[Detmold, GK, Wagman, Warrington **PRD102 (2020) 014514**, 2003.05914]
[Detmold, GK, Lamm, Wagman, Warrington **PRD103 (2021) 094517**, 2101.12668]

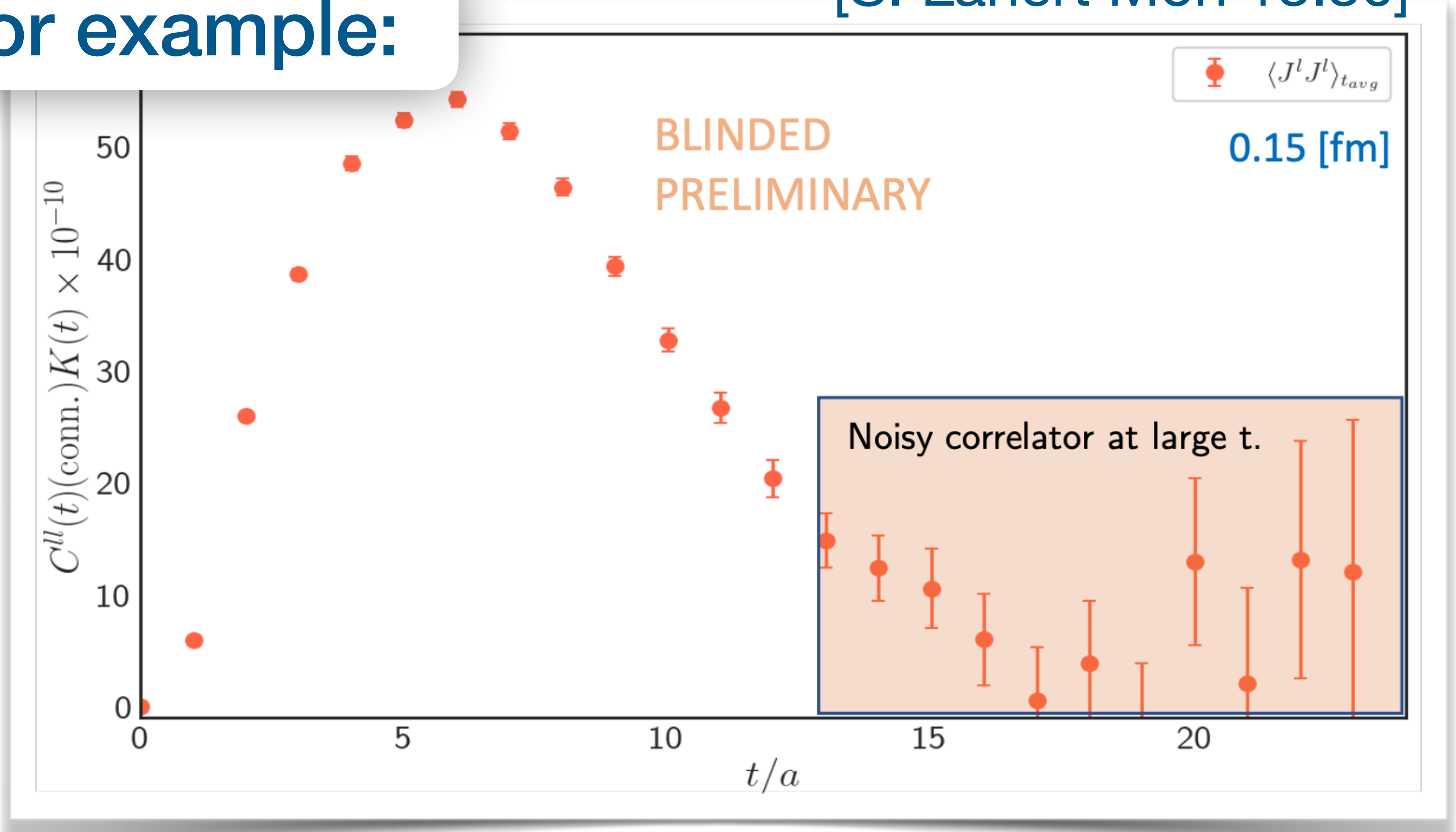
Massachusetts Institute of Technology

Observifolds:

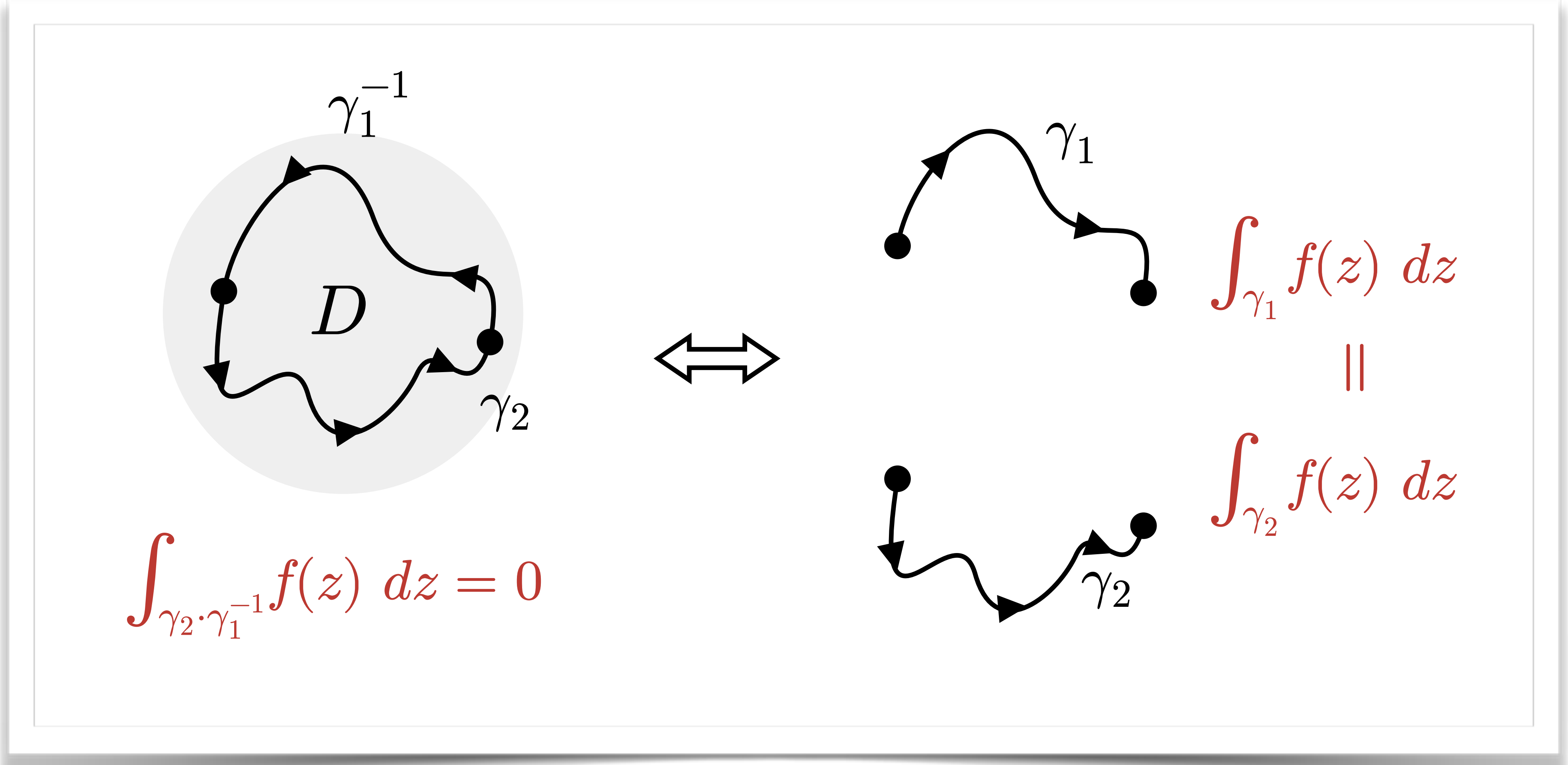
Taming the signal-to-noise problem via contour deformations

For example:

[S. Lahert Mon 13:30]



[GK PhD Thesis, 2106.01975]



Gurtej Kanwar (MIT)
July 27, 2021

38th International Symposium on Lattice Field Theory
MIT | Boston, MA | July 26-30, 2021

