Life Outside the Golden Window: Statistical Angles on the LQCD Signal-to-Noise Problem

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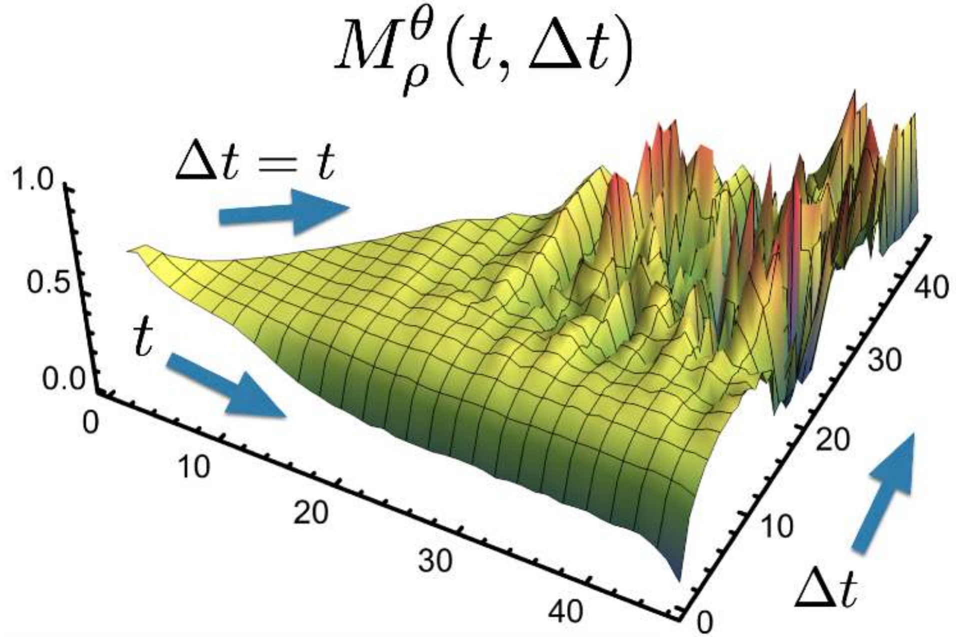
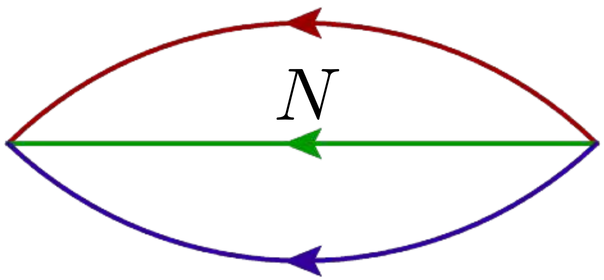


with Martin Savage and the NPLQCD collaboration

MW and Savage, arXiv:1611.07643; MW and Savage, arXiv:1704.07356

The Signal-to-Noise Problem

Noise in Monte Carlo calculations arises from quantum fluctuations in observables

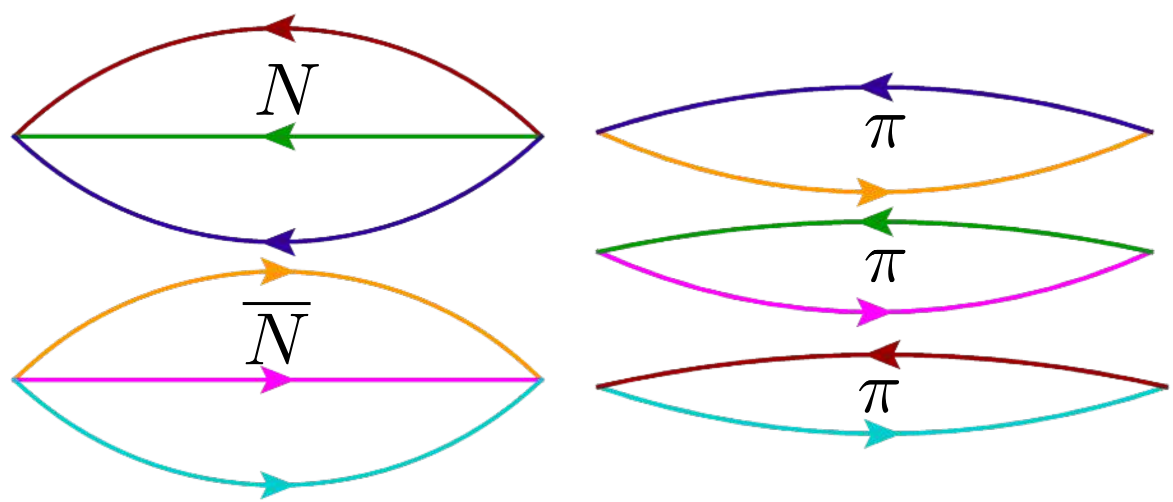


$$G(t) = \langle C_i(t) \rangle \sim e^{-m_N t}$$

Late-time behavior of nucleon variance fixed by lowest energy state with the right quantum numbers to contribute to variance

$$\mathrm{Var}(G(t)) \sim \langle |C_i(t)|^2 \rangle$$

$$\sim e^{-3 m_\pi t}$$



Parisi-Lepage signal-to-noise

$$\mathrm{StN} \sim e^{-\left(m_N - \frac{3}{2} m_\pi\right) t}$$

G. Parisi. Phys. Rept. 103 (1984), P. Lepage. TASI (1989)

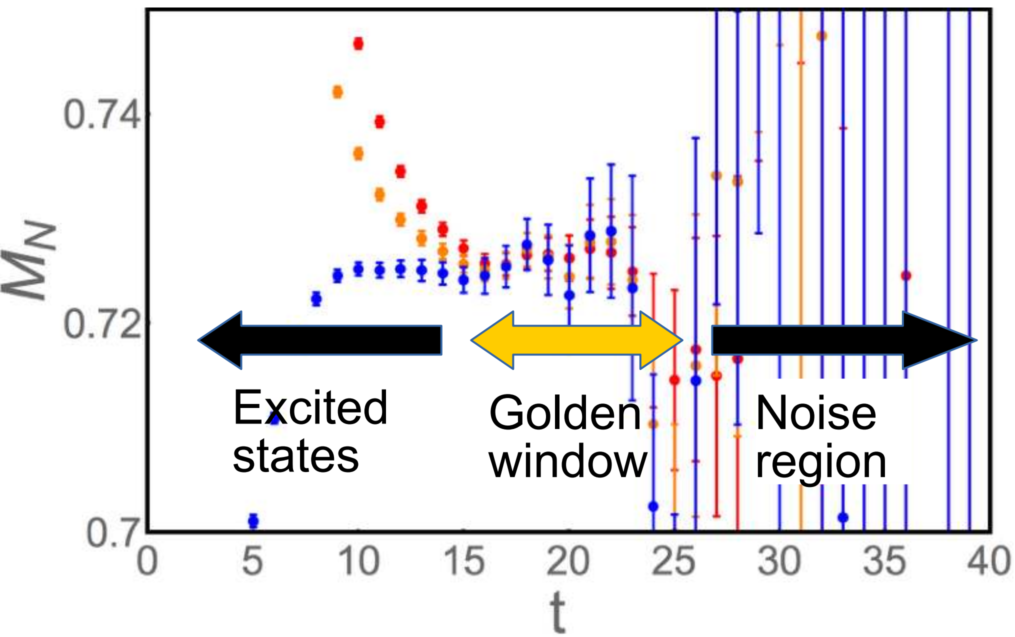
The Golden Window

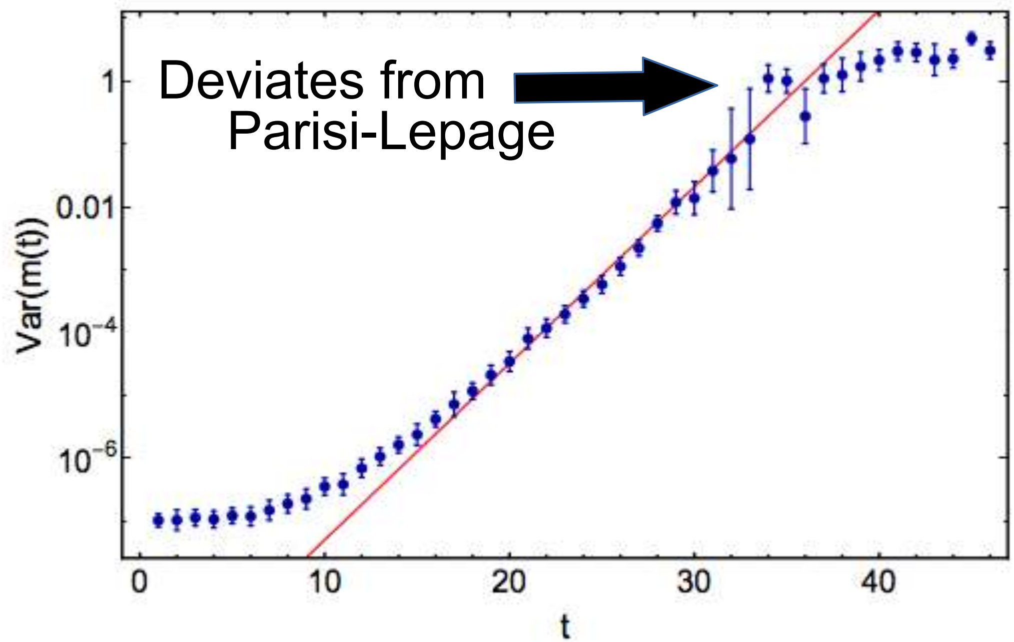
LQCD calculations of baryons rely on a golden window where excited state contamination is small but StN is still manageable

