SIGN25 Workshop in Bern, Switzerland

# Towards Real-Time Observables from First Principles: Correlators in 3+1D Yang-Mills Theory

In collaboration with Kirill Boguslavski and David I. Müller

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Paul Hotzy, 24.01.2025

# Content

1. Real-time simulations via Complex Langevin:
   Motivation and introduction

2. Complex Langevin for Yang-Mills field theory

3. Criteria of correctness, stabilization methods,
   and the role of kernels

4. Introduction and benchmarks for an anisotropic kernel

5. Real-time correlation function from CL

6. Limitation, conclusion, and outlook

# Motivation

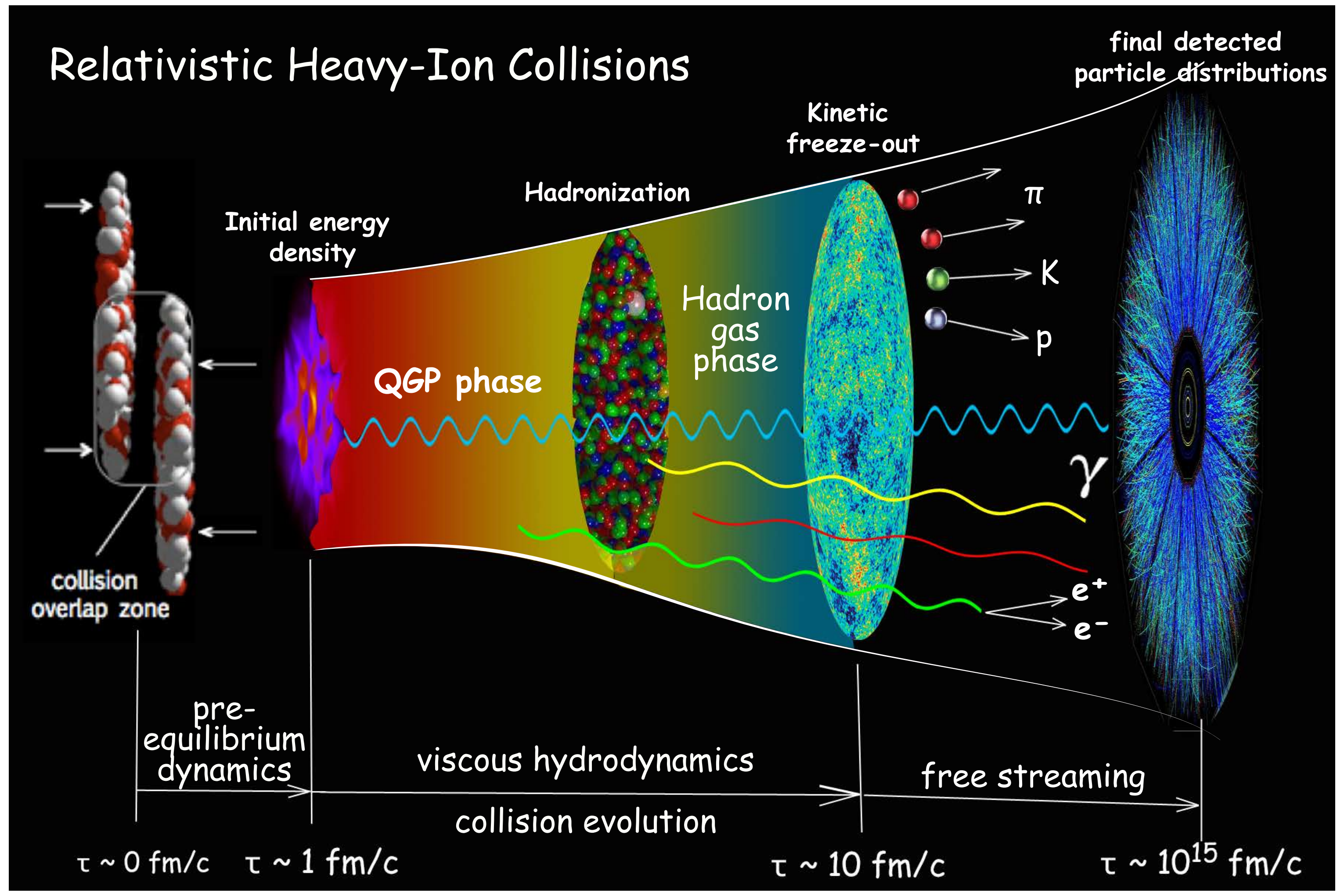
# A major roadblock for theoretical physics

## No first principle access of fundamental quantities for heavy-ion collisions

- There is **no first principle description** of the quark-gluon plasma (QGP) after heavy-ion collisions

- Various stages with different assumptions: classical statistical approximation, kinetic theory, holography, . . .

- **Ab-initio description** of real-time dynamics allows a coherent understanding of the QGP-dynamics




C. Shen, U. Heinz [arxiv:1507.01558]

- Direct computations of **QCD real-time observables** are difficult due to the **sign problem** (next slide)

- The **sign problem limits many different fields** — progress may impact other research areas (QCD at finite chemical potential, cold quantum gases, compact stars, many-body physics, . . . .)

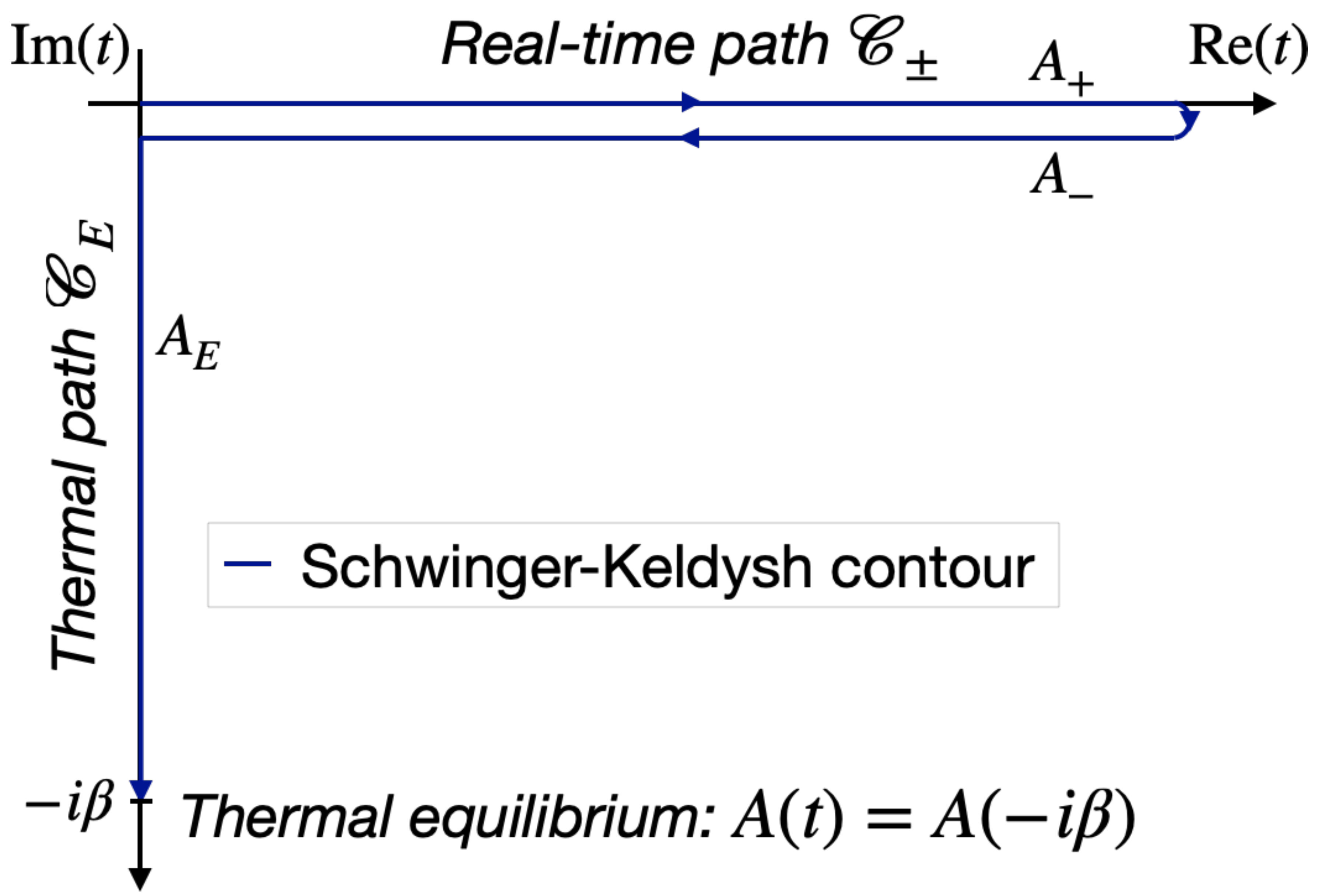
# Real-time sign problem

## Action becomes complex when physical time is not Wick rotated

- Yang-Mills action — integration along contour: $S_{\text{YM}} = -\frac{1}{4}\int_{\mathscr{C}_\pm, \mathscr{C}_E} d^4x\, F_a^{\mu\nu} F^a_{\mu\nu}$
- Path integral along the Schwinger-Keldysh contour

$$\langle \mathcal{O}[A] \rangle = \frac{1}{Z}\int \mathscr{D}A e^{-S[A]}\,\mathcal{O}[A]$$
$$= \frac{1}{Z}\int \mathscr{D}A_E\, e^{-S_E[A_E]} \int \mathscr{D}A_+ \mathscr{D}A_-\, \mathbf{e}^{\mathbf{iS[A_+,A_-]}}\, \mathcal{O}\left[A_+, A_-, A_E\right]$$

*This is the bad guy; the phase factor leads to an oscillatory integrand — sign problem!*




- Thermal path $\mathscr{C}_E$: periodic boundary encodes **thermal equilibrium** and temperature $T = 1/\beta$
- Real-time path $\mathscr{C}_\pm$: encodes physical time — **dynamical properties** of the gauge fields

# Introduction to complex Langevin

# Introduction to complex Langevin (1/2)

## A naive generalization of real Langevin

- **Langevin equation**:

$$\partial_\theta A^a_{x,\mu}(\theta) = K^a_{x,\mu}[A(\theta)] + \eta^a_{x,\mu}(\theta)$$

auxiliary time $\theta$

  - Drift term — describes classical evolution: $K^a_{x,\mu}[A(\theta)] = -\,\delta S \big/ \delta A^a_{x,\mu}$
  - Gaussian noise — encodes the quantum fluctuations: $\eta^a_{x,\mu}(\theta), \qquad \langle \eta^a_{x,\mu}(\theta)\eta^a_{y,\nu}(\theta)\rangle = 2\delta^{ab}\delta^{\mu\nu}\delta(x-y)\delta(\theta-\theta')$

- **Real action S:** dyn. variables $x$ are characterized by the limiting probability density $P(\theta \to \infty) \propto e^{-S}$
- **Complex action S:** drift term is complex — we need to complexify the dyn. variables

$$\mathfrak{su}(N_c) \ni A \to A = A_r + iA_i \in \mathfrak{sl}(N_c, \mathbb{C})$$

✳ CL yields (provided it is stable) a real density $P(A_r, A_i) \in \mathbb{R}$, but is it the one we are looking for?

$$\int \mathscr{D}A\, \mathcal{O}(A) e^{-S(A)} = \int \mathscr{D}A_r \mathscr{D}A_i\, P(A_r, A_i)\, \mathcal{O}(A_r + iA_i)$$

*Does that even exist?*

[D. Weingarten: Phys. Rev. Lett. **89**, 240201]

# Introduction to complex Langevin (2/2)

## A *less* naive generalization of real Langevin

- **Criteria of correctness** — we know when it fails:

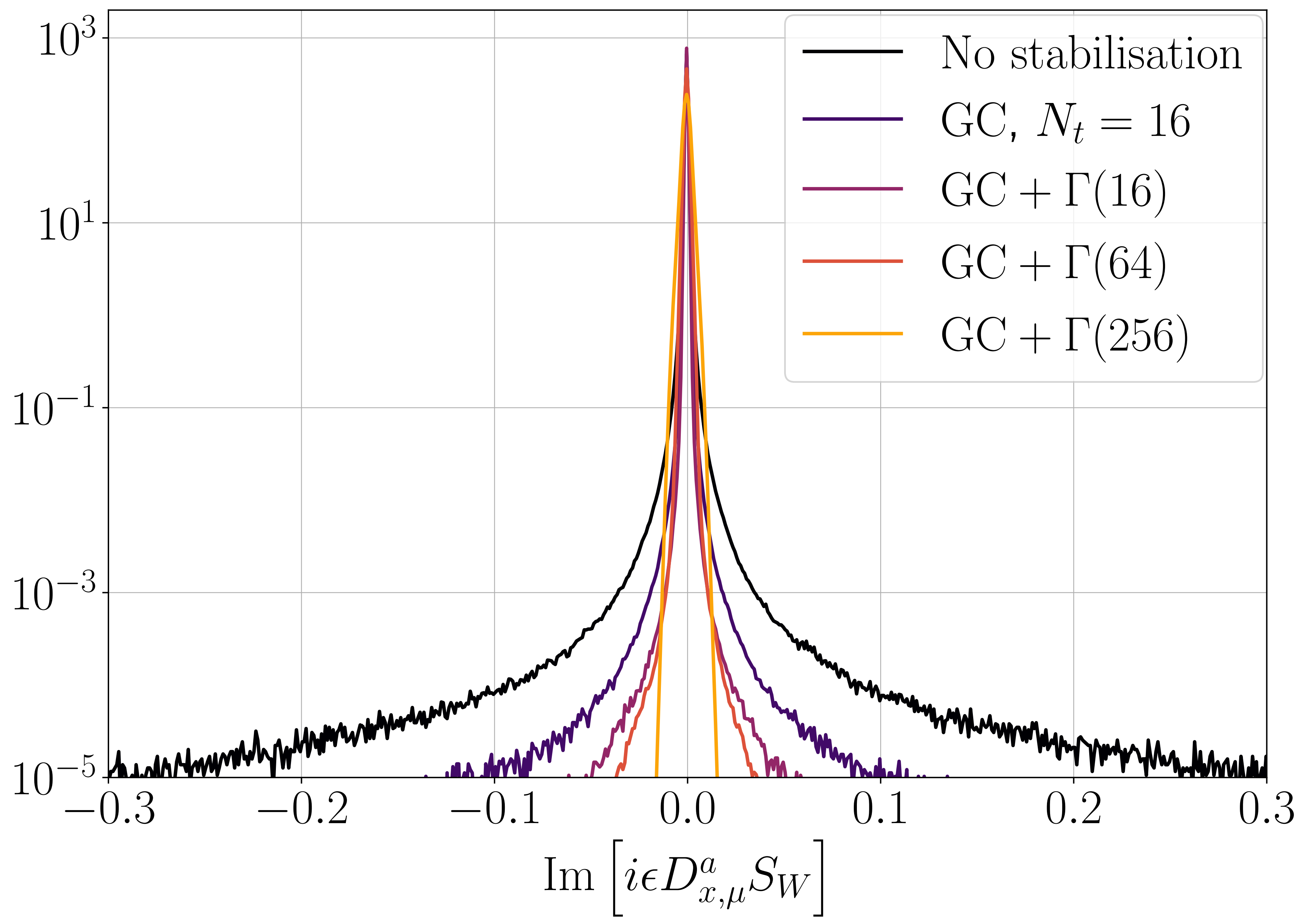
    1. Density of drift magnitude has to decay exponentially
    [K. Nagata et al: *Phys.Rev.D* 94 (2016) 11, 114515]

    $$p(u;\theta) = \int \mathcal{D}A_r \int \mathcal{D}A_i\, \delta(u - u(A_r + iA_i))P(A_r, A_i;\theta)$$
    $$u(A) = \|K(A)\|$$

