Sign problem time

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From Euclidean spectral densities to real-time physics

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Highly preliminary work in collaboration with

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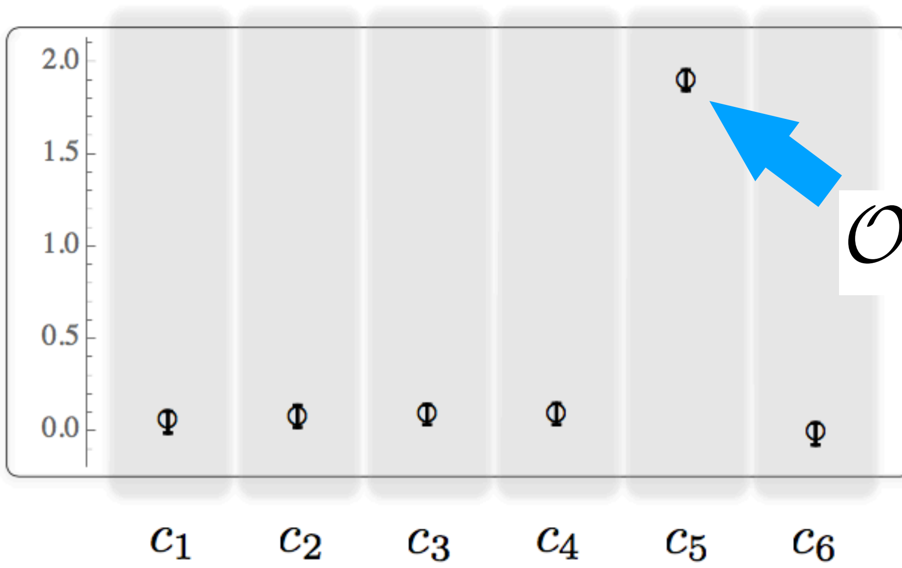
Real results with imaginary time

$$\mathcal{L}_{EFT(\not\pi)} = c_i \mathcal{O}_i$$

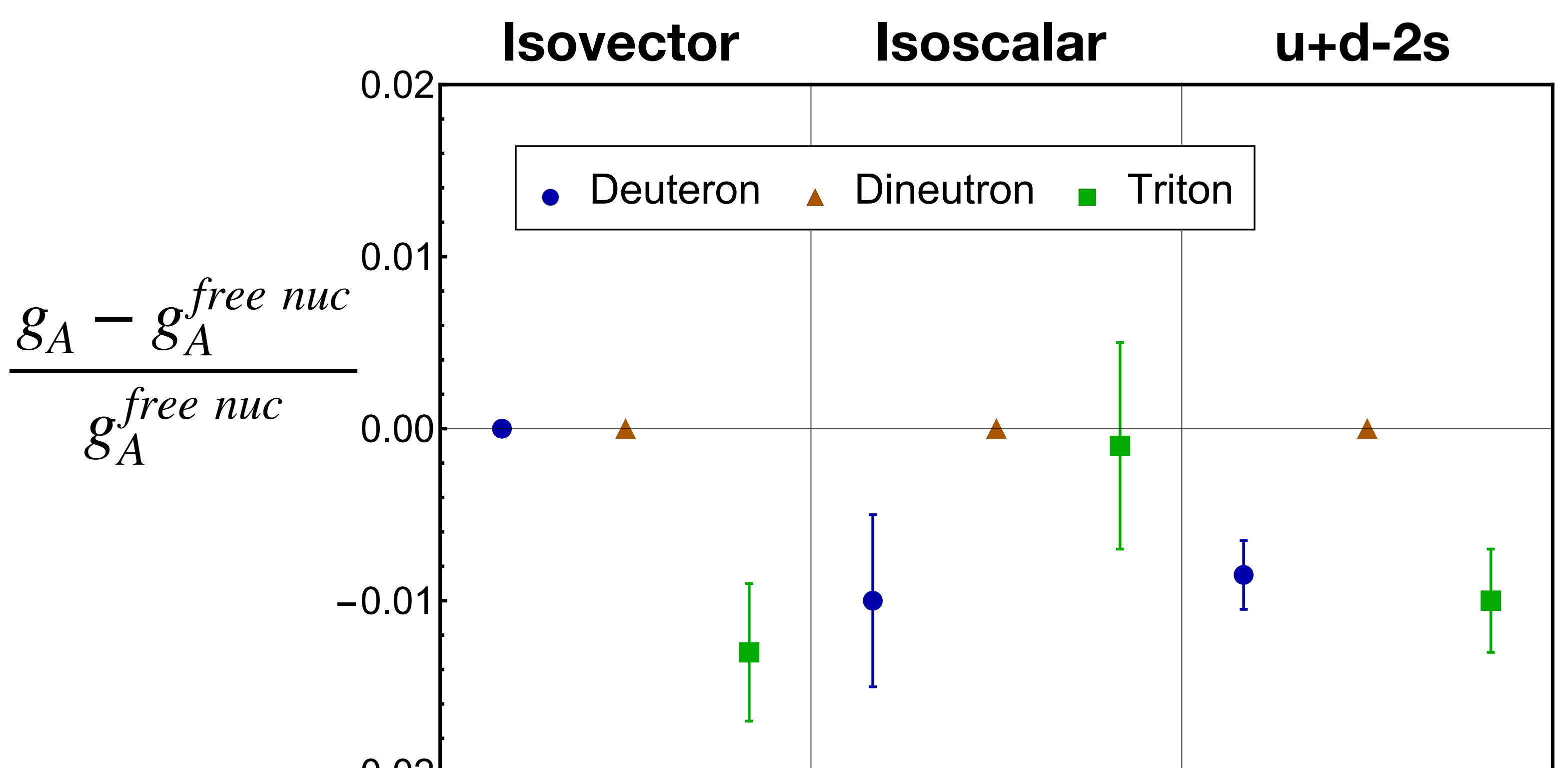
Baryon-baryon interactions have large scattering lengths and little spin-flavor dependence



$$\mathcal{O}_5 = (\overline{B}B)^2$$

$$N_f = 3,\ m_\pi = 806(9)\ \text{MeV},\ a = 0.145(2)\ \text{fm}$$

MW + NPLQCD, PRD 96 (2017)



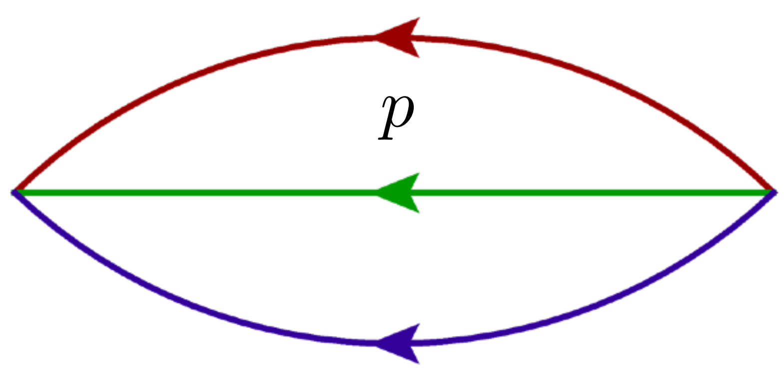
MW + NPLQCD, PRL 120 (2018)

Light nuclei "look like" non-interacting nucleons plus few-percent QCD effects

Larger QCD effects in larger nuclei needed to interpret BSM physics searches

The signal-to-noise problem

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



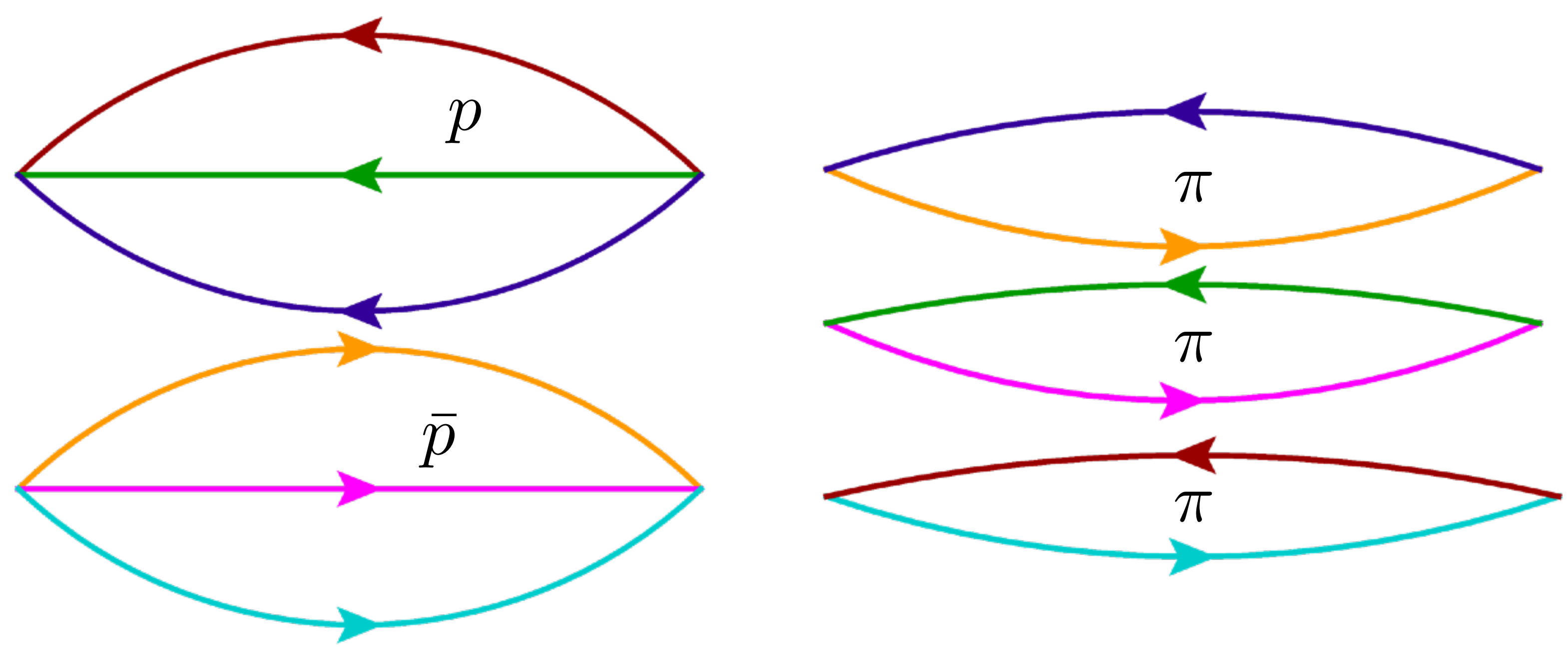
$$G_N(t) = \left\langle N(t) N(0)^\dagger \right\rangle \sim e^{-M_N t}$$

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

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

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

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



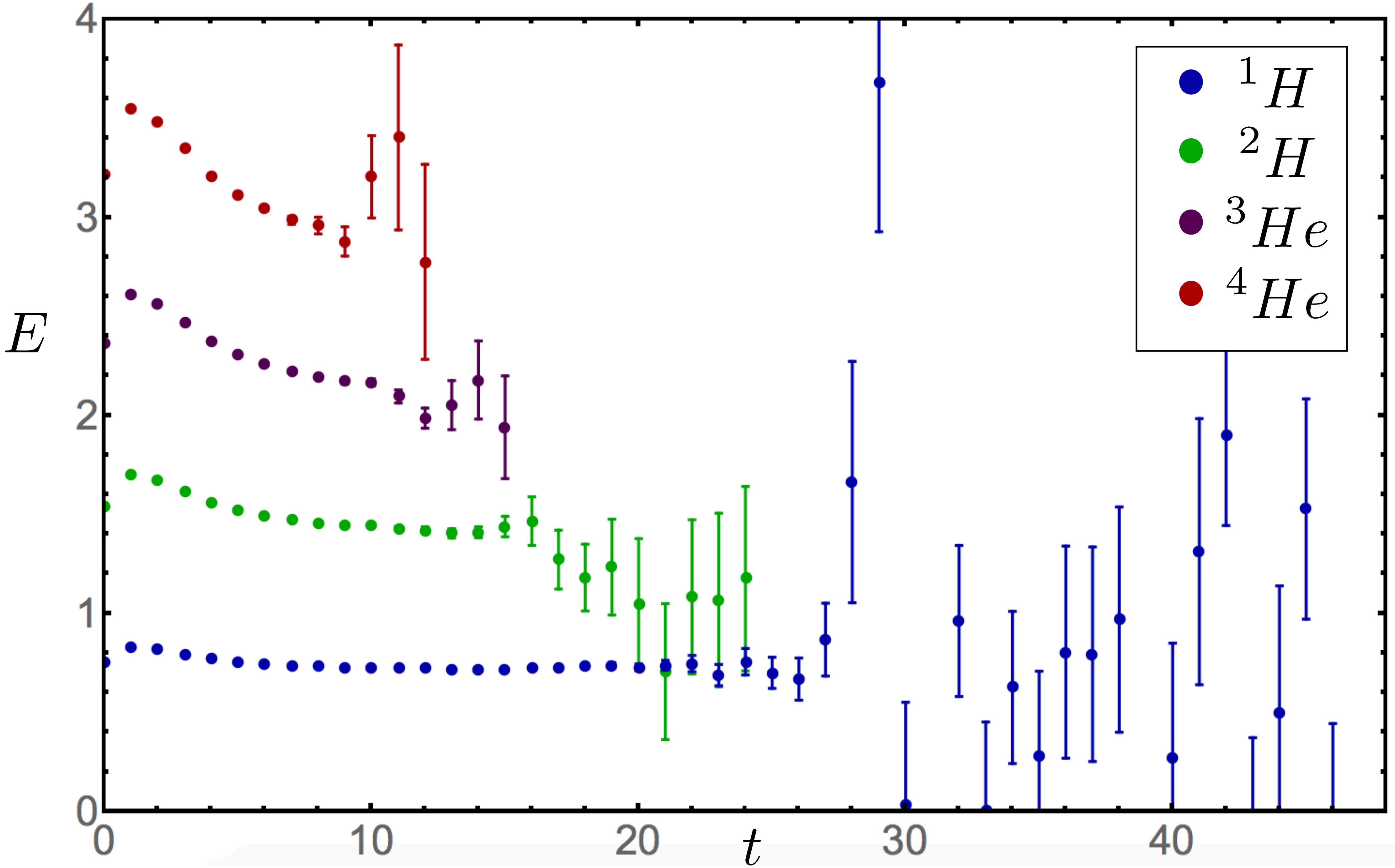
Signal-to-noise problem:

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

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

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

The signal-to-noise problem



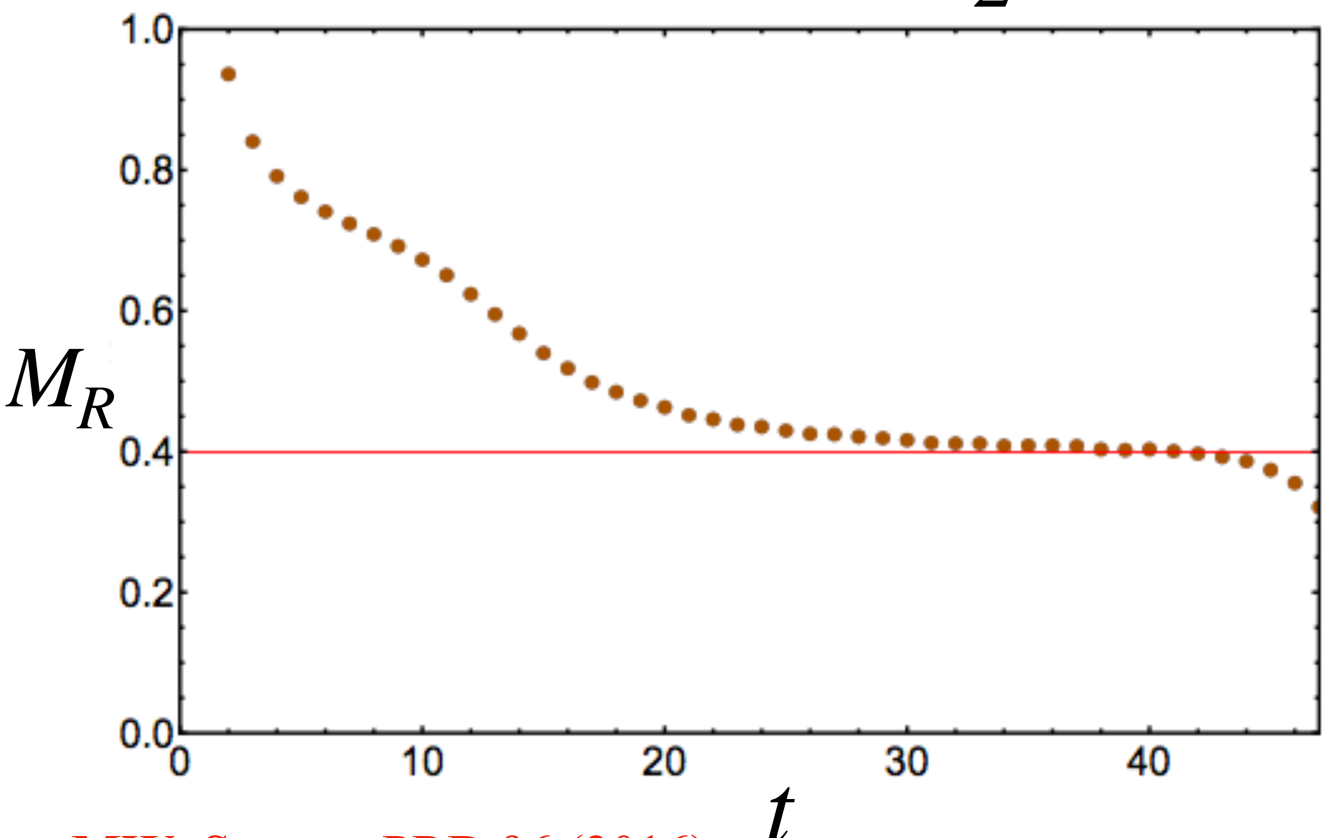
The (sign)al-to-noise problem

Quark propagators and generic hadron correlators have complex phases in background gauge fields

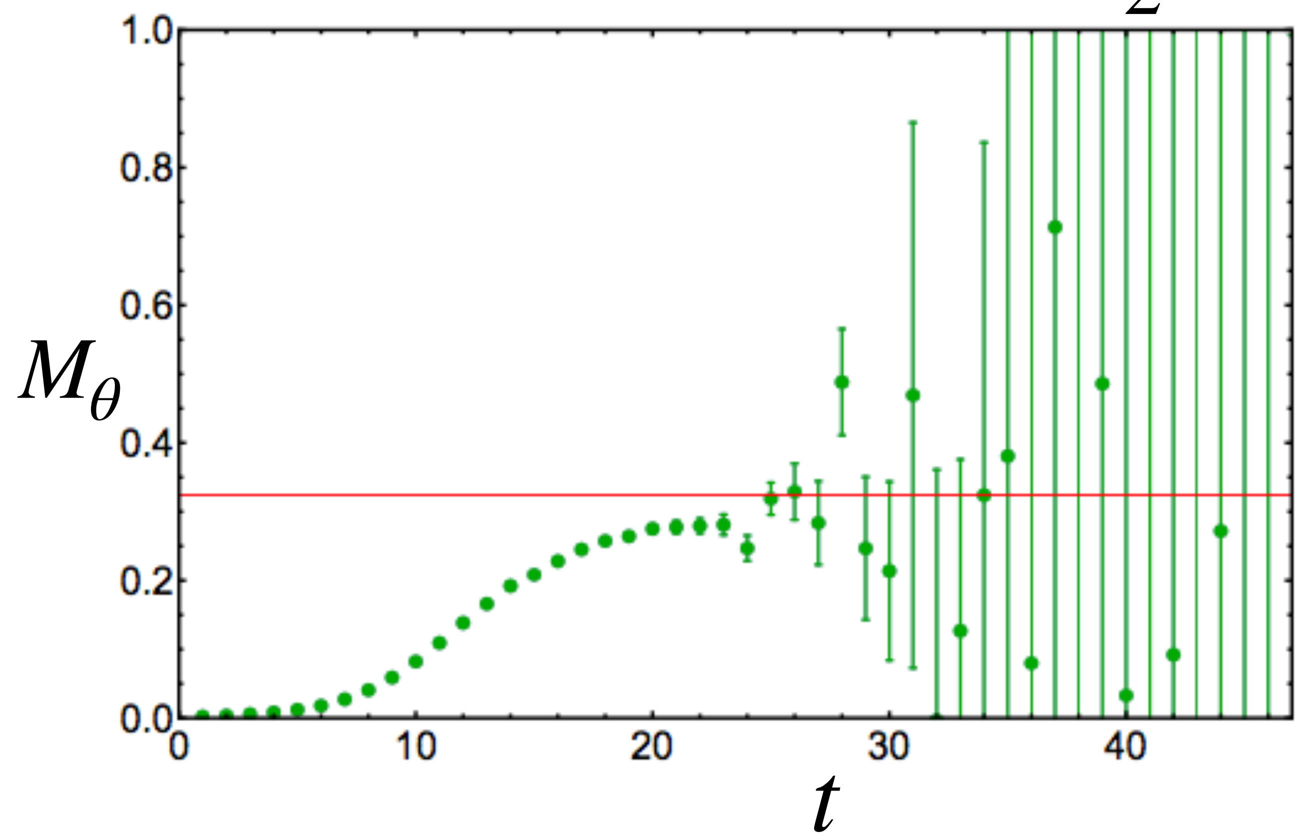
$$Z^{-1}\int \mathcal{D}U\ e^{-S_E(U)}C(t,U) = Z^{-1}\int \mathcal{D}U\ e^{-S_E(U)+R(t,U)+i\,\theta(t,U)}$$

Phase leads to sign problems for path integrals defining correlation functions, also responsible for baryon signal-to-noise problem

$$M_R = -\,\partial_t \ln \left\langle e^{R(t)} \right\rangle \sim \frac{3}{2} m_\pi$$



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



MW, Savage, PRD 96 (2016)

Phase fluctuations

Correlation function phases for large source/sink separations are sums of many random phase differences

$$\langle \mathcal{O}(t)\mathcal{O}(0)^\dagger \rangle_U = Z_0^2 \prod_s < 0(U, s+1)|e^{-H}|0(U,s) > + \ldots$$

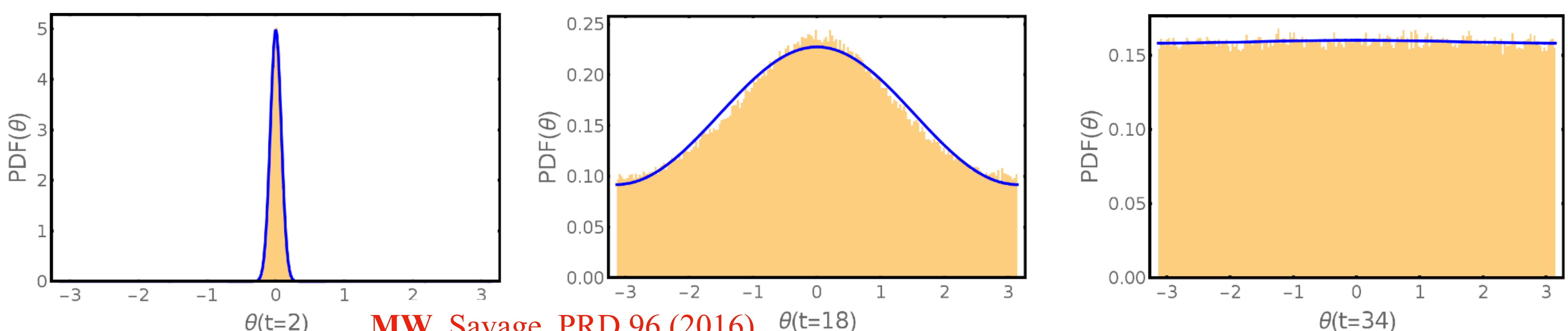
Log-normal for pions: Hamber, Marinari, Parisi and Rebbi, Nucl Phys B225 (1983)
Endres, Kaplan, Lee and Nicholson, PRL 107 (2011)

Central limit theorem for random phases: increasingly broad "wrapped normal distribution" approaches uniform distribution

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

$$\mathcal{P}(\theta(t)) \approx \frac{1}{\sqrt{2\pi\sigma^2(t)}} \sum_k e^{-(\theta(t)-2\pi k)^2/(2\sigma(t)^2)} \qquad \sigma^2(t) \sim 2\left(M_N - \frac{3}{2}m_\pi\right)t$$

QCD nucleon phase with wrapped normal fit



MW, Savage, PRD 96 (2016)

Real time (imaginary results…)

Minkowski gauge action linear combination of many plaquettes, expect approximately (wrapped) normal for large volume

$$S_G^M = \frac{1}{g^2} \sum_x \left\{ \sum_k \mathrm{Re\ Tr}[1 - \mathcal{P}_{k4}] - \sum_{i<j} \mathrm{Re\ Tr}[1 - \mathcal{P}_{ij}] \right\}$$

Universal toy sign problem

$$\int \mathcal{D}U\ e^{-S_E(U) + R(t,U) + i\,\theta(t,U)} \qquad\qquad \int \mathcal{D}U\ e^{iS_M(U)}$$

$$\int d\theta\ e^{i\theta\ -\ \theta^2/(2\sigma^2)\ +\ \dots}$$

Toy model: Gaussian random phase

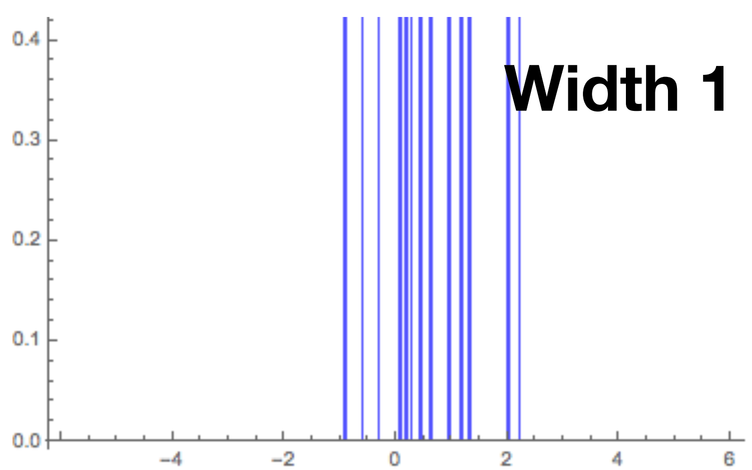
Calculating variance of random phase has a sign(al-to-noise) problem

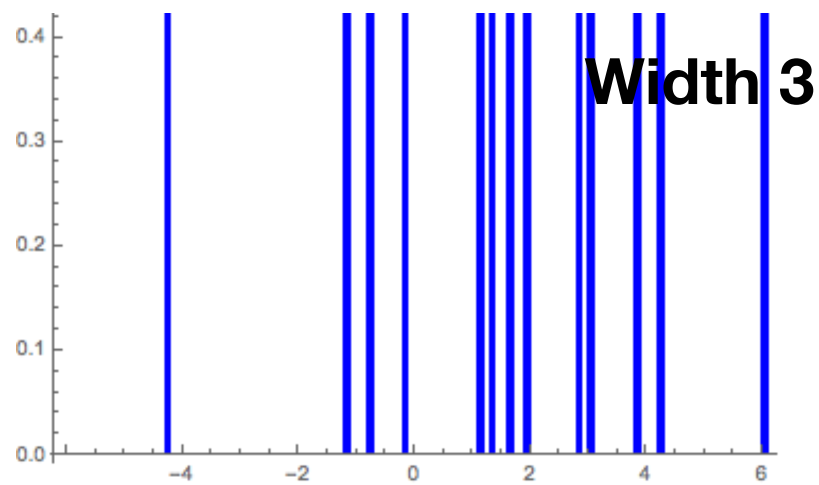
$$\sigma^2 = \langle x^2 \rangle \qquad \sigma^2 = -\ln \langle \cos\theta \rangle$$

$$\mathrm{StN}(x^2) \sim \frac{\langle x^4 \rangle}{\langle x^2 \rangle^2} \sim 1$$

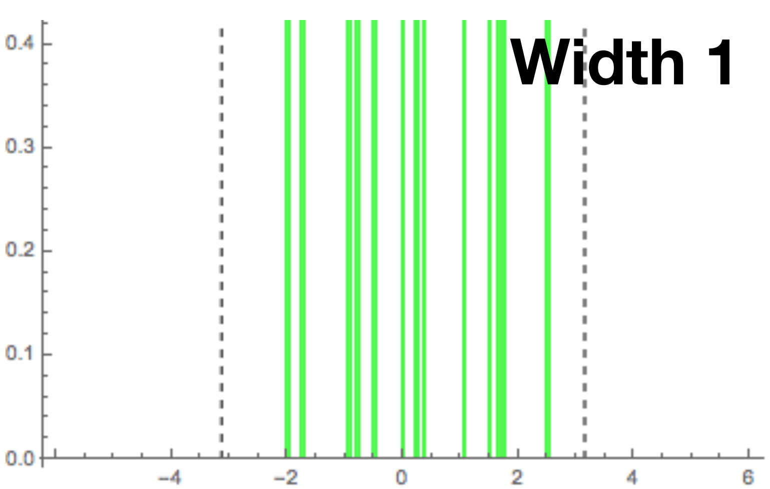
$$\mathrm{StN}(\cos\theta) \sim \frac{\langle \cos\theta \rangle}{1 - \langle \cos 2\theta \rangle} \sim e^{-\sigma^2}$$

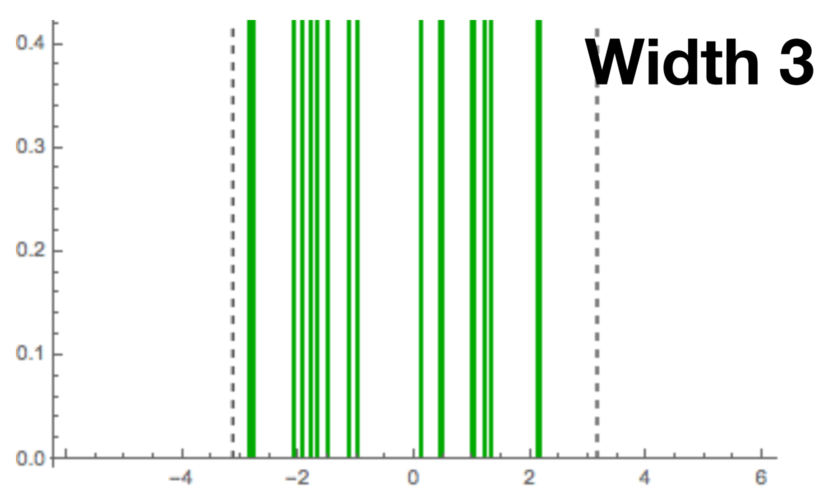
Normal random variables

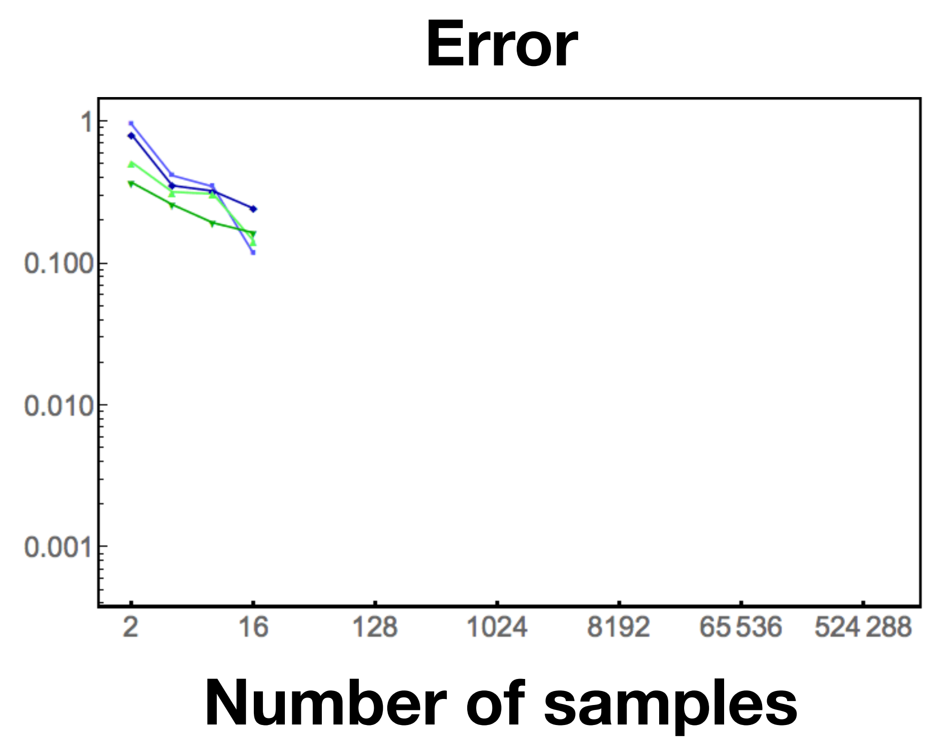




Wrapped normal random phases





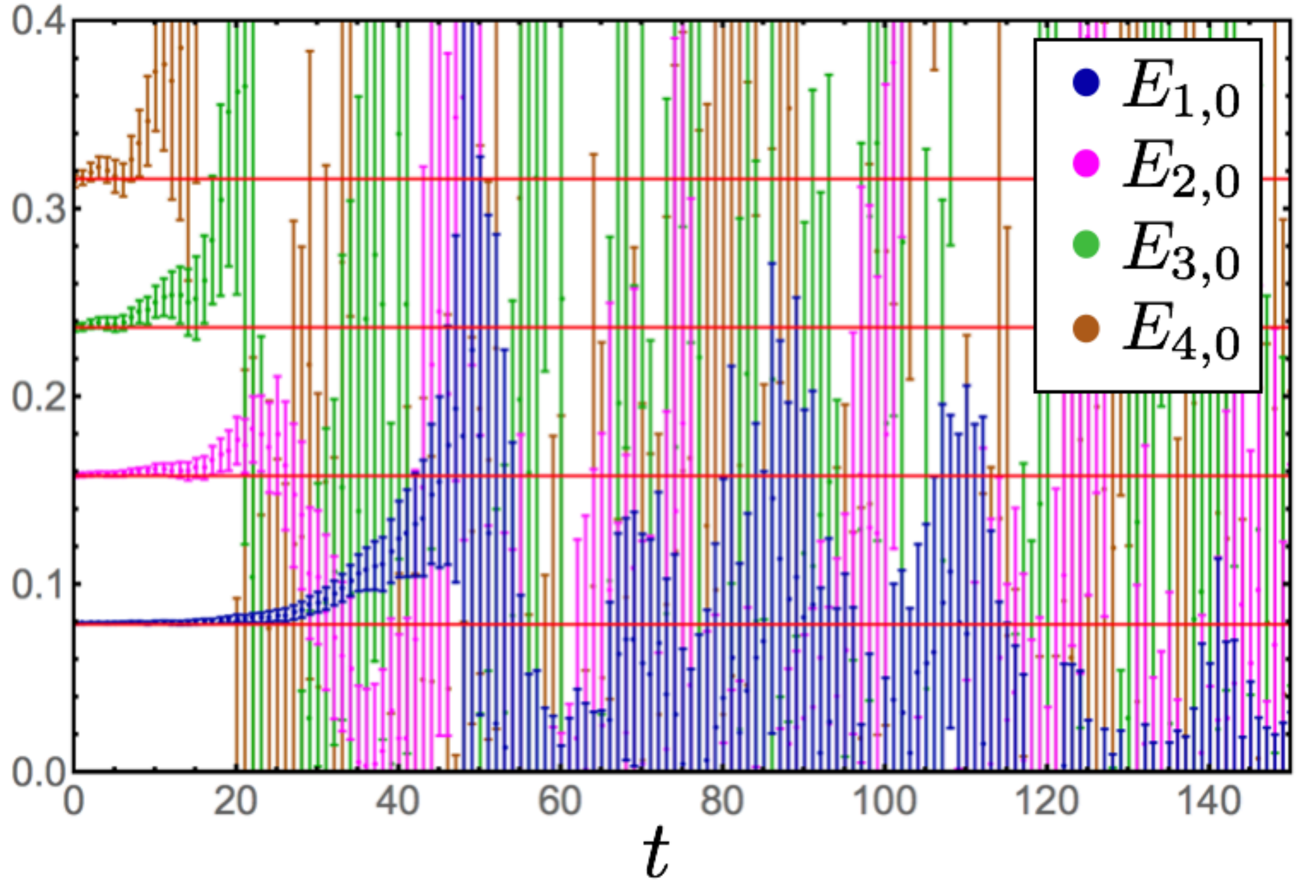


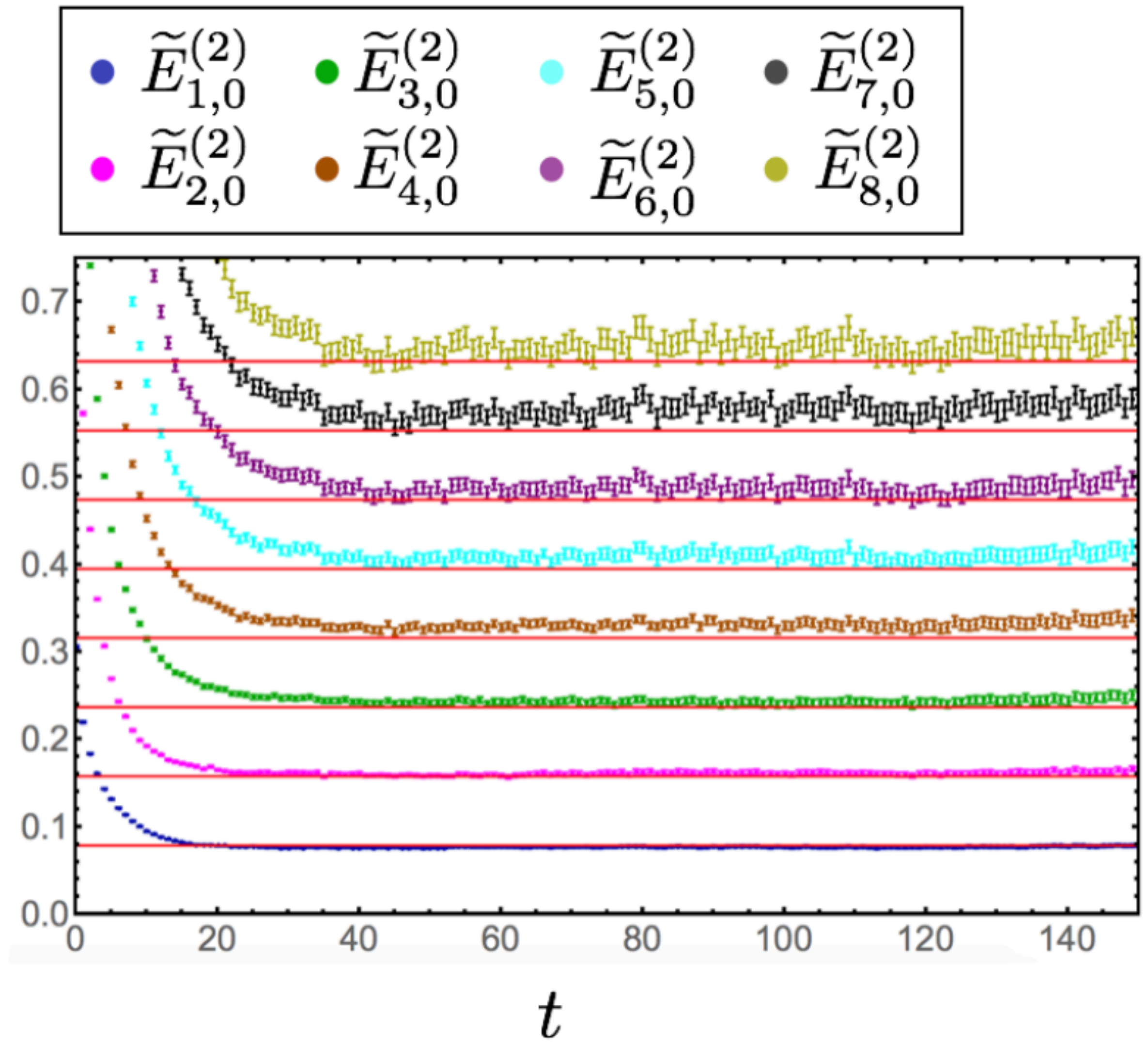
Bigger toy: free scalar field theory

Complex scalar: U(1) charge signal-to-noise problem

Under Gaussian assumptions, exponential noise avoided by sampling a non-compact (unwrapped) phase instead of compact phase

Detmold, Kanwar, **MW**, PRD 98 (2018)





Systematically improvable but noise re-appears in higher cumulants

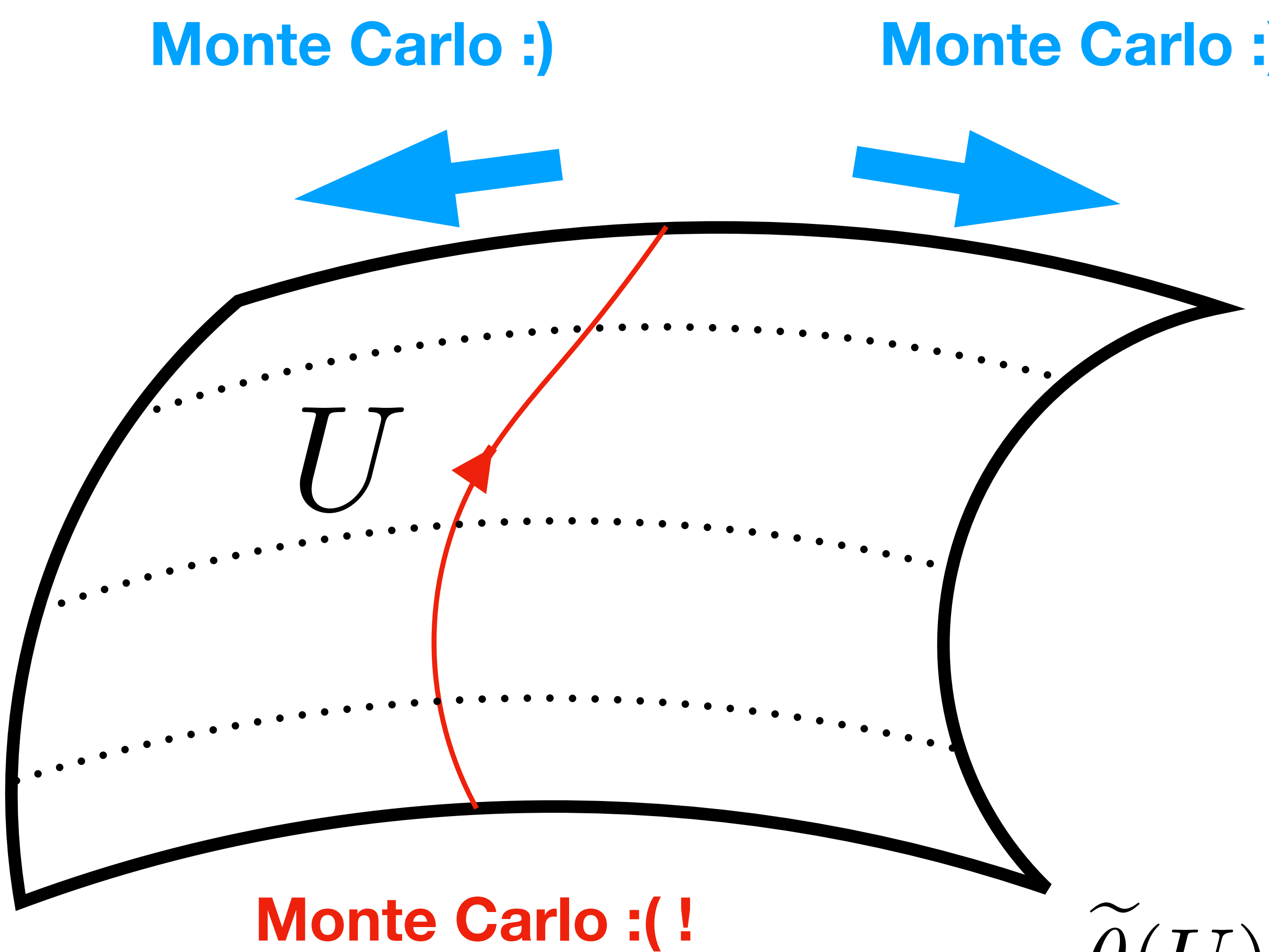
Similar ideas for baryon chemical potential: Ejiri, PRD 77 (2008)

Don't Monte Carlo sample phases

$$\int \mathcal{D}U \; e^{-S_E(U)+i\widetilde{\theta}(U)}$$

Smooth non-compact phase defines one-dimensional line in configuration space

Monte Carlo without sign problem possible on level sets with fixed non-compact phase



$$\widetilde{\theta}(U) = \widetilde{\theta}_{max}$$

Need different method for one-dimensional integral along line of varying phase

$$\widetilde{\theta}(U) = -\widetilde{\theta}_{max}$$

Density-of-states methods

Rewrite path integral to separate out 1D phase integral

$$Z = \int \mathcal{D}U e^{-S_E(U)+iS_M(U)} = \int dS_M \int \mathcal{D}U\ \delta(S_M - S_M(U))\ e^{-S_E(U)+iS_M(U)}$$

$$\equiv \int dS_M\ \rho(S_M)\ e^{iS_M}$$

Log-linear-relaxation (LLR) anstatz, piecewise linear polynomial

$$\frac{\partial \log \rho(S_M)}{\partial S_M} \approx \sum_i a_i \Theta_i\left(S_M\right)$$

Controlled fractional error

$$\left| \frac{\rho_{LLR}(S_M)}{\rho(S_M)} - 1 \right| = O(\delta S_M)^2$$

$$\delta S_M = S_M^{i+1} - S_M^i$$

Wang, Landau, PRL 86 (2001)

Langfeld Lucini Rago, PRL 109 (2012)

Lucini, Francesconi, Holzmann Rago, arXiv 1901.07602

SK density-of-states

Defining path integrals including LLR density of states,

$$\langle\langle O(U)\rangle\rangle_i \equiv \frac{\int \mathcal{D}U\ O(U) e^{-a_i S_M - S_E}\Theta_i(S_M)}{\int \mathcal{D}U\ e^{-a_i S_M - S_E}\Theta_i(S_M)}$$

LLR coefficients can be found by solving constraint equation

$$0 = \langle\langle S_M - (S_M^i + S_M^{i+1})/2\rangle\rangle_i$$

stochastically using e.g. iterative Robbins-Monroe method

$$a_i^{(n+1)} = a_i^{(n)} + \frac{12\epsilon_i}{n\left(S_M^{i+1} - S_M^i\right)^2}$$

Completely analogous to LLR for Euclidean density-of-states!

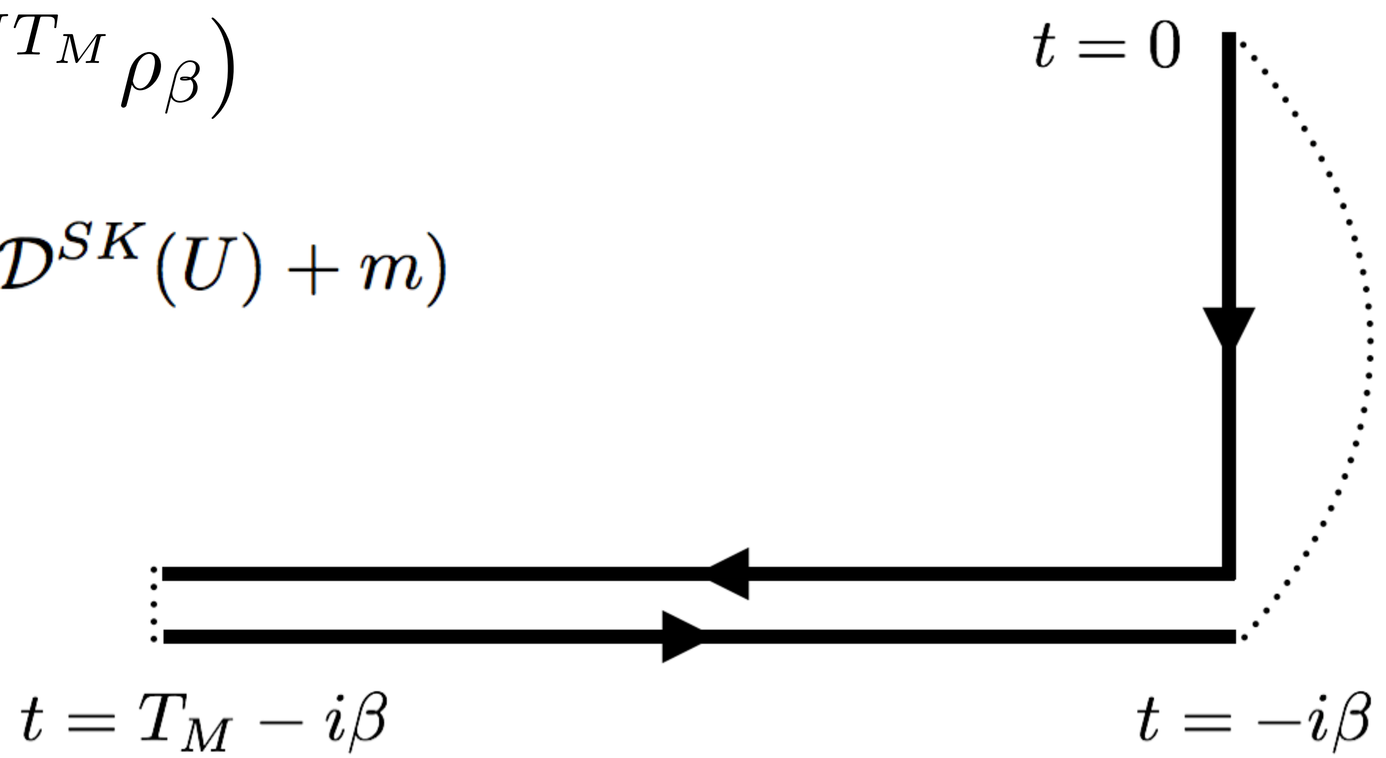
Langfeld Lucini Rago, PRL 109 (2012)

Going out of equilibrium

Schwinger-Kelydsh partition function

$$Z = \mathrm{Tr}\left(\rho_\beta\right) = \mathrm{Tr}\left(e^{iHT_M} e^{-iHT_M}\rho_\beta\right)$$

$$= \int \mathcal{D}U\ e^{-S_G^E(U)+iS_G^M(U)}\ \det(\mathcal{D}^{SK}(U)+m)$$



Extensive phase trivially obtained by summing plaquettes on real-time contour segments

Operator insertions on real-time contour segments allow advanced/retarded Green's functions, etc., to be constructed

Real-time lattice fermions

Analytic continuation of Euclidean Wilson fermion action:

$$-iS_F^M = \sum_{\mathbf{x},t,\mathbf{x}',t'} \bar{\psi}(\mathbf{x},t) \Big[\frac{i}{2}(D_k - D_k^\dagger)_{\mathbf{x},t,\mathbf{x}',t'}\gamma^k + \frac{1}{2}(D_4 - D_4^\dagger)_{\mathbf{x},t,\mathbf{x}',t'}\gamma^4 + \frac{ir_k}{2}(D_k^\dagger D^k)_{\mathbf{x},t,\mathbf{x}',t'} - \frac{ir_4}{2}(D_4^\dagger D_4)_{\mathbf{x},t,\mathbf{x}',t'} + im\delta_{\mathbf{x}',\mathbf{x}}\delta_{t,t'} \Big] \psi(\mathbf{x}',t')$$

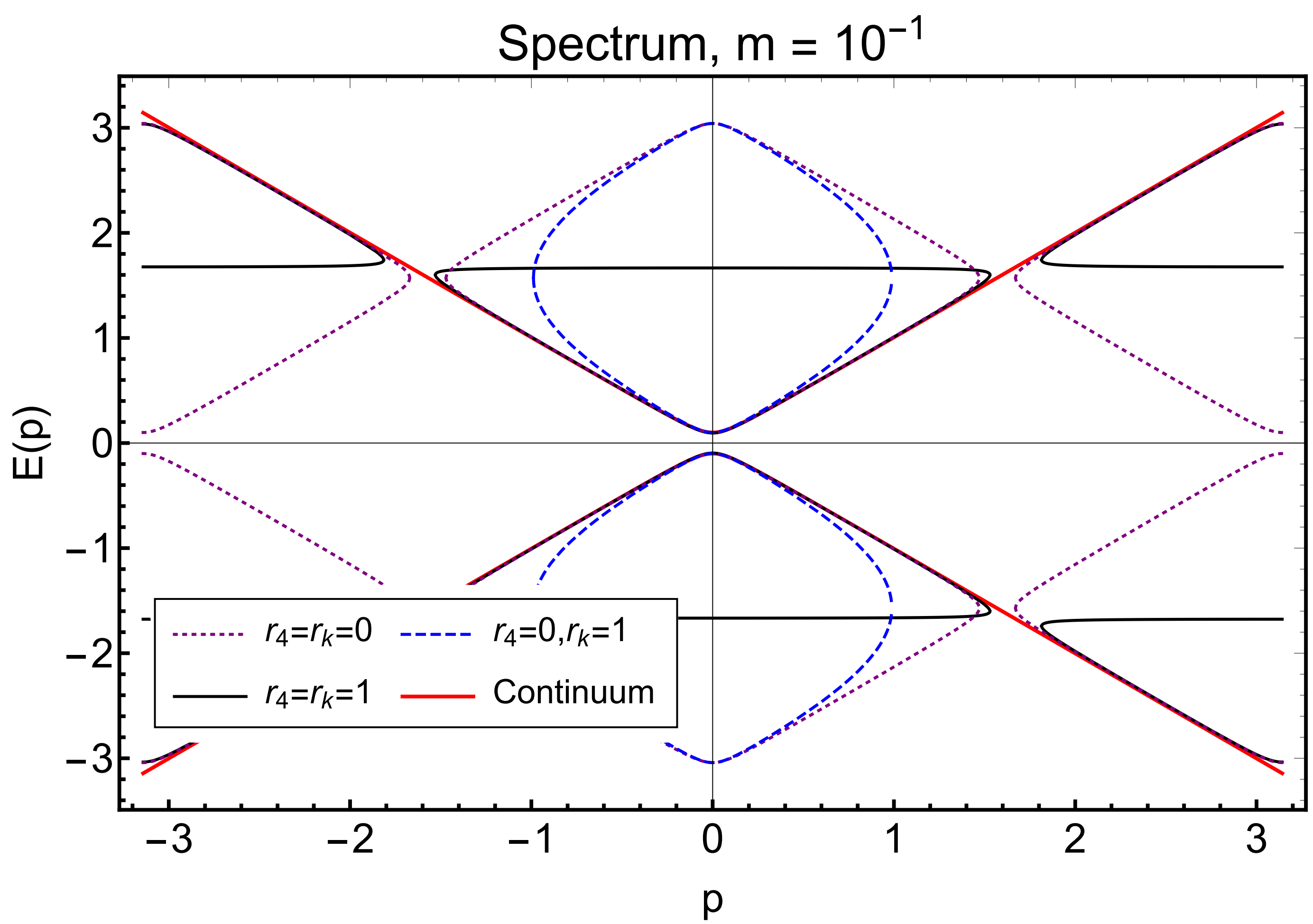
Semi-classical studies including anomalous fermion number violation:

Aarts, Smit, Nucl. Phys. B 555 (1999)

Saffin Tranberg, JHEP 1107 (2011)

Mace, Mueller, Schlichting, Sharma, PRD 95 (2017)

…



Spacelike doublers can be completely removed by Wilson term

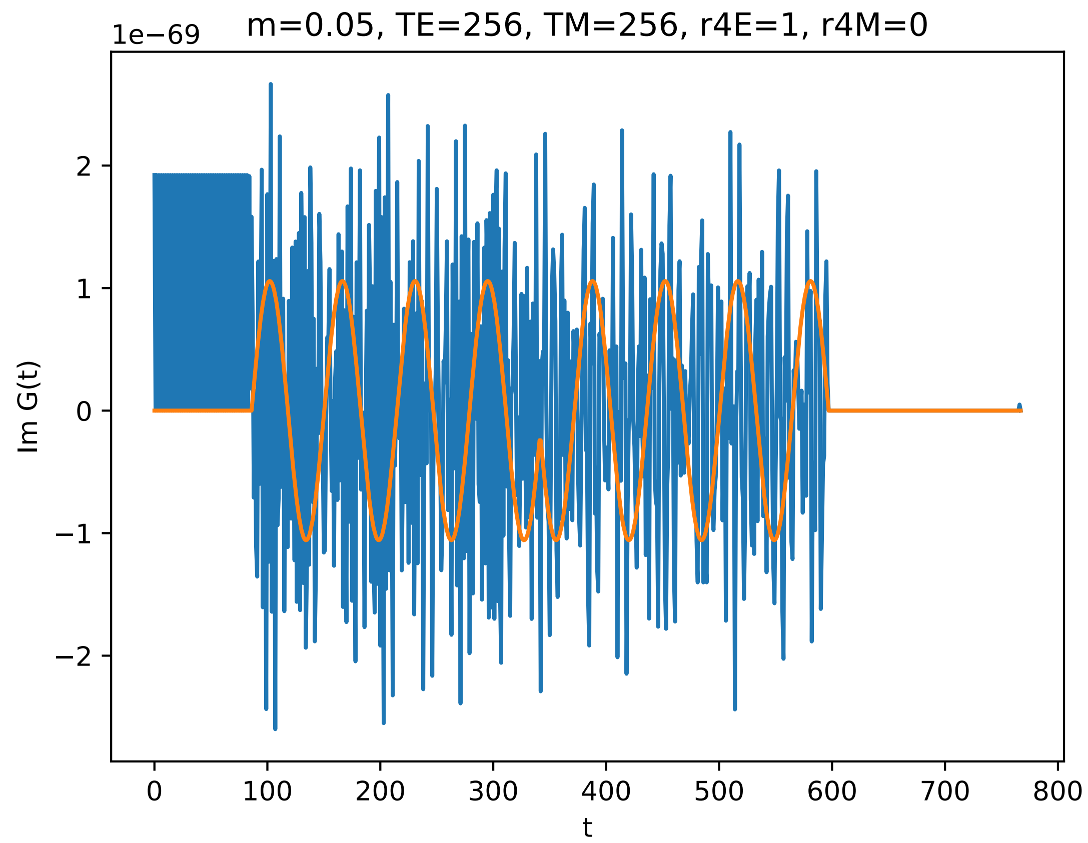
Temporal doublers cannot, unlike Euclidean spacetime

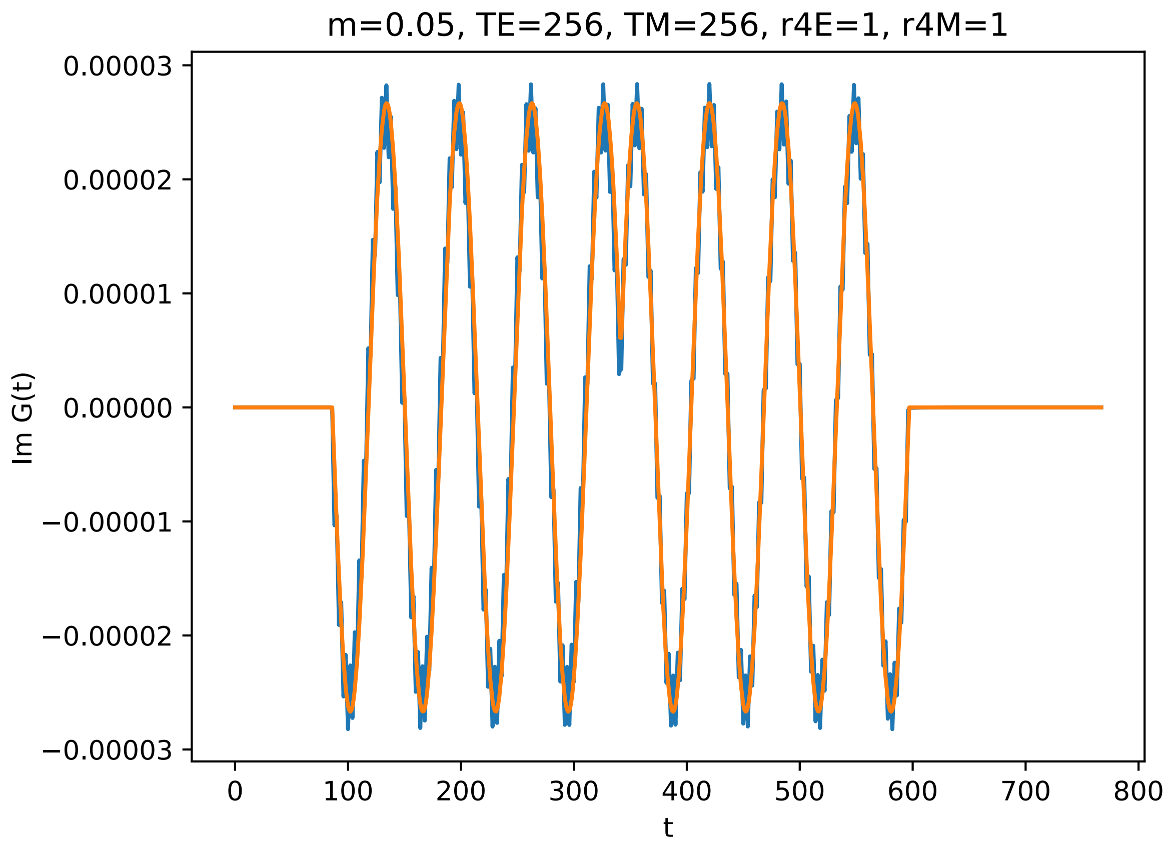
SK free fermion doublers

Semi-classical studies have only included spatial Wilson term, choose initial conditions with time doublers un-excited

Aarts, Smit, Nucl. Phys. B 555 (1999)

On SK contour, doubler modes present in thermal equilibrium

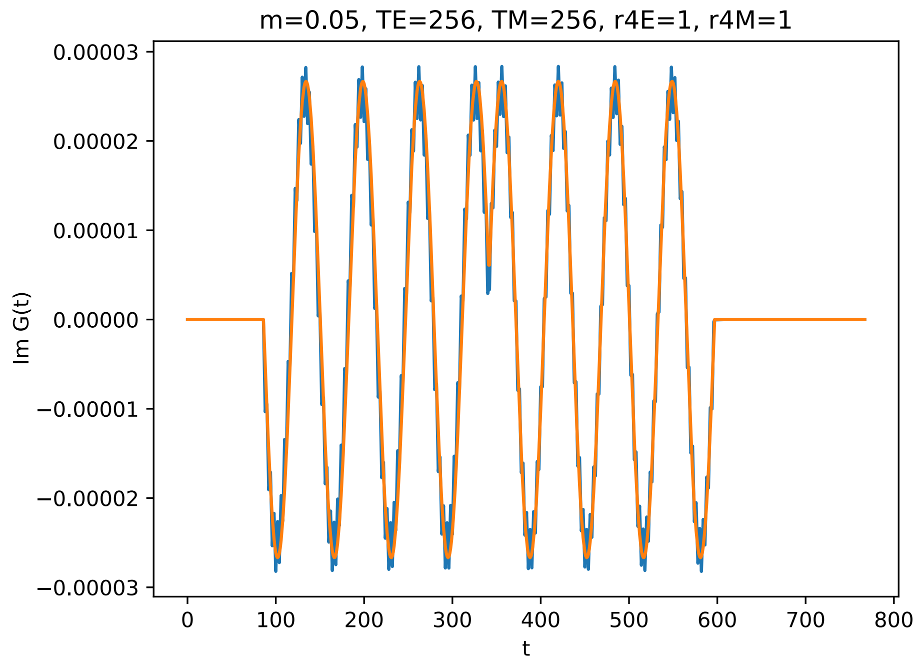




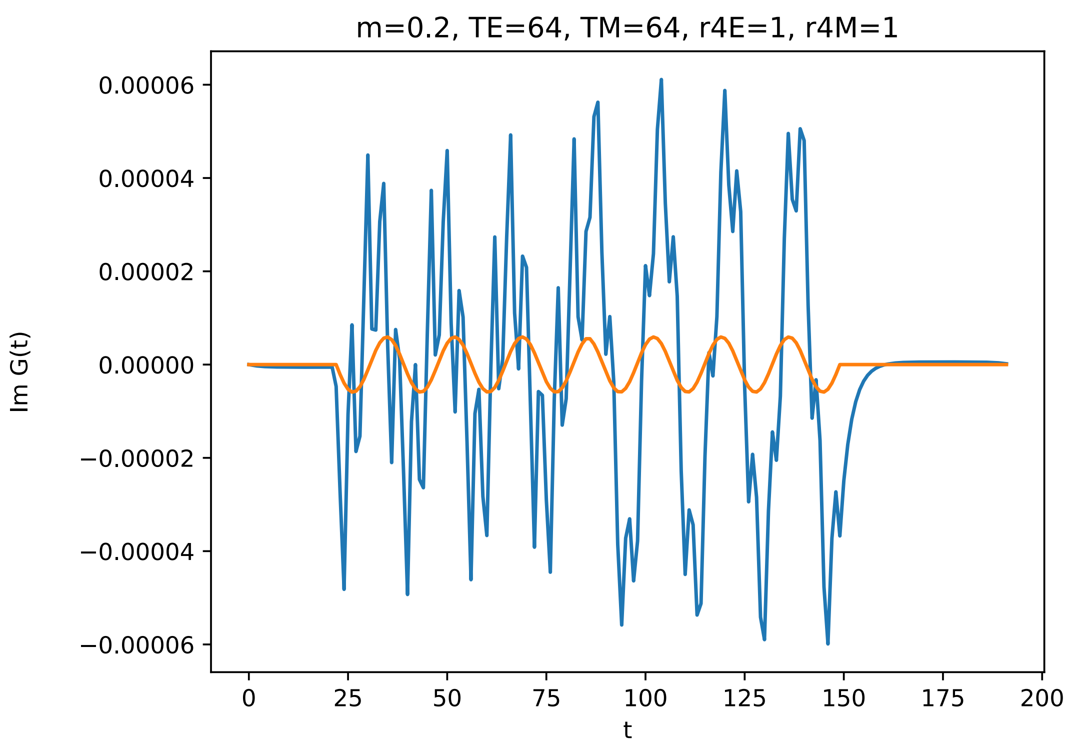
Temporal Wilson term suppresses doublers provided Euclidean extent large in lattice units

SK free fermion doublers

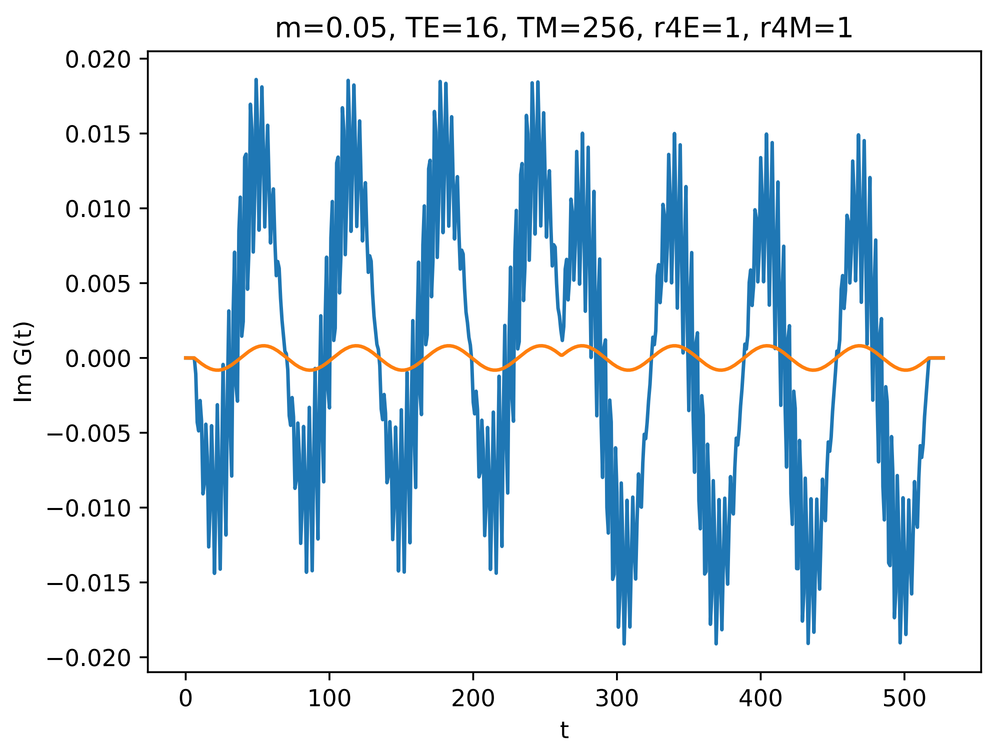
Doublers Suppressed



Too coarse



Too hot (in lattice units)