Beane et al (NPLQCD). Phys. Rev. D79 (2009)

$$m(t) = \ln\left[\frac{\langle C_i(t)\rangle}{\langle C_i(t+1)\rangle}\right]$$

$$\mathrm{Var}\,(m(t)) \sim e^{2\left(m_N - \frac{3}{2}m_\pi\right)t}$$

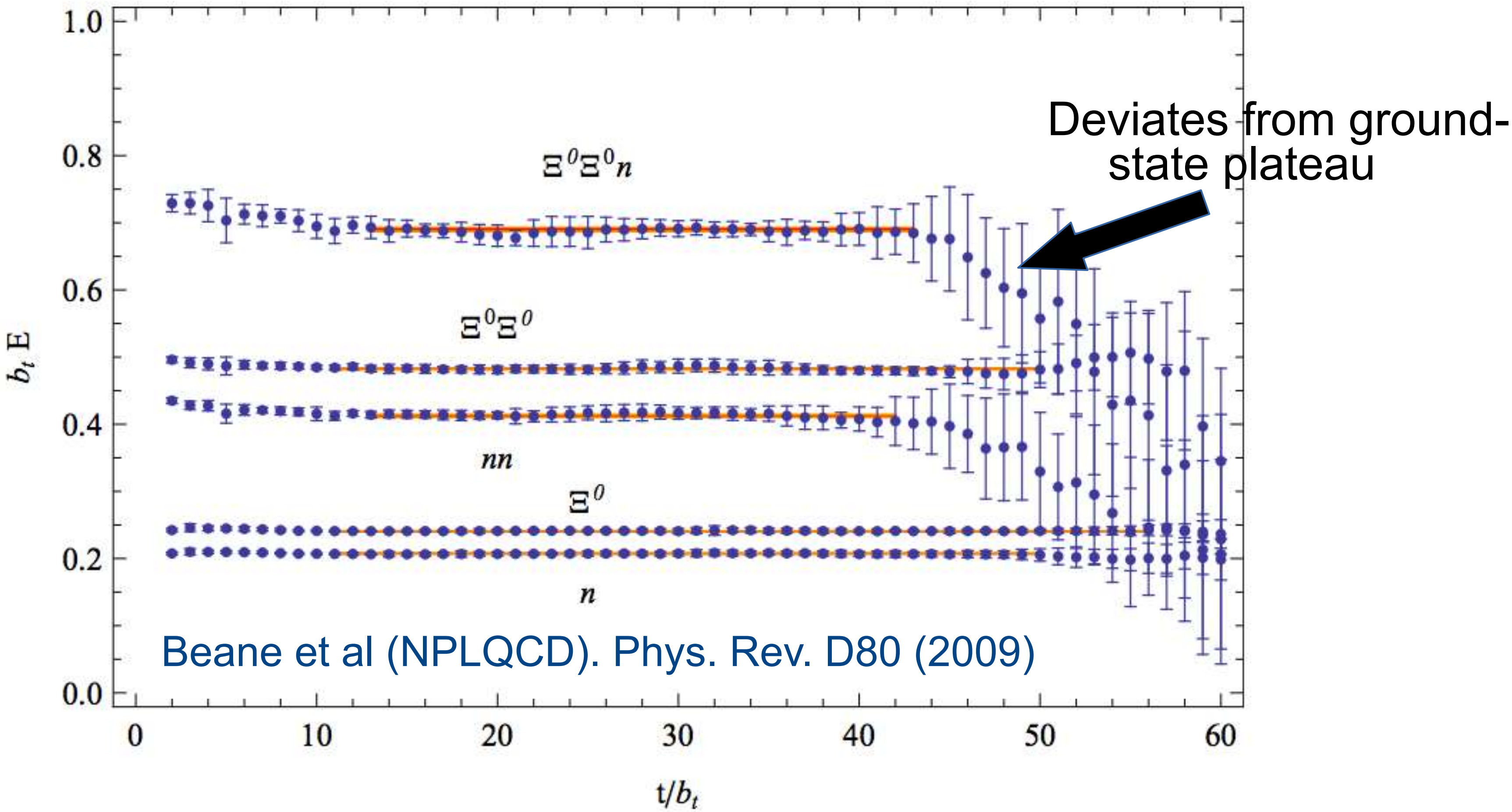




Late time noise region disobeys general quantum field theory principles

Widening the Golden Window

Optimizing linear combinations of sink operators found by e.g. Matrix-Prony or variational methods reduces excited state overlap, extending the golden window to earlier times



Different linear combinations minimize variance ground-state overlap and delay noise region. Cannot affect Parisi-Lepage scaling asymptotically

Detmold and Endres, Phys. Rev. D 90 (2014)

The Sign(al-to-Noise) Problem

Statistical estimation of an exponentially decaying average phase always has exponential StN degradation

$$\mathrm{StN}(e^{i\theta_i(t)}) \sim \frac{\left\langle e^{i\theta_i(t)} \right\rangle}{\sqrt{\left\langle \left| e^{i\theta_i(t)} \right|^2 \right\rangle}} \sim \left\langle e^{i\theta_i(t)} \right\rangle \sim e^{-m_\theta t}$$

Average correlation functions are real. Individual correlation functions in generic gauge fields are complex

$$C_i(t) = e^{R_i(t)+i\theta_i(t)}$$

Standard LQCD methods equivalent to reweighting a complex action

$$G(t) = \langle C_i(t) \rangle = \int \mathcal{D}U \; e^{-S(U)+R(t,U_i)+i\theta(t,U_i)} \;\; = \frac{1}{N}\sum_{i=1}^{N} e^{R_i(t)+i\theta_i(t)}$$

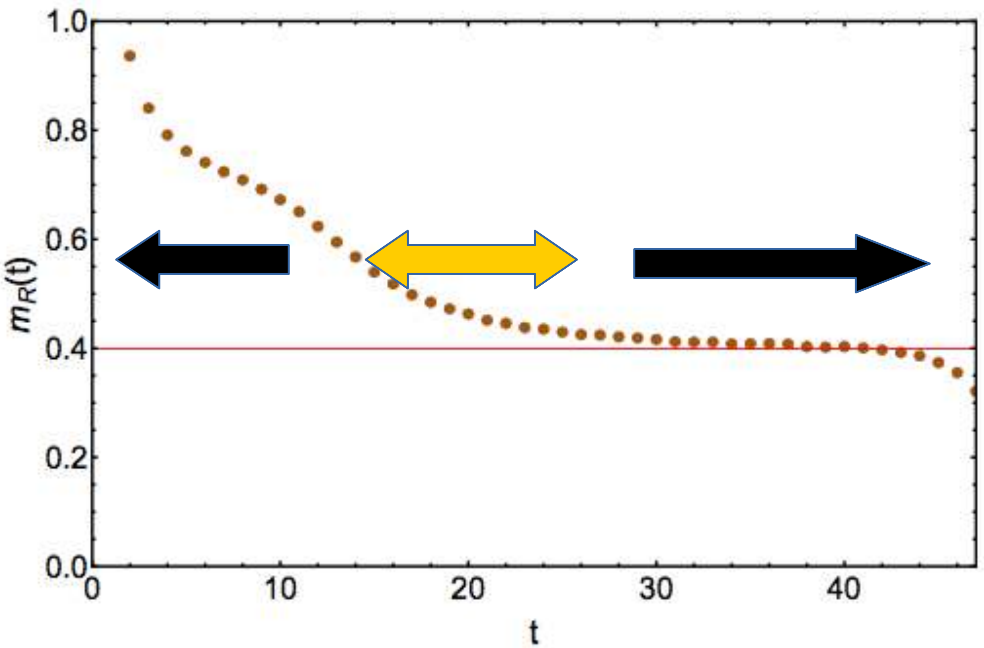
Is the LQCD signal-to-noise problem in all or part a sign problem?