    2. Vanishing boundary terms [D. Sexty et al: *Phys.Rev.D* 99 (2019) 1, 014512]

- Aposteriori checks — mostly diagnostic

***What shall we do if the criterion is not satisfied?***




*Computation expectation values with complex Langevin*

$$\langle \mathcal{O} \rangle = \frac{1}{Z}\int_D \mathcal{D}A \exp[-S(A)]\mathcal{O}(A) = \lim_{\Theta\to\infty}\int_{\theta_0}^{\theta_0+\Theta} d\theta\, \mathcal{O}(A(\theta))$$

# What can we do if the criterion is not fulfilled?

## Need for alternation of sampling algorithm to obtain correct (real) probability density

- CL was found give to wrong results ➞ interest crumbled after 80s

- Development of stabilization methods reinvigorated the interest

➞ *Adaptive stepsize*, *gauge cooling*, dynamical stabilization, regularization methods, **kernels**,...

$$\epsilon(\theta) = \min\left[\epsilon, B/\|K(A(\theta))\|\right]$$

$$\sum_{x,\mu} Tr\left[U^V_{x,\mu} U^{V\dagger}_{x,\mu} - 1\right] \rightarrow \min\,, \quad U^V_{x,\mu} = V_x U_{x,\mu} V^{-1}_{x+\mu}, \quad V \in SL(N_c, \mathbb{C})$$

Kernel transformations $\Gamma$ in one box

Kernelled CLE

$$\partial_\theta A_R(x) = K^\Gamma_R[A(x;\theta)] + \sqrt{\Gamma}\eta(x;\theta)$$

$$\partial_\theta A_I(x) = K^\Gamma_I[A(x;\theta)], \quad K^\Gamma = \int dx' \, \Gamma(x,x') K(x')$$

**?** ➞

Kernelled complex FPE

$$\partial_\theta \rho(A;\theta) = L^T_{c,\Gamma}\rho(A;\theta)$$

$$\rho(A;\theta \rightarrow \infty) \propto \exp\left(-S[A]\right)$$

*Depends on how the* ***real*** $P$ *changed*
*via the* ***kernelled real FPE*** ➞ *not fully understood!*

# CL for Lattice Yang-Mills theory (1/2)

## Complexification of the Wilson plaquette action

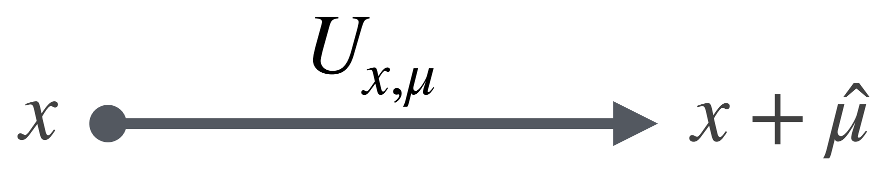
Yang-Mills action

$$S_{\mathrm{YM}} = -\frac{1}{4}\int d^4x\, F_a^{\mu\nu} F_{\mu\nu}^a$$

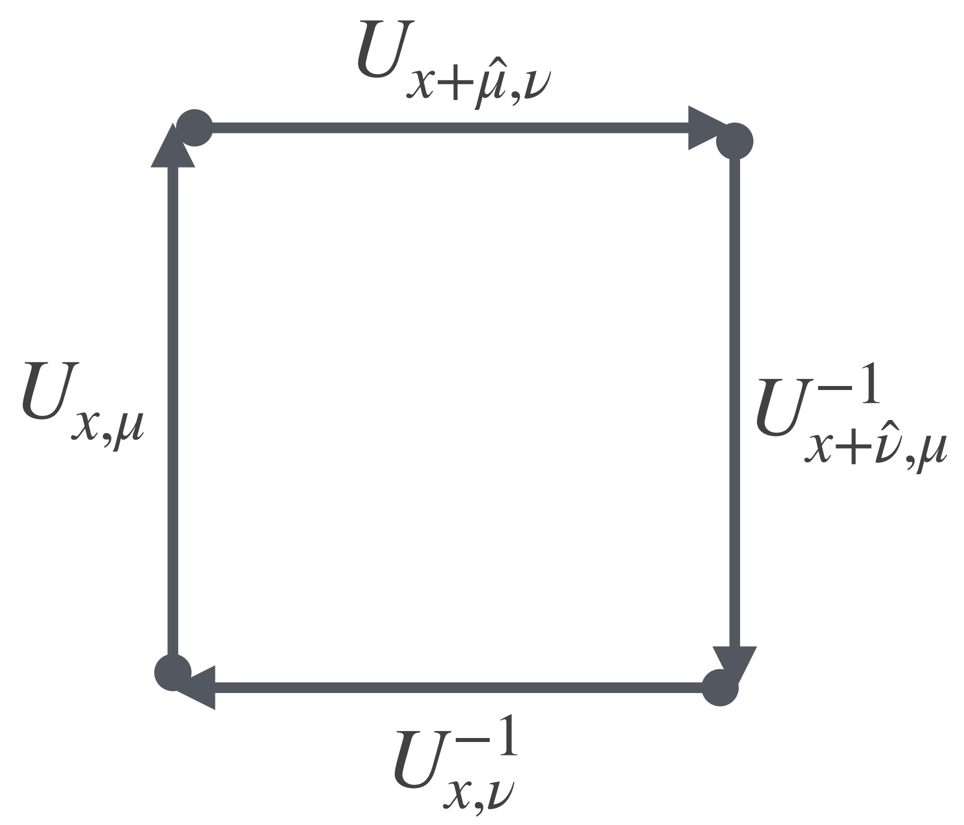
Wilson plaquette action

$$S_{\mathrm{w}} = \frac{1}{g^2} \sum_{x,\mu\neq\nu} \rho_{\mu\nu}(x) \mathrm{Tr}\left[U_{\mu\nu}(x) - 1\right]$$

$$\rho_{0i}(x) = -\frac{a_s}{a_t},\ \rho_{ij}(x) = \frac{a_t}{a_s}$$




$$U_{x,\mu} \simeq \exp\left[iga_\mu A_\mu(x+\hat{\mu}/2)\right] \in SL(N_c, \mathbb{C})$$




$$U_{x,\mu\nu} = U_{x,\mu} U_{x+\hat{\mu},\nu} U^{-1}_{x+\hat{\nu},\mu} U^{-1}_{x,\nu}$$

- Lattice spacing defines a *UV momentum cutoff* that vanishes for $a \to 0$ (scale setting required — not discussed in this talk!)
- Complex time contour is **encoded in complex temporal lattice spacing** $a_t \in \mathbb{C}$
- Complexification of link variables and plaquette (right figures)

# CL for Lattice Yang-Mills theory (2/2)

Introduction of an anisotropic kernel and the discretized CL equation

- CLE is numerically solved by the Euler-Maruyama scheme

$$U_{x,\mu}(\theta+\epsilon) = \exp\left[it^a\left(i\Gamma_\mu \epsilon\, D^a_{x,\mu} S_{\mathrm{W}} + \sqrt{\Gamma_\mu \epsilon}\, \eta^a_{x,\mu}(\theta)\right)\right] U_{x,\mu}(\theta)$$

field-independent kernel

- Anisotropic field-independent kernel:

$$\Gamma_0(t) = |a_0(t)|^2/a_s^2, \quad \Gamma_s = 1$$

- Temporal and spatial links are updated differently — direction-dependent time step

$$\rightarrow \quad \epsilon_0 = |a_t|^2/a_s^2\,\epsilon, \quad \epsilon_i = \epsilon$$

Autocorrelation time grows slower than stable sampling interval

→

**Higher anisotropies lead to greater stability!**

(see K. Boguslavski, PH, D. I. Müller: 10.1007/JHEP06(2023)011)

# Systematics
# of the anisotropic kernel

# Benchmarking of stabilizing effect (1/3)

## Comparision of one-point functions with Euclidean results

- Time translation invariance in thermal equilibrium allows **comparison of one-point fcts. with Euclidean results** (no sign problem)
- First results on isosceles contours already in 2006 [D. Sexty et al: hep-lat/0609058]
- Gauge cooling is not enough!
- Expectation values of spatial plaquette:

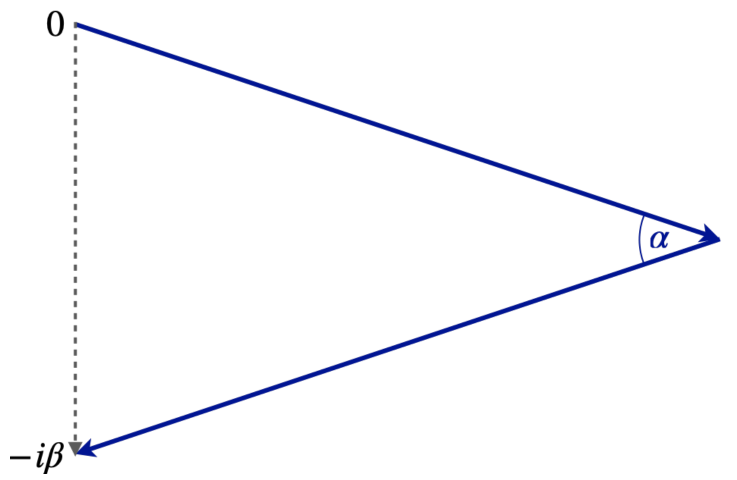
$$\mathcal{O}[U] = \frac{1}{6N_cN_x} \sum_{x,i\neq j} \mathrm{Tr}\left[U_{x,ij}\right]$$

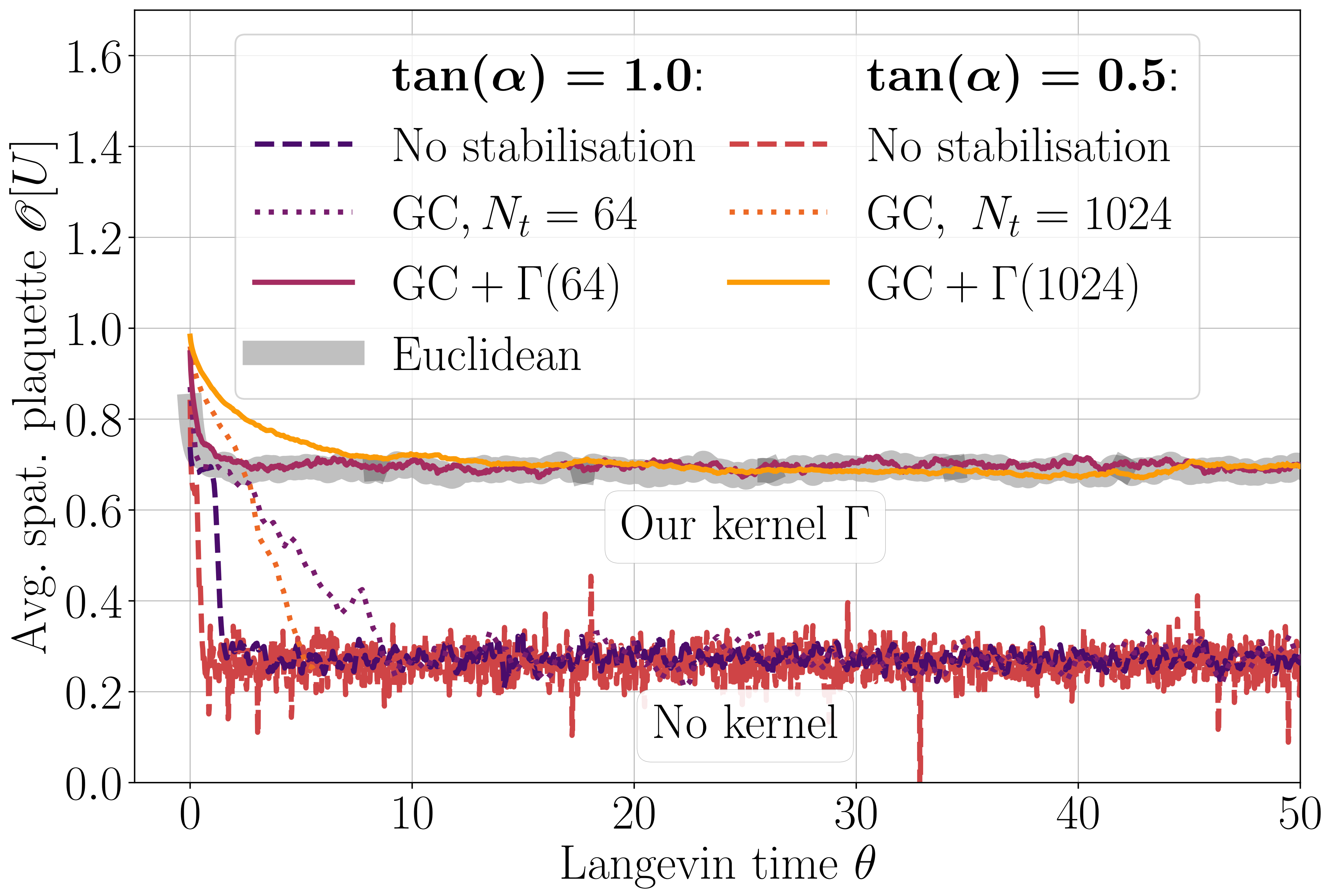
**Our kernel reproduces the Euclidean result!**

1+3D SU(2) Yang-Mills:

$L = 16 \times 4^3, N_c = 2,$

$g = 1, \beta = 1/T = 4$



# Benchmarking of stabilizing effect (2/3)

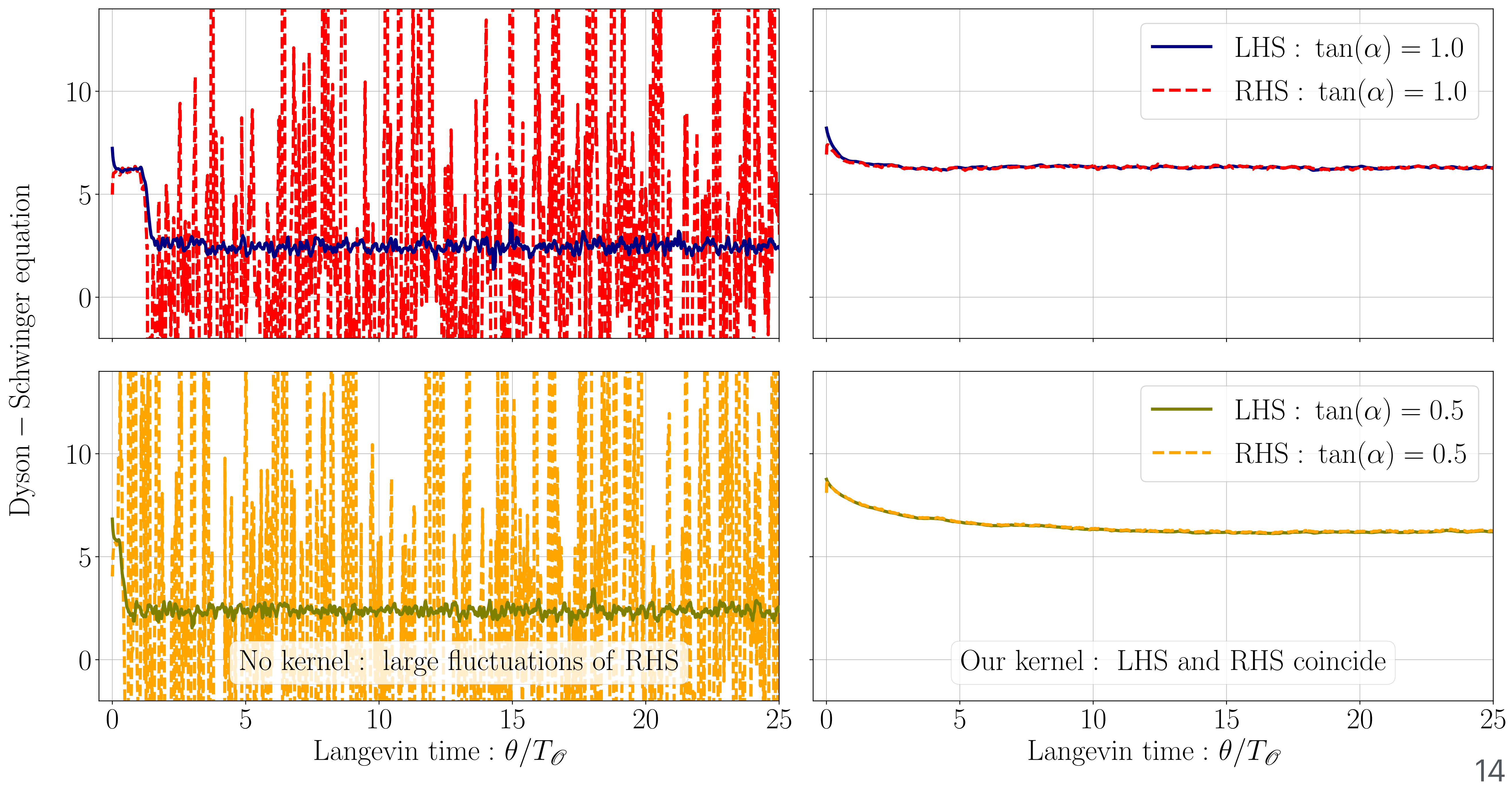
## Fluctuations of RHS of Dyson-Schwinger equations are sensitive to wrong convergence

- Dyson-Schwinger equations of trace of spatial plaquette variables $\mathrm{Tr}(U_{x,ij})$
- Provides elf-consistency check of the validity of link configuration
- RHS of Dyson-Schwinger equations is very sensitive to instabilities
  ➞ good probe for stability

**Kernel leads to satisfied DSE!**

$$\frac{2(N_c^2-1)}{N_c}\left\langle \mathrm{Tr}(U_{x,ij})\right\rangle = \frac{i}{2N_c}\sum_{|\rho|\neq i}\beta_{i\rho}\left\langle \mathrm{Tr}\left[(U_{x,i\rho}-U_{x,i\rho}^{-1})U_{x,ij}\right]\right\rangle$$

*No kernel* *Our kernel*



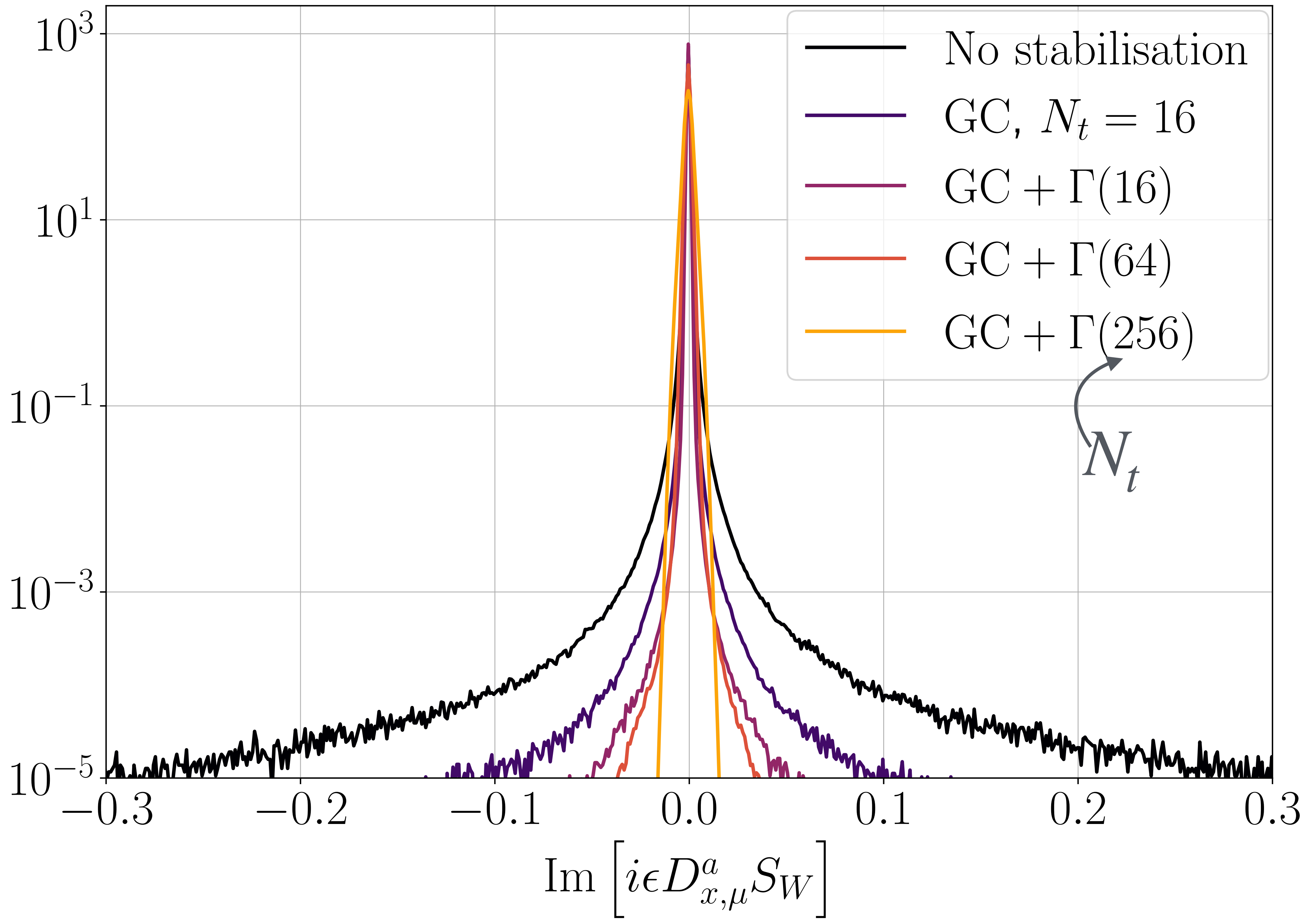
# Benchmarking of stabilizing effect (3/3)

## Direct check of criterion of correctness

- If the density of the drift magnitude decays exponentially
  ➞ CL converges correctly

- Compact support of histogram ➞ criterion is satisfied

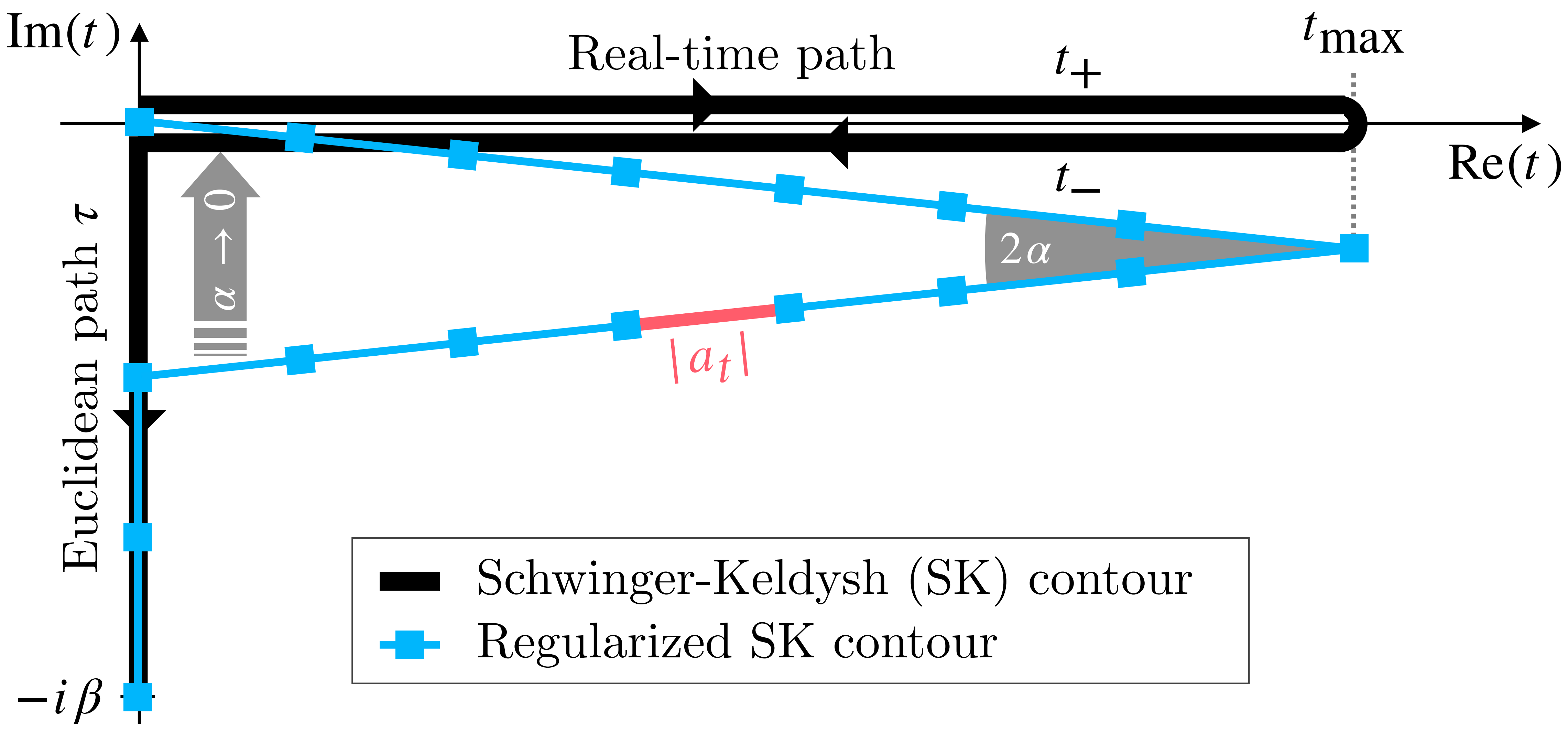
**Kernel systematically localizes the histogram for growing $N_t$ or larger anisotropies $a_s / |a_t|$ !**



# Results for unequal real-time correlation functions

# Simulation strategy

- **Path integral along SK-contour: temporal continuum limit $a_t \to 0$ is ill-defined**
  - → Regularization by tilt angle $\alpha$ needed
    - → Extrapolation to real-time contour $\alpha \to 0$

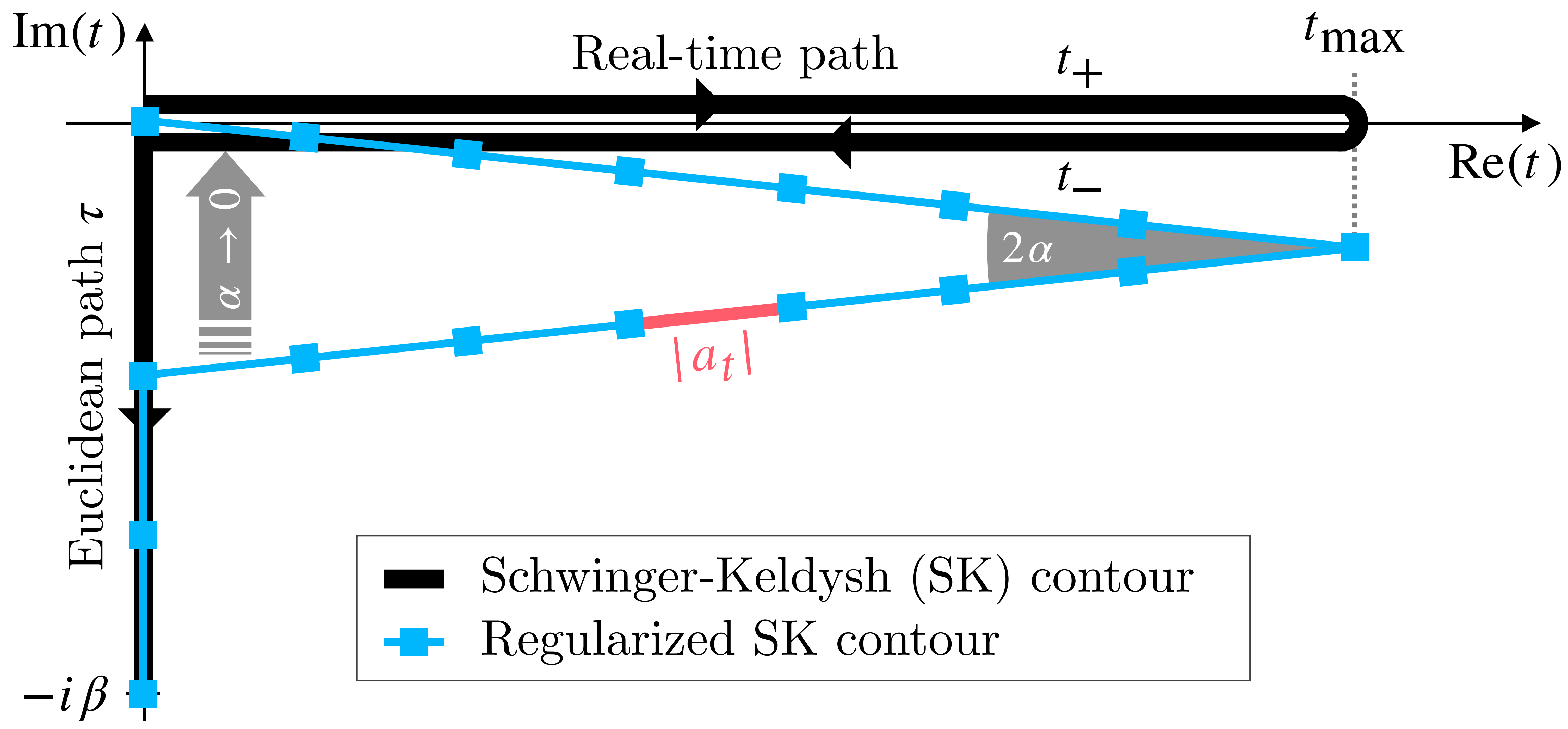



- **Smaller tilt angles lead to aggravated instabilities**
  - → Anisotropic kernel counteracts instability by tuning the lattice anisotropy $a_t/a_s \to 0$
    - → Kernel in the temporal continuum limit **naturally and systematically stabilizes** simulations
      - → Extrapolation $\alpha \to 0$ at sufficiently small $a_t$ (stable simualtions)