Signal-to-noise problems and the variance correlator

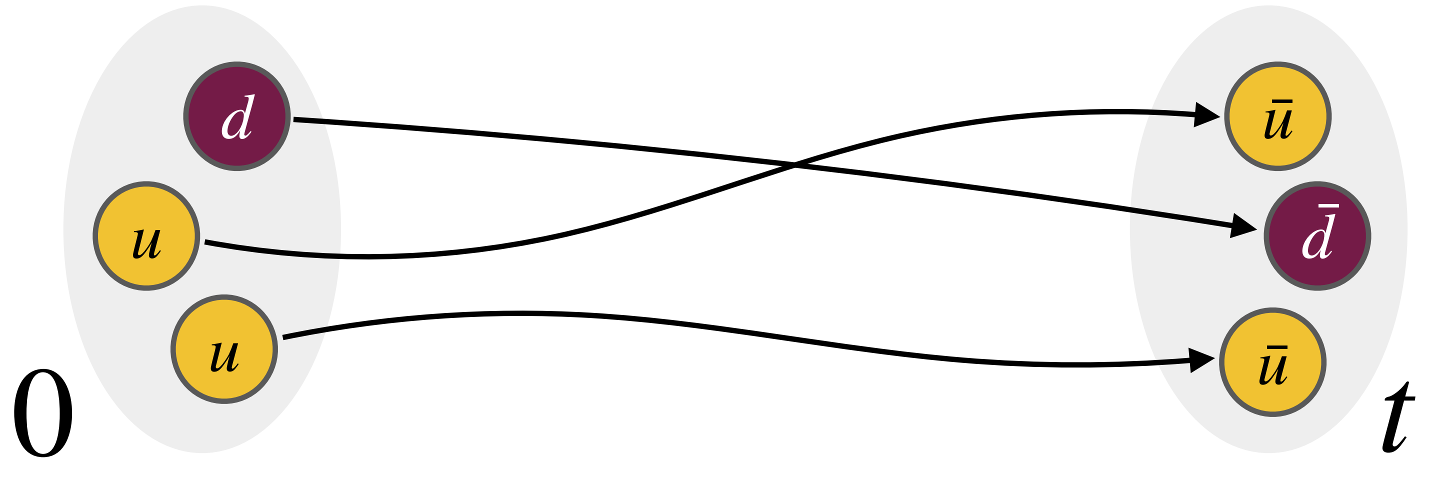
Parisi & Lepage: variance scaling related to physical states

$$\text{Var}[\mathscr{A}(t)\mathscr{A}^\dagger(0)] \sim \left\langle \underline{\mathscr{A}(t)\mathscr{A}^\dagger(t)}\,\underline{\mathscr{A}^\dagger(0)\mathscr{A}(0)} \right\rangle \sim e^{-M_{A^\dagger A}t}$$

Interpret as annihilating / creating a physical state

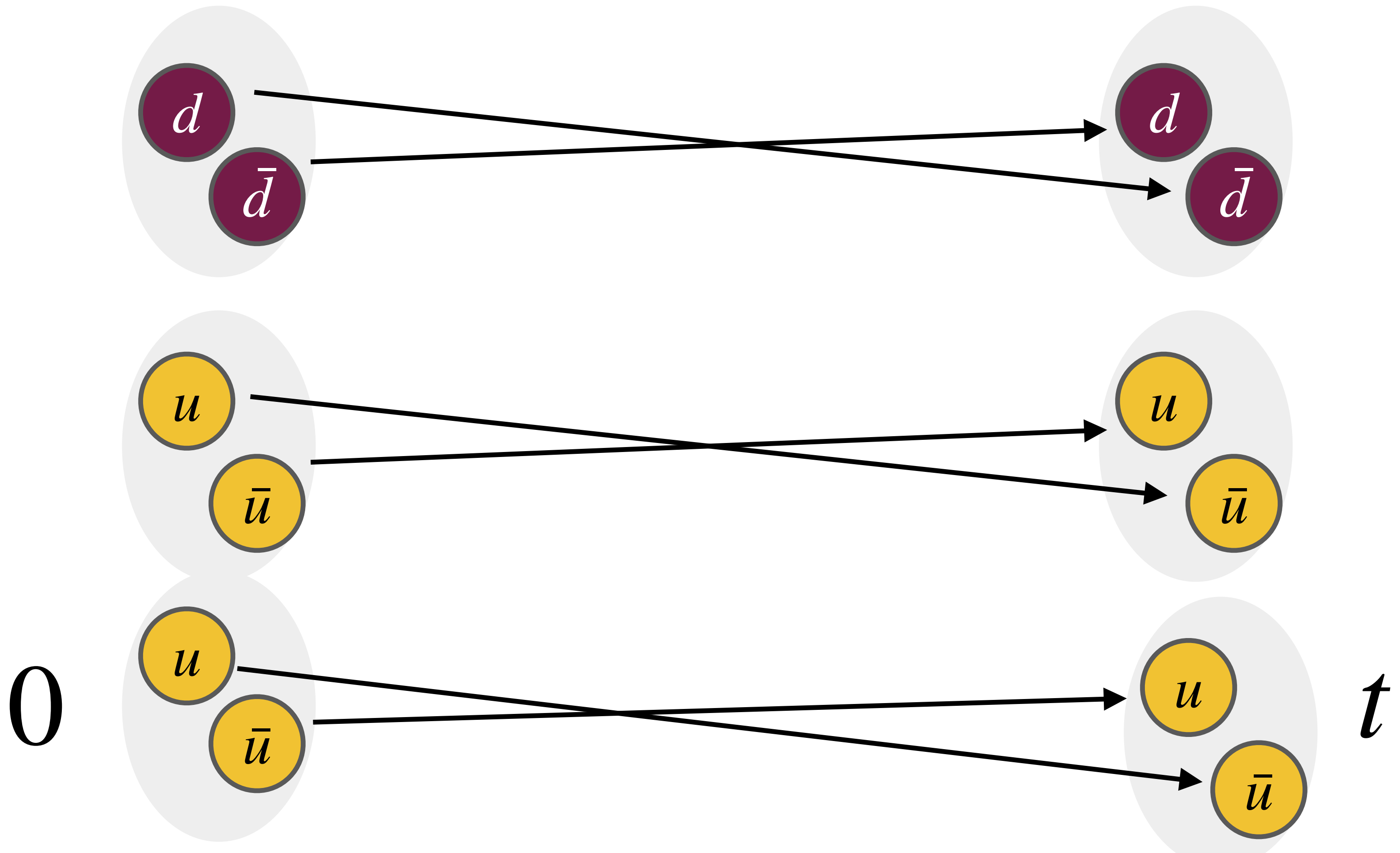
Example: StN of the nucleon given by

Signal:



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

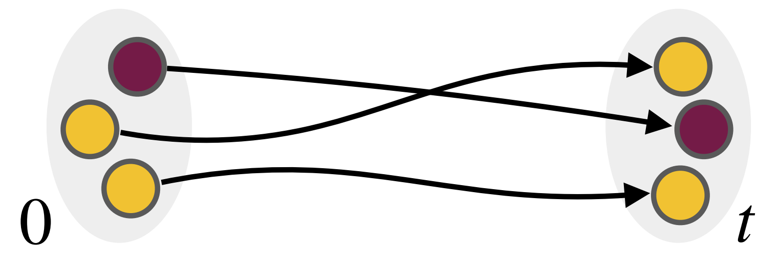
Variance:



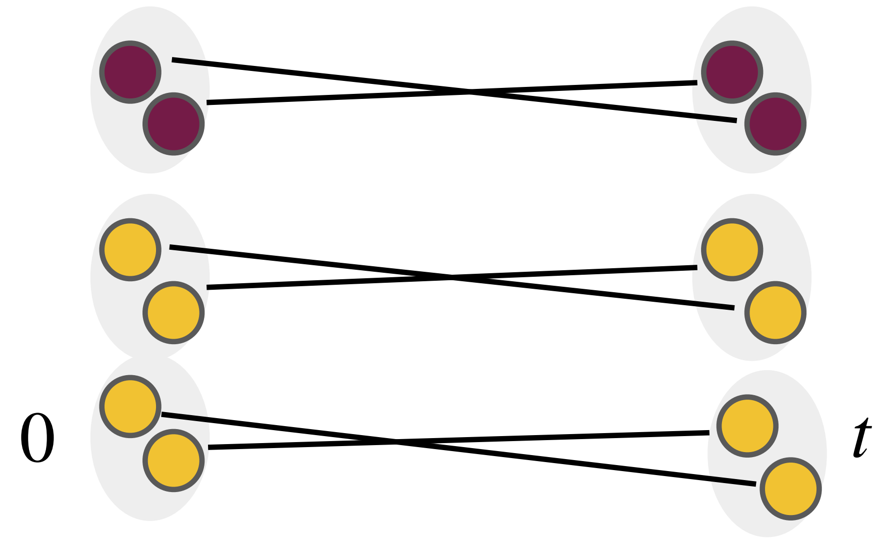
$$\text{Var}[\mathscr{N}(t)\mathscr{N}^\dagger(0)] \sim e^{-3M_\pi t}$$

Variance correlator ~ 3 pions

Signal-to-noise problems and the variance correlator



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



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

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

Exponentially bad!