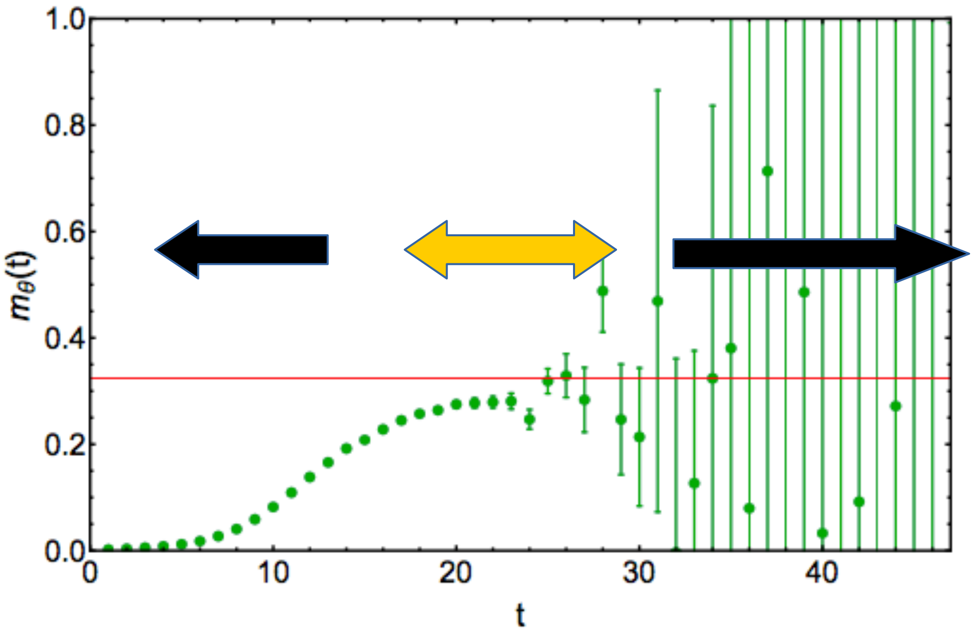
Magnitude - Phase Decomposition

Magnitude and phase of generic hadron correlation functions are (empirically) approximately decorrelated

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

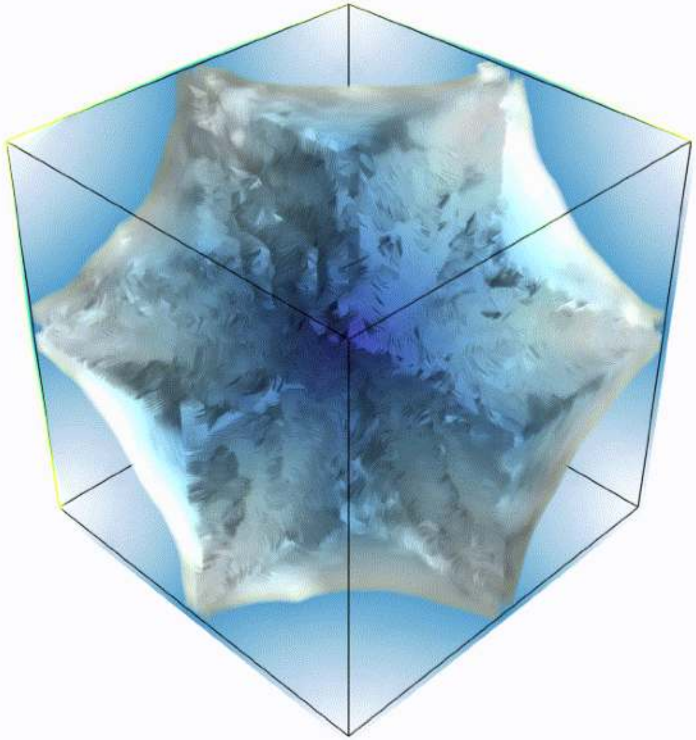
$$m_\theta(t) = \ln\left(\frac{\langle e^{i\theta_i(t)}\rangle}{\langle e^{i\theta_i(t+1)}\rangle}\right) \sim m_N - \frac{3}{2}m_\pi$$





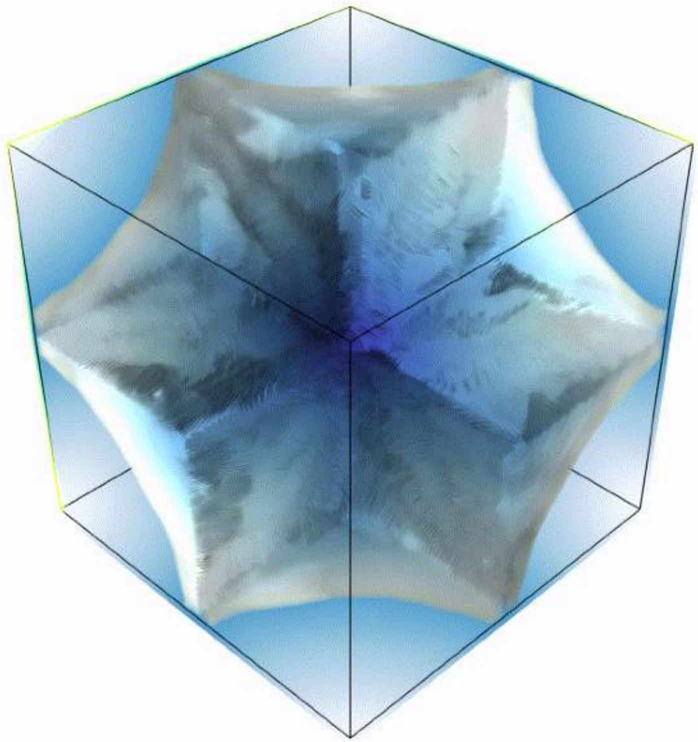
MW and Savage, arXiv:1611.07643

Nucleon Magnitude



Similar long-range structures in log-magntiude of nucleon and pion correlation functions

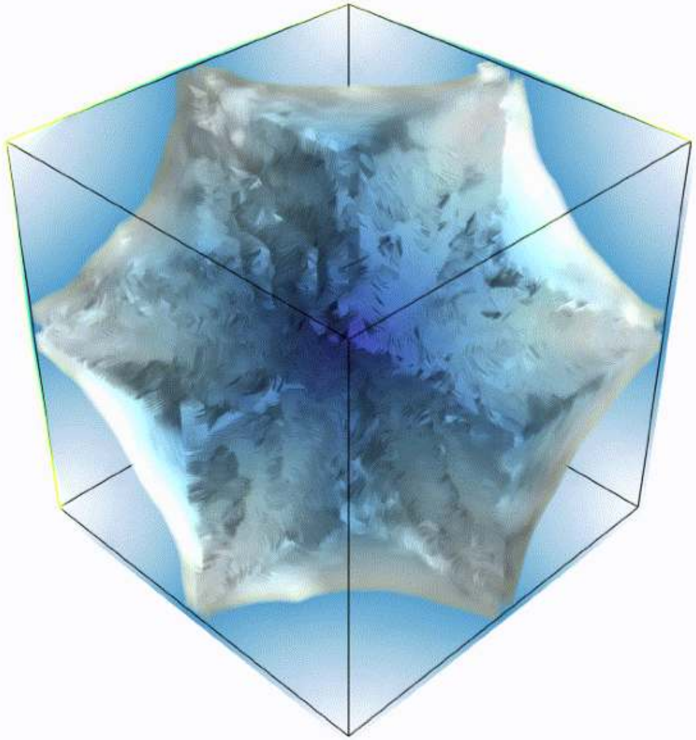
$$\ln C_i^{\pi}(t)$$



$$\ln |C_i(t)|$$

Animations by Daniel Trewartha (JLab)

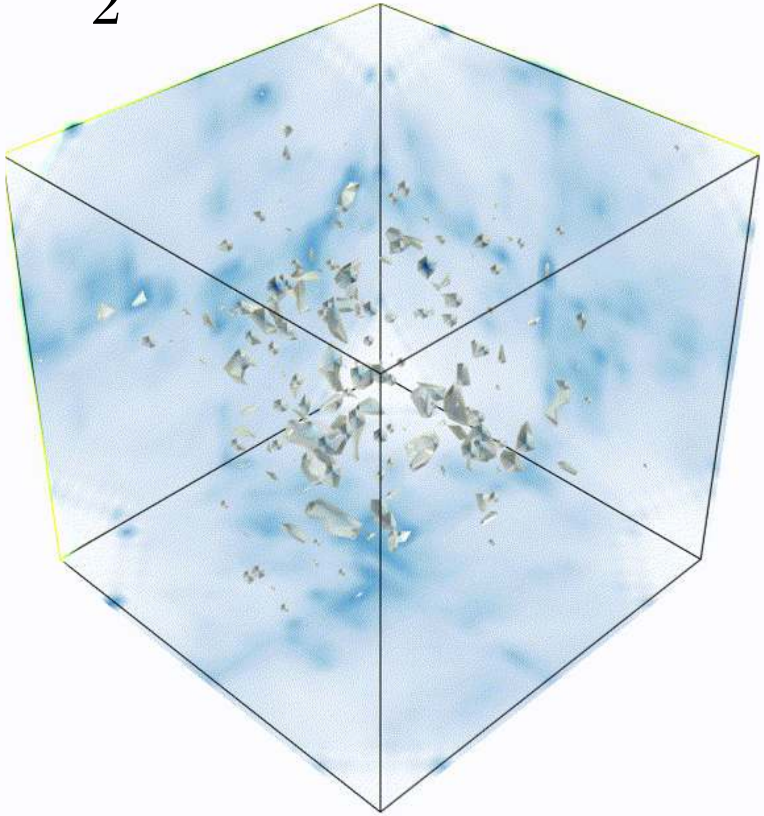
Nucleon Magnitude



$$\ln|C_i(t)|$$

Similar long-range structures in log-magntiude of nucleon and pion correlation functions

