“Observifolds”: Deforming the Path Integral to Improve Noisy Observables

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[Detmold, GK, Wagman, Warrington PRD102 (2020) 014514]
[Detmold, GK, Lamm, Wagman, Warrington 2101.xxxxx]

U. Heidelberg | Cold Quantum Coffee (January 12, 2021)

Lattice field theories

1. Non-perturbative regulator: lattice spacing a cuts off UV modes $\gg 1/a$

$$\langle \mathcal{O} \rangle = \frac{1}{Z}\int \mathcal{D}U\, \mathcal{O}[U]\, e^{-S[U]} \quad \rightarrow \quad \left\langle \mathcal{O}_{reg.} \right\rangle = \frac{1}{Z}\int \prod_i dU_i\, \mathcal{O}[U]\, e^{-S[U]}$$

(in Euclidean spacetime) (on Euclidean spacetime lattice)

2. Criticality / universality: access well-defined continuum limit

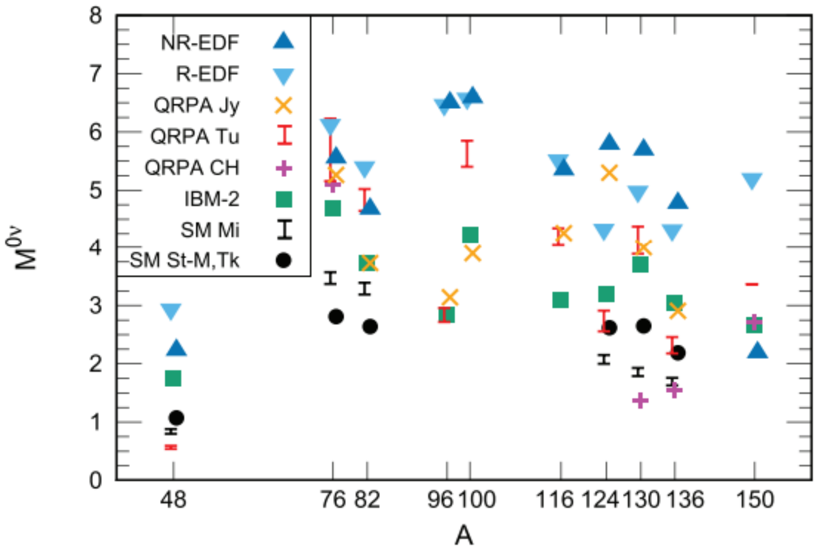
3. Gauge theories: exact gauge invariance preserved

(Just one) Motivation for LQFT

- Many experiments for new physics rely on nuclear targets / samples

- Need to know SM predictions for nuclear matrix elements

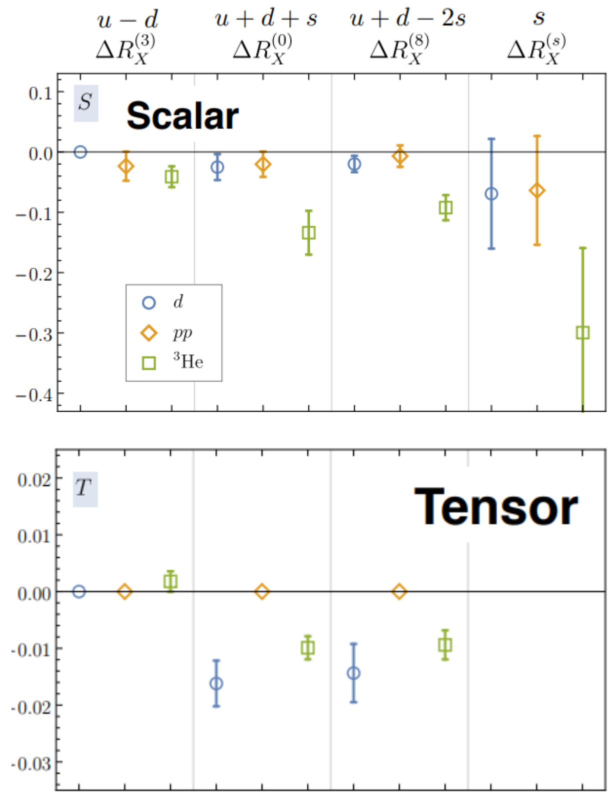
- Models disagree: **ab initio is key!**



[Engel & Menéndez, Rep Prog Phys 2017, 046301]

(Just one) Motivation for LQFT

- Lattice Quantum Chromodynamics (LQCD) gives ab initio theory inputs
- LQCD matrix elements from QCD → LECs for many-body methods
- Complementary to experiment



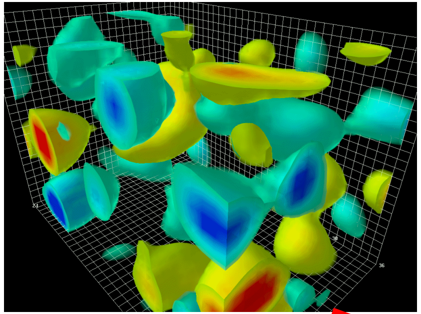
[Chang et al, PRL120 (2018) 152002]
[Shanahan, INT-18-70]

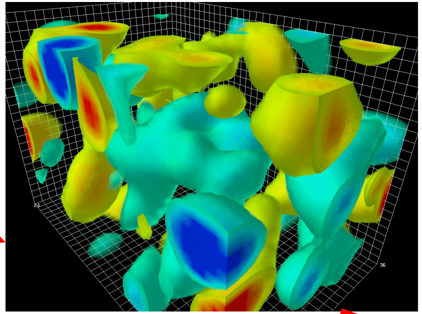
Lattice QFT

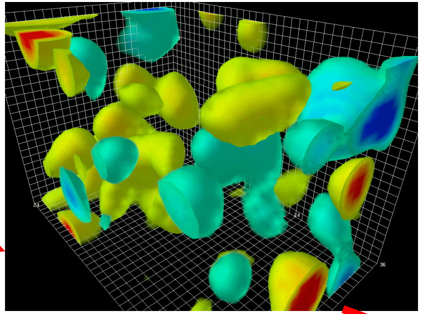
- Approximate the Euclidean path integral using Markov chain Monte Carlo