Similar problems affect 3-point and higher correlation functions!

(or complex phase)

Noise problem = sign problem

Intuition:

$$\mathrm{Var}[C(t)] \sim \langle |C(t)|^2 \rangle \sim \mathrm{Var}[|C(t)|]$$

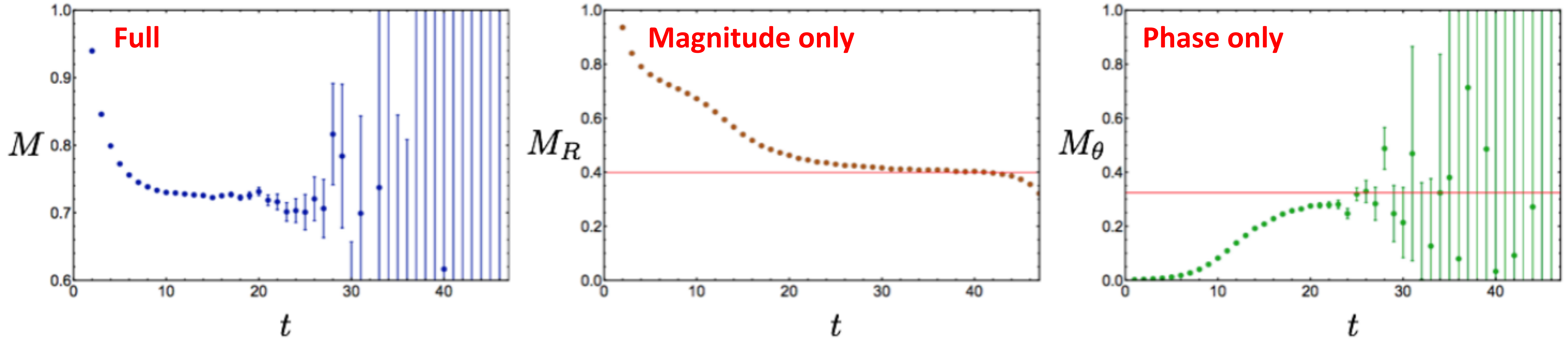
Variance scaling set by magnitude…

$$\langle C(t) \rangle \ll \langle |C(t)| \rangle$$

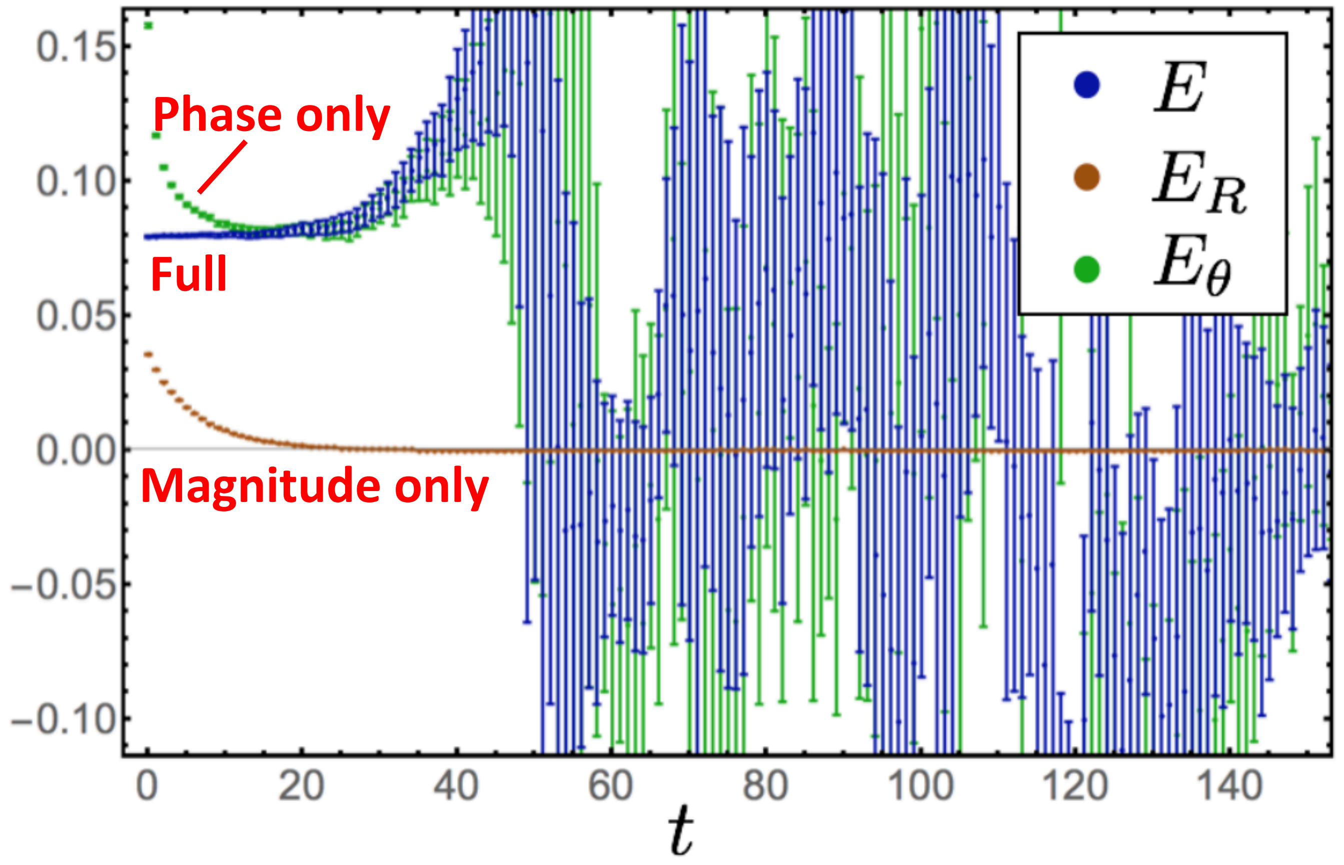
… but phase fluctuations generically give exponentially smaller signal.

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

Nucleon effective mass: [Wagman & Savage, PRD96 (2017) 114508]



Scalar theory effective mass:



[Detmold, GK, Wagman, PRD98 (2018) 074511]

Can we leverage contour deformations to shrink Var[$\mathcal{O}$] while preserving $\langle \mathcal{O} \rangle$?

Can we leverage contour deformations to shrink Var$[\mathcal{O}]$ while preserving $\langle \mathcal{O} \rangle$?

