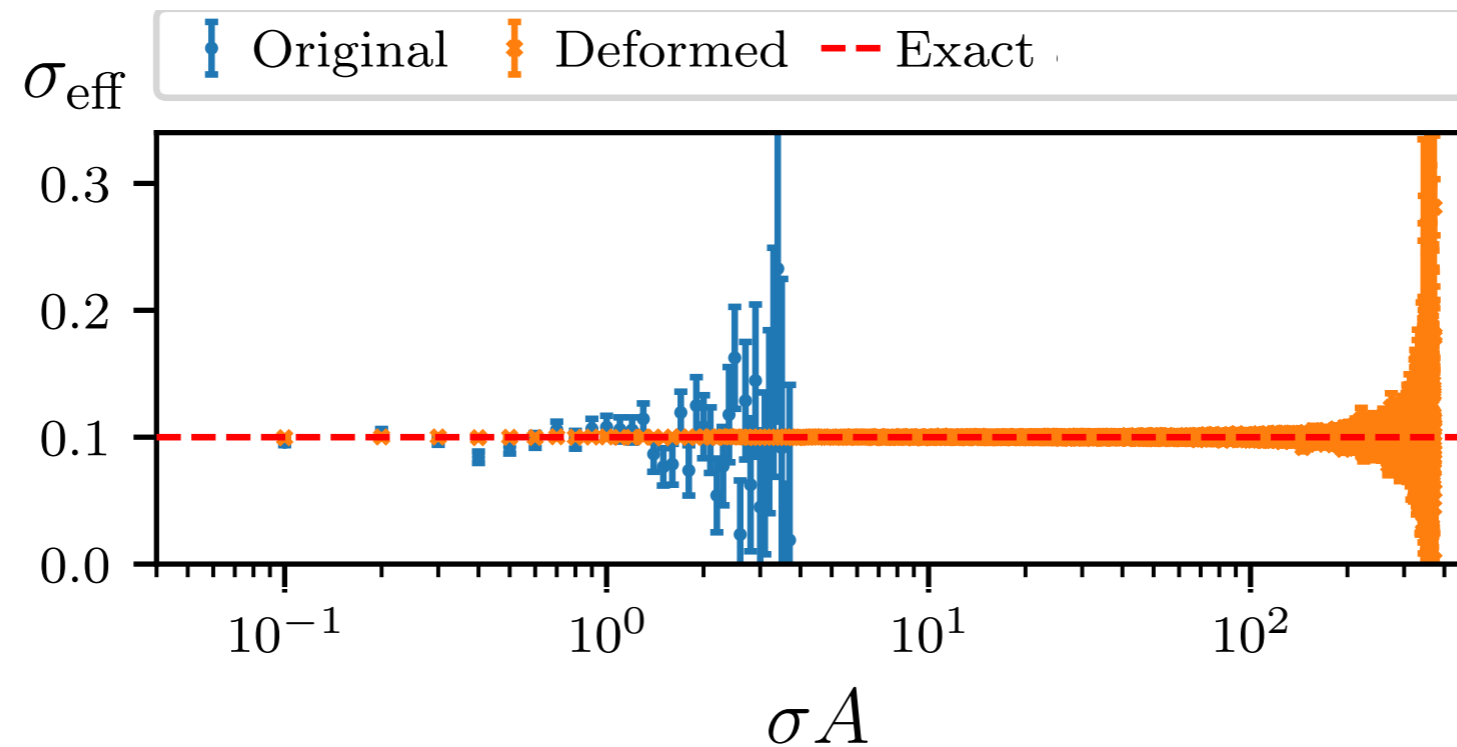


Sign(al-to-noise) Problems in Lattice Gauge Theory

Michael Wagman



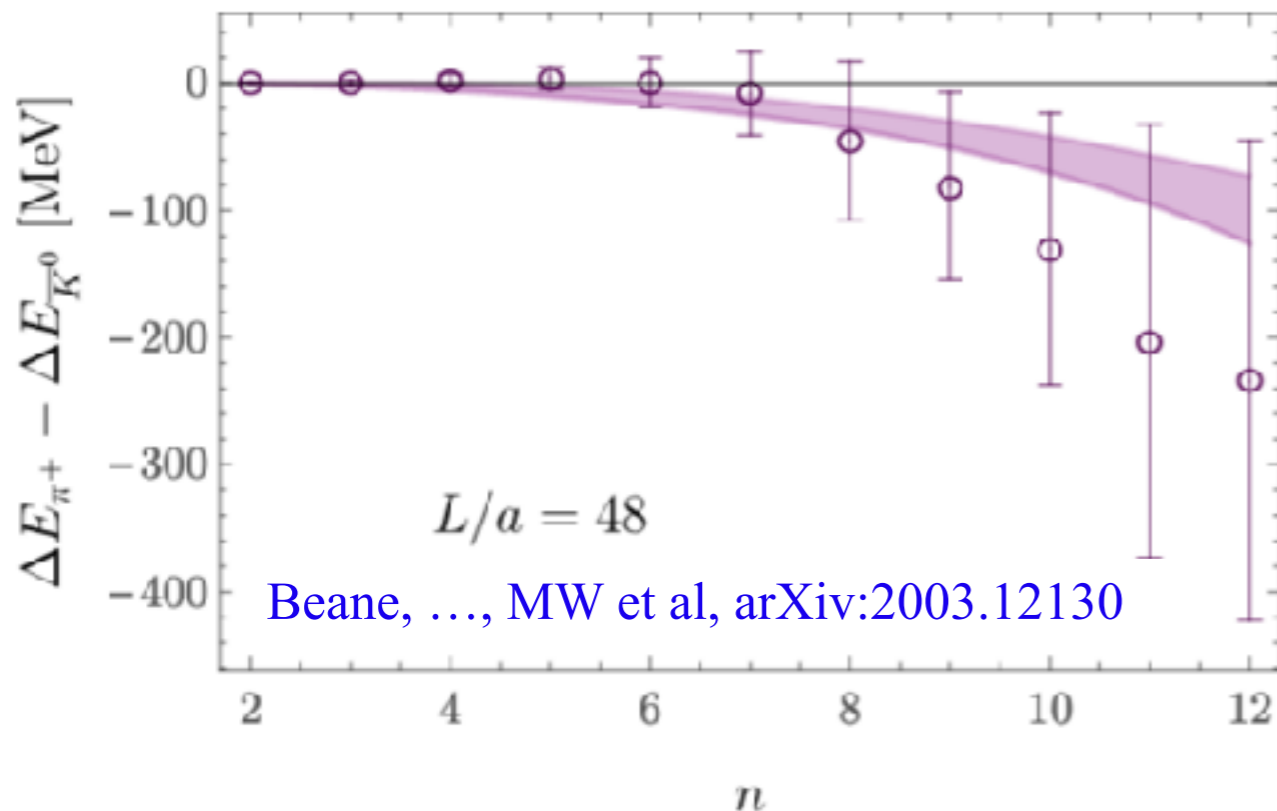
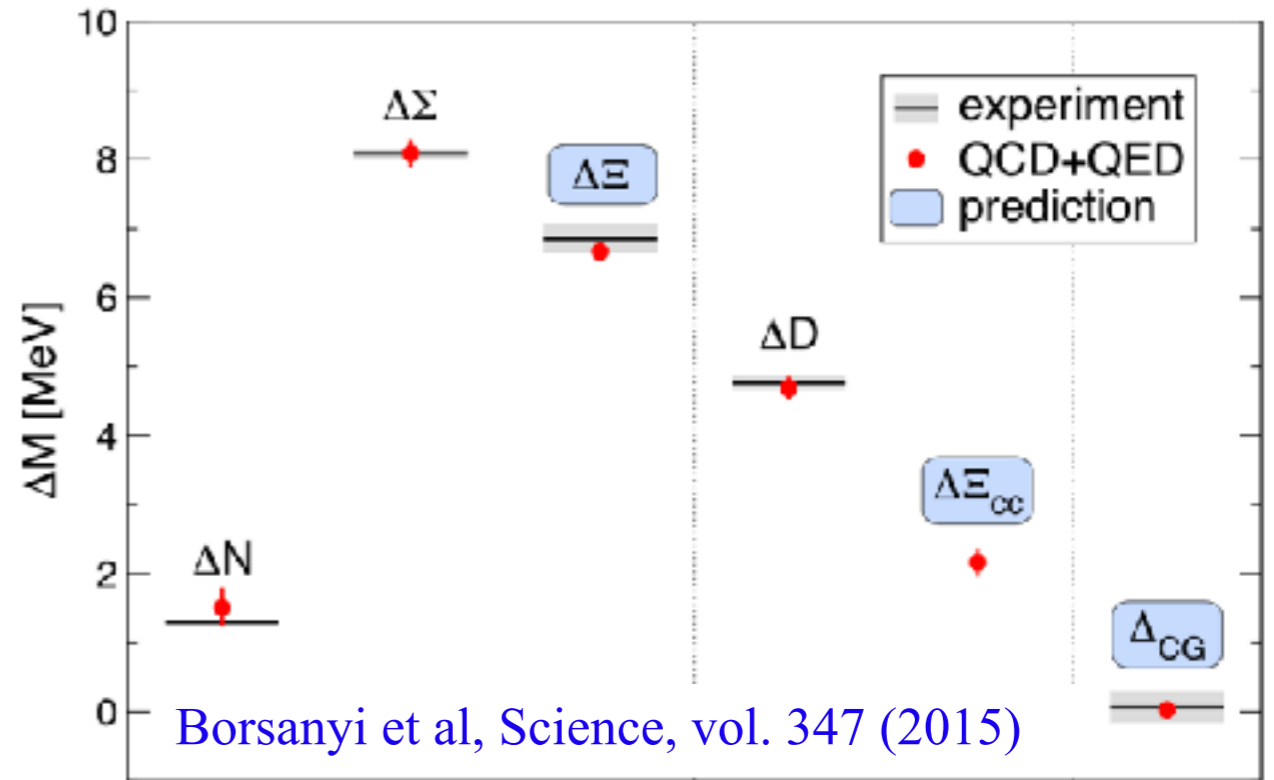
Fermilab

University of Iowa
Nuclear and Particle Physics Seminar

Feb 8, 2021

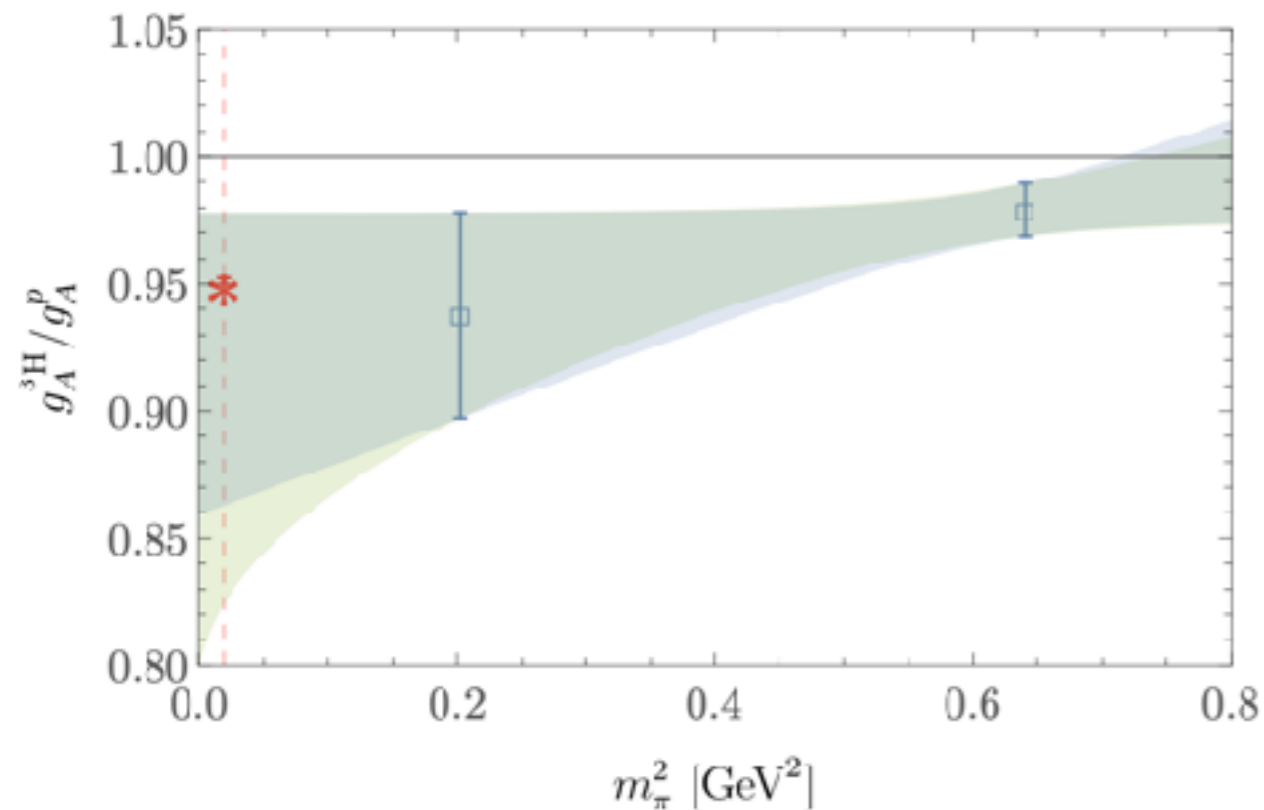
Solving the Standard Model

Simple quantities like the proton-neutron mass difference have been computed with percent-level precision in lattice QCD+QED



Increasingly complex effects such as QED effects on charged multi-meson systems are being explored

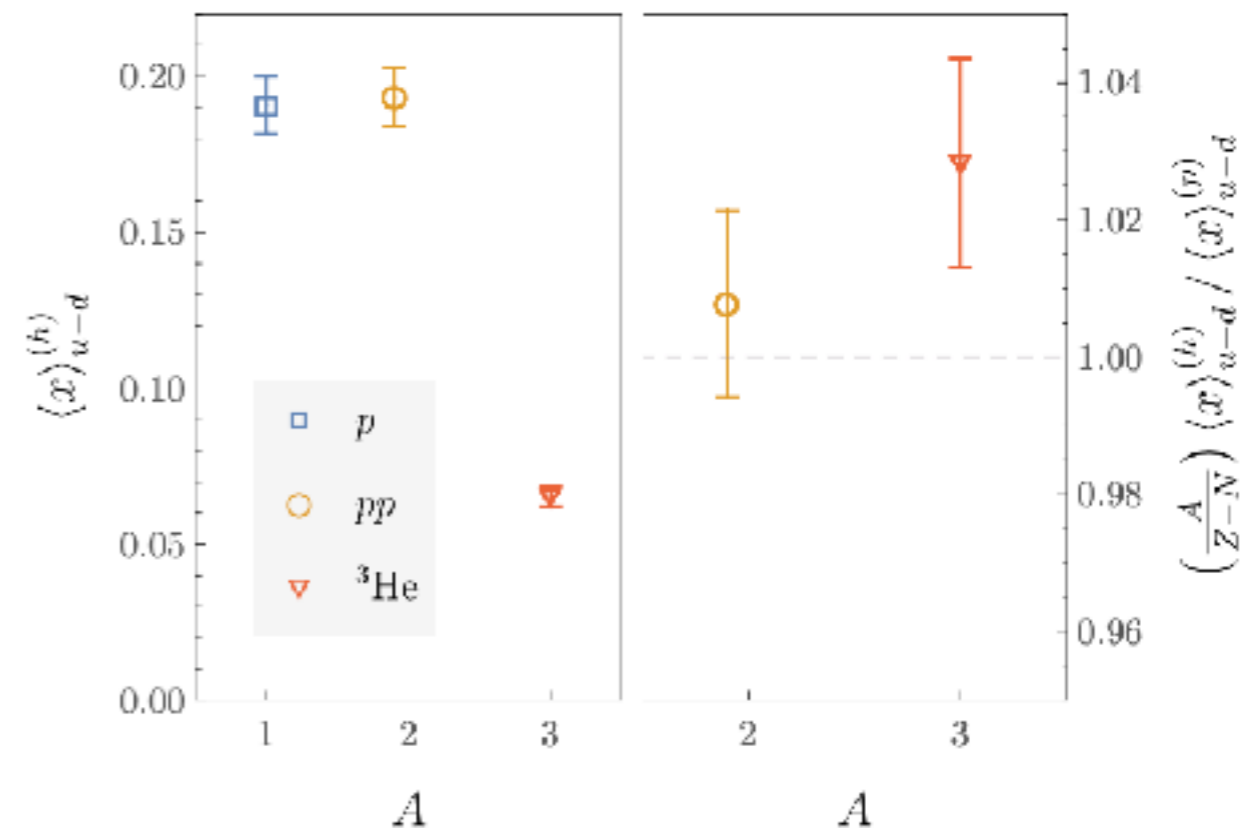
Nuclear matrix elements from LQCD



Parreño, ..., MW, et al [NPLQCD] arXiv:2102.xx

The u - d quark momentum fractions of light nuclei have been computed in exploratory calculations at heavier-than-physical quark masses

