Phase Fluctuations and Sign Problems

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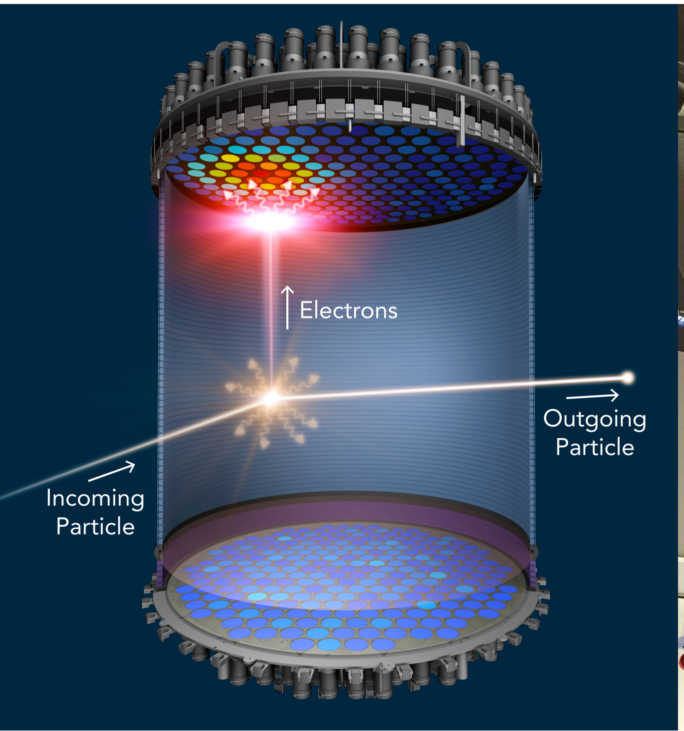
Lattice QCD and Nuclei

Nuclear theory predictions are needed to extract or constrain new physics from intensity frontier experiments

Lattice QCD can inform and test EFT power counting and models of heavy nuclei by calculating properties of simple nuclei

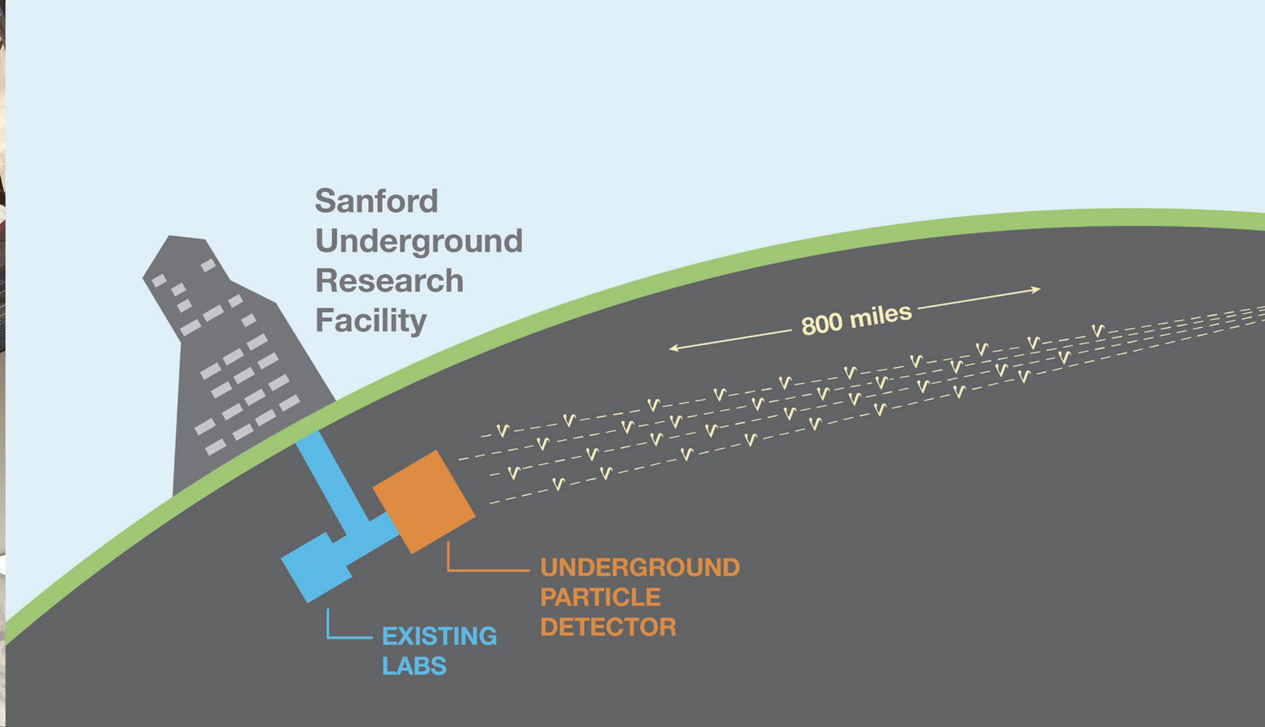
Increasing the range of nuclei directly accessible to LQCD will increase the reliability of low-energy nuclear theory predictions

LUX



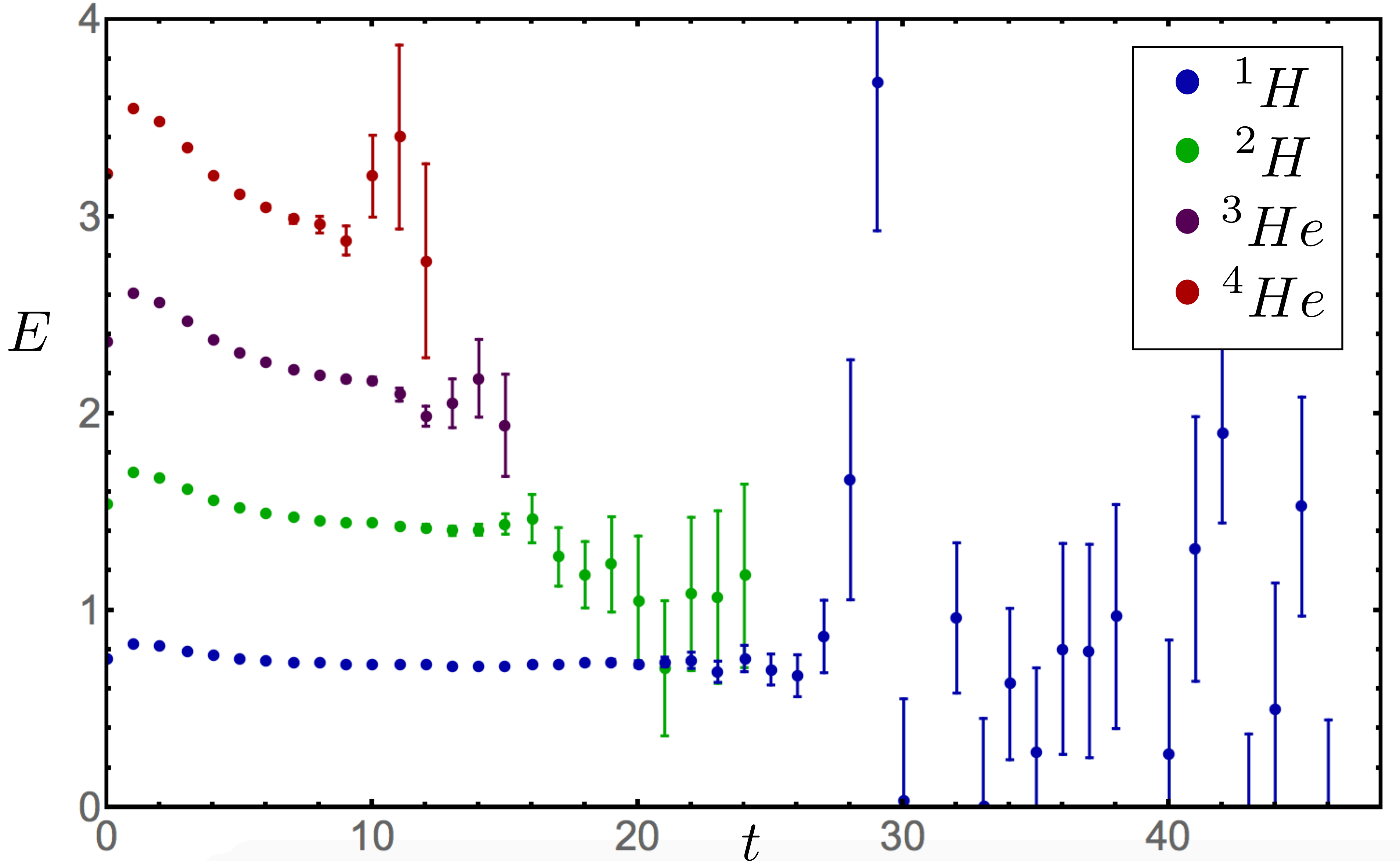
CUORE

DUNE



The Signal-to-Noise Problem

LQCD nuclear correlation functions have StN ratios that decrease exponentially with increasing baryon number

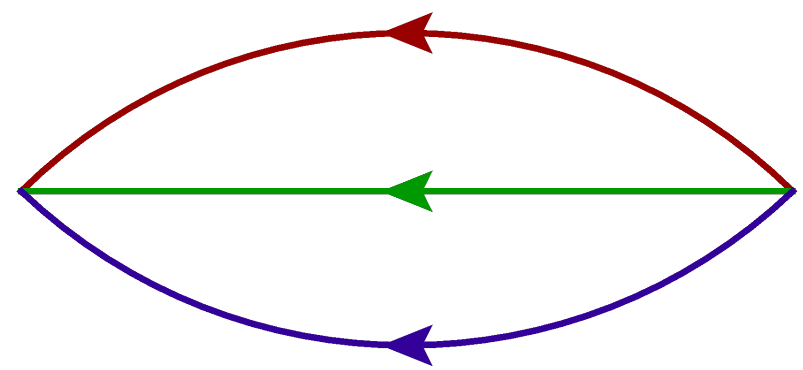


Parisi, Phys Rept 103 (1984), Lepage, TASI (1989), NPLQCD, PRD 79 (2009), Detmold and Endres, PRD 90 (2014), …

The Sign(al-to-Noise) Problem

Average correlators are real. Individual correlators in generic gauge fields are complex

$$G_N(\mathbf{p},t) = \left\langle C_N(\mathbf{p},t) \right\rangle = \left\langle e^{R_N(\mathbf{p},t)+i\theta_N(\mathbf{p},t)} \right\rangle$$



Complex phase fluctuations give path integrals representing correlators sign problems

$$G_N(\mathbf{p},t) = \int \mathscr{D}U \; e^{-S(U)+R_N(\mathbf{p},t;U)+i\theta_N(\mathbf{p},t;U)} = \frac{1}{N}\sum_{i=1}^{N} e^{R_N(\mathbf{p},t;U_i)+i\theta_N(\mathbf{p},t;U_i)}$$

