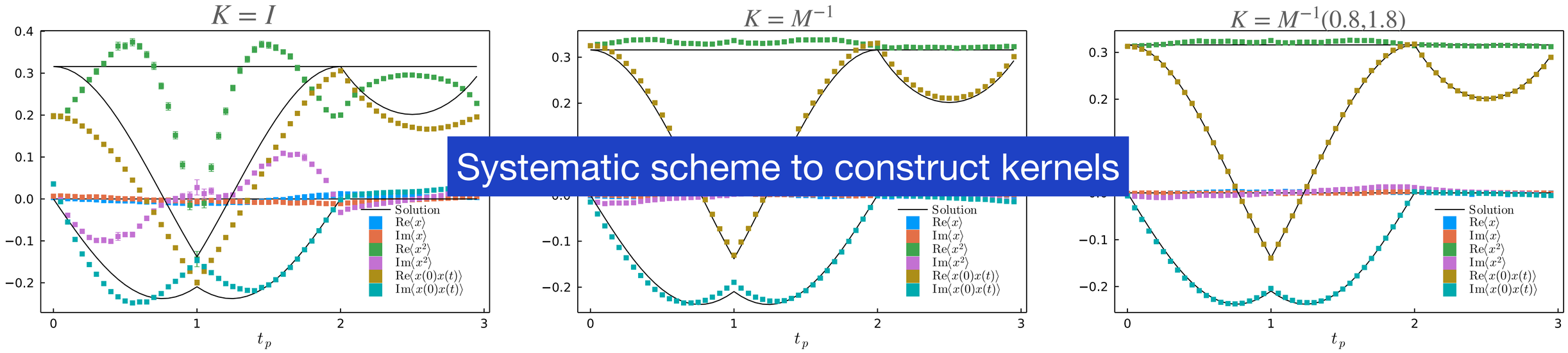
Fixing the problem

- 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)

Kernelled complex Langevin

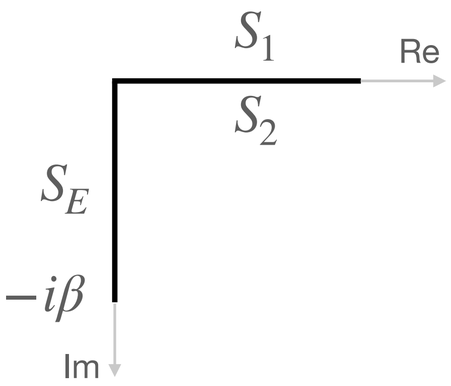
- Interactive theory: $d\phi = K\, i\frac{\partial S[\phi]}{\partial \phi} d\tau_L + \sqrt{K} dW, \quad i\frac{\partial S[\phi]}{\partial \phi} = iM\phi - i\frac{\lambda}{6}\phi^3$
- Free theory propagator kernel for interactive theory: $K = iM^{-1}$

$$d\phi = -\phi + M^{-1}\frac{\lambda}{6}\phi^3 + \sqrt{iM^{-1}}dW$$

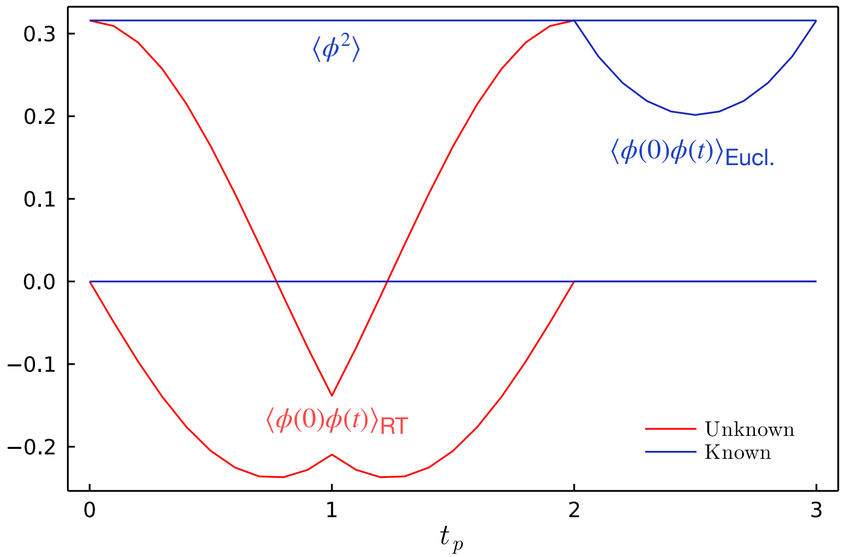


Systematic scheme to construct kernels

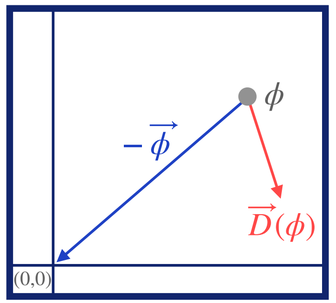
Construct kernel using prior knowledge



- 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
  - Contour symmetries (Forward-backwards real-time)
  - Fokker-Planck eigenvalues?
- 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 (Work in progress)



Low cost update



- Boundary terms accumulate with too slow falloff in the distribution.
- Minimising the drift out from origin
- Fast evaluation of the gradient $\nabla_K L_D(\{\phi\})$
- Gradient descent optimisation
- Use L^{Sym}, L^{Eucl}, L^{BT} to test result from minimising L_D

$$L_D = \left| D(\phi)\cdot(-\phi) - |D(\phi)||\phi| \right|^{\xi},$$

where $\quad D = K\dfrac{\partial S}{\partial \phi}$

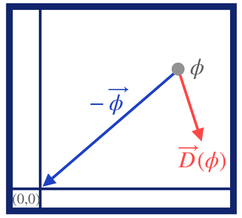
Boundary terms (L^{BT}) are minimised when we minimise L_D