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

Deforming the path integral

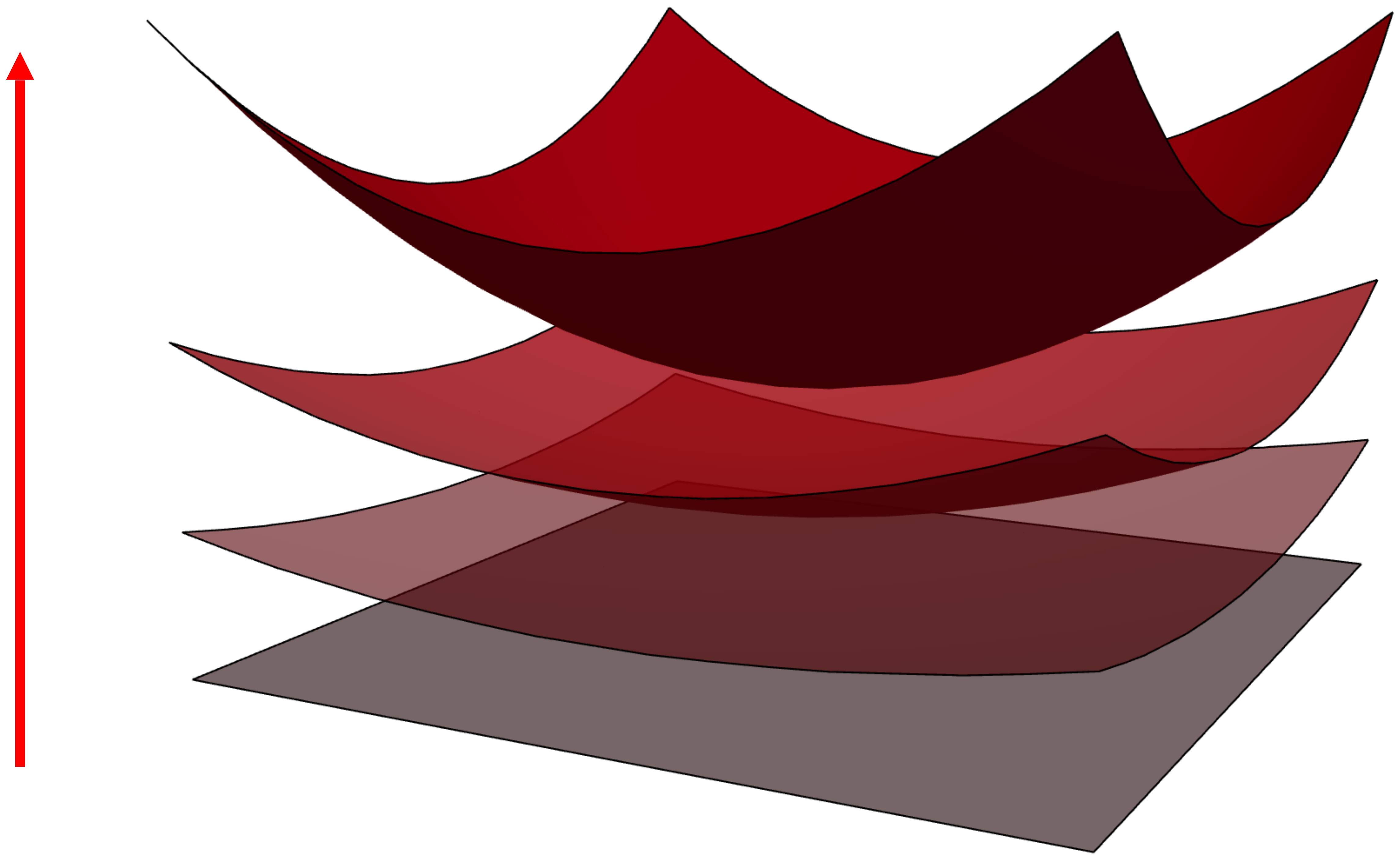
See previous talk by Neill Warrington!

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



[Image credit: Neill Warrington]

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**

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

Measure "deformed observable", use **original Monte Carlo weights**

$$\mathcal{Q}(U) \equiv e^{-[S_{\text{eff}}(U) - S(U)]} \mathcal{O}(\tilde{U}(U))$$

… where $S_{\text{eff}}(U) \equiv S(\tilde{U}(U)) - \log J(U)$

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

This is key!

Path integral deformations for observables (“observifolds”)

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

$$\langle \mathcal{O} \rangle = \int_{\tilde{\mathcal{M}}} e^{-S} \quad \ldots \quad e^{-S(\tilde{U}(U))}\mathcal{O}(\tilde{U}(U))$$

Measure “deforme … **eights**

However:

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

$$\mathcal{Q}(U) \equiv e^{-[S_{\text{eff}}(U) - S(U)]}\mathcal{O}(\tilde{U}(U))$$

… where $S_{\text{eff}}(U) \equiv S(\tilde{U}(U)) - \log J(U)$

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

This is key!

Optimizing the variance

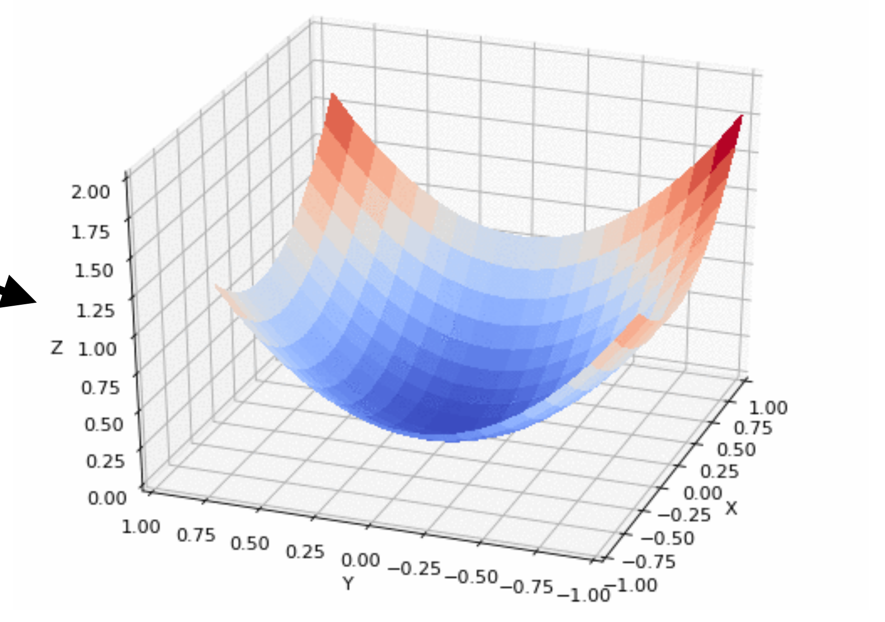
Choice of $\tilde{U}(U)$ defines $\mathcal{Q}(U)$ → Deformation determines variance.

Write expressive parameterizations, then **numerically minimize variance.**

- Gradients of variance defined using **existing MC samples**:

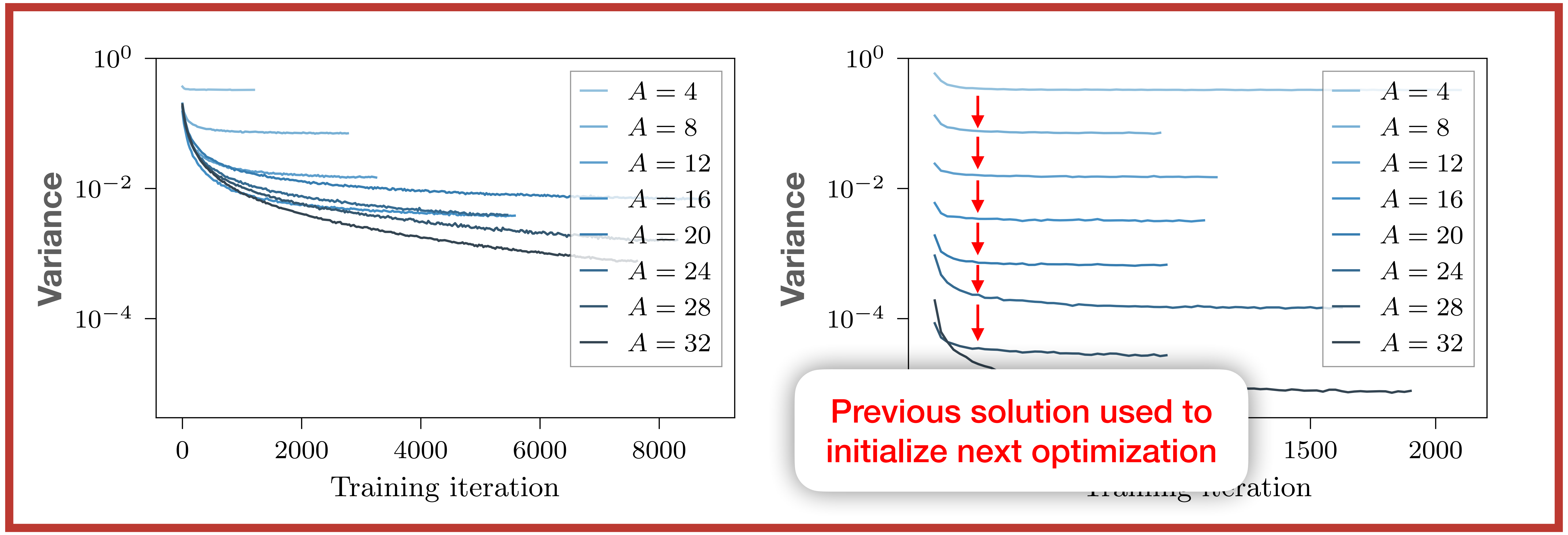
$$\nabla_{\vec{\omega}} \mathrm{Var}[\mathrm{Re}\,\mathcal{Q}] = \langle \nabla_{\vec{\omega}} (\mathrm{Re}\,\mathcal{Q})^2 \rangle = 2 \langle \mathrm{Re}\,\mathcal{Q}\,\mathrm{Re}\,\nabla_{\vec{\omega}} \mathcal{Q} \rangle$$