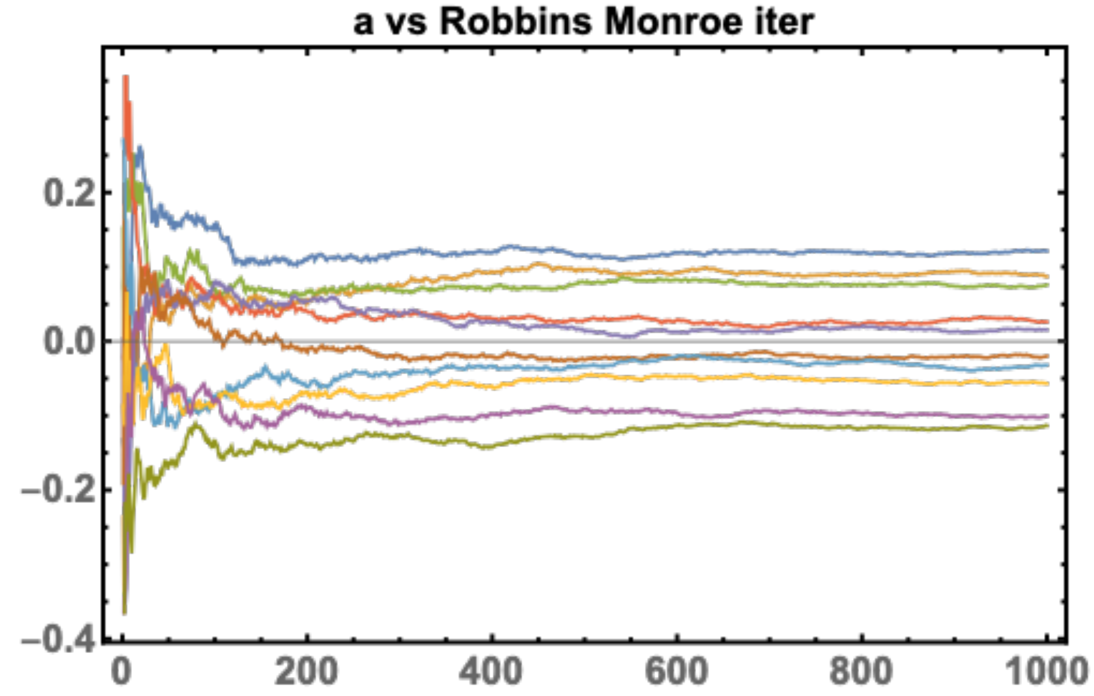


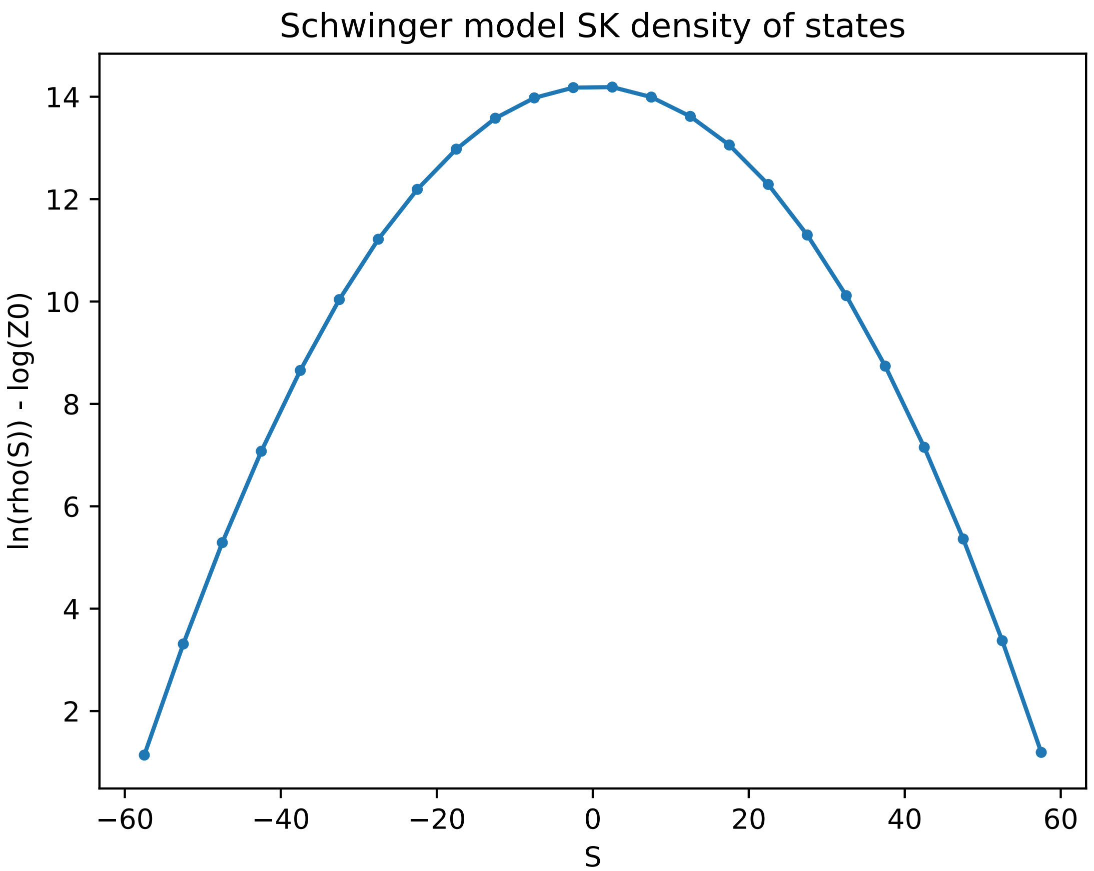
Towards SK Schwinger model

Toy model for non-equilibrium lattice gauge theory: (1+1)D QED

Robbins-Monroe method used to estimate for LLR density of states for (1+1)D QED on SK contour

$$T_E = T_M = 32 \qquad L = 4$$





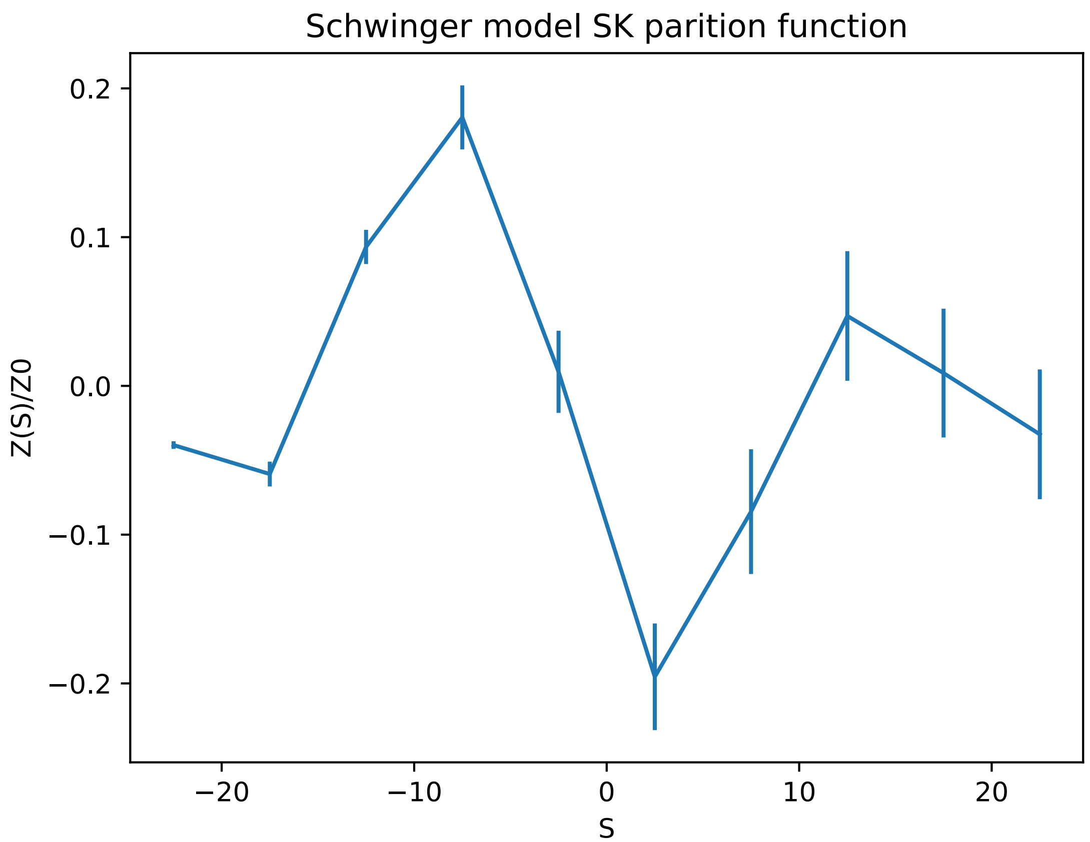
Resulting density of states very close to Gaussian

Width scales with volume as expected by central limit theorem

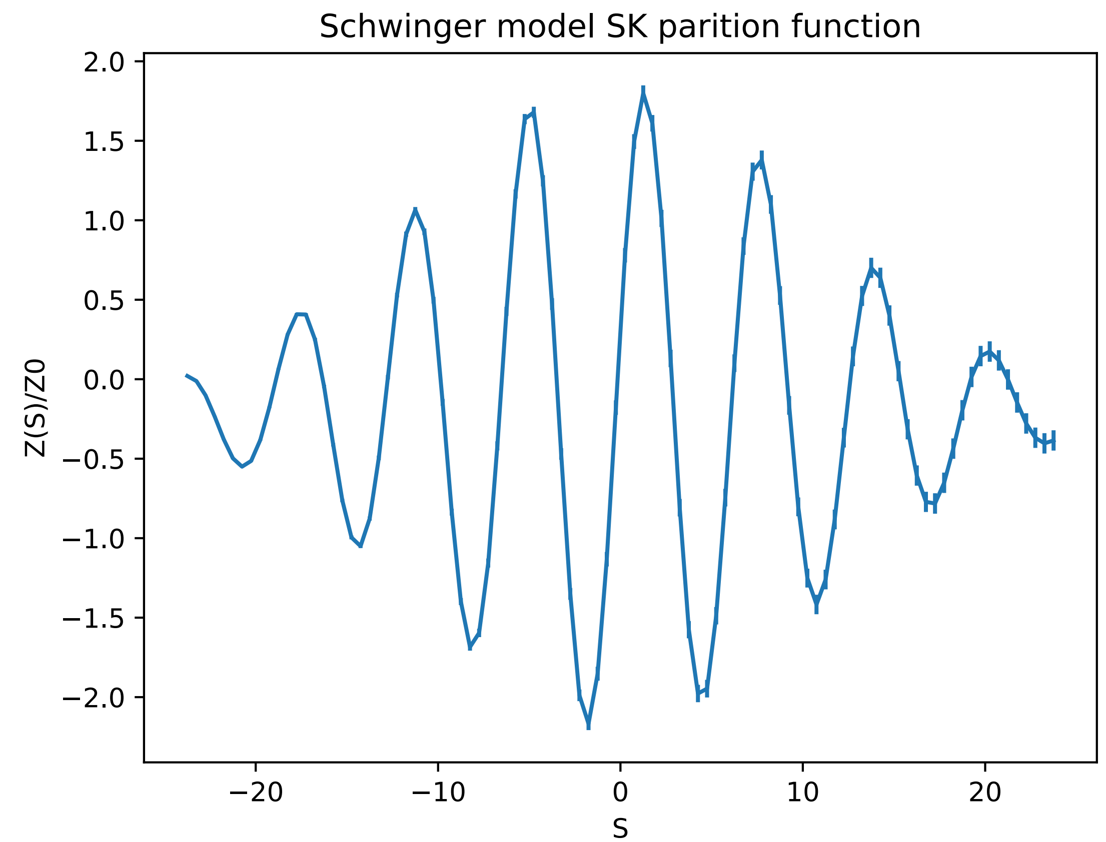
Towards SK Schwinger model

Decreasing bin size with fixed total ensemble size leads to increasingly accurate estimate of density of states

Width 5



Width 0.5



Phase fluctuations of real-time correlation function obstruct accurate correlation function reconstruction, more to be done!