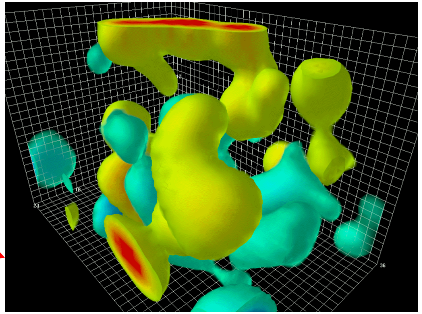
$$\langle \mathcal{O} \rangle = \int \mathcal{D}U e^{-S(U)} \mathcal{O}(U) \approx \frac{1}{N} \sum_{i}^{N} \mathcal{O}(U_i)$$

where $U_i \sim e^{-S(U)}$









[Leinweber, "Visualizations of Quantum Chromodynamics", 2004]

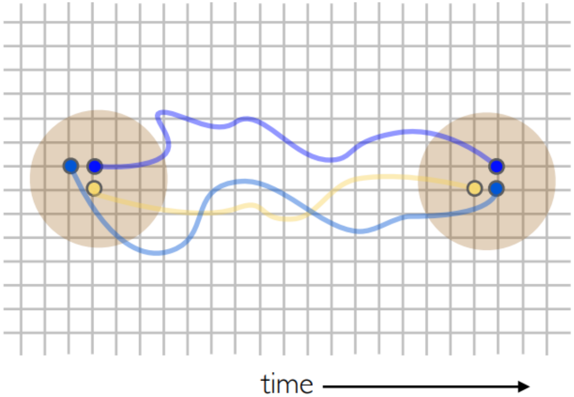
Lattice QFT

- Imaginary-time correlation functions inform us of the spectrum of the theory

$$\left\langle \mathcal{O}(t)\mathcal{O}^\dagger(0) \right\rangle = \sum_n Z_n e^{-E_n t} \sim Z_0 e^{-E_0 t}$$

$$m_{\text{eff}}(t) \equiv -\partial_t \log \left\langle \mathcal{O}(t)\mathcal{O}^\dagger(0) \right\rangle$$

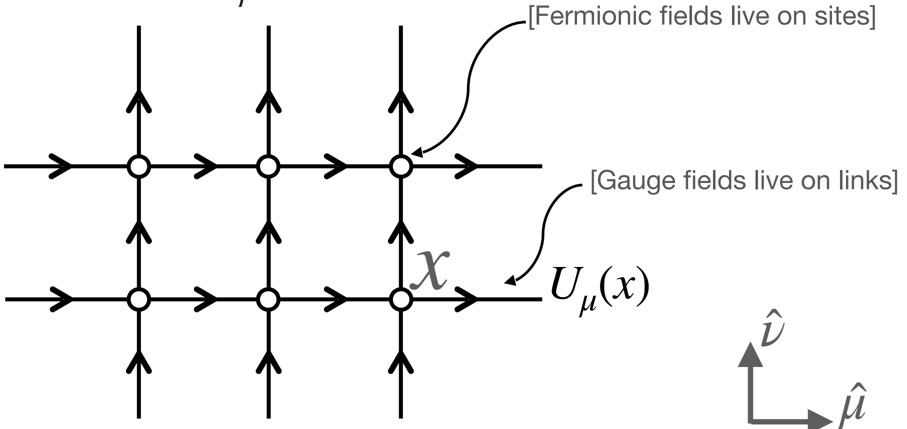
[Detmold, INT-14-57W]



E.g. for the nucleon in lattice QCD

Lattice gauge theory

- Exact **gauge invariance** preserved by discretizing gauge field onto links (short parallel transporters): $U_\mu(x) \in G$



[Image credit: Dan Hackett]

- $G = SU(N)$ relevant from a phenomenological standpoint

Signal-to-noise problem in observables

- Sample mean of observable is **noisy**

$$\sigma = \sqrt{\mathrm{Var}[\mathcal{O}]/N} \gg \langle \mathcal{O} \rangle$$

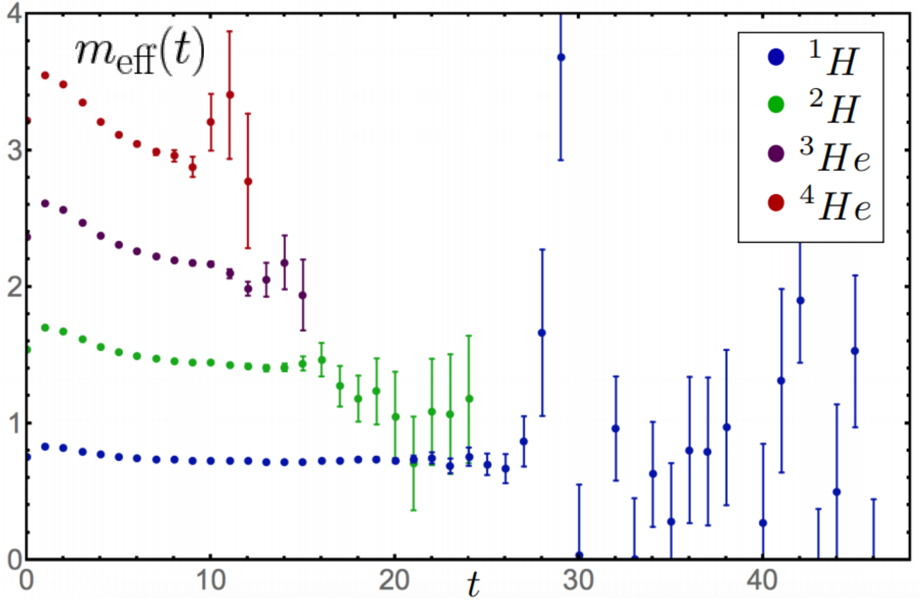
- Signal-to-noise (StN) problem

$$\mathrm{StN} = \frac{\langle \mathcal{O} \rangle}{\sigma} \ll 1$$

Noisy correlation functions

- **Large t:** StN falls exponentially
- **Small t:** Excited state effects
- To extract physical information, fit plateau at intermediate t
  (if it exists!)

[Wagman, Lattice 2018]



Noise problem driven by variance correlator

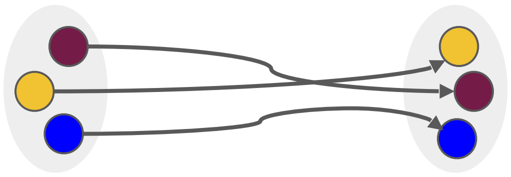
- Parisi & Lepage: variance related to physical states

$$\mathrm{Var}[\mathscr{A}(t)\mathscr{A}^\dagger(0)] = \left\langle \underline{\mathscr{A}(t)\mathscr{A}^\dagger(t)}\,\underline{\mathscr{A}^\dagger(0)\mathscr{A}(0)} \right\rangle$$

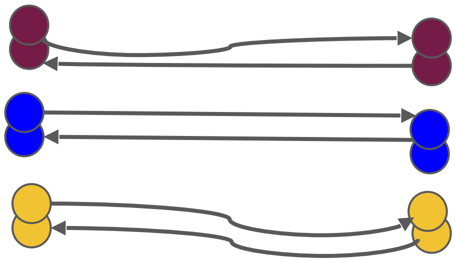
Interpret as creating / annihilating a physical state

- For the nucleon,

$$\left\langle \mathscr{N}(t)\mathscr{N}^\dagger(0) \right\rangle \sim e^{-M_N t}$$

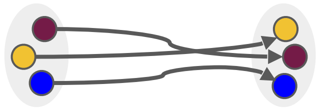


$$\mathrm{Var}[\mathscr{N}(t)\mathscr{N}^\dagger(0)] \sim e^{-3M_\pi t}$$

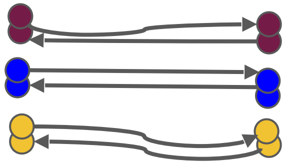


Variance correlator
~ 3 pions

Noise problem driven by variance correlator



$$\left\langle \mathcal{N}(t)\mathcal{N}^\dagger(0)\right\rangle \sim e^{-M_N t}$$



$$\mathrm{Var}[\mathcal{N}(t)\mathcal{N}^\dagger(0)] \sim e^{-3M_\pi t}$$

$$\mathrm{StN}[\mathcal{N}(t)\mathcal{N}^\dagger(0)] = \frac{\left\langle \mathcal{N}(t)\mathcal{N}^\dagger(0)\right\rangle}{\sqrt{\mathrm{Var}[\mathcal{N}(t)\mathcal{N}^\dagger(0)]}} \sim e^{-(M_N - 3M_\pi/2)t}$$

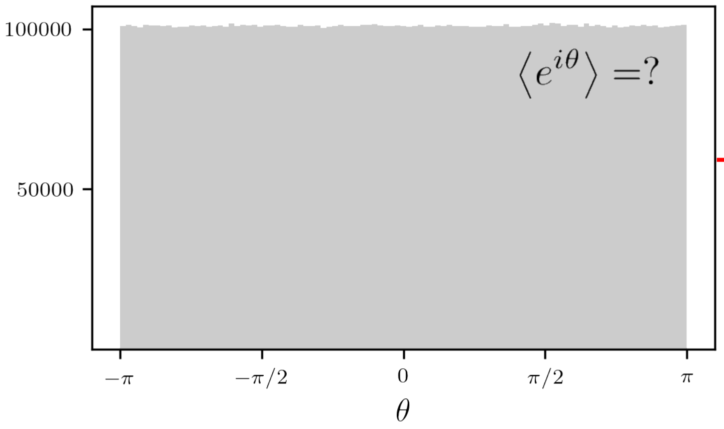
Exponentially bad!

Noise problem = sign problem

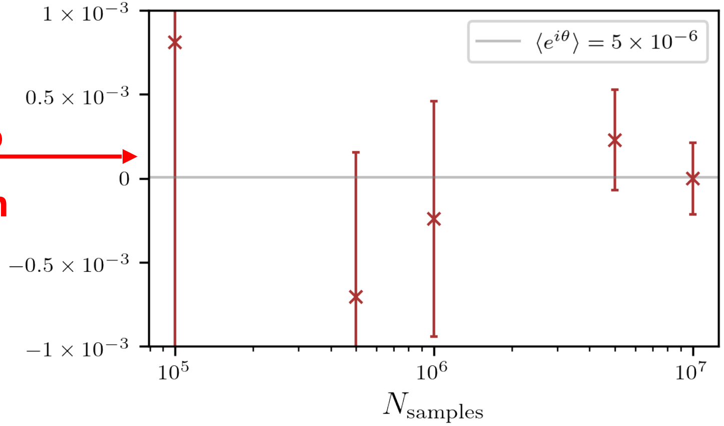
(actually, phase)

- Even for observables with real expectation, $\mathrm{Arg}\left[\mathcal{O}_i\right] \neq 0$

- **Sign problem:** when phase distribution is nearly uniform, precise near-cancellation of phases determines the mean



Monte Carlo breaks down

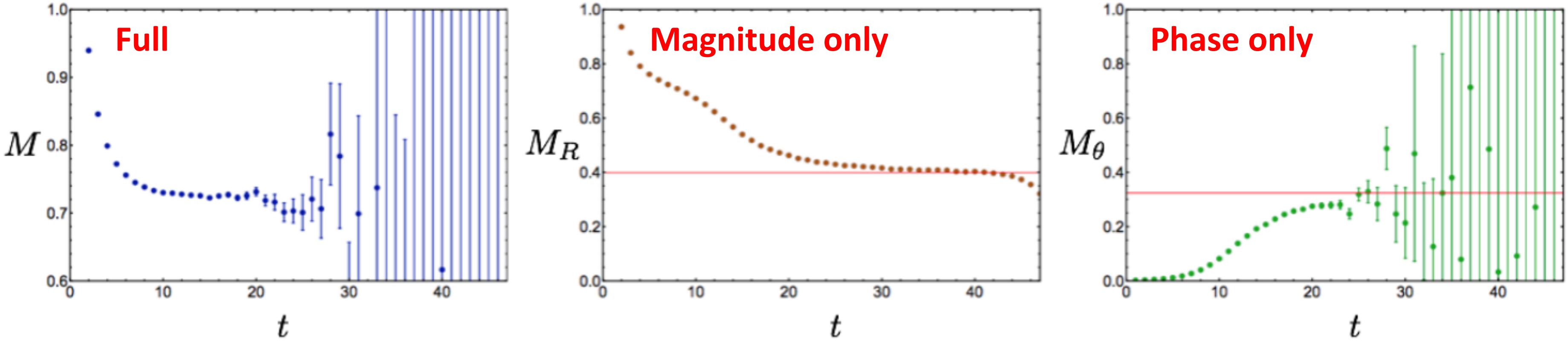


Noise problem = sign problem

(actually, phase)

- Empirically observed (e.g. nucleon, nuclei, Wilson loops in lattice QCD)

Nucleon Effective Mass



[Wagman & Savage, PRD96 (2017) 114508]

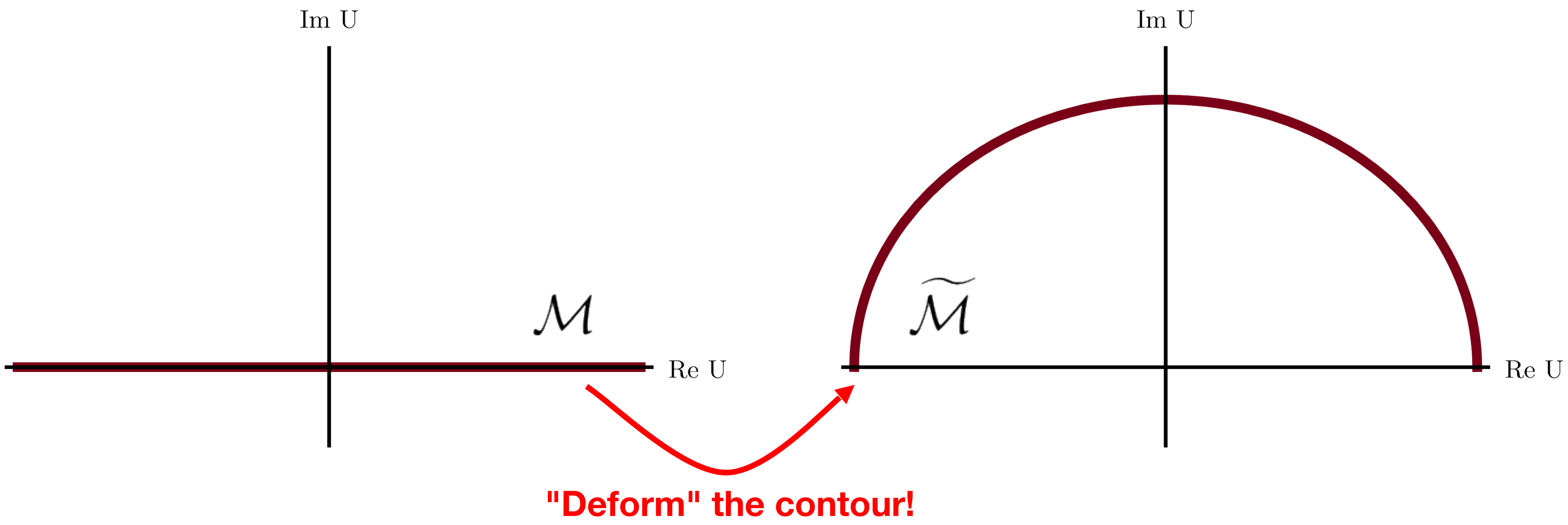
Can we make $\text{Var}[\mathcal{O}]$ smaller while preserving $\langle \mathcal{O} \rangle$?

Observifolds: Yes, and (often) without changing Monte Carlo sampling

Complex contour deformations

Original integral: $\mathcal{I} = \int_{\mathcal{M}} \mathcal{D}U \; f(U)$

If $f(U)$ is holomorphic: $\mathcal{I} = \int_{\widetilde{\mathcal{M}}} \mathcal{D}\widetilde{U} \; f(\widetilde{U})$



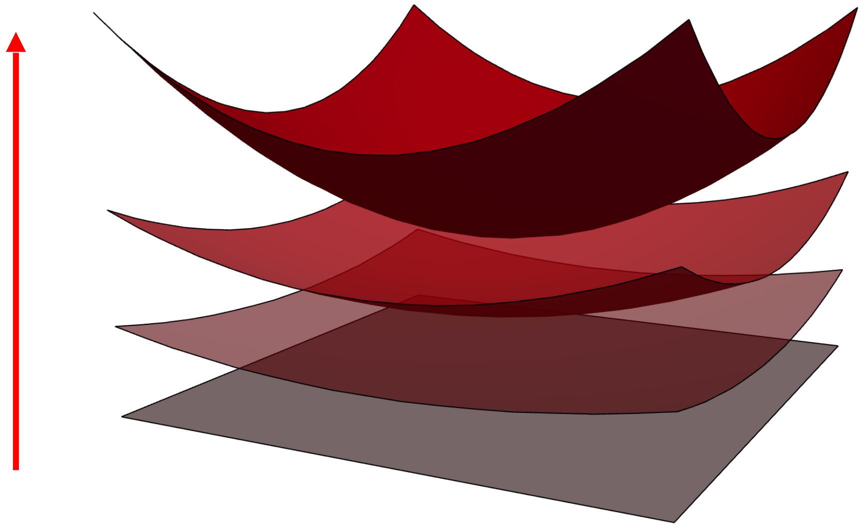
Deforming the path integral

Just high-dimensional contour deformation...

$$\langle \mathcal{O} \rangle = \int_{\mathcal{M}} \mathcal{D}U e^{-S(U)} \mathcal{O}(U) = \int_{\widetilde{\mathcal{M}}} \mathcal{D}\widetilde{U} e^{-S(\widetilde{U})} \mathcal{O}(\widetilde{U})$$

Integral value unchanged!

Deform all variables in high-dimensional configuration space



Holomorphic?

- Write Boltzmann weight e^{-S} and observable $\mathcal{O}$ in terms of real field variables.

  E.g. $$S_\phi = \ldots + m^2 \sum_n \phi_n^* \phi_n \quad \rightarrow \quad S_\phi = \ldots + m^2 \sum_n (a_n - ib_n)(a_n + ib_n),$$

  where $\phi_n = a_n + ib_n$, path integral holomorphic over $a_n, b_n \in \mathbb{R}$

- Lattice gauge theory: **angular parameterizations** give the needed real field variables

- Deforming angular params into complexified group, we are effectively treating

$$U^\dagger \to U^{-1}$$

Many related works on path integral deformations

Simulating theories with complex actions

- Non-zero density [Cristoforetti, et al. PRD86(074506), PRD88(051501), PRD89(114505); Aarts PRD88(094501); Alexandru, et al. PRD93(014504), JHEP05(053), PRD96(094505), PRD98(054514), PRD98(034506), PRD97(094510), PRL121(191602); Fujii, et al. JHEP12(125); Tanizaki, et al. NJP18(033002); Mori, et al. PTEP2018(023B04), PRD99(014033); ...]
- Real-time evolution [Alexandru, et al. PRL117(081602), PRD95(114501); Mou, et al. JHEP11(135)]

... and related to complex Langevin approaches [Aarts, et al. JHEP10(159); Sexty NPA931(856)]

Path integral deformations for observables ("observifolds")

Action is **real**, observable is **complex**

$$\langle \mathcal{O} \rangle = \int_{\widetilde{\mathcal{M}}} e^{-S(\widetilde{U})} \mathcal{O}(\widetilde{U}) \xrightarrow{\text{manifold coordinates}} \langle \mathcal{O} \rangle = \int_{\mathcal{M}} J(U) e^{-S(\widetilde{U}(U))} \mathcal{O}(\widetilde{U}(U))$$

Deformed observable with respect to **original Monte Carlo sampling**

$$\mathcal{Q}(U) \equiv e^{-[S_{\text{eff}}(U) - S(U)]} \mathcal{O}(\widetilde{U}(U)) \qquad \langle \mathcal{Q}(U) \rangle = \langle \mathcal{O}(U) \rangle$$

Note: $S_{\text{eff}}(U) \equiv S(\widetilde{U}(U)) - \log J(U)$

The big picture

$$\langle \mathcal{Q}(U) \rangle = \langle \mathcal{O}(U) \rangle$$

$$\mathrm{Var}[\mathcal{Q}(U)] \neq \mathrm{Var}[\mathcal{O}(U)]$$

Optimizing the variance

Either use **intuition** about good deformations, or **numerically optimize**.

Gradients can be estimated using existing MC samples,

$$\nabla_{\vec{\omega}} \operatorname{Var}(\operatorname{Re} \mathcal{Q}) = \left\langle \nabla_{\vec{\omega}} (\operatorname{Re} \mathcal{Q})^2 \right\rangle = 2 \left\langle \operatorname{Re} \mathcal{Q} \operatorname{Re} \nabla_{\vec{\omega}} \mathcal{Q} \right\rangle$$

$$= 2 \left\langle (\operatorname{Re} \mathcal{Q}) \operatorname{Re} \left(\mathcal{Q} \left[-\nabla_{\vec{\omega}} S_{\text{eff}} + \frac{\nabla_{\vec{\omega}} \mathcal{O}(\widetilde{U})}{\mathcal{O}(\widetilde{U})} \right] \right) \right\rangle .$$

Application: 1+1 U(1) gauge theory

[Detmold, GK, Wagman, Warrington PRD102 (2020) 014514]

Pure-gauge Schwinger model

1+1 U(1) gauge theory is the **quenched** limit of the Schwinger model (QED 1+1)

$$U_x^\mu \in U(1) \longrightarrow P_x = U_x^1 U_{x+\hat{1}}^2 (U_{x+\hat{2}}^1)^\dagger (U_x^2)^\dagger \longrightarrow \theta_x \equiv \arg P_x$$

links **plaquettes** **plaq phase**

Action is **holomorphic** in angular parameters

$$S_G(\theta) \equiv -\beta \sum_x \cos\theta_x$$

Note: theory with this action solvable for open BCs

Wilson loops

Closed loops of links, for $x \times t$ rectangle gives access to static quark correlation function, **string tension**

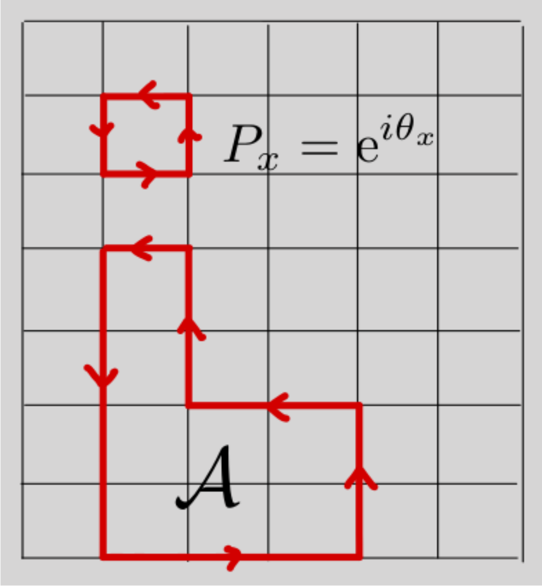
StN exponentially bad with Wilson loop area

$$\langle W_{\mathcal{A}} \rangle \equiv \left\langle \prod_{x \in \mathcal{A}} e^{i\theta_x} \right\rangle = e^{-\sigma A}$$

where $\sigma = \ln \left[\frac{I_0(\beta)}{I_1(\beta)} \right]$

$$\mathrm{StN}(W_{\mathcal{A}}) = \frac{e^{-\sigma A}}{\sqrt{\frac{1}{2} + \frac{1}{2} e^{-\sigma' A} - e^{-2\sigma A}}}$$

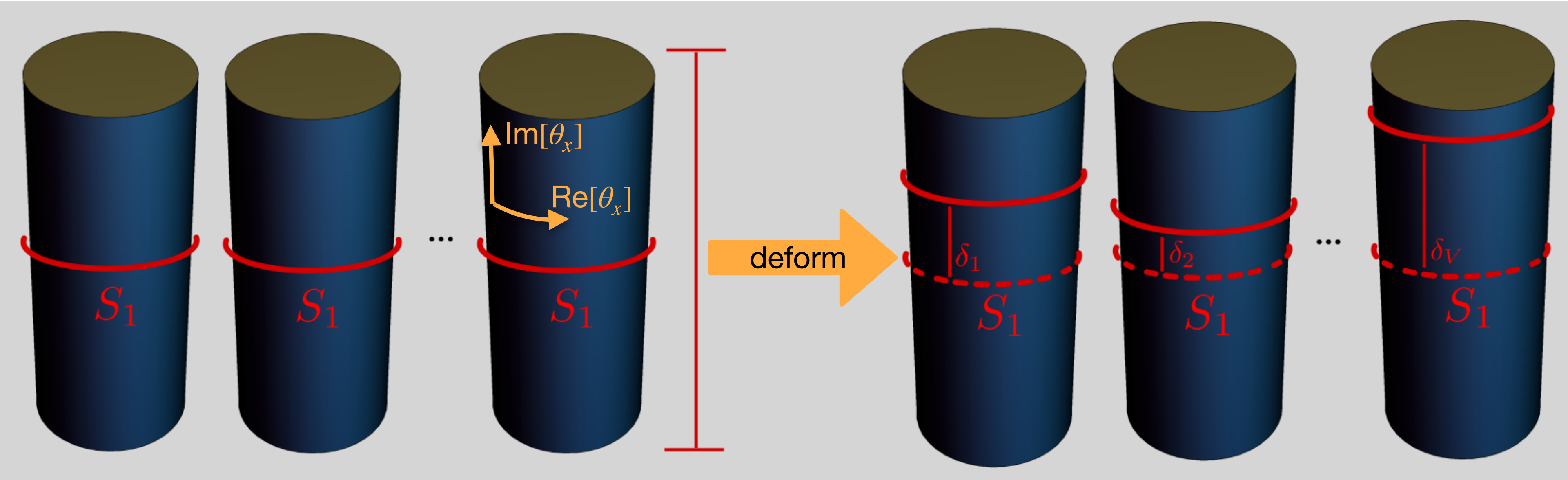
1+1 U(1) plaquettes / loops



Deformation

Shift plaquette integral in complex direction

$$\widetilde{\theta}_x = \theta_x + i\delta_x$$



Deformation

For all plaquettes inside loop, $\delta_x = \delta$, otherwise 0

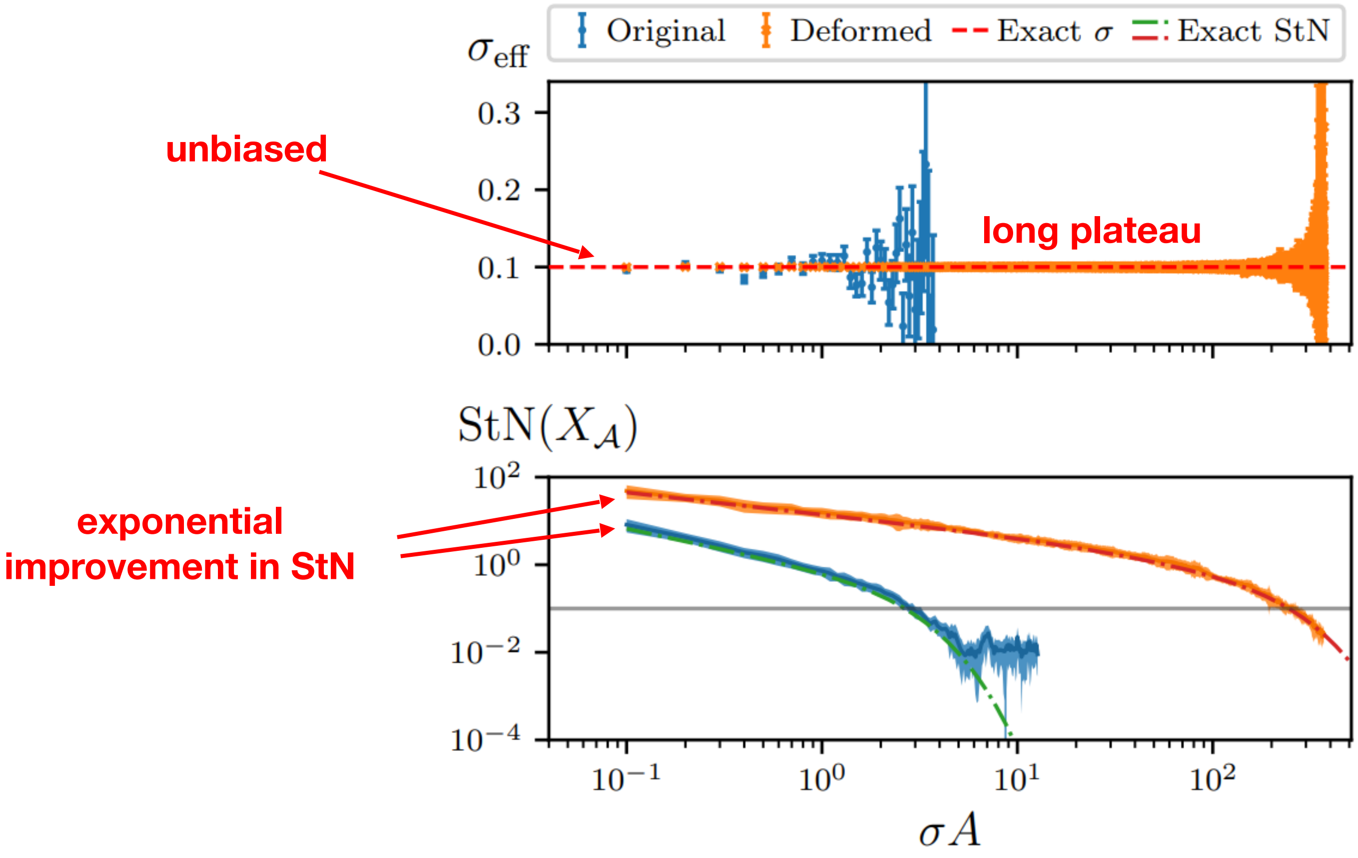
$$\widetilde{\theta}_x = \theta_x + i\delta_x$$

Intuition: make observable magnitude small sample-by-sample…

$$e^{i\theta_x} \to e^{i\theta_x} e^{-\delta}$$

… holomorphy guarantees expectation unchanged, so less phase cancellation required!

It works!


Original
Deformed
Exact σ
Exact StN
σ_eff
0.3
0.2
0.1
0.0
unbiased
long plateau
StN(X_A)
10^2
10^0
10^-2
10^-4
exponential
improvement in StN
10^-1
10^0
10^1
10^2
σA

Application: 1+1 SU(N) gauge theory

[Detmold, GK, Lamm, Wagman, Warrington 2101.xxxxx]

Pure-gauge $SU(N)$ theory

Links $U_\mu(x) \in SU(N)$, plaquettes and Wilson loops constructed like Schwinger

$$P_x = U_x^1 U_{x+\hat{1}}^2 (U_{x+\hat{2}}^1)^\dagger (U_x^2)^\dagger \in SU(N) \qquad\qquad W_{\mathscr{A}} = \prod_{x \in \mathscr{A}} P_x$$

Wilson gauge action written in terms of plaquettes

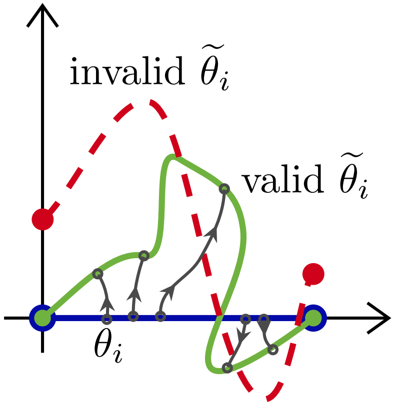
$$S = -\frac{1}{g^2} \sum_x \mathrm{tr}(P_x + P_x^{-1})$$

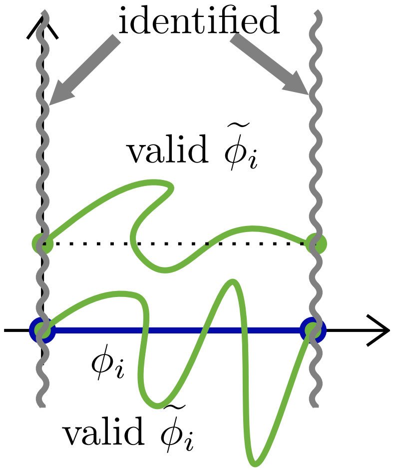
Angular parameterization of $SU(N)$

[Bronzan PRD38 (1988) 1994] gives an explicit construction for $SU(3)$ and generalized approach for $SU(N)$

- Azimuthal angles $\phi_j \in [0,2\pi]$
- Zenith angles $\theta_i \in [0,\pi/2]$
- $\Omega \equiv (\phi_1, \ldots, \theta_1, \ldots)$

Deform collection of angles, dealing appropriately with **endpoints**





Deformation

Vertical deformations $\widetilde{\Omega} = \Omega + if(\Omega)$

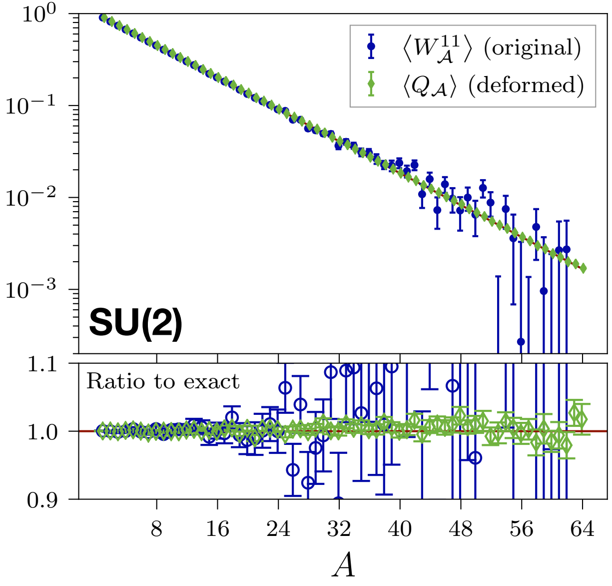
Fourier series definition of $f(\Omega)$, using a subset of all possible terms

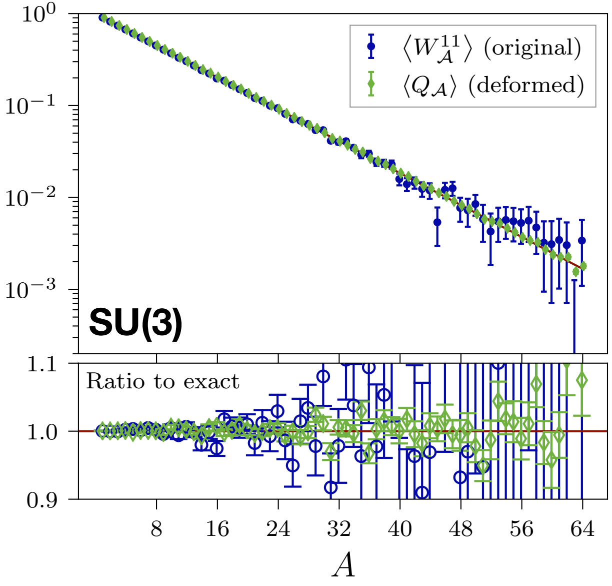
- Care with **endpoints**: For θ_i use modes $\sin(2\theta_i m_i)$ preserving fixed endpoints, for ϕ_i use modes $\sin(\phi_i n_i + \chi_i)$ preserving endpoint identification
- Cutoff Λ labels highest mode included

Results

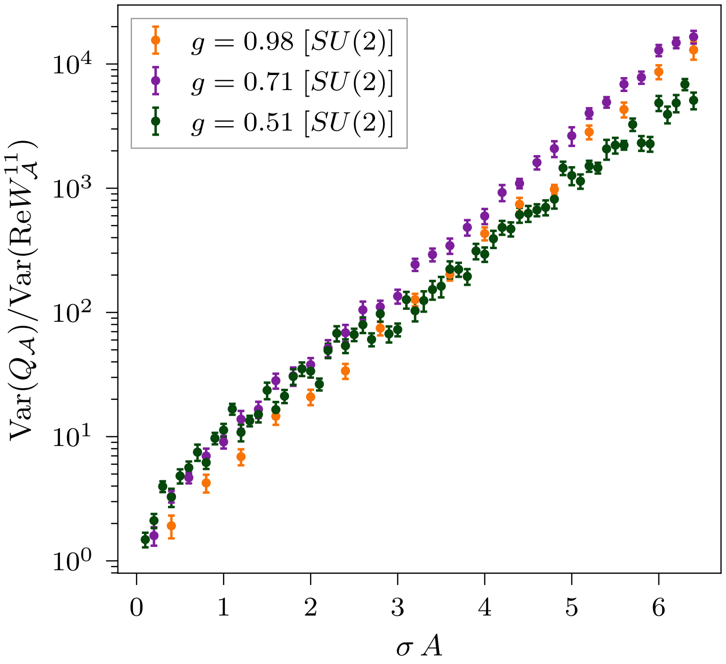
- Tested on $SU(2)$ and $SU(3)$ gauge theory
- 3 choices of coupling, coarse / med / fine lattices with fixed physical volume

Fine lattices:

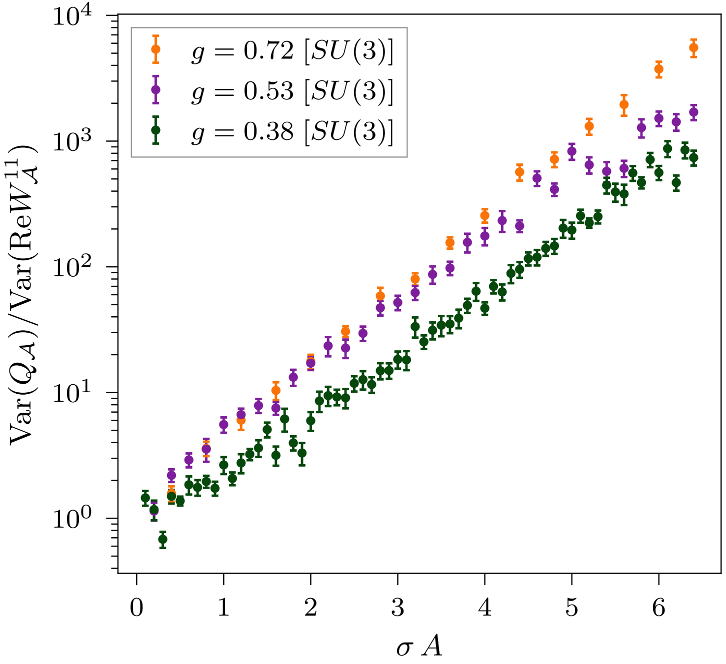




Results

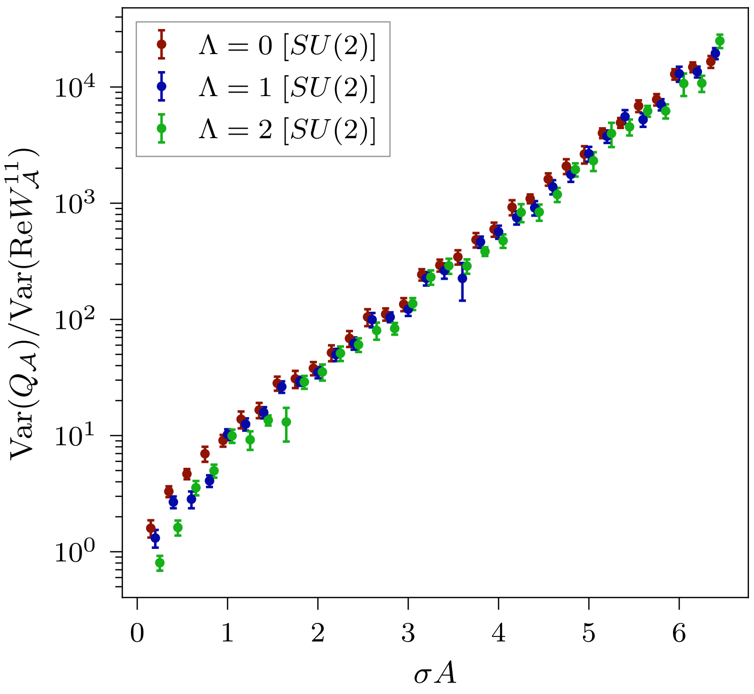


$g = 0.98$ $[SU(2)]$
$g = 0.71$ $[SU(2)]$
$g = 0.51$ $[SU(2)]$
$\mathrm{Var}(Q_{\mathcal{A}})/\mathrm{Var}(\mathrm{Re}W^{11}_{\mathcal{A}})$
σA

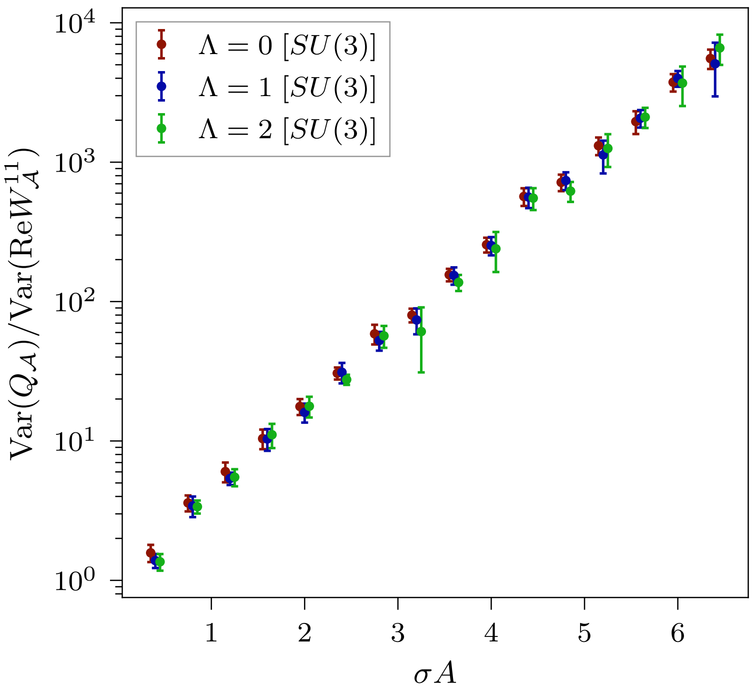


$g = 0.72$ $[SU(3)]$
$g = 0.53$ $[SU(3)]$
$g = 0.38$ $[SU(3)]$
$\mathrm{Var}(Q_{\mathcal{A}})/\mathrm{Var}(\mathrm{Re}W^{11}_{\mathcal{A}})$
σA

Results



$\Lambda = 0\ [SU(2)]$
$\Lambda = 1\ [SU(2)]$
$\Lambda = 2\ [SU(2)]$
$\mathrm{Var}(Q_\mathcal{A})/\mathrm{Var}(\mathrm{Re}W_\mathcal{A}^{11})$
10^0
10^1
10^2
10^3
10^4
0
1
2
3
4
5
6
σA



$\Lambda = 0\ [SU(3)]$
$\Lambda = 1\ [SU(3)]$
$\Lambda = 2\ [SU(3)]$
$\mathrm{Var}(Q_\mathcal{A})/\mathrm{Var}(\mathrm{Re}W_\mathcal{A}^{11})$
10^0
10^1
10^2
10^3
10^4
1
2
3
4
5
6
σA

Conclusions / Outlook

1. Deforming holomorphic path integral preserves mean
2. Use this to our advantage: find better observables, **provably** identical mean
3. Both $U(1)$ and $SU(N)$ lattice gauge theory in 1+1D promising
4. No theoretical obstacle to higher dims… practical results?
5. Fermionic observables?

Towards LQCD and other relevant LQFTs!

Backup Slides

Application: 0+1 complex scalar theory

Complex scalar theory

Use phase-magnitude decomposition for variables $\phi_t = R_t e^{i\theta_t}$

Holomorphic: $$S = -2\sum_{t=0}^{L-1} R_t R_{t+1}\cos(\theta_{t+1} - \theta_t) + V(R)$$

$$V(R) \;=\; \sum_t (2 + m^2)R_t^2 + \lambda R_t^4$$

Interested in correlation functions

$$G_t = \left\langle R_t R_0 e^{i\theta_t - i\theta_0} \right\rangle \equiv \langle C_t(R,\theta)\rangle$$

Deformation for scalar theory

Intuition: phase differences appear in action similarly to phases of Schwinger, use shifts into imaginary direction

$$\tilde{\theta}_t = \theta_t + i\delta_t^{(1)} + i\delta_t^{(2)} f_c(R_t R_{t+1}) + i\delta_t^{(3)} f_c(R_{t-1} R_t)$$

Extra terms inspired by small phase fluctuation expansion.

Results

Experiments with numerical optimization as well as simple one-parameter hand tuning