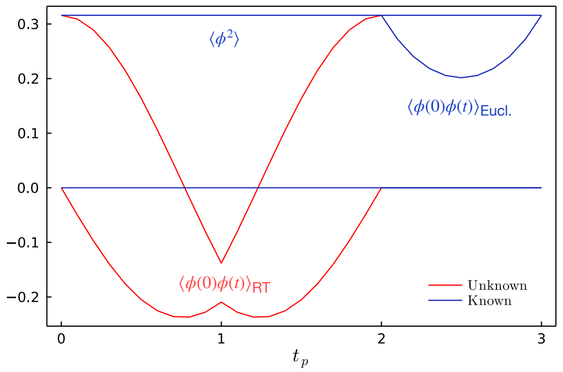
Holomorphic CL: Correctness criterion

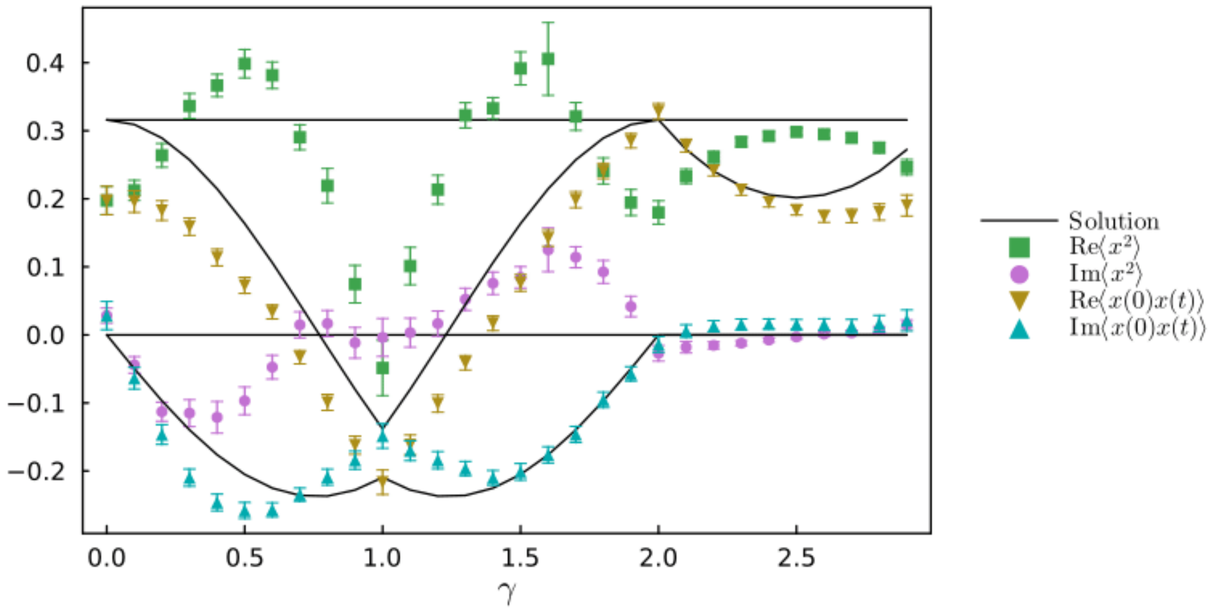
Real-time interactive theory

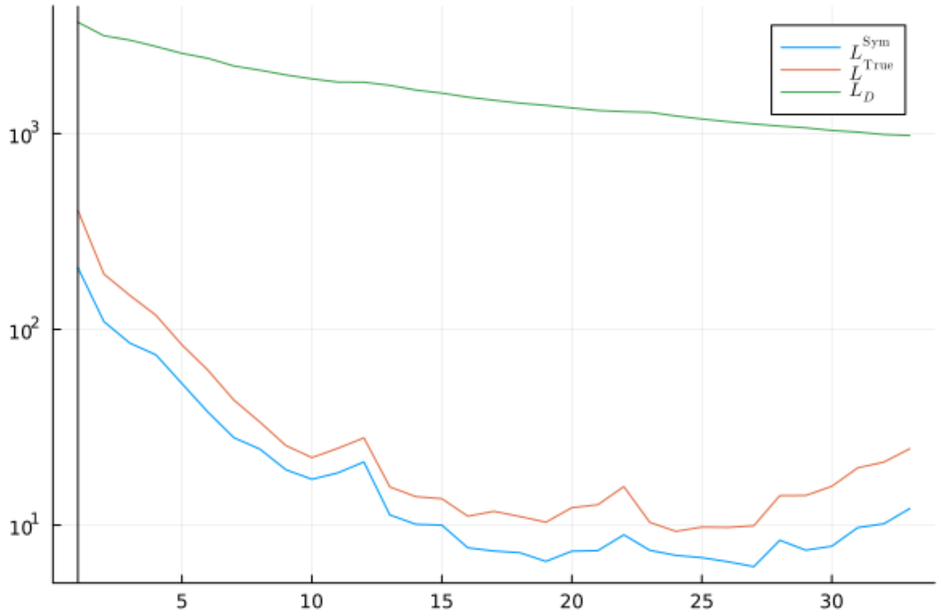
$$L_D = \left| D(\phi)\cdot(-\phi) - |D(\phi)||\phi| \right|^{\xi},$$