$$\frac{3}{2}\ln C_i^{\pi}(t) - \ln|C_i(t)|$$

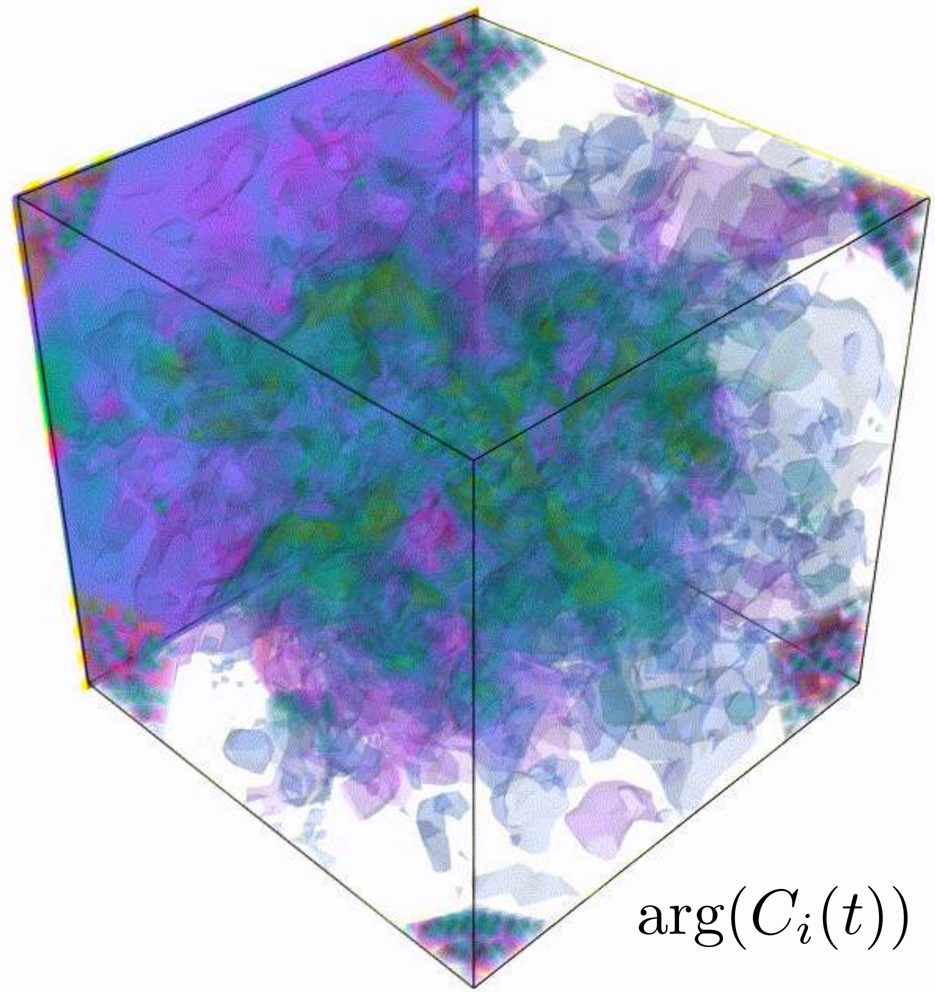


Animations by Daniel Trewartha (JLab)

Nucleon Phase

Difference between nucleon and (rescaled) pion correlation functions comes from destructively interfering phase fluctuations

Understanding the statistics of phase fluctuations critical to understand StN problem



Animations by Daniel Trewartha (JLab)

LQCD Correlation Function Statistics

Generic real, positive correlation functions, as well as early-time nucleons in LQCD, are log-normally distributed

Hamber, Marinari, Parisi and Rebbi, Nucl. Phys. B 225 (1983)

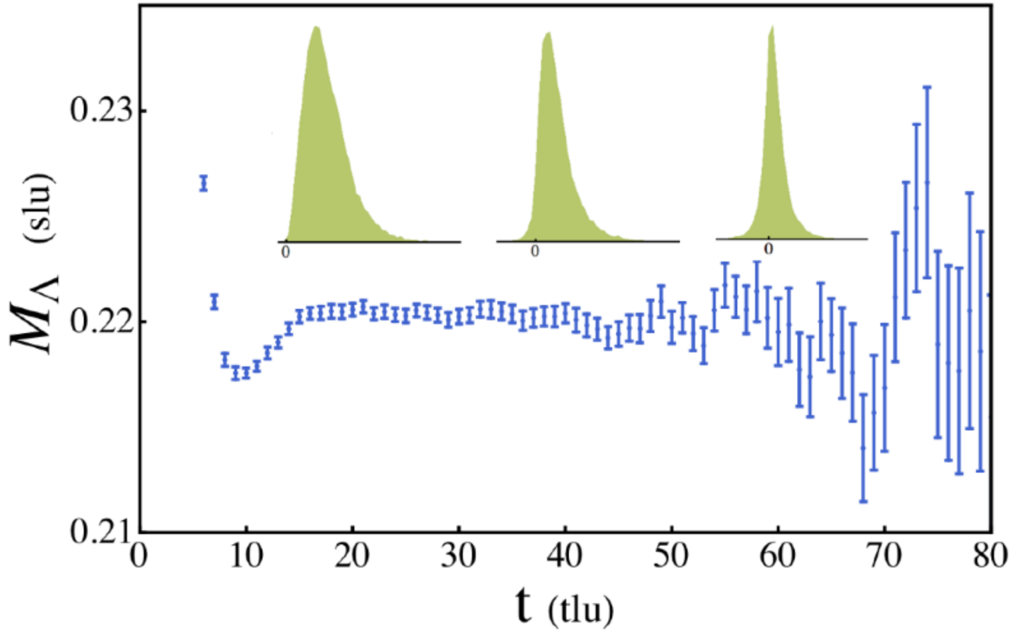
Guagnelli, Marinari, and Parisi, Phys. Lett. B 240 (1990)

Endres, Kaplan, Lee and Nicholson, Phys. Rev. Lett. 107 (2011)

DeGrand, Phys. Rev. D 86 (2012)

Log-normal distributions arise in models with only two-body interactions and products of generic random numbers

Late-time nucleon real part is not log-normal. Moment analysis by Savage predicts broad, symmetric distribution



Beane, Detmold, Orginos, Savage (NPLQCD) J. Phys. G 42 (2015)

