Cold Quantum Coffee Seminar

# Stabilizing complex Langevin for real-time YM theory

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# Outline

# Motivation

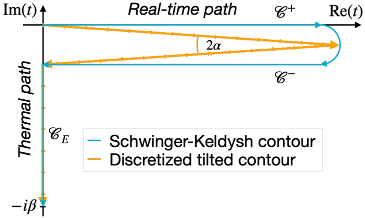
- Field theoretic and many-body systems are not solvable analytically
  - Heavy ion collisions, neutron stars, condensed matter, cold atoms, ...
- Calculations often have to be done have to be done numerically or approximations are used (or both)
- Standard numerical integration methods fail for oscillatory integrals
  - Based on sampling according to some weight function $\rightarrow$ not applicable for complex weights
  - Improving accuracy leads to exponentially many samples needed $\rightarrow$ computationally not feasible
- We miss methods that calculate observables from first principles!

# Schwinger-Keldysh formalism for Yang-Mills theory

## Expectation values in terms of path integrals

$$\langle \mathscr{O}[A] \rangle = \frac{1}{Z} \int \mathcal{D}A_E \, e^{-S_E[A_E]} \int \mathcal{D}A_+ \, \mathcal{D}A_- \, e^{iS[A_+,A_-]} \, \mathcal{O}(x)$$

- Expectation values of non-local observables in thermal equilibrium
  - $\langle \mathcal{O}_1(t)\mathcal{O}_2(t') \rangle = \mathrm{Tr}\left[ e^{-\beta H} \mathcal{O}_1(t) \mathcal{O}_2(t') \right]$
  - Only dependent on $t - t'$ due to time translation invariance
  - Transport coefficients, viscosities, spectral functions, ...
  - Periodic boundary conditions:
    $A^a_\mu(t = 0) = A^a_\mu(t = -i\beta)$
  - Yang-Mills action:
    $S_{\mathrm{YM}} = -\frac{1}{4} \int_{\mathcal{C}} d^4x F^{\mu\nu}_a F^a_{\mu\nu}$



# Sign problem of real-time YM theory

## Complex weight function leads to the sign problem

- Real-time contour leads to complex weight function

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

- Direct calculation of oscillatory integrals is not feasible
- Numerical integration methods exponentially costly

## Alternative integration methods needed

- Reweighting, Contour deformation, Analytic continuation, Taylor expansion, Lefschetz thimbles, **Complex Langevin method**, ...

# Reweighting not applicable

- Ideas of reweighting:
  - Split the action in imaginary $S_R + iS_I = -iS$
  - Reinterprete the observable by multiplying the phase $\mathcal{O} \rightsquigarrow \mathcal{O}e^{-iS_I}$

$$\begin{aligned}\langle \mathcal{O}_1(t)\mathcal{O}_2(t')\rangle &= \frac{\int \mathcal{D}x e^{-S_R} e^{-iS_I} \mathcal{O}_1(t)\mathcal{O}_2(t)}{\int \mathcal{D}x e^{-S_R} e^{-iS_I}} \\ &= \frac{\int \mathcal{D}x e^{-S_R} e^{-iS_I} \mathcal{O}_1(t)\mathcal{O}_2(t)}{\int \mathcal{D}x e^{-S_R}} \frac{\int \mathcal{D}x e^{-S_R}}{\int \mathcal{D}x e^{-S_R} e^{-iS_I}} \\ &= \frac{\langle \mathcal{O}_1(t)\mathcal{O}_2(t')e^{-iS_I}\rangle_{S_R}}{\langle e^{-iS_I}\rangle_{S_R}}\end{aligned}$$

- Enumerator and denominator can be estimated by MC
  - for the SK integral the average phase vanishes identically, reweighting is not applicable
- Assumption: $\langle e^{-iS_I}\rangle_{S_R} \neq 0$ (in practice sufficiently large)
  - measure of how “hard” the sign problem is

# Outline

# Introduction of the real Langevin method

## Correspondence of Langevin and Fokker-Planck equations

Equivalence by same stationary solution: $P(\mathbf{x}, \theta \to \infty) = \exp\left[-S(\mathbf{x})\right]$

$$\overbrace{d\mathbf{x} = \mathbf{K} d\theta + d\mathbf{w}}^{SDE} \quad \overset{\text{Itô's lemma}}{\Longleftrightarrow} \quad \overbrace{\partial_\theta P(\mathbf{x}, \theta) = \nabla(\nabla - \mathbf{K}) P(\mathbf{x}, \theta)}^{PDE} \tag{1}$$