Triton beta-decay rate computed from lattice QCD, effects of axial two-body currents visible



Detmold, ..., MW, et al [NPLQCD], arXiv:2101.12668

Excited-state effects

Euclidean correlation functions have spectral representation

$$\begin{aligned} G(\tau) &= \langle N(\tau) \bar{N}(0) \rangle = \sum_n \langle 0 | N | n \rangle e^{-E_n \tau} \langle n | \bar{N} | 0 \rangle \\ &\equiv \sum_n Z_n e^{-E_n \tau} \end{aligned}$$

Precise studies of multi-nucleon systems face challenges from unbound finite-volume excited states

$$\vec{p} = \frac{2\pi\vec{n}}{L} \quad E_{NN} \approx 2\sqrt{M_N^2 + \left(\frac{2\pi n}{L}\right)^2}$$

Analogous issues with $N\pi$ excited-states may impact axial form factor calculations

Jang, Gupta, Yoon, Bhattacharya, PRL 124 (2020)

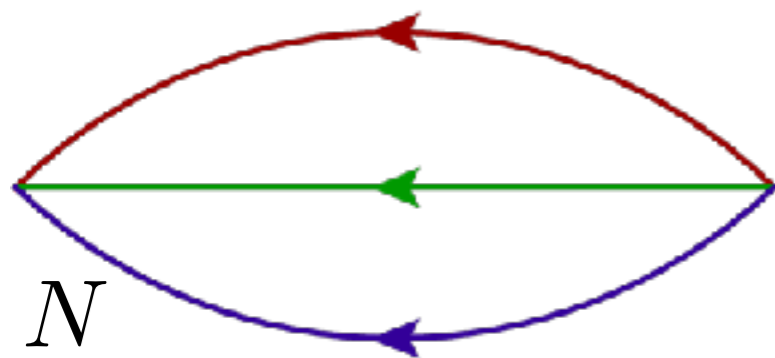
Alexandrou et al [ETMC], arXiv:2011.13342

Better tools for needed for dealing with multi-hadron excited states

The signal-to-noise problem

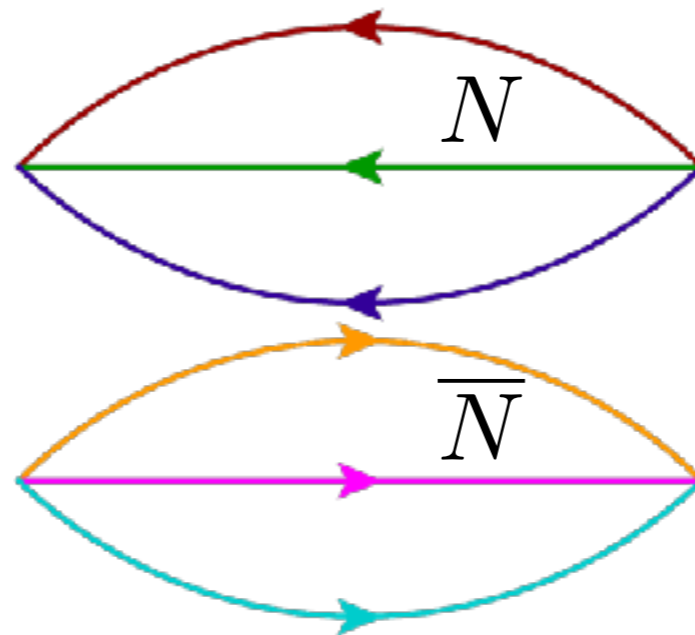
Monte Carlo noise in nucleon/nuclear correlation functions grows exponentially with Euclidean time separation

Correlation function variance can be analyzed as a correlation function

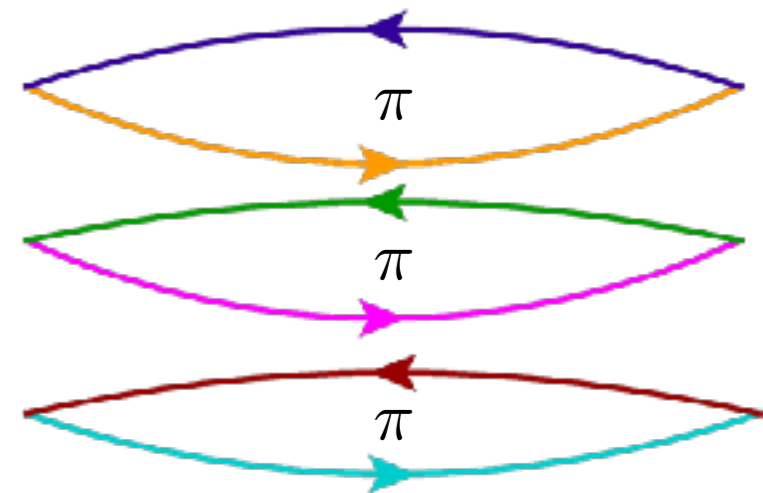


$$G_N \sim e^{-M_N t}$$

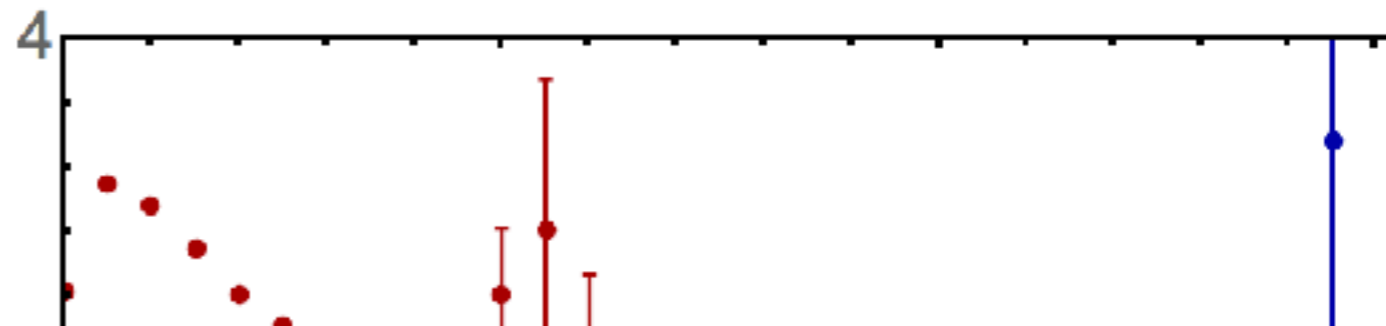
$$\text{Var}(G_N) \sim \langle |N(t)N(0)^\dagger| \rangle \sim e^{-3m_\pi t}$$



$$\frac{G_N}{\sqrt{\text{Var}(G_N)}} \sim e^{-(M_N - \frac{3}{2}m_\pi)t}$$



$$\text{Multi-nucleon: } \sim e^{-A(M_N - \frac{3}{2}m_\pi)t}$$



The sign(al-to-noise) problem

Nucleon correlation functions are real on average but complex in generic gauge field backgrounds

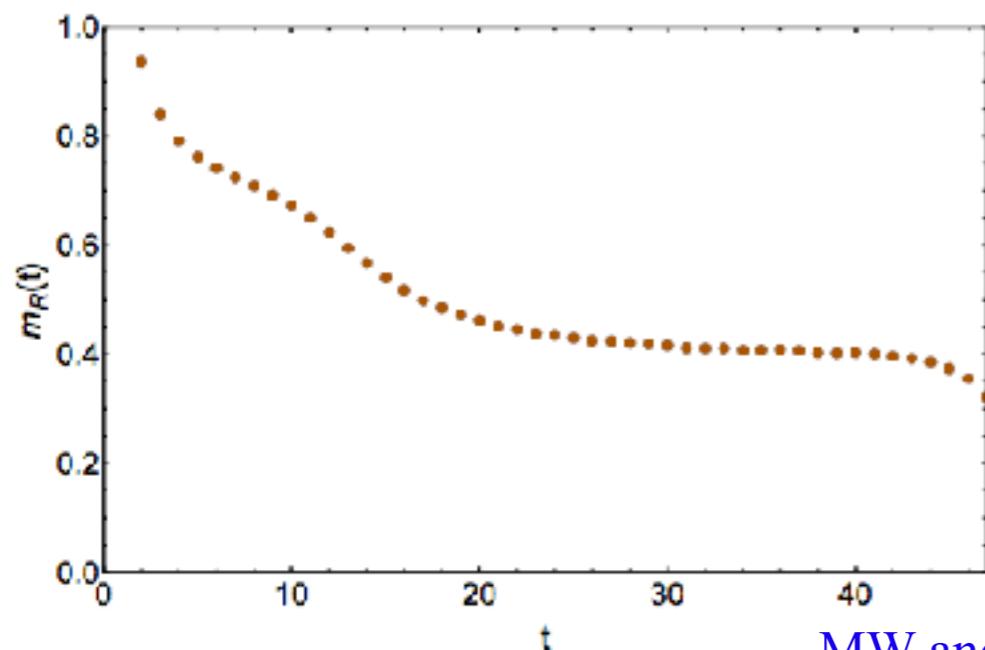
$$G_N(t) = \left\langle e^{R(t)+i\theta(t)} \right\rangle$$

Contributions to the energy from phase fluctuations lead to StN problems

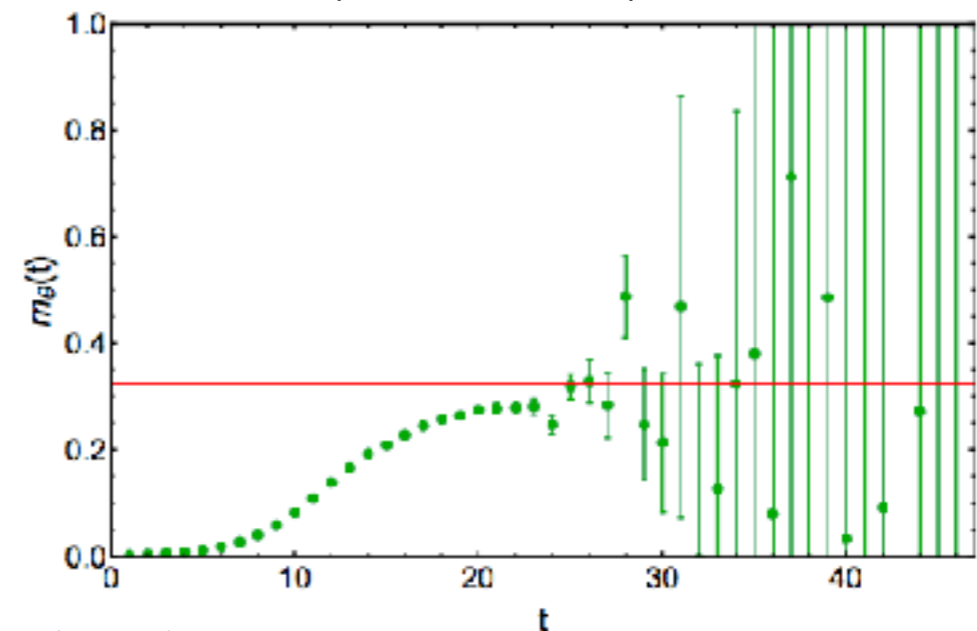
$$\text{StN}(e^{i\theta(t)}) \sim \frac{\langle e^{i\theta(t)} \rangle}{\langle |e^{i\theta(t)}|^2 \rangle} = \langle e^{i\theta(t)} \rangle \sim e^{-m_\theta t}$$

Empirically, phase fluctuations (“sign problem”) reproduce the Parisi-Lepage signal-to-noise problem

$$m_R(t) = \ln \left(\frac{\langle e^{R(t)} \rangle}{\langle e^{R(t+1)} \rangle} \right) \sim \frac{3}{2} m_\pi$$



$$m_\theta(t) = \ln \left(\frac{\langle e^{i\theta(t)} \rangle}{\langle e^{i\theta(t+1)} \rangle} \right) \sim M_N - \frac{3}{2} m_\pi$$

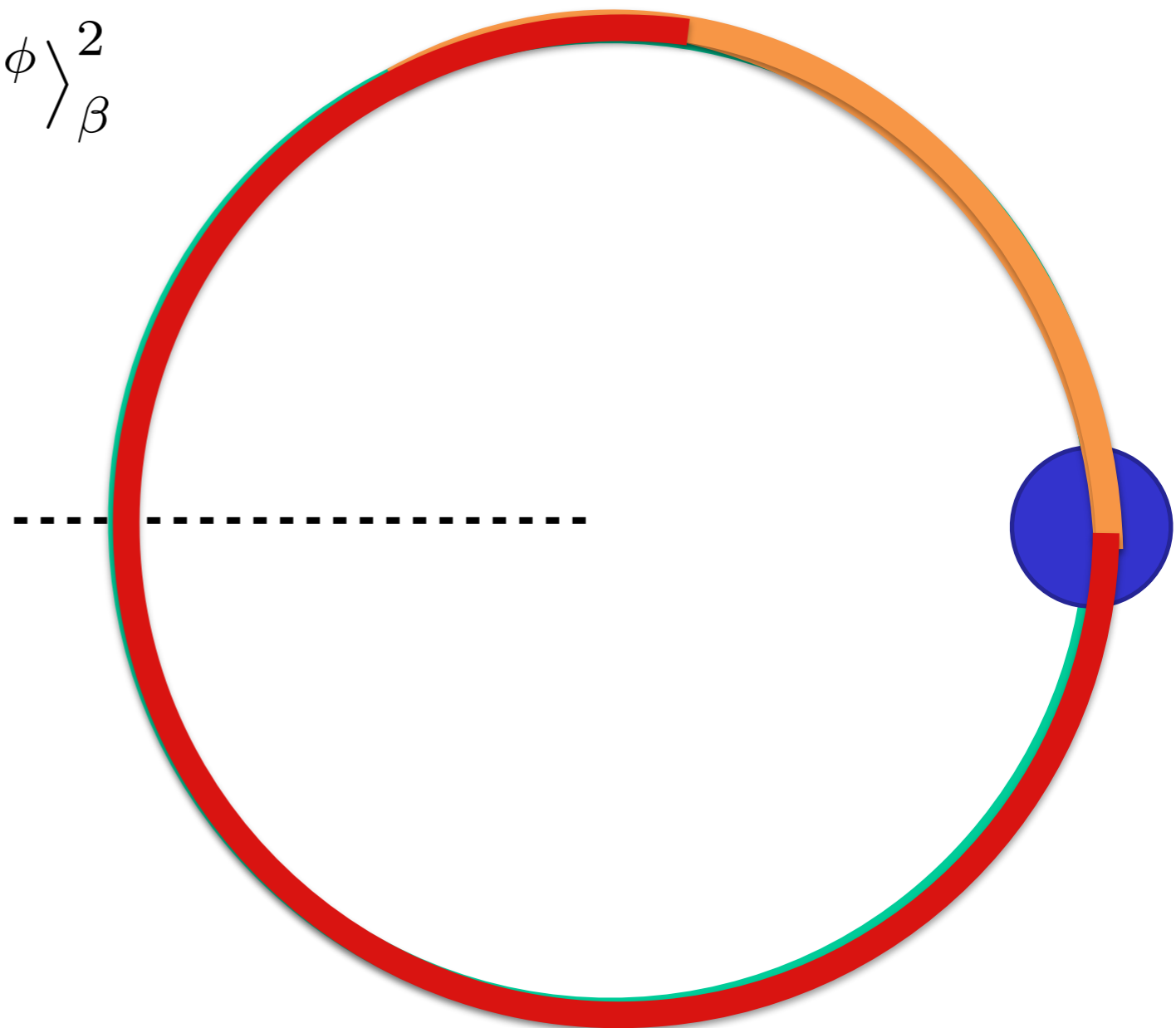


A nice toy sign problem

$$\int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{i\phi} e^{\beta \cos(\phi)} = I_1(\beta) = \langle e^{i\phi} \rangle_{\beta} I_0(\beta)$$

$$\begin{aligned} \text{Var}_{\beta}[\text{Re } e^{i\phi}] &= \langle \cos^2(\phi) \rangle_{\beta} - \langle e^{i\phi} \rangle_{\beta}^2 \\ &= \frac{1}{2} \left[1 + \frac{I_2(\beta)}{I_0(\beta)} \right] - \left[\frac{I_1(\beta)}{I_0(\beta)} \right]^2 \end{aligned}$$

