Hadronic Structure, Conformal Maps, & Analytic Continuation

Thomas Bergamaschi
William I. Jay
Patrick R. Oare

Based on arXiv:2305.16190
Hadronic Structure

The role of spectral functions

\[ e^+ e^- \rightarrow \text{hadrons} \]

\[ e^- p^+ \rightarrow e^- X \]

\[ \rho_{\mu\nu}(q) = \frac{1}{2\pi} \int d^4 x e^{iq\cdot x} \langle \emptyset \left| [j^\text{EM}_\mu(x), j^\text{EM}_\nu(0)] \right| \emptyset \rangle \]

\[ \rho_{\mu\nu}(q) = (q_\mu q_\nu - q^2 g_{\mu\nu}) \rho(q^2) \]

\[ W_{\mu\nu}(p, q) = \int \frac{d^4 x}{4\pi} e^{iq\cdot x} \langle p \left| [j^\text{EM}_\mu(x), j^\text{EM}_\nu(0)] \right| p \rangle \]

\[ W_{\mu\nu} = F_1 \times (\text{Lorentz projectors}) + F_2 \times (\text{Lorentz projectors}) \]
Hadronic Structure

The role of spectral functions

- Lattice QCD calculations occur in Euclidean time:

\[ G(\tau) = \sum_n \left| \langle 0 | \mathcal{O} | n \rangle \right|^2 \left( e^{-E_n \tau} + e^{-E_n(\beta - \tau)} \right) \]

- In frequency space (take \( a \ll 1 \)):

\[ G(i\omega_\ell) = \int d\tau e^{i\omega_\ell \tau} G(\tau) \]

\[ = \sum_n \left| \langle 0 | \mathcal{O} | n \rangle \right|^2 \left( \frac{1}{E_n + i\omega_\ell} + \frac{1}{E_n - i\omega_\ell} \right) \]

- General relation: \( \rho(\omega) = \frac{1}{\pi} \text{Im} \ G(\omega) \)

\[ \frac{1}{\pi} \text{Im} \left( \frac{1}{x + i\epsilon} \right) \rightarrow \delta(x) \]
Analytic Continuation

Problem description

Euclidean data at Matsubara frequencies $i\omega_\ell$

Analytic continuation

$\Leftrightarrow$

Infer behavior of $G(z)$ near the real line given Euclidean data on the imaginary axis

Finite-volume energy levels
Analytic Continuation

Problem description

Euclidean data at Matsubara frequencies $i\omega_n$

Analytic continuation

Infer behavior of $G(z)$ near the real line given Euclidean data on the imaginary axis

Finite-volume energy levels

$\rho^\epsilon(\omega) \equiv \frac{1}{\pi} \text{Im} G(\omega + i\epsilon)$ can be viewed as smeared spectral function in the spirit of Hansen, Meyer, and Robaina [arXiv:1704.08993].
Analytic Continuation

Challenges and hopes

• The received wisdom:

  • “Excited states decay away exponentially.” Analytic continuation to the real line amounts to an inverse Laplace transform. This problem is ill-defined.

  • “Little can be said from a finite set of points.” Complex functions are uniquely defined by analytic continuation given data for the function on a full open set, e.g., an open interval on the imaginary axis.

• Causes for cautious optimism:

  • “Causal Green functions are remarkably rigid.” Causality dictates that Green functions in QFT must be analytic in the upper half plane, with poles and branch cuts appearing only on the real line.

  • Carlson’s theorem. Roughly, complex functions which do not grow quickly at infinity are uniquely specified by their value on the integers.
Recall: analytic functions are defined by convergent power series in an open set around each nonsingular point.

Radius of convergence is determined by the location of the nearest pole.

Difficult to “see past the first pole” in these coordinates.
Analytic Continuation

Conformal maps

- Recall: analytic functions are defined by convergent power series in an open set around each nonsingular point.
- Radius of convergence is determined by the location of the nearest pole.

So change coordinates!

\[ C(z) = \frac{z - i}{z + i} \]
Analytic Continuation

The technical problem

- Recall: analytic functions are defined by convergent power series in an open set around each nonsingular point.
- Radius of convergence is determined by the location of the nearest pole.
- The Cayley transform maps the problem to the unit disk.
- Given Euclidean data

\[
\{ i \omega_\ell \} \rightarrow \zeta_\ell \subset \mathbb{D},
\]

\[
\{ G(i \omega_\ell) \} \mapsto w_\ell \subset \mathbb{D},
\]

construct an analytic function \( f(\zeta) \)

on the disk such that \( f(\zeta_\ell) = w_\ell \).
Analytic Continuation

Nevanlinna’s Theorem

- Theorem (Nevanlinna, 1919/1929):

  - Any solution to the interpolation problem with \( N \) points can be written in the form

  \[
  f(\zeta) = \frac{P_N(\zeta)f_N(\zeta) + Q_N(\zeta)}{R_N(\zeta)f_N(\zeta) + S_N(\zeta)}
  \]

  where the coefficient functions \( P_N, Q_N, R_N, S_N \) are calculable using an inductive formula in terms of the input data \( \{\zeta_\ell\} \) and \( \{w_\ell\} \) and an arbitrary analytic function \( f_N(\zeta) : \mathbb{D} \to \mathbb{D} \).