- Langevin time $\theta$
- Wiener increment/noies term: $d\mathbf{w}$
- Drift term: $\mathbf{K} = -\nabla S$
- Averages of some random variable $X$ depending on $x$ reduces to sampling from stochastic process

$$\langle X \rangle_P \approx \lim_{\theta_0 \to \infty} \frac{1}{T} \int_{\theta_0}^{\theta_0 + T} d\theta \, X(\theta)$$

# Introduction of the complex Langevin method

**Idea:** Generalization of correspondence of Langevin and Fokker-Planck equations

Complexification of degrees of freedom: $\mathcal{M} \ni \mathbf{x} \to \mathbf{z} = \mathbf{x} + i\mathbf{y} \in \mathcal{M}_c$

$$\left.\begin{aligned} d\mathbf{x} &= \mathbf{K}_x d\theta + d\mathbf{w} \\ d\mathbf{y} &= \mathbf{K}_y d\theta \end{aligned}\right\} \Longleftrightarrow \left\{\begin{aligned} &\partial_\theta P(\mathbf{x},\mathbf{y},\theta) = L^T P(\mathbf{x},\mathbf{y},\theta) \\ &L = \nabla_x(\nabla_x + \mathbf{K}_x) + \nabla_y \mathbf{K}_y \end{aligned}\right.$$

$$\stackrel{?}{\Longleftrightarrow} \left\{\begin{aligned} &\partial_\theta \rho(\mathbf{x},\theta) = L_c^T \rho(\mathbf{x},\theta) \\ &L_c = \nabla_x(\nabla_x + \mathbf{K}) \end{aligned}\right.$$

Complex action leads to weigth function $\rho(\mathbf{x},\theta) \to \exp\left[-S(x)\right]$

- Holomorphic drift term
- Spectrum of $L_c$ is in the left half plane and 0 is non-degenerate
- Vanishing boundary terms for all (!) moments imply

$$\langle \mathcal{O} \rangle = \int dxdy \mathcal{O}(x+iy) P(x,y,\theta\to\infty) = \int dx \mathcal{O}(x)\rho(x,\theta\to\infty)$$

# Complex Langevin method for gauge fields

- CL equation for gauge fields

$$\partial_\theta A^a_\mu(\theta, x) = i\frac{\delta S_{\mathrm{YM}}}{\delta A^a_\mu(t,x)} + \eta^a_\mu(\theta, x)$$

- Complexification of the Lie algebra $\mathfrak{su}(N_c, \mathbb{C}) \to \mathfrak{sl}(N_c, \mathbb{C})$
- Gaussian distributed noise term

$$\langle \eta^a_\mu(\theta, t, \mathbf{x})\rangle = 0,$$
$$\langle \eta^a_\mu(\theta, t, \mathbf{x})\eta^b_\nu(\theta', t', \mathbf{x}')\rangle = 2\delta(\theta-\theta')\delta(t-t')\delta^{(d-1)}(\mathbf{x}-\mathbf{x}')\delta^{ab}\delta_{\mu\nu}$$

**Goal:** Overcoming the sign problem

- CL bypasses the sign problem by sampling at late $\theta$

$$\langle \mathcal{O}[A]\rangle \approx \lim_{\theta_0\to\infty}\frac{1}{T}\int_{\theta_0}^{\theta_0+T} d\theta\, \mathcal{O}[A(\theta)]$$

# Outline

# Three major Problems of CL for real-time YM

1. Discretized path integral along Schwinger-Keldysh contour is non-analytic w.r.t lattice spacing

   $\rightarrow$ we tilt the contour to regularize

2. Complex contours give rise to unambiguities in the CL formulation because of the noise correlator (Dirac delta)

   $\rightarrow$ we introduce parametrization dependent CL equation

3. CL suffers from instabilities and wrong convergence issues

   $\rightarrow$ stabilization techniques needed, we introduce an anisotropic kernel

# Tilted SK contour - Problem 1 ✓

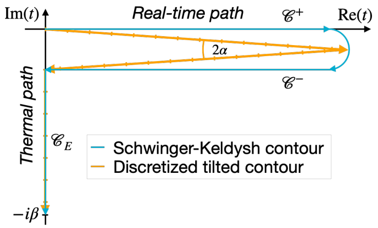
**Path integral for Wilson action on a Minkowski time contour has an ill-defined continuum limit!**