where $D = K\dfrac{\partial S}{\partial \phi}$





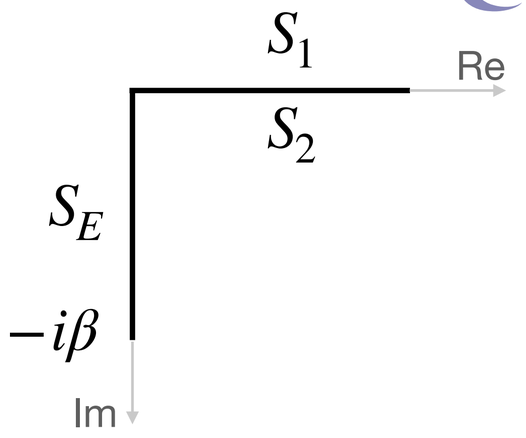


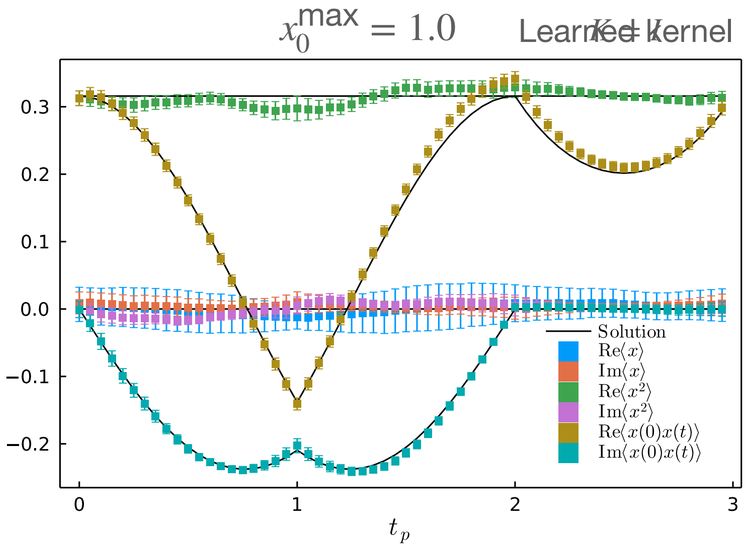


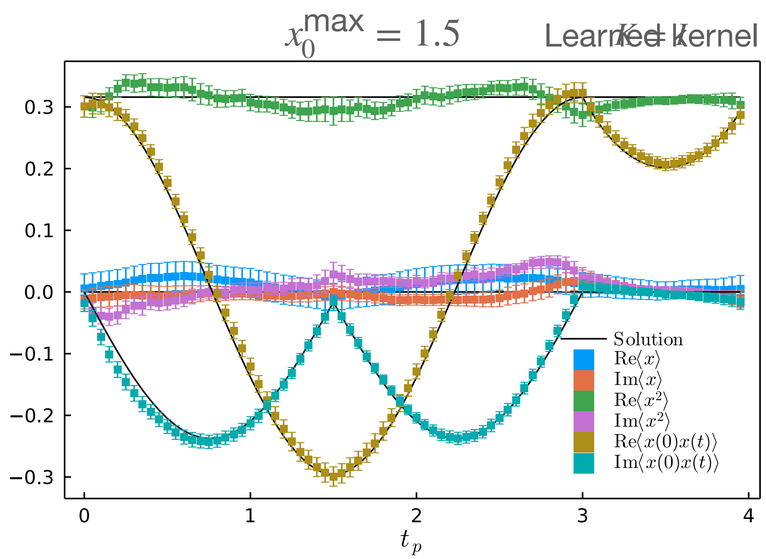
Optimisation using L_D, selecting iteration with best L^{Sym}

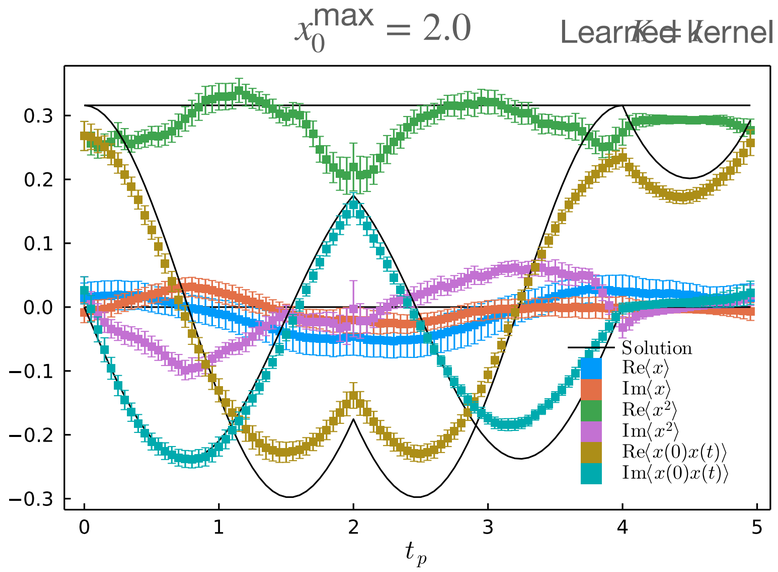
Real-time interactive theory results

- 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: $\dfrac{dS[\phi]}{d\phi} = 0$ (Free theory OK)







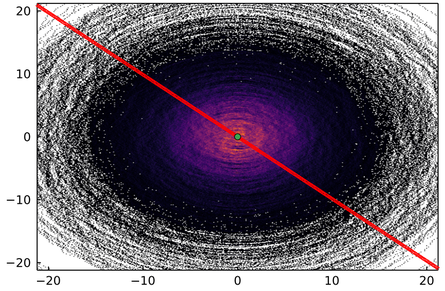


$L_{\text{True}} = |\langle x\rangle - \langle x\rangle_{\text{True}}| + |\langle x^2\rangle - \langle x^2\rangle_{\text{True}}|$

Connection with thimbles

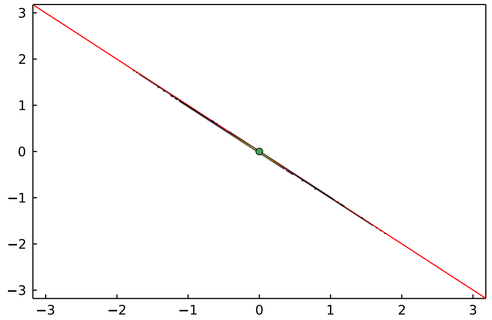
- Lefschetz thimbles: $\dfrac{d\phi}{d\tau} = \overline{\dfrac{dS[\phi]}{d\phi}}$
- Simplest model: $S = \dfrac{1}{2} i x^2$

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



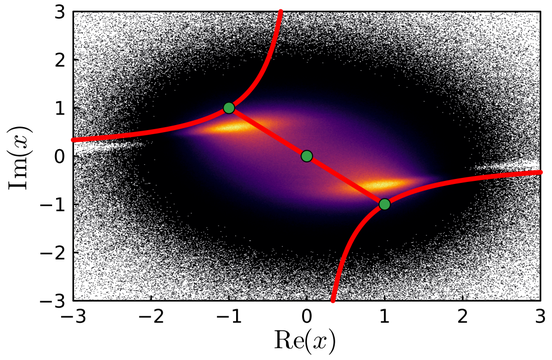
Optimising L_D=0 →

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



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

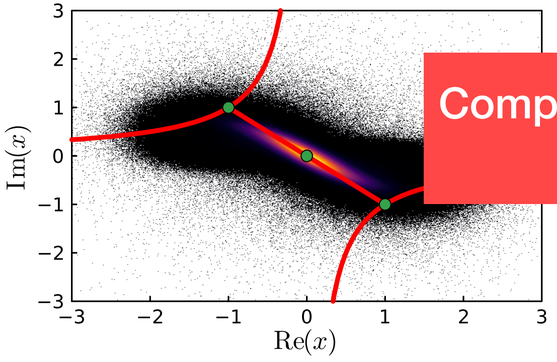
- Models with more than one critical point $S = 2i\phi^2 + \dfrac{1}{2}\phi^4$



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

Two minimas

Converges to correct solution



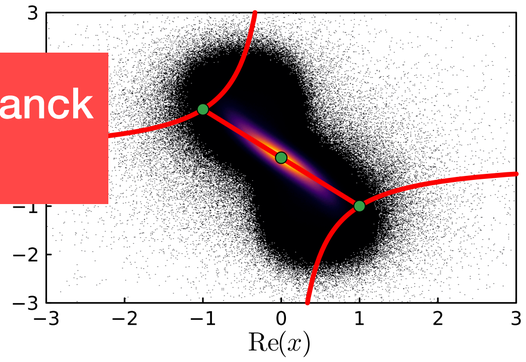
$K_N \dfrac{dS[\phi]}{d\phi} = e^{-i\frac{\pi}{3}}(4i\phi + 2\phi^3)$

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

Complex Fokker-Planck eigenvalues

And

Converges to wrong solution



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

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

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

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

Correctness cycle

Aarts, James, Seiler, Stamatescu (2011)

Real Action

Fokker-Planck for real action

$$\partial_t P_R = \partial_x K(\partial_x - \nabla S) P_R$$

Equilibrium distribution e^{-S}

$-S \in \mathbb{R}$

Real Langevin equation

$$d\phi = -K \nabla S \, d\tau + H dW$$

Complexification

$\phi \to \phi_R + i\phi_I$

Complex Action

$iS \in \mathbb{C}$

Complex Langevin equation

$$d\phi = iK \nabla S \, d\tau + H dW$$

Complex Action

$iS \in \mathbb{C}$

Complex Fokker-Planck

$$\partial_t \rho = \partial_x K(\partial_x + i \nabla S)\rho = L_0^T \rho$$

Equilibrium distribution e^{iS} ?

