Numerical Analytic Continuation for Lattice Field Theory

William I. Jay

william.jay@colostate.edu

Colorado State University

ECT*, Trento, Italy 26-30 May 2025

The complex structure of strong interactions in Euclidean and Minkowski space





Work in progress with:



Fernando Romero-López



Miguel Salg

Coming soon to an arXiv near you...





Motivation and Context



- Experimentally, most hadrons appear as resonances, i.e., "bumps" in scattering cross sections.
 - Location of the bump \iff Mass of the resonance
 - Width of the bump \iff Lifetime of the resonance

- Ex: $\pi^{-}\Sigma^{+}$ spectrum below $K^{-}p$ threshold (~ 1442 MeV)
 - More than 60 years of experimental and theoretical study
 - What is the nature of the resonance?
 - Can it be understood from QCD?



Data - CLAS 2014

Dalitz & Tuan, PRL 2 (1959) 425-428

Dalitz & Tuan, Annals Phys. 10 (1960) 307-351

CLAS Collaboration, PRL 112 (2014) 8, 082004

Hyodo & Jido, Prog. Part. Nucl. Phys. 67, 55 (2012)

Hyodo & Niiyama, Prog. Part. Nucl. Phys. 120, 103868 (2021)

• Ex: Exotic "XYZ" hadrons - a renaissance in hadron spectroscopy



- Theoretically, we want to calculate the properties of resonances directly from the underlying degrees of freedom: QCD
 - Provide predictions/postdictions to test our understanding of low-energy QCD
 - Help characterize the nature of resonances seen in experiment

- Resonances are identified with poles of scattering amplitudes *M* in the complex plane.
- Ex: Breit Wigner

$$\mathcal{M}(E) \sim \frac{\Gamma/2}{(E_R - E) - i\Gamma/2}$$

• Pole at complex $E = E_R - i\Gamma/2$

- Resonances are identified with poles of scattering amplitudes \mathcal{M} in the complex plane.
- <u>But</u>, analytic structure of scattering amplitudes is tightly constrained by causality and unitarity
 - Causality: No poles away from the real line on first ("physical") Riemann sheet
 - Unitarity: Complex poles come in conjugate pairs on higher Riemann sheets
 - Multi-particle thresholds: Branch cuts on the real line



PDG Review: #50 *Resonances,* Asner, Hanhart, Mikhasenko

- Resonances are identified with poles of scattering amplitudes \mathcal{M} in the complex plane.



- Resonances are identified with poles of scattering amplitudes \mathcal{M} in the complex plane.







- Scattering amplitudes are defined in infinite volume:
 - Begin with asymptotically separated initial states
 - Particles interact
 - Compute phase shift in outgoing waves at asymptotic separation.
- Conceptual complication in finite-volume:
 - A periodic, few-fm box does *not* have asymptotic states



Finite volume

Infinite volume





Finite volume

Infinite volume



Lüscher, Commun.Math.Phys. 104 (1986) 177 Lüscher, Commun.Math.Phys. 105 (1986) 153-188 Lellouch and Lüscher, Commun.Math.Phys. 219 (2001) 31-44 + many, many other contributors!

Aside: Origin of Quantization Condition

Case 1: Infinite volume

- Consider 2 bosons in non-relativistic QM.
- Consider a finite-range potential V(r) = 0, r > R
- Look for scattering (E > 0) solutions to the Schrödinger equation
 - $\psi_p(r) \sim \cos\left(pr + \delta(p)\right)$
 - Matching solutions at r = R to find phase shift $\delta(p)$
- Note: momentum *p* is a continuous

Aside: Origin of Quantization Condition Case 2: Finite volume

• Look for scattering (E > 0) solutions to the Schrödinger equation

•
$$\psi_p(r) \sim \cos\left(pr + \delta(p)\right)$$

- Compute phase shift $\delta(p)$ by matching solutions at r = R
- Enforce periodicity at boundary: $\psi_p(r) \Big|_{r=L/2} = 0$

•
$$\implies p_n \frac{L}{2} + \frac{2}{L} \delta(p_n) = \pi n$$

• Quantization condition: discrete momenta satisfy this equation



Lattice QCD

 $\langle \hat{\mathcal{O}}(\tau) \hat{\mathcal{O}}(0) \rangle$

Pipeline of ideas

1.) Compute finite-volume spectrum E_n (lattice QCD)

2.) Solve quantization condition for $K^{-1}(E_n)$

3.) Locate poles using analytic continuation

$$\det_{\ell m} \left[\frac{F(E,L) + K^{-1}(E)}{E} \right] \Big|_{E=E_n} = 0$$

Real line: $\operatorname{Re} \mathscr{M}^{-1}(E) = K^{-1}(E)$

 $\mathcal{M}^{-1}(E) \to \mathcal{M}^{-1}(z)$



State of the art: Step 1



- Choose a variational basis of N operators $\hat{\mathcal{O}}_i$ with the quantum numbers of the desired states (e.g., I=1 $\pi\pi$)
- Compute the $N \times N$ matrix of correlation functions $\langle \hat{\mathcal{O}}_i(\tau) \hat{\mathcal{O}}_i(0) \rangle$
- Solve generalized eigenvalue problem to find N energy levels E_n