- \( P_N, Q_N, R_N, S_N \leftrightarrow \text{“Nevanlinna coefficients”} \)

- Arbitrary function \( f_N(\zeta) \leftrightarrow \text{“Freedom to specify further Euclidean data to constrain the interpolating function”} \)

- Applicability to field-theory problems first recognized by condensed-matter theorists Fey, Yeh, and Gull [arXiv:2010.04572]
Analytic Continuation
The full space of solutions

• Question: For fixed $N$ and $\zeta$, what are the possible values that an interpolating function $f(\zeta)$ can take, by varying possible values of the arbitrary function $f_N(\zeta) \in \mathbb{D}$?

  • The size of this set $\iff$ ambiguity in the analytic continuation

  • Remarkably, this set can be parameterized explicitly for each, $N$ and $\zeta \in \overline{\mathbb{D}}$
Analytic Continuation

The full space of solutions

- Question: For fixed $N$ and $\zeta$, what are the possible values that an interpolating function $f(\zeta)$ can take, by varying possible values of the arbitrary function $f_N(\zeta) \in \mathbb{D}$?

- Answer: The space of possible values is given by the Wertevorrat $\Delta_N(\zeta)$, which is the disk of radius $r_N(\zeta)$ and centered at $c_N(\zeta)$.

$$c_N = \frac{P_N(-R_N/S_N) + Q_N}{R_N(-R_N/S_N) + S_N} \quad r_N = \frac{|P_NS_N - Q_NR_N|}{|S_N|^2 - |R_N|^2}$$

- The Wertevorrat $\Delta_N(\zeta)$ rigorously contains the full infinite family of all possible analytic continuations at each point $\zeta \in \mathbb{D}$.
Finally we need to map the Wertevorrat back to the upper half plane. Use the inverse Cayley transform $z = C^{-1}(\zeta)$.

\[ \rho^\epsilon(\omega) = \frac{1}{\pi \text{Im} G(\omega + i\epsilon)} \]

\[ \delta \rho^\epsilon(\omega) = \frac{1}{\pi} \left[ \max \text{Im} \partial D_N(\omega + i\epsilon) - \min \text{Im} \partial D_N(\omega + i\epsilon) \right] \]
Analytic Continuation

The Algorithm

1. Start with a Euclidean correlation function $G(t)$
2. Evaluate the Fourier coefficients to obtain $G(i\omega_\ell)$
3. Map the Euclidean data to the unit disk
4. Solve the interpolation problem
   - Evaluate the Nevanlinna coefficients
   - Compute the Wertevorrat
5. Map the Wertevorrat back to the upper half-plane
6. For each point $\omega + i\epsilon$, evaluate the space of possible smeared spectral densities $\delta\rho^e(\omega)$
Numerical Example
The R-ratio — reconstructing a parameterization

• Bernecker and Meyer [arXiv:1107.4388] give a useful parameterization of R-ratio data

• This parameterization can serve as input for a spectral reconstruction

• Can easily convert:
\[ R(s) \iff \rho(\omega) \iff G(i\omega \ell) \]

Formula from beginning of talk

“Laplace transform”

\( \rho(770), \omega(782), \phi(1020) \)

\( s \text{ [GeV}^2\text{]} \)

W.I. Jay — MIT

Figure from [arXiv:1107.4388]
Numerical Example

The R-ratio — reconstructing a parameterization

- Energies rescaled to line in unit interval $\longrightarrow$ lattice units with $a \approx 0.07$ fm, so $am_\rho \approx 0.25$

- Euclidean data generated for $\beta = 96$ total points on the imaginary-energy axis

✓ Spectral peaks from $\rho(770)/\omega(782)$ and $\phi(1020)$ clearly visible in reconstructions

✓ Exact answer is contained within the bounding envelope of the Wertevorrat

\[ \epsilon \downarrow 0 \]
Summary

- Today’s spectral reconstruction algorithm:
  - Leverages a century-old theorem due to Nevanlinna
  - Builds off of work in the condensed matter community by Fey, Yeh, and Gull [arXiv:2010.04572]
  - Applies to diagonal correlation functions of bosonic/fermionic operators
    - Bosonic operators (alternative view by Nogaki and Shinaoka [arXiv:2305.03449])
    - Fermionic operators [arXiv:2010.04572]
- Our method:
  - Admits interpretation as a smeared spectral density in the spirit of Hansen, Meyer, and Robaina [arXiv:1704.08993]
  - Bound errors rigorously with Nevanlinna’s Wertevorrat
    - Wertevorrat ⇔ Full space of functions consistent with the input data and analyticity
- Next steps: understanding interplay with statistical uncertainties
  - Important existing work in this direction by Huang, Gull, and Lin [arXiv:2210.04187]
Backup
The Pick Criterion

Existence of an Interpolating Function

• Question: When does an interpolating function, analytic on $\mathbb{D}$, exist for the input data $\{\zeta_l\}, \{w_\ell\}$ such that $f(\zeta_\ell) = w_\ell$ for all $\ell$?