$\langle L^n \mathcal{O} \rangle = 0$

?

True if no boundary terms present

Fokker-Planck for complexified Langevin

$$\partial_t P = \left[(\partial_x H_R + \partial_y H_I)^2 + \partial_x Re(iK \nabla S) + \partial_y Im(iK \nabla S) \right] P = L^T P$$

? $L_0^T \Phi = \lambda \Phi$

$Re(\lambda) \leq 0$

$$\lim_{t \to \infty} \langle \mathcal{O} \rangle_{\rho(t)} = \langle \mathcal{O} \rangle_{\rho(\infty)}, \quad \rho \propto e^{iS}$$

Modification to CLE necessary when $Re(\lambda) \nleq 0$

Klauder, Petersen (1985)

Boundary terms and kernels

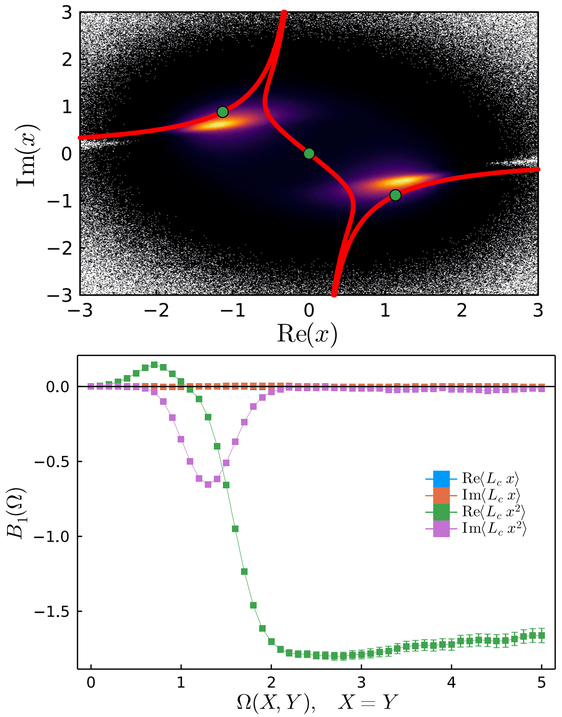
$$S = \frac{1}{2}\sigma x^2 + \frac{\lambda}{4}x^4$$

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

- Minimising L_D minimise the boundary terms:
  - $B_1(Y) = \left\langle L_c \mathcal{O}(x+iy)\right\rangle = \left\langle (\nabla_x + \nabla S) K \nabla_x \mathcal{O}(x+iy)\right\rangle_Y$
- No boundary terms $\neq$ true solution when using a kernel; equilibrium distribution not e^{-S}

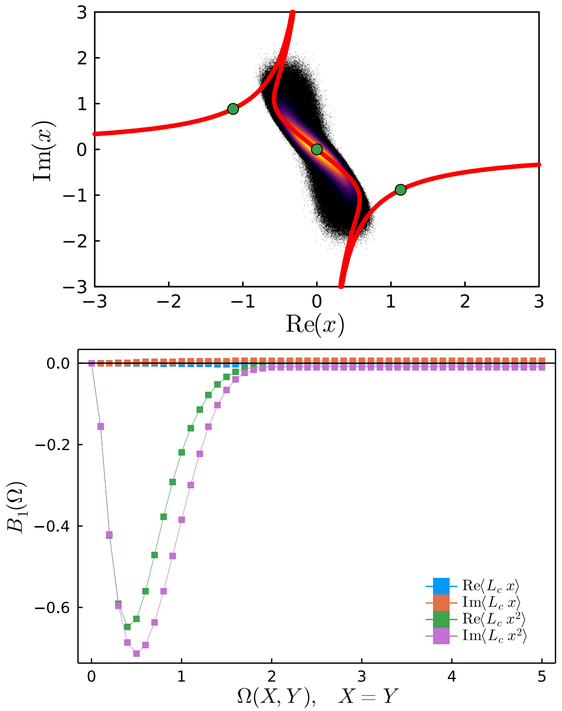
$L_{\text{True}} = |\langle x\rangle - \langle x\rangle_{\text{True}}| + |\langle x^2\rangle - \langle x^2\rangle|$

$K = 1$



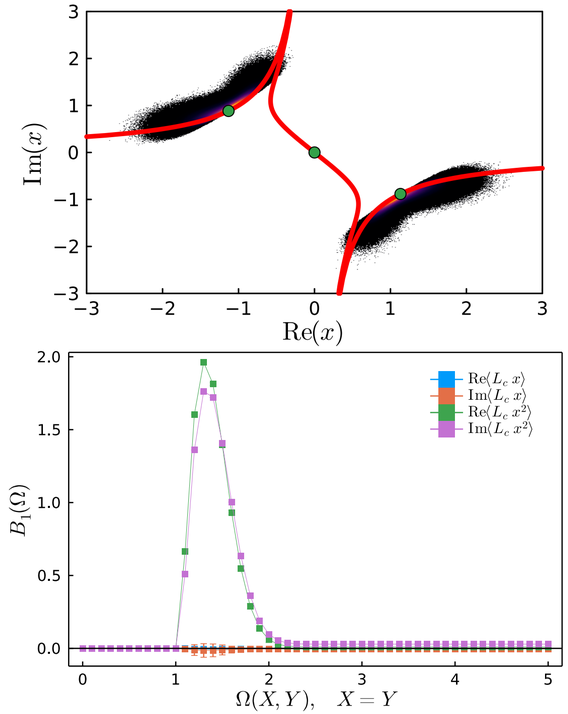
$L_{\text{True}} = 0.888 \pm 0.008$

$K = e^{-i\frac{3\pi}{4}}$



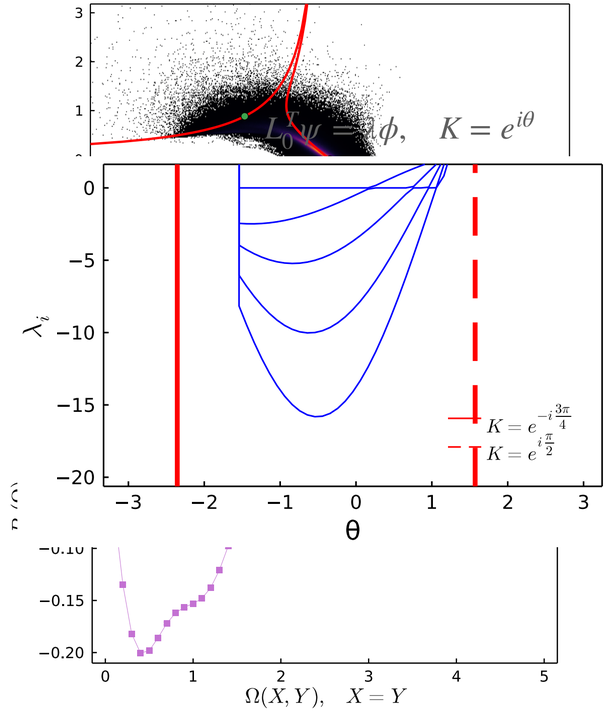
$L_{\text{True}} = 0.486 \pm 0.002$

$K = e^{-i\frac{6\pi}{4}} = e^{i\frac{\pi}{2}}$



$L_{\text{True}} = 2.15 \pm 0.11$

Field dependent kernel
Okano, Schülke, Zheng (1991)