$$= 2 \left\langle (\mathrm{Re}\,\mathcal{Q}) \mathrm{Re} \left(\mathcal{Q} \left[-\nabla_{\vec{\omega}} S_{\mathrm{eff}} + \frac{\nabla_{\vec{\omega}} \mathcal{O}(\tilde{U})}{\mathcal{O}(\tilde{U})} \right] \right) \right\rangle$$



Stochastic gradient descent

- Different manifold for each observable, but **transfer learning** allows efficient optimization:



Application to $SU(N)$ gauge theory

Write Wilson gauge action written in terms of **plaquettes**

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

Analytic continuation of $P_x^\dagger$

Complexification:
$SU(N) \to SL(N,\mathbb{C})$

Three lattice spacings:

		$SU(2)$		$SU(3)$	
σ	V	g	β	g	β
0.4	16	0.98	4.2	0.72	11.7
0.2	32	0.71	8.0	0.53	21.7
0.1	64	0.51	15.5	0.38	41.8

Parameters chosen to fix σV

Study **Wilson loops** as an example observable:

$$W_{\mathcal{A}}^{11} = [\prod_{x\in\mathcal{A}} P_x]^{11}$$

$$\langle W_{\mathcal{A}}^{11}\rangle = \frac{1}{N}\mathrm{tr}\langle W_{\mathcal{A}}\rangle \sim e^{-\sigma A}, \quad \mathrm{Var}[W_{\mathcal{A}}^{11}] \sim 1$$

Exponentially bad StN problem

Useful to …

- Gauge fix
- Write Wilson loop using plaqs.
- Select a diag component, here (1,1)

Angular parameterization of $SU(N)$

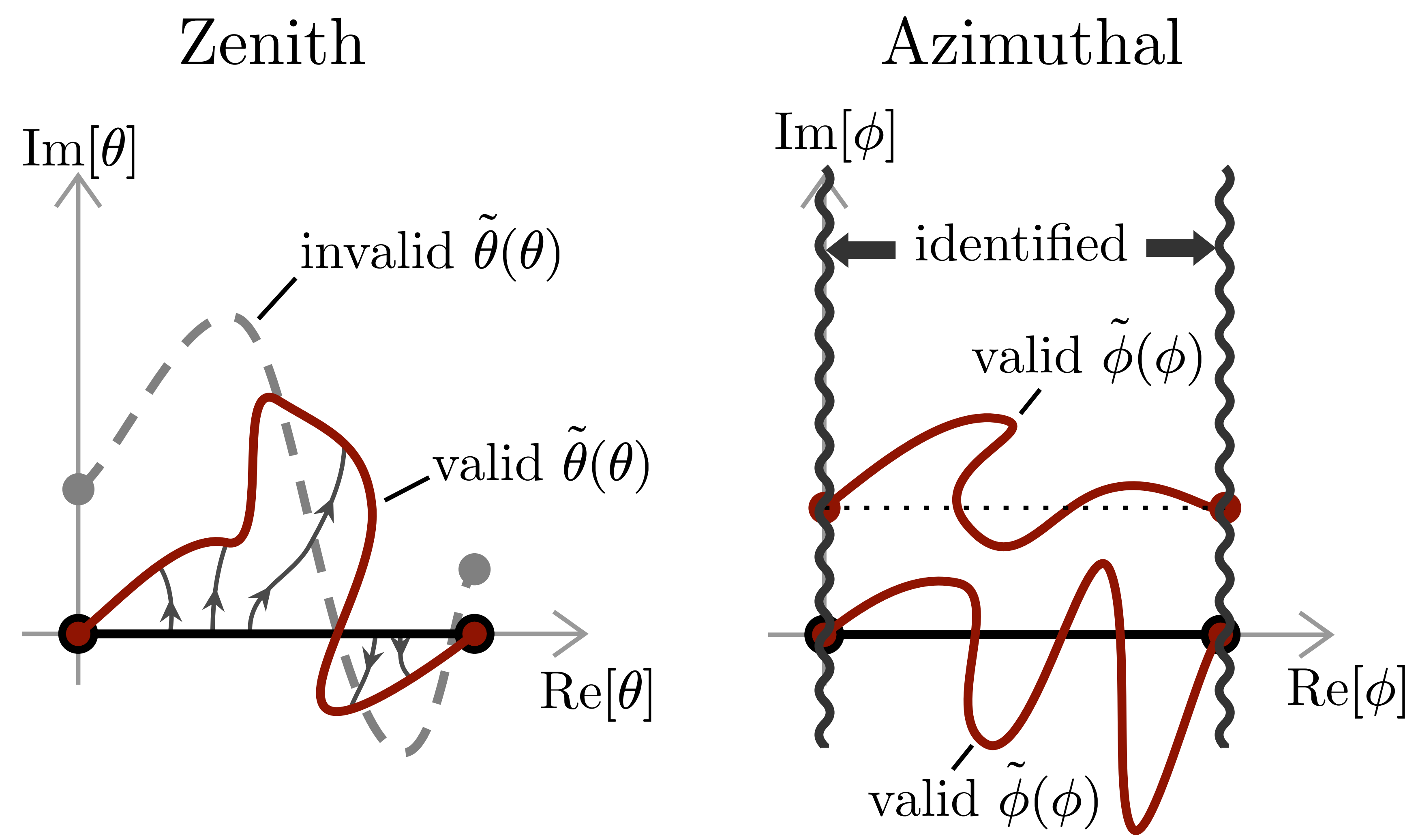
[Bronzan PRD38 (1988) 1994] gives an explicit construction for $SU(3)$ and generalized approach for $SU(N)$

- **Azimuthal** angles $\phi_j \in [0,2\pi]$
- **Zenith** angles $\theta_i \in [0,\pi/2]$
- $\Omega \equiv \underbrace{(\phi_1, \ldots, \theta_1, \ldots)}_{(N^2-1)\text{ angles}}$

$$U(\Omega) = \begin{pmatrix} c_1 c_2 e^{i\phi_1} & s_1 e^{i\phi_3} & c_1 s_2 e^{i\phi_4} \\ s_2 s_3 e^{-i(\phi_4+\phi_5)} - s_1 c_2 c_3 e^{i(\phi_1+\phi_2-\phi_3)} & c_1 c_3 e^{i\phi_2} & -c_2 s_3 e^{-i(\phi_1+\phi_5)} - s_1 s_2 c_3 e^{i(\phi_2-\phi_3+\phi_4)} \\ -s_1 c_2 s_3 e^{i(\phi_1-\phi_3+\phi_5)} - s_2 c_3 e^{-i(\phi_2+\phi_4)} & c_1 s_3 e^{i\phi_5} & c_2 c_3 e^{-i(\phi_1+\phi_2)} - s_1 s_2 s_3 e^{-i(\phi_3-\phi_4-\phi_5)} \end{pmatrix}$$

where $s_i \equiv \sin(\theta_i)$, $c_i \equiv \cos(\theta_i)$.