- Contour deformation resolves non-analyticity

$$\beta_0 \to e^{+i\alpha}\beta_0, \quad \beta_s \to e^{-i\alpha}\beta_s$$

- For a SK contour we effectively tilt the real-time paths

$$a_{t,k} \to e^{-i\alpha}a_{t,k} \qquad \text{for} \quad t_k \in \mathscr{C}^+,$$
$$a_{t,k} \to e^{+i\alpha}a_{t,k} \qquad \text{for} \quad t_k \in \mathscr{C}^-$$




- **Order of limits is crucial:**
  - **First $a_{t,k} \to 0$ then $\alpha \to 0$.**

# Parametrization dependent CL equation - Problem 2 ✓

## Parametrization dependent CL equation

Introduce curve parameter $\lambda$ for $t(\lambda)$ leads to

$$\partial_\theta A^a_\mu(\theta, \lambda, \mathbf{x}) = i \left. \frac{\delta S_{\mathrm{YM}}}{\delta A^a_\mu(\lambda, \mathbf{x})} \right|_{A=A(\theta)} + \eta^a_\mu(\theta, \lambda, \mathbf{x}),$$

$$\langle \eta^a_\mu(\theta, \lambda, \mathbf{x}) \eta^b_\nu(\theta', \lambda', \mathbf{x}') \rangle = 2\delta_{\mu\nu}\delta^{ab}\delta(\theta - \theta')\delta(\lambda - \lambda')\delta^{(3)}(\mathbf{x} - \mathbf{x}')$$

- Complex time contours leads to ambiguous noise correlator expression ($\delta$-distribution for complex arguments)
  - Ambiguities are resolved by a parametrization dependent CL formulation

$$t : [a, b] \mapsto \mathbb{C}, \qquad t(a) = 0, \quad t(b) = -i\beta$$

  - Noise correlator in terms of $\lambda$

$$\delta(t(\lambda) - t(\lambda')) \rightsquigarrow \delta(\lambda - \lambda')$$

- Solution is however independent of the chosen parametrization
- Limiting cases (Minkowski and Euclidean contour) are consistent with new formulation

# Some lattice QCD...

- Link variables and plaquette variables

$$U_{x,\mu} \simeq \exp\left[ig a_\mu A_\mu\big(x+\hat{\mu}/2\big)\right] \in \mathrm{SU}(N_c) \rightsquigarrow \mathrm{SL}(N_c,\mathbb{C}),$$
$$U_{x,\mu\nu} = U_{x,\mu} U_{x+\hat{\mu},\nu} U^{-1}_{x+\hat{\nu},\mu} U^{-1}_{x,\nu}$$

- Wilson plaquette action

$$S_{\mathrm{W}}[U] = \frac{1}{2N_c} \sum_{k,\mathbf{x},\mu\neq\nu} \beta_{\mu\nu} \mathrm{Tr}\left[U_{x,\mu\nu} - 1\right],$$

- Coupling constants

$$\beta_{0i} = -\frac{2N_c}{g^2}\frac{a_s}{a_{t,k}}, \qquad \beta_{ij} = +\frac{2N_c}{g^2}\frac{\bar{a}_{t,k}}{a_s}$$

- Time reversibility is retained by averaged spacing (turning points of the SK contour!)

$$\bar{a}_{t,k} = (a_{t,k} + a_{t,k+1})/2$$

# Euler-Maruyama for numerical solution of the CLE

## CL update step for link variables on a SK-contour

- Discretization of contour parameter
- Additional lattice spacing factors compared to common CL-step [1]

$$U_{x,t}(\theta+\epsilon) = \exp\left( it^a \left[ i\epsilon \frac{\mathbf{a}_{\lambda,\mathbf{k}}}{\mathbf{a}_\mathbf{s}} \left.\frac{\delta S_\mathrm{W}}{\delta \tilde{A}^a_{x,t}}\right|_\theta + \sqrt{\epsilon}\sqrt{\frac{\mathbf{a}_{\lambda,\mathbf{k}}}{\mathbf{a}_\mathbf{s}}}\,\eta^a_{x,\lambda}(\theta) \right] \right) U_{x,t}(\theta)$$

$$U_{x,i}(\theta+\epsilon) = \exp\left( it^a \left[ i\epsilon \frac{\mathbf{a}_\mathbf{s}}{\bar{\mathbf{a}}_{\lambda,\mathbf{k}}} \left.\frac{\delta S_\mathrm{W}}{\delta \tilde{A}^a_{x,i}}\right|_\theta + \sqrt{\epsilon}\sqrt{\frac{\mathbf{a}_\mathbf{s}}{\bar{\mathbf{a}}_{\lambda,\mathbf{k}}}}\,\eta^a_{x,i}(\theta) \right] \right) U_{x,i}(\theta)$$

