## State of the Art of Time Series Analysis in LQFT George T. Fleming

## The Big Picture

- Tremendous advances in algorithms (thanks QCDNA) and computing have made generating large lattices O(1004) feasible.
- Latest preconditioners enable $O\left(10^{5}\right)$ solves per lattice. New observables can be constructed.
- Getting to a physics result usually requires one more step: analysis.
- Despite all the effort on the first two steps, often the bottle neck to publication is the third step.


## The Big Picture

- The LHC discovered a Higgs boson. Nobel prizes were awarded.
- Some theorists imagine that the Higgs boson could be a composite particle made of something like quarks and gluons of QCD.
- To compute the properties of such a Higgs boson would be a very hard observable calculation, naively involving $\mathrm{O}(\mathrm{Vol})$ linear solves per config, on an ensemble of $\mathrm{O}(1,000)$ independent configs.


## Computing the Composite

## Higgs Mass

- The Higgs mass would be extracted from a correlation function with "disconnected contributions

$$
C\left(\vec{p},\left|t-t^{\prime}\right|\right)=\int d^{3} x d t d^{3} x^{\prime} d t^{\prime}\left\langle\bar{\psi} \psi(\vec{x}, t) \bar{\psi} \psi\left(\vec{x}^{\prime}, t^{\prime}\right)\right\rangle e^{-i \vec{p} \cdot \vec{x}} e^{i \vec{p} \cdot \vec{x}^{\prime}}
$$

- Written in terms of Dirac matrices

$$
\begin{gathered}
C\left(\vec{p},\left|t-t^{\prime}\right|\right)=\int d^{3} x d t d^{3} x^{\prime} d t^{\prime}\left\langle\operatorname{Tr}\left[M^{-1}\left(x, t ; x^{\prime}, t^{\prime}\right) M^{-1}\left(x^{\prime}, t^{\prime} ; x, t\right)\right]\right. \\
\left.-\operatorname{Tr}\left[M^{-1}(x, t ; x, t)\right] \operatorname{Tr}\left[M^{-1}\left(x^{\prime}, t^{\prime} ; x^{\prime}, t^{\prime}\right)\right]\right\rangle e^{-i \vec{p} \cdot \vec{x}} e^{i \vec{p} \cdot \vec{x}^{\prime}}
\end{gathered}
$$

- Translation invariance symmetry allows us to compute the first term from a single point but the second term is $\mathrm{O}(\mathrm{Vol})$ harder.


## Fast Convolution Theorem

- 1965: Cooley-Tukey (FFT), 1966: Stockham, Helms, Sande
$C_{i j}(x-y)_{c}=\left\langle O_{i}(x) O_{j}(y)\right\rangle_{c}=\left\langle O_{i}(x) O_{j}(y)\right\rangle-\left\langle O_{i}(x)\right\rangle\left\langle O_{j}(y)\right\rangle$
- Use FFT on $\mathrm{O}_{\mathrm{i}}(\mathrm{x})$

$$
\widetilde{C}_{i j}(q)=\left\langle\widetilde{O}_{i}^{*}(q) \widetilde{O}_{j}(q)\right\rangle=\widetilde{C}_{i j}(q)_{c}+c_{0} \delta_{q, 0}
$$

- Disconnected piece only at $\mathrm{q}=0$, easily subtracted.
- For composite Higgs $\mathrm{O}(\mathrm{x})=\left[\mathrm{M}^{-1}\right]_{\mathrm{x}, \mathrm{x}}$. Is there an efficient way to estimate just the diagonal part of the inverse without doing $\mathrm{O}(\mathrm{Vol})$ linear solves?
- Perfect for autocorrelation. Why isn't it used more?


## Got $\mathrm{C}_{\mathrm{ij}}(\mathrm{x}-\mathrm{y})$, now what?

- Euclidean time hadron correlator in infinite box

$$
C\left(t_{n}\right)=\sum_{m=1}^{M} A_{m} e^{-a n E_{m}}, \quad n \geq 0, A_{m} \in \mathbb{R}, 0 \leq E_{1} \leq \cdots
$$

- Vandermonde system of $N=2 M$ time slices given $M$ states, $\mathbf{y}=\mathbf{V}(x) \mathbf{a}, \quad y_{n} \equiv C\left(t_{n}\right), x_{m} \equiv e^{-a E_{m}}, a_{m} \equiv A_{m}$

$$
\left(\begin{array}{l}
y_{1} \\
y_{2} \\
y_{3} \\
y_{4} \\
\vdots \\
y_{2 M}
\end{array}\right)=\left(\begin{array}{llll}
1 & 1 & \cdots & 1 \\
x_{1} & x_{2} & \cdots & x_{M} \\
x_{1}^{2} & x_{2}^{2} & \cdots & x_{M}^{2} \\
x_{1}^{3} & x_{2}^{3} & \cdots & x_{M}^{3} \\
\vdots & \vdots & \ddots & \vdots \\
x_{1}^{2 M-1} & x_{2}^{2 M-1} & \cdots & x_{M}^{2 M-1}
\end{array}\right)\left(\begin{array}{l}
a_{1} \\
\vdots \\
a_{M}
\end{array}\right)
$$

- Could use NLLS to fit, but exponential fits can be unstable. Or solve the Vandermonde system.


## Vandermonde solution

- Successful collaboration from previous QCDNA.
- Find the roots of the polynomial below.
- Easy to get many solutions.
- Note the left block is a Hankel matrix.

$$
\left|\begin{array}{cccc:c}
y_{1} & y_{2} & \cdots & y_{M} & 1 \\
y_{2} & y_{3} & \cdots & y_{M+1} & x_{1} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
y_{M+1} & y_{M+2} & \cdots & y_{2 M} & x_{1}^{M}
\end{array}\right|=0 .
$$

## Even More Solutions

- We can get lots of solutions. But, most are spurious due to overfitting noise.
- The challenge is to find the few physically relevant states among many irrelevant ones.
- The general polynomial equation for $K$ correlators:

- A determined system requires $M=\sum_{k=1}^{K} M_{k}$ and $N=M+1$ as before.


## Correlator Matrices, Matrix Polynomials

- Treat $\mathrm{C}_{\mathrm{ij}}(\mathrm{t})$ as a NxN Hermitian matrix $\mathbf{C}(\mathrm{t})$.
- Matrix pencil: $\mathbf{C}(\mathrm{t}+1)=\mathrm{x}_{\mathrm{n}} \mathbf{C}(\mathrm{t})$.
- Why stop there: $2 \mathbf{C}(\mathrm{t}+2)-\mathrm{x} \mathbf{C}(\mathrm{t}+1)-\mathrm{x}^{2} \mathbf{C}(\mathrm{t})=0$.
- In general can always form a matrix polynomial equation of order $\mathrm{N}_{\mathrm{t}}$.

Matrix Polynomials
\& C

$$
\begin{array}{r}
\text { I. Gohberg } \\
\text { P. Lancaster } \\
\text { L. Rodman }
\end{array}
$$



## Yet Even More solutions

- If the $y_{m}=\mathbf{C}(\mathrm{t})$ are matrix-valued, one can form many polynomials, what's a good suggestion?
- The Vandermonde polynomial with Matrix-valued coefficients.
- Obviously, more statistics helps because it suppresses the spurious solutions.
$\left|\begin{array}{cccc:c}y_{1} & y_{2} & \cdots & y_{M} & 1 \\ y_{2} & y_{3} & \cdots & y_{M+1} & x_{1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ y_{M+1} & y_{M+2} & \cdots & y_{2 M} & x_{1}^{M}\end{array}\right|=0$.