# Model and simulation parameters

*Depends on tilt angle, as length of contour!*

- **Lattice SU(2) Yang-Mills theory:**
  - 1+3D lattice with $N_t \times N_s^3 \approx 64 \times 16^3$
  - Various regularization angles $\tan(\alpha) \in [1/3, 1/96]$
  - *Real-time extent of* $\max[Re(t)] = 1.5\beta = 1.5$
  - *Very, very small bare coupling* $g = 0.5$




- **Simulation parameters:**
  - Langevin step size $\epsilon = 10^{-4}$
  - Sampling interval $\theta \in [10, 20]$ (cold start)
  - Adaptive step size $B = 10^3$ (just catches outliers)
  - Gauge cooling $N_{GC} = 1, \alpha_{GC} = 0.05$
  - Anisotropic kernel factor $\Gamma_0 = |a_t|^2 / a_s^2 = 1/16^2,\ \Gamma_i = 1$

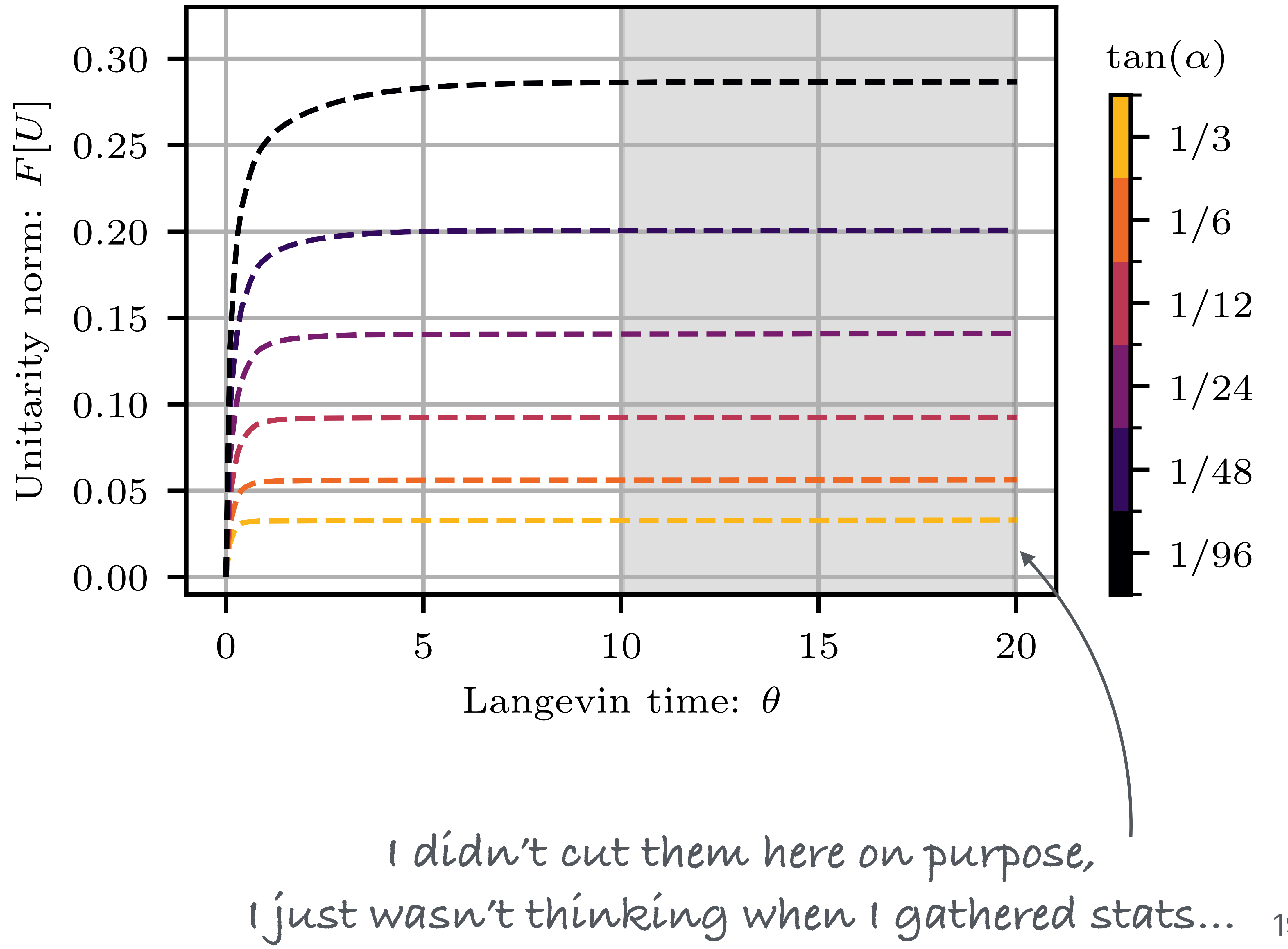
# Constant unitarity norm (1/2)

## Sampling from trajectory intervals with constant unitarity norm

- We sample in a Langevin time interval, where the unitarity norm is constant
  → **no broadening of distribution in complex space**

- Various tilt angles $\alpha$ all lead to a plateau
  → **plateau height depends on the angle $\alpha$**

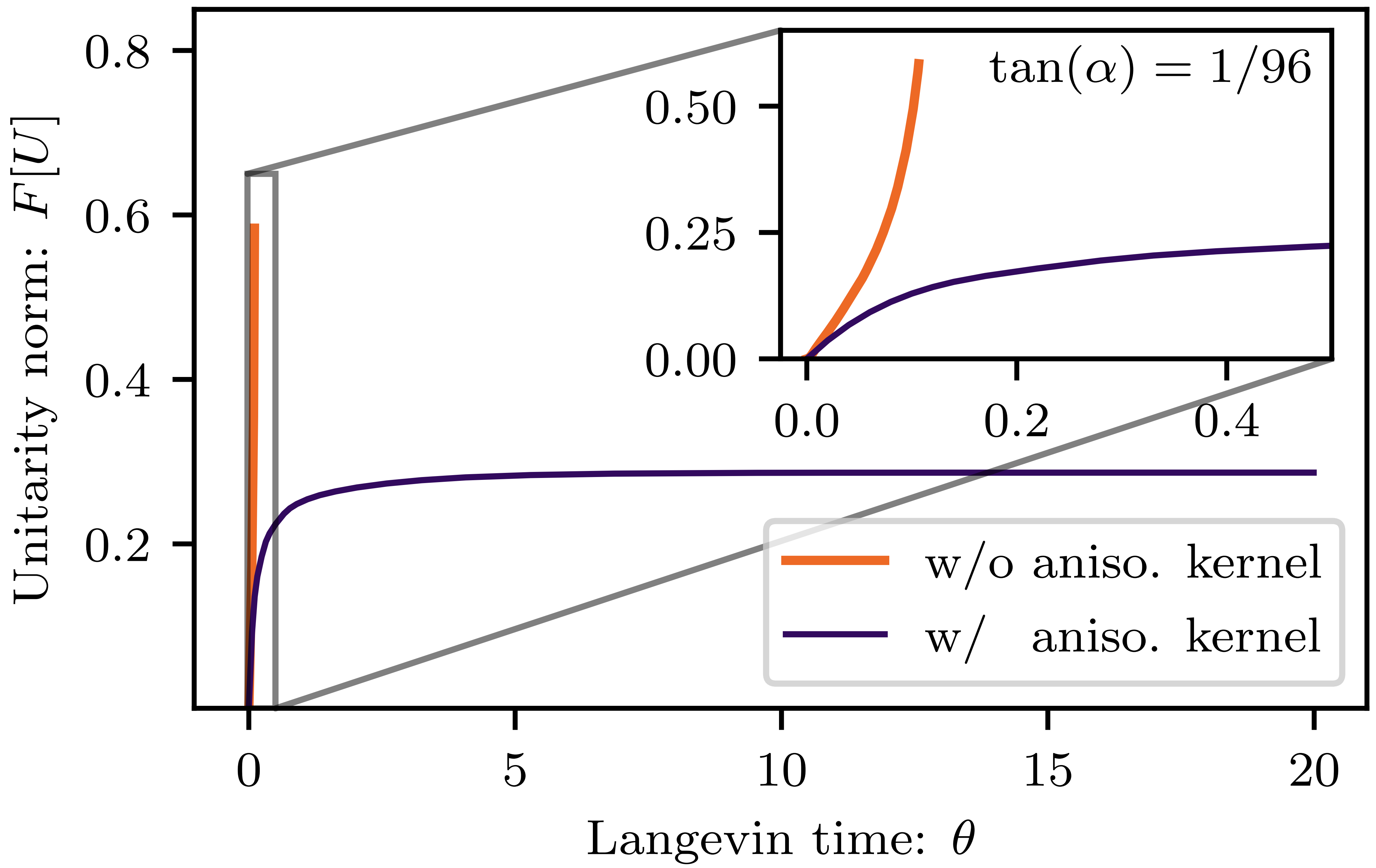
- Simulations are **not indefinitely stable**
  →. Stable until at least $\theta = 30$
  → Healthy margin to avoid instability effects



# Constant unitarity norm (2/2)

## Effectiveness of kernel becomes evident at small tilt angles

- At such a small bare coupling…
  wouldn't this work anyway regardless of the kernel?
  — No.
- For smaller tilt angles $\alpha$ the effect of the anisotropic kernel becomes evident
- *Without kernel:* **exponential growth of unitarity norm**
- *With kernel:* **plateau at a moderate level is reached**



# Correlators of the magnetic energy density

- Magnetic energy density on the lattice

$$B^2(t,x) = \frac{1}{4}\sum_{i<j} F_{ij}^2(t,x) \approx -\sum_{i<j}\frac{1}{a_i^2 a_j^2}\,\mathrm{Tr}\left\{\mathscr{P}_A(C_{ij}(x))^2\right\}$$

- Clover leafs

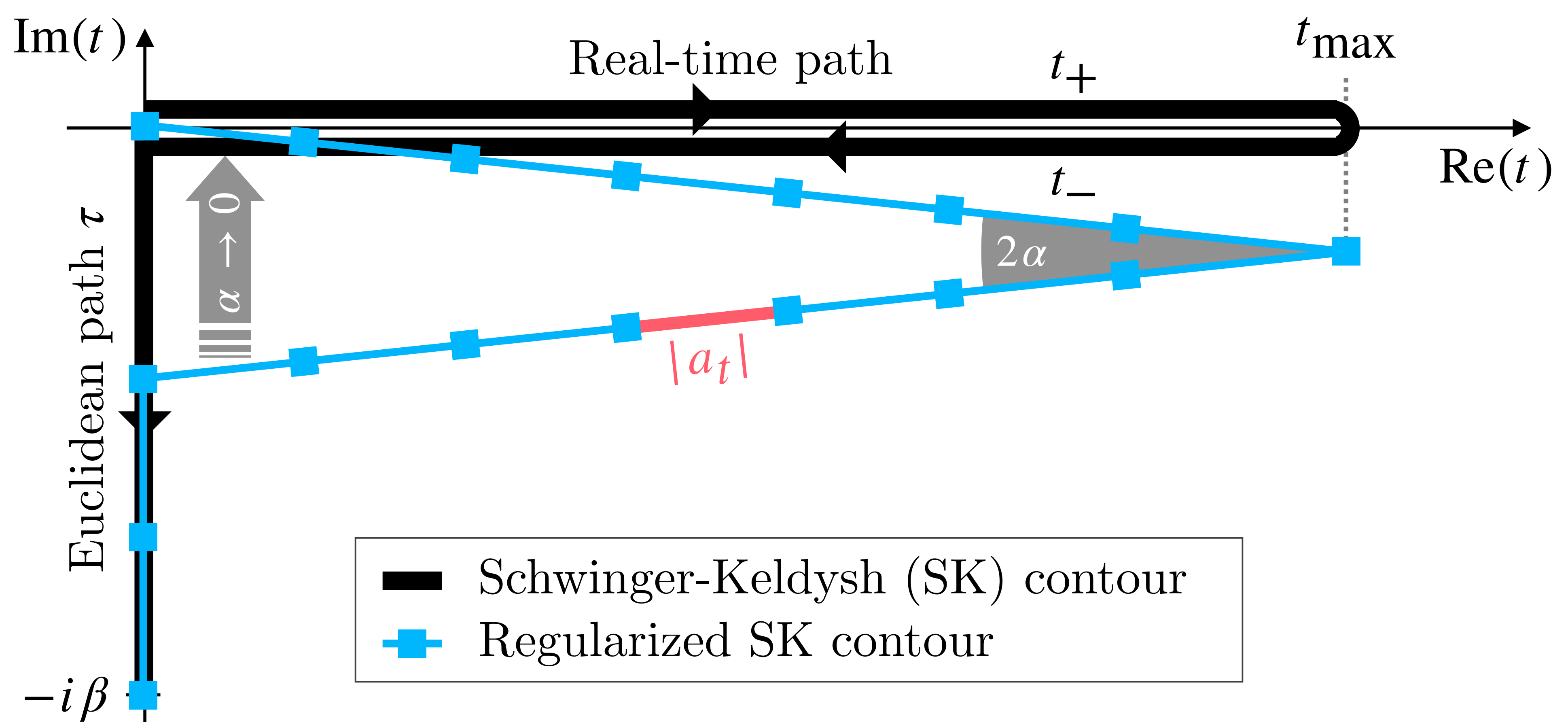
$$C_{\mu\nu}(x) = \frac{1}{4}[U_{\mu\nu}(x) + U_{\nu(-\mu)}(x) + U_{(-\mu)(-\nu)}(x) + U_{(-\nu)\mu}(x)]$$