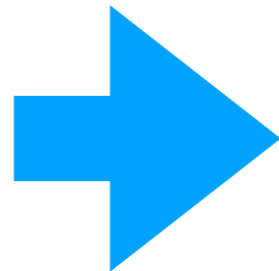
For uniform phase
fluctuations, average
phase vanishes but
variance is always $O(1)$



Contour deformations

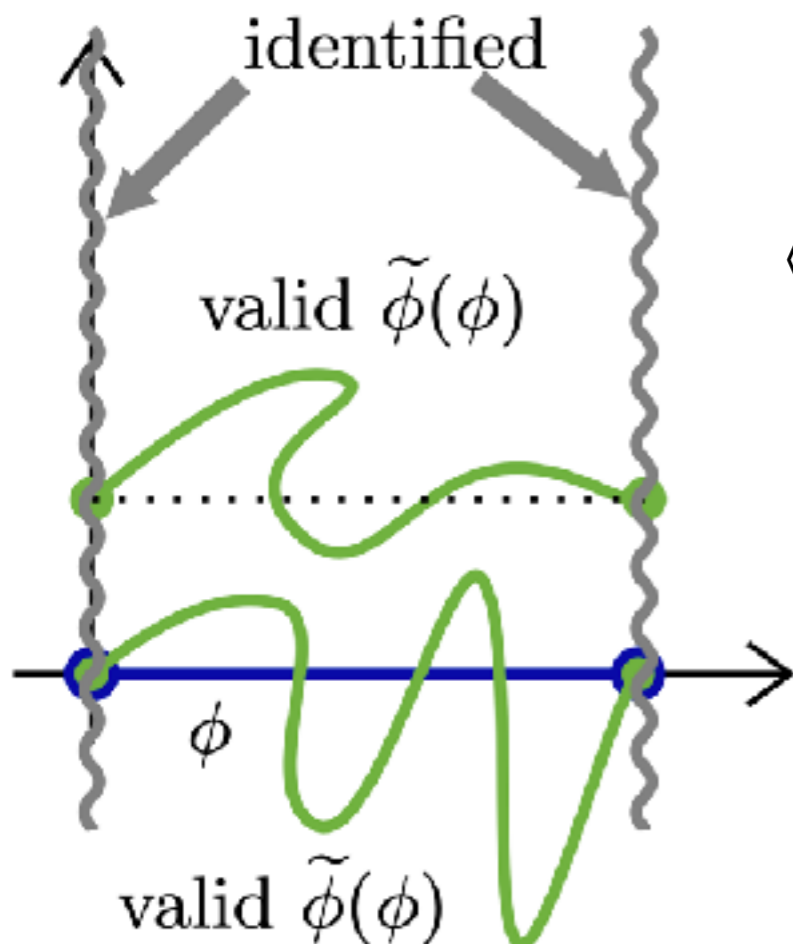
$$\int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{i\phi} e^{\beta \cos(\phi)} = I_1(\beta) = \langle e^{i\phi} \rangle_{\beta} I_0(\beta)$$

Stokes' theorem +
holomorphic integrand



integral result unaffected by
contour deformation

Constant vertical deformation:



$$\langle e^{i\phi} \rangle_{\beta} = \int_{-\pi+if}^{\pi+if} \frac{d\phi}{2\pi I_0(\beta)} e^{i\phi} e^{\beta \cos(\phi)}$$

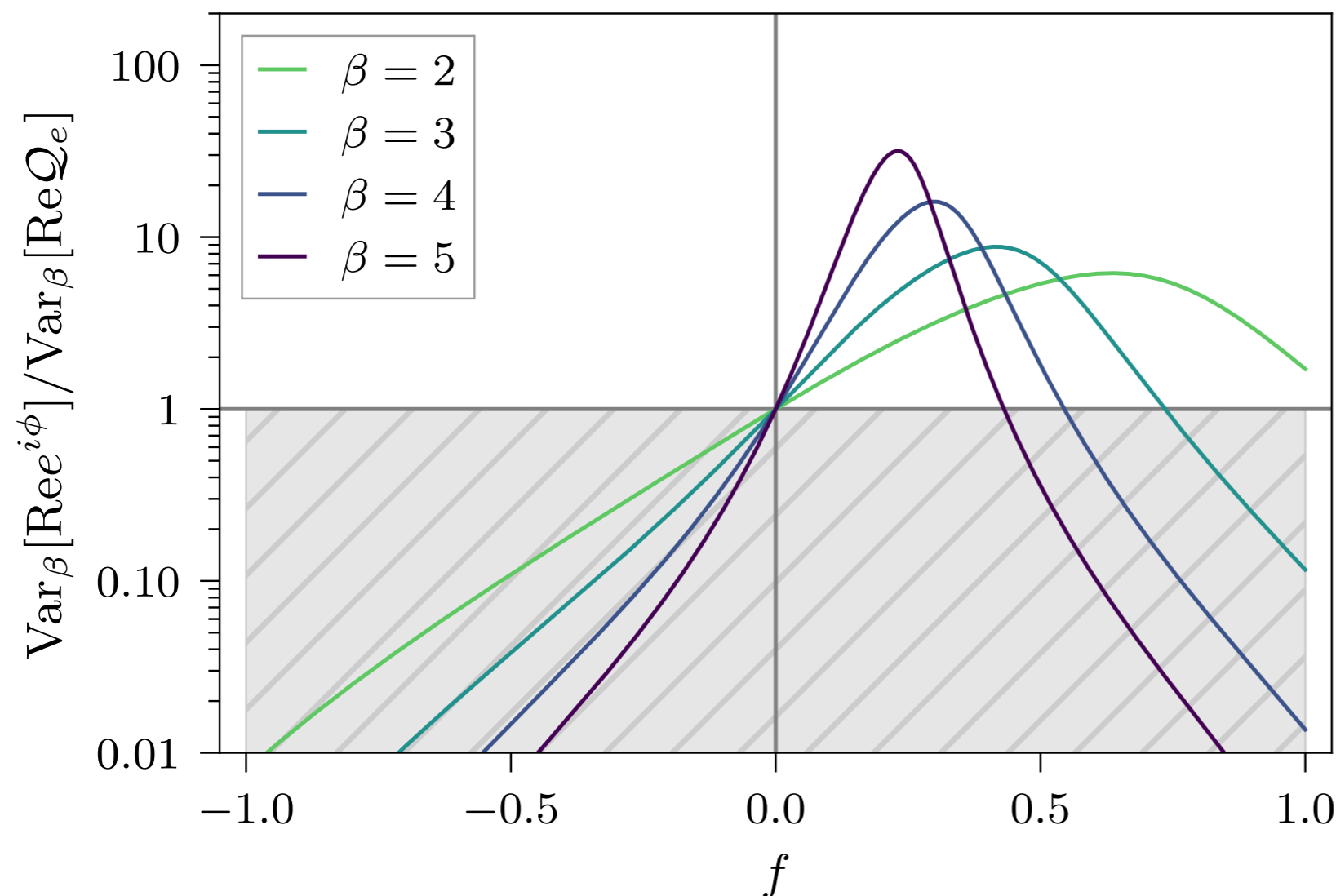
$$= \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{i\phi-f} e^{\beta \cos(\phi+if)}$$

$$= \left\langle e^{i\phi-f} e^{\beta \cos(\phi+if) - \beta \cos(\phi)} \right\rangle_{\beta} \equiv \langle \mathcal{Q}_e \rangle_{\beta}$$

Variance reduction

The variance involves non-holomorphic integrands

$$\text{Var}_\beta[\text{Re } \mathcal{Q}_e] = \langle (\text{Re } \mathcal{Q}_e)^2 \rangle_\beta - \langle e^{i\phi} \rangle_\beta^2 \neq \text{Var}_\beta[\text{Re } e^{i\phi}]$$



$$\mathcal{Q}_e = e^{-f} e^{i\phi} e^{\Delta S}$$

Path integral contour deformations

Consider a path integral with a sign problem

$$\langle \mathcal{O} \rangle_M = \frac{1}{Z_M} \int_{\mathcal{M}} \mathcal{D}U \, e^{iS_M(U)} \mathcal{O}(U)$$

Witten, AMS/IP
Stud.Adv.Math. 50 (2011)

Cristoforetti, Di Renzo,
Scorzato, PRD 86 (2012)

...

Deform the integration contour

$$= \frac{1}{Z_M} \int_{\tilde{\mathcal{M}}} \mathcal{D}U \, e^{iS_M(\tilde{U})} \mathcal{O}(\tilde{U})$$

$$= \frac{1}{Z_M} \int_{\mathcal{M}} \mathcal{D}U \, J(U) \, e^{iS_M(\tilde{U}(U))} \mathcal{O}(\tilde{U}(U))$$

Review:

Alexandru, Basar, Bedaque,
Warrington, arXiv:2007.05436

Deformed integrand can have less severe sign problem

$$= \frac{1}{Z_M} \int_{\mathcal{M}} \mathcal{D}U \, |J(U)| \, e^{-\text{Im}[S_M(\tilde{U}(U))]} \mathcal{O}(\tilde{U}(U)) \\ \times e^{i\text{Re}[S_M(\tilde{U}(U))] + i\arg[J(U)]}$$

Observifolds

Deformed observables method: contour deformations
without modifying Monte Carlo sampling

$$\begin{aligned}\langle \mathcal{O} \rangle &= \frac{1}{Z} \int_{\mathcal{M}} \mathcal{D}U \, e^{-S(U)} \, \mathcal{O}(U) \\&= \frac{1}{Z} \int_{\tilde{\mathcal{M}}} \mathcal{D}\tilde{U} \, e^{-S(\tilde{U})} \, \mathcal{O}(\tilde{U}) \\&= \frac{1}{Z} \int_{\mathcal{M}} \mathcal{D}U \, e^{-S(U)} \, \det \left(\frac{\partial \tilde{U}}{\partial U} \right) e^{-S(\tilde{U}(U)) + S(U)} \, \mathcal{O}(\tilde{U}(U)) \\&\equiv \frac{1}{Z} \int_{\mathcal{M}} \mathcal{D}U \, e^{-S(U)} \, \mathcal{Q}(U)\end{aligned}$$

$$\langle \mathcal{O} \rangle = \langle \mathcal{Q} \rangle$$

$$\text{Var}[\mathcal{O}] \neq \text{Var}[\mathcal{Q}]$$

Lattice gauge theory

Gauge transformations act on matter fields as

$$\psi_x^a \rightarrow \Omega_x^{ab} \psi_x^b$$

$$\Omega_x \in SU(N), U(1)$$

Gauge field acts as parallel transporter in color space

$$D_\mu^{ab} \psi_x^b = U_{x,\mu}^{ab} \psi_{x+\hat{\mu}}^b - \psi_x^a$$

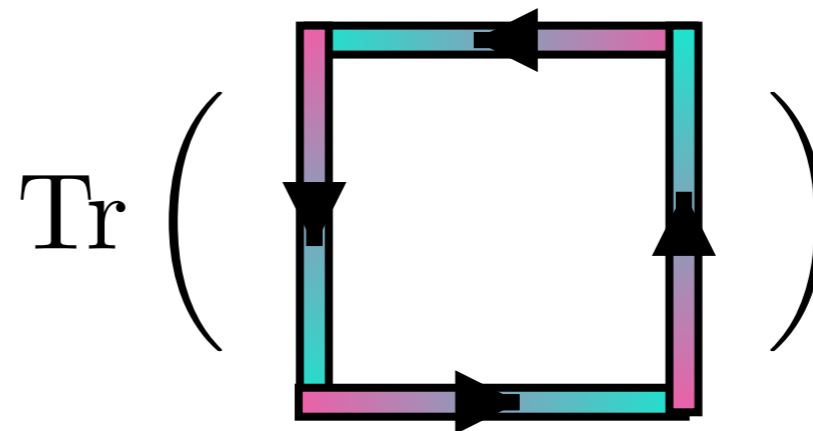
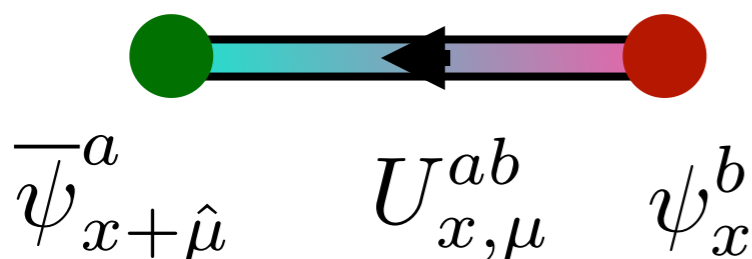
$$D_\mu \psi_x^a \rightarrow \Omega_x^{ab} D_\mu \psi_x^b$$

$$U_{x,\mu} \in SU(N), U(1)$$

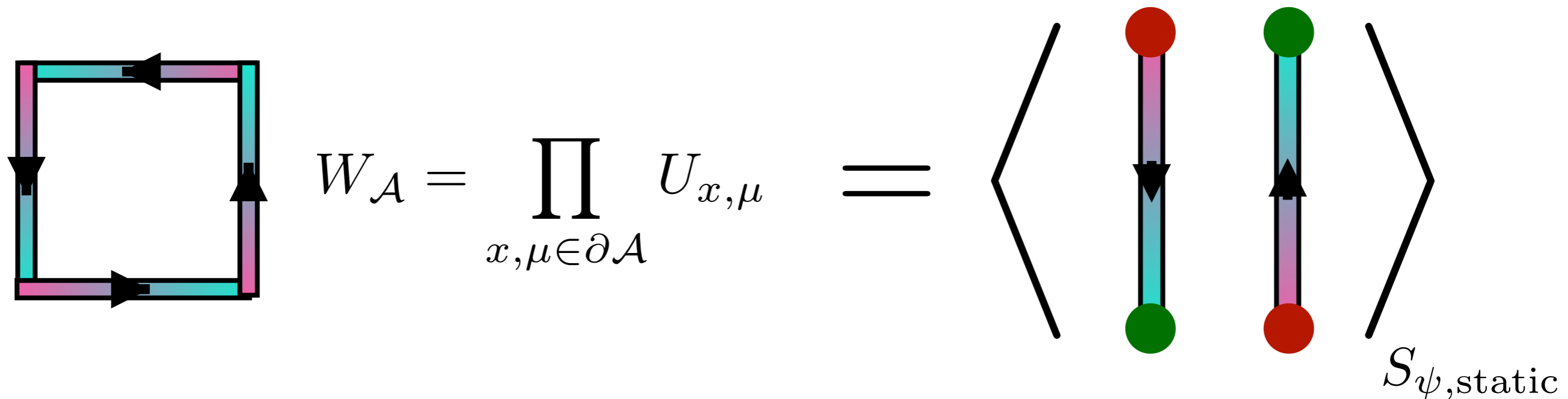
$$U_{x,\mu} = e^{i \int_x^{x+\hat{\mu}} dy A_\mu(y)}$$

$$U_{x,\mu} \rightarrow \Omega_x U_{x,\mu} \Omega_{x+\hat{\mu}}^\dagger$$

Gauge invariant building blocks:



Wilson loops



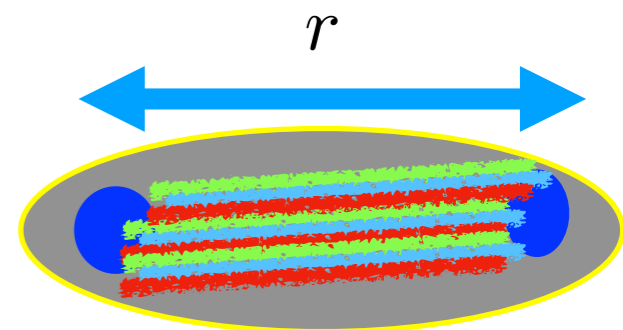
Wilson loops are equivalent to static quark propagators

$$S_{\psi, \text{static}} = \sum_x \bar{\psi}_x D_4 \psi_x = \sum_x \bar{\psi}_x (U_{x,4} \psi_{x+\hat{4}} - \psi_x)$$

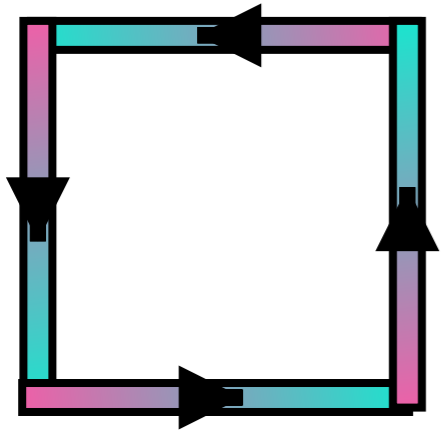
Since by equations of motion $\psi(\vec{x}, \tau) = \prod_{\tau'=0}^{\tau} U_{(\vec{x}, \tau'), 4}^{-1} \psi(\vec{x}, 0)$

Static quark potential accessible from Wilson loops

$$\langle W_{r \times \tau} \rangle = \sum_n Z_n e^{-E_n(r) \tau} = e^{-V(r) \tau} + \dots$$



Plaquettes



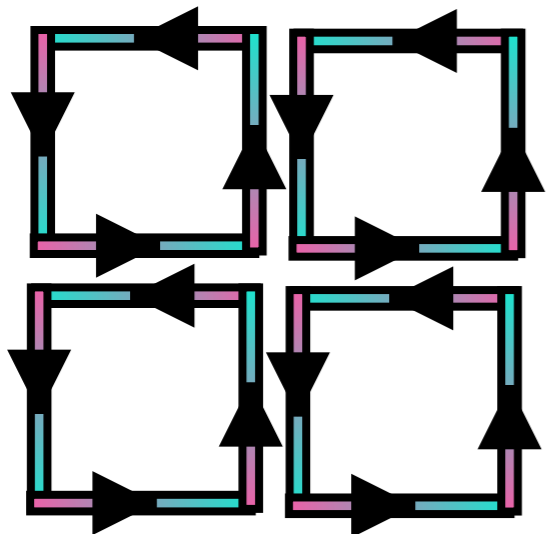
“Plaquettes” are 1x1 Wilson loops

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

Wilson action provides simple, gauge-invariant action with correct naive continuum limit

$$S_W(U) = \frac{1}{g^2} \sum_x \sum_{\mu < \nu} \text{Tr} [2 - P_{x,\mu\nu} - P_{x,\mu\nu}^{-1}]$$

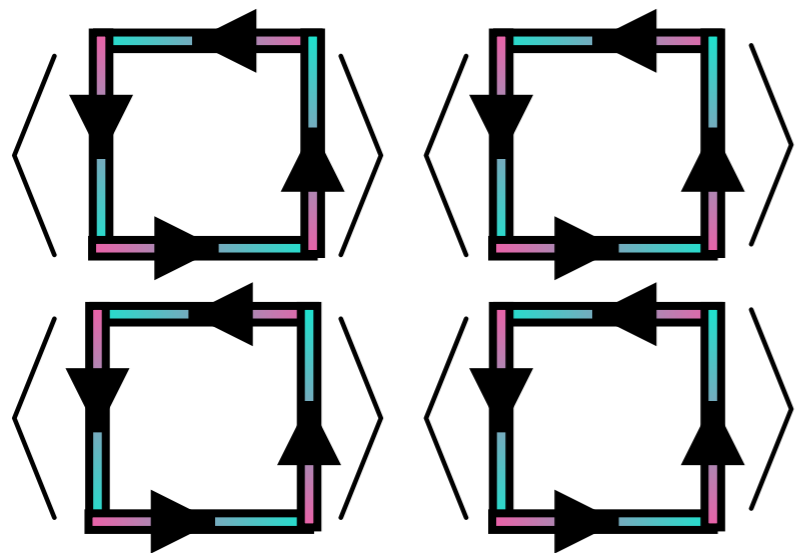
Wilson loops can be expressed using plaquettes, most simply taking open boundary conditions and gauge-fixing $U_{x,\nu} = 1$



$$W_{\mathcal{A}} = \prod_{x,\mu \in \partial \mathcal{A}} U_{x,\mu} = \prod_{x \in \mathcal{A}} P_{x,\mu\nu}$$

2D Confinement

In 2D, Wilson loop expectation values further factorize into products of single-plaquette expectation values



$$\langle \text{Tr}(W_{\mathcal{A}}) \rangle = \prod_{x \in \mathcal{A}} \langle \text{Tr}(P_x) \rangle = \langle \text{Tr}(P) \rangle^A$$

Implies confinement, static quark potential

$$V(r) = \sigma r$$

String tension:

$$\sigma = -\ln \left\langle \frac{1}{N} \text{Tr}(P) \right\rangle$$

Confining potential arises for any gauge group in 2D from factorization

$$\sigma_{U(1)} = \ln \left(\frac{I_0(1/e^2)}{I_1(1/e^2)} \right)$$

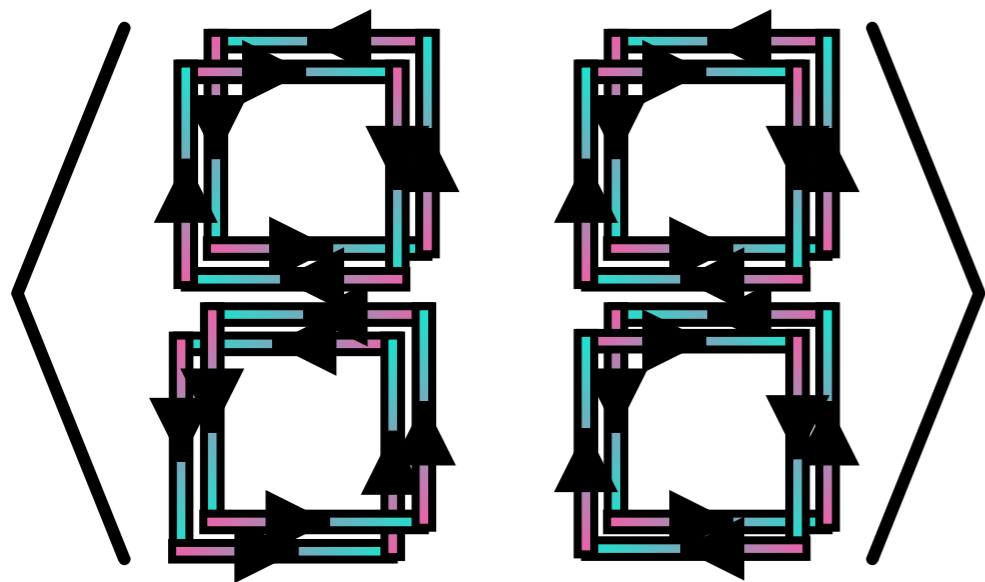
$$\sigma_{SU(2)} = \ln \left(\frac{I_1(4/g^2)}{I_2(4/g^2)} \right)$$

Gross and Witten, PRD 21 (1980)

Wadia, arXiv:1212.2906 (1979)

2D Wilson loop noise

Squared traces also factorize, but differently



$$\langle |\text{Tr}(W_{\mathcal{A}})^2| \rangle = 1 + (N^2 - 1) \langle \chi_{1,-1} \rangle^A$$

$$\langle \text{Tr}(W_{\mathcal{A}})^2 \rangle = \frac{N(N+1)}{2} \langle \chi_2 \rangle^A + \frac{N(N-1)}{2} \langle \chi_{1,-1} \rangle^A$$

Detmold, Kanwar, Lamm, MW, Warrington, arXiv:2101.12668

Phase (sign in $N=2$) fluctuations of Wilson loop traces lead to exponential StN problem

$$\text{Var} \left[\frac{1}{N} \text{Re Tr}(W_{\mathcal{A}}) \right] = \frac{1}{2N^2} + \dots$$

$$\text{StN} \left[\frac{1}{N} \text{Re Tr}(W_{\mathcal{A}}) \right] = \sqrt{2} N n e^{-\sigma A} + \dots$$

2D U(1) contour deformations

Using the parameterization

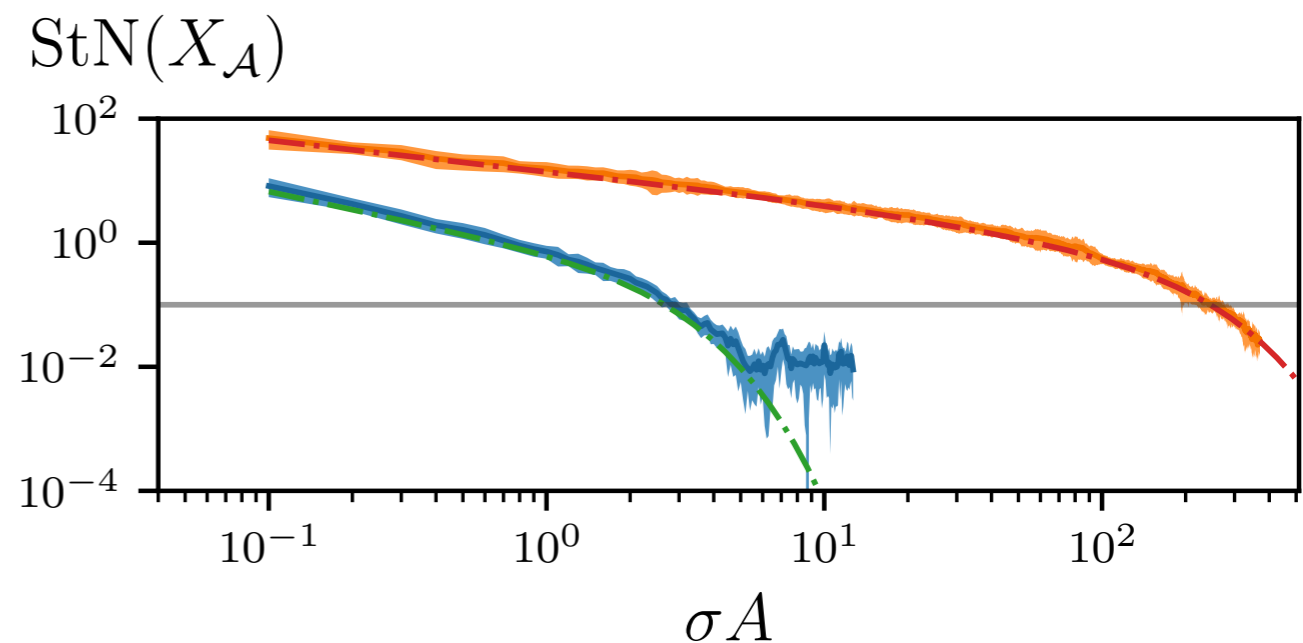
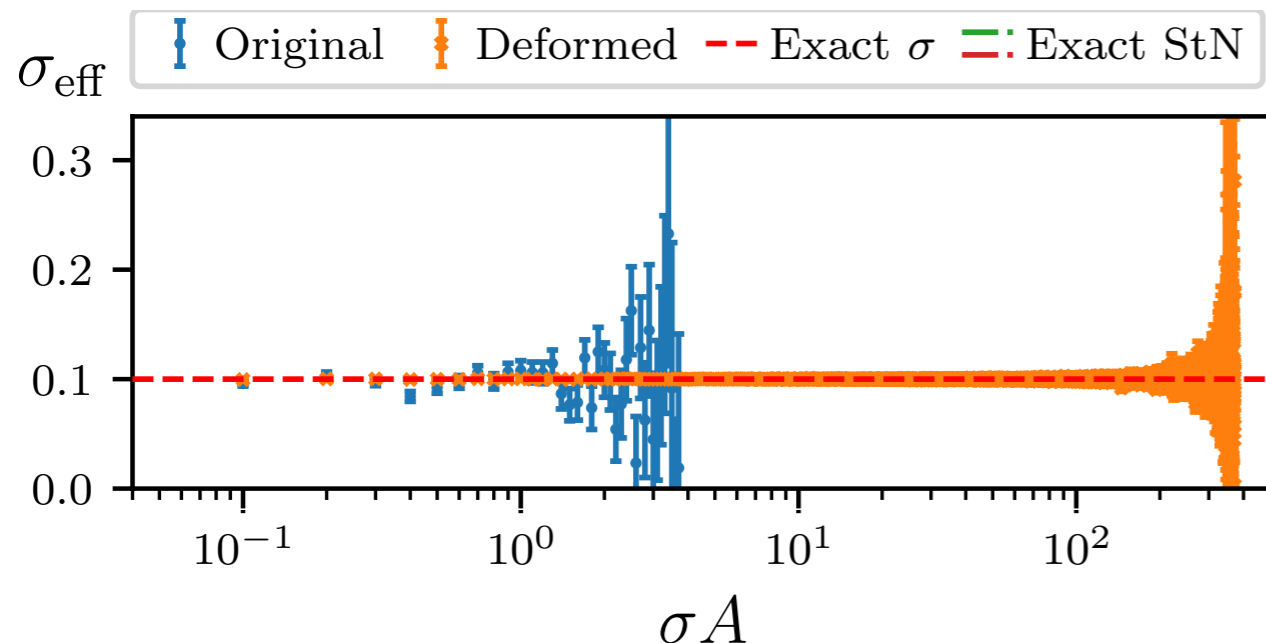
$$P = e^{i\phi} \in U(1)$$

U(1) Wilson loops are products of toy sign problem integrals

$$\begin{aligned} \langle W_{\mathcal{A}} \rangle &= \left(\int \frac{dP}{2\pi I_0(1/e^2)} P e^{\frac{1}{2e^2}(P+P^{-1})} \right)^A \\ &= \left(\int_{-\pi}^{\pi} \frac{d\phi}{2\pi I_0(1/e^2)} e^{i\phi} e^{\frac{1}{e^2} \cos(\phi)} \right)^A \end{aligned}$$

Contour deformation analogous to toy problem for U(1) Wilson loops

$$e^{i\phi} \rightarrow e^{i(\phi+if)}$$

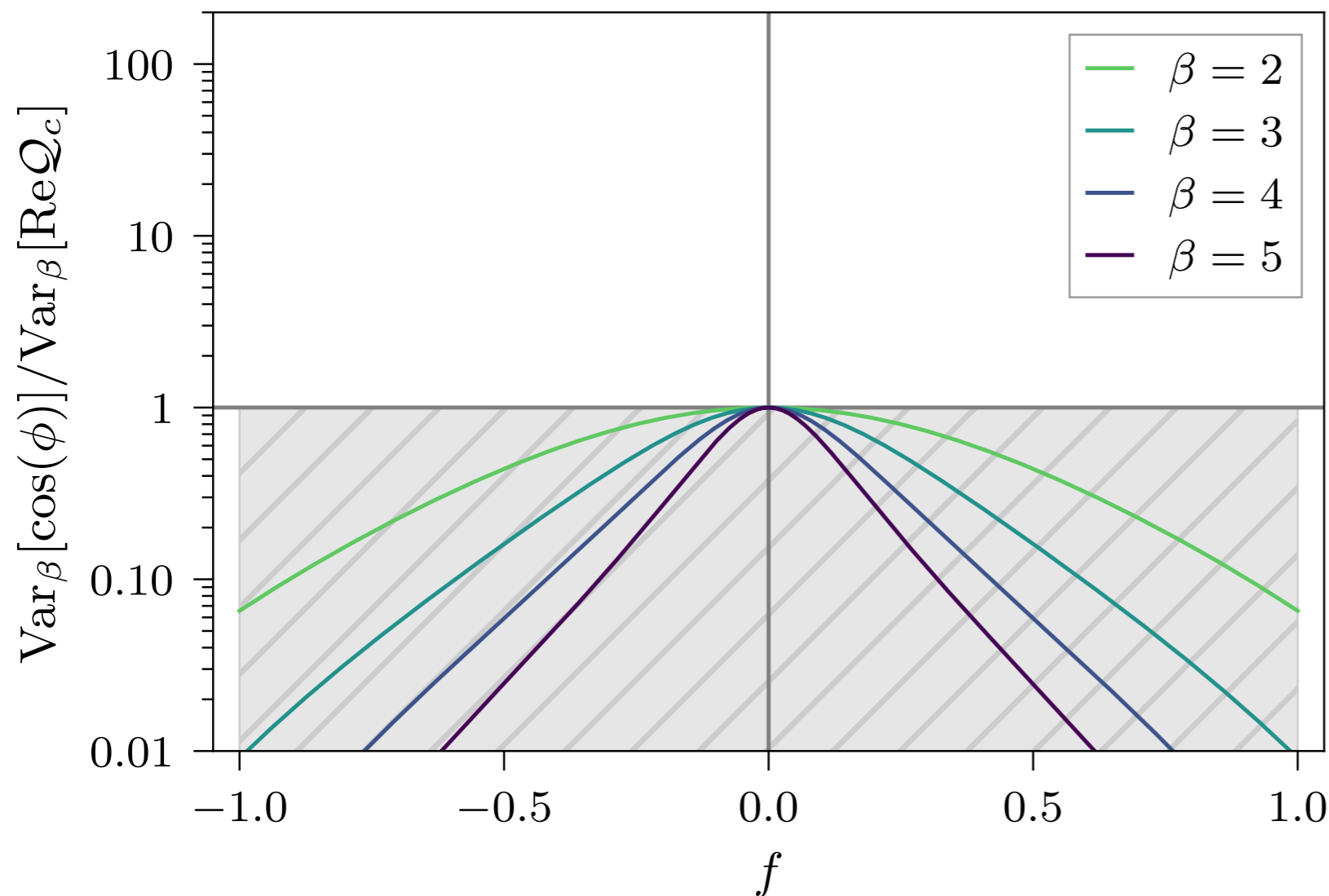


A mean toy sign problem

An alternative expression of the same expectation value

$$\langle \cos(\phi) \rangle_\beta = \int_{-\pi}^{\pi} \frac{d\phi}{2\pi I_0(\beta)} \cos(\phi) e^{\beta \cos(\phi)} = \frac{I_1(\beta)}{I_0(\beta)} = \langle e^{i\phi} \rangle_\beta$$

has identical variance but different contour deformation possibilities



$$Q_c = \cos(\phi + if) e^{\Delta S}$$

Parameterizing SU(2)

Mean toy sign problem — SU(2) Wilson loops parameterized as

$$P = \cos(\alpha/2) + i \sin(\alpha/2) \hat{n} \cdot \sigma$$

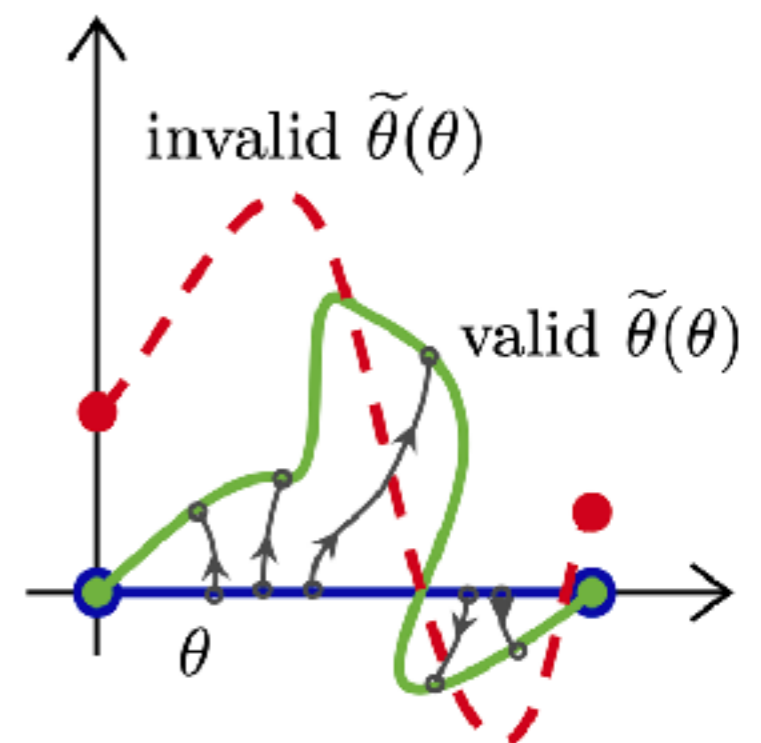
$$\frac{1}{2} \text{Tr}(P) = \cos(\alpha/2)$$

Useful to instead use angular parameterization

$$P = \begin{pmatrix} \sin(\theta)e^{i\phi_1} & \cos(\theta)e^{i\phi_2} \\ -\cos(\theta)e^{-i\phi_2} & \sin(\theta)e^{i\phi_1} \end{pmatrix}$$

Nice toy sign problem — (1,1) component only

$$\left\langle \frac{1}{2} \text{Tr}(P) \right\rangle = \langle P_{11} \rangle = \left\langle \sin(\tilde{\theta}) e^{i\tilde{\phi}} e^{\Delta S} J(\theta, \phi) \right\rangle$$



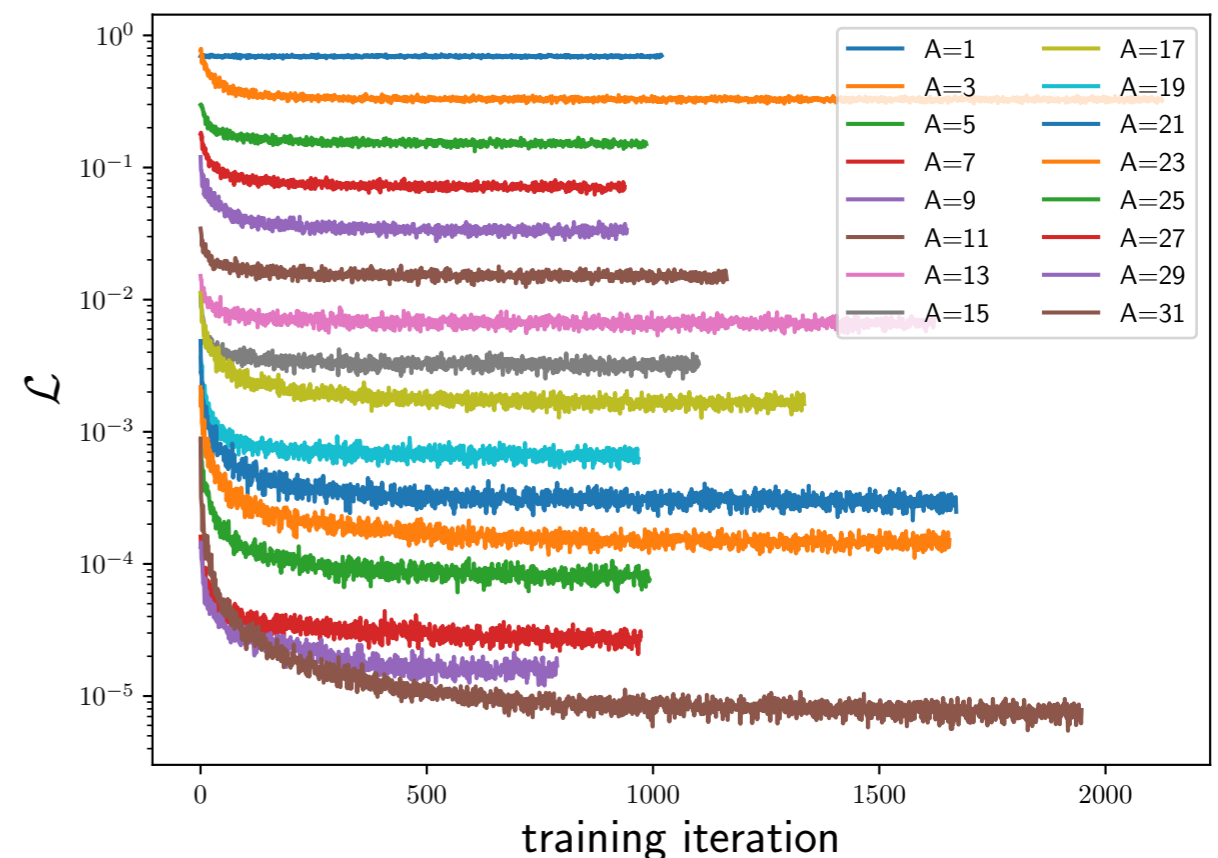
Parameterizing SU(2) contours

More general manifolds can be parameterized using gauge-field-dependent vertical deformations (ordered in spacetime)

$$\tilde{\Omega} = \Omega + i \sum_{\{n_i\}=0}^{\Lambda} \sum_{\{m_j\}=1}^{\Lambda} \lambda_{n_1 \dots m_K} \prod_{i=1}^J \sin(\phi_i n_i + \chi^i) \prod_{j=1}^K \sin(2\theta_j m_j)$$

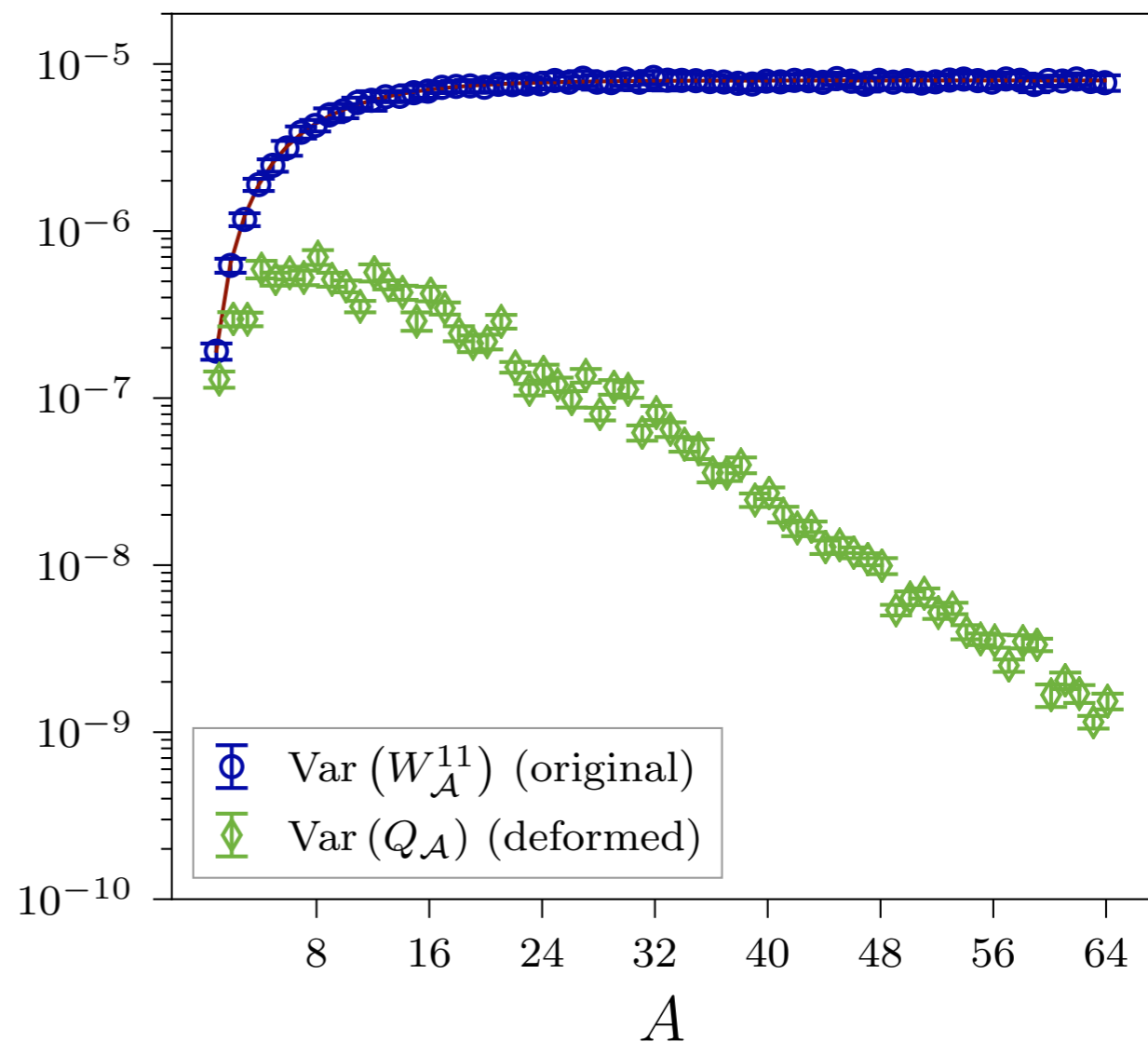
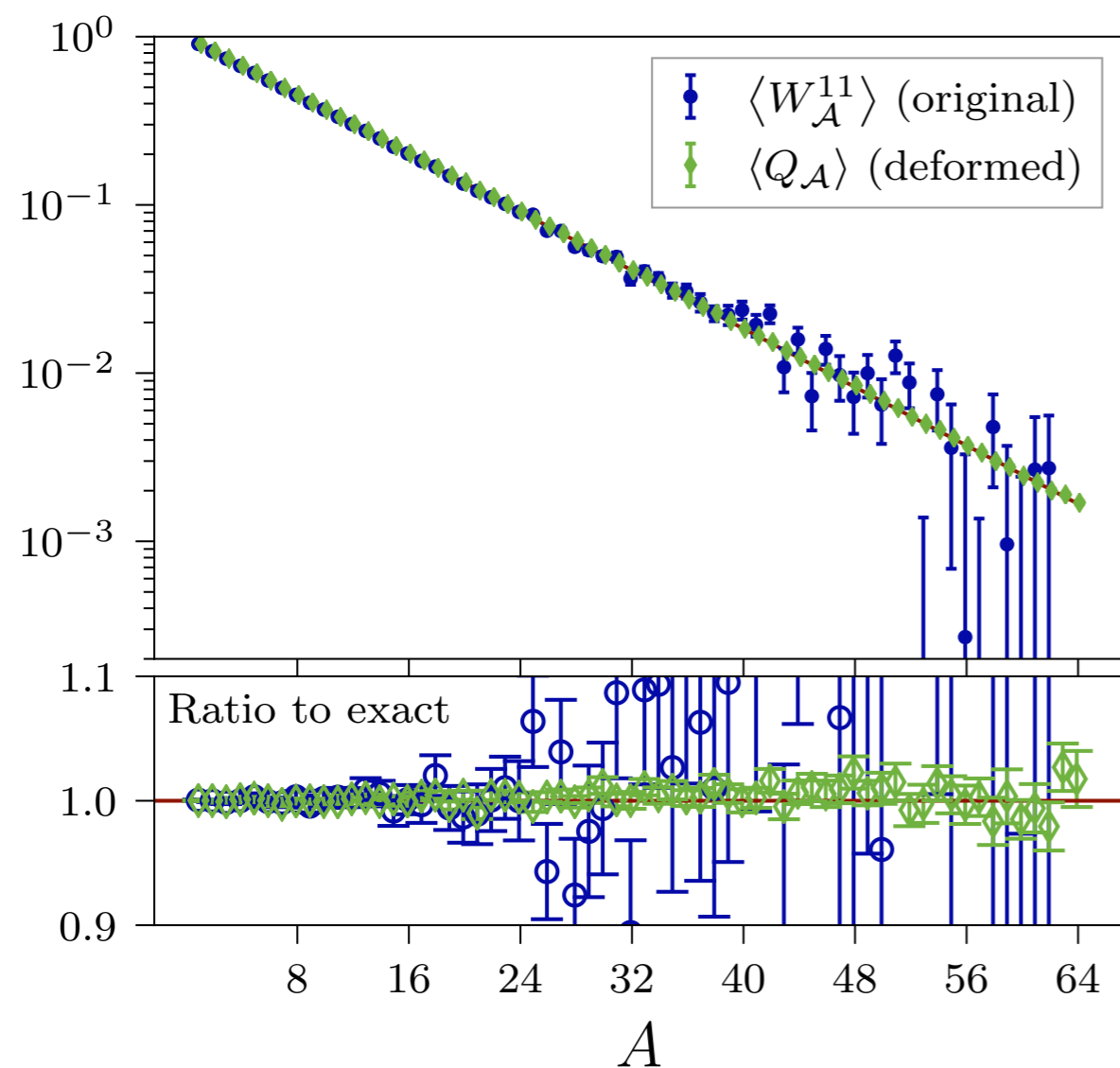
Variance minimization is a well-posed optimization problem suitable for machine learning techniques

Overtraining on sample variance avoided using resampling (mini-batches) and using a separate test set for train rate scheduling



SU(2) deformation results

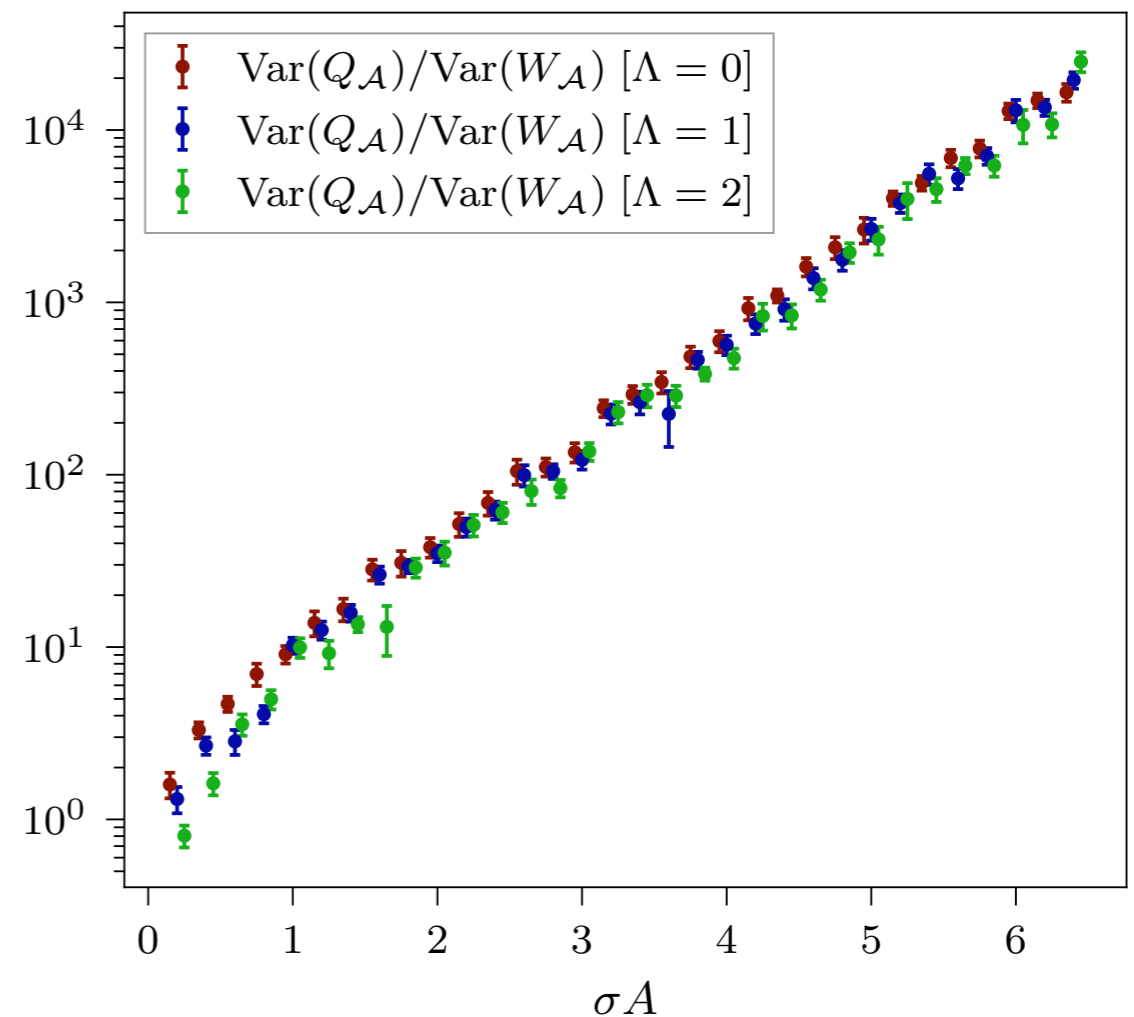
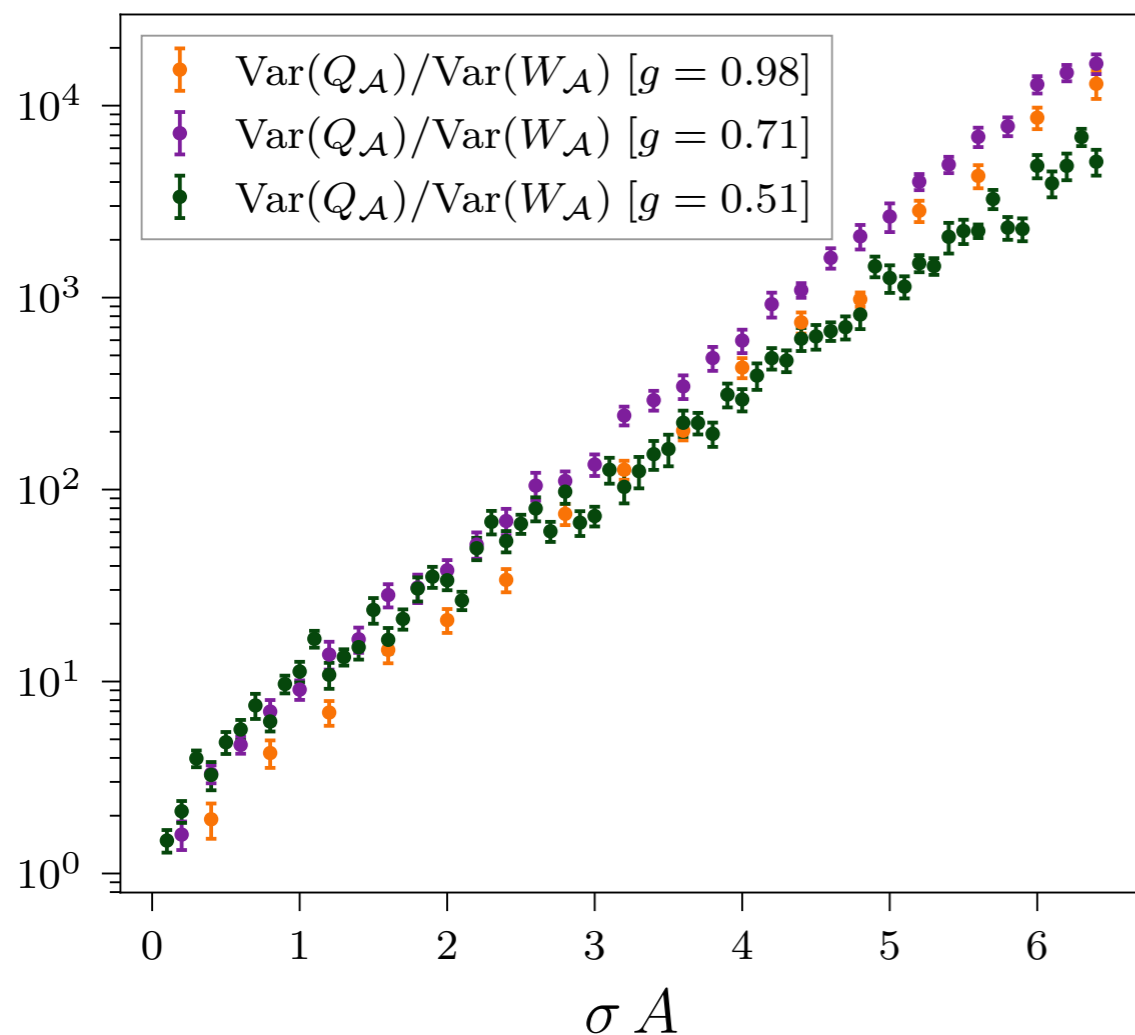
Optimized manifolds lead to exponentially increasing variance reduction for large area Wilson loops



SU(2) deformation results

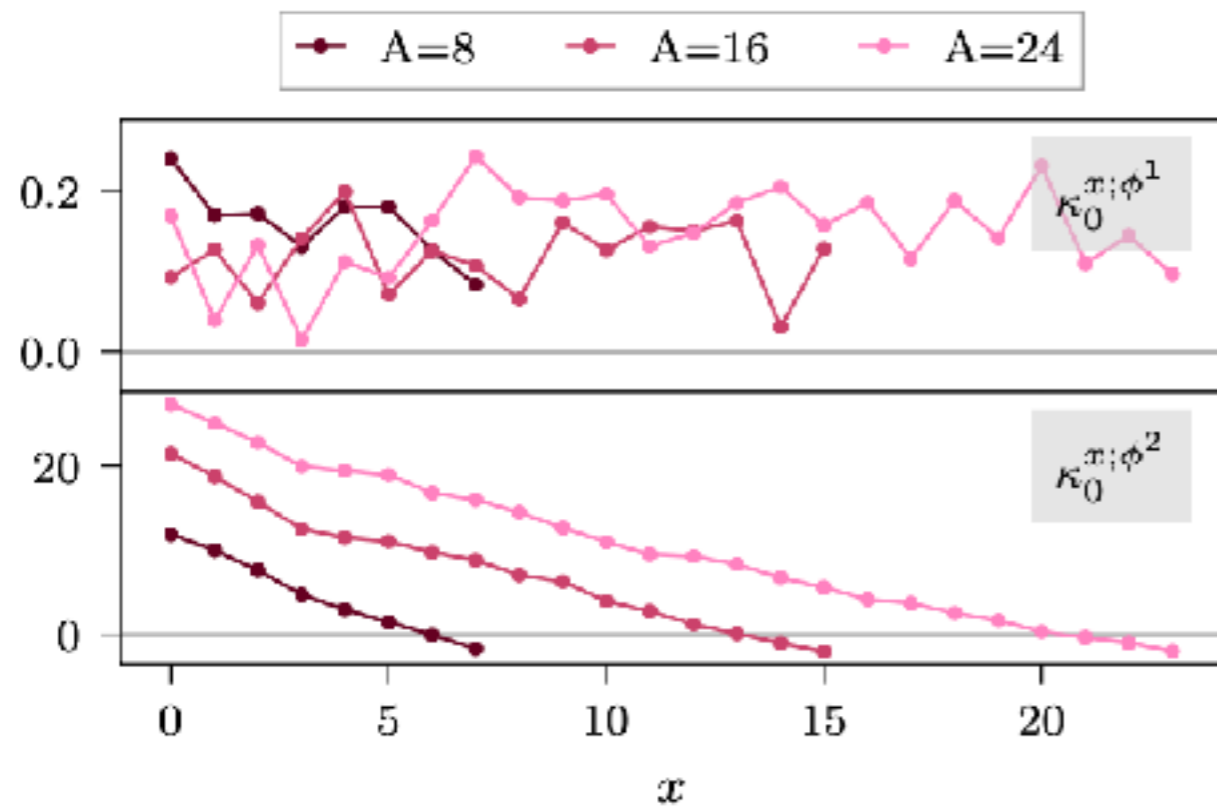
Variance reduction scales in physical units as gauge coupling is decreased towards continuum limit

Gains predominantly coming from zeroth order Fourier cutoff (constant vertical deformations)



SU(2) deformation results

Optimal manifold resembles a constant magnitude deformation of diagonal phase throughout Wilson loop, linearly decreasing deformation of off-diagonal phase



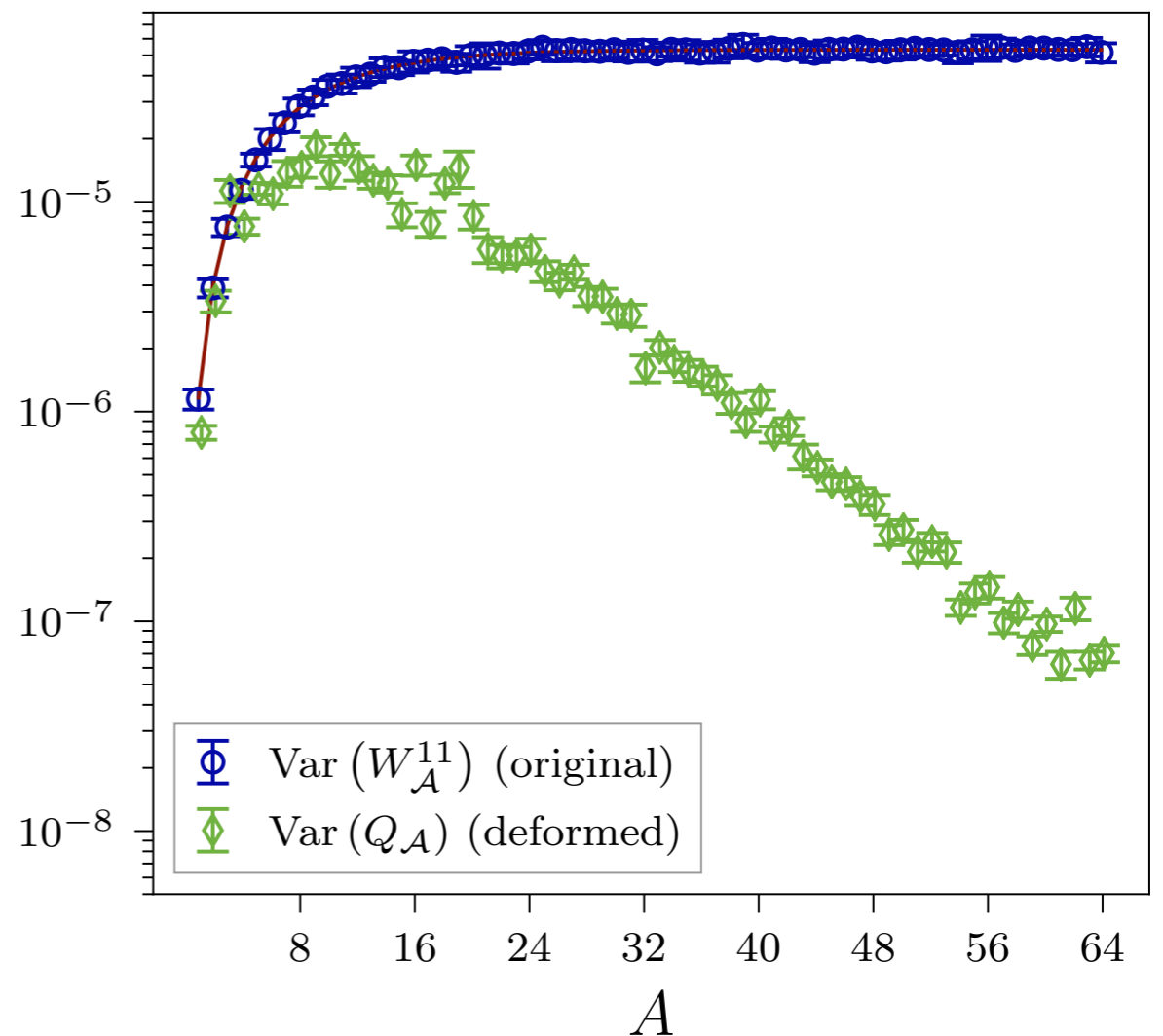
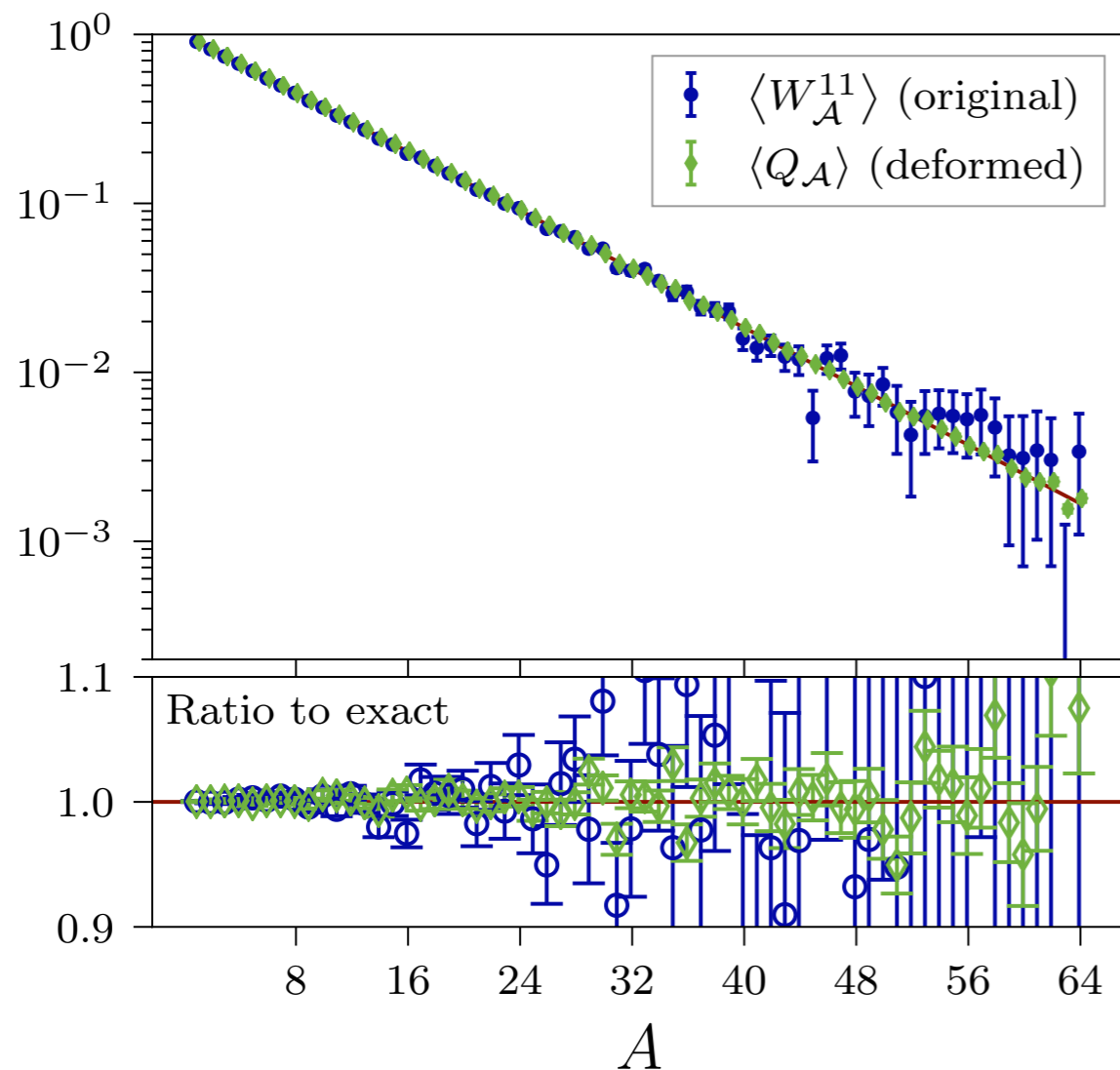
Qualitative features follow from minimizing magnitude of product of two plaquettes

$$(P_x P_{x'})^{11} = \sin \theta_x \sin \theta_{x'} e^{i\phi_x^1 + i\phi_{x'}^1} + \cos \theta_x \cos \theta_{x'} e^{i\phi_x^2 - i\phi_{x'}^2},$$

SU(3) contour deformations

Analogous angular parameterization of SU(3) matrices

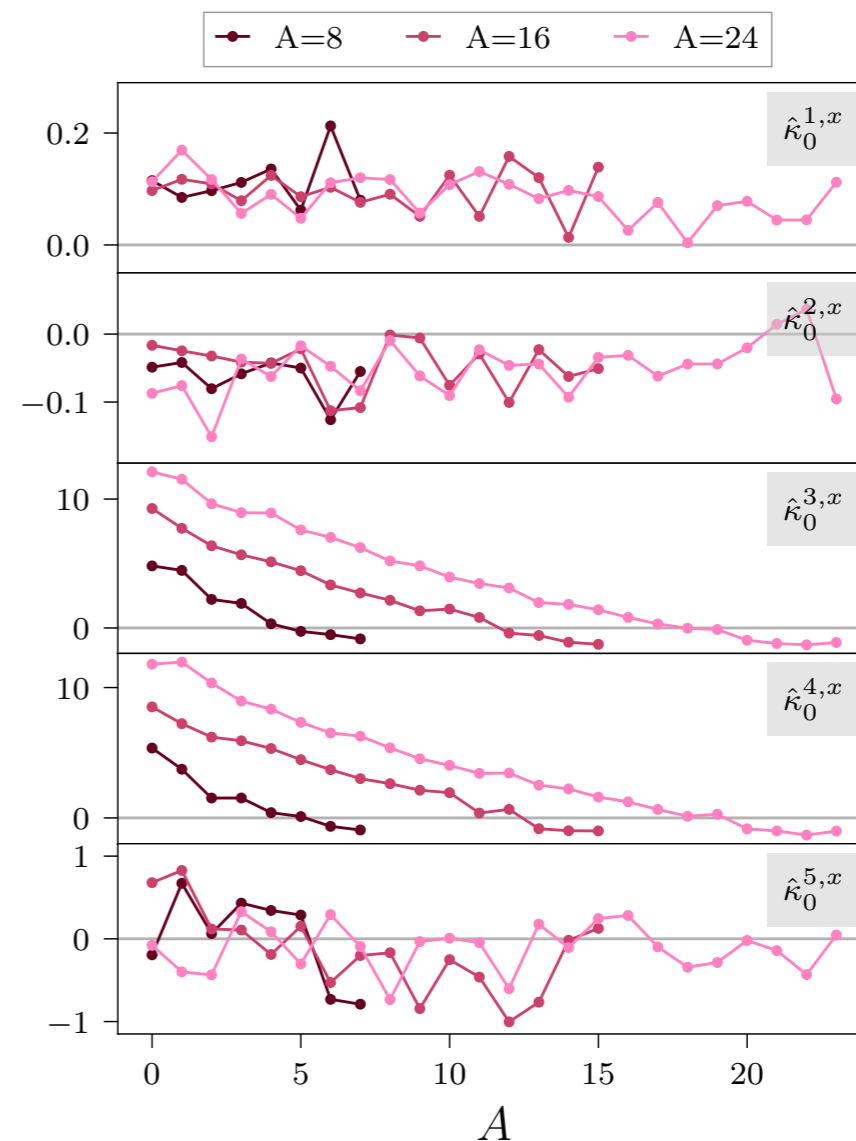
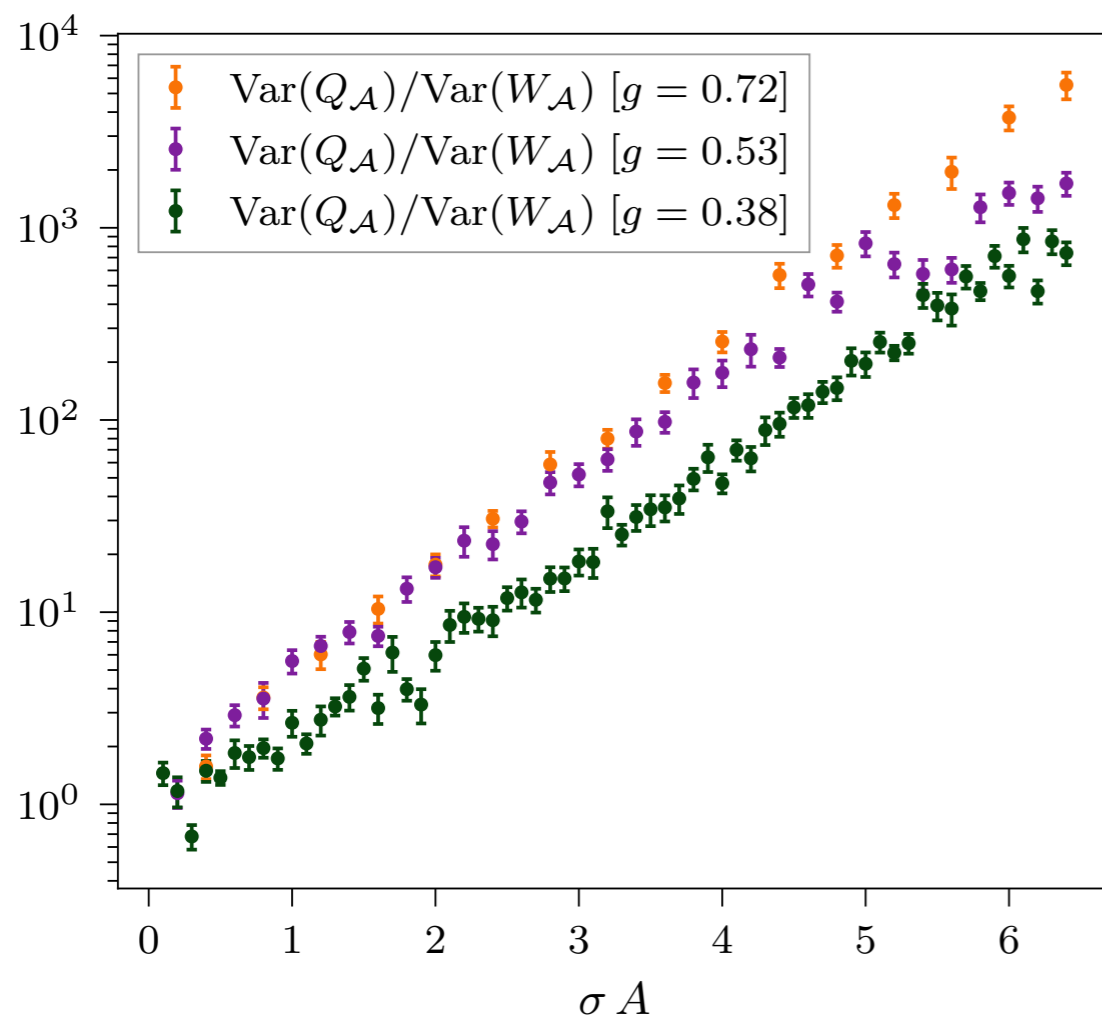
$$\phi_x^1, \dots, \phi_x^5, \theta_x^1, \dots, \theta_x^3$$



SU(3) deformation results

Variance reduction roughly scales in physical units as gauge coupling is decreased towards continuum limit (training?)

Gains predominantly coming from zeroth order Fourier cutoff, qualitatively consistent with loop magnitude minimization



Sign problem time

Real-time evolution faces a notorious sign problem

$$\langle \mathcal{O} \rangle_M = \frac{1}{Z_M} \int \mathcal{D}U \, e^{iS_M(U)} \mathcal{O}(U)$$

Can trade sign for StN problem (compact gauge group) $p(U)dU = dU$

$$\langle \mathcal{O} \rangle_M = \frac{\int \mathcal{D}U p(U) \mathcal{O}(U) e^{iS_M(U)}}{\int \mathcal{D}U p(U) e^{iS_M(U)}}$$

Still a problem, e.g. 2D U(1) $\text{StN}(e^{iS_{M,U(1)}}) \approx \sqrt{n} e^{-2.3Vt}$

Improve with contour deformations $p(U)dU = e^{-\text{Im}[S_M(\tilde{U}(U))]} |J(U)| dU$

$$\langle \mathcal{O} \rangle_M = \frac{\int \mathcal{D}U p(U) \mathcal{O}(U) e^{i\text{Re}[S_M(\tilde{U}(U))] + i\arg[J(U)]}}{\int \mathcal{D}U p(U) e^{i\text{Re}[S_M(\tilde{U}(U))] + i\arg[J(U)]}}$$

Real-time lattice gauge theory

A more basic question: what's the action?

$$S_{E,W}(U) = \frac{2}{g^2} \sum_x \sum_{\mu < \nu} \text{Tr}(2 - P_{x,\mu\nu} - P_{x,\mu\nu}^{-1})$$

Identifying time-space (space-space) plaquette terms as kinetic and potential energies and performing usual Wick rotation gives

$$S_{M,W}(U) = \frac{2}{g^2} \sum_x \sum_k \text{Tr}(2 - P_{x,0k} - P_{x,0k}^{-1}) \\ - \frac{2}{g^2} \sum_x \sum_{i < j} \text{Tr}(2 - P_{x,ij} - P_{x,ij}^{-1})$$

(1+1)D Minkowski Wilson loops

Wick rotate action

$$g^2 \rightarrow ig^2$$

$$\left\langle \frac{1}{2} \text{Tr}(W_{\mathcal{A}}) \right\rangle_{M,W,SU(2)} = \left[\frac{I_1(4i/g^2)}{I_2(4i/g^2)} \right]^{-Lt}$$

$$\left\langle \frac{1}{2} \text{Tr}(W_{\mathcal{A}}) \right\rangle_{E,W,SU(2)} = \left[\frac{I_1(4/g^2)}{I_2(4/g^2)} \right]^{-L\tau}$$

Non-unitary time evolution

No continuum limit

Analytically continue time

$$\tau \rightarrow it$$

$$\left\langle \frac{1}{2} \text{Tr}(W_{\mathcal{A}}) \right\rangle_{M,HFK,SU(2)} = \left[\frac{I_1(4/g^2)}{I_2(4/g^2)} \right]^{-iLt}$$

The HFK action

A unitarity time-evolution operator exists for the Wilson action

$$\hat{T} = e^{-\hat{H}} \qquad \hat{U} = e^{-i\hat{H}} = \hat{T}^i$$

However, \hat{U} is not the lattice time-evolution operator

An alternative action proposed by Hoshina, Fujii, and Kikukawa using character expansion leads to a unitary lattice time-evolution operator

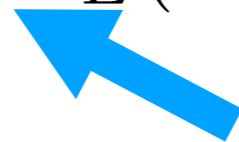
$$e^{iS_{M,HKF}(U)} = e^{-\frac{i}{e^2} \sum_x \sum_{i<j} (1 - \cos(\phi_{x,ij}))} \prod_{x,k} \left[\sum_{r=-\infty}^{\infty} [I_r(-i/e^2)]^i e^{i/e^2} e^{ir\phi_{x,0k}} \right]$$

$$P_{x,\mu\nu} = e^{i\phi_{x,\mu\nu}}$$

The heat-kernel action

An alternative Euclidean action starts from “heat-kernel” equation

$$\partial_\tau \mathcal{K}_E(U, \tau) = \Delta \mathcal{K}_E(U, \tau)$$



Laplace-Beltrami operator for gauge group

Solution for U(1): $\mathcal{K}_{E,U(1)}(e^{i\phi}, -e^2) = \sum_{n=-\infty}^{\infty} \exp \left[-\frac{1}{2e^2} (\phi + 2\pi n)^2 \right]$

Generalization to SU(N) gives heat-kernel action

Analytic continuation gives Schrödinger equation

$$i\partial_t \mathcal{K}_M(U, t) = -\Delta \mathcal{K}_M(U, t)$$

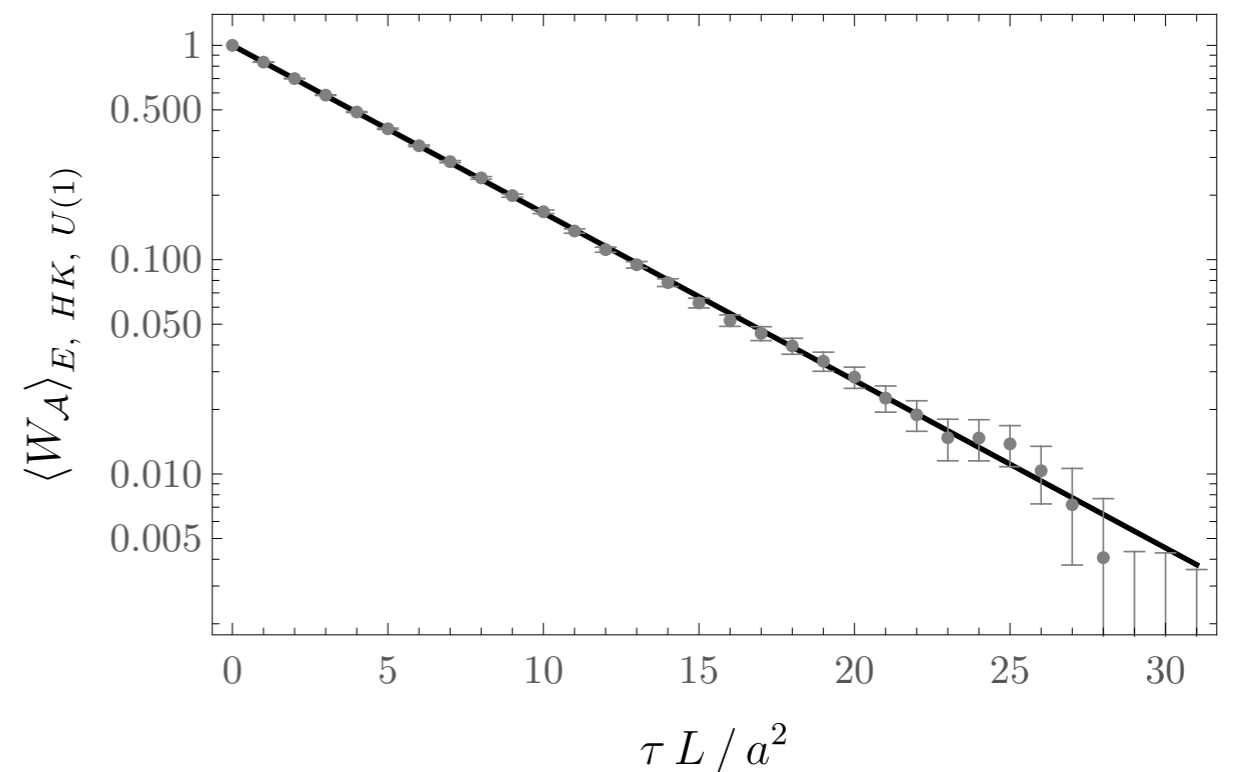
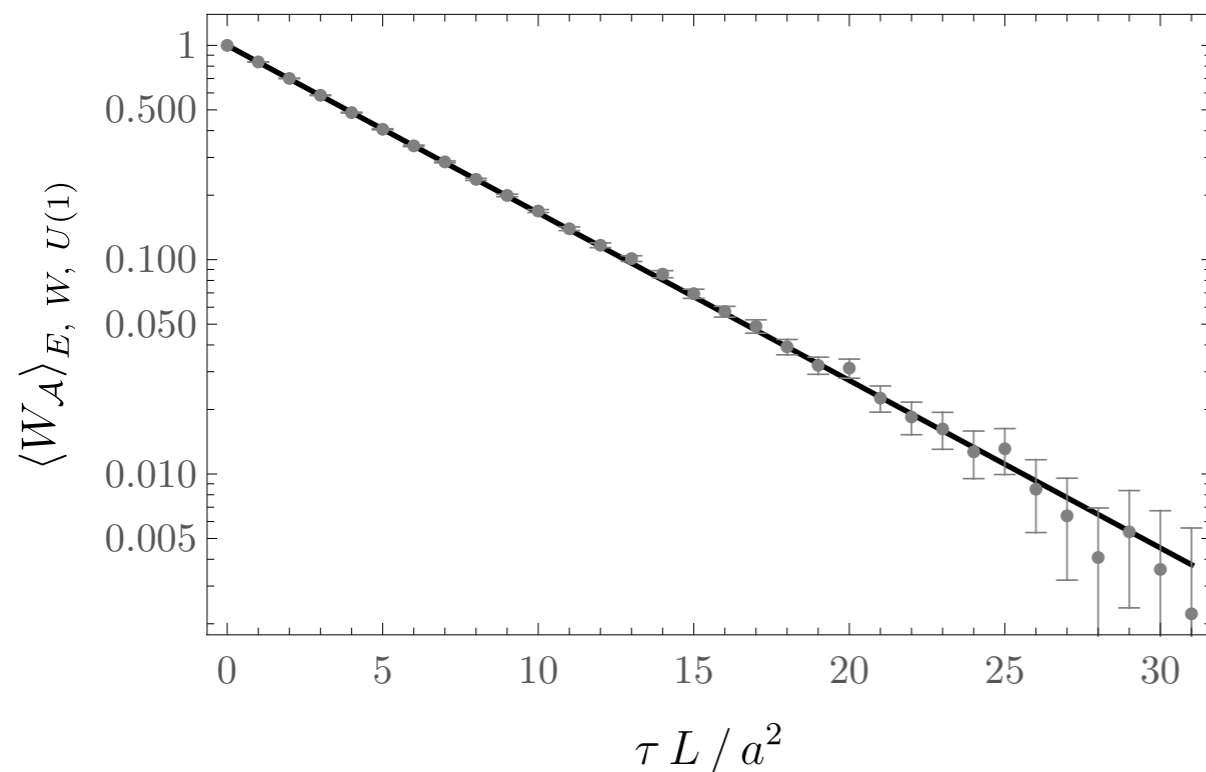
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Euclidean U(1) heat-kernel results

Infinite sum in Euclidean heat-kernel action can be performed stochastically by introducing integer-valued auxiliary field

$$\int \mathcal{D}U e^{-S(U)} = \left(\int \mathcal{D}U \sum_{n=-\infty}^{\infty} \right) e^{-S(U,n)}$$

Monte Carlo results for 2D Wilson loops with heat-kernel action with appropriately tuned coupling identical to Wilson action



Real-time U(1) lattice gauge theory

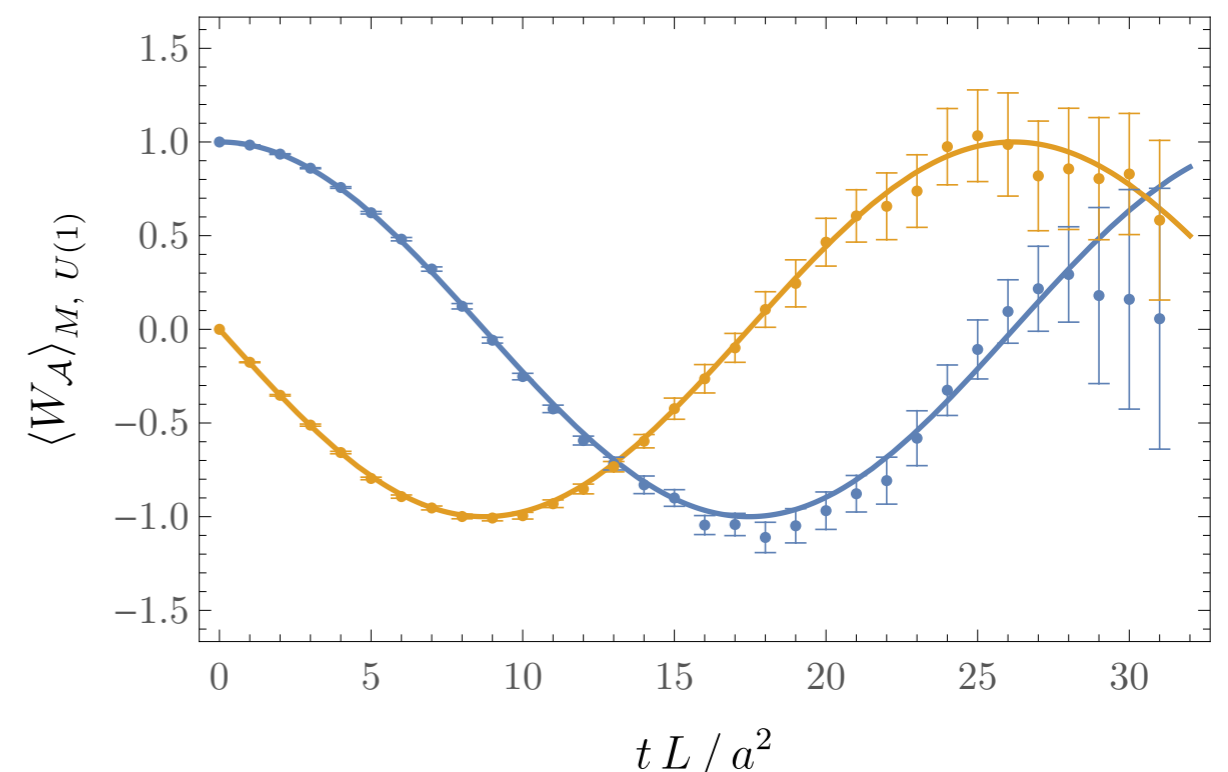
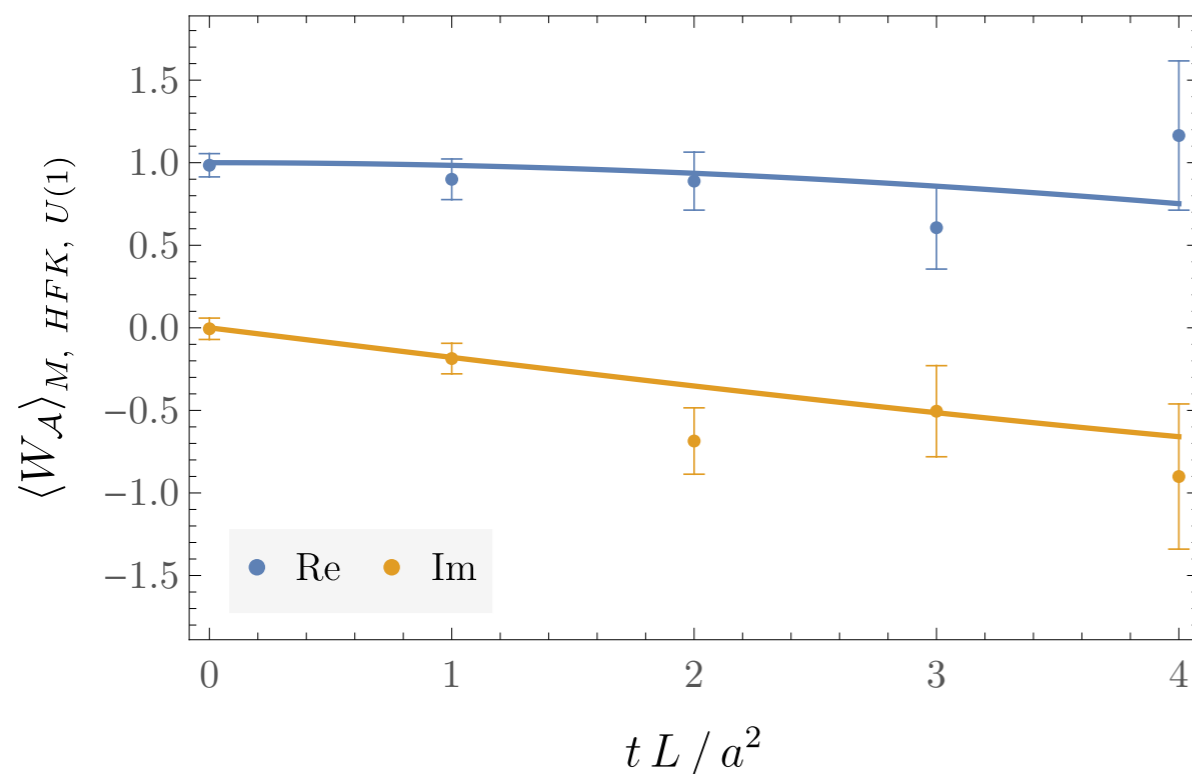
In Minkowski spacetime, the sums defining both the HFK and heat-kernel actions diverge

Path integral contour deformations can improve convergence

$$U \rightarrow \tilde{U}(U, n)$$

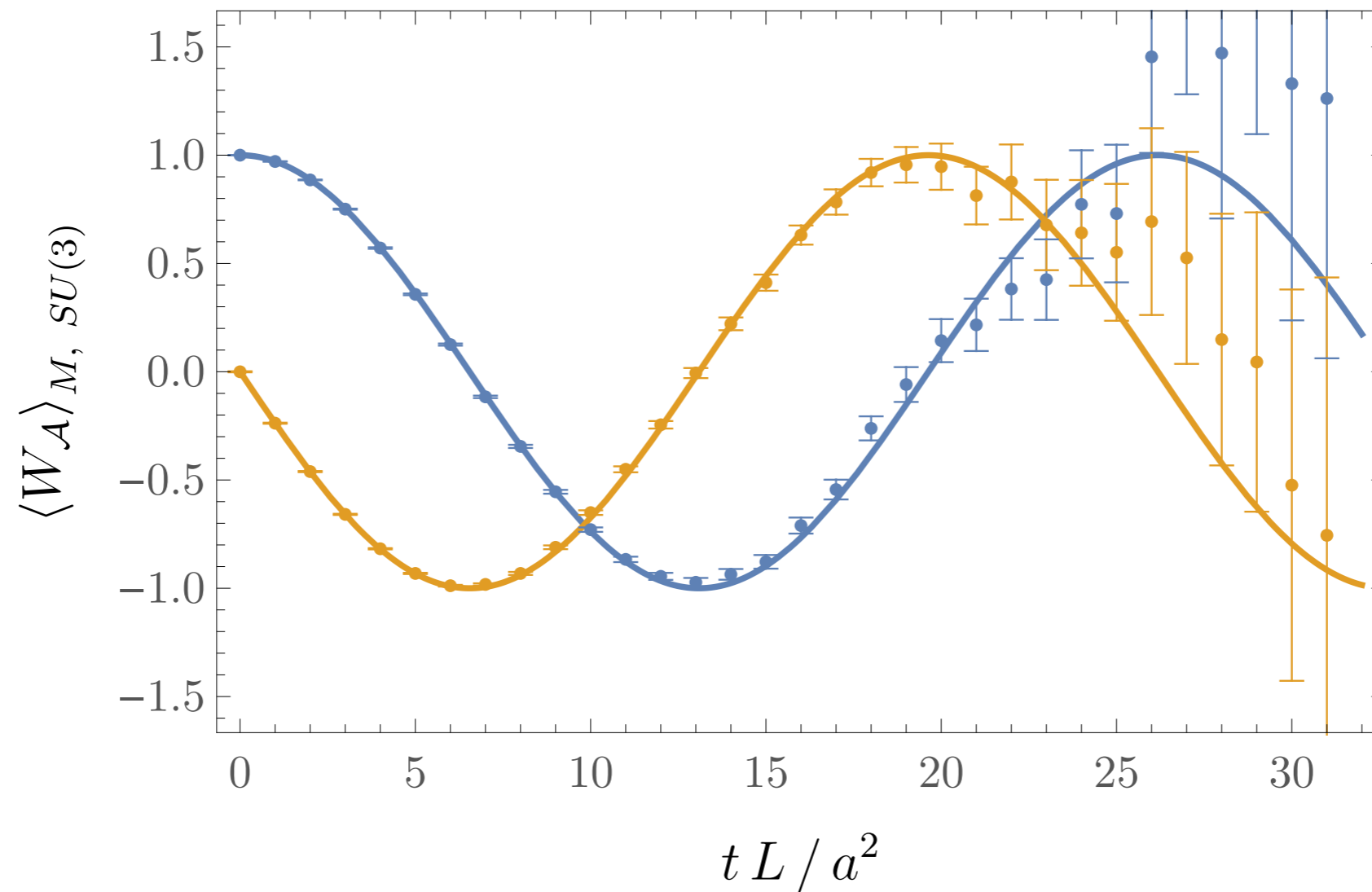
With the heat-kernel action, they also “solve” the sign problem

$$e^{\frac{i}{2e^2}(\phi+2\pi n)^2} \rightarrow e^{-\frac{1}{2e^2}(\phi+2\pi n)^2}$$



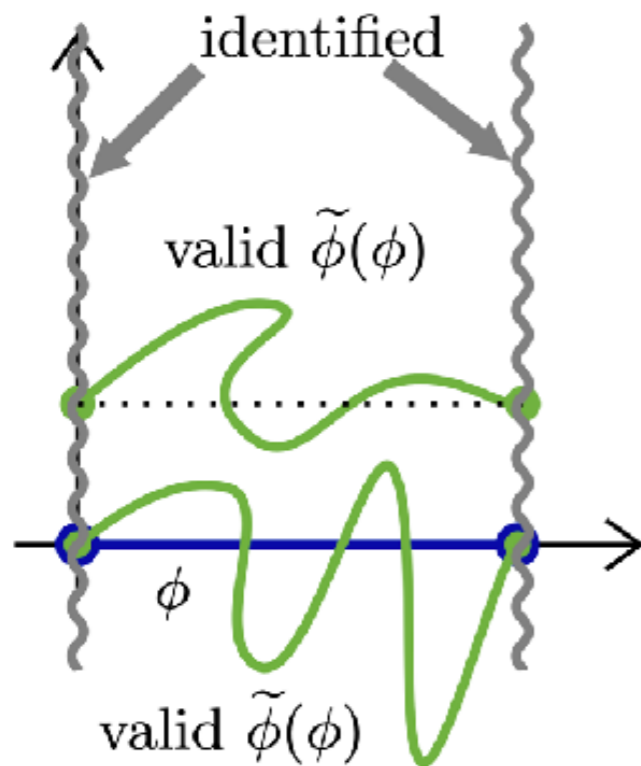
Real-time SU(3)

Works in (1+1)D



Conclusions

Lattice QCD is increasingly important for HEP/NP problems; sign(al-to-noise) problems present challenges



Path integral contour deformations have been shown to tame sign(al-to-noise) problems in 2D lattice gauge theory

Monte Carlo simulations of real-time lattice gauge theory are possible with the right action and contour deformation