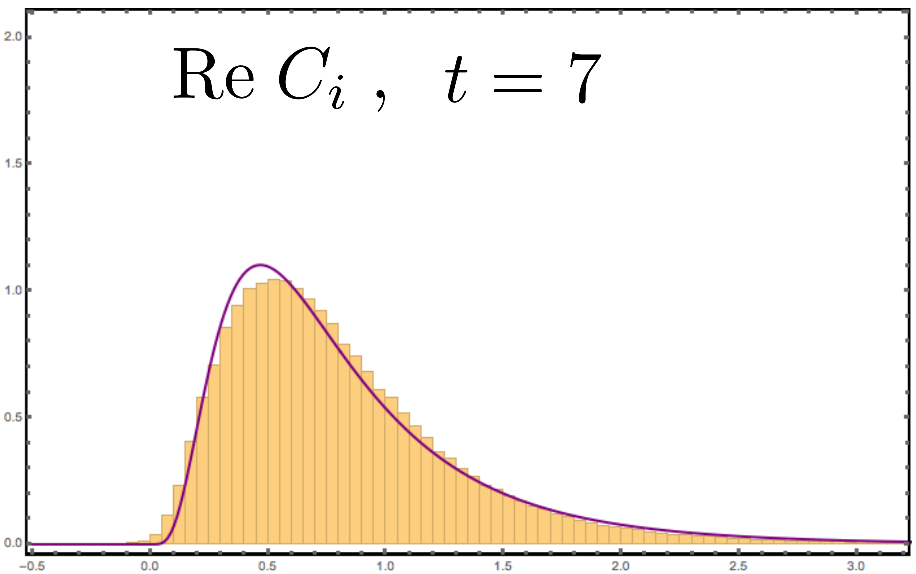
Complex Log-Normal Distributions

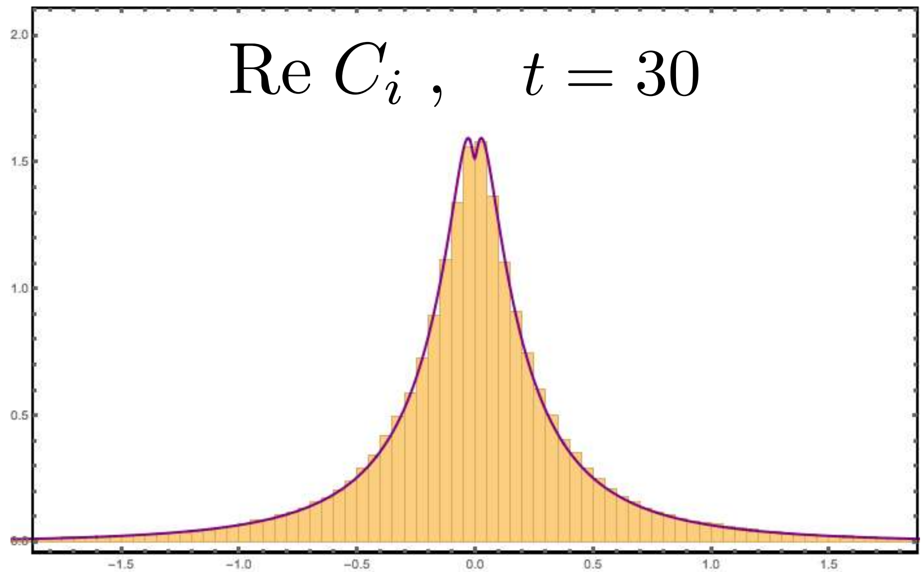
Phase is a circular random variable only defined modulo 2π

Summing over periodic images of Gaussian provides a wrapped normal distribution suitable for a circular random variable
See e.g. N. I. Fisher, "Statistical Analysis of Circular Data" (1995)

Real part of nucleon correlation functions well-described by marginalization of "complex log-normal distribution"

$$C_i(t) = e^{R_i(t) + i\theta_i(t)} \qquad \mathcal{P}(R_i, \theta_i) = e^{-(R_i - \mu_R)^2/(2\sigma_R^2)} \sum_{n=-\infty}^{\infty} e^{-n^2\theta_i^2/(2\sigma_\theta^2)}$$





MW and Savage, arXiv:1611.07643

Circular Statistics and the Noise Region

Circular random variables have different properties than random real numbers. Finite sample effects obstruct parameter inference unless

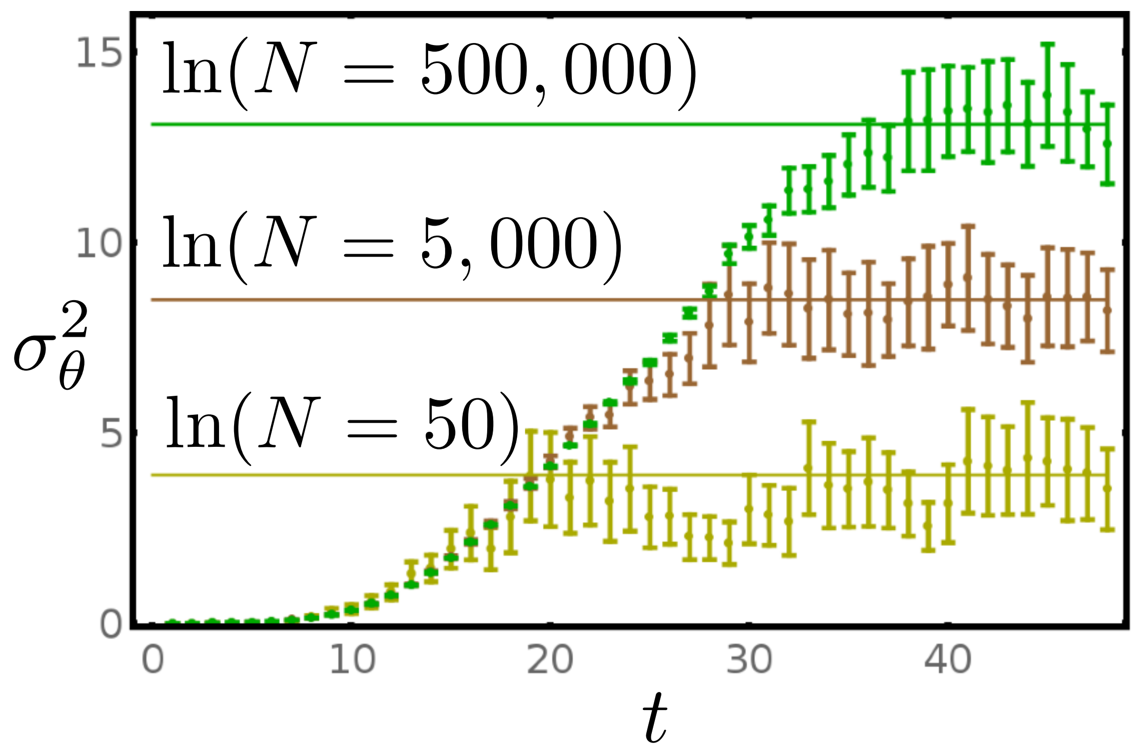
$$\frac{1}{N}\sum_{i=1}^{N}\cos\theta_i > \frac{1}{\sqrt{N}}$$

N. I. Fisher, “Statistical Analysis of Circular Data” (1995)

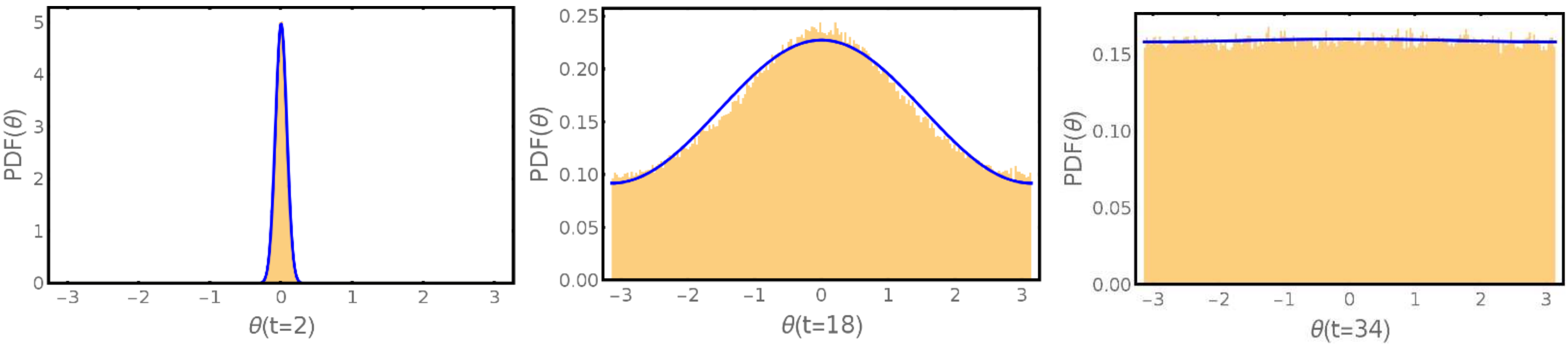
Avoiding finite sample effects requires

$$N > e^{\sigma_\theta^2} \sim e^{2(m_N - \frac{3}{2}m_\pi)t}$$

This will violated in a late-time “noise region” where standard estimators become unreliable



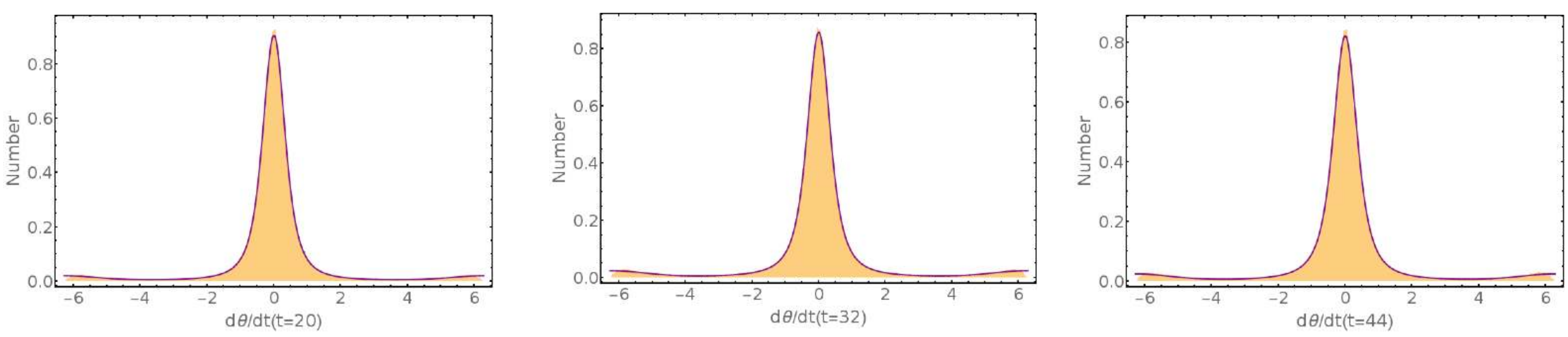
Lévy Flights on the Unit Circle



Phase wrapped normally distributed at all times

Phase and log-magnitude time derivatives approach time independent, heavy-tailed wrapped stable distributions at late times