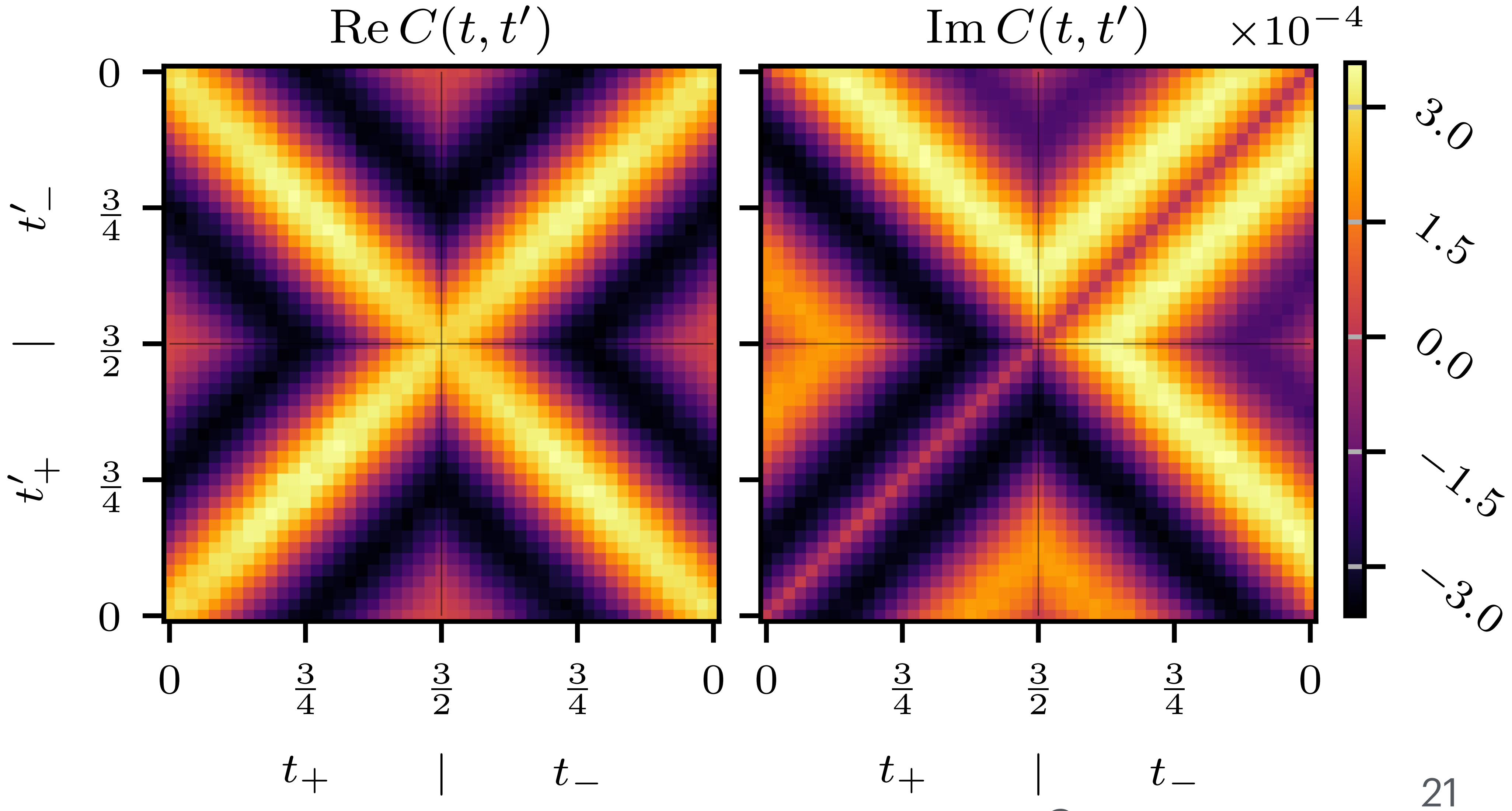
- Connected part of the integrated correlation function

$$C(t,x;t',x) = \langle B^2(t,x)B^2(t',x')\rangle - \langle B^2(t,x)\rangle\langle B^2(t',x')\rangle,$$

$$C(t,t') = \frac{1}{N_s^3}\sum_x C(t,x;t',x)$$

→ Integration over spatial lattice: - less statistics needed
- shorter runtimes



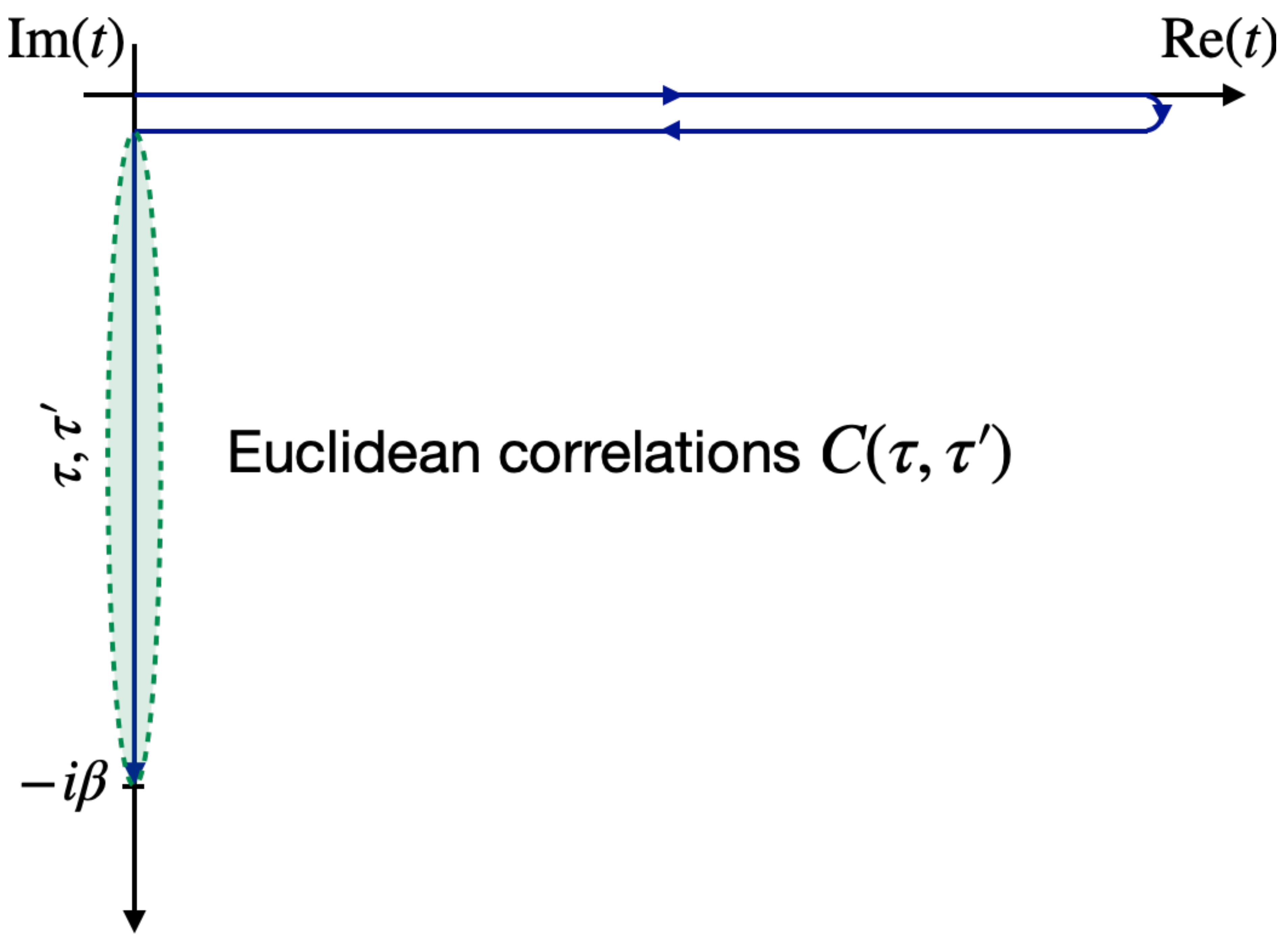



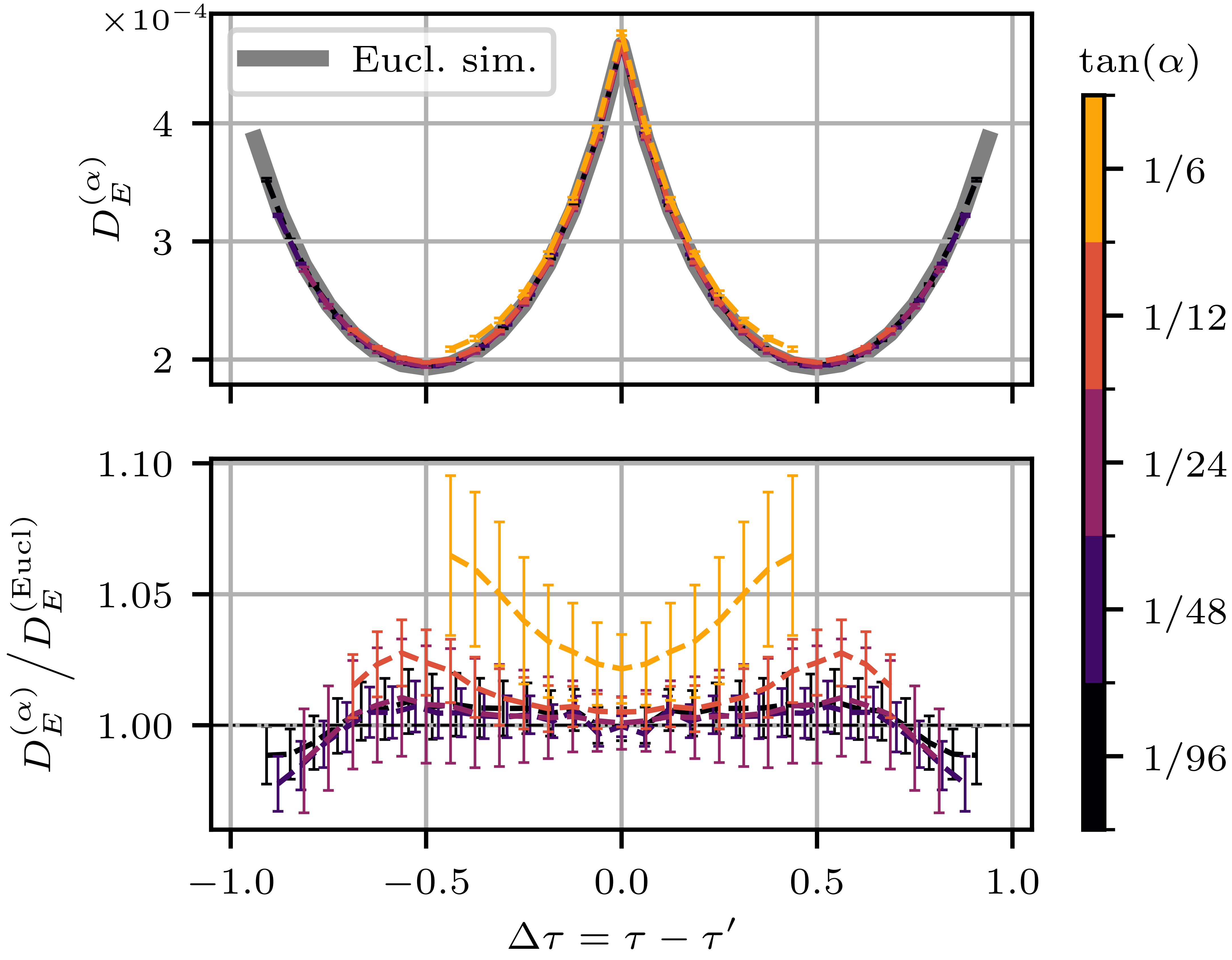

(extrapolated $\alpha \to 0$)

# Reproduction of Euclidean Correlator

Direct check of 'non-local' observable — stronger than one-point functions

- Euclidean correlator is correctly reproduced for sufficiently small tilt angles $\alpha$
- Reference data obtained on a Euclidean lattice in the absence of a sign problem



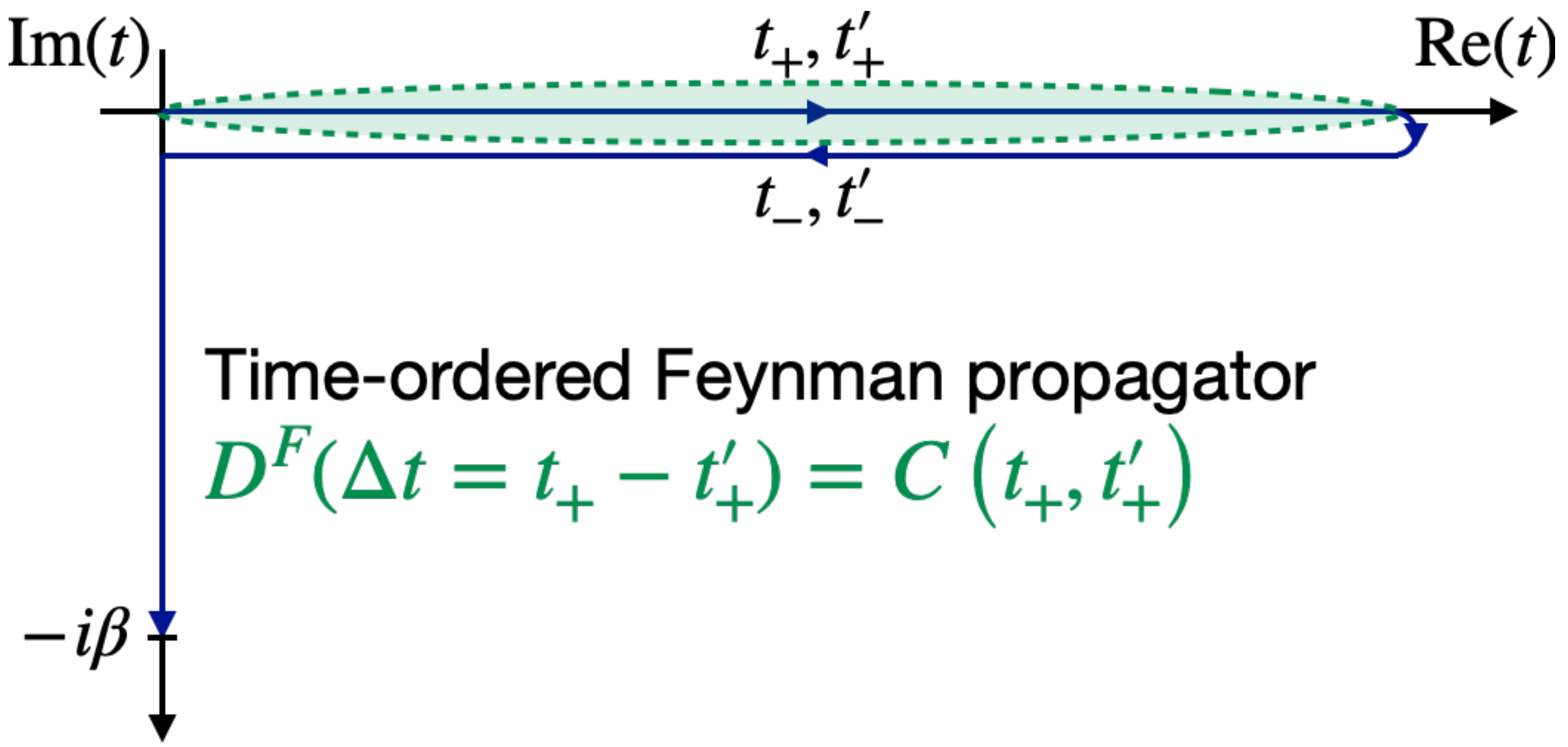



# Does the extrapolation converge?

Computing the spectral and statistical correlation function for various angles

- Statistical correlation function: $F = \mathrm{Re}\, D^F$
- Spectral function: $\rho = -\,\mathrm{sgn}(\Delta t)\, \mathrm{Im}\, D^F$