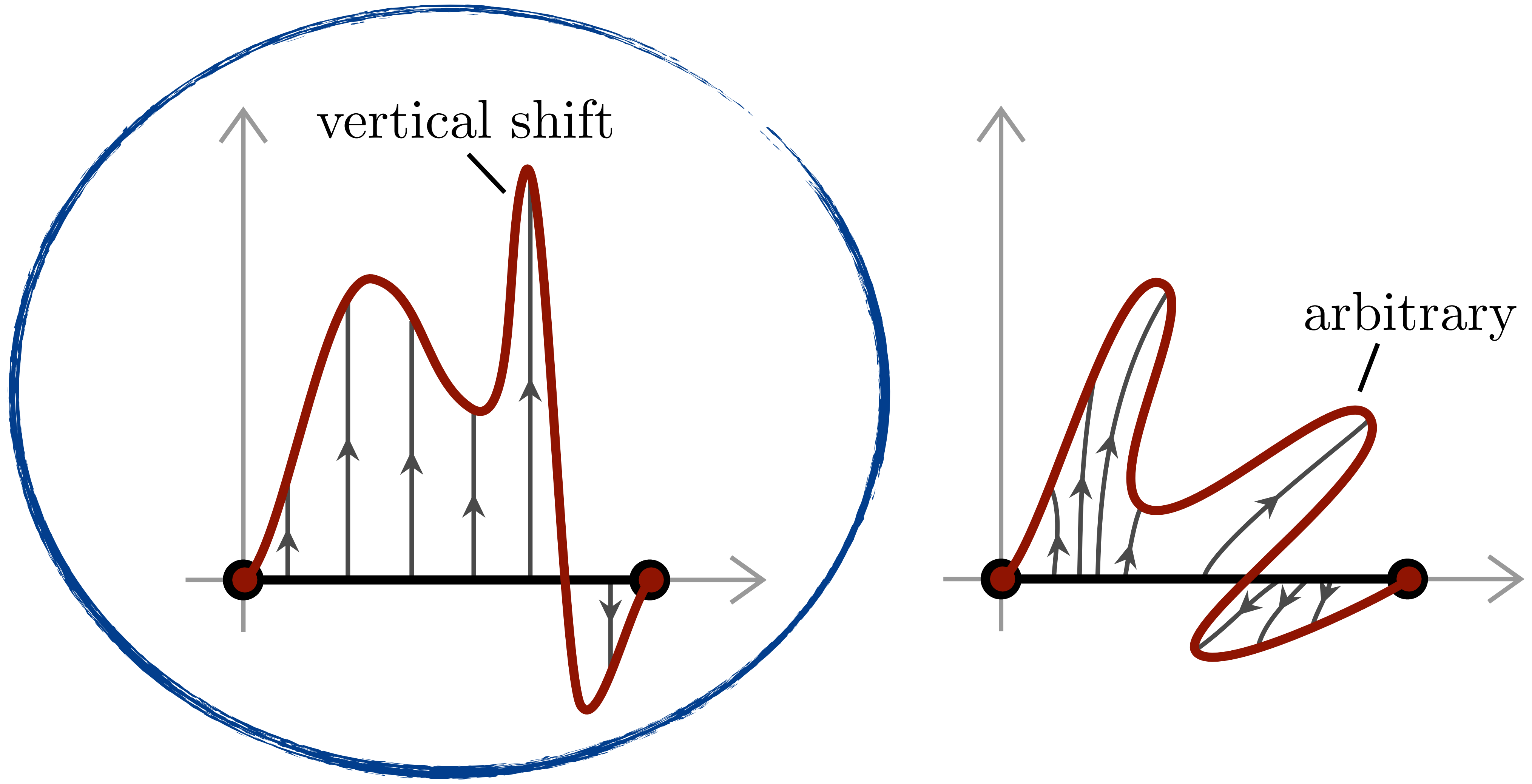
Deform collection of angles, dealing appropriately with **endpoints**



Action & observables are holomorphic functions of complexified angles.

Deformation

Vertical deformations $\tilde{\Omega}_x = \Omega_x + if(\Omega)$



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

$$\tilde{\phi}^a_x = \phi^a_x + i\kappa_0^{x;\phi^a} + i\sum_{y\leq x} f_{\phi^a}(\Omega_y; \kappa^{xy}, \lambda^{xy}, \chi^{xy}, \zeta^{xy}),$$

$$\tilde{\theta}^a_x = \theta^a_x + i\sum_{y\leq x} f_{\theta^a}(\Omega_y; \kappa^{xy}, \lambda^{xy}, \chi^{xy})\,.$$

Original real part

Parameterized imaginary shift

$$f_{\theta^a} = \sum_{m=1}^{\Lambda} \kappa_m^{xy;a} \sin(2m\theta^a_y)\Big\{1 + \sum_{n=1}^{\Lambda}\Big[\sum_{\substack{r\neq a\\ r=1}}^{3} \lambda_{mn}^{xy;ar}\sin(2n\theta^r_y) + \sum_{s=1}^{5}\eta_{mn}^{xy;as}\sin(n\phi^s_y + \chi_{mn}^{xy;as})\Big]\Big\},$$

$$f_{\phi^a} = \sum_{m=1}^{\Lambda} \kappa_m^{xy;a} \sin(m\phi^a_y + \zeta_m^{xy;a})\Big\{1 + \sum_{n=1}^{\Lambda}\Big[\sum_{r=1}^{3} \lambda_{mn}^{xy;ar}\sin(2n\theta^r_y) + \sum_{\substack{s\neq a\\ s=1}}^{5}\eta_{mn}^{xy;as}\sin(n\phi^s_y + \chi_{mn}^{xy;as})\Big]\Big\}.$$

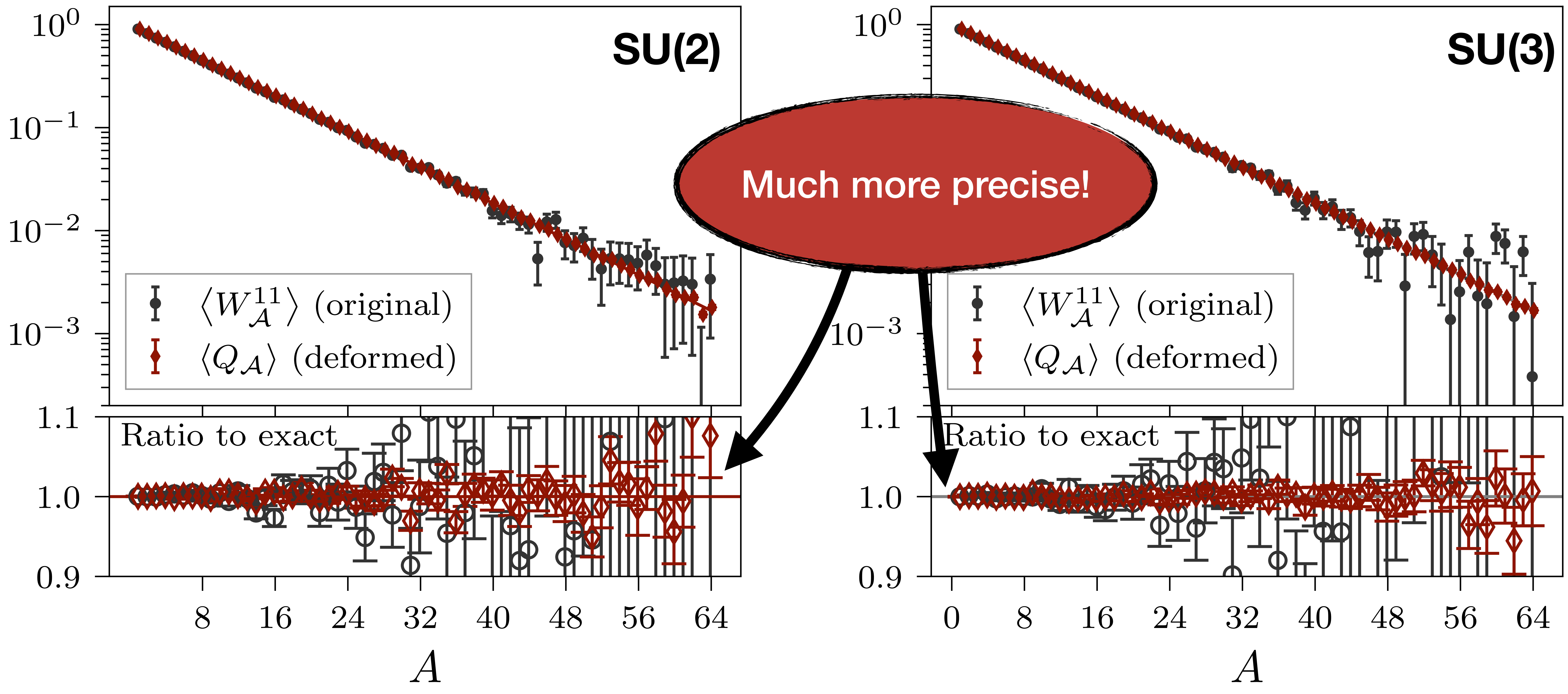
Triangular Jacobian: $f(\Omega)$ only allowed to depend on $y \leq x$. Jacobian determinant calculable in $O(V)$.