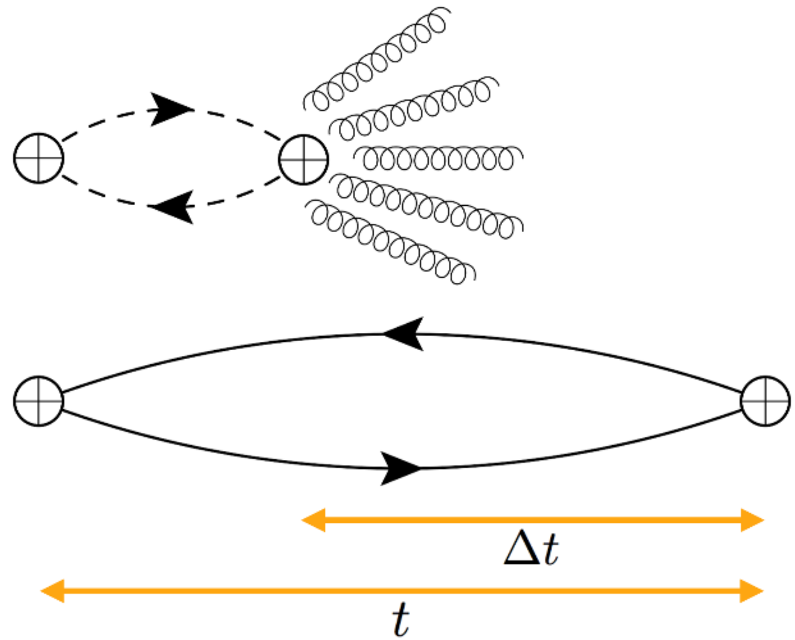
Independent samples from these distributions describe Lévy flights



Phase Reweighting

“Phase-reweighted correlation function” measures fixed-length phase differences

$$G^{\theta}(t, \Delta t) = \left\langle C_i(t) e^{-i\theta_i(t-\Delta t)} \right\rangle$$



Exponent of StN problem set by number of steps in random walk of the phase included in measurement

$$\mathrm{StN} \sim e^{-(m_N - \frac{3}{2} m_\pi)\Delta t}$$

MW and Savage, arXiv:1704.07356

Reduces to standard correlation function in limit $\Delta t \to t$

$$G^{\theta}(t, t) = \langle C_i(t) \rangle = G(t)$$

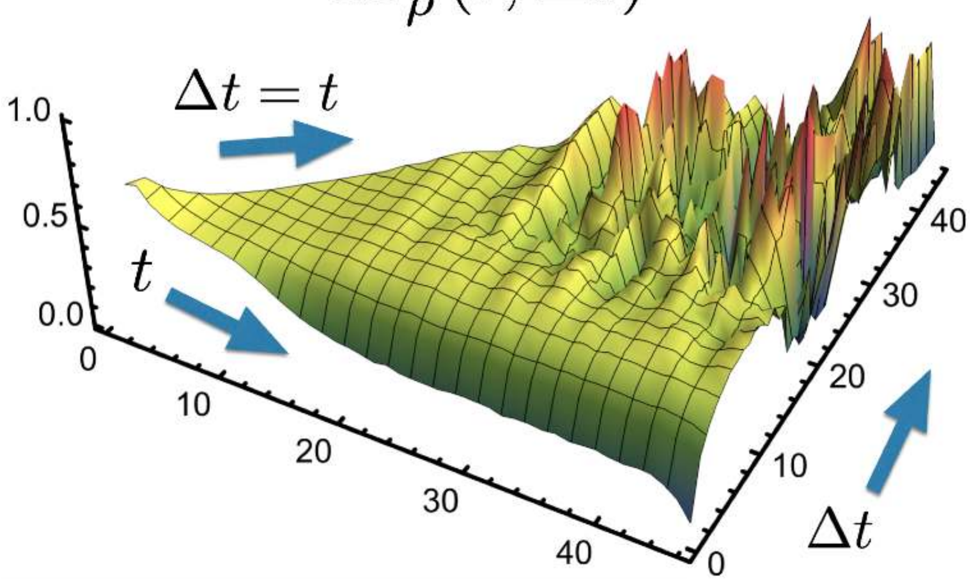
Phase Reweighted Effective Mass

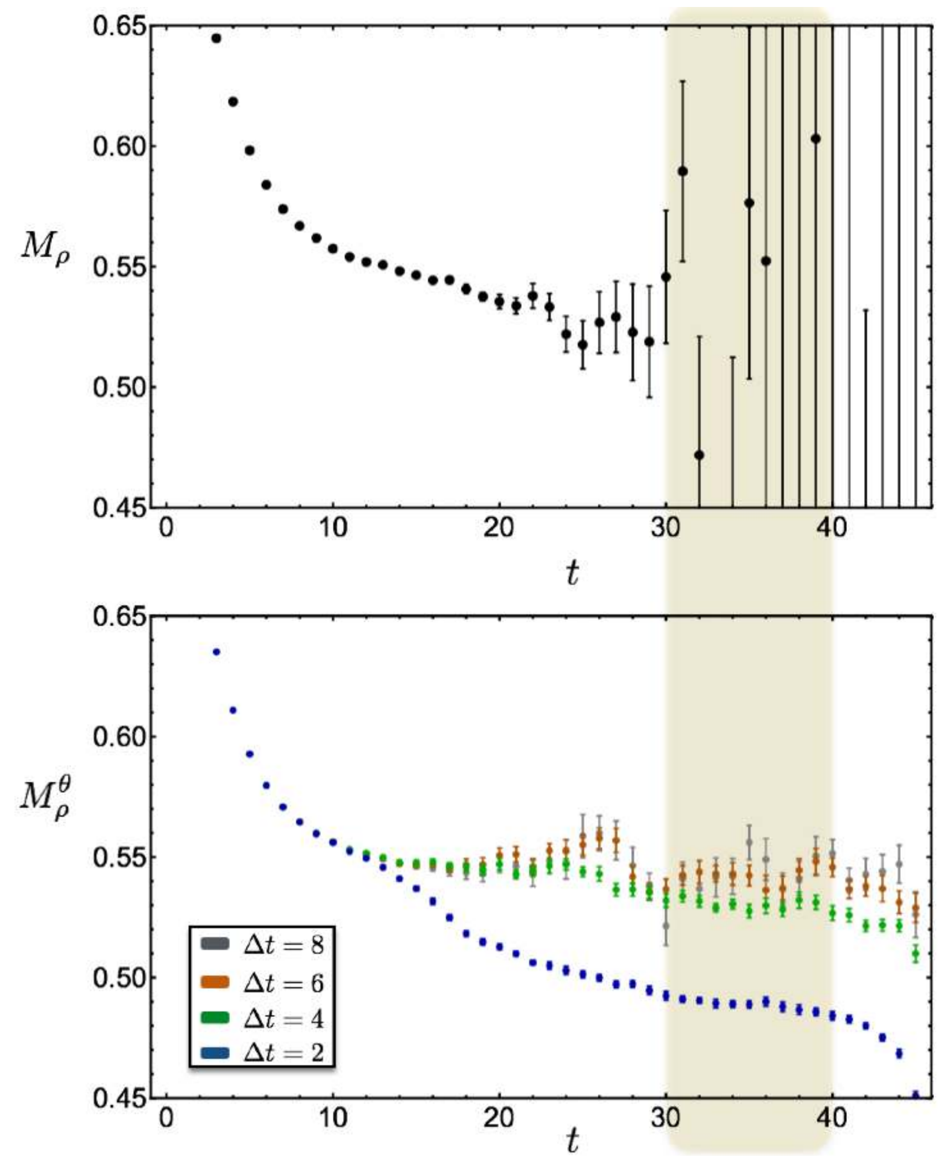
$$G^{\theta}(t, \Delta t) = \left\langle C_i(t) e^{-i\theta_i(t-\Delta t)} \right\rangle$$

$$m^{\theta}(t) = \ln\left(\frac{G^{\theta}(t, \Delta t)}{G^{\theta}(t+1, \Delta t+1)} \right)$$