- Langevin time step $\epsilon \to 0$
- Noise $\eta^a_{x,i}$ is approximated by a Gaussian distribution
- $\sqrt{\frac{a_s}{\bar{a}_{\lambda,k}}}$ leads to issues in the $N_t \to \infty$ limit

# Instabilities of the CL method

**CL suffers from instabilities**

- Runaway instabilities

  → numerical blow-up due to excursions into the non-compact manifold
- Wrong-convergence issues

  → distorted expectation values due to violation of the criterion of correctness

**Bad:** We are facing both types of instabilities for YM on a SK contour
***Even worse:*** Severity of the instabilities drastically increases with shrinking tilt-angles → limit to SK contour difficult

# Existing stabilization techniques

- **Gauge cooling [2]:** Exploit gauge freedom to minimize non-unitarity measured by a functional $F[U]$

$$U_{x,\mu} \mapsto U^V_{x,\mu} = V_x U_{x,\mu} V^{-1}_{x+\mu}, \qquad F[U] \geq F[U^V]$$

- **Adaptive stepsize [3]:** Regulate large drift terms which lead to instabilities

$$\epsilon \mapsto \tilde{\epsilon} = \epsilon \min\left(1, \frac{B}{\max\limits_{x,\mu,a} |K^a_{x,\mu}|}\right)$$

- **Dynamical stabiliziation [4]:** Penalize drift terms depending on the local non-unitary of the configuration

$$K^a_{x,\mu} \mapsto \tilde{K}^a_{x,\mu} = K^a_{x,\mu} + i\alpha_{\mathrm{DS}} M^a_x,$$
$$M^a_x = b^a_x \left(\sum_c b^c_x b^c_x\right), \quad b^a_x = \sum_\mu \mathrm{Tr}[t^a U_{x,\mu} U^\dagger_{x,\mu}]$$

# Kernel freedom of the CL method

## Field-independent kernel freedom

- *Kerneled Langevin equation* yields same limiting density function

$$\partial_\theta A^a_\mu(\theta, x) = i \int dx' \, \Gamma^{ab}_{\mu\nu}(x, x') \frac{\delta S}{\delta A^b_\nu(x')} + \int dx' \, \tilde{\Gamma}^{ab}_{\mu\nu}(x, x') \eta^b_\nu(\theta, x')$$

- $\Gamma^{ab}_{\mu\nu}(x, x')$ is required to be factorizable

$$\Gamma^{ab}_{\mu\nu}(x, x') = \int dx'' \, \tilde{\Gamma}^{ac}_{\mu\sigma}(x, x'') \tilde{\Gamma}^{bc}_{\nu\sigma}(x', x'')$$

- Kerneled Langevins equations correspond to the same Fokker-Planck equations (equivalence classes)
- *In practice:* Kernels may aggravate or mitigate instabilities

# Anisotropic kernel - Problem 3 ✓

## Kerneled CL update step

- Rescaling of Langevin time for temporal and spatial d.o.f.

$$U_{x,t}(\theta+\epsilon) = \exp\left( it^a \left[ i\epsilon \left( \frac{a_{\lambda,k}}{a_s} \right)^2 \frac{\delta S_{\mathrm{W}}}{\delta \tilde{A}^a_{x,t}}\bigg|_\theta + \sqrt{\epsilon}\frac{a_{\lambda,k}}{a_s}\eta^a_{x,\lambda}(\theta) \right] \right) U_{x,t}(\theta)$$

$$U_{x,i}(\theta+\epsilon) = \exp\left( it^a \left[ i\epsilon \frac{\delta S_{\mathrm{W}}}{\delta \tilde{A}^a_{x,i}}\bigg|_\theta + \sqrt{\epsilon}\eta^a_{x,i}(\theta) \right] \right) U_{x,i}(\theta)$$

**Empirical motivation for chosen kernel:**

- Noise of spatial update blows up for $a_{\lambda,k} \to 0$ $\quad\rightsquigarrow\quad$ $\theta \mapsto \frac{\bar{a}_{\lambda,k}}{a_s}\theta$
- Slow down dynamics of temporal plaquettes $\quad\rightsquigarrow\quad$ $\theta \mapsto \frac{a_{\lambda,k}}{a_s}\theta$

# Comparison

## Commonly used CL update step [1]

$$U_{x,\mu}(\theta+\epsilon) = \exp\left(it^a\left[i\epsilon\,\frac{\delta S_{\mathrm{W}}}{\delta A^a_{x,\mu}}\bigg|_\theta + \sqrt{\epsilon}\eta^a_{x,\mu}(\theta)\right]\right)U_{x,\mu}(\theta)$$

## New kerneled CL update step

$$U_{x,t}(\theta+\epsilon) = \exp\left(it^a\left[i\epsilon\left(\frac{a_{\lambda,k}}{a_s}\right)^2\frac{\delta S_{\mathrm{W}}}{\delta \tilde{A}^a_{x,t}}\bigg|_\theta + \sqrt{\epsilon}\frac{a_{\lambda,k}}{a_s}\eta^a_{x,\lambda}(\theta)\right]\right)U_{x,t}(\theta)$$

$$U_{x,i}(\theta+\epsilon) = \exp\left(it^a\left[i\epsilon\,\frac{\delta S_{\mathrm{W}}}{\delta \tilde{A}^a_{x,i}}\bigg|_\theta + \sqrt{\epsilon}\eta^a_{x,i}(\theta)\right]\right)U_{x,i}(\theta)$$

# Great interconnection of methods - Problem 1,2,3 ✓

**We see great interconnection of the three proposed solutions:**

- Path integral regularization is done by contour deformation (tilting)
- Tilted contours (non-real, non-imaginary) can be dealt with by parameterized CL formulation
- Calculation of physical observables requires a double-extrapolation

$$\Rightarrow \text{first } a_t \to 0, \text{ second } \alpha \to 0$$

- Kernel systematically improves stability for smaller $a_t$

**Instabilities get worse for $\alpha \to 0$ and are counteracted by our kernel for $a_t \to 0$!**

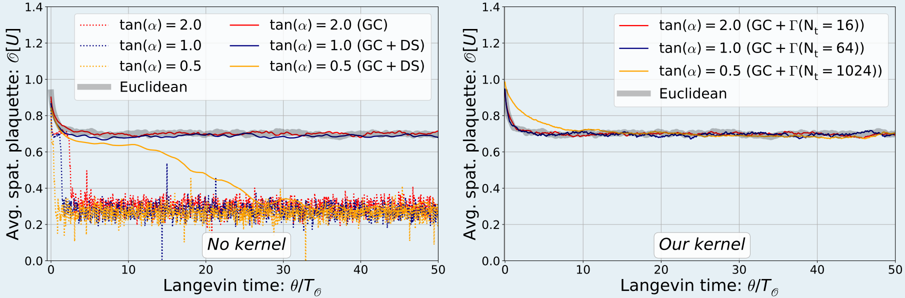
# Outline

# Numerical setup

- We simulate $SU(2)$ gauge theory on a $N_t \times 4^3$ lattice
- Kernel is controlled by number of temporal lattice points $N_t$
- Inverse temperature $\beta = 4.0$, coupling constant $g = 1$
  - We are in the deconfined phase ($\langle |P| \rangle \neq 0$).
- Simulations are initialized with identity matrices
- Same seed for random number generator for noise
- Langevin time is rescaled by the autocorrelation time

# Correct expectation values of one-point functions

## Trace of average spatial plaquette




- Avg. spatial plaquette (considered in earlyier studies [1]):

$$\mathscr{O}[U] = \frac{1}{N_t N_s^3} \sum_x \frac{1}{3} \sum_{i<j} \frac{1}{N_c} \mathrm{Re}\,\mathrm{Tr}\, U_{x,ij}$$

- Existing methods not enough for stabilizing simulations
- **Kernels successfully stabilizes even small tilt angles**

# Expectation values from CL

**Results for average spatial plaquette $\mathscr{O}$ via CL:**

| $\tan(\alpha)$ | Stabilization techniques | $N_t$ | $\langle \mathscr{O} \rangle$ |
|---|---|---|---|
| (Euclidean) | None | 16 | 0.6992(3) |
| 2.0 | AS, GC | 16 | 0.6981(2) |
| 1.0 | AS, GC, DS | 16 | 0.6858(1) |
| 0.5 | AS, GC, DS | 16 | 0.2801(3) |
| 2.0 | AS, GC, $\Gamma$ | 16 | 0.6987(3) |
| 1.0 | AS, GC, $\Gamma$ | 64 | 0.6977(5) |
| 0.5 | AS, GC, $\Gamma$ | 1024 | 0.6973(8) |
| 0.4 | AS, GC, $\Gamma$ | 8192 | 0.6968(6) |

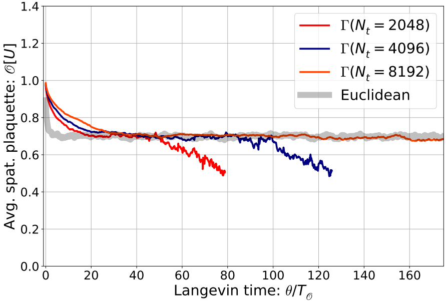
# Systematic improvement of CL instabilities

## Anisotropic kernel systematically stabilizes CL

- Our kernel allows simulations even for $\max \mathrm{Re}(t) > \beta$
- Stability is systematically improved for partial continuum limit

$\Rightarrow$ **Calculation of real-time observables might be feasible!**

- Stability region grows faster then auto-correlation time w.r.t. $N_t$
- Computational cost grows linearly with $N_t$



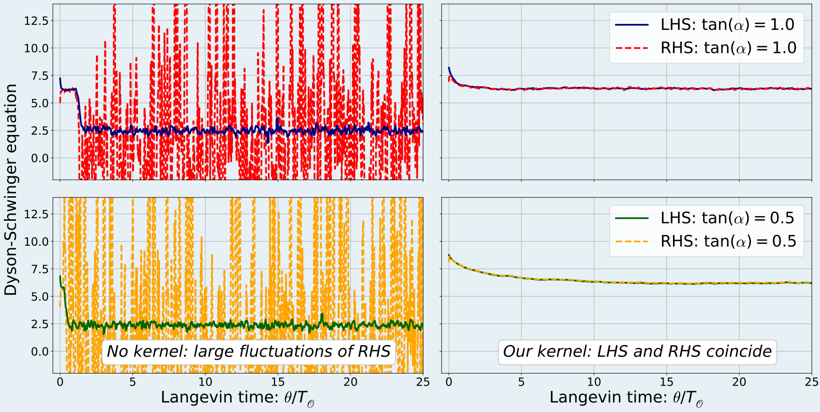

*Tilt angle:* $\tan(\alpha) = 0.4$

# Dyson-Schwinger equations

## DSE for spatial plaquettes

- Self-consistency check of link configuration

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

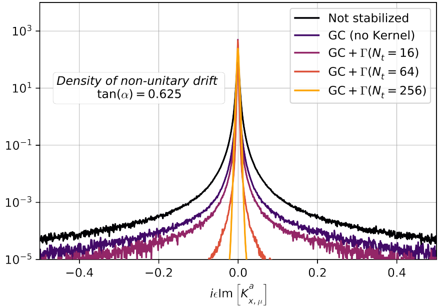


# Localized histogram of the drift terms

## Anisotropic kernel and the criterion of correctness

- We implicitly assume that $K_y PO$ decay sufficiently fast
- Localised histograms of the $K_y$ should lead to vanishing boundary terms

- Gauge cooling helps, but skirts are still present
- No skirts of histograms using our kernel with sufficiently large $N_t$



# Outline

# Conclusion & Outlook

## Conclusion

- Stabilization techniques extend the applicability of CL
- We found an approach to systematically improve stability
- Anisotropic kernel enables simulations of $\max \mathrm{Re}(t) > \beta$

$\rightsquigarrow$ Extrapolation to Schwinger-Keldysh contour might be possible

- What I have shown you
  - Average spatial plaquette
  - Dyson-Schwinger equations
  - Histograms of the drift term

- What I have *not* shown you
  - Larger Wilson loops ($W_{n \times n}$)
  - Polyakov loop
  - Unitarity norm
  - Euclidean correlators

# Teaser of our most recent results

## Outlook

- Checks of mathematical features of correlation function
  - Independence $\frac{t+t'}{2}$
  - Relations of Wightman functions and Propagators
  - Fluctuation-dissipation relation

- Calculation of physical lattice spacing (ongoing)
  - Renormalization needed for physical observables

- Bulk and shear spectral function (ongoing)
  - We carry out the double extrapolation
  - We are able to simulate real-time extents of $t_{\max} = 4\beta$

- Far-future prospect: Non-thermal quantum systems

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