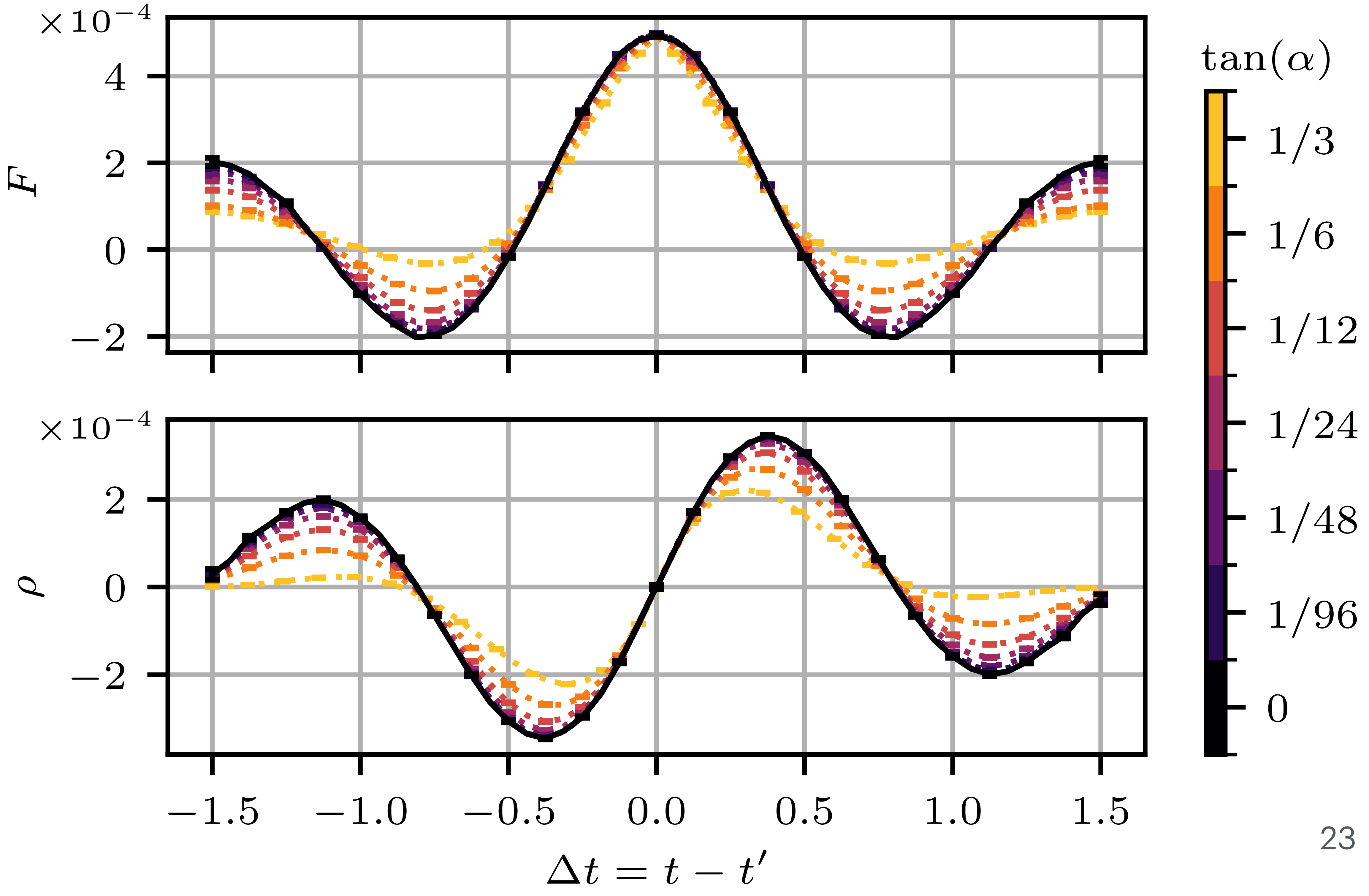
*Encode fundamental, microscopic excitation of the observables*




Time-ordered Feynman propagator

$D^F(\Delta t = t_+ - t'_+) = C\left(t_+, t'_+\right)$

**Converge to finite quantity for $\alpha \to 0$!**

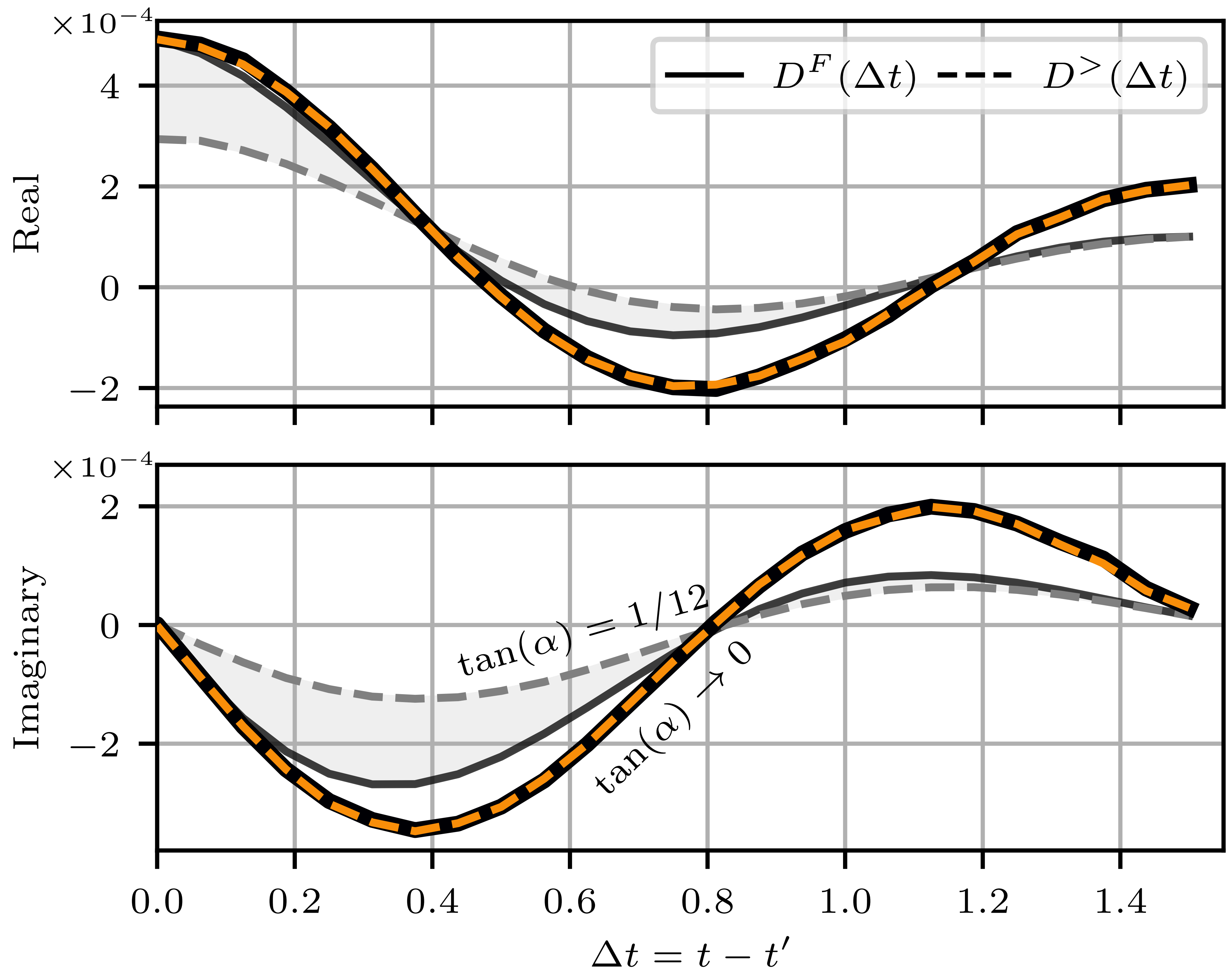


# Does it converge correctly?

## Consistency between different correlation function emerges at $\alpha \to 0$

- Relation of time-order Feynman propagator $D^F$ and Wightman functions $D^>(t,t') = C(t_-, t'_+)$:

$$D^F(t,t') = \Theta(t-t')D^>(t,t') + \Theta(t'-t)D^<(t,t')$$




- Valid for extrapolated data but NOT for finite tilt angles

  → requires vanishing regularization, non-trivial relation

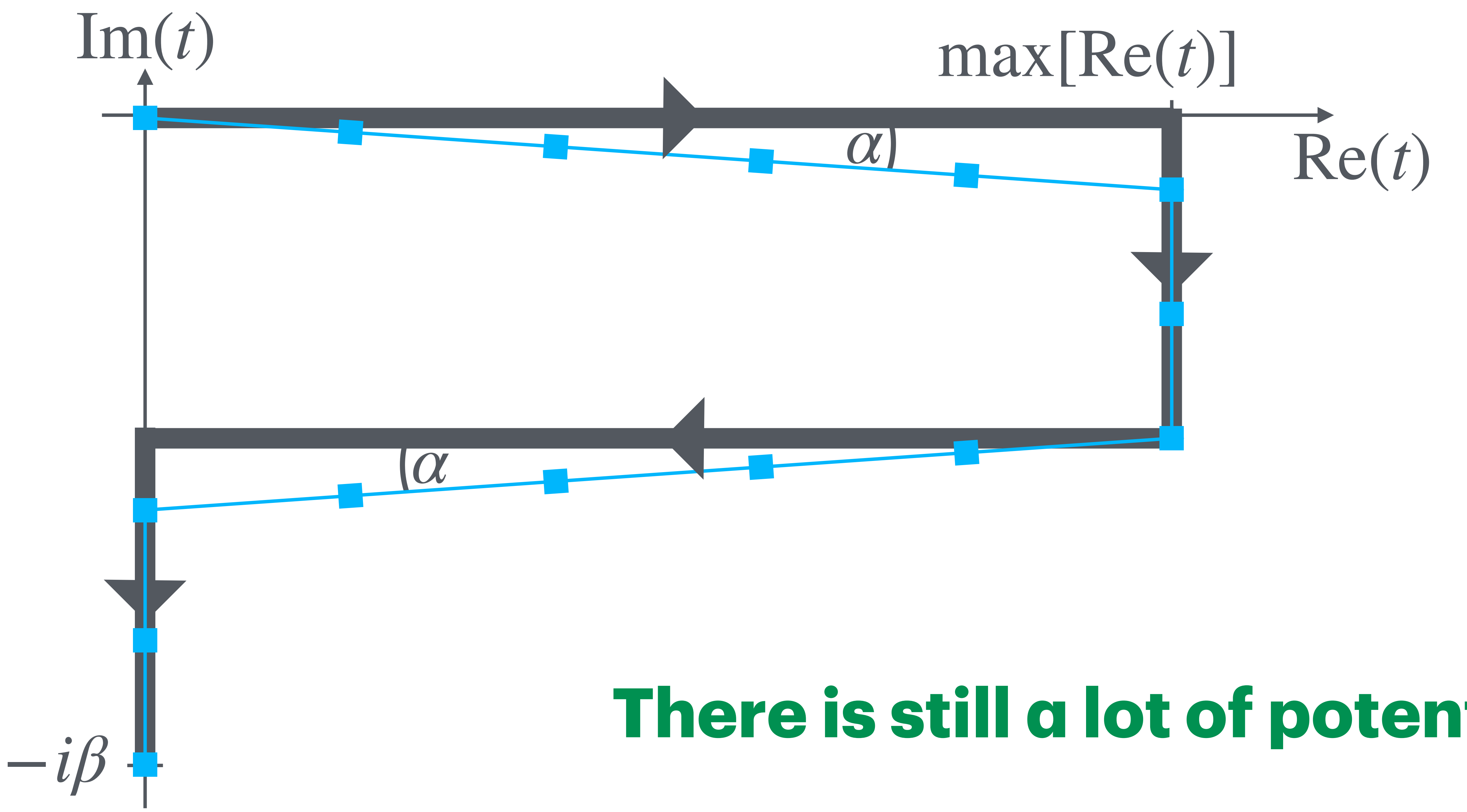
  → **sizable dampening of the oscillation**

  → **confirmation of our approach!**

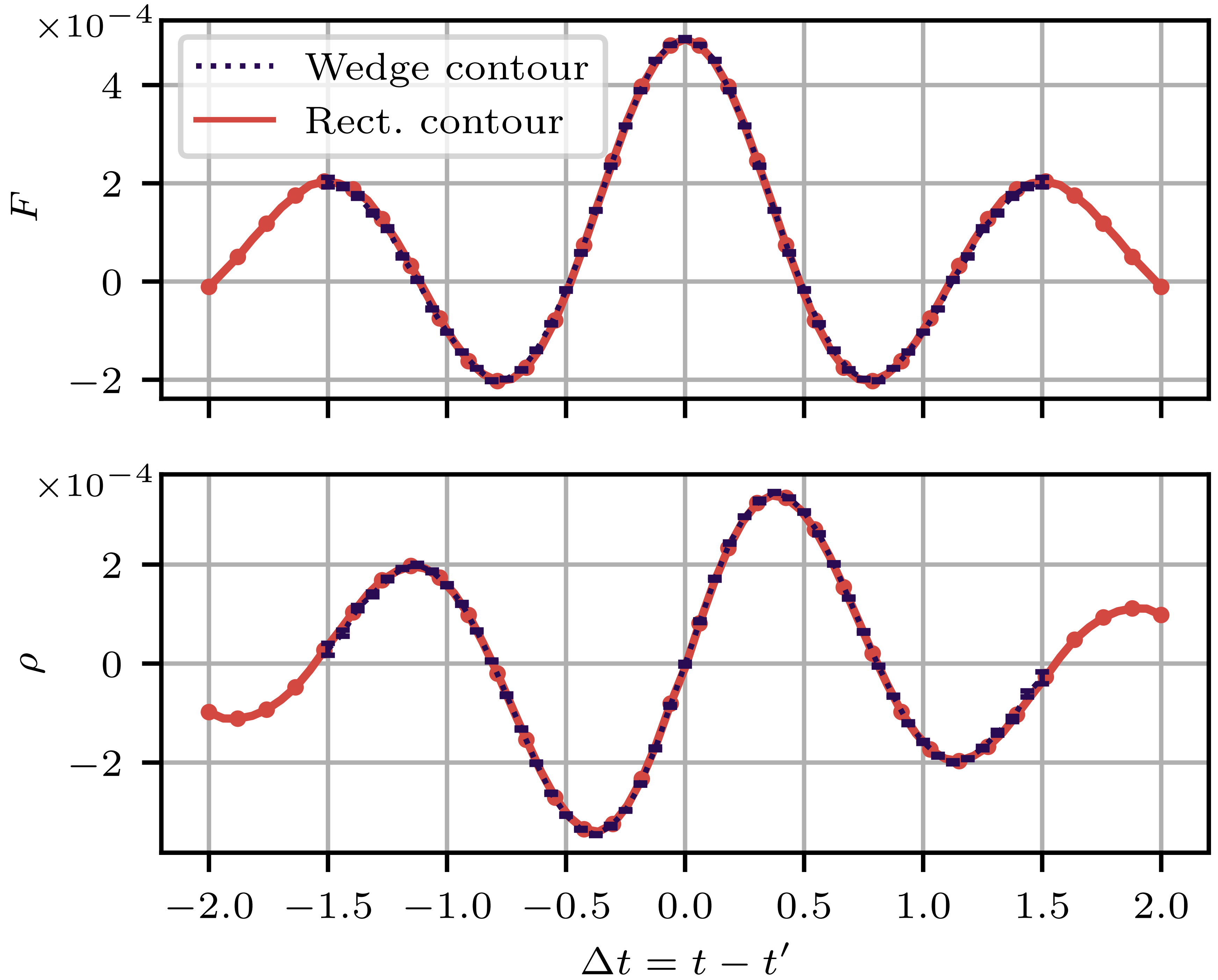
# Extending real-time range by different contour