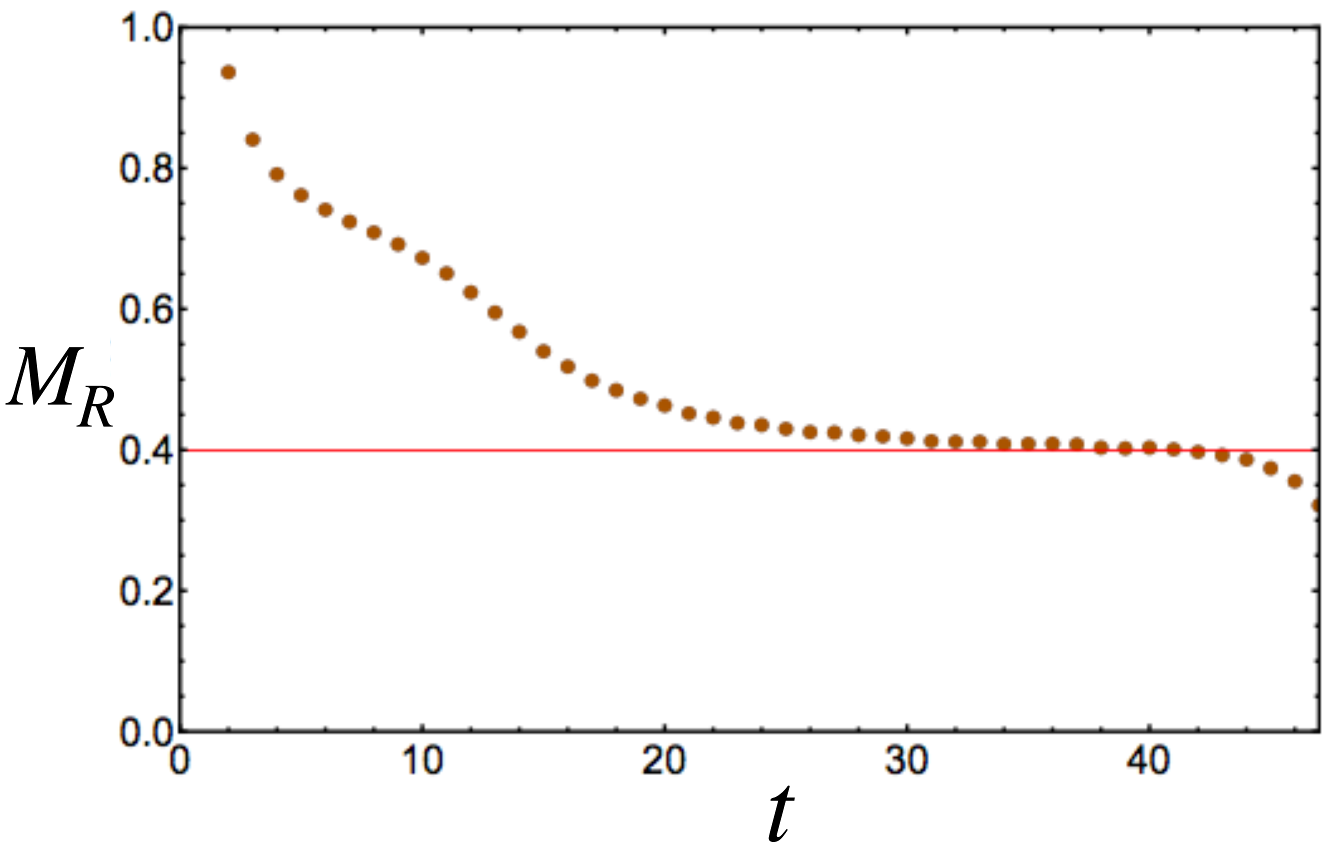
An exponentially decaying average phase always has exponential StN degradation

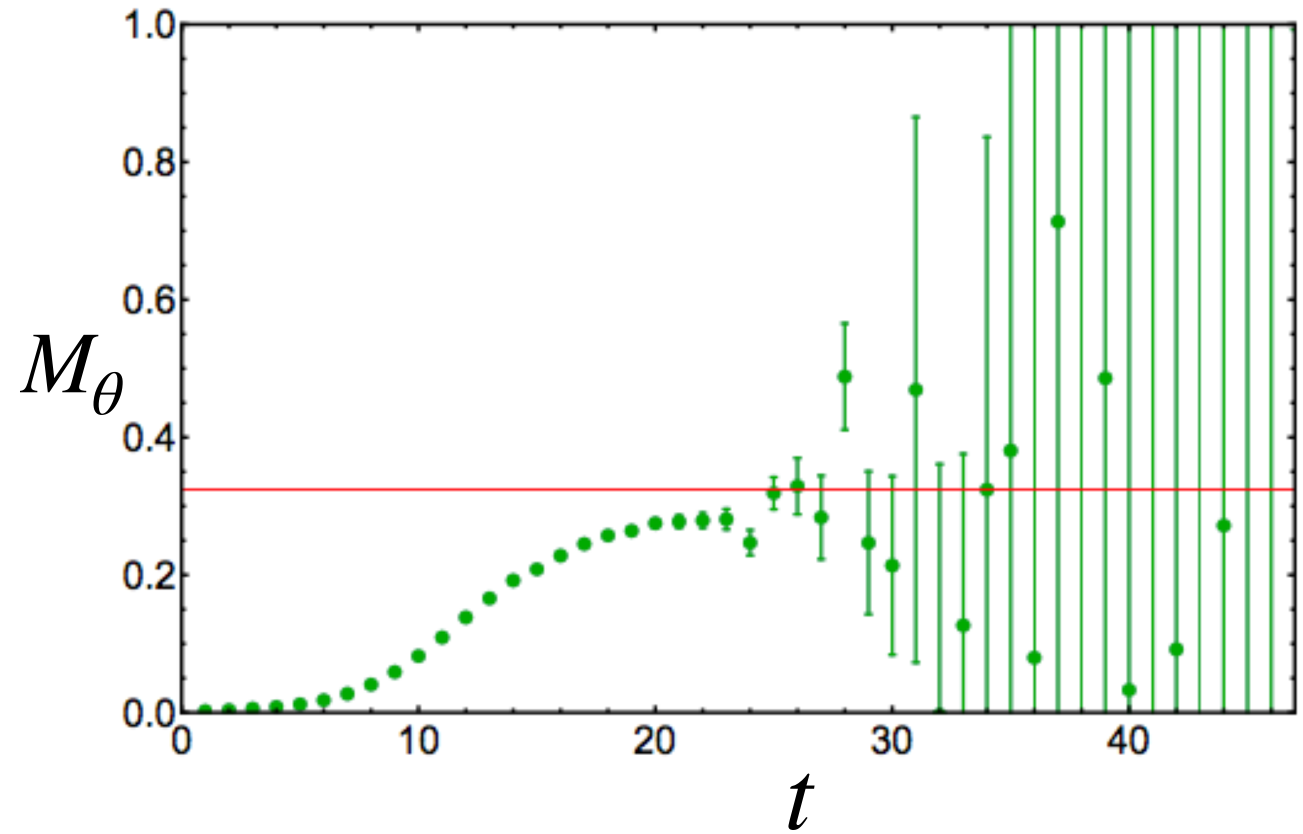
$$StN(Re[e^{i\theta(t)}]) = \frac{\left\langle e^{i\theta} \right\rangle}{\sqrt{\frac{1}{2}+\frac{1}{2}\left\langle e^{2i\theta} \right\rangle - \left\langle e^{i\theta} \right\rangle^2}} \sim \left\langle e^{i\theta} \right\rangle \sim e^{-M_\theta\, t}$$

Correlation Function Phases

Empirically, correlator magnitudes decay at a rate set by the pion mass, phase factors contribute remaining effective mass

$$M_R = -\partial_t \ln \left\langle e^{R(\mathbf{0},t)} \right\rangle \sim \frac{3}{2} m_\pi \qquad M_\theta = -\partial_t \ln \left\langle e^{i\theta(\mathbf{0},t)} \right\rangle \sim M_N - \frac{3}{2} m_\pi$$





MW and Savage, PRD 96 (2016)

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 B225 (1983)

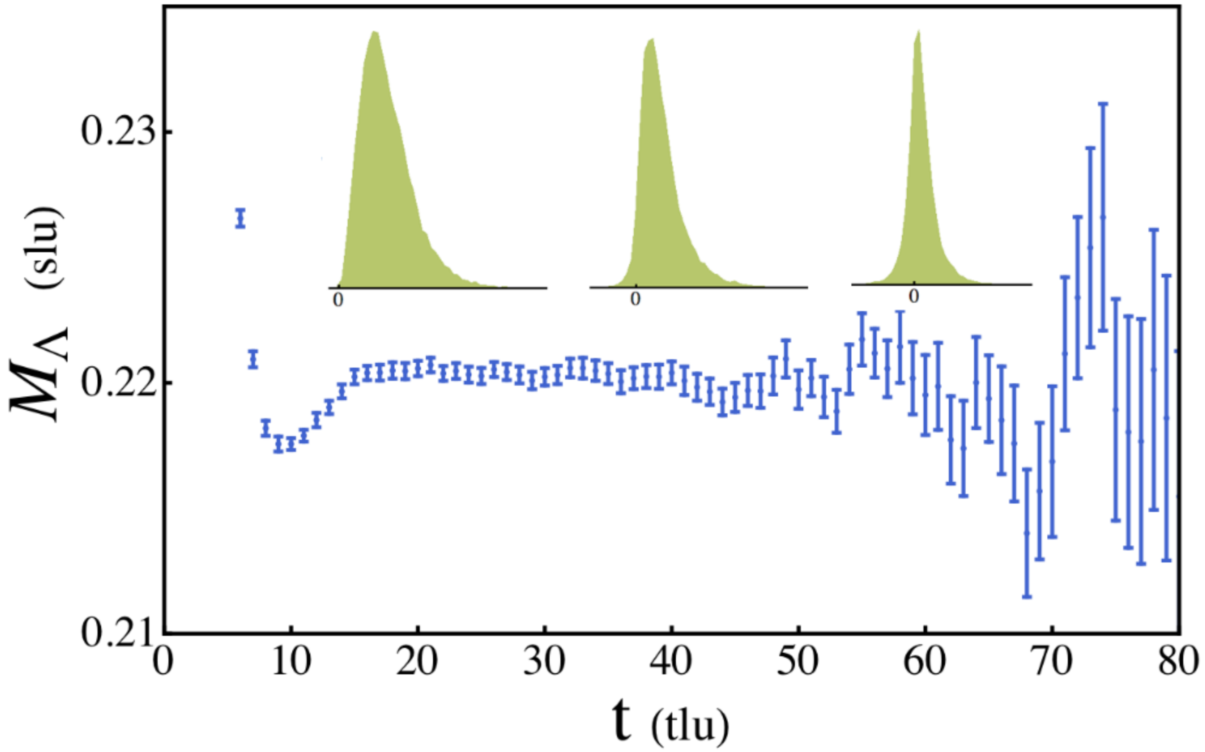
Guagnelli, Marinari, and Parisi, PLB 240 (1990)

Endres, Kaplan, Lee and Nicholson, PRL 107 (2011)

Grabowska, Kaplan, and Nicholson, PRD 87 (2012)

DeGrand, PRD 86 (2012)

Porter and Drut, PRE 93 (2016)



Beane, Detmold, Orginos, Savage, J Phys G42 (2015)

Log-normal distributions arise in two-body potential models and products of generic random positive numbers

Kaplan showed large-time nucleon correlators are better described by heavy-tailed stable distributions

Broad, symmetric large-time distributions consistent with moment analysis by Savage

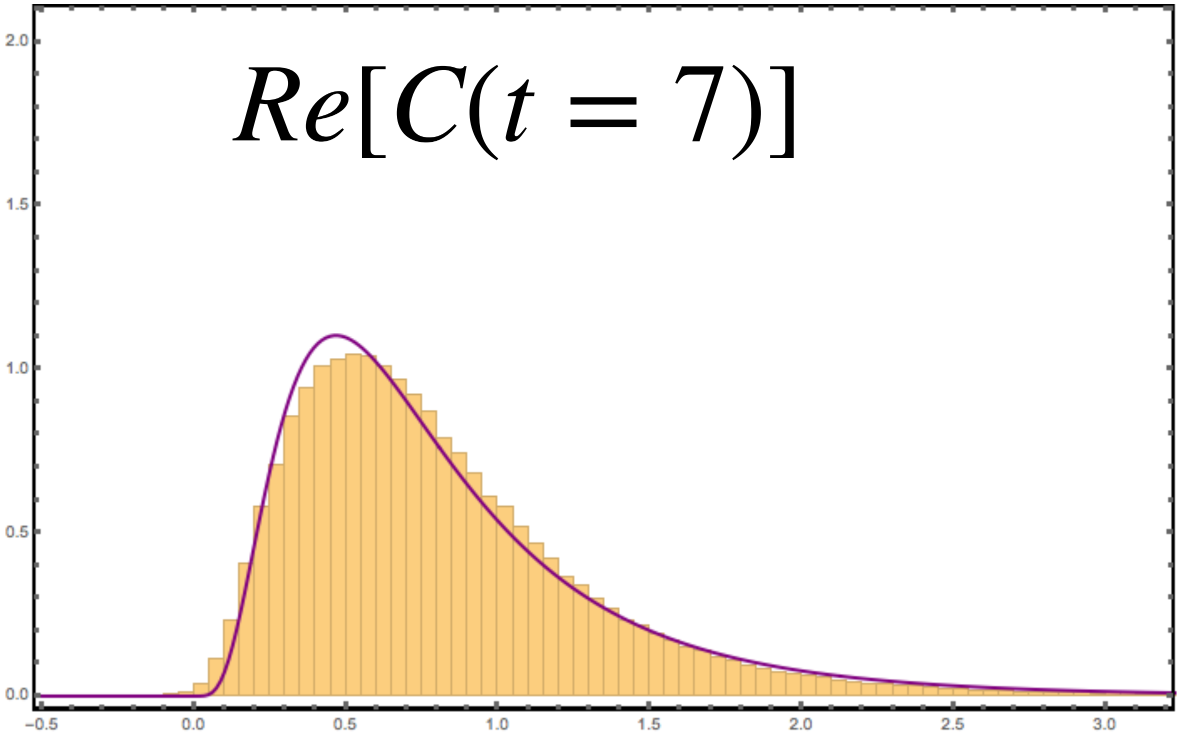
Complex Log-Normal Distributions

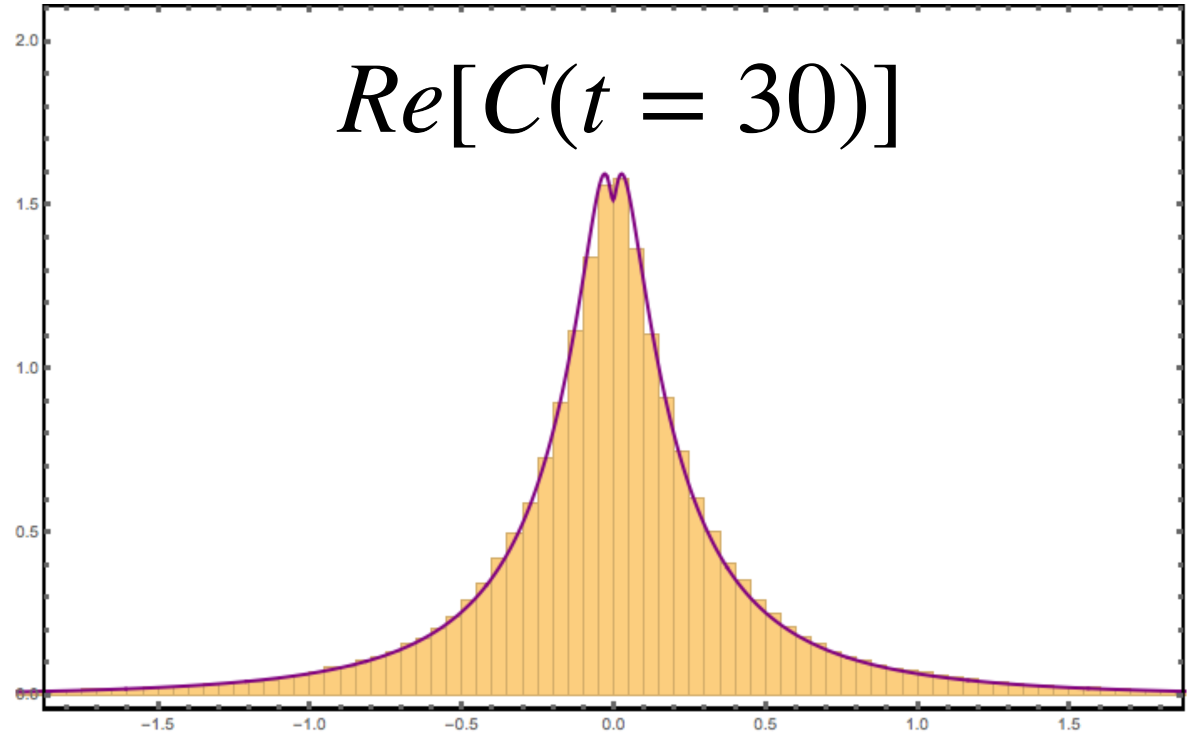
Products of phase factors have different central limit theorems, approach "wrapped normal" and eventually uniform distributions

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"

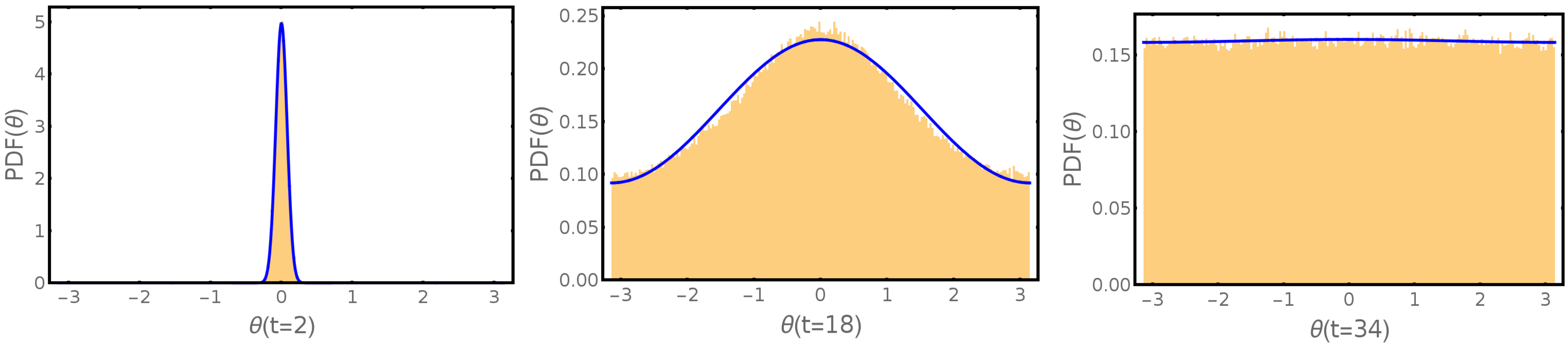
$$PDF(R,\theta) = e^{-(R-\mu_R)^2/(2\sigma_R^2)} \sum_{n=-\infty}^{\infty} e^{-n^2\theta^2/(2\sigma_\theta^2)}$$





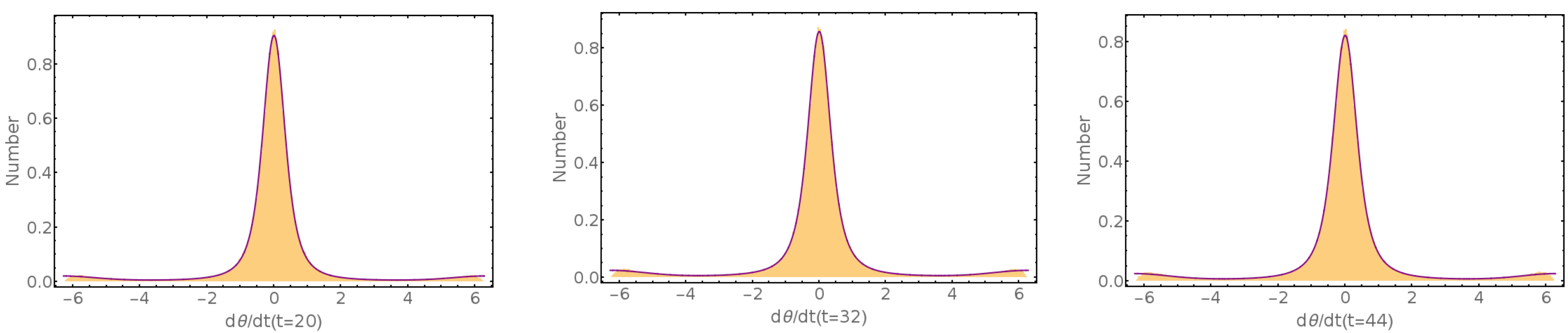
MW and Savage, PRD 96 (2016)   MW, LATTICE 2017

Heavy-Tailed Phase Velocity



Nucleon phase empirically well-described by wrapped-normal distribution

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

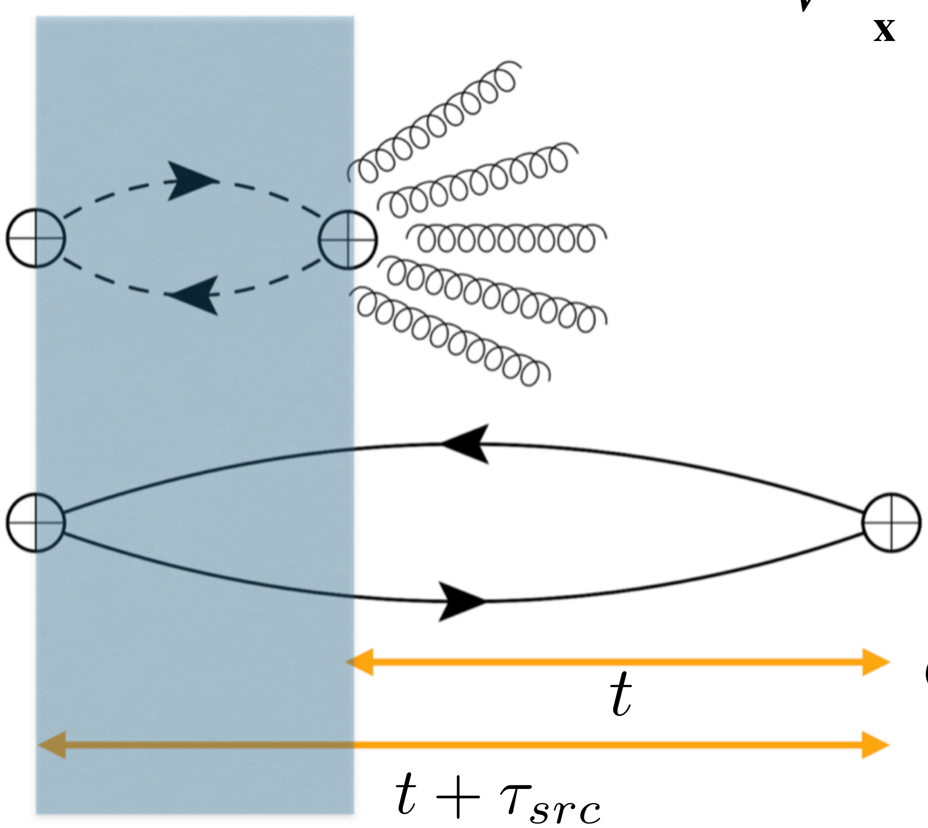


Dynamical Source Construction

Generalized pencil-of-functions (GPoF): an interpolating operator that has been time evolved is still a good interpolating operator

$$G_N(\mathbf{p},t,\tau_{src}) = \frac{1}{V}\sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}}\Gamma_{\alpha\beta}\left\langle N_\alpha(\mathbf{x},t)e^{H\tau_{src}}\overline{N}_\beta(0)e^{-H\tau_{src}}\right\rangle = G_N(\mathbf{p},t+\tau_{src})$$

Aubin and Orginos (2010)



Generalized GPoF (GGPoF): an interpolating operator time evolved with a modified Hamiltonian is still a good interpolating operator

$$G_N^{(\theta_N)}(\mathbf{p},t,\tau_{src}) = \frac{1}{V}\sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}}\Gamma_{\alpha\beta}\left\langle e^{i\theta_N(\mathbf{p},0)-i\theta_N(\mathbf{p},-\tau_{src})}N_\alpha(\mathbf{x},t)\overline{N}_\beta(\mathbf{0},-\tau_{src})\right\rangle$$

Phase fluctuations during source construction can be removed by adding phase reweighting to the time evolution operator used