Calculable by re-analyzing existing correlation functions

$$M_{\rho}^{\theta}(t, \Delta t)$$





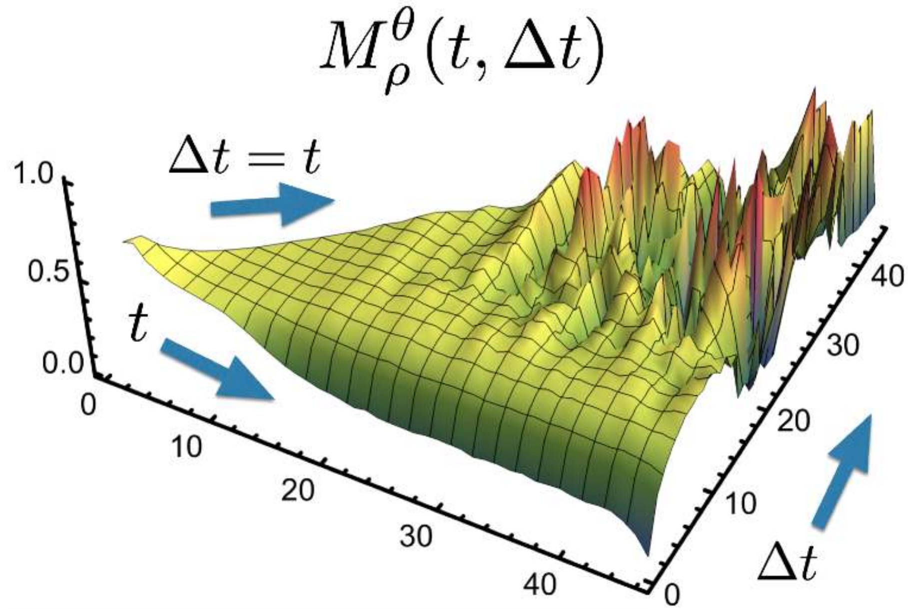
MW and Savage, arXiv:1704.07356

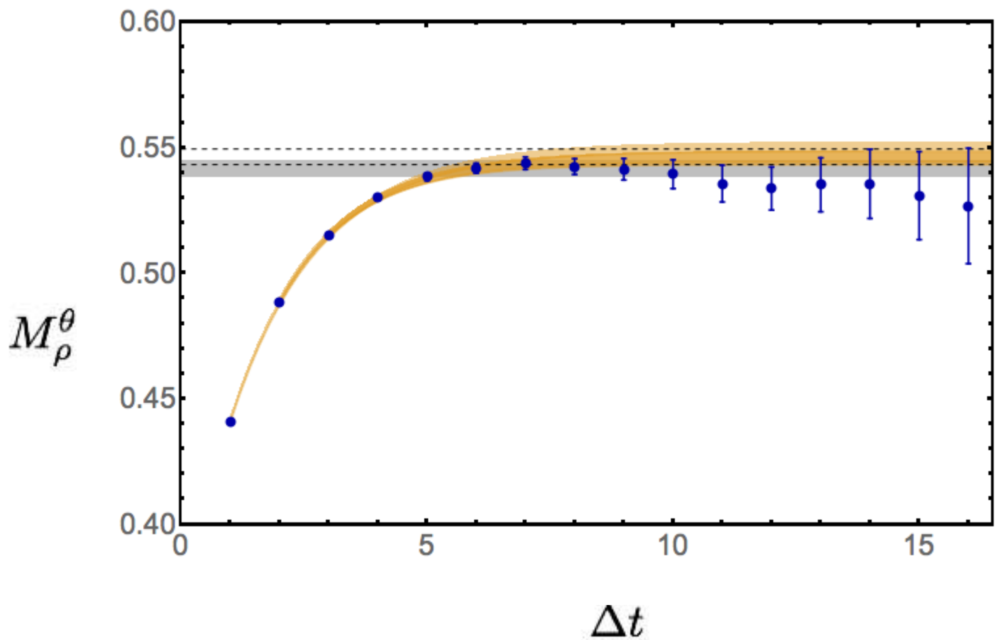
Data from Orginos et al, Phys.Rev. D92 (2015)

Phase Reweighting Extrapolation

Known results for simple systems correctly recovered after extrapolation $\Delta t \to t$

$$M_\rho^\theta(t,\Delta t) \;=\; M_\rho \;+\; c\,\delta M_\rho e^{-\delta M_\rho \Delta t} \;+\; \ldots$$





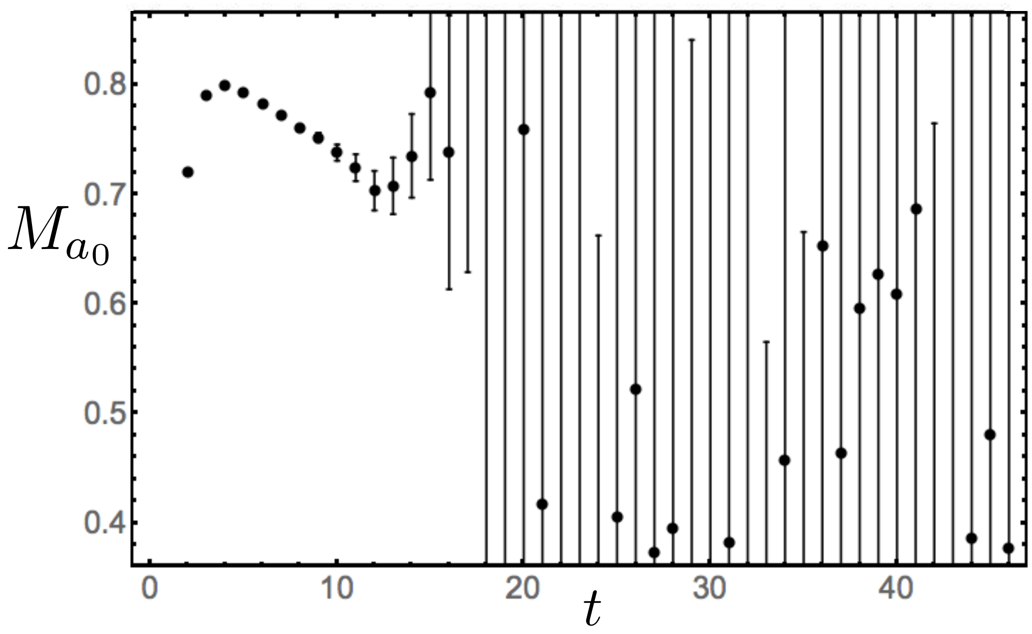
Phase-reweighted effective mass exactly reproduces standard EM if correlation functions at t and Δt are decorrelated. Exploits same physics of approximate factorization as

Cè, Giusti, and Schaefer, Phys.Rev. D93 (2016)

Signals from Noise

State-of-the-art spectroscopy relies on optimized sources that plateau at early times

Alternatively, ground-state spectrum accessible to simple $\overline{q}\Gamma q$ sources by extrapolating phase reweighted results from very late times



Future calculations will combine complimentary approaches of phase reweighting and source optimization using e.g. variational methods

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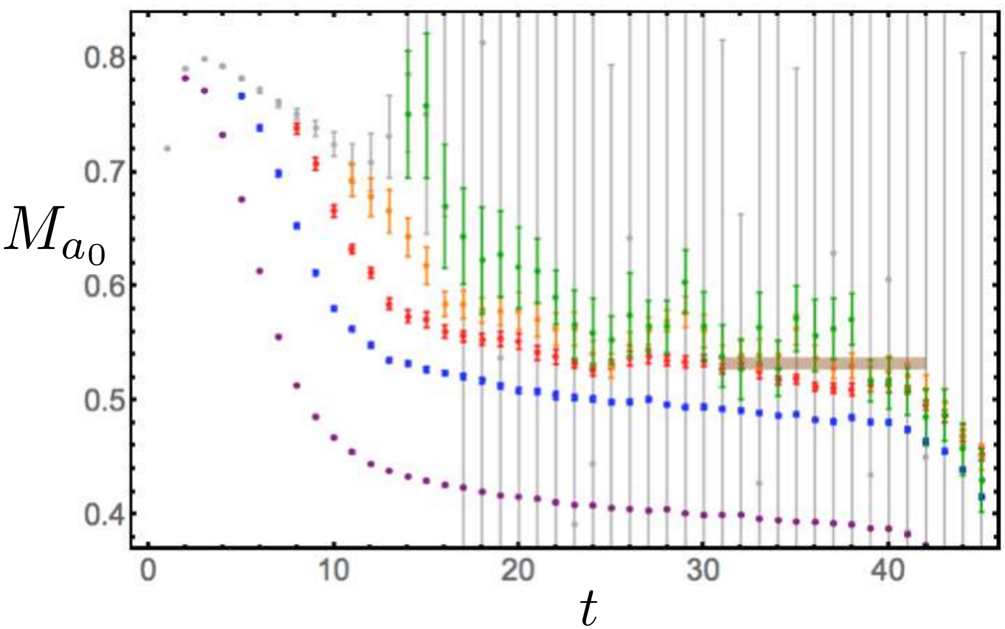
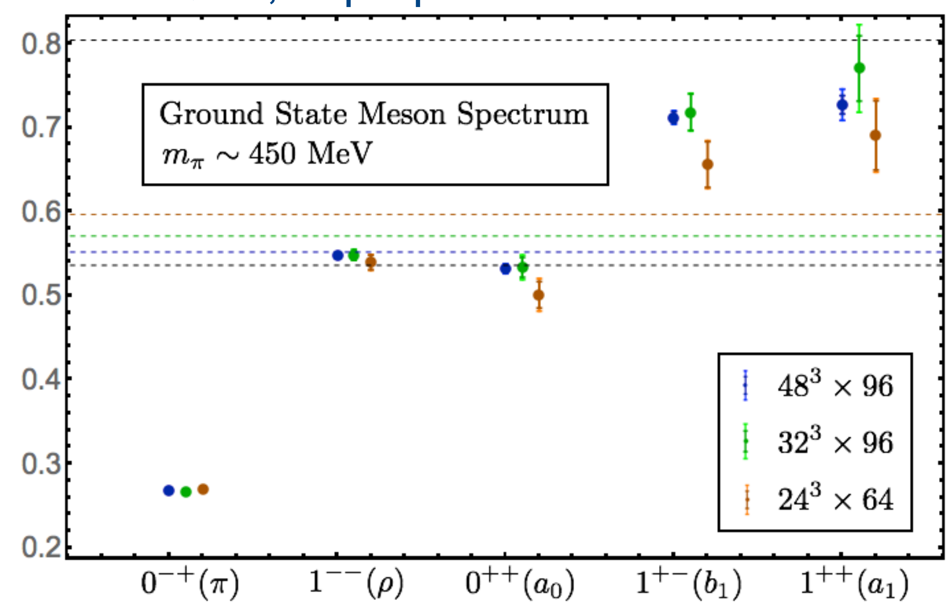


NPLQCD, in preparation



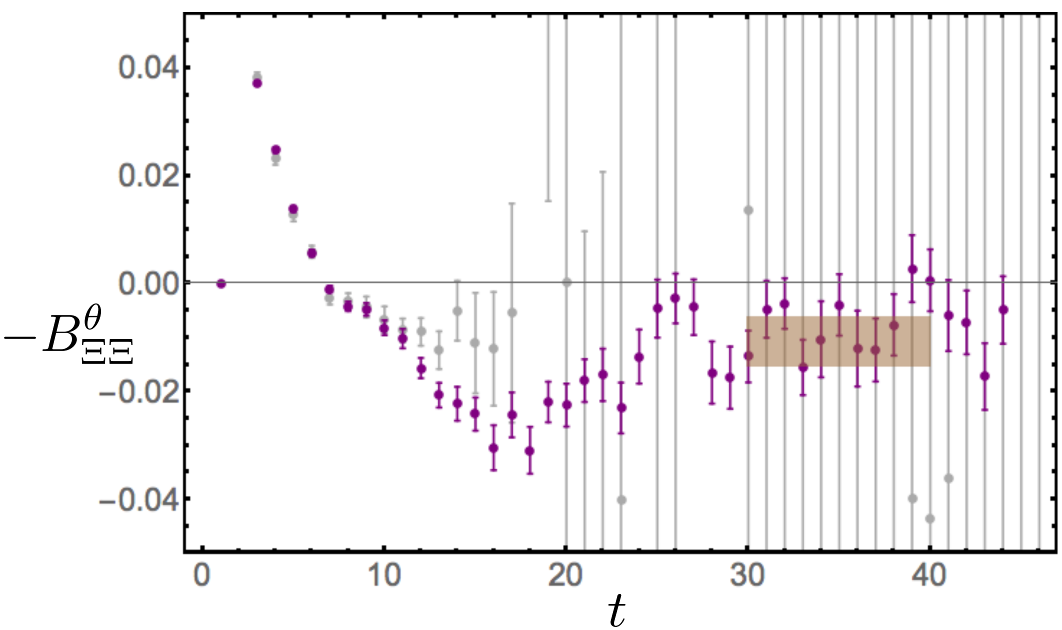
Future calculations will combine complimentary approaches of phase reweighting and source optimization using e.g. variational methods

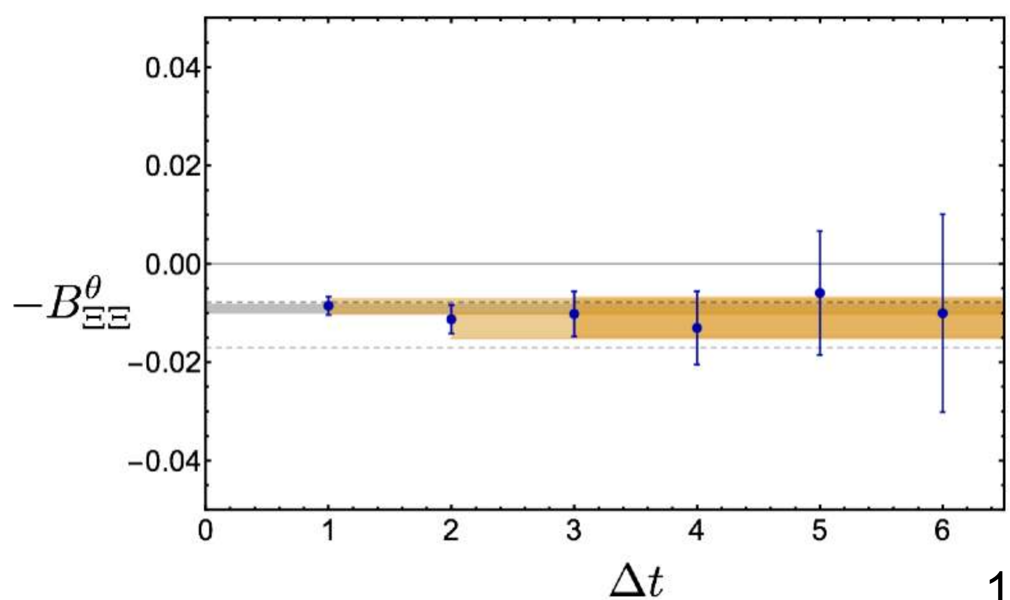
Towards Nuclear Physics

Bias at $\Delta t < t$ means phase reweighting is **not** a "general solution to the sign problem" that would prove P=NP, violate Cramer-Rao bounds in circular statistics, and provide free lunches

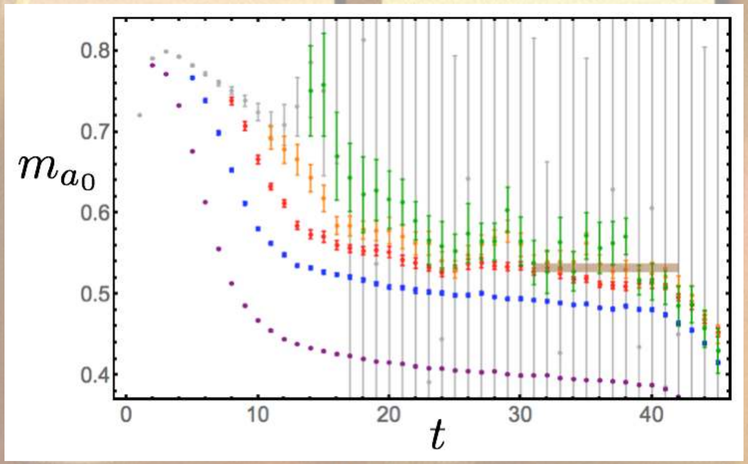
Preliminary results suggest bias can be removed from phase reweighted nuclear binding energies with accessible statistics

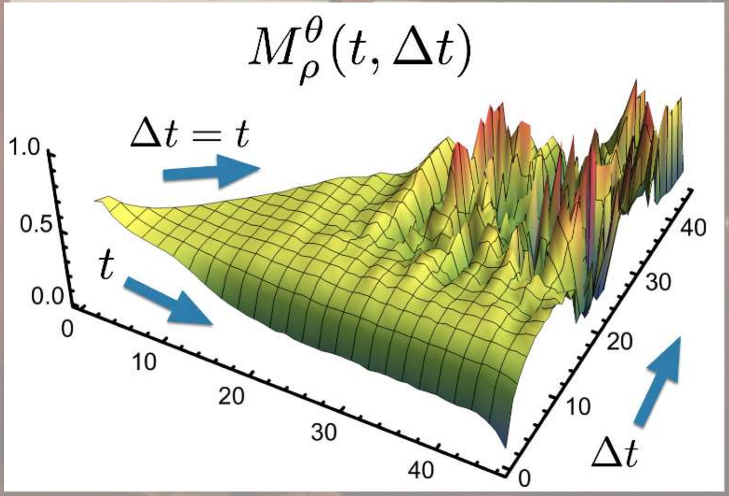
Precision of phase reweighting increases indefinitely compared to standard measurements as the time extent of the lattice is increased





Summary





The LQCD StN problem is a sign problem

Generic correlation functions have approximately complex log-normal distributions that time evolve with heavy-tailed random walks

Phase reweighting provides constant StN at the cost of a bias that can be removed by extrapolation