## Split source of instability into two islands (forward/backward paths)

- 'Rectangular' contour is **more stable** than 'wedge' contour and yields the same information
- **Tilting is still necessary** (blue line) to regularize the path integral
- Extending $\max[\mathrm{Re}(t)] = 1.5\beta$ to $2\beta$ with the **same simulation and model parameters**




**There is still a lot of potential!**



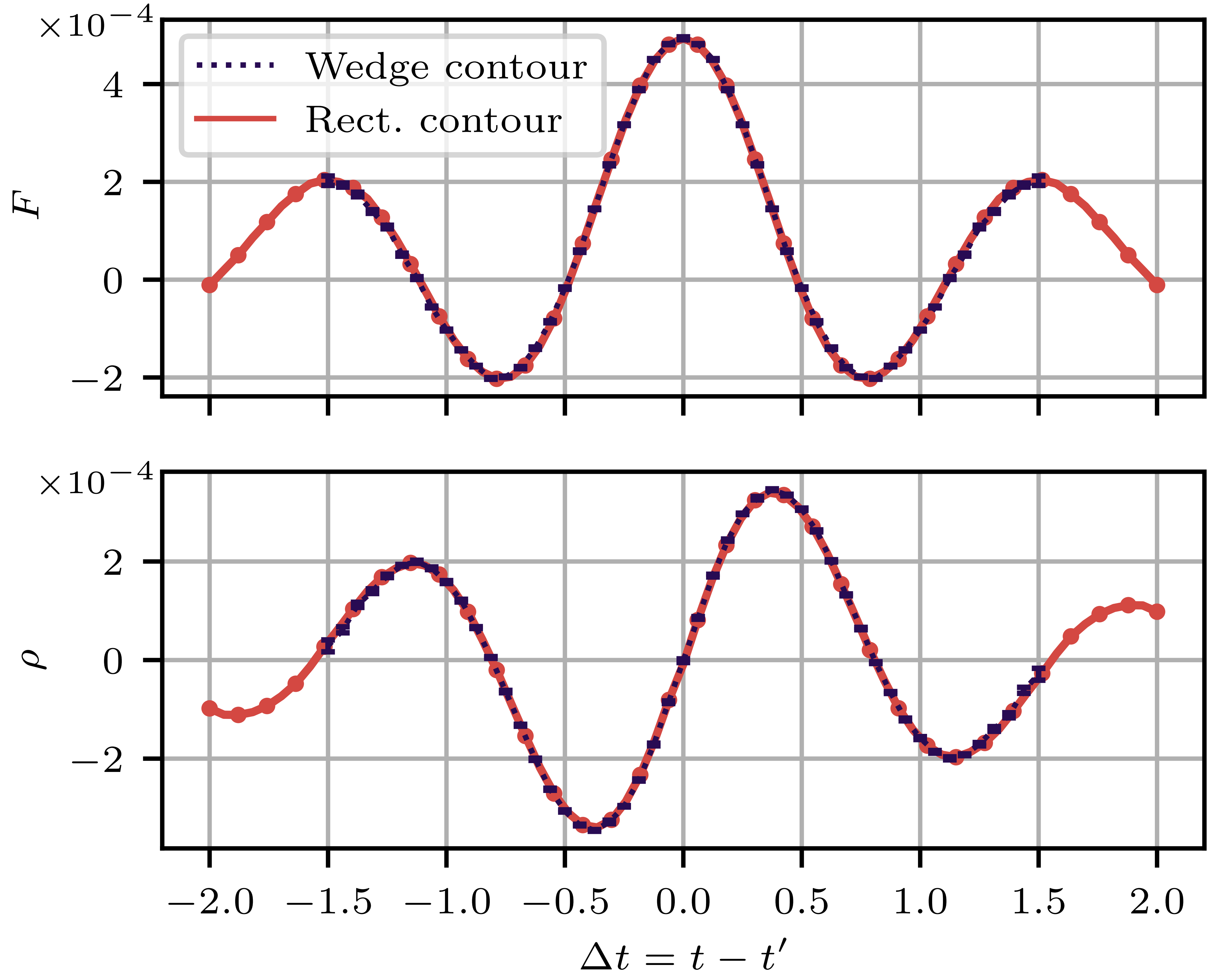
# Fitting the correlation function (1/2)

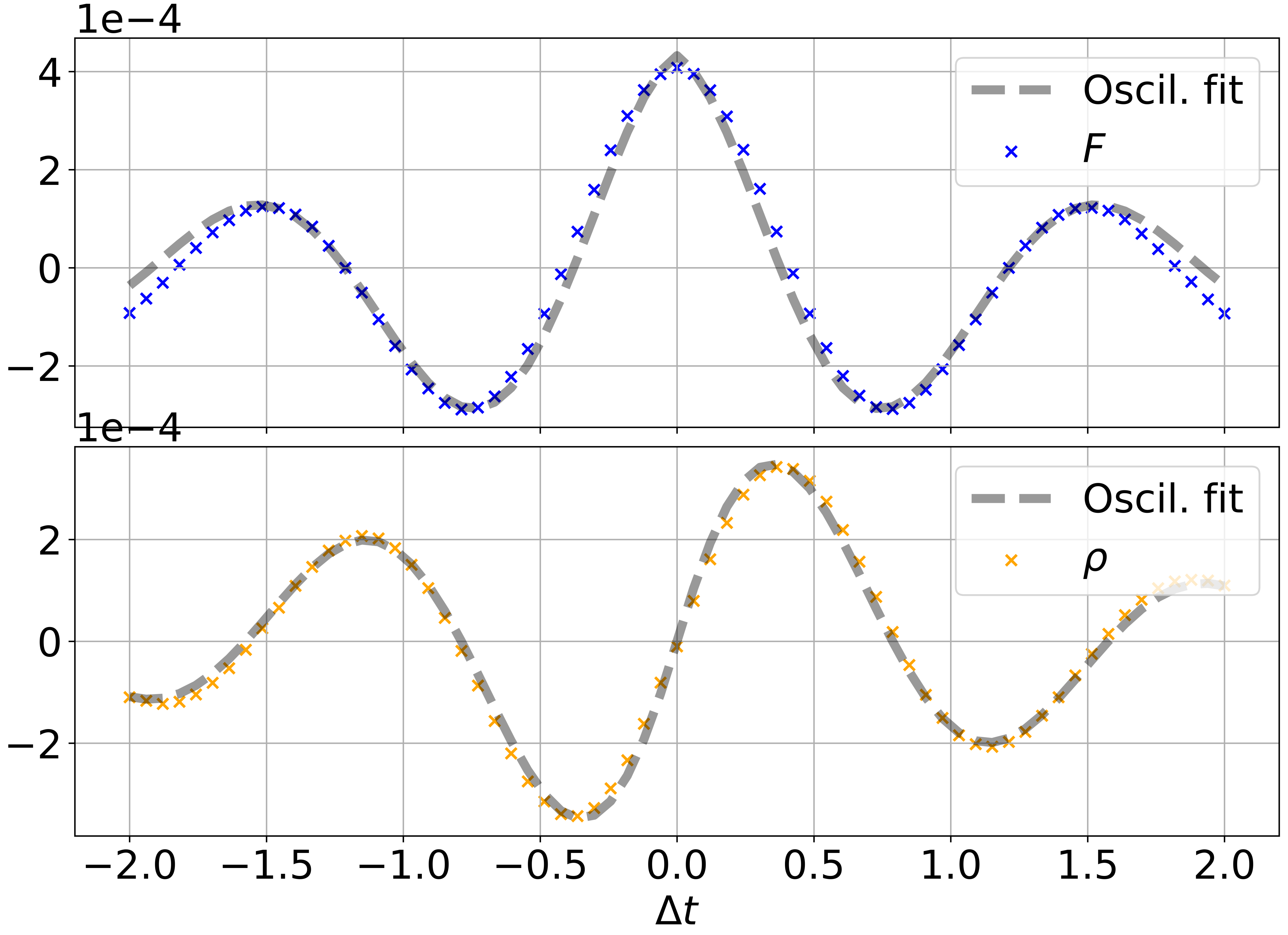
Small-frequency behavior only accessible with sufficient real-time extent

Preliminary

- Fitting damped oscillation to analyse the fluctuation-dissipation relation

$$F(\Delta t) \approx Ae^{\gamma|\Delta t|}\cos(\omega\Delta t),\ \ \rho(\Delta t) \approx Ae^{\gamma|\Delta t|}\sin(\omega\Delta t)$$



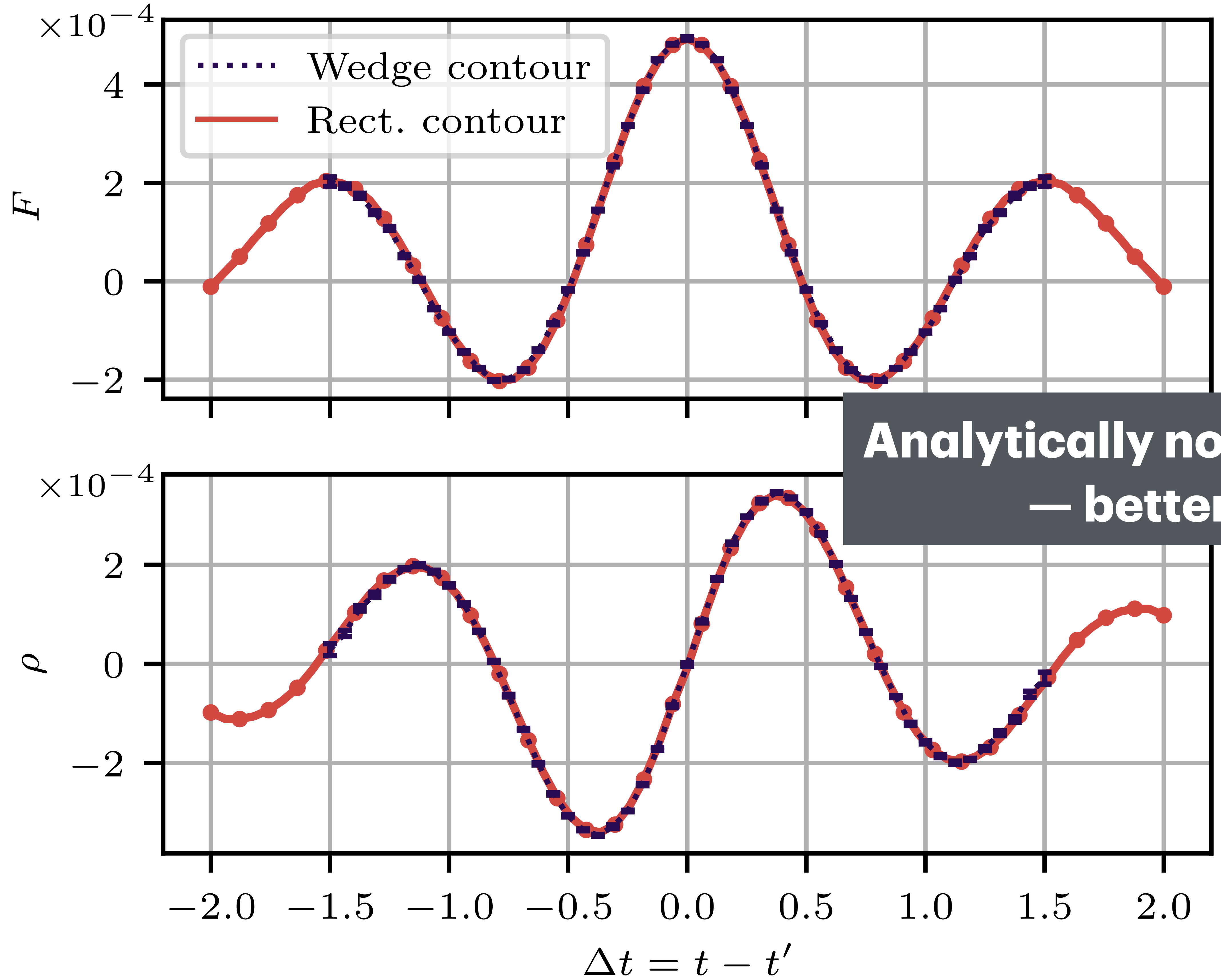
Preliminary

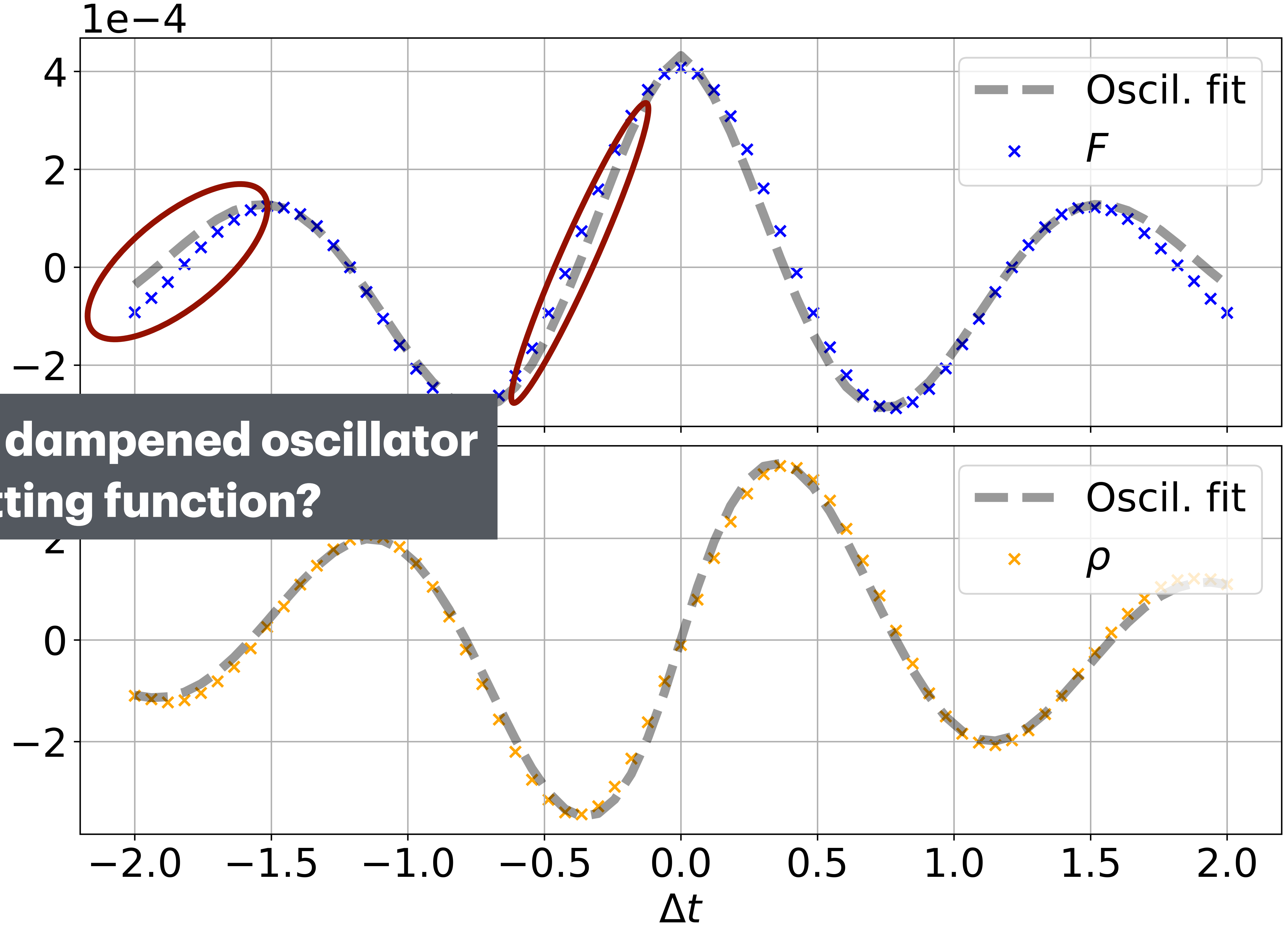
# Fitting the correlation function (2/2)

## Analytical form of integrated correlation function is unclear but not harmonic oscillation

- Fitting damped oscillation to analyse the fluctuation-dissipation relation

$$F(\Delta t) \approx A e^{\gamma|\Delta t|} \cos(\omega \Delta t), \;\; \rho(\Delta t) \approx A e^{\gamma|\Delta t|} \sin(\omega \Delta t)$$




**Analytically not a dampened oscillator — better fitting function?**

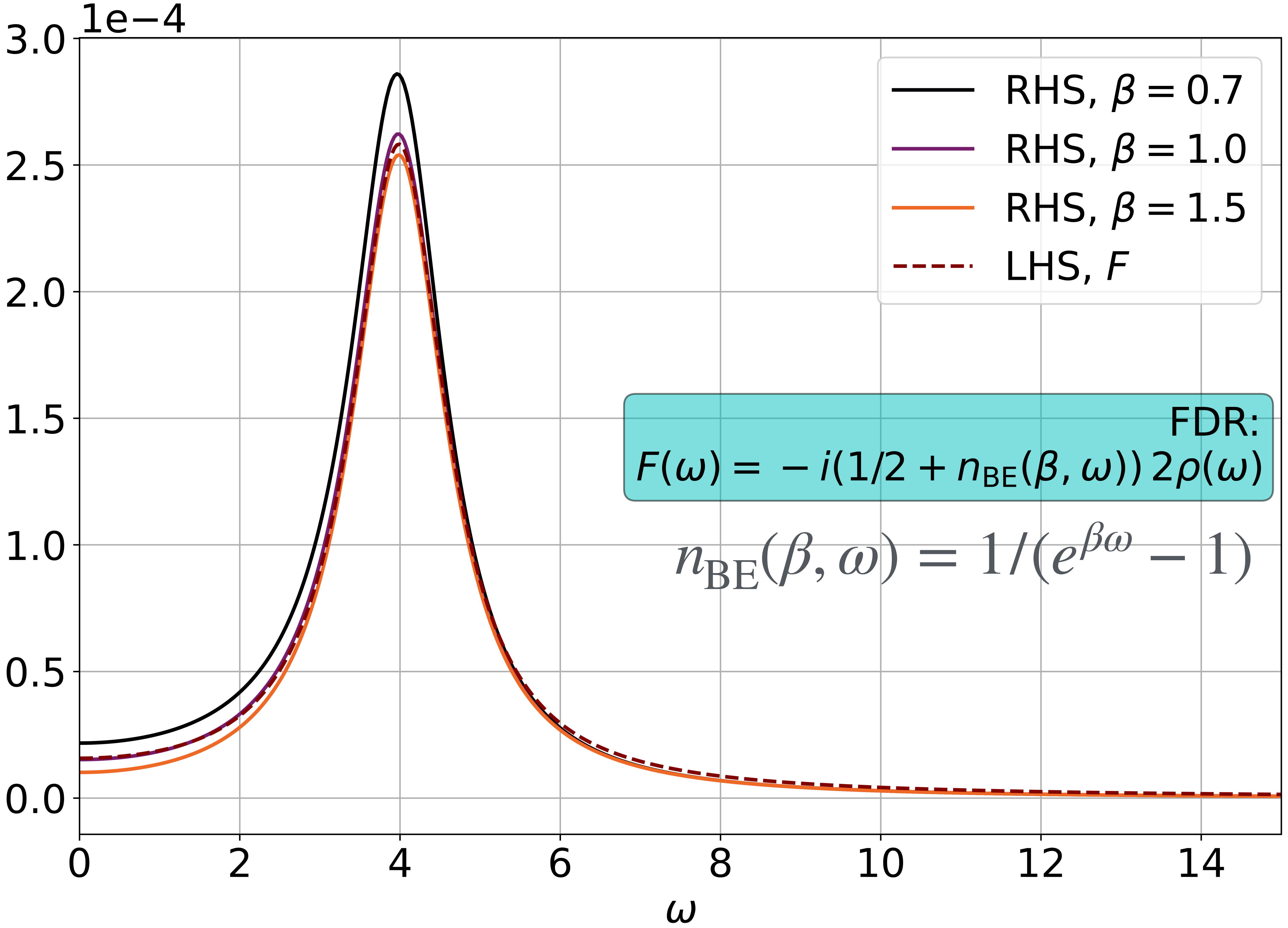
# Fluctuation-dissipation relation

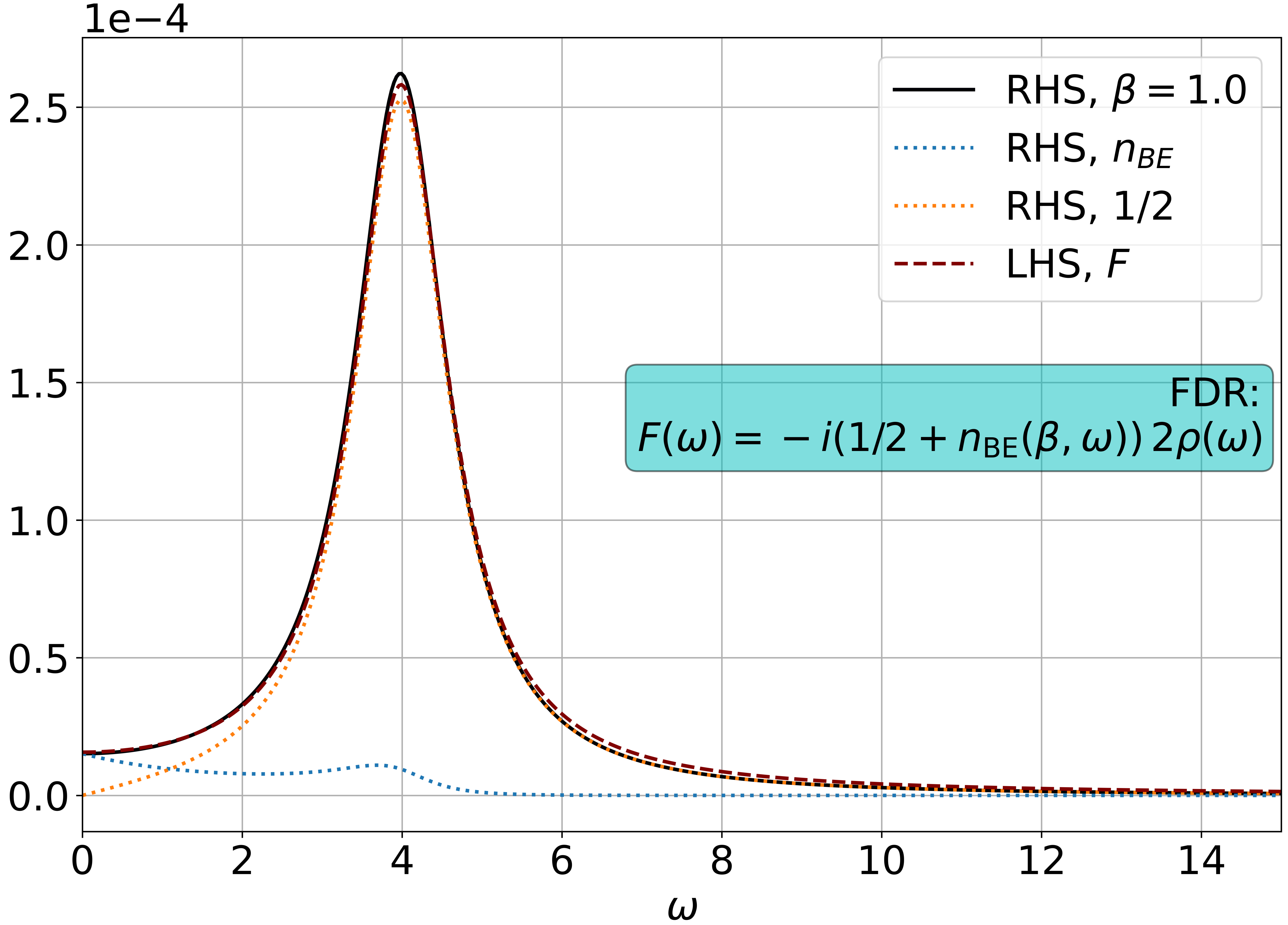
Preliminary

Fitting allows to verify fluctuation-dissipation relation to good accuracy

- Varying $\beta$ in Bose-Einstein stat. $n_{\mathrm{BE}}$ indirectly determines temperature → $\beta \approx 1$ (left)

- Quantum $1/2$ is essential to obtain agreement over whole $\omega$ range



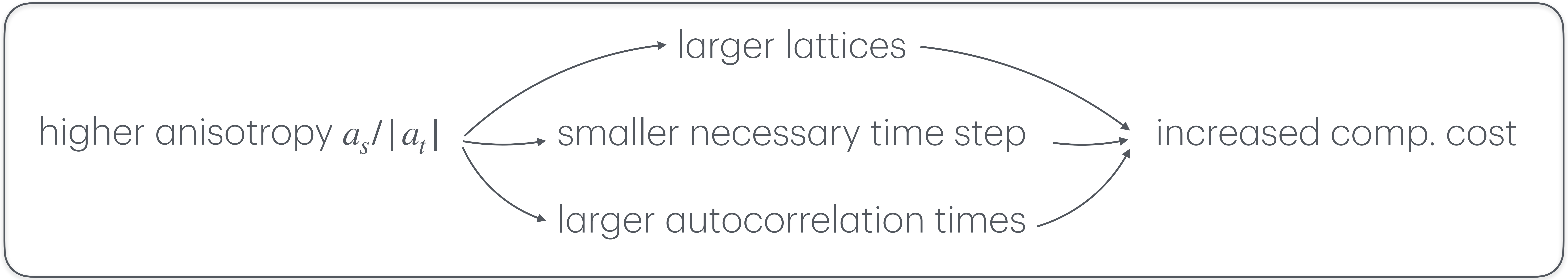



# Limitation, outlook and conclusion

# Limitations of our approach

- Systematic improvement of stability for larger anisotropy

✔ extension of time extend and stronger couplings




- Larger coupling $g$ severely worsens the instabilities → necessary anisotropy is huge

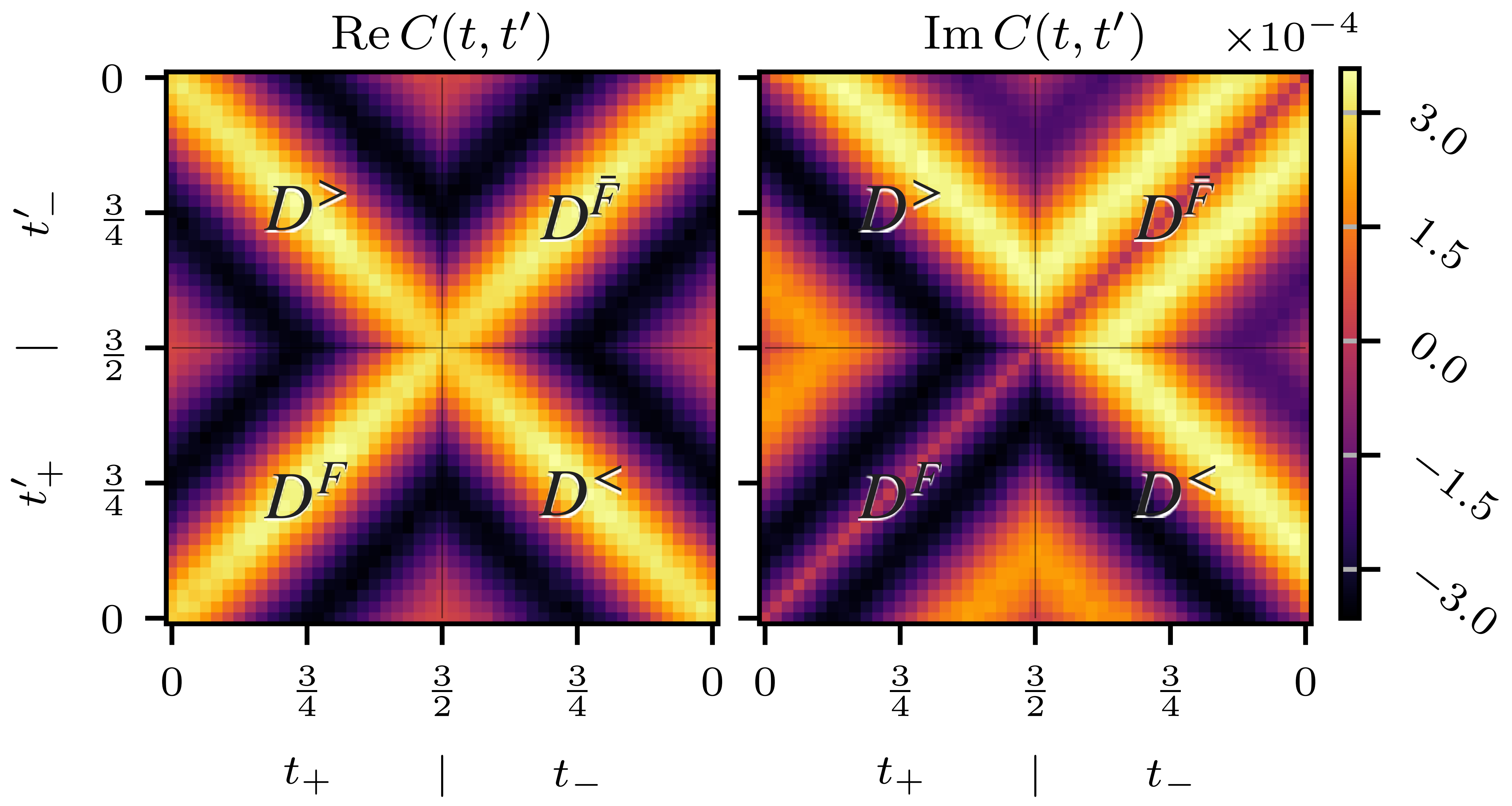
✘ not the solution for the sign problem in gauge theories in real-times

***BUT: We can build on it and use it as a basis or in combination for future developments!***

# Conclusion and outlook

- Sign problem impedes direct access to real-time dynamics of field theories
  - Spectral functions
  - Transport properties
  - Pre-equilibrium dynamics

- Complex Langevin tries to overcome that issue
  - Recent conceptional and practical progress
  - Development of kernels for greater stability
  - Correlation function in 1+3D SU(2) Yang-Mills
  - Numerical reproduction of fluct.-diss. rel.




- How to overcome current limitations?
  - Combination of kernel ideas?
  - Design of field-dependent kernels based on Lefschet thimbles?
- How do we set the scale on SK-contours?
- Further application?
  - Non-thermal systems? Incl. fermions?

Thank you for your attention!