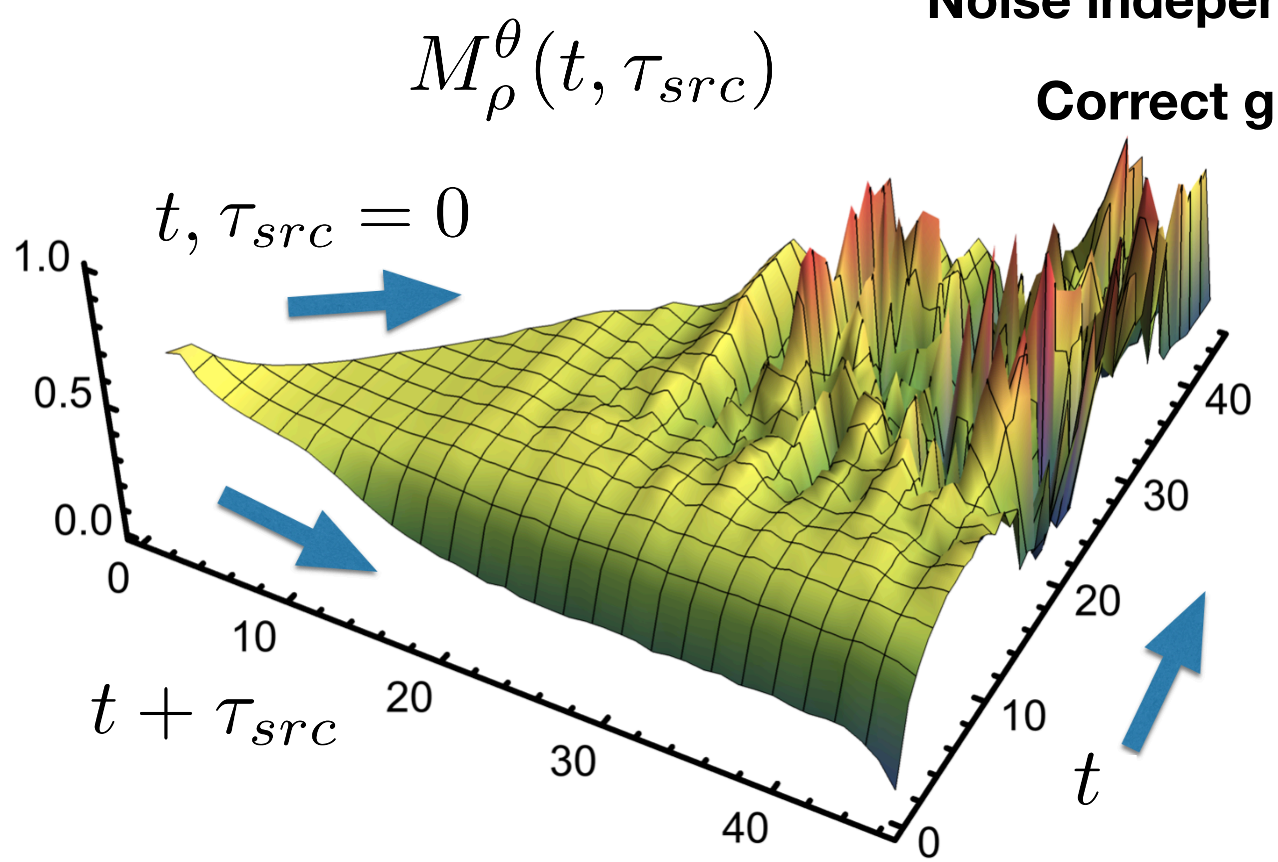
$$StN\left[G_N(\mathbf{p},t,\tau_{src})\right] \sim e^{-(E(\mathbf{p})-\frac{3}{2}m_\pi)(t+\tau_{src})} \qquad StN\left[G_N^{(\theta_N)}(\mathbf{p},t,\tau_{src})\right] \sim e^{-(E(\mathbf{p})-\frac{3}{2}m_\pi)t}$$

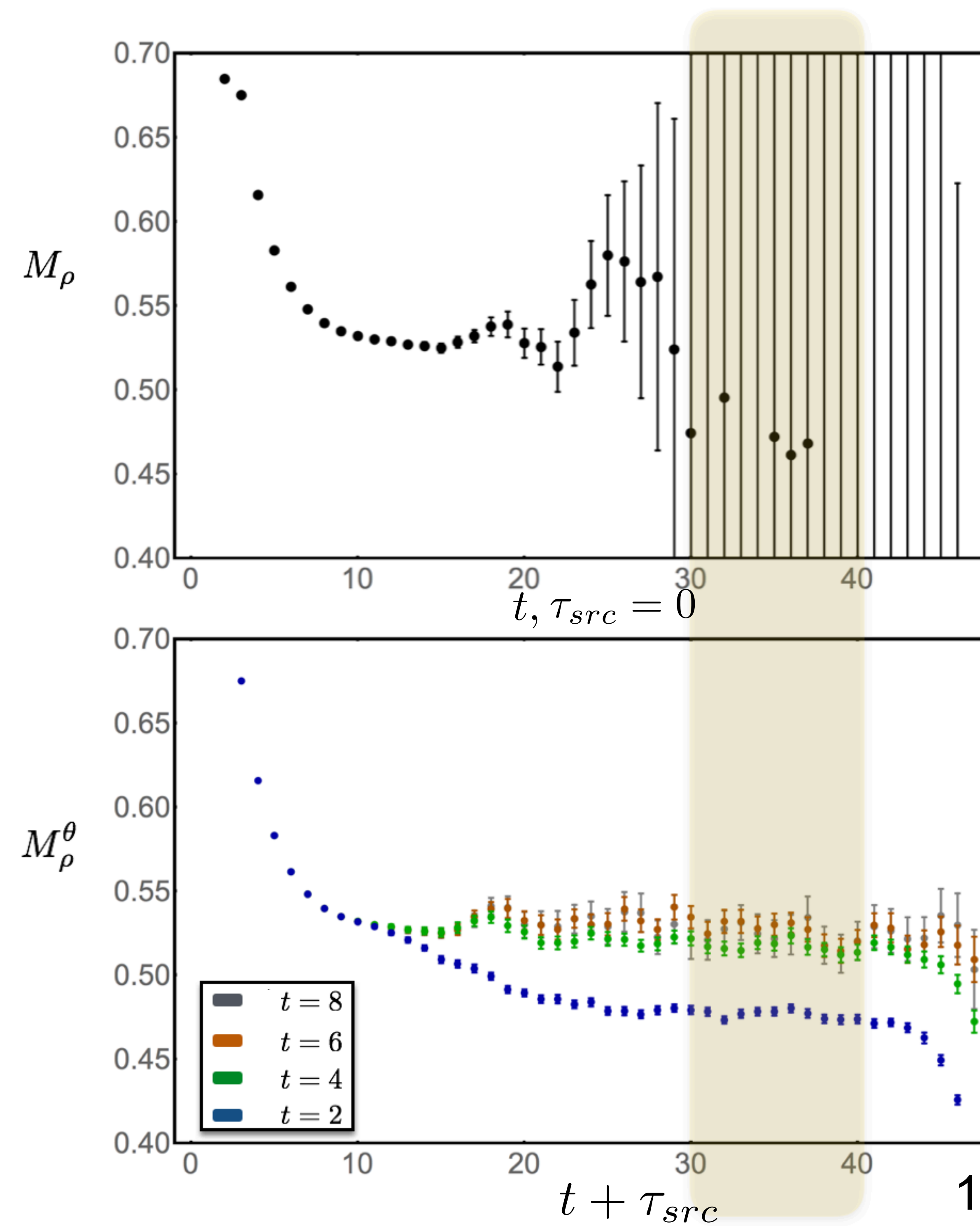
MW and Savage (2017)

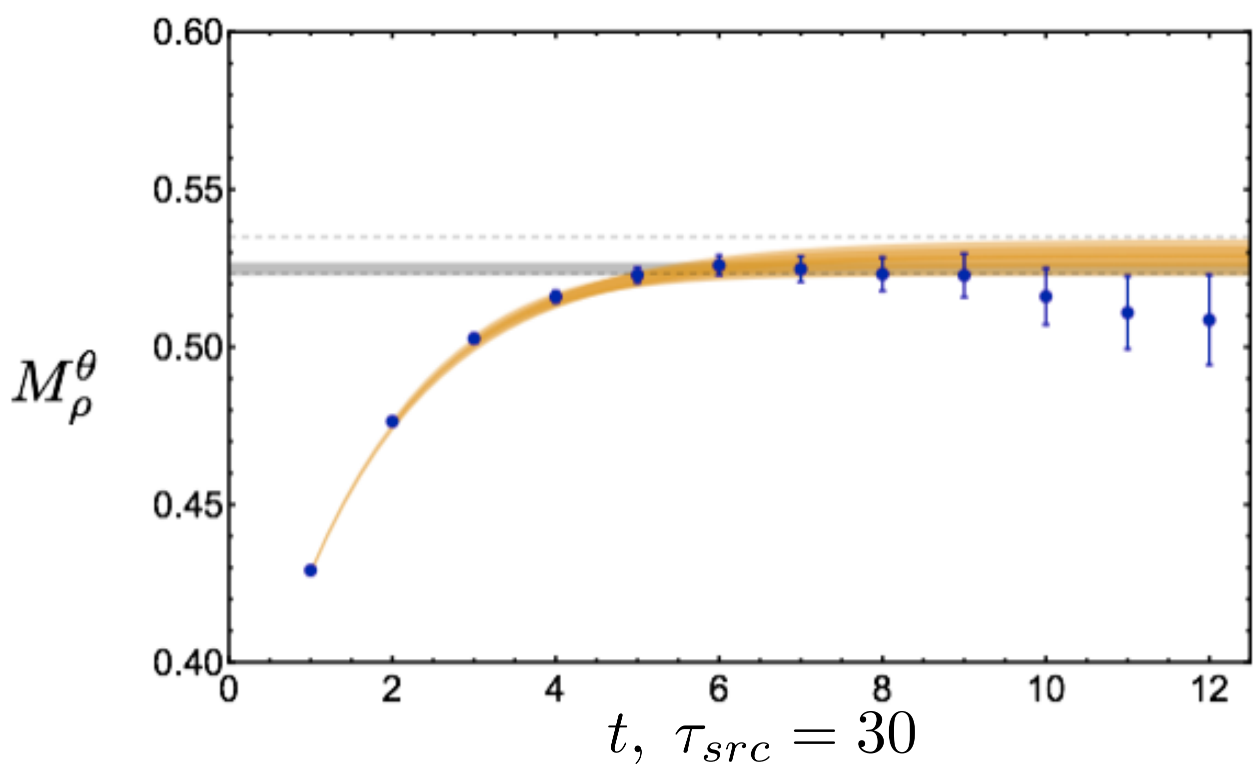
Phase Reweighted GGPoF

Noise independent of τ_{src} after variance excited-state region

Correct ground-state energies empirically reproduced* **







Phase Reweighted GGPoF

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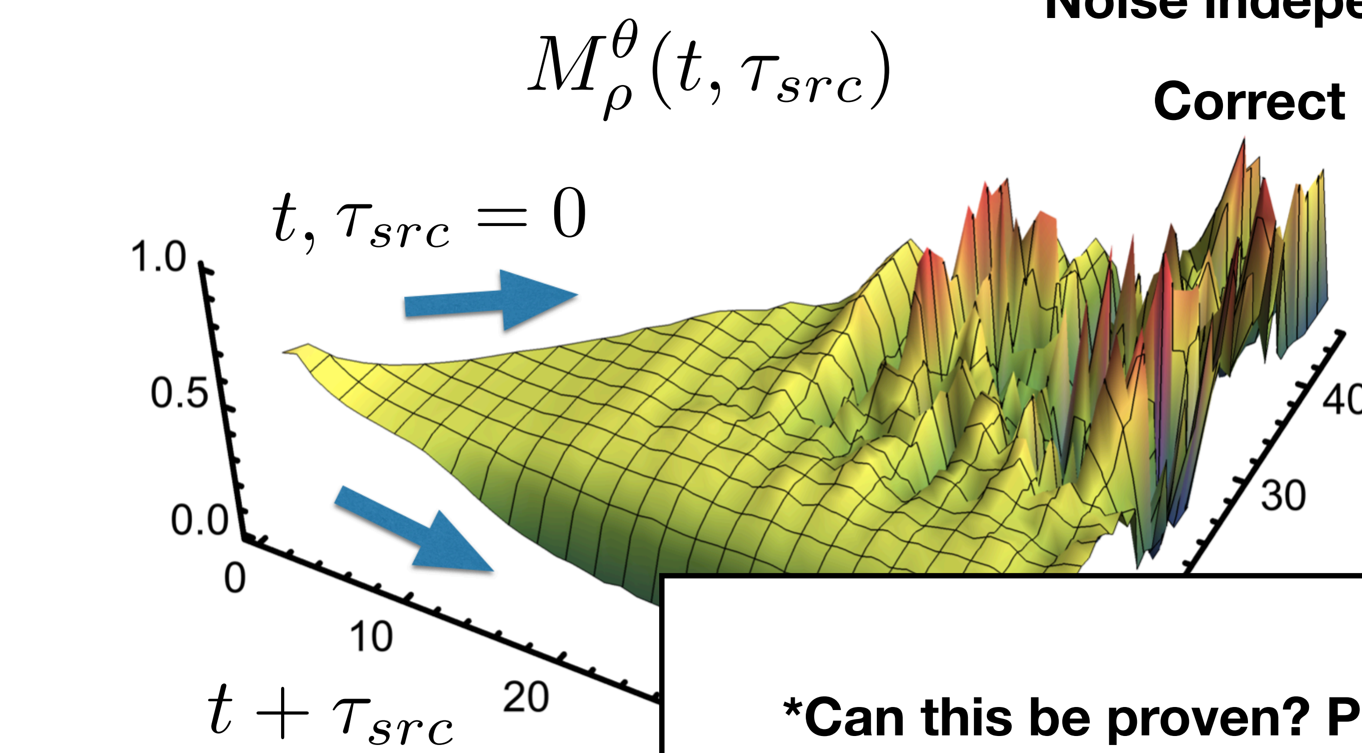
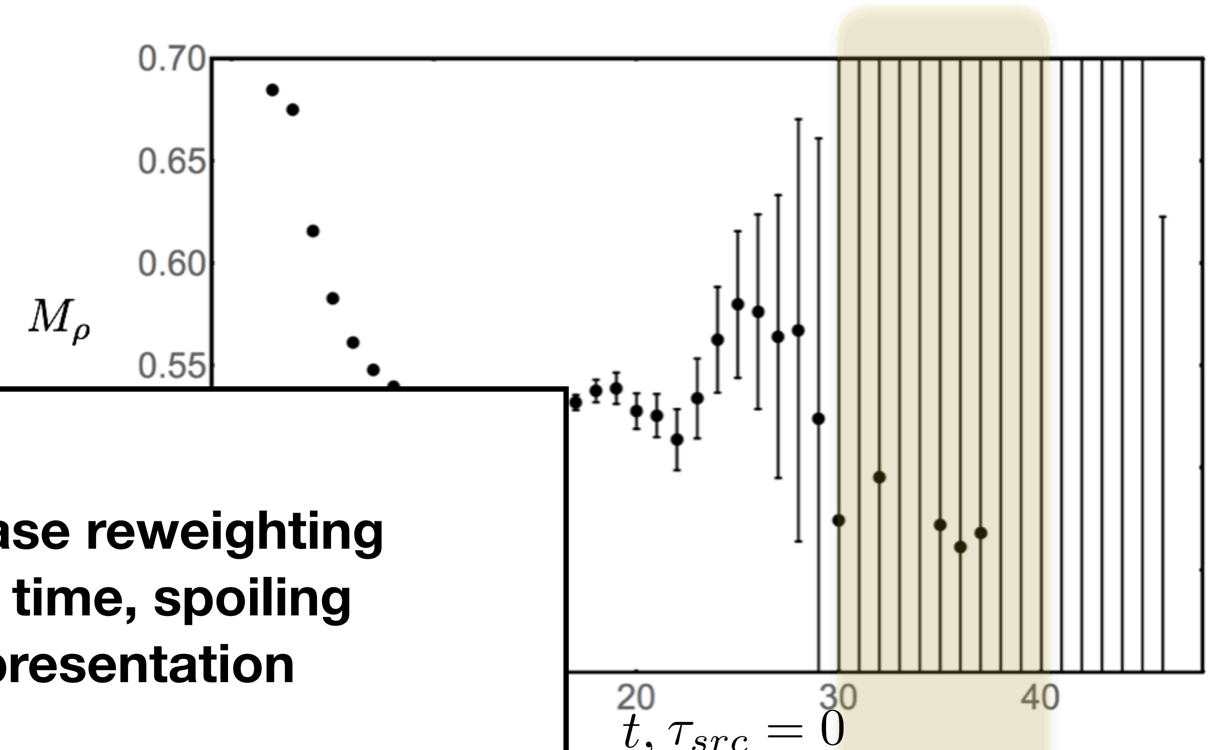
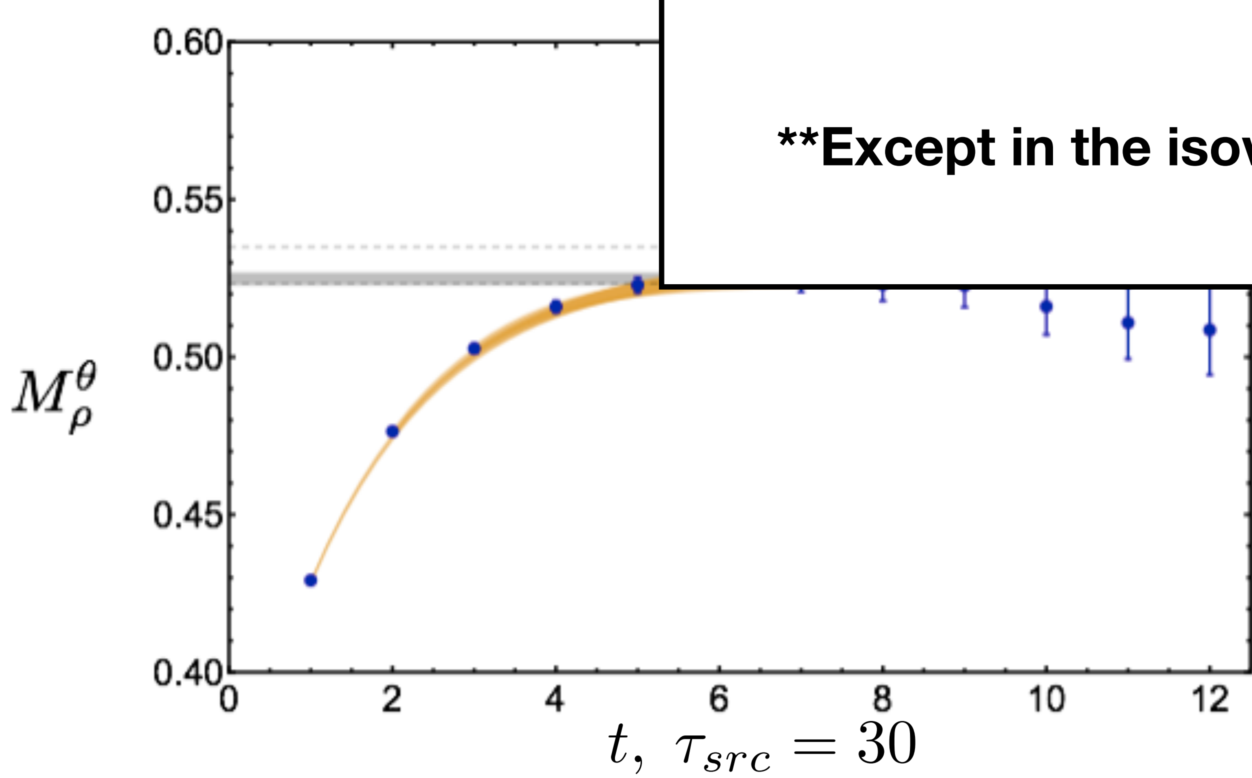
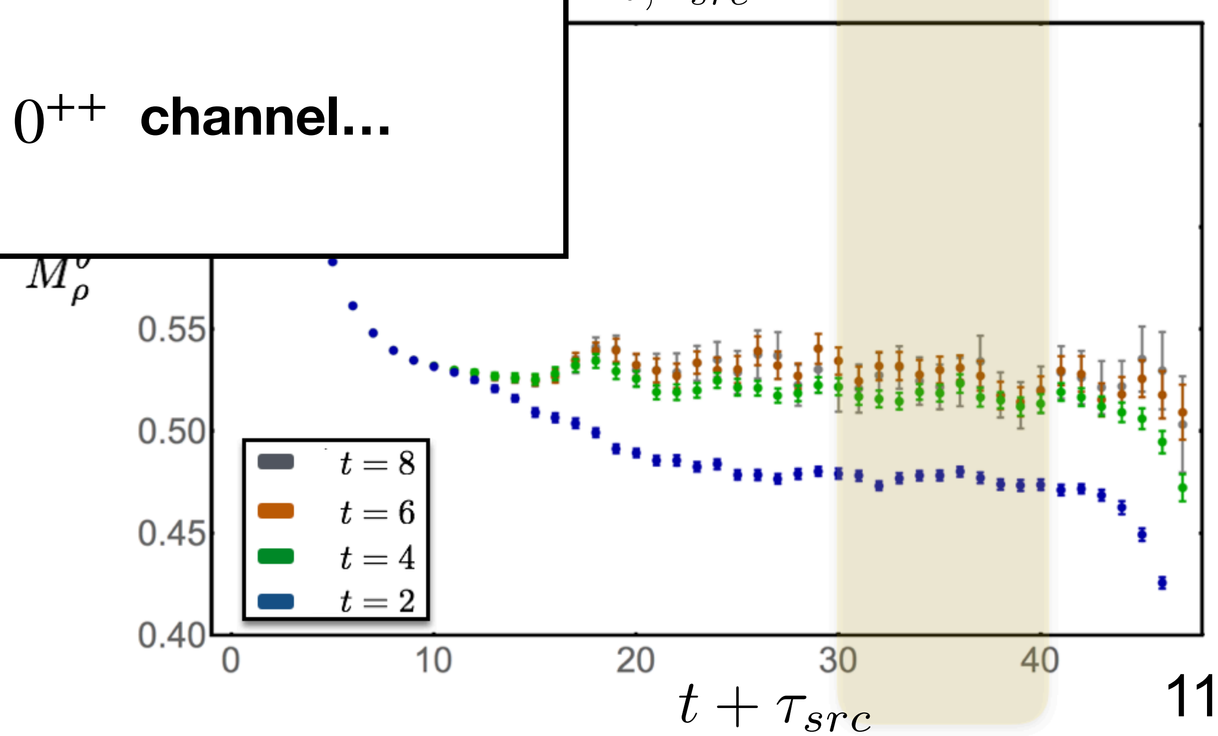




***Can this be proven? Phase reweighting factors are non-local in time, spoiling standard spectral representation**

****Except in the isovector 0^{++} channel…**





Auxiliary Charged Static Fermions

Auxiliary fields representing static quarks and an Abelian gauge field in the zero-coupling limit can be freely added to path integrals

$$1 = \lim_{e\to 0} \int \mathscr{D}V \mathscr{D}\overline{H} \mathscr{D}H \; e^{-\sum_x \overline{H}(x)\left[e^{iV_4(x)} H(x+\hat{4}) - H(x)\right] + \frac{1}{4e^2} V_{\mu\nu}(x) V_{\mu\nu}(x)} \delta\left(\partial_\mu V_\mu - \partial^2 f(x)\right)$$

$$= \int \mathscr{D}\overline{H} \mathscr{D}H \; e^{-\sum_x \overline{H}(x)\left[e^{if(x+\hat{\mu}) - if(x)} H(x+\hat{4}) - H(x)\right]}$$

Static fermion two-point function given by auxiliary field Wilson line, depends on auxiliary function gauge-fixing function

$$G_H(t,f) = \left\langle H_s(\mathbf{x},t) \overline{H}_{s'}(0) \right\rangle = \delta_{\mathbf{x},\mathbf{y}} \delta_{s,s'} e^{if(\mathbf{0},t) - if(\mathbf{0},0)}$$

The spectrum of auxiliary-charge zero states is independent of the auxiliary field gauge-fixing function

GGPoF with Auxiliary Fields

Spectral representation for correlators with hadrons and auxiliary fermions depends on gauge-fixing function (only) between auxiliary source/sink

$$G_N^{(f)}(\mathbf{p}, t, \tau_{src}) = \frac{1}{V} \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \Gamma_{\alpha\beta} \left\langle N_\alpha(\mathbf{x}, t) H_1(0) \overline{H}_1(\mathbf{0}, -\tau_{src}) \overline{N}_\beta(\mathbf{0}, -\tau_{src}) \right\rangle^{(f)}$$

$$= \Gamma_{\alpha\beta} \sum_{\mathfrak{n},\mathfrak{k}} \langle 0 | N_\alpha | \mathfrak{n}(\mathbf{p}) \rangle \, e^{-E_{\mathfrak{n}}(\mathbf{p})t} \langle \mathfrak{n}(\mathbf{p}) | H_1 | \mathfrak{k}^{(f)} \rangle \, e^{-E_{\mathfrak{k}}^{(f)}\tau_{src}} \left\langle \mathfrak{k}^{(f)} | \overline{H}_1 \overline{N}_\beta | 0 \right\rangle$$

$$= \sum_{\mathfrak{n}} Z_{\mathfrak{n}}(\mathbf{p}) Z_{\mathfrak{n}}^{(f)}(\mathbf{p}, \tau_{src}) e^{-E_{\mathfrak{n}}(\mathbf{p})t}$$

GGPoF nucleon two-point function reproduced by choosing a gluon-field dependent auxiliary gauge-fixing function

$$f(t) = \theta_N(t, U) = \arg C_N(t, U)$$

$$G_N^{(\theta_N)}(\mathbf{p}, t, \tau_{src}) = \frac{1}{V} \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \Gamma_{\alpha\beta} \left\langle e^{i\theta_N(\mathbf{p},0) - i\theta_N(\mathbf{p},-\tau_{src})} N_\alpha(\mathbf{x}, t) \overline{N}_\beta(\mathbf{0}, -\tau_{src}) \right\rangle = \sum_{\mathfrak{n}} Z_{\mathfrak{n}}(\mathbf{p}) Z_{\mathfrak{n}}^{(\theta_N)}(\mathbf{p}, \tau_{src}) e^{-E_{\mathfrak{n}}(\mathbf{p})t}$$

Meson GGPoF Results

Identical construction for generic hadrons, e.g. isovector mesons

$$G_{\Gamma}^{(\theta_\Gamma)}(\mathbf{p}, t, \tau_{src}) = \frac{1}{V}\sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \left\langle e^{i\theta_\Gamma(0) - i\theta_\Gamma(\tau_{src})}[\bar{d}\Gamma u](\mathbf{x}, t)[\bar{u}\Gamma d](\mathbf{0}, -\tau_{src})\right\rangle = \sum_{\mathfrak{n}} Z_{\mathfrak{n}}^{\Gamma}(\mathbf{p}) Z_{\mathfrak{n}}^{\Gamma,(\theta_N)}(\mathbf{p}, \tau_{src}) e^{-E_{\mathfrak{n}}(\mathbf{p})t}$$

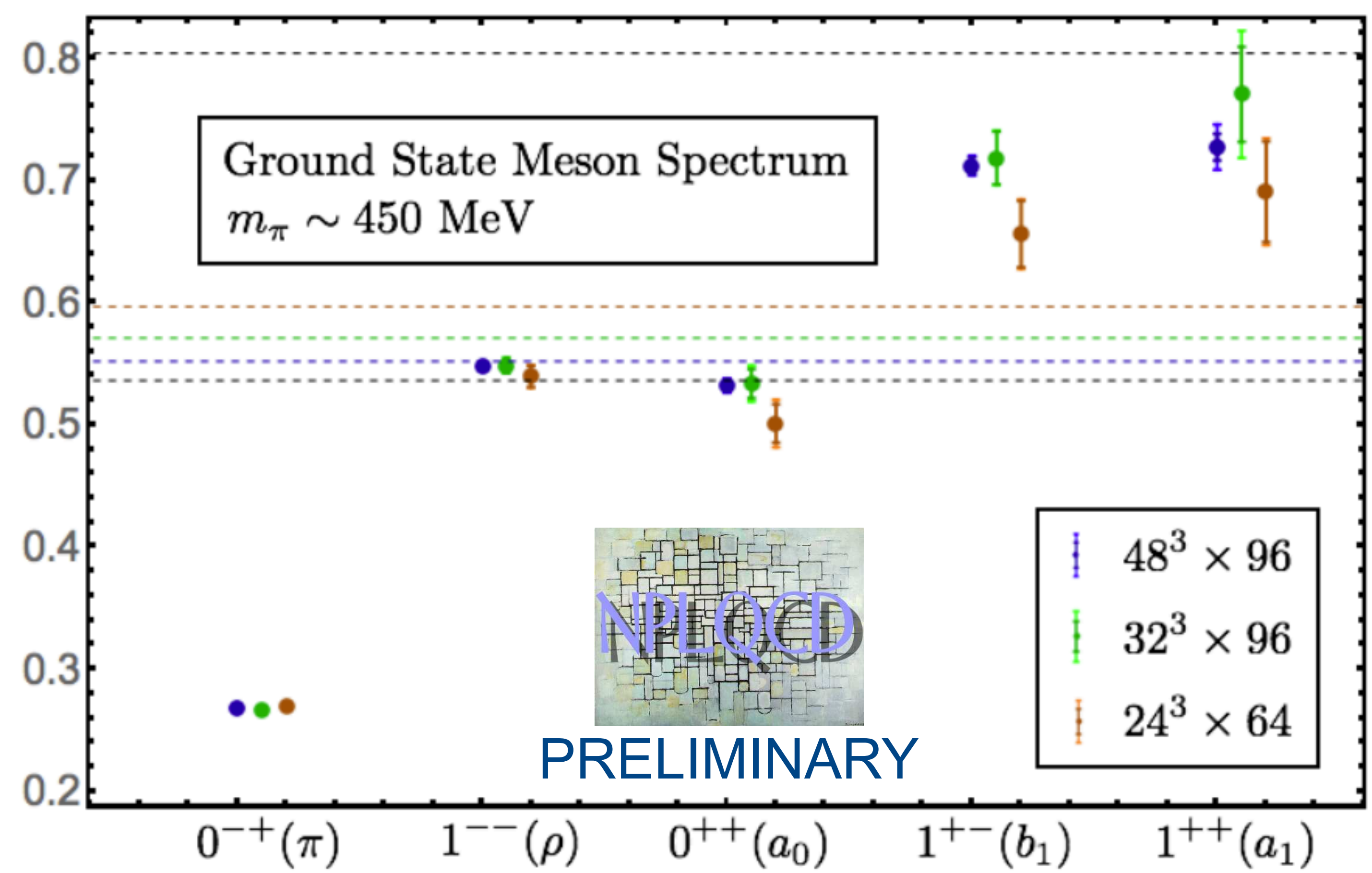
Possible for $Z_{\mathfrak{n}}^{\Gamma}(\mathbf{p}) Z_{\mathfrak{n}}^{\Gamma,(\theta_N)}(\mathbf{p}, \tau_{src})$ to be non-zero in cases where $Z_{\mathfrak{n}}^{\Gamma}(\mathbf{p}) Z_{\mathfrak{n}}^{\Gamma}(\mathbf{p}) = 0$

Isovector mesons:

$\bar{u}d \to e^{i\theta}\bar{u}d$ equivalent to $U(1)_{u-d}$ background field: breaks conservation of total isospin!

Baryons and nuclei:

$qqq \to e^{i\theta}qqq$ equivalent to $U(1)_B$ background field: preserves all symmetries of interest



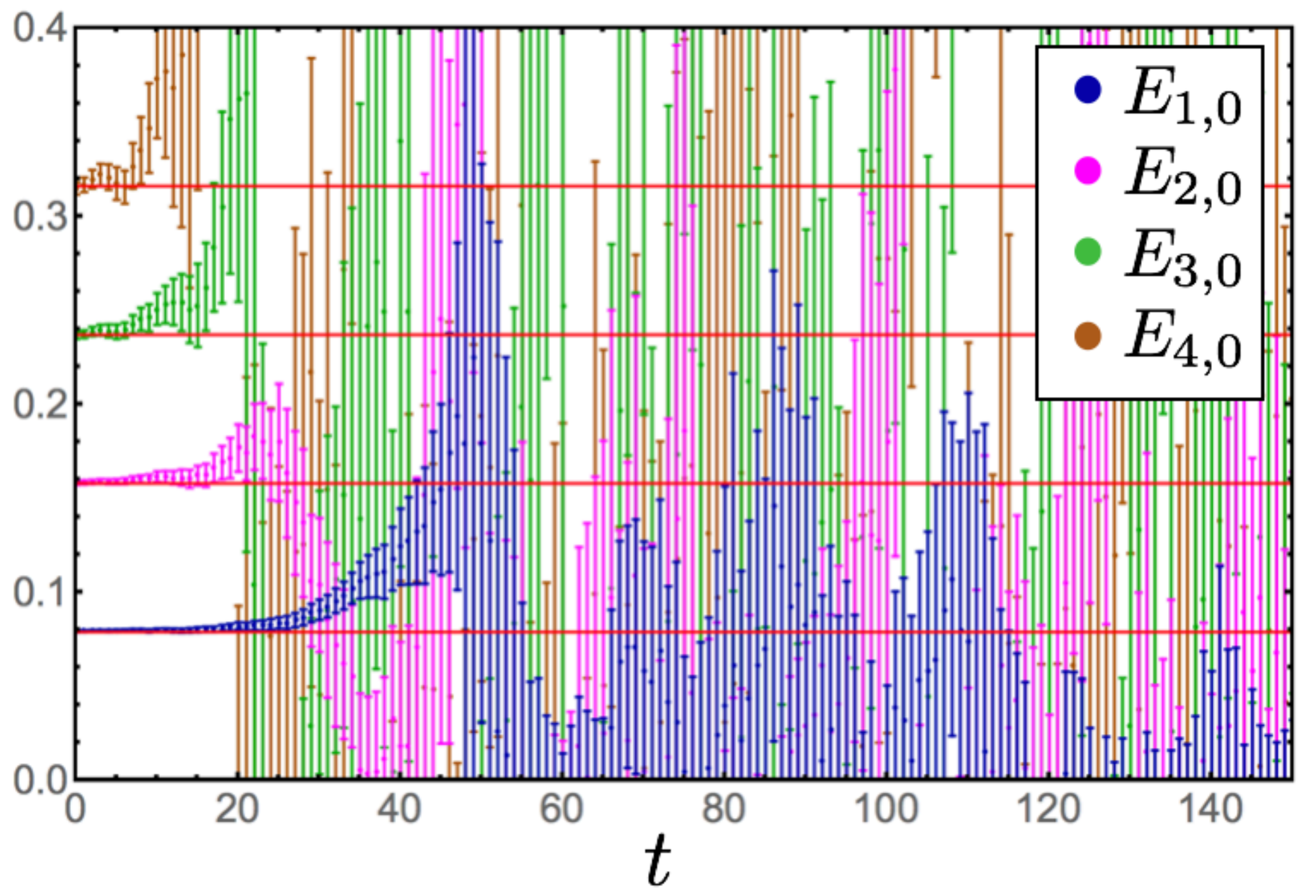
Scalar Signal-to-Noise Problems

Is exponential StN degradation of complex correlators inevitable?

Toy model: free (or interacting) complex scalar field theory in (0+1)D

$$S = \sum_{t=0}^{L-1} (\varphi^*(t+1) - \varphi^*(t))(\varphi(t+1) - \varphi(t)) - M^2 |\varphi^2|$$

$$G_{Q,2P} = \left\langle \varphi(t)^Q |\varphi(t)|^{2P} \varphi^*(t)^Q |\varphi(0)|^{2P} \right\rangle \sim e^{-E_{Q,2P}\, t}$$



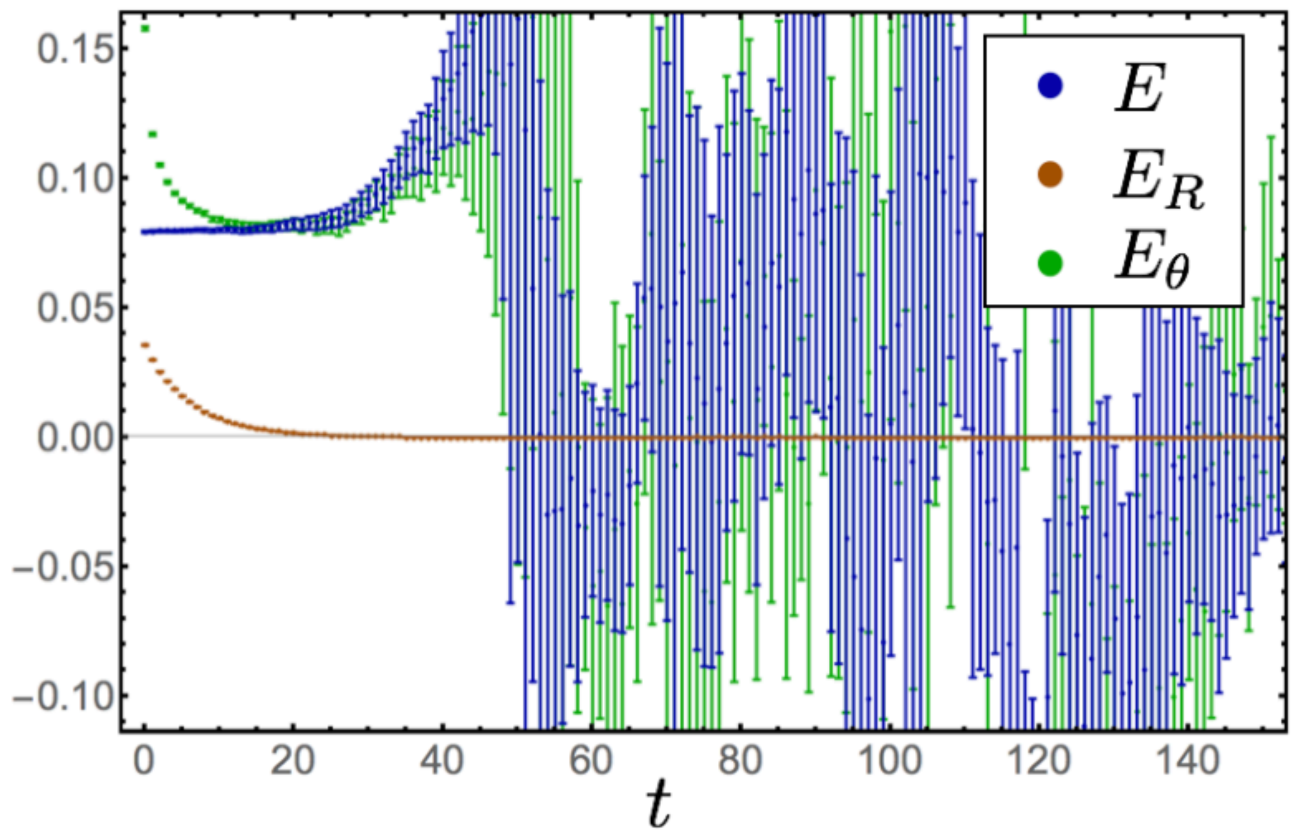
Scalar correlators have exponential StN degradation set by total charge contained in spacetime volume

$$StN[G_{Q,2P}] \sim e^{-E_{Q,0}\, t} \sim e^{-M|Q|t}$$

Scalar Sign(al-to-Noise) Problems

Scalar field phase gives correlation function path integrals a sign problem, responsible for exponential StN problem

$$G_{1,0} = \left\langle e^{\mathscr{R}(t)+i\Theta(t)} \right\rangle$$
$$= \int \mathscr{D}\varphi^* \mathscr{D}\varphi \; e^{-S+\mathscr{R}(t)+i\Theta(t)}$$



Distribution of phase fluctuations approximately wrapped normal

$$PDF(\Theta) = \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} e^{-in\Theta} \prod_{t'=1}^{t} \left[\frac{I_{|n|}(\kappa(t))}{I_0(\kappa(t))} \right] \approx \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} e^{-in\Theta} e^{-tn^2/(2\langle \kappa \rangle)}$$

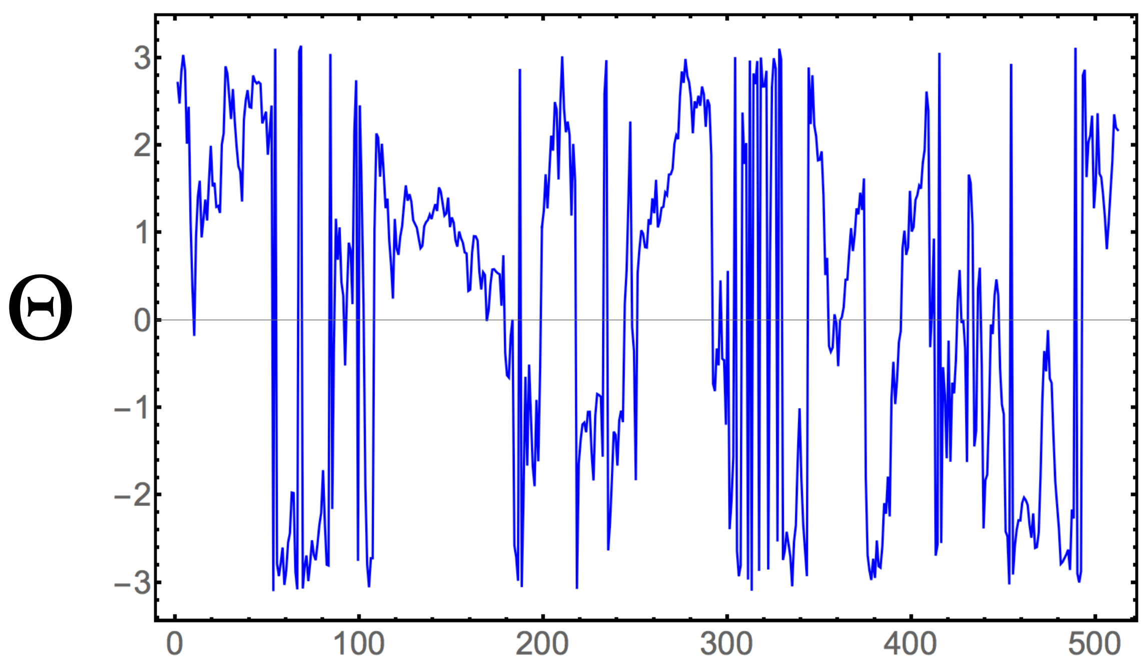
No magnitude fluctuations, small phase fluctuations

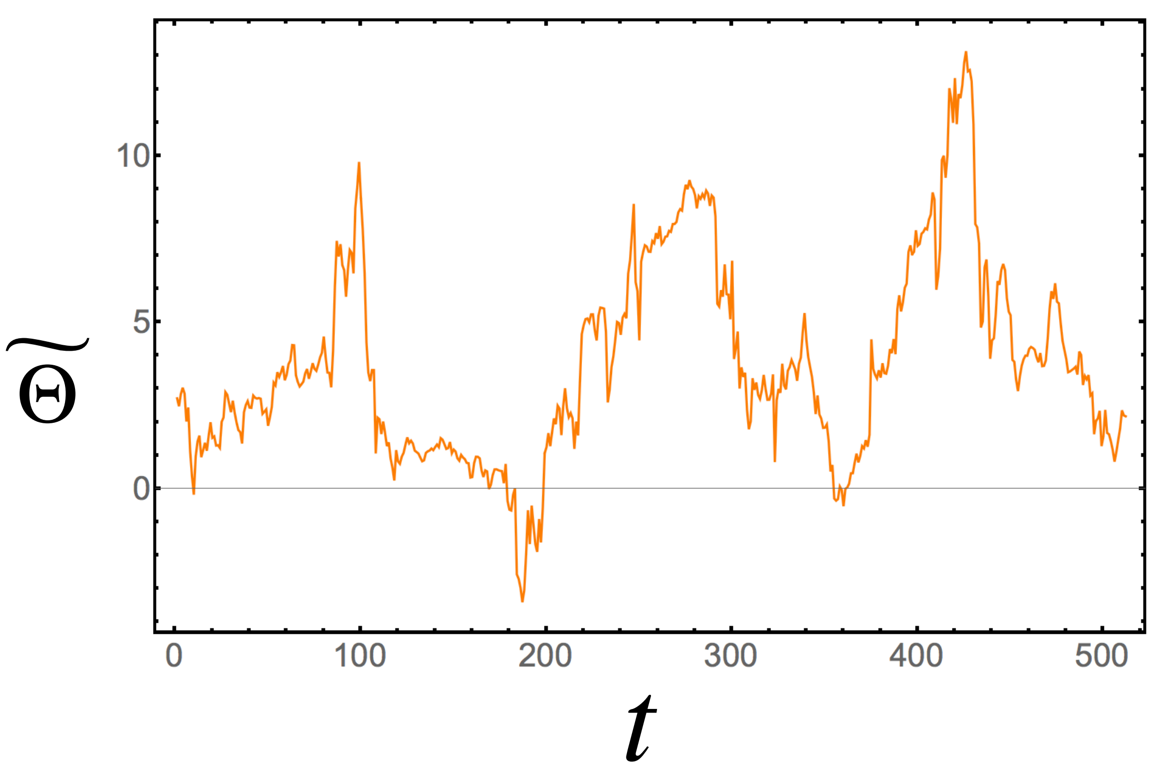
$$\kappa(t) = 2\,|\varphi(t)|\,|\varphi(t-1)|$$

Phase Unwrapping

Wrapped normal approximation has exponential StN problem

$$StN[\langle \cos\Theta \rangle] \sim e^{-t/(2\kappa)}$$





What if we "unwrap" the phase?

$$\widetilde{\Theta}(t) = \sum_{t'=1}^{t} \Theta(t') - \Theta(t'-1) + 2\pi\nu(t')$$

Average phase can be reconstructed from unwrapped phase cumulants

$$\langle \cos\Theta \rangle = \left\langle \cos\widetilde{\Theta} \right\rangle = e^{\sum_{n=1}^{\infty} \kappa_n(\widetilde{\Theta})/n!}$$

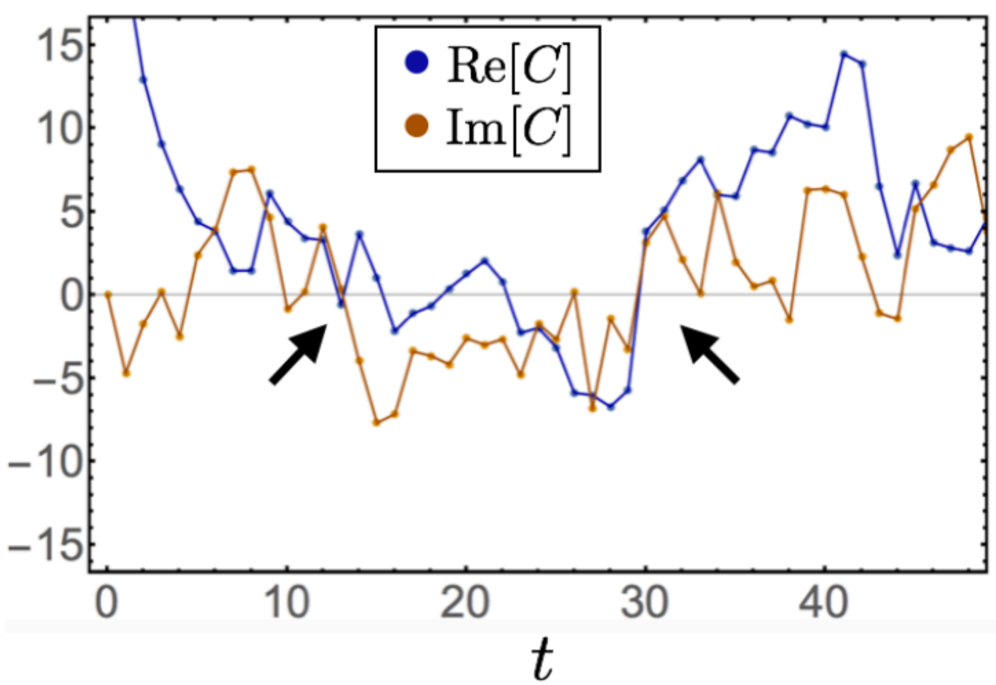
Unwrapped cumulants avoid exponential StN problem

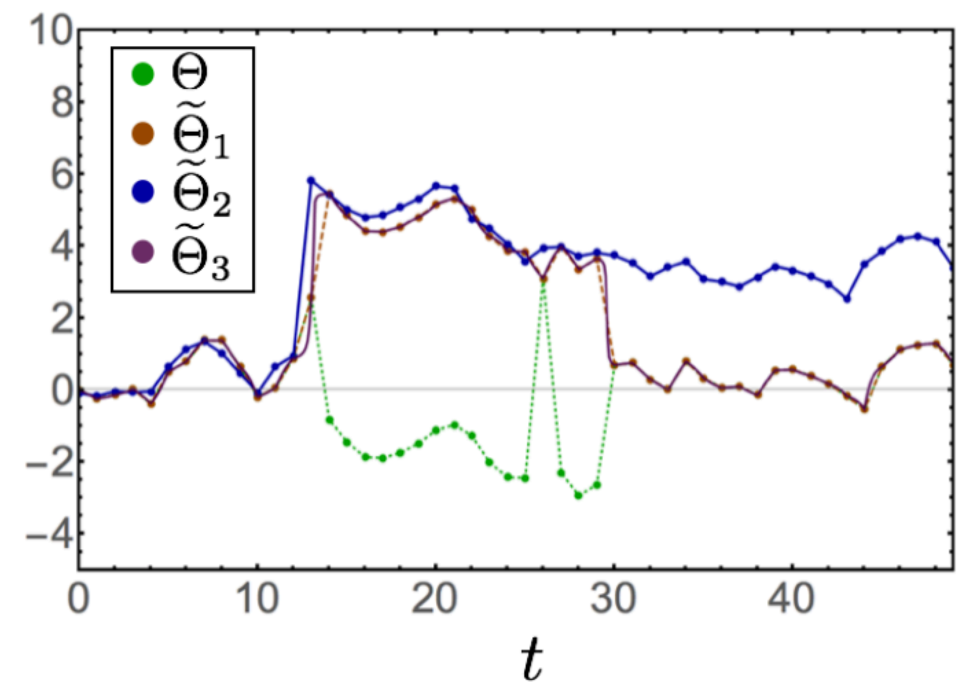
$$StN[e^{-\widetilde{\Theta}^2/2}] \sim \frac{\sqrt{2}\kappa}{t}$$

Detmold, Kanwar, MW (2018)

Phase Unwrapping Systematics

Large phase jumps in regions of small magnitude lead to ambiguities in phase unwrapping





Different definitions lead to large numerical discrepancies for all points after a large phase jump

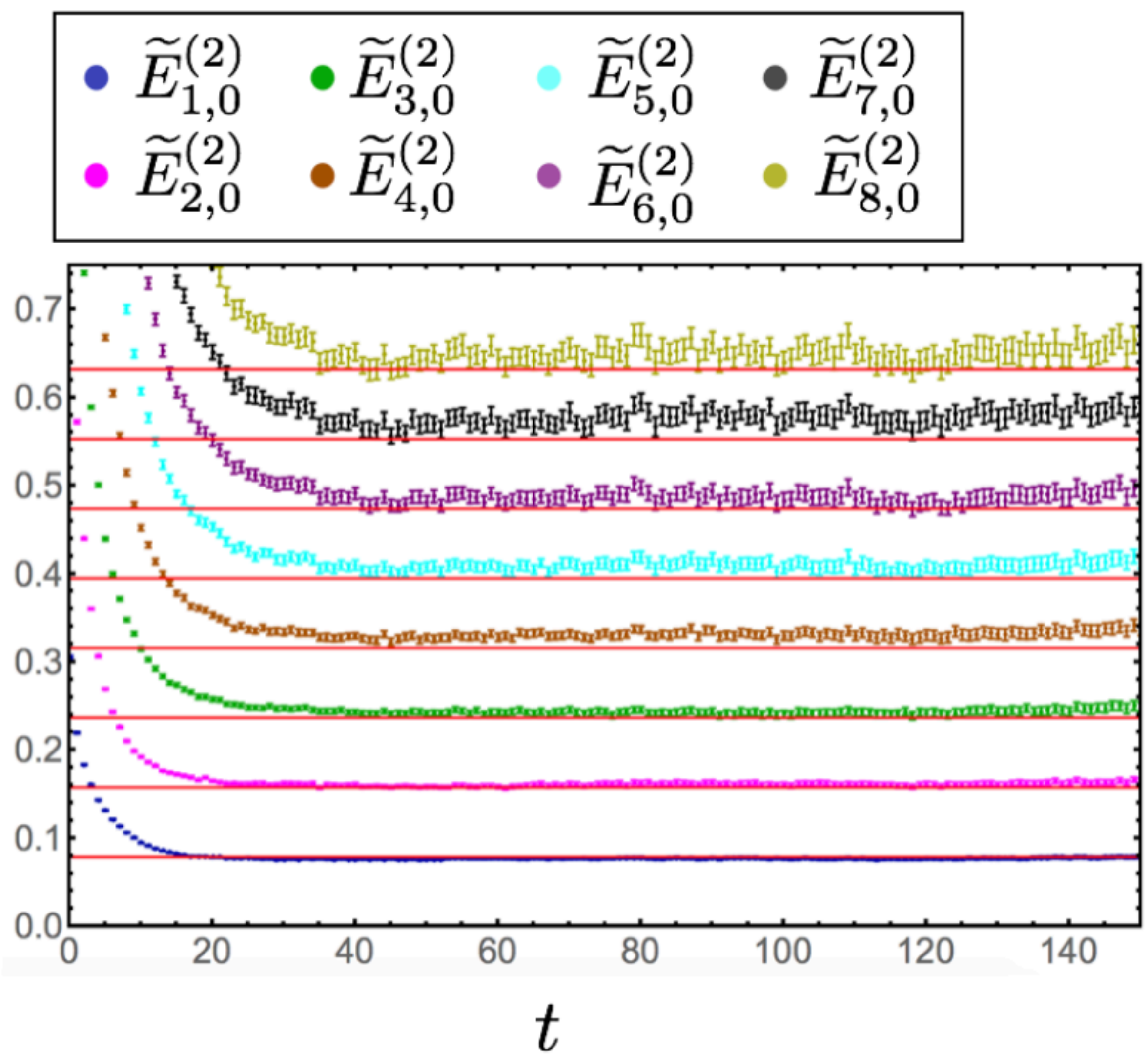
Heavy-tailed phase jump distributions appear in 1D scalar field correlators as well as LQCD baryons

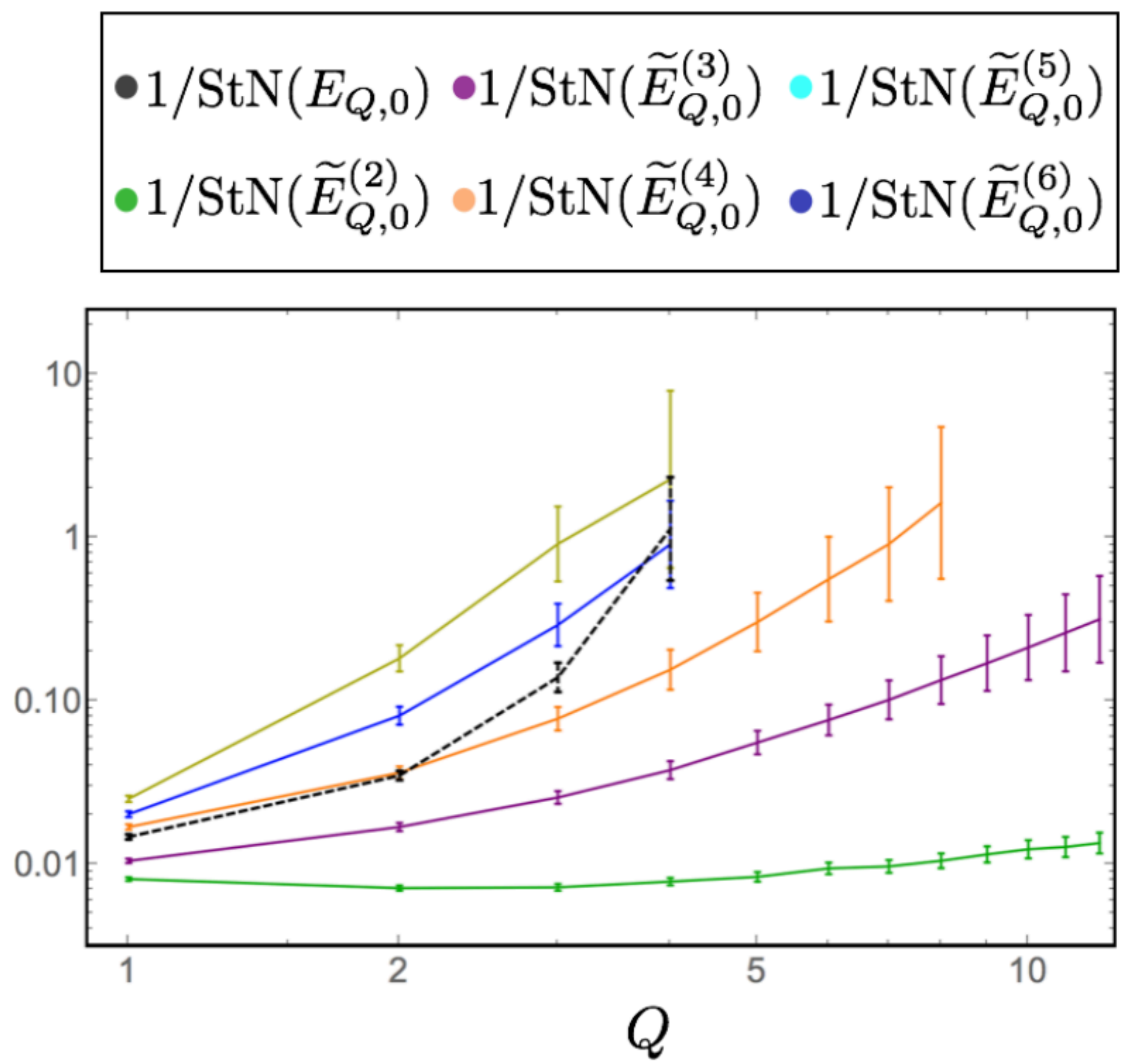
— Are large phase jumps a generic feature of LQFT?

Phase Unwrapping Precision

Accuracy of leading-order result depends sensitively on definition, best to assume smoothness on physical scales

Leading-order unwrapped cumulant results avoid exponential StN degradation, higher-order cumulants noisier





Outlook

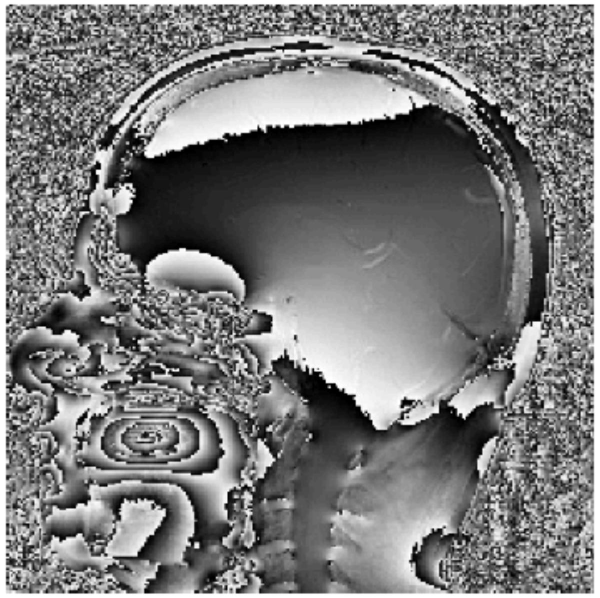
The baryon StN problem arises from phase fluctuations

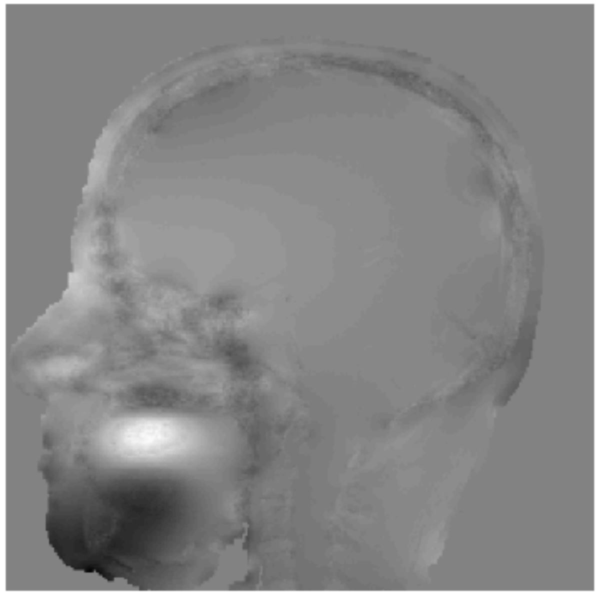
Removing phase fluctuations allows sources to be dynamically evolved towards the ground state without additional StN degradation

Phase unwrapping provides correlator estimates that avoid exponential StN degradation but systematic errors are not fully controlled

Stay tuned for Gurtej Kanwar's talk, up next

Multi-dimensional phase unwrapping in other applications can be more robust, work to control LQFT phase unwrapping systematics in progress





Ying (2006)