Prony Methods for Extracting Excited States

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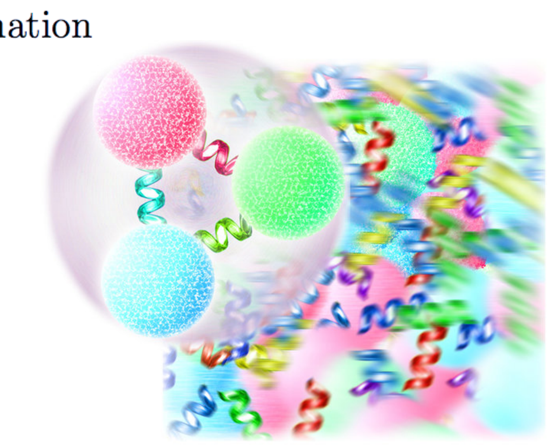
Motivation

Estimating low lying eigenstates of Hamiltonians in a finite box

- Resolving close lying states can be challenging and expensive
- Enhancement of statistical accuracy of ground state where S/N is high
- Insight into two particle elastic scattering to yield structural information
- Observed excited state baryons and mesons are poorly understood
- Lattice input could help determine composition of exotic states
  - tetra- or penta-quarks
  - hadronic molecules
  - unbound resonances



Problem

$$C_{ij}(t) = \langle 0|\mathcal{O}_i^\dagger(t)\mathcal{O}_j(0)|0\rangle = \sum_m^\infty \langle 0|\mathcal{O}_i^\dagger|E_m\rangle\langle E_m|\mathcal{O}_j|0\rangle \sigma_m^t e^{-E_m t} \approx \sum_m^M a_{ij\,m}\sigma_m^t e^{-E_m t}$$

$\sigma_m = 1$ using Wilson type fermions
$\sigma_m = \pm 1$ using staggered fermions

Time reversal symmetry for mesons i.e. $C(t) = C(N_t - t) \;\Rightarrow\; e^{-E_m t} \to [e^{-E_m t} + e^{-E_m(N_t - t)}]$

Exponential form

$$y_n(t) = \sum_m^M a_m \sigma_m^{t+n} e^{-E_m t} e^{-E_m n} \quad \text{for } 0 < t \ll \tfrac{N_t}{2}$$

$$y_n(t) = \sum_m^M a_m \sigma_m^{t+n} e^{E_m t} e^{E_m n} \quad \text{for } \tfrac{N_t}{2} \ll t < N_t$$

$$m_{eff} = \mp\log\left(\frac{y_{n+1}(t)}{y_n(t)}\right)$$

Hyperbolic cosine form

$$y_0 = C(t) \qquad y_{n+1}(t) = \frac{1}{2}[y_n(t+1) + y_n(t-1)]$$

$$y_n(t) = \sum_m^M a_m \sigma_m^{t+n} e^{-E_m \frac{N_t}{2}} \cosh(E_m(t - \tfrac{N_t}{2}))\cosh^n(E_m)$$

$$m_{eff} = \cosh^{-1}\left(\frac{y_{n+1}(t)}{y_n(t)}\right)$$

Both forms $y_n(t) = \sum_m^M A_m(t) z_m^n$

Theory

$2M \times M$ Vandermonde matrix $V(z)$

$$y_n(t) = \sum_m^M A_m(t) z_m^n \;\Leftrightarrow\; y(t) = V(z)a$$

$$\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{2M-1} \end{pmatrix} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_M \\ z_1^2 & z_2^2 & \cdots & z_M^2 \\ \vdots & \vdots & \ddots & \vdots \\ z_1^{2M-1} & z_2^{2M-1} & \cdots & z_M^{2M-1} \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_M \end{pmatrix}$$

Prony's Method [1][2][3]

Solve non-linear system by finding roots of **Hankel Matrix determinant**

Find roots $\{z_m\}$ then solve linear problem $y(t) = V(z)a$

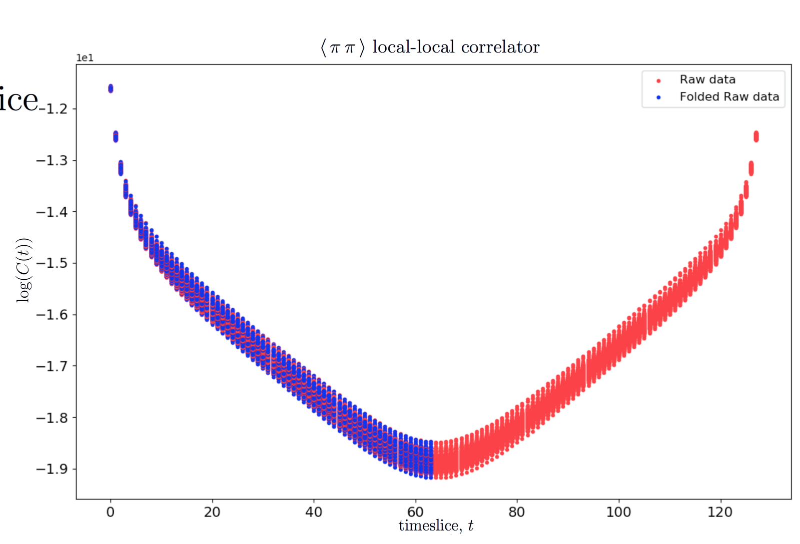
$$0 = \begin{vmatrix} y_0 & y_1 & \cdots & y_{M-2} & y_{M-1} & 1 \\ y_1 & y_2 & \cdots & y_{M-1} & y_M & z \\ y_2 & y_3 & \cdots & y_M & y_{M+1} & z^2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ y_M & y_{M+1} & \cdots & y_{2M-2} & y_{2M-1} & z^M \end{vmatrix}$$

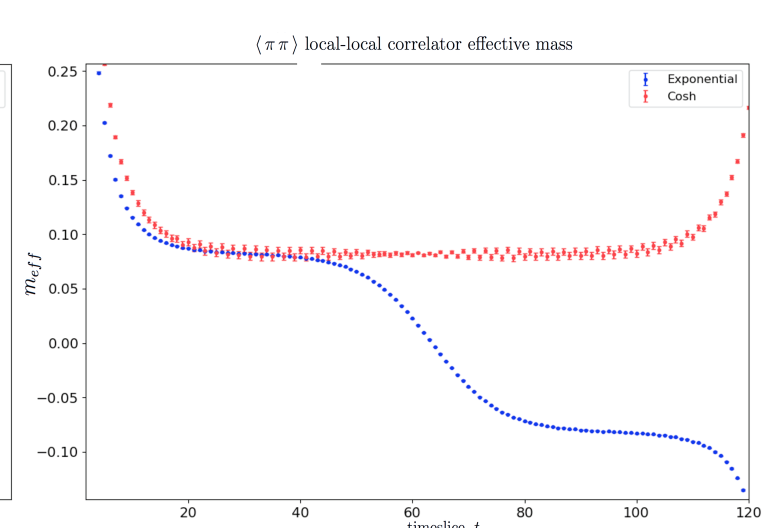
Analysis with $SU(3)$ $N_f = 8$ Ensembles

Application to near conformal gauge theory [4] (see Ethan Neil's talk)

Pre-binned correlators to explore spectrum of Goldstone Boson and determine F_π

- $64^3 \times 128$ lattice
- $m_\pi/m_\rho \approx 0.48$
- $m_\pi L \approx 5.25$

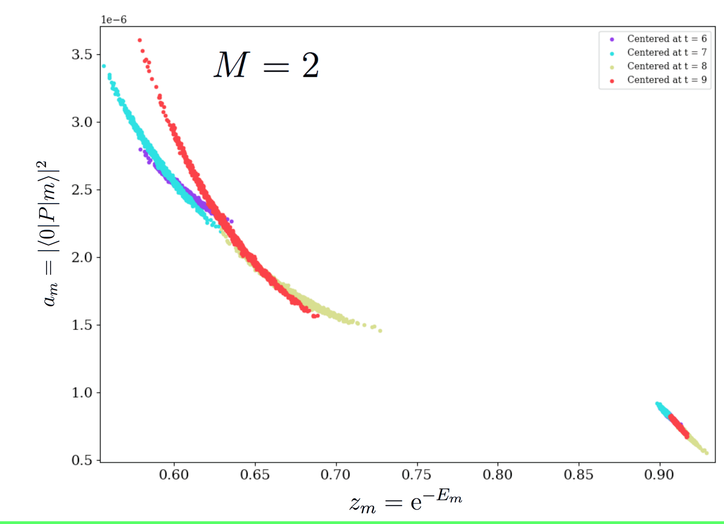


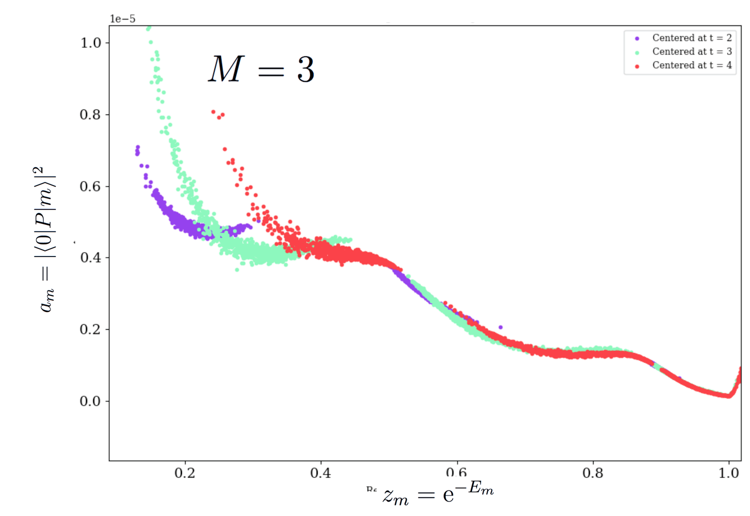


Extracting Amplitudes and Roots

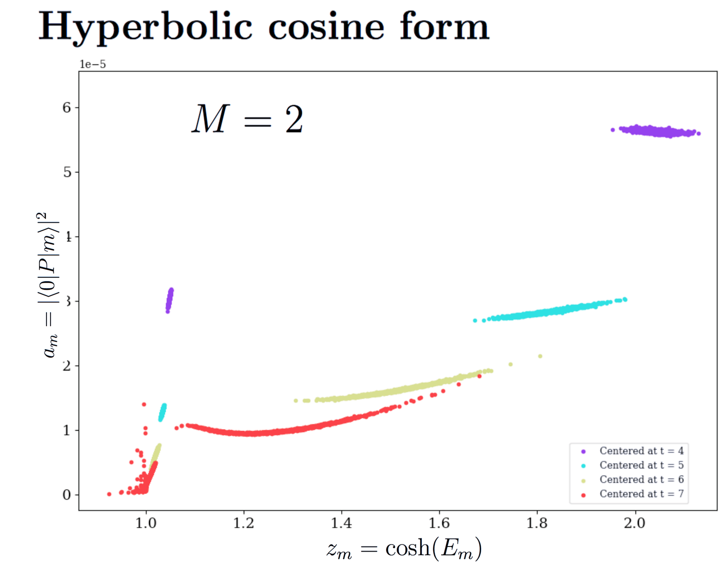
1000 random Bootstrap samples generated from 232 data points of correlation functions $C(t)$

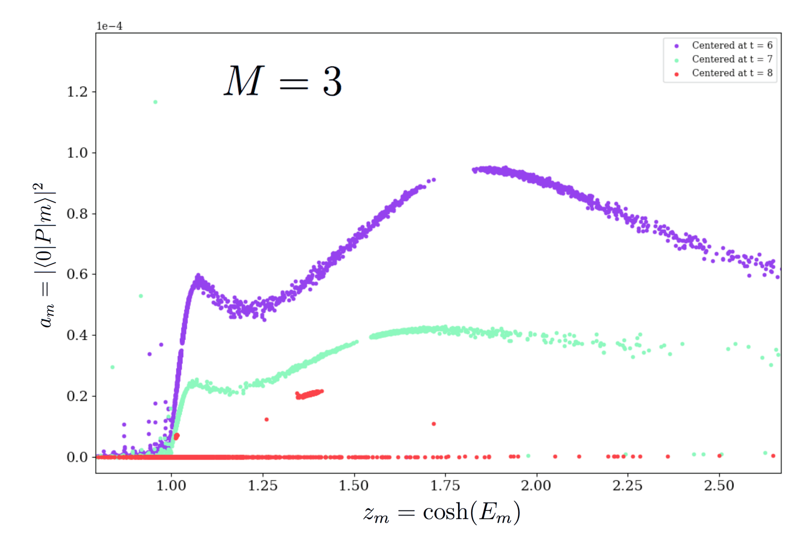
Exponential form





Hyperbolic cosine form





Clustering

Approximate bivariate normal distribution of $\log(a_m)$ vs. $\log(z_m)$

$$\text{const}_m = A_m(t) z_m^n \;\Rightarrow\; \log(\text{const}_m) = \log(a_m) + (t+n)\log(z_m)$$

Expectation maximization $\leftrightarrow$ Log- likelihood minimization [5]

$$P(x) = \frac{\exp[-\frac{1}{2}(\vec{x}-\vec{\mu})^\dagger \Sigma (\vec{x}-\vec{\mu})]}{2\pi\sqrt{|\Sigma|}} \qquad \vec{\mu} = \begin{pmatrix} \langle z \rangle \\ \langle a \rangle \end{pmatrix} \quad \Sigma = \begin{pmatrix} \langle |z - \langle z \rangle|^2 \rangle & \langle (z-\langle z\rangle)(a - \langle a \rangle)^* \rangle \\ \langle (z - \langle z \rangle)^*(a - \langle a \rangle) \rangle & \langle |a - \langle a \rangle|^2 \rangle \end{pmatrix}$$

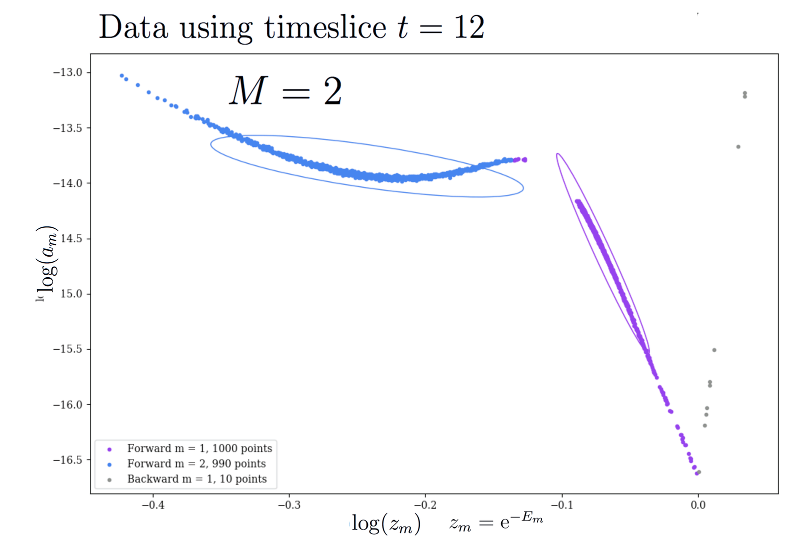
K-means cluster algorithm, with constraint: M points in M distinct clusters

1. Assign initial cluster assignments
2. Compute mean μ and covariance Σ of each cluster
3. Reassign each point to a cluster to minimize $(\vec{x}-\vec{\mu})^\dagger \Sigma (\vec{x}-\vec{\mu})$
4. Repeat 2 & 3 until steady state is reached

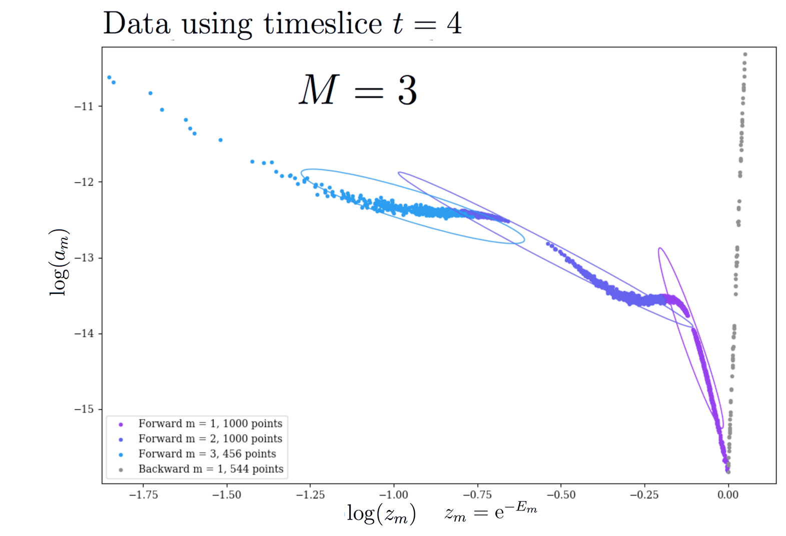
Initial cluster assigments by magnitude of z_m for each set of roots calculated from Bootstrap sample

Exponential form

Data using timeslice $t = 12$



Data using timeslice $t = 4$



Future Work

- Improve empirical estimation of cluster distribution to account for apparent non-Gaussian features
- Include clusters for backward propagating states
- Investigate uncertainties from cluster ellipses as a function of time to make $m_{\rm eff}$ plots
- Multiple correlation functions with same quantum numbers (including correlation matrices)

- Disconnected contributions: $\langle \mathcal{O} \rangle \neq 0 \Rightarrow \langle 0|\mathcal{O}_i^\dagger \mathcal{O}_j|0\rangle = a_{ij\,0} + \cdots$

$$\Delta_f(t + \tfrac{1}{2}) = \frac{1}{2}[C(t+1) - C(t)] \sim \sinh(\tfrac{E_m}{2})$$

$$\Delta_c(t) = \frac{1}{2}[C(t+1) - C(t-1)] \sim \sinh(E_m)$$

- Non-oscillating form of $y_n(t)$ to reduce error and time dependent correlations

$$y_n(t) = \sum_m^M a_m \sigma_m^t e^{-E_m t} e^{-2E_m n} \quad \text{for } 0 < t \ll \tfrac{N_t}{2}$$

$$m_{eff}^2 = \mp\log\left(\frac{y_{n+1}(t)}{y_n(t)}\right)$$

$$y_n(t) = \sum_m^M \sigma_m^t e^{-E_m \frac{N_t}{2}} \cosh(E_m(t - \tfrac{N_t}{2}))\cosh^n(2E_m)$$

$$m_{eff} = \frac{1}{2}\cosh^{-1}\left(\frac{y_{n+1}(t)}{y_n(t)}\right)$$

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[1] G. C. F. M. R. de Prony, J. Ecole Poly. 1, 24 (1795), partial translation available in [3]

[2] G. T. Fleming, S. D. Cohen, H.-W. Lin, and V. Pereyra, Phys. Rev. D80, 074506 (2009), [0903.2314].

[3] Vandevoorde, Ph.D. thesis, Rensselaer Polytechnic Institute, Troy, New York, USA (1996), http://wwwlib.umi.com/dissertations/fullcit/9806112

[4] LSD collaboration, Appelquist, T. et al., Lattice simulations with eight flavors of domain wall fermions in SU(3) gauge theory, Phys. Rev. D90 (2014) 114502, [1405.4752].

[5] Dempster, A.P.; Laird, N.M.; Rubin, D.B. (1977). "Maximum Likelihood from Incomplete Data via the EM Algorithm". Journal of the Royal Statistical Society, Series B. 39 (1): 1-38.