• Theorem (Pick, 1915):

  Such a function exists if and only if the Pick matrix

  $\begin{bmatrix}
  1 - w_i \bar{w}_j \\
  \frac{1}{1 - \zeta_i \bar{\zeta}_j}
  \end{bmatrix}$

  is positive semidefinite.

• This condition can fail for noisy data (observed already in arXiv:2010.04572). See also arXiv:2210.04187 for work toward robust reconstructions.
Nevanlinna Coefficients
Concrete Formulae

Convenient notation for manipulating Möbius transformations:

\[
\begin{pmatrix}
a(\zeta) & b(\zeta) \\
c(\zeta) & d(\zeta)
\end{pmatrix} h(\zeta) \equiv \frac{a(\zeta)h(\zeta) + b(\zeta)}{c(\zeta)h(\zeta) + d(\zeta)}
\]

The Nevanlinna coefficients:

\[
f(\zeta) = U_1(\zeta)U_2(\zeta)\cdots U_N(\zeta)f_N(\zeta)
\equiv \left( \begin{array}{c}
P_N(\zeta)Q_N(\zeta) \\
R_N(\zeta)S_N(\zeta)
\end{array} \right) f_N(\zeta)
\]

Inductive blocks:

\[
U_n(\zeta) = \frac{1}{\sqrt{1 - |w_n^{(n-1)}|^2}} \begin{pmatrix}
b_{\zeta_n}(\zeta) & w_n^{(n-1)} \\
w_n^{(n-1) *} b_{\zeta_n}(\zeta) & 1
\end{pmatrix}
\]

Blaschke factors:

\[
b_a(\zeta) = \frac{|a|}{a} \frac{a - \zeta}{1 - \bar{a}\zeta}
\]

“The nth interpolant \(f_n\) evaluated at the \(m\)th zero”

\[
w_m^{(n)} \equiv f_n(\zeta_m)
\]
Analytic Continuation

Computing properties of the \textit{Wertevorrat}

- Question: For fixed $N$ and $\zeta$, \textbf{what are the possible values that an interpolating function $f(\zeta)$ can take}, by varying possible values of the arbitrary function $f_N(\zeta) \in \mathbb{D}$?

- Answer: For fixed $N$ and $\zeta$, consider the auxiliary function $T : \mathbb{D} \rightarrow \mathbb{D}$

\[
T(w) = \frac{P_Nw + Q_N}{R_Nw + S_N}
\]

- We want to evaluate the image of this map.

- First, observe that $T(\omega)$ is a Möbius transformation, which maps circles to circles. Therefore $T(\mathbb{D})$ must be also be disk $\Delta_N(\zeta)$.

- Since $T(-S_N/R_N) = \infty$, the reflection property of Möbius transformations says that disk is centered at the point $c_N$. A calculation gives the radius $r_N$.

\[
c_N = \frac{P_N(-R_N/S_N) + Q_N}{R_N(-R_N/S_N) + S_N} \quad r_N = \frac{|P_NS_N - Q_NR_N|}{|S_N|^2 - |R_N|^2}
\]
Bosons and fermions

• Can consider two possibilities:
  • Fermionic: $\rho(-\omega) = \rho(\omega)$ [+ from anti-commutator]
  • Bosonic: $\rho(-\omega) = -\rho(\omega)$ [- from commutator]

• Technical detail: slightly different conformal maps used to transform the problem to the unit disk. See our arXiv:2305.16190

• For finite smearing $\epsilon$, $\rho^\epsilon_+(\omega) \neq \rho^\epsilon_-(\omega)$.

• BUT they converge to the same function: $\lim_{\epsilon \to 0} \rho^\epsilon_{\pm}(\omega) = \rho(\omega)$, $\omega > 0$
Numerical Examples
Discrete poles

- For $\omega > 0$: $\rho(\omega) = \delta(\omega - 0.2) + \delta(\omega - 0.5) + \delta(\omega - 0.8)$
- Euclidean data generated for $\beta = 64$ total points on the imaginary-energy axis
- The exact answer is always contained with bounding envelope of the Wertevorrat

Fermionic

Bosonic