$L_{\text{True}} = 0.023 \pm 0.024$

Summary and Outlook

- Implicit scheme; Stabilise and regularise real-time CL

- Goal: extending real-time convergence CL
- Kernel controlled complex Langevin:
  - Free scalar theory: ok with kernel
  - Optimised kernel in real-time thermal ϕ^4 theory

- Minimising drift loss L_D minimise boundary terms
- Kernels can alter Fokker-Planck eigenvalue spectrum

- Implicit scheme for gauge models

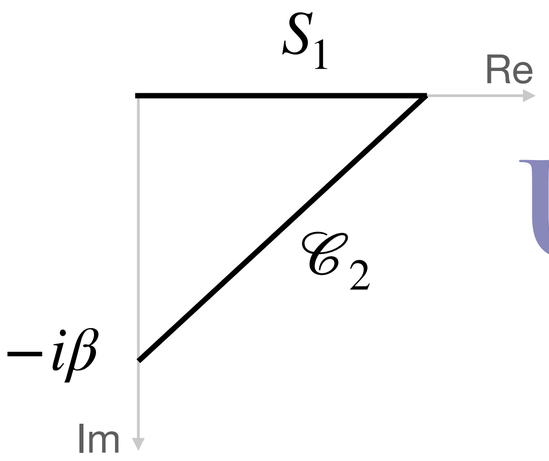
- Kernel as appropriately parameterised function
  - Field dependent kernel

- Improved loss function including more than one of the critical points

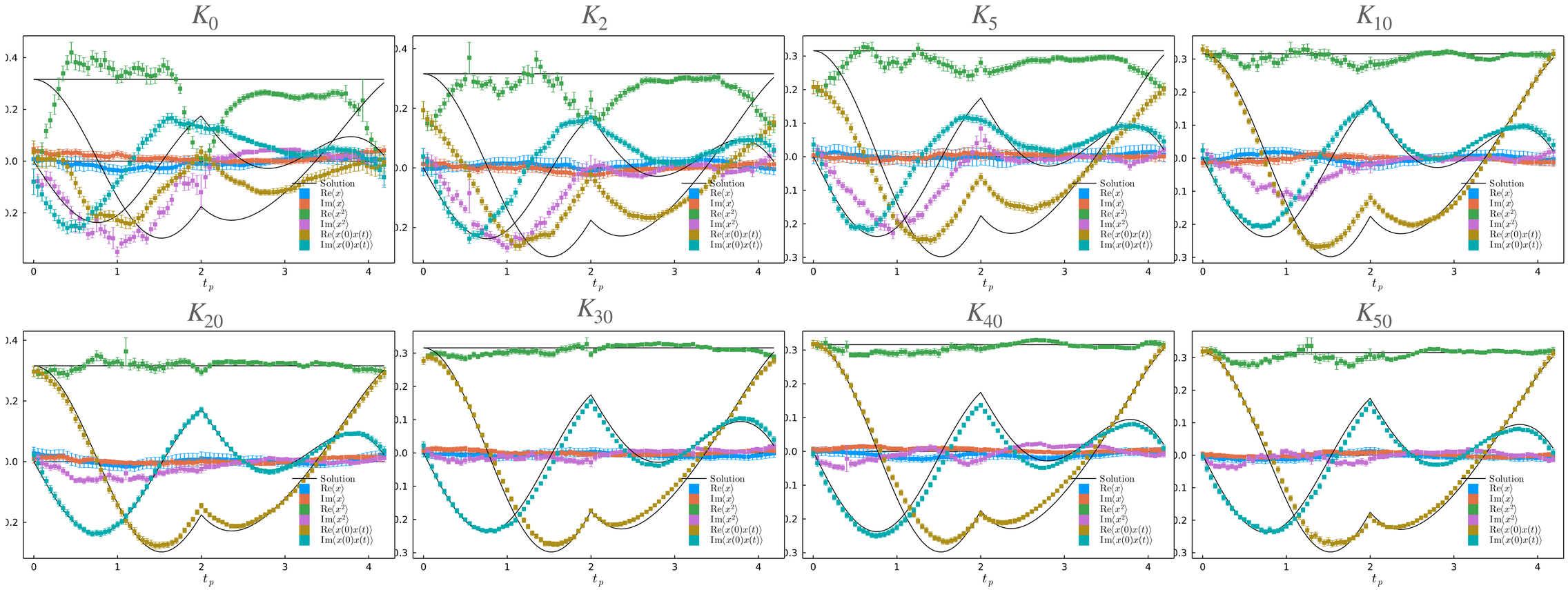
- Sensitivity analysis of full complex Langevin simulation

Thank you

Backward tilted contour

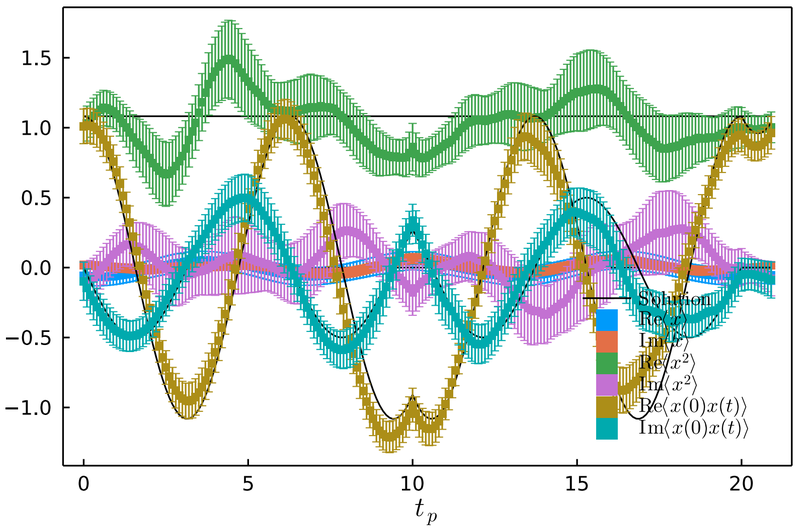


- Follow real axis up to $x_0^{\text{max}} = 2.0$
- Using $\beta = 1.0$, $m = 1$, $\lambda = 24$
- Form of the kernel $K = e^{A+iB}$