This is key for scalability!

Results

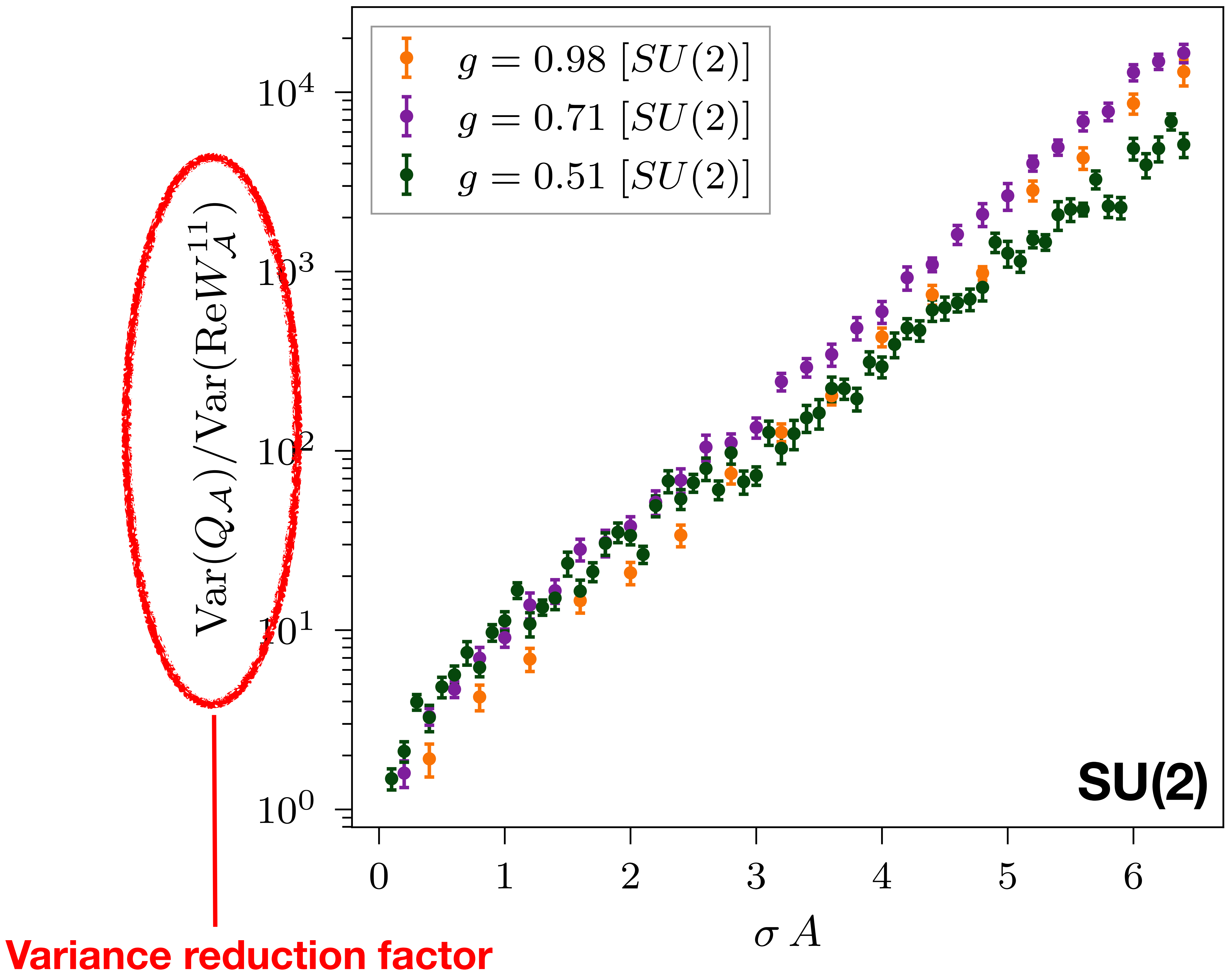
Significant variance reduction at large $\mathscr{A}$, no bias.

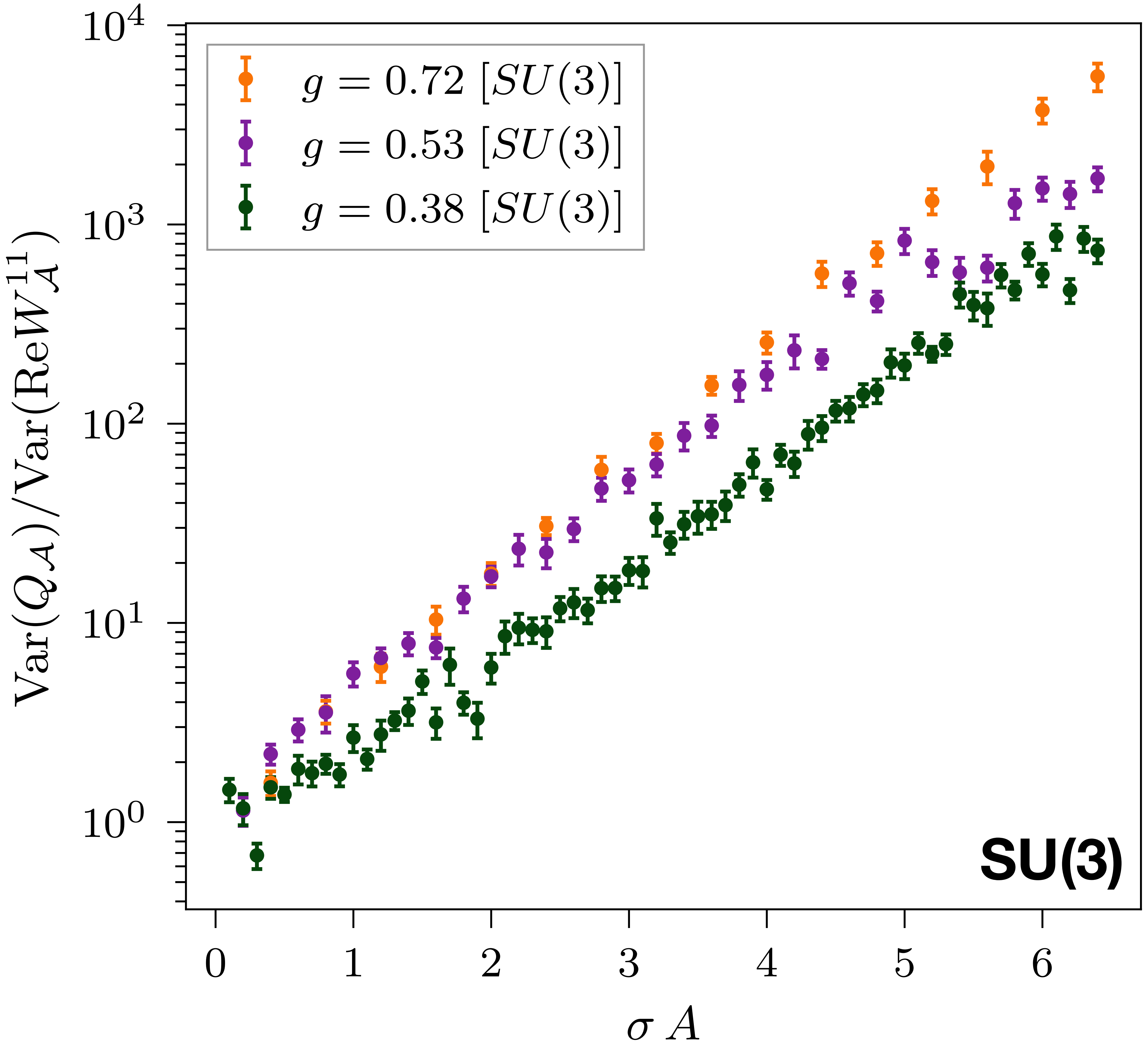
Fine lattice spacing:



Results

Similar variance reduction effects across all 3 lattice spacings:





Conclusions / Outlook

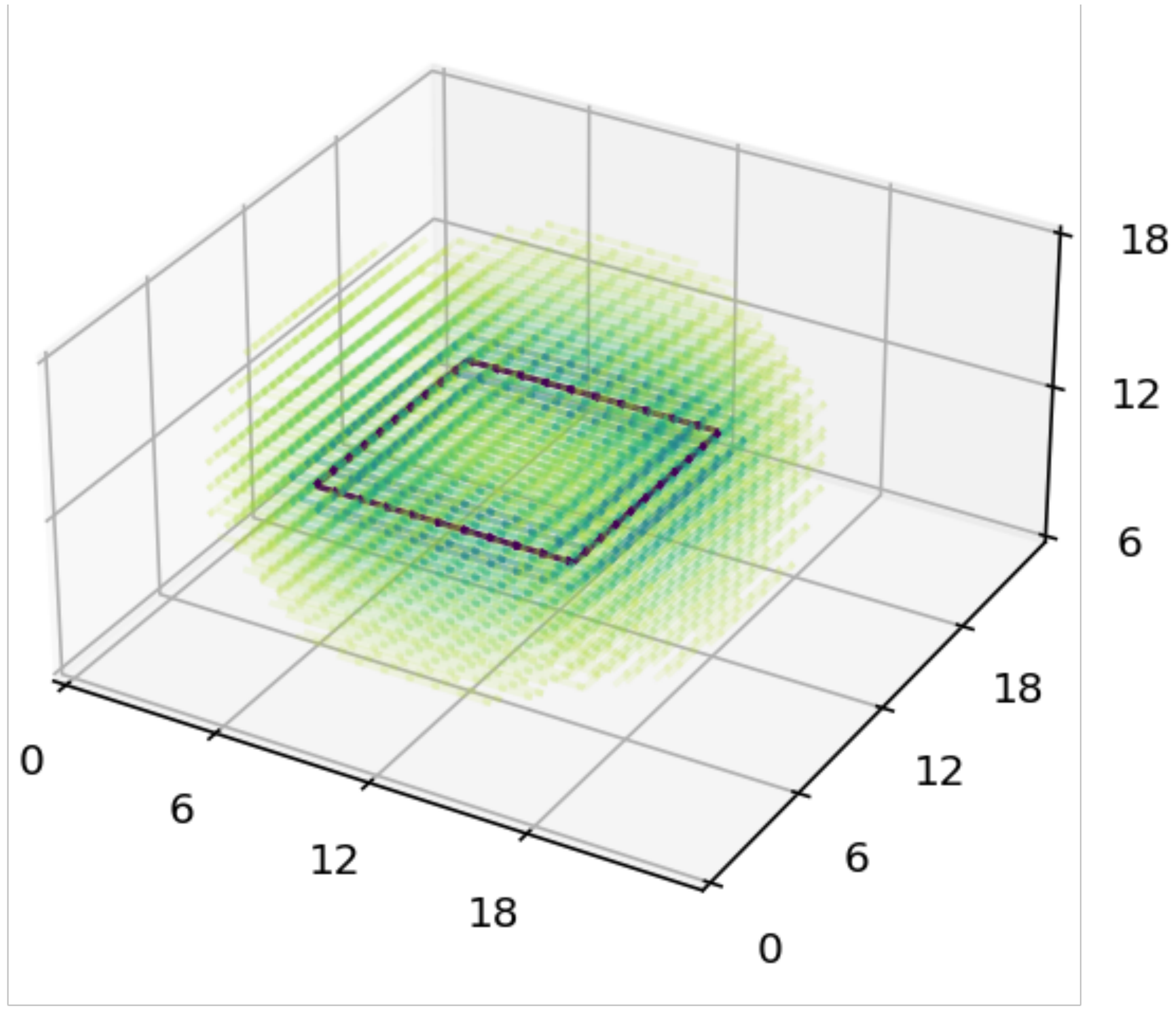
Contour deformations allow …

- **Deforming observables** $\mathcal{O} \to \mathcal{Q}$, where $\langle \mathcal{O} \rangle = \langle \mathcal{Q} \rangle$ but $\mathrm{Var}[\mathcal{O}] \neq \mathrm{Var}[\mathcal{Q}]$.

  No systematic error!

- **Minimizing variance numerically** (using existing MC samples).

- **Far more precise** measurements in proof-of-principle applications to gauge theory.



Preview: Approximate analytical solution for $\Lambda = 0$ deformation of 3D $U(1)$ giving optimal Wilson loop variance reduction.

Next: Higher dimensions and fermions. Analytic methods?

Backup Slides

Analytical hints

Expand about the **classical solution**, expand in **small deform parameters**.

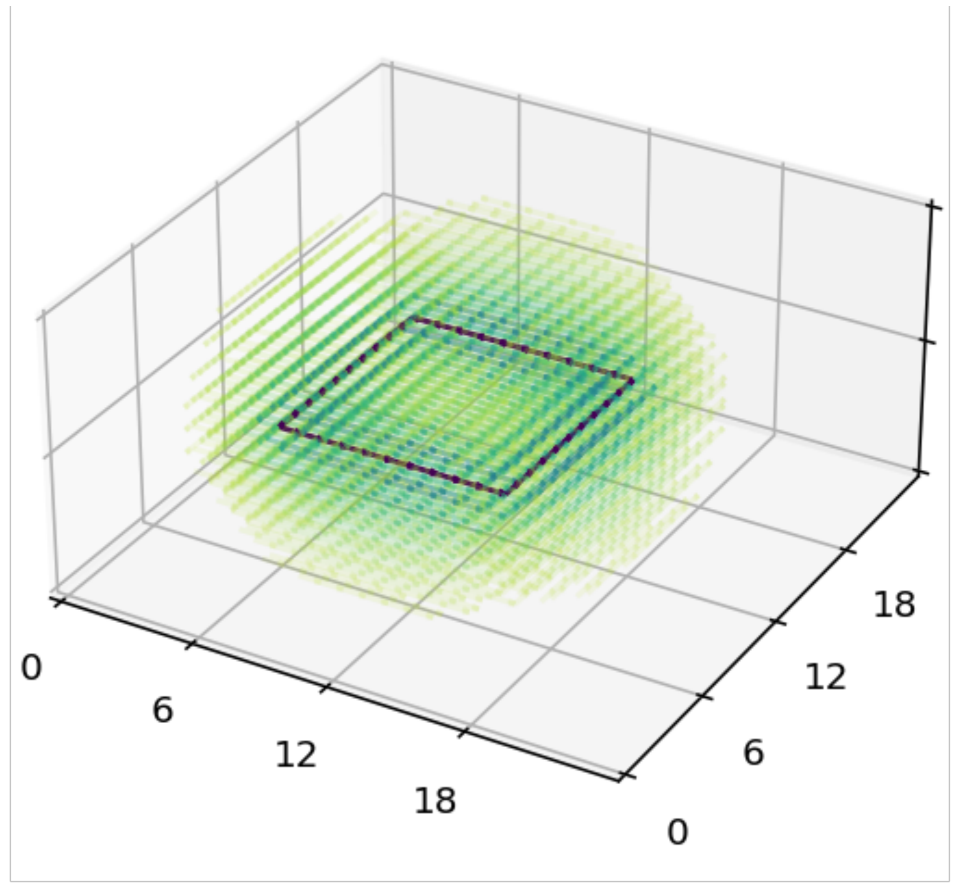
Solve for deform params producing anti-correlated phase fluctuations.

XY model:

- Two-point function $\langle e^{i\theta(x)} e^{-i\theta(y)} \rangle$
- $\widetilde{\theta}(x) = \theta(x) + i\delta(x)$
- Result: heat kernel constraint on $\delta(x)$

U(1) gauge theory:

- Wilson loops, $\widetilde{\theta}_\mu(x) = \theta_\mu(x) + i\delta_\mu(x)$
- Result: Local flux constraint on $\delta_\mu(x)$



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

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

Fourier cutoff effects

Higher Fourier cutoffs do not appear useful in this parameterization: