Phase Unwrapping and One-Dimensional Sign Problems

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Overview

Path integrals with complex integrands have sign problems, even when the "action" is real and the "observable" is complex

$$
\begin{aligned}
\langle \mathcal{O} \rangle &= \frac{1}{Z} \int \mathcal{D}U \; e^{-S(U)} \; \mathcal{O}(U) \\
&= \frac{1}{Z} \int \mathcal{D}U \; e^{-S(U) + \ln|\mathcal{O}(U)| + i \arg \mathcal{O}(U)} \\
&\equiv \frac{1}{Z} \int \mathcal{D}U \; e^{-\mathfrak{R}[S_{eff}(U)] - i\mathfrak{I}[S_{eff}(U)]}
\end{aligned}
$$

1) "Complex observable" sign problems arise in LQCD calculations of hadronic and nuclear correlation functions

MW and Savage, PRD 96 (2016)

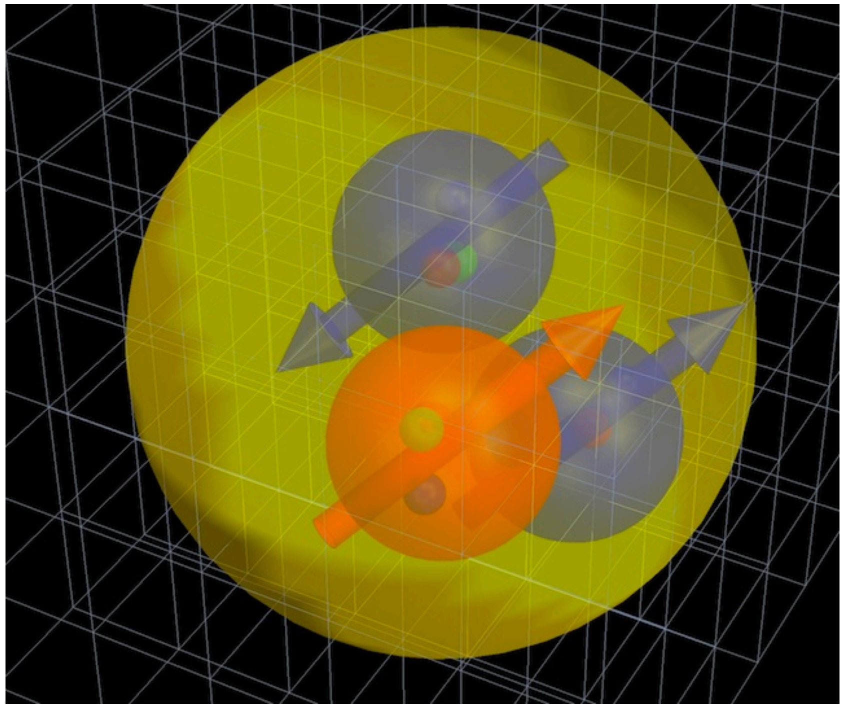
2) Complex scalar field theory provides interesting toy models of complex observable sign problems

Detmold, Kanwar, MW (2018)

3) Phase unwrapping techniques exploiting phase fluctuation smoothness can approximately(!) solve toy sign problems

Nuclear Physics from Lattice QCD

The structure of light nuclei at heavy pion mass is being determined from lattice QCD

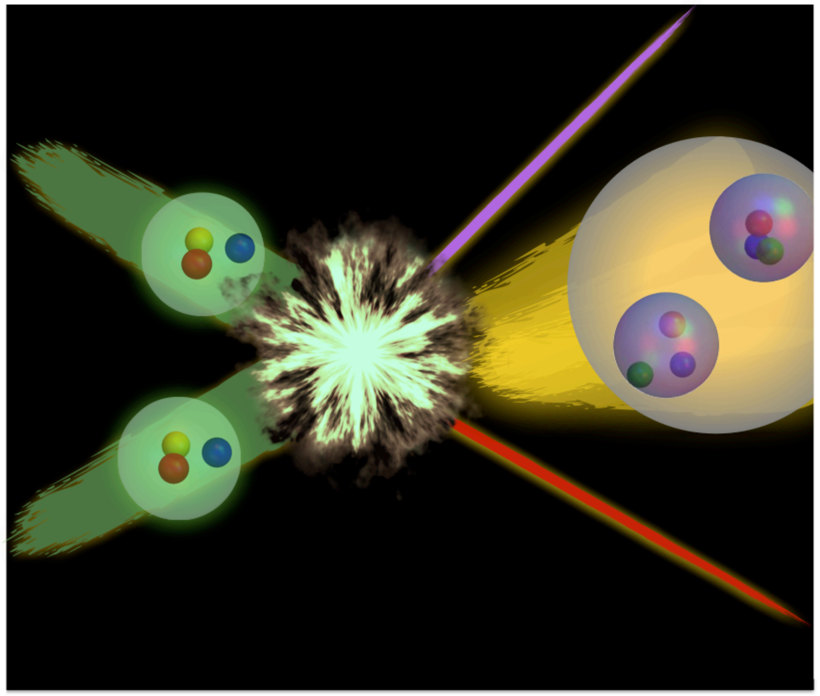


Naive shell model good first approximation to nuclear physics, even at heavy pion mass

Beane, Chang, Cohen, Detmold, Lin, Orginos, Parreno, Savage, Tiburzi, PRL 113 (2014)

Chang, Davoudi, Detmold, Gambhir, Orginos, Savage, Shanahan, Tibuzri, MW, Winter, PRL 120 (2018)

Relative large nuclear modifications of scalar matrix elements could be important for dark matter direct detection



Electroweak fusion and single- and double-beta decay reaction rates computed in lattice QCD (for light nuclei at heavy pion mass)

Beane, Chang, Detmold, Orginos, Parreno, Savage, Tiburzi, PRL 113 (2014)

Savage, Shanahan, Tiburzi, MW, Winter, Beane, Chang, Davoudi, Detmold, Orginos, PRL 119 (2017)

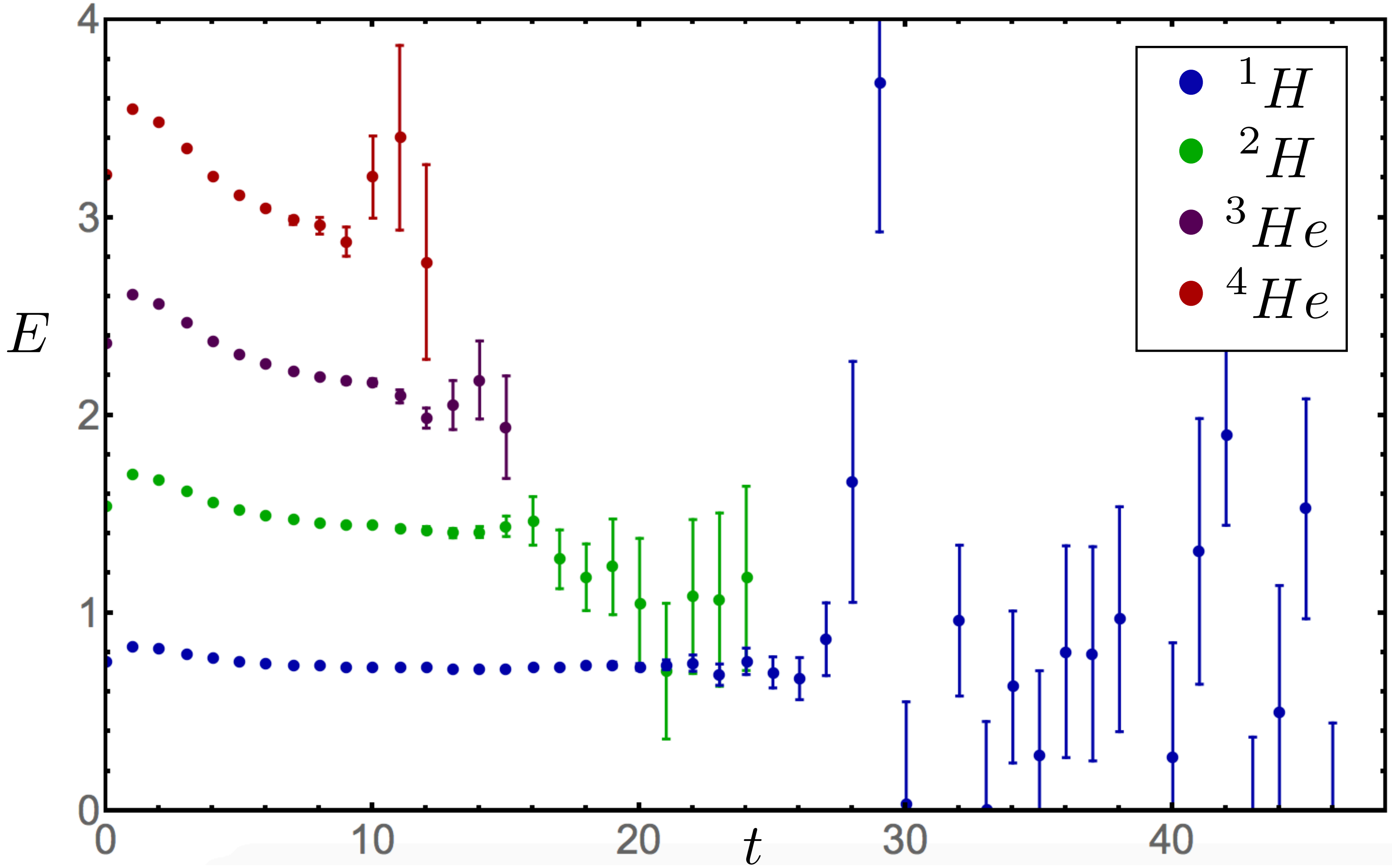
Shanahan, Tiburzi, MW, Winter, Chang, Davoudi, Detmold, Orginos, Savage, PRL 119 (2017)

The Signal-to-Noise Problem

Nuclear correlation functions can be computed using gauge field configurations sampled with (positive!) zero-density weights

$$G_A(t) = \left\langle N(t)^A N^\dagger(0)^A \right\rangle$$

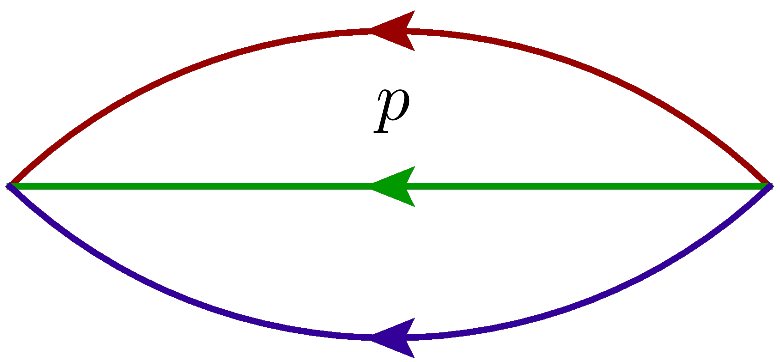
StN ratios of LQCD nuclear correlation functions decrease exponentially with increasing baryon number



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

The Signal-to-Noise Problem

"Noise" in Monte Carlo measurements represents quantum fluctuations in observables, determined by physical properties of quantum system



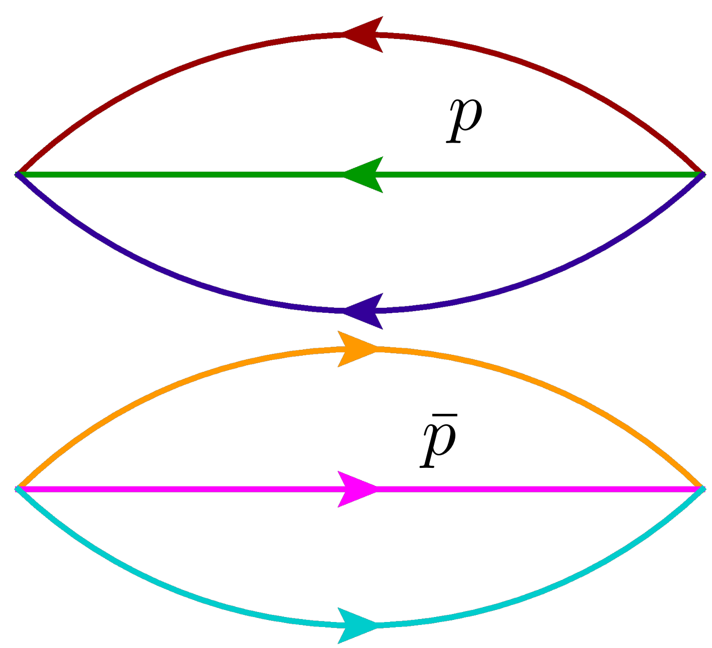
$$G_N(t) = \langle N(t) N(0)^\dagger \rangle \sim e^{-M_N t}$$

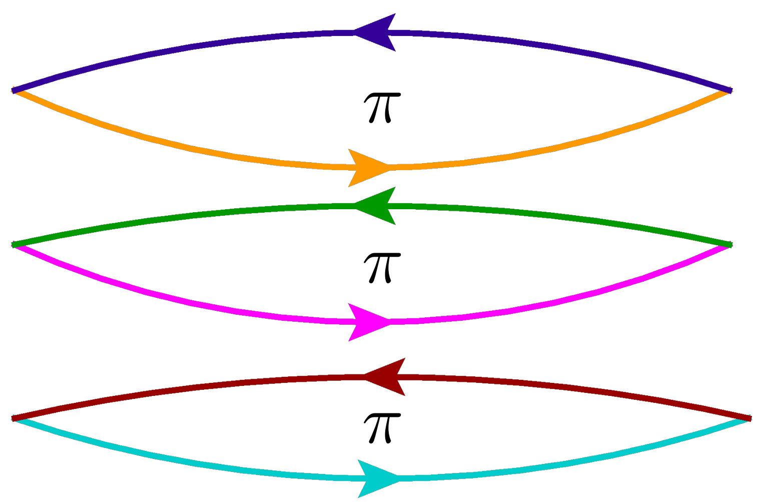
$$\overline{G}_N(t) = \sum_{i=1}^{N} C_N(t; U_i) = G_N(t) + O(N^{-1/2})$$

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

$$Var[\overline{G}_N(t)] \sim \sqrt{N} \left\langle \, | N(t) N(0)^\dagger |^2 \right\rangle$$

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





Signal-to-noise problem:

$$\frac{\langle \overline{G}_N(t) \rangle}{Var[\overline{G}_N(t)]} \sim \sqrt{N} \; e^{-(M_N - \frac{3}{2} m_\pi) t}$$

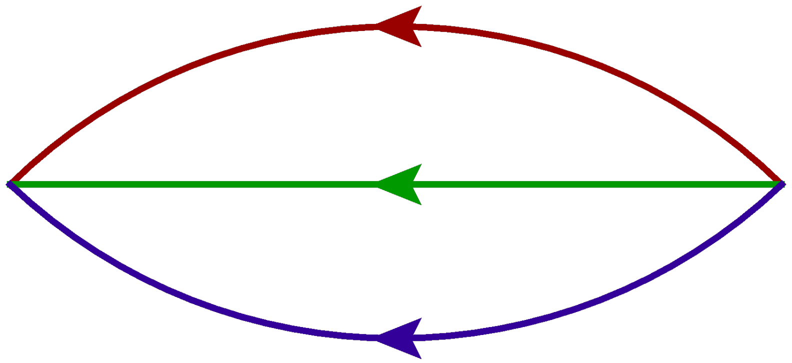
$$\frac{\langle \overline{G}_A(t) \rangle}{Var[\overline{G}_A(t)]} \sim \sqrt{N} \; e^{-A(M_N - \frac{3}{2} m_\pi) t}$$

Parisi, Phys Rept 103 (1984), Lepage, TASI (1989)

The Sign(al-to-Noise) Problem

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

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



Complex phase fluctuations give path integrals representing correlators sign problems

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

An exponentially decaying average phase always has exponential StN degradation

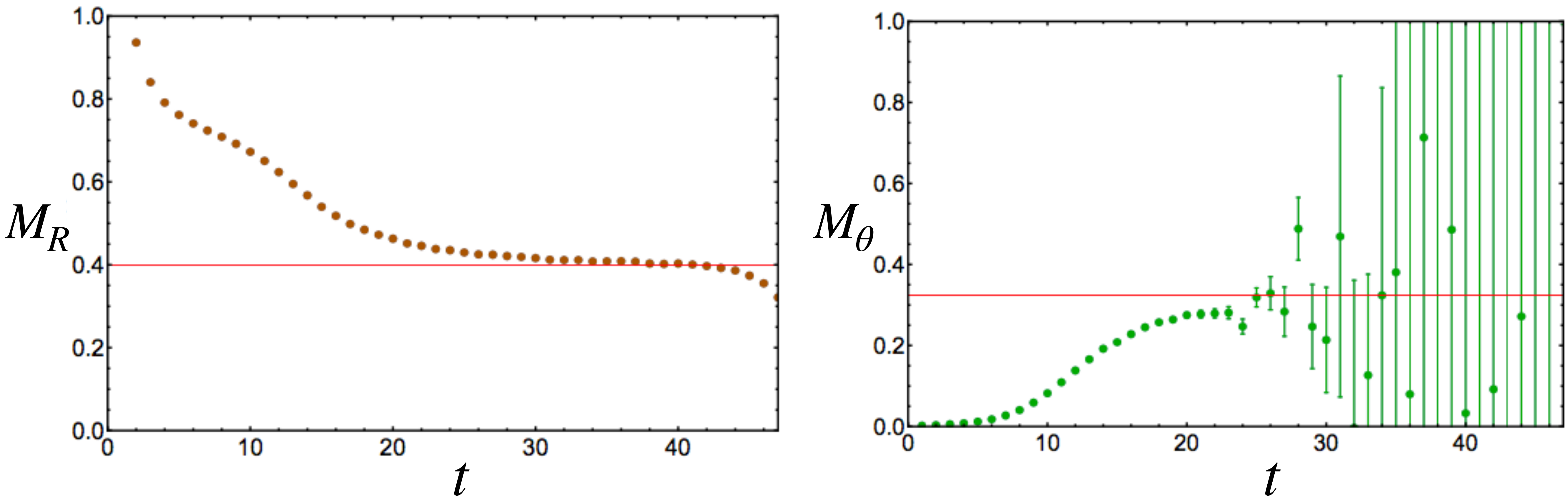
$$StN(Re[e^{i\theta_N(t)}]) = \frac{\left\langle e^{i\theta_N} \right\rangle}{\sqrt{\frac{1}{2}+\frac{1}{2}\left\langle e^{2i\theta_N} \right\rangle - \left\langle e^{i\theta_N} \right\rangle^2}} \sim \left\langle e^{i\theta_N} \right\rangle \sim e^{-M_\theta t}$$

MW and Savage, PRD 96 (2016)

Correlation Function Phases

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

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



Circular Statistics

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

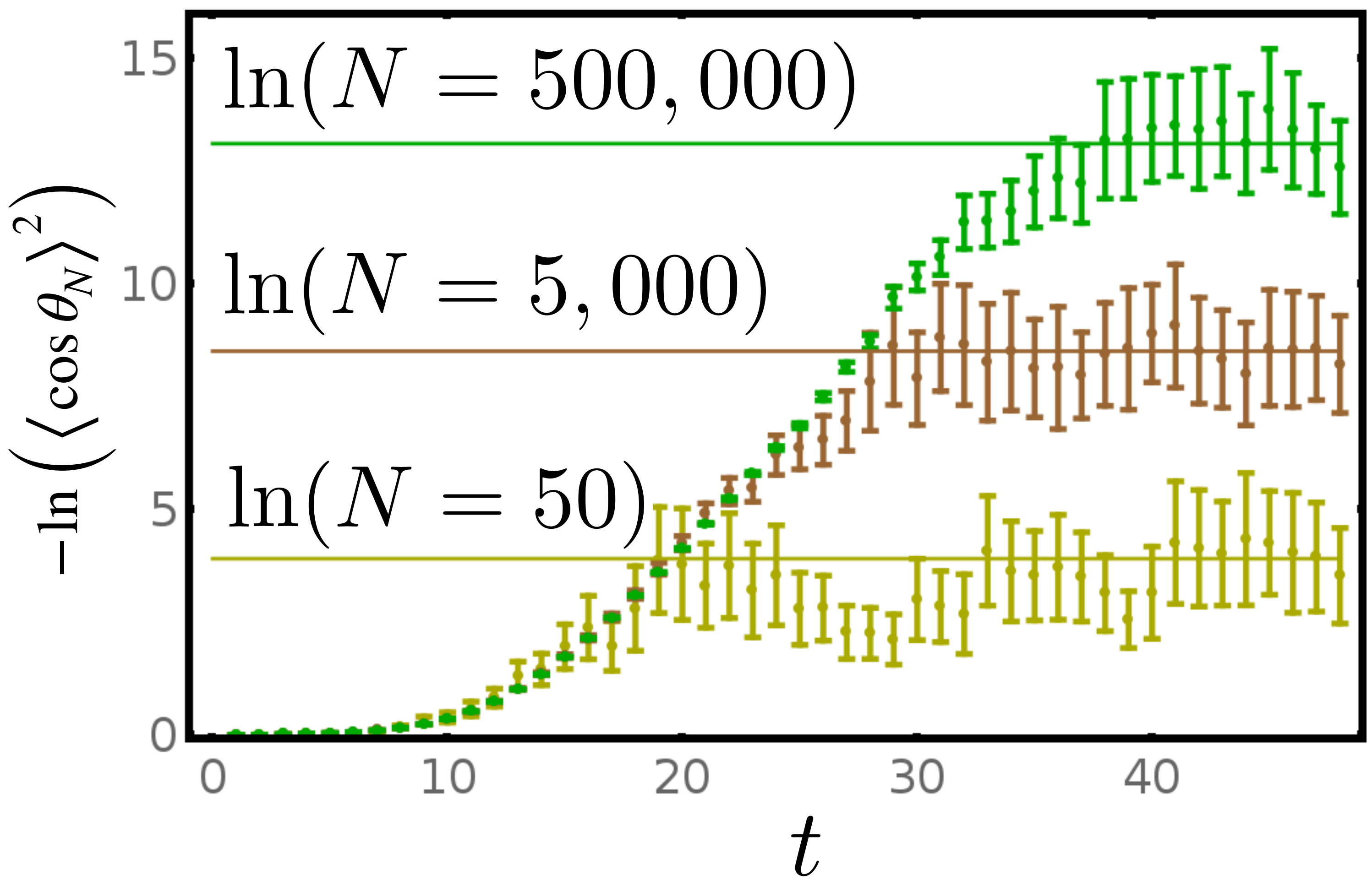
$$\frac{1}{N}\sum_{i=1}^{N}\cos\theta_N(U_i) \gtrsim \frac{1}{\sqrt{N}}$$

See e.g. Fisher, Statistical Analysis of Circular Data (1995)

Avoiding finite sample effects requires

$$N \gtrsim \left\langle e^{2i\theta_N(t)} \right\rangle \sim e^{2(M_N - \frac{3}{2}m_\pi)t}$$

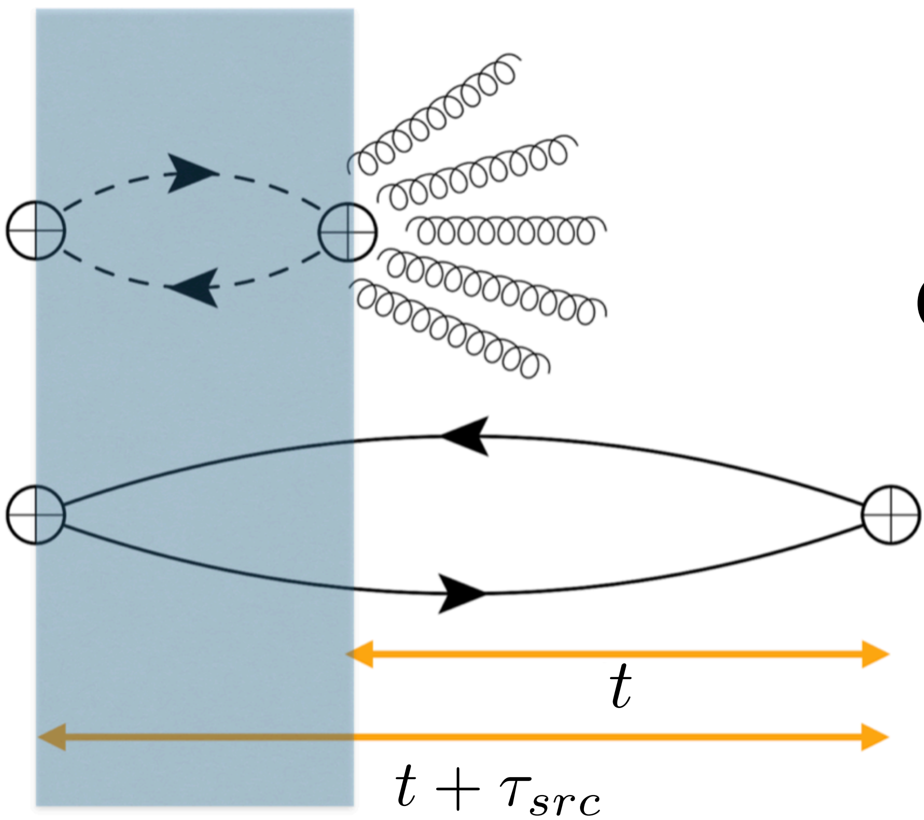
Bound will be violated in a late-time "noise region" where standard estimators become unreliable



Dynamical Source Construction

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

Aubin and Orginos AIP Conf. Proc. 1374 (2011)



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

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

MW and Savage (2017)

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

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

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

Analogous to constrained-phase/fixed-node evolution in QMC

Zhang, Shiwei, Carlson, PRB 55 (1997) Wiringa, Pieper, Carlson, Pandharipande PRC 62 (2000)

Meson GGPoF

Spectral representation for phase reweighted correlator given by

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

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:

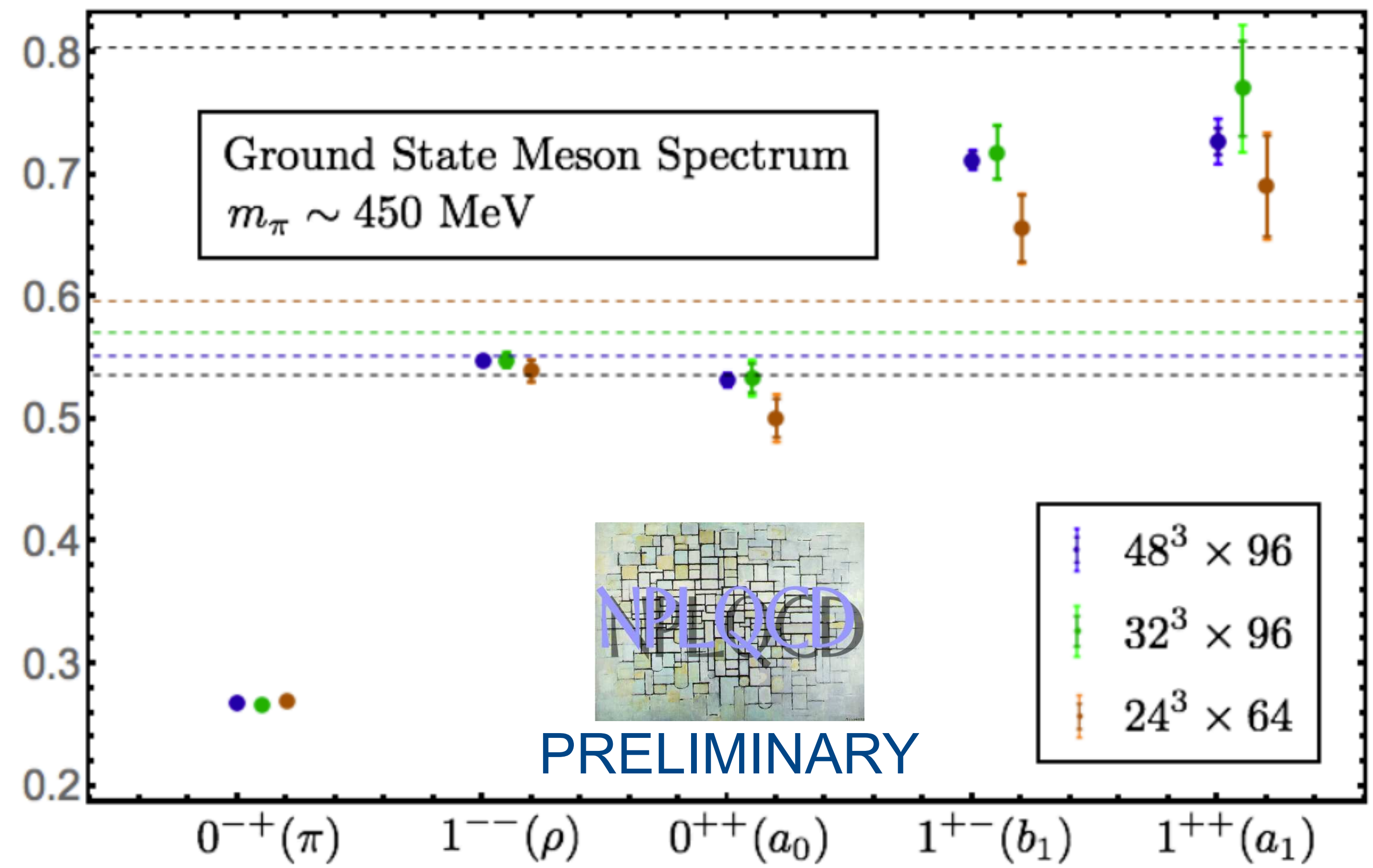
$\bar{u}d \rightarrow e^{i\theta}\bar{u}d$ equivalent to $U(1)_{u-d}$

Background field breaks conservation of total isospin

Baryons and nuclei:

$qqq \rightarrow e^{i\theta}qqq$ equivalent to $U(1)_B$

Background field preserves all symmetries of interest



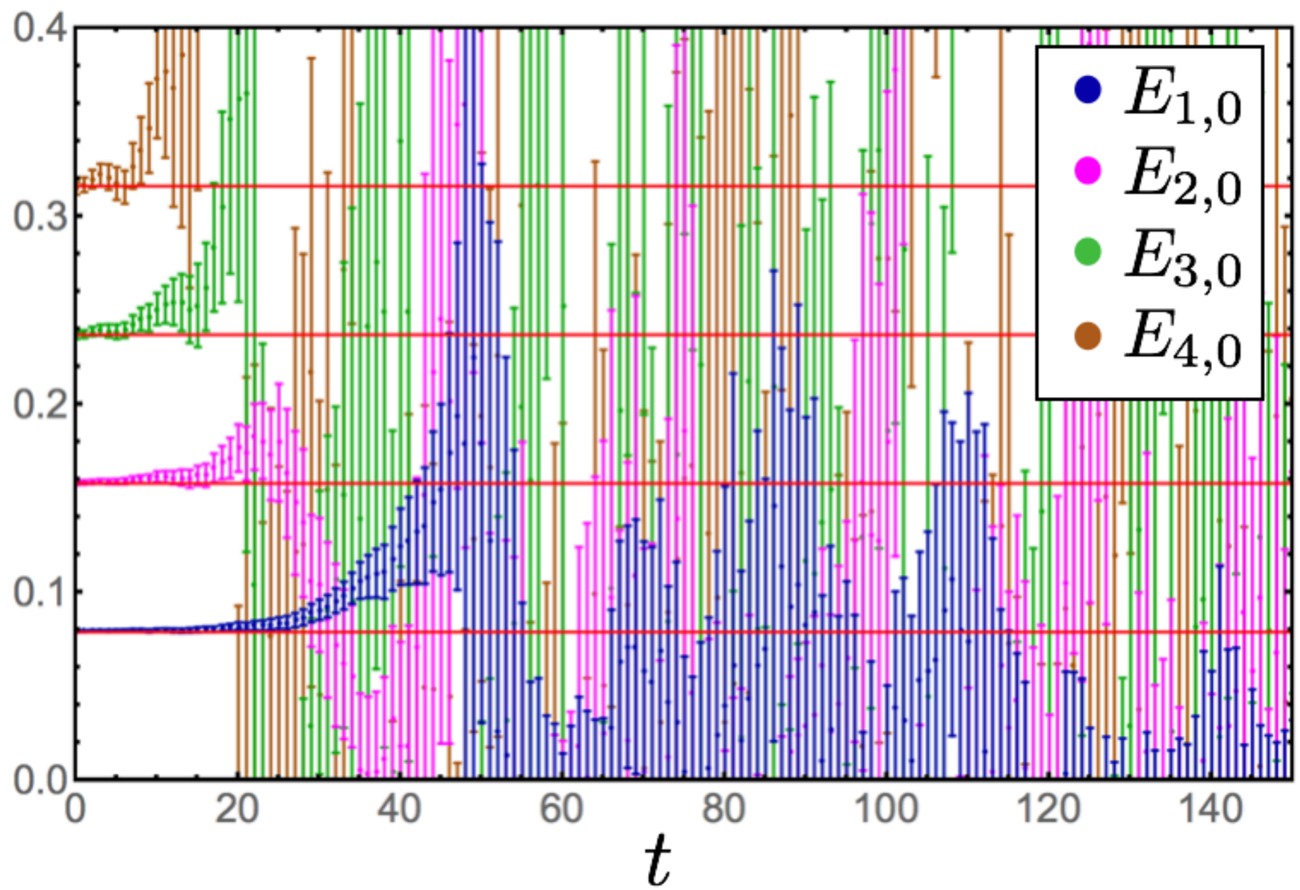
Scalar Signal-to-Noise Problems

Is exponential StN degradation of complex correlators inevitable?

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

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

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



Exponential StN problem set by U(1) charge

$$Var[\Re G_{Q,2P}] = \frac{1}{2} G_{0,2|Q|+4P} + \frac{1}{2} G_{2Q,4P} - G_{Q,2P}^2$$

$$\sim 1$$

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

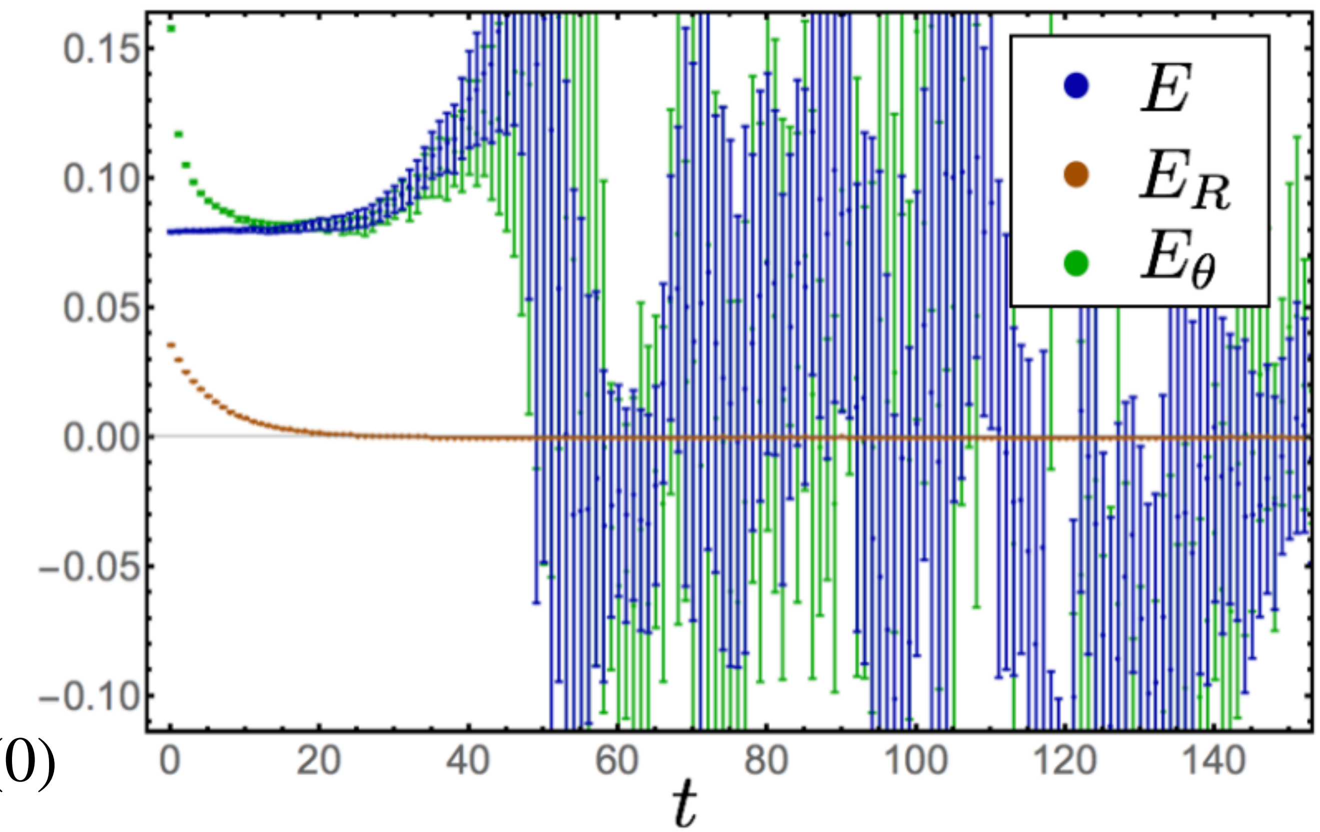
Detmold, Kanwar, MW (2018)

Scalar Sign(al-to-Noise) Problems

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

$$G_{1,0} = \left\langle e^{\mathscr{R}(t)+i\Theta(t)} \right\rangle$$

$$= \int \mathscr{D}\varphi^* \mathscr{D}\varphi \; e^{-S+\mathscr{R}(t)+i\Theta(t)}$$



$$\mathscr{R}(t) = \ln|\varphi(t)| + \ln|\varphi(0)|$$

$$\Theta(t) = \theta(t) - \theta(0) = \arg\varphi(t) - \arg\varphi(0)$$

Any correlation function with non-zero U(1) charge has phase fluctuations and StN problems set by size of charge

$$G_{Q,2P} = \left\langle e^{(|Q|+2P)\mathscr{R}(t)+iQ\Theta(t)} \right\rangle = \int \mathscr{D}\varphi^* \mathscr{D}\varphi \; e^{-S+(|Q|+2P)\mathscr{R}(t)+iQ\Theta(t)}$$

Phase fluctuations needed to project on to U(1) charge sectors

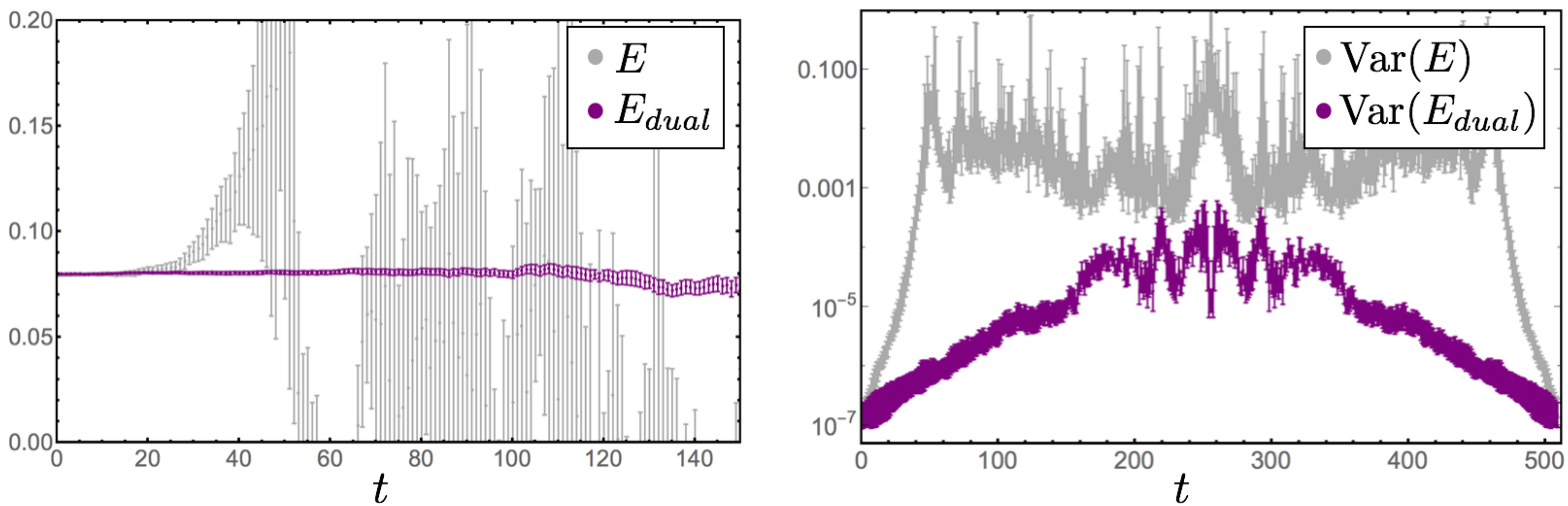
Integrating Out Phase Noise

Analytically integrating out phase fluctuations using dual variables solves sign problem and Parisi-Lepage StN problem

Same scalar field dual variables introduced in Endres, PRD 75 (2006)

$$Z = \int_0^\infty \prod_{t=0}^{L-1} \left[d|\varphi(t)|\,|\varphi(t)|\, e^{-2|\varphi(t)|^2 - V(|\varphi(t)|)} \right] \int_{-\pi}^{\pi} \prod_{t=0}^{L-1} \left[\frac{d\theta}{\pi} e^{\kappa(t)\cos\left(\theta(t) - \theta(t-1)\right)} \right]$$

$$= 4 \sum_{q\in\mathbb{Z}} \int_0^\infty \prod_{t=0}^{L-1} \left[d|\varphi(t)|\,|\varphi(t)|\, e^{-2|\varphi(t)|^2 - V(|\varphi(t)|)} \right] I_{|q|}(\kappa(t)) \qquad \kappa(t) = 2|\varphi(t)\varphi(t-1)|$$



Mild residual StN problem arises from estimating average product of many positive random variables

Elegant solution for interacting scalars, hard to generalize to QCD

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)

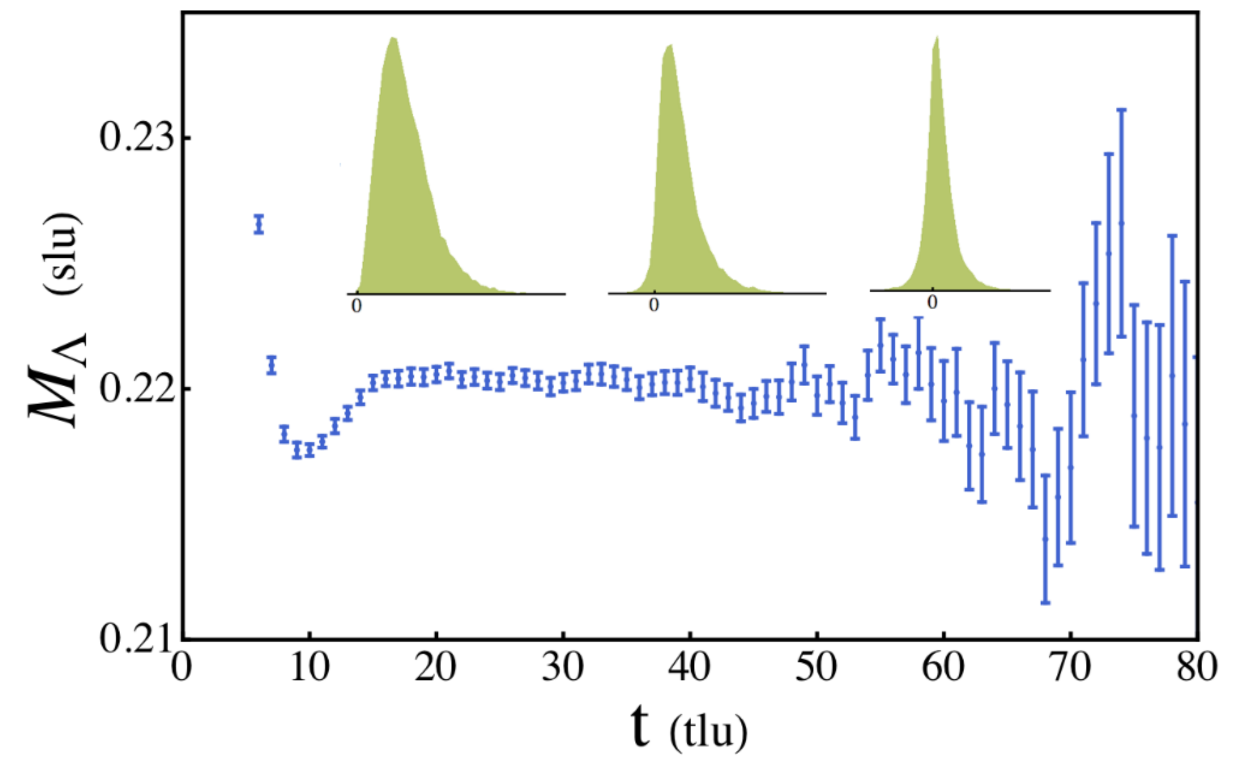
Endres, Kaplan, Lee and Nicholson, PRL 107 (2011)

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

DeGrand, PRD 86 (2012)

Porter and Drut, PRE 93 (2016)

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



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

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

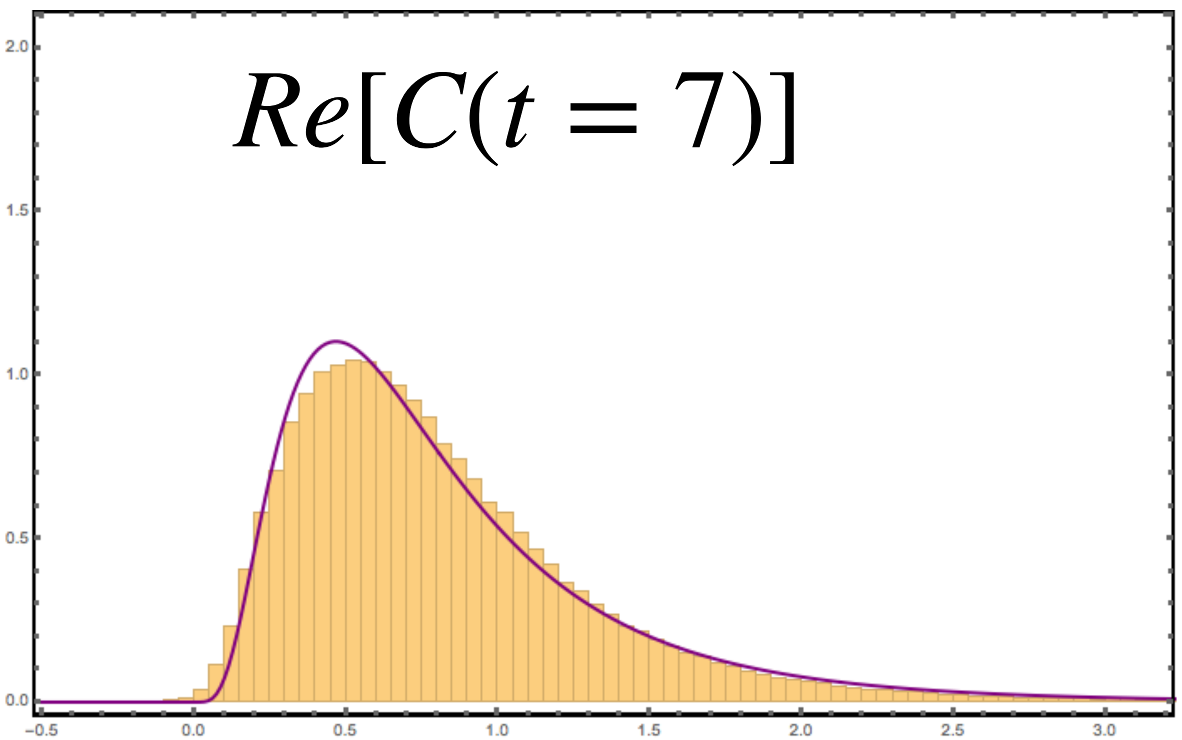
Broad, symmetric large-time distributions consistent with moment analysis by Savage

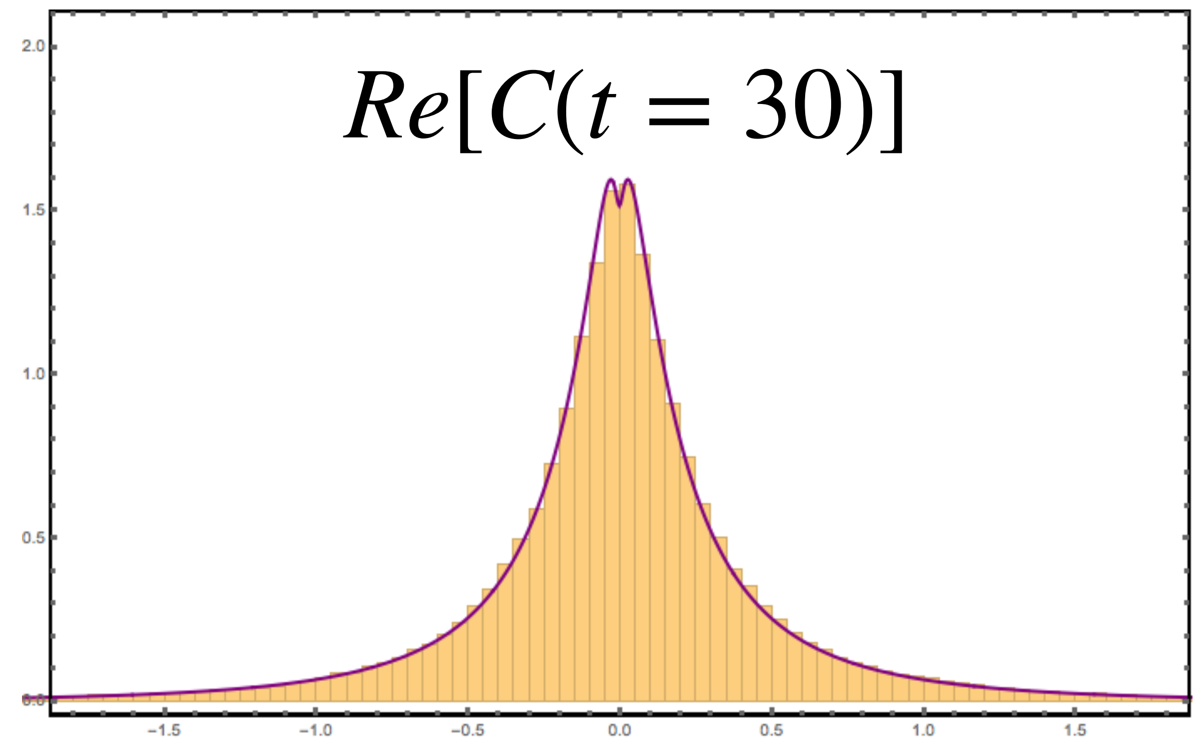
Complex Log-Normal Distributions

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

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

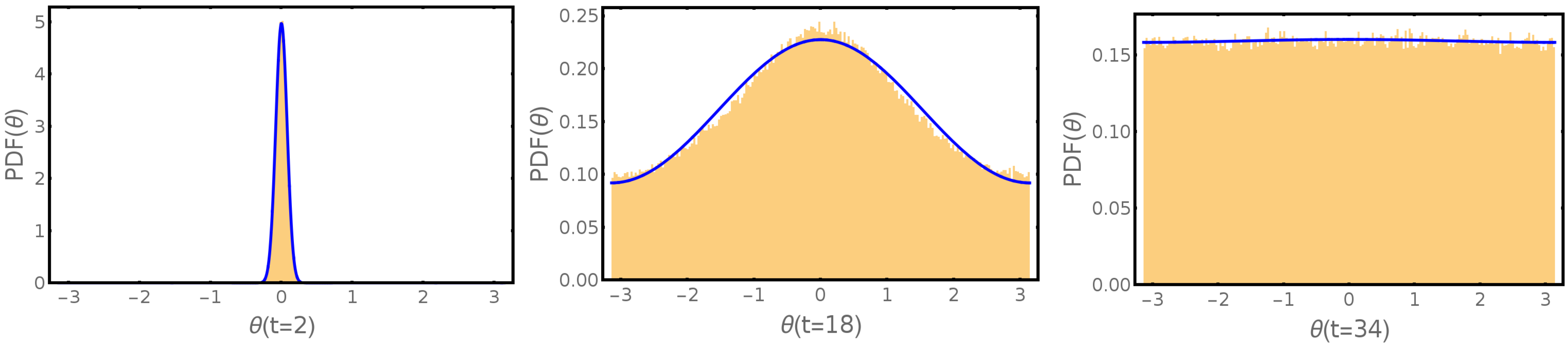
$$PDF(R,\theta) = e^{-(R-\mu_R)^2/(2\sigma_R^2)} \sum_{n=-\infty}^{\infty} e^{-n^2\theta^2/(2\sigma_\theta^2)}$$





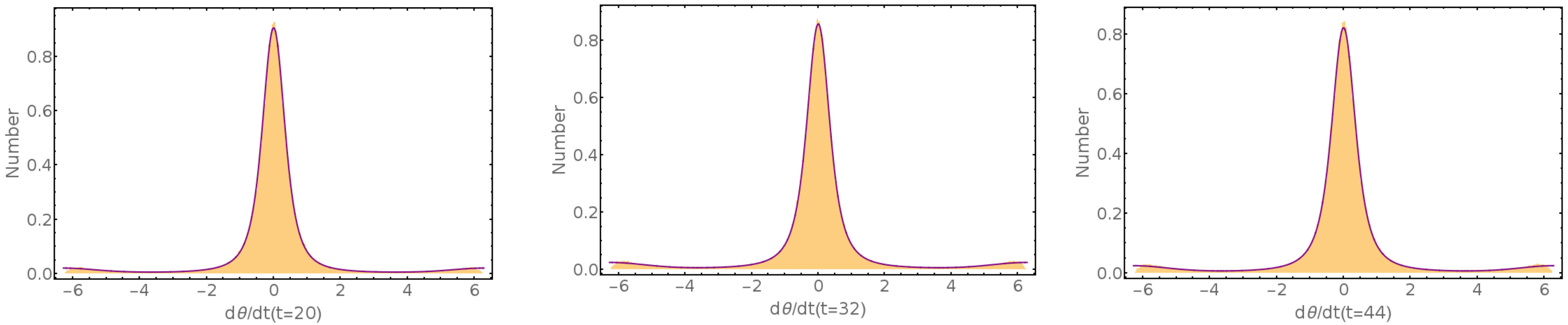
MW and Savage, PRD 96 (2016) MW, LATTICE 2017

Large Phase Jumps



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

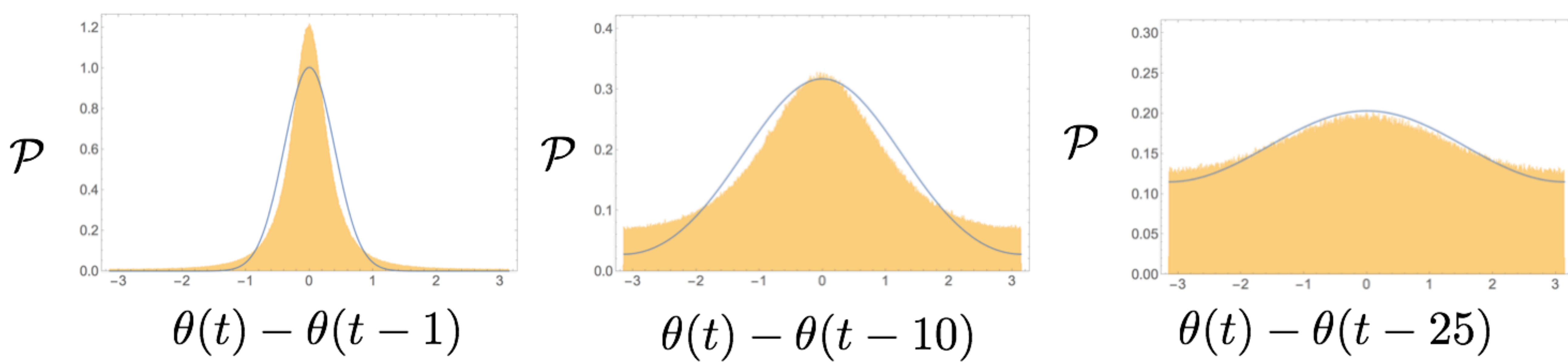


Scalar Field Phase Distributions

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



MC phase distributions show heavy-tails not present if magnitude fluctuations are ignored — even in free field theory!

Detmold, Kanwar, MW (2018)

Wrapped Normal Noise

Wrapped normal approximation (ignoring magnitude fluctuations giving rise to large phase jumps) still has full StN problem

$$PDF(\Theta) \approx \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} e^{-in\Theta} e^{-n^2 Et} \qquad \langle \overline{G} \rangle \approx Z e^{-Et}$$

$$Var[\overline{G}(t)] \approx \left[\left\langle \left(\frac{1}{N} \sum_i \cos(\Theta_i) \right)^2 \right\rangle - \left\langle \frac{1}{N} \sum_i \cos(\Theta_i) \right\rangle^2 \right] \approx \frac{1}{2N} \left(1 - e^{-2Et}\right)$$

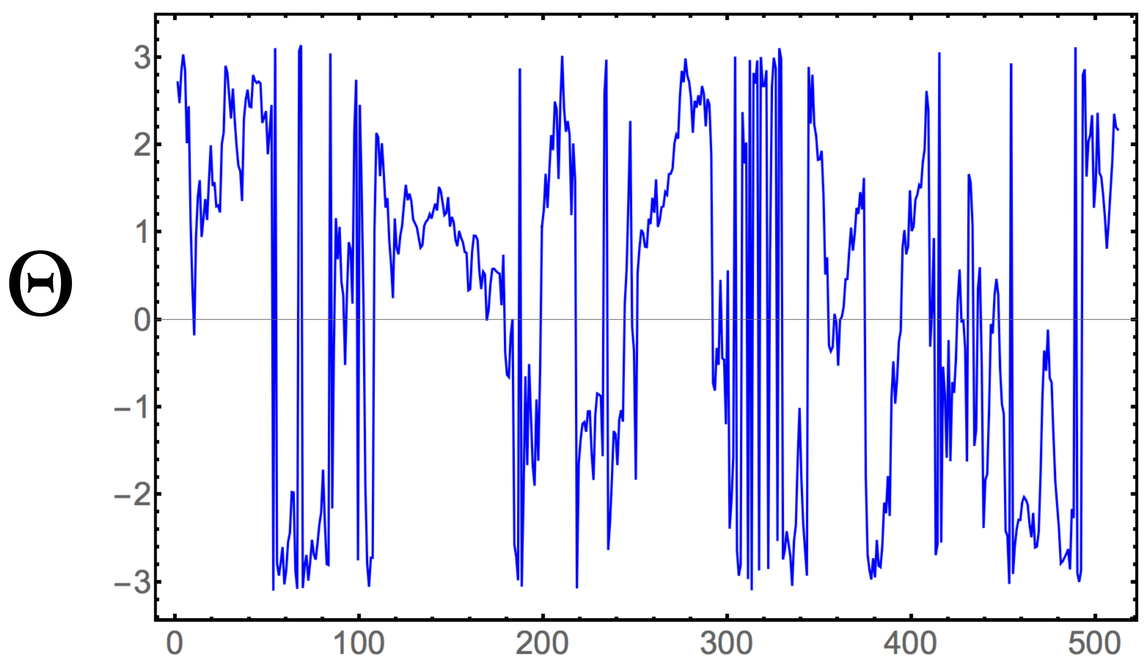
$$StN[\overline{G}(t)] \approx \sqrt{2N} \frac{e^{-Et}}{\sqrt{1 - e^{-2Et}}}$$

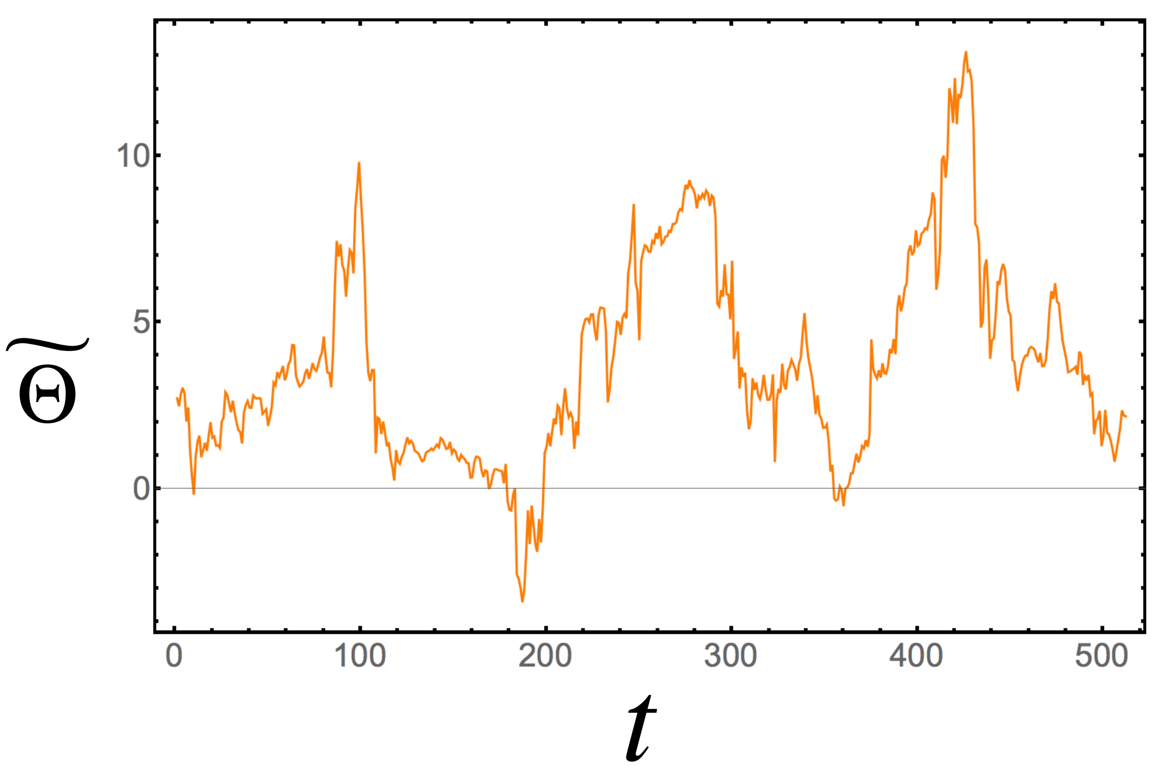
Exponential StN degradation is inevitable for a time series of wrapped normal compact random variables

Central limit theorem for compact random variables suggests approximately wrapped normal phases are generic

Phase Unwrapping

"Phase unwrapping" maps compact random variables to real random variables by adding winding numbers





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

Winding number defined by smoothness assumption, e.g. single lattice site smoothness

$$\left|\widetilde{\Theta}(t) - \widetilde{\Theta}(t-1)\right| < \pi$$

Windowed integration: assumes smoothness only on "physical" length scales

$$\left|\widetilde{\Theta}(t) - \frac{1}{min(w,t)} \sum_{t'=max(t-w,0)}^{t-1} \widetilde{\Theta}(t')\right| < \pi$$

Unwrapped Normal Noise

A wrapped normal phase can be associated with a normally distributed unwrapped phase

$$PDF(\widetilde{\Theta}) \approx \sqrt{\frac{1}{\pi E t}} e^{-\widetilde{\Theta}^2/(4Et)}$$

Correlator estimated from unwrapped normal phase variance has exponentially better StN than wrapped normal estimate

$$\widetilde{G}(t) = \sum_{i=1}^{N} |\varphi_i(t)\varphi_i(0)| \exp\left(-\frac{1}{2N}\sum_{i=1}^{N}\widetilde{\Theta}_i(t)^2\right)$$

$$\left\langle \widetilde{G}(t) \right\rangle = Z e^{-Et}$$

$$StN[\widetilde{G}(t)] \approx \sqrt{N}\frac{1}{\sqrt{2}Et}$$

Unwrapped phase squared is positive-definite for each field configuration, avoids sign problem facing usual correlator

Unwrapped Cumulant Expansion

Cumulant expansion provides correlator/energy estimates for an arbitrary wrapped phase distribution (assuming finite moments)

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

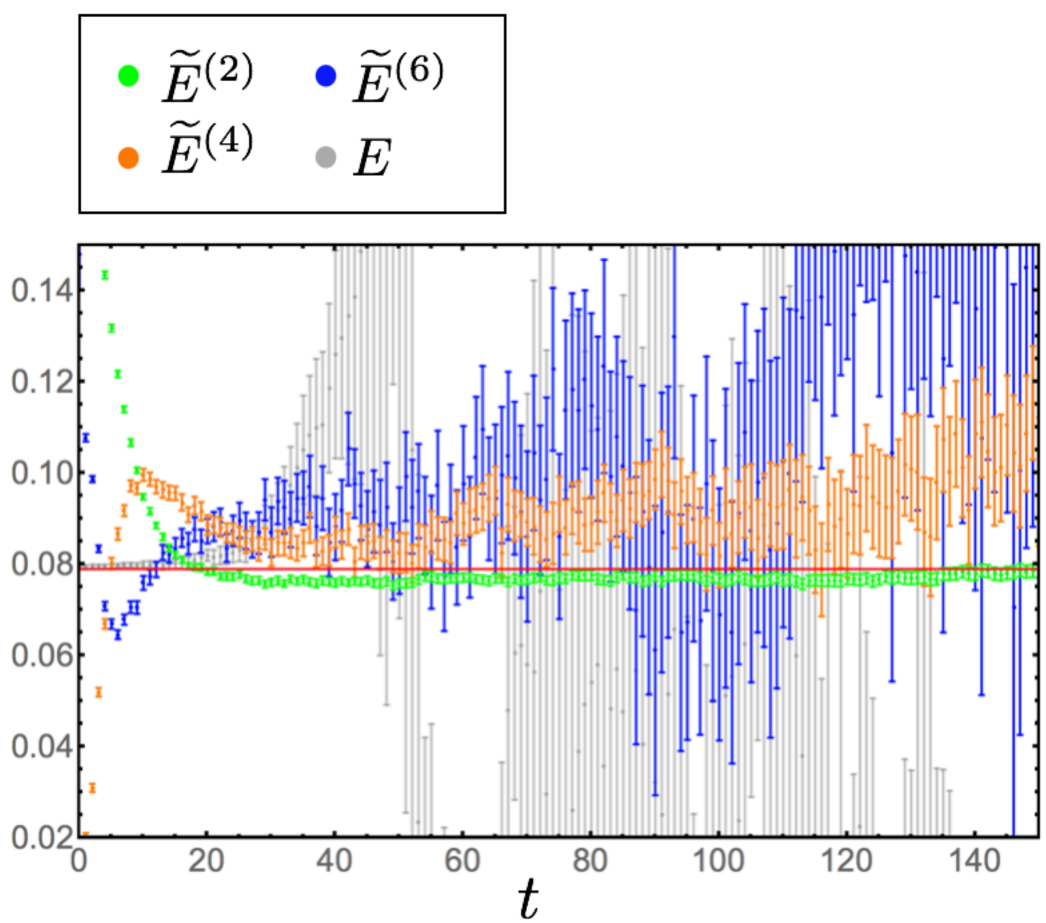
$$\widetilde{E}^{(n_{max})} = -\sum_{n=1}^{n_{max}} \frac{1}{n!} \partial_t \kappa_n \left(\mathscr{R} + i\widetilde{\Theta} \right)$$

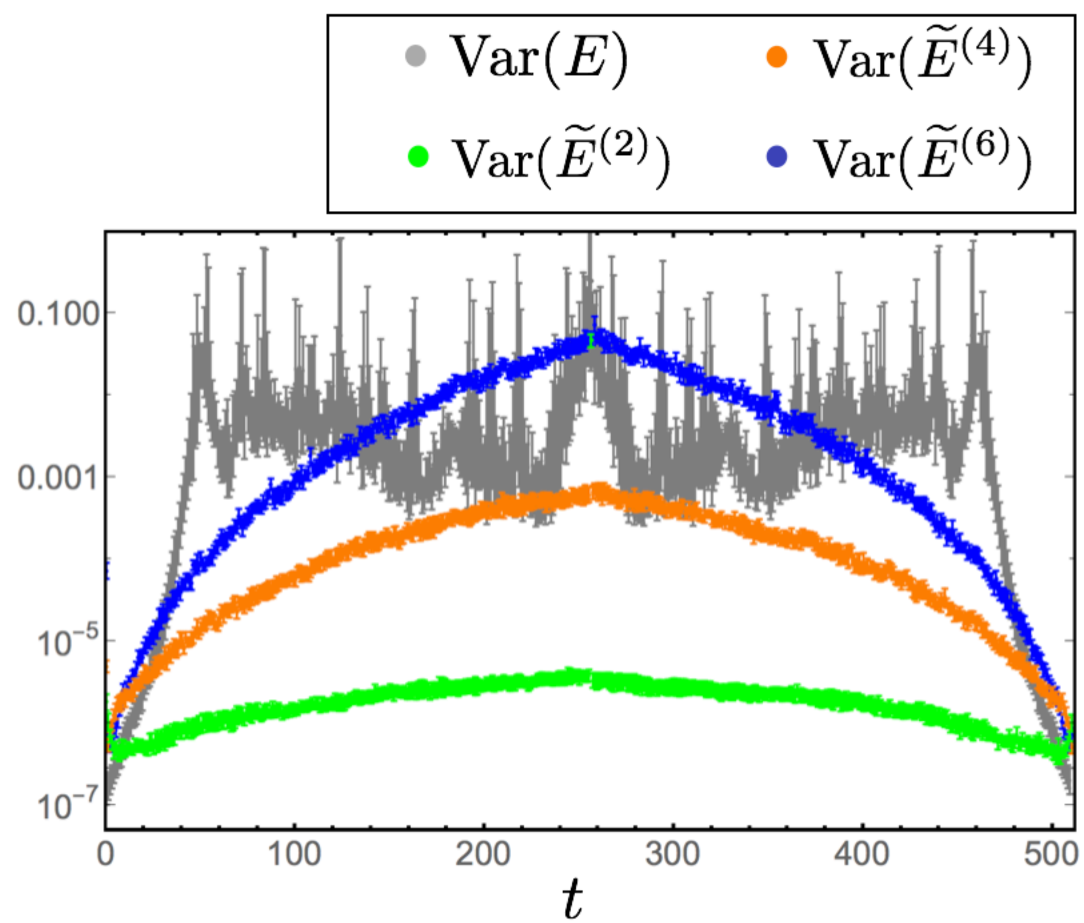
Based on cumulant expansion for real correlators,

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

Moments of normal random variables avoid exponential StN decay with *t*

$$StN\left[\widetilde{\Theta}^n\right] = \sqrt{N}\ 2^{-n+1/4}\ [1 + O(N^{-1}) + O(n^{-1})]$$

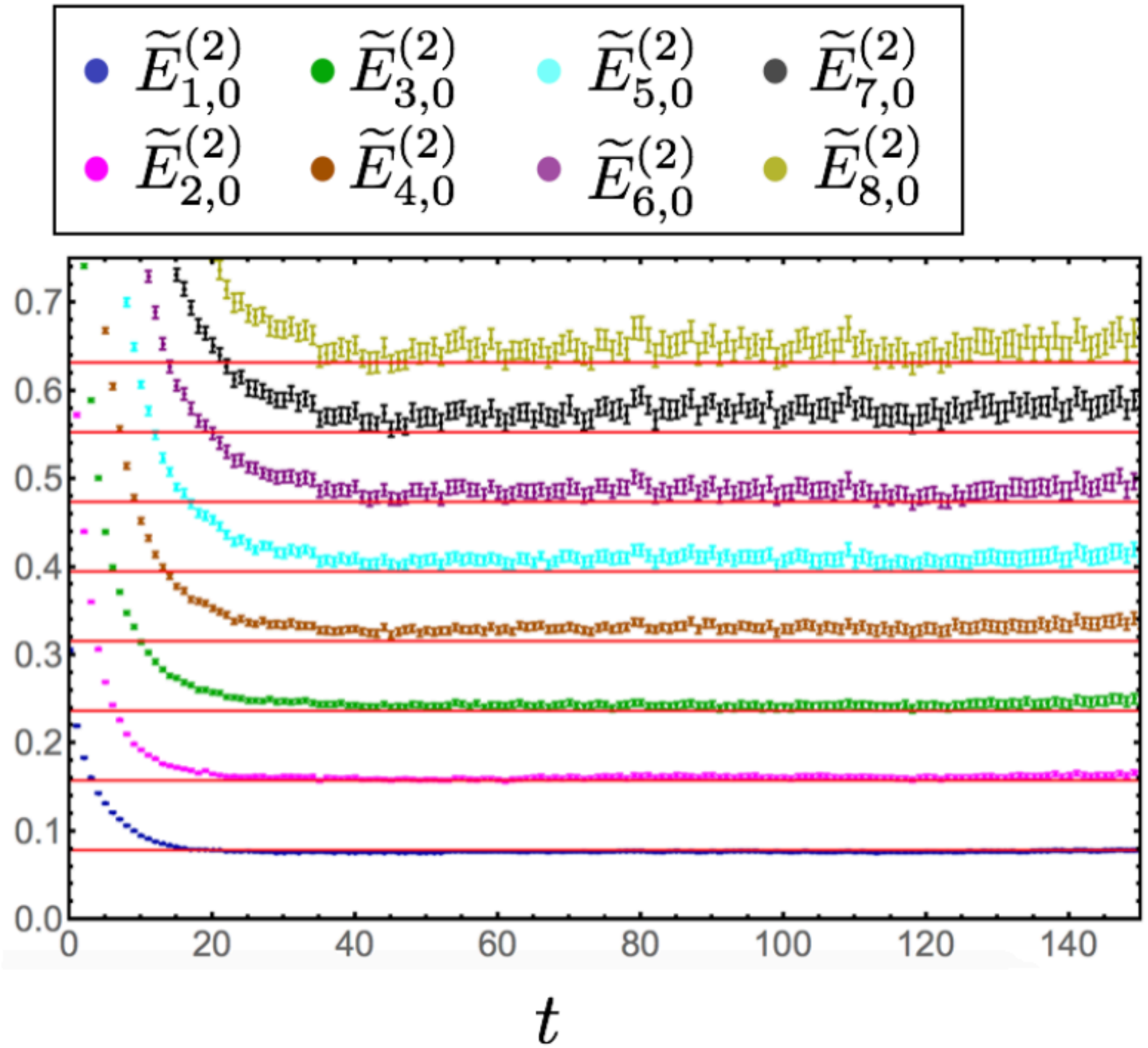


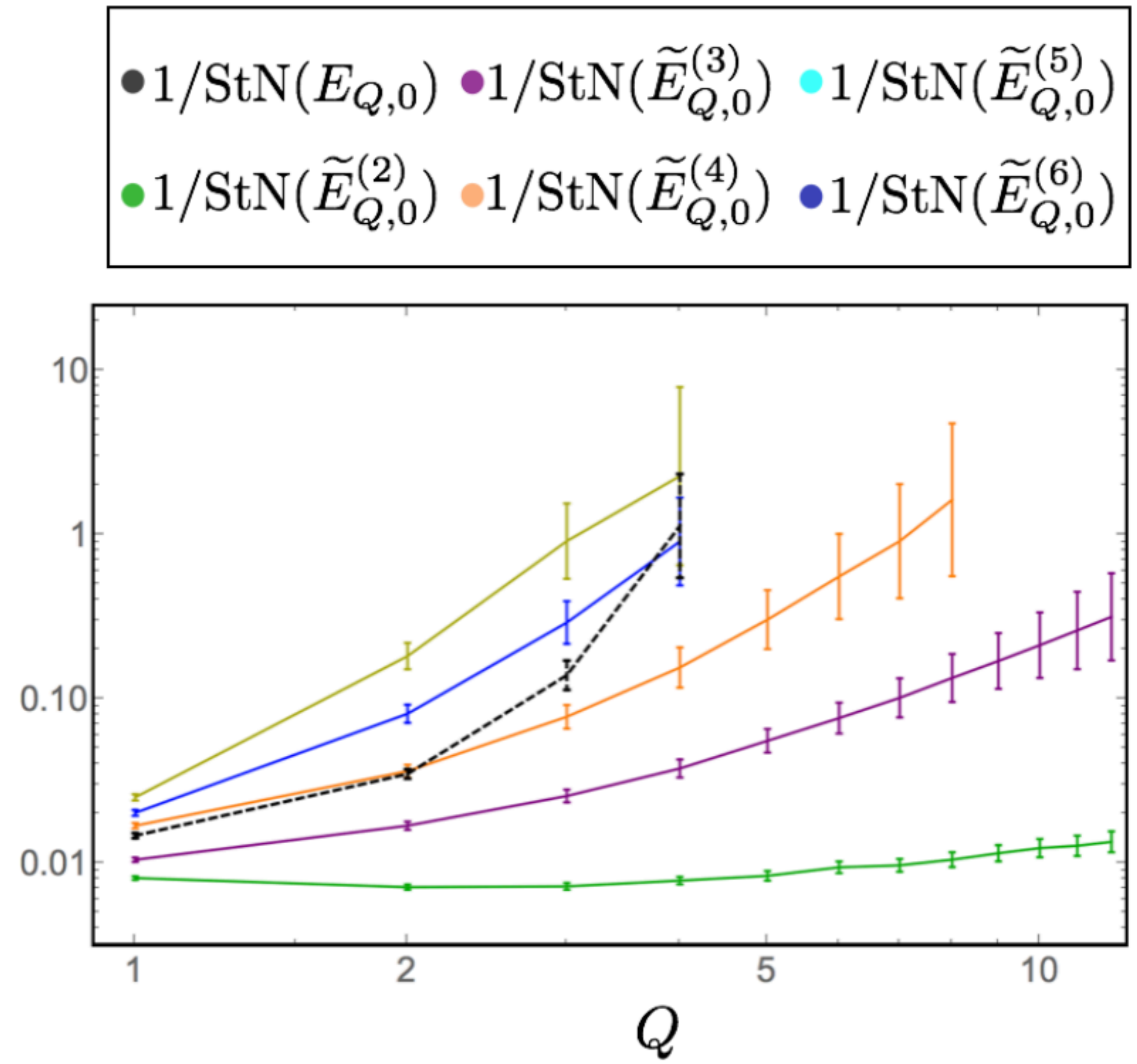


Phase Unwrapping Precision

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

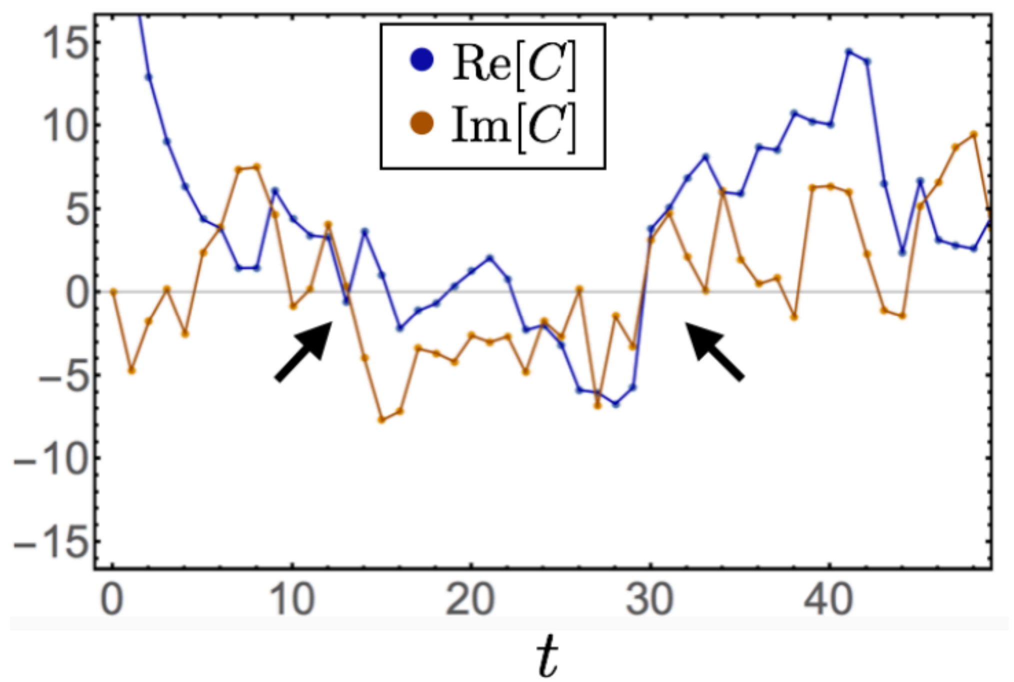


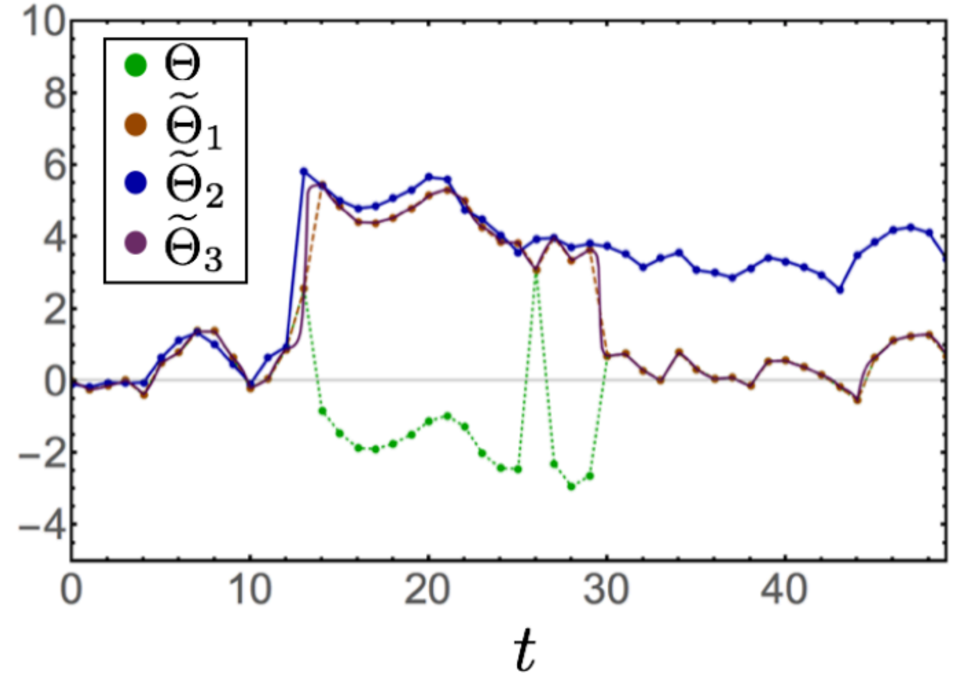


Large Phase Jump Ambiguities

Large phase jumps in regions of small magnitude are not Boltzmann suppressed and lead to ambiguities in phase unwrapping

$$S = 2\,|\,\varphi(t)\varphi(t-1)\,|\cos(\theta(t)-\theta(t-1)) + \ldots$$





Different definitions lead to large numerical discrepancies for all points after a large phase jump, accumulation of errors problem

Heavy-tailed phase jump distributions appear in 1D scalar field correlators as well as LQCD baryons, generic feature of LQFT?

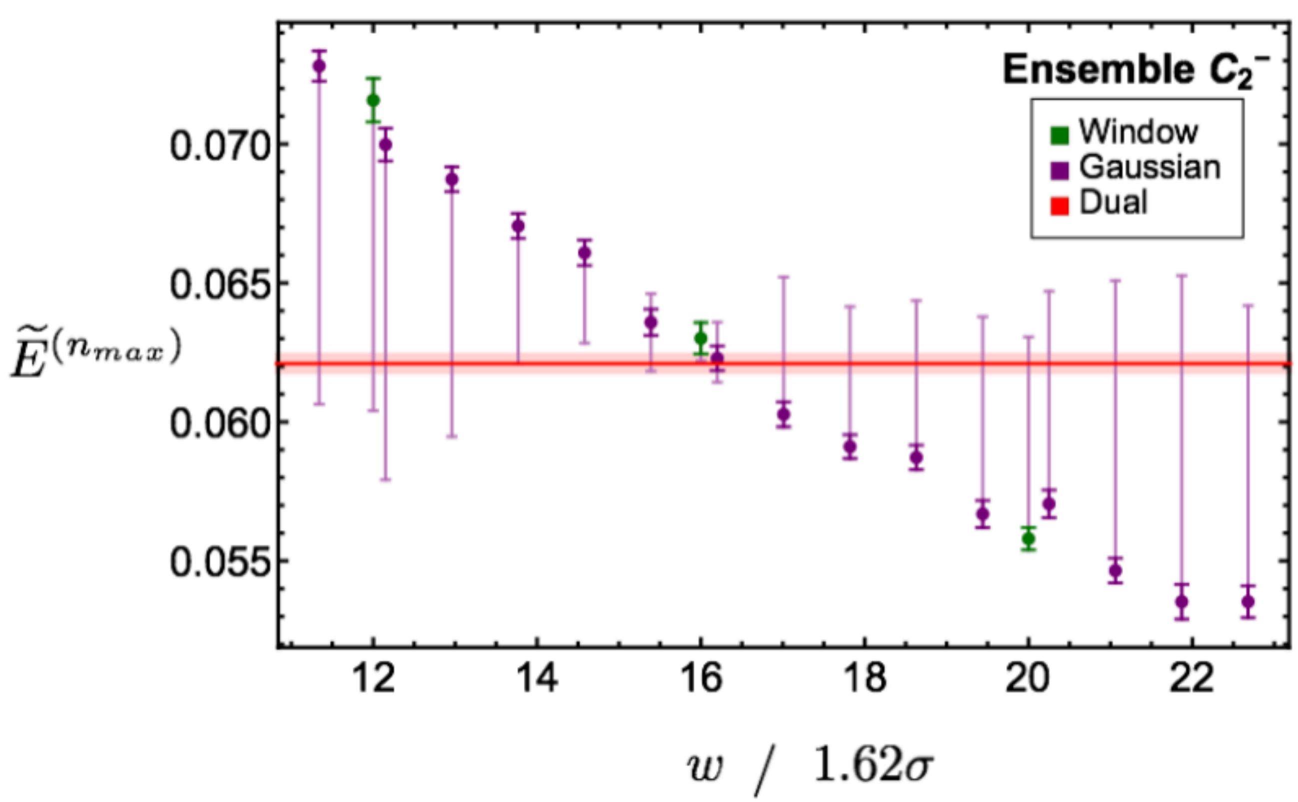
Adding Interactions

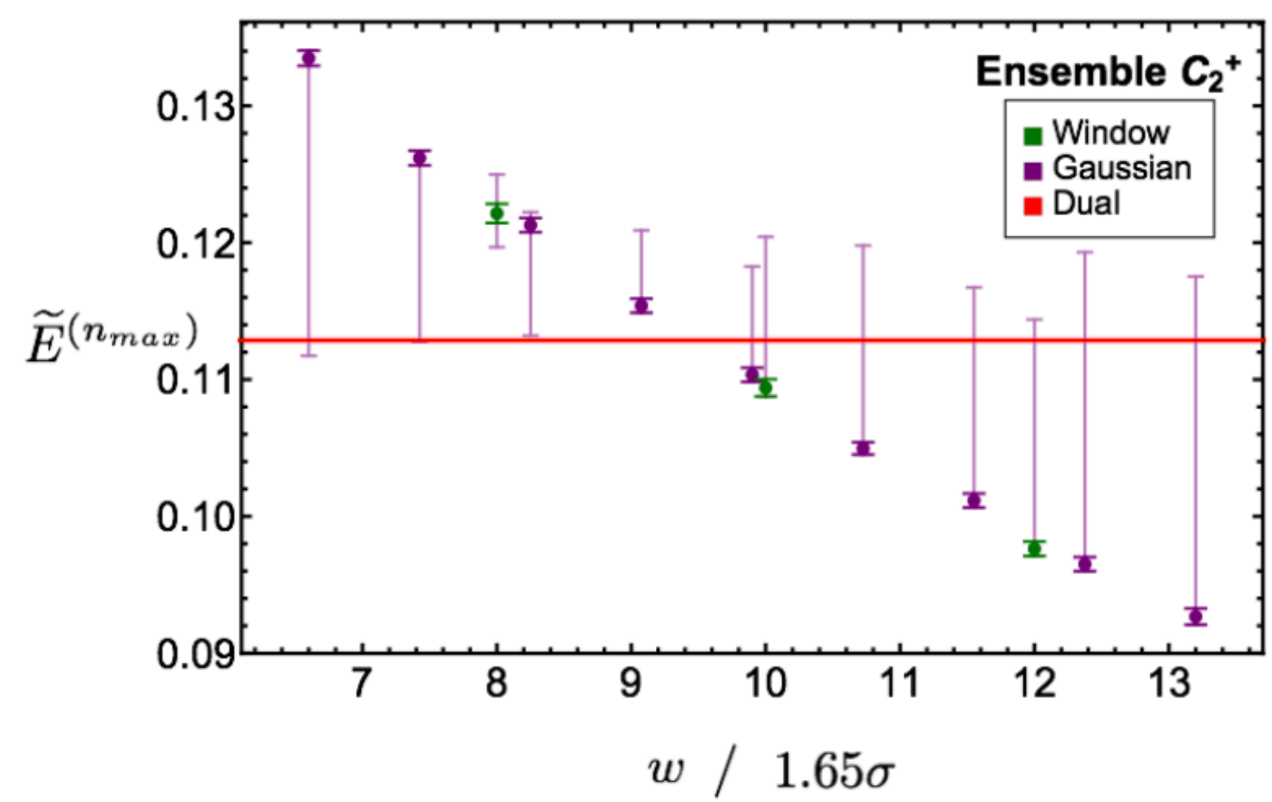
Phase unwrapping (and dual variable integration) can be immediately applied to interacting (0+1)D scalar field theory

$$S = \sum_{t=0}^{L-1} (\varphi^*(t+1) - \varphi^*(t))(\varphi(t+1) - \varphi(t)) \pm M^2|\varphi^2| + \lambda|\varphi^4|$$

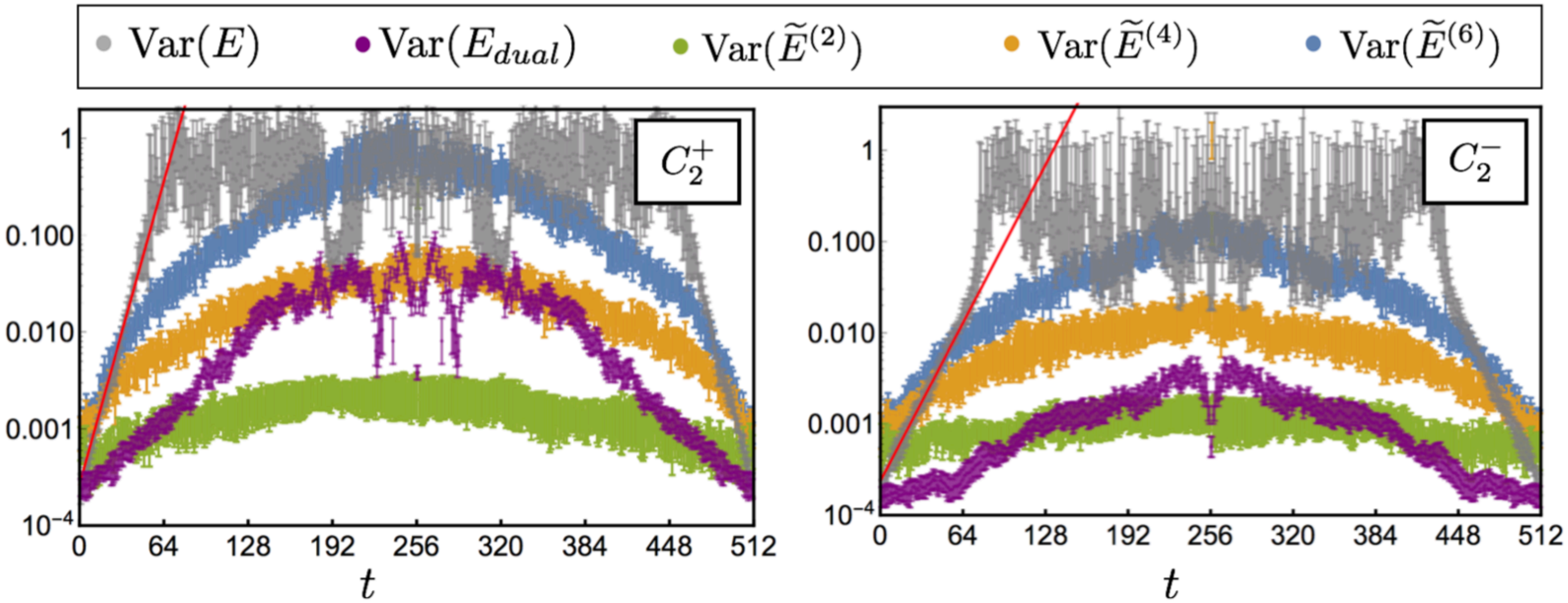
Large phase jump ambiguities appear for positive and negative mass

Accurate results obtained at leading order in cumulant expansion if integration window is (self-consistently) tuned to correlation length

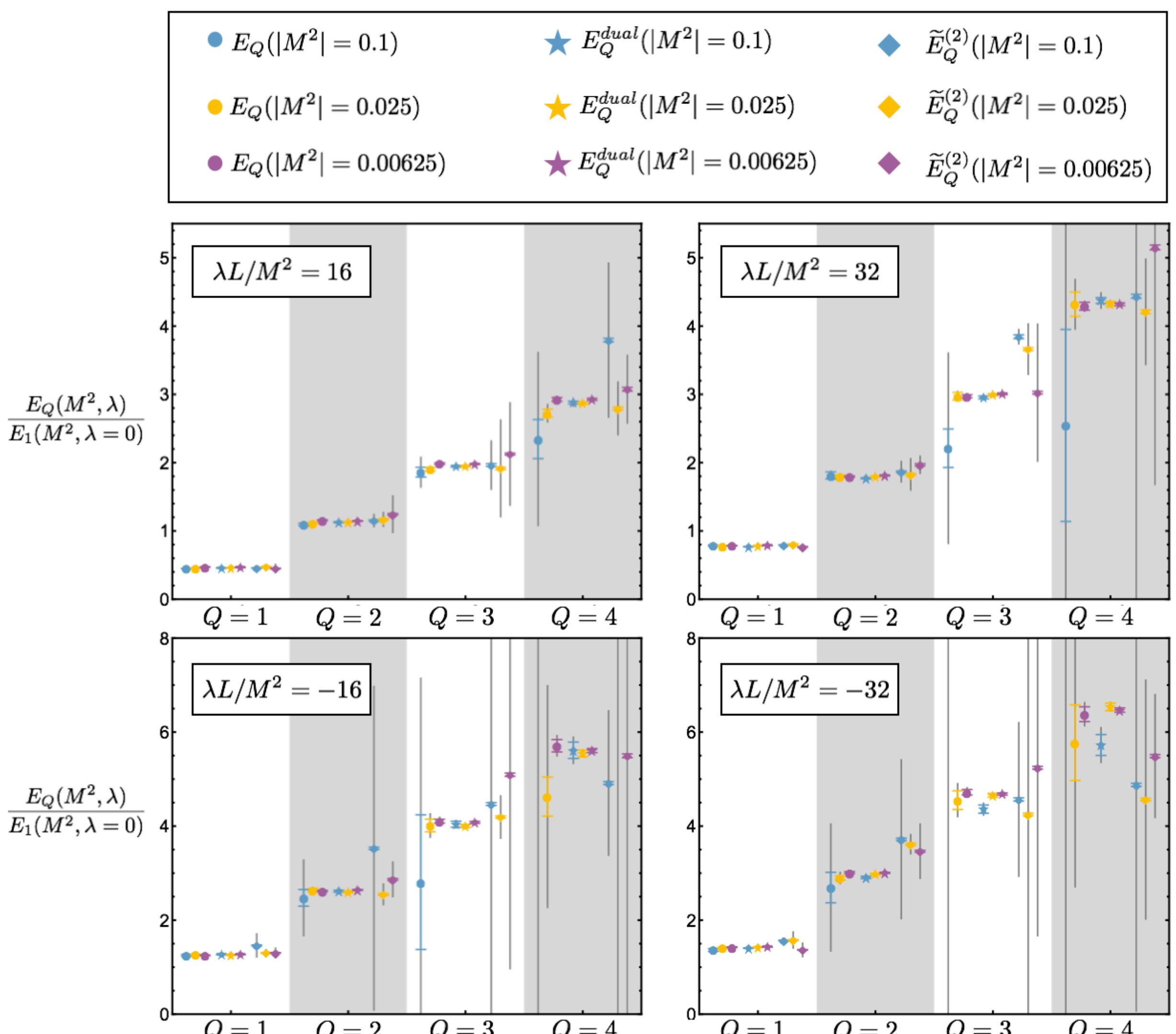




One-Dimensional Results



Leading order unwrapped phase cumulant expansion has even better StN than dual variable estimate



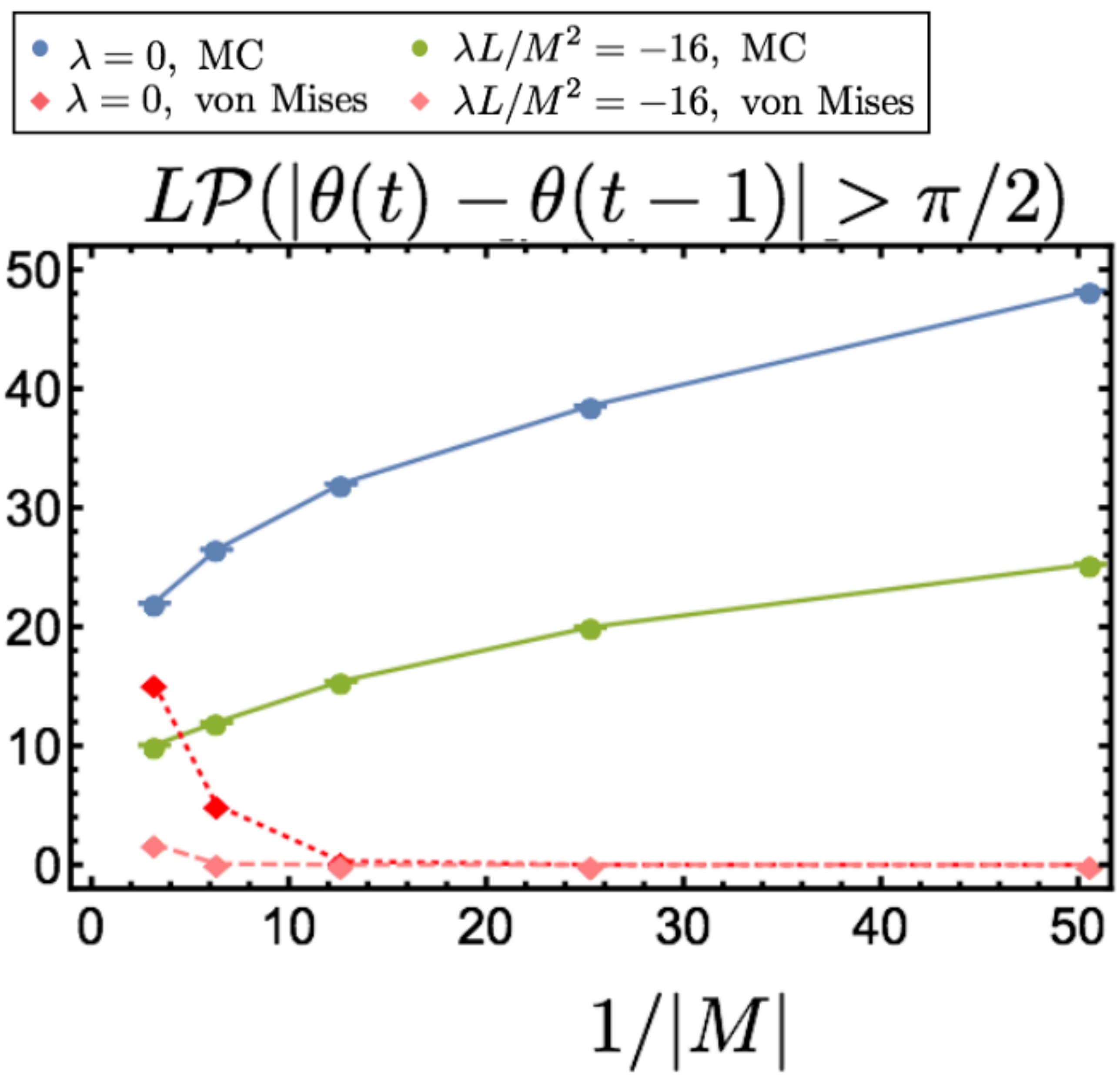
Higher order cumulants add noise (exponentially) quickly

When systematic uncertainty estimates for truncation errors are included, phase unwrapping does not provide precise results

One-Dimensional Obstacles

Ignoring magnitude fluctuations, large phase jumps become rare as the lattice spacing becomes smaller than physical scales

$$Prob[\,|\,\partial_t\Theta\,|\, > \pi - \epsilon) = \frac{2}{I_0(\kappa)} \int_{\pi-\epsilon}^{\pi} \frac{d\Delta}{2\pi} e^{2|\varphi(t)\varphi(t-1)|\cos(\Delta)}$$



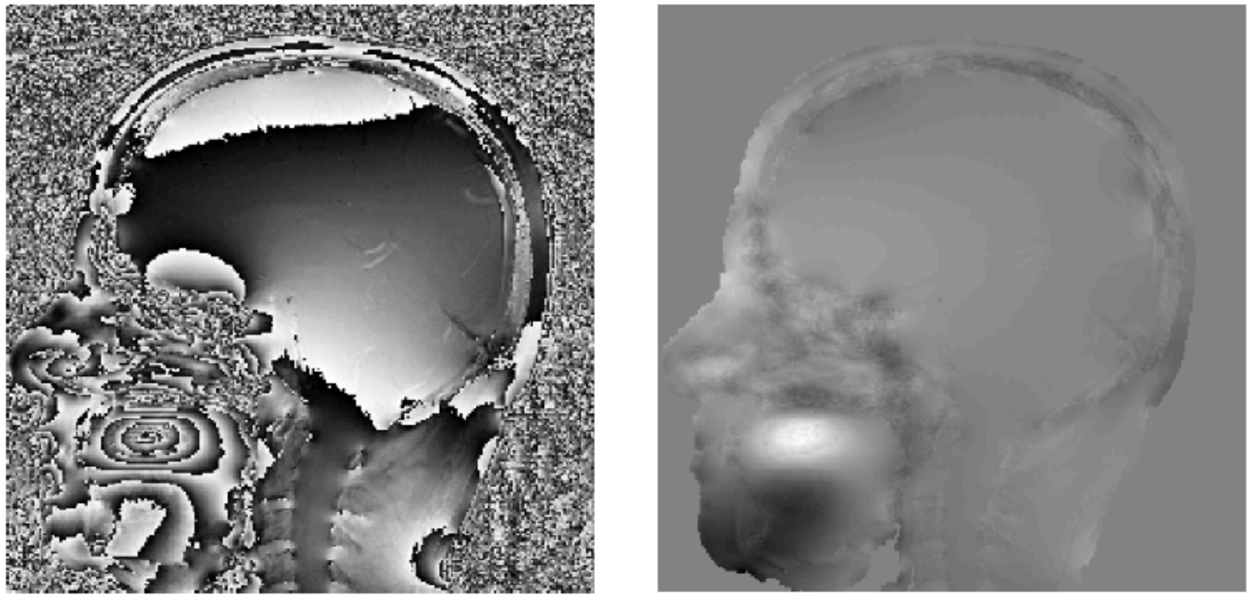
In MC data including magnitude fluctuations, probability of a large phase jump somewhere in lattice volume ***increases*** as the lattice spacing is reduced

Large phase jumps and 1D accumulation of errors appear insurmountable obstacles

Higher Dimensional Outlook

Multidimensional phase unwrapping has been explored in signal processing, radar, MRI, etc. for decades

Enforcing consistency between multiple unwrapping paths allows error correction, numerically robust algorithms in higher dimensions

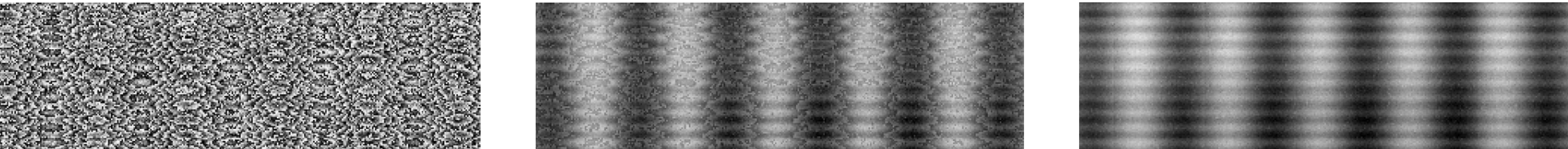


Ying (2006)

Alternatives to truncated cumulant expansions — reweighting correlator path integrals with low-order unwrapped cumulant estimators?

Much more to explore!

Detmold, Kanwar, MW, *in progress*



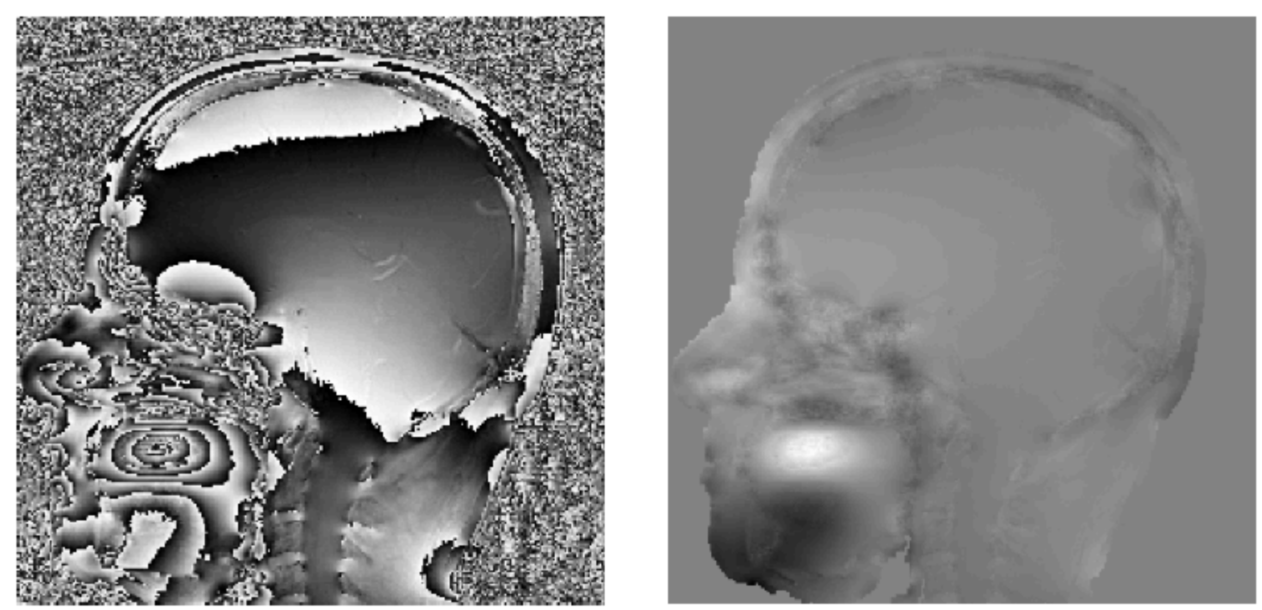
Conclusions

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

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



Ying (2006)