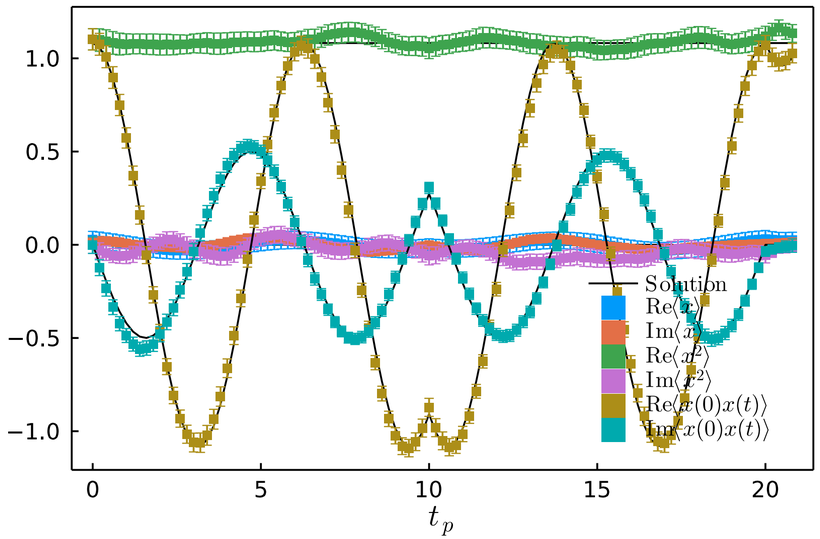
Learning free theory kernel

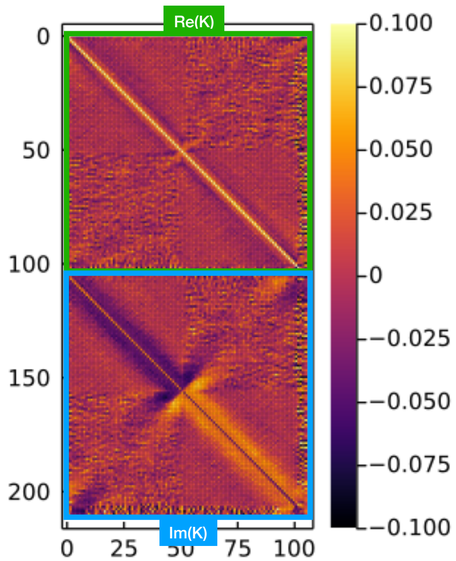
- Able to find kernel for all real-times when only one critical point at the origin
- Kernel form $K = e^{A+iB}$



Optimising L_D using constant kernel

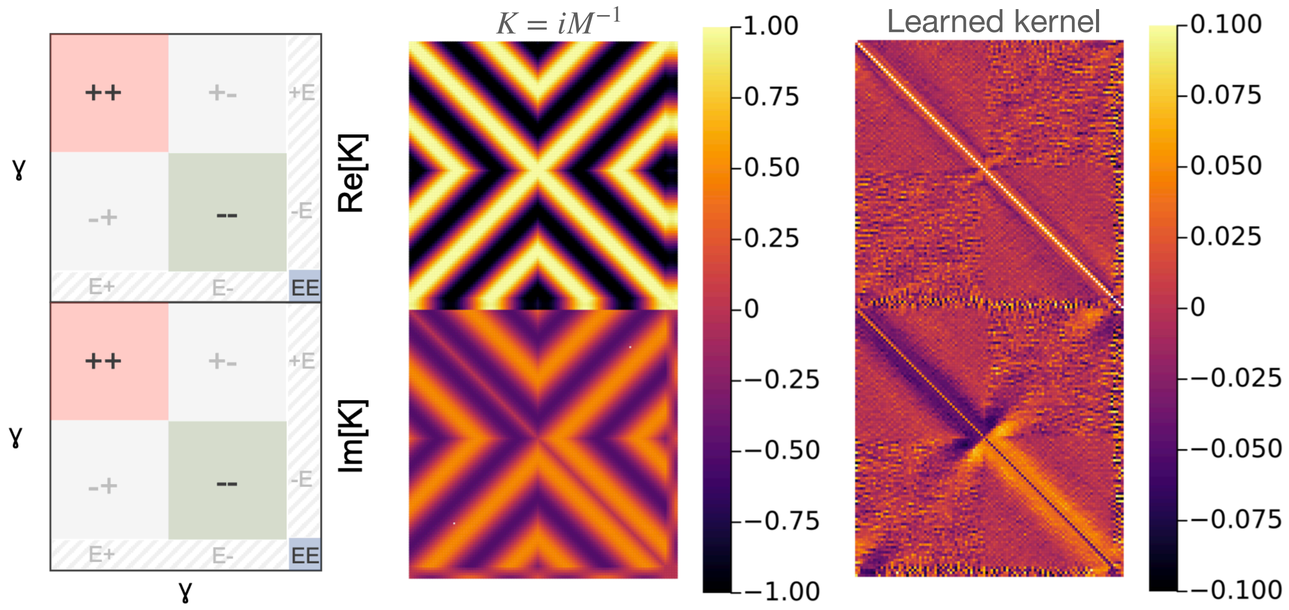
30 iterations

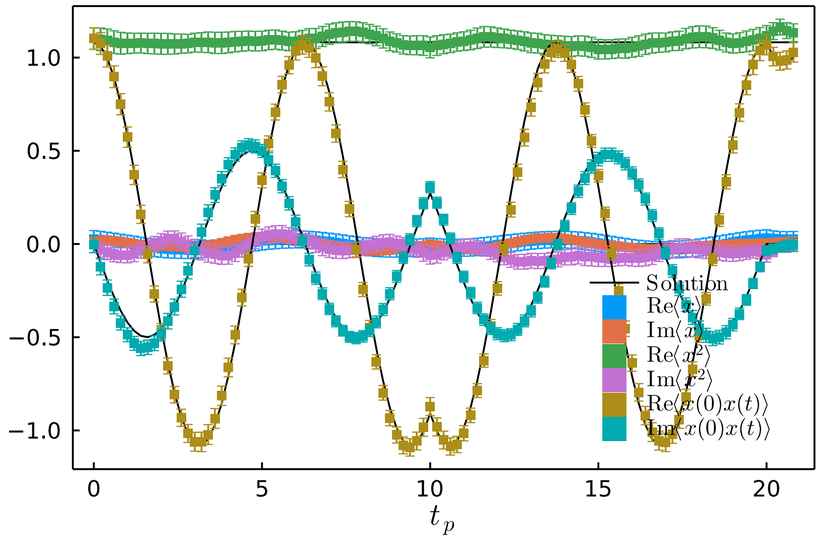




Kernel form after optimisation

- Free theory up to 10 in real-time





Field dependent kernel

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

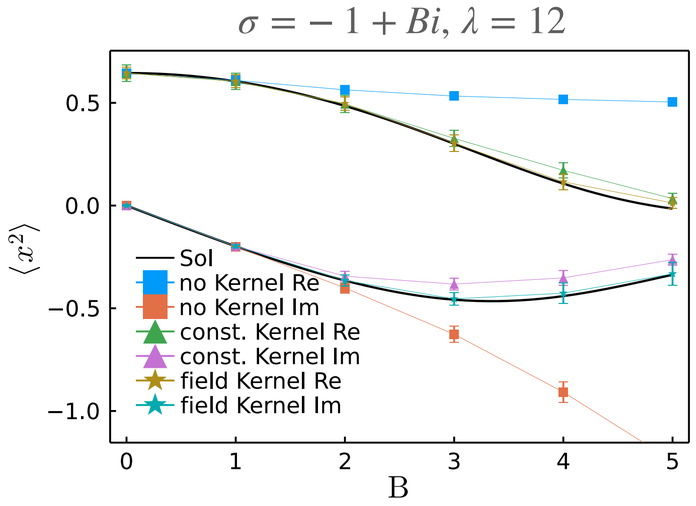
- Need to add extra derivative term

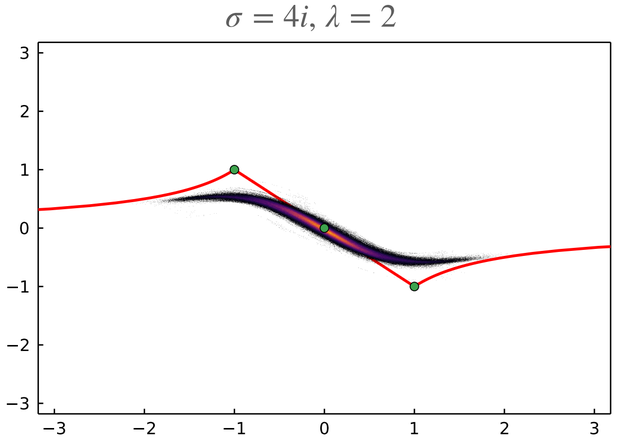
$$\frac{d\phi}{d\tau_0} = K[\phi]\frac{\delta S[\phi]}{\delta\phi} + \frac{\partial K[\phi]}{\partial\phi} + \sqrt{K[\phi]}\xi$$

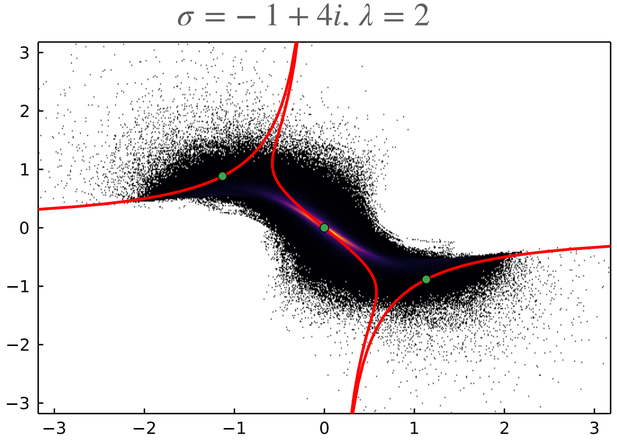
$$K = \frac{1}{|\sigma|}f(x^2)e^{-i\theta_\sigma} + \frac{1}{|\lambda|}(1 - f(x^2))e^{-i\theta_\lambda}$$

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

Okano, Schülke, Zheng (1991)

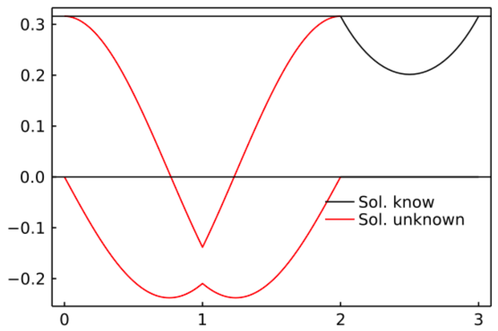


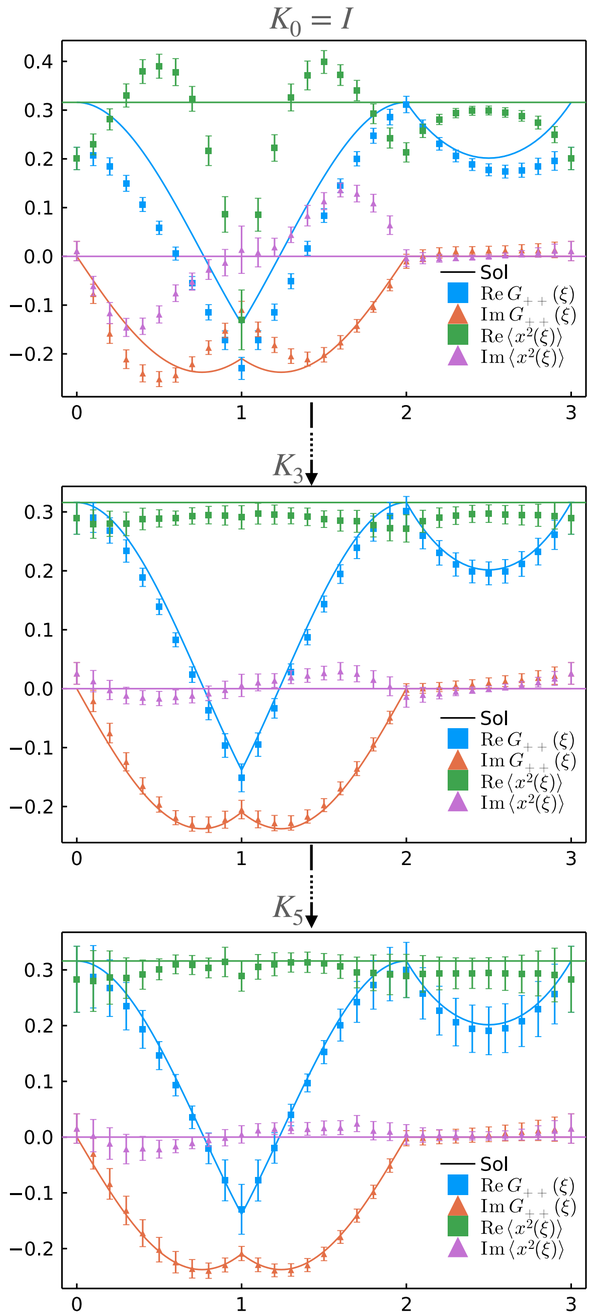




Construct kernel

- 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



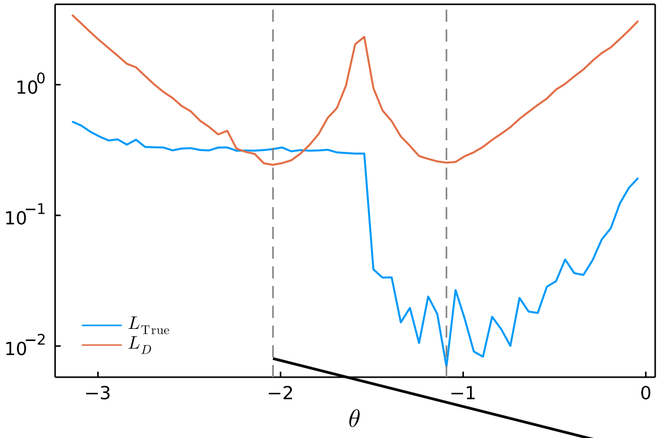


More info about simple model results

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

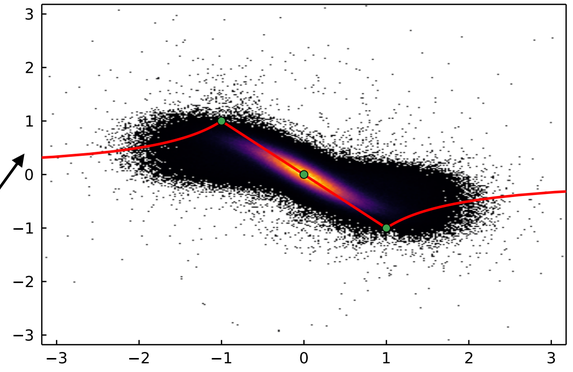
$\sigma = 4i,\ \lambda = 2$

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



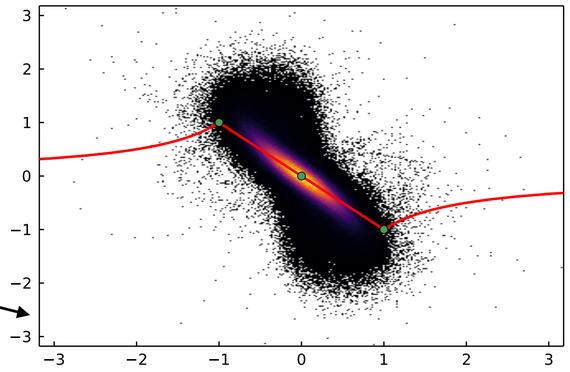
$K = e^{-i\frac{\pi}{3}}$

$\langle x^2 \rangle = 0.154 \pm 0.005 - i(0.306 \pm 0.005)$

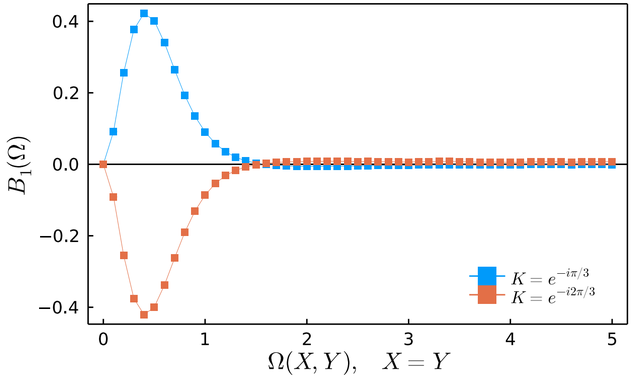


$K = e^{-i\frac{2\pi}{3}}$

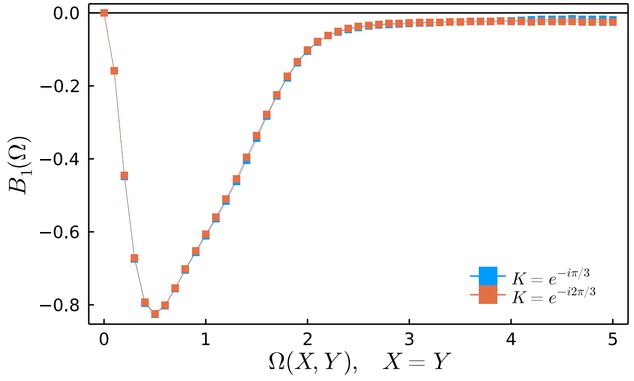
$\langle x^2 \rangle = -0.160 \pm 0.004 - i(0.314 \pm 0.004)$



$\mathrm{Re}\langle L_c\, x^2 \rangle$

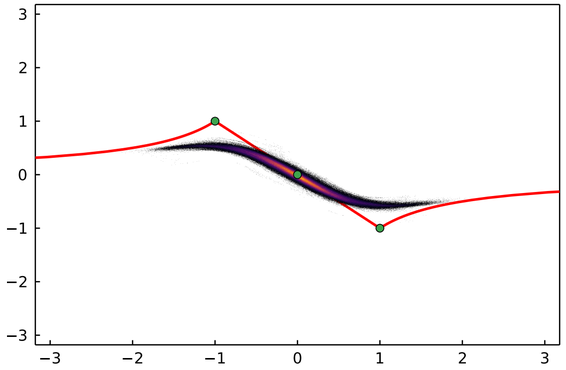


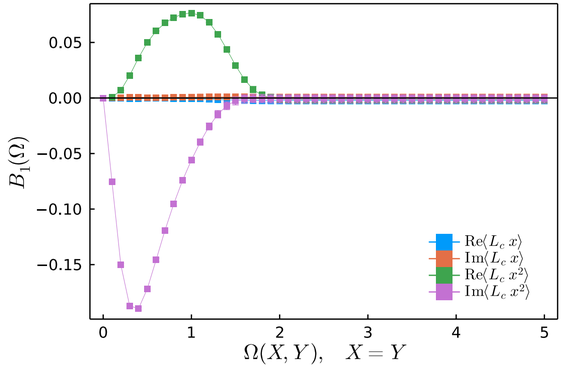
$\mathrm{Im}\langle L_c\, x^2 \rangle$



Field dependent

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

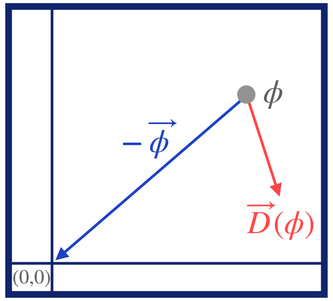




Low cost update scheme

$$L_D = \left| D(\phi)\cdot(-\phi) - |D(\phi)|\,|\phi| \right|^{\xi}$$

where $D = K\dfrac{\delta S}{\delta \phi}$



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}