State of the art: Steps 2 and 3

2.) Solve quantization condition for $K^{-1}(E_n)$

3.) Locate poles using analytic continuation

$$\det_{\mathscr{C}m} \left[K^{-1}(E) + F(E, \mathbf{P}, L) \right] \Big|_{E=\mathbf{E}_n} = 0$$
$$\mathscr{M}^{-1}(E) \to \mathscr{M}^{-1}(Z)$$

- Assume an explicit parametric model for the K-matrix to relate solutions of the quantization condition at different energies.
- Fix parameters of model with a least-squares fit.
- Solve for poles using the best-fit parameters
- Check parameterization dependence of result to quantify systematic uncertainties

State of the art: Steps 2 and 3

2.) Solve quantization condition for $K^{-1}(E_n)$

3.) Locate poles using analytic continuation

$$\det_{\mathcal{C}m} \left[K^{-1}(E) + F(E, \mathbf{P}, L) \right] \Big|_{E=\mathbf{E}_n} = 0$$
$$\mathcal{M}^{-1}(E) \to \mathcal{M}^{-1}(Z)$$

Today's talk:

 New non-parametric approach to solving quantization condition and finding poles via analytic continuation

Solving the quantization condition

Useful to get concrete: Single-channel s-wave ($\ell = 0$) scattering

Ex: $\pi\pi \to \sigma \to \pi\pi$ below $K\bar{K}$ threshold.

det
$$[K^{-1} + F] = 0$$

 $\implies q \cot \delta_0(q^2) = (\text{kinematics}) \times \mathcal{Z}_{00}(q^2, L, \mathbf{P})$

Determinant simplifies to a single line.

 \mathscr{Z}_{00} - Lüscher zeta function (transcendental function for finite volume)

Solving the quantization condition

Useful to get concrete: s-wave multi-channel scattering

Ex: $\pi \Sigma \to \Lambda(1405) \to \overline{K}N$

$$\det \begin{bmatrix} K^{-1} + F \end{bmatrix} = 0$$

$$\Longrightarrow \det \begin{bmatrix} \begin{pmatrix} K_{\pi\Sigma;\pi\Sigma}^{-1}(E) & K_{\pi\Sigma;\bar{K}N}^{-1}(E) \\ K_{\bar{K}N;\pi\Sigma}^{-1}(E) & K_{\bar{K}N;\bar{K}N}^{-1}(E) \end{pmatrix} + \begin{pmatrix} F_{\pi\Sigma}(E) & 0 \\ 0 & F_{\bar{K}N}(E) \end{pmatrix} \end{bmatrix} = 0$$

For each energy E, the quantization condition is a real equation in three unknowns: $K_{ii}^{-1}(E)$

Solving the quantization condition - usual method

- Parameterize the K-matrix
- Solve for discrete energies
- Compare to known energies
- Construct χ^2 function
- Define best-fit parameters

Ansatz
$$K^{-1}(E) = \sum_{m} \theta_{m} E^{m}$$

Solution $E_{\text{QC}}(\theta)$

$$E_{\text{LQCD}}: \Delta E = E_{\text{LQCD}} - E_{QC}(\theta)$$

$$\chi^2(\theta) = \Delta E^T \Sigma_{\rm LQCD}^{-1} \Delta E$$

$$\theta^{\star} = \operatorname{argmin}_{\theta} \chi^2(\theta)$$



A "non-parametric" proposal



Solving the quantization condition - a Bayesian approach

Goal: non-parametric model for K-matrix at nodes on the real line

- Consider interpolating a smooth function $u(E) : \mathbb{R} \to \mathbb{R}$ at a discrete set of "nodes" **E** and "values" **u**
- If typical variations in u(E) occur at scale longer than node spacing, the error from interpolating a discrete set "ought to be small."

Solving the quantization condition - a Bayesian approach

Goal: non-parametric model for K-matrix at nodes on the real line

• Bayesian approach \implies need "prior" distribution for values $\mathbf{u} = K_{\ell}^{-1}(\mathbf{E})$:

$$p(\mathbf{u} | \mathbf{u}_0) \propto \exp\left[-\frac{1}{2}(\mathbf{u} - \mathbf{u}_0)^T \Sigma_p^{-1}(\mathbf{u} - \mathbf{u}_0)\right]$$

 $p(\mathbf{E}_{\text{LQCD}} | \mathbf{u}) \propto \exp \left| -\frac{1}{2} \chi^2(\mathbf{u}) \right|$

multivariate Gaussian distribution

$$\Sigma_p(E, E') = \sigma(E, E')^2 \exp\left[-\frac{(E - E')^2}{2\ell_c^2}\right] + \epsilon \delta_{E, E'}$$

Radial Basis Function (RBF) kernel

Likelihood - usual χ^2

Solving the quantization condition - a Bayesian approach

Goal: non-parametric model for K-matrix at nodes on the real line

• Bayes Theorem:

 $(posterior) = (likelihood) \times (prior)$

 $p(\mathbf{u} | \mathbf{E}_{LQCD}, \mathbf{u}_0) = p(\mathbf{E}_{LQCD} | \mathbf{u}) \times p(\mathbf{u} | \mathbf{u}_0)$

Note: Similar, but not identical, to a Gaussian process.

 $E_{\rm OC}(\mathbf{u})$ has important nonlinearities in \mathbf{u} from singularities in zeta function \mathcal{Z}_{00}

Solving the quantization condition - a Bayesian approach

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• Bayes Theorem:

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 $p(\mathbf{u} | \mathbf{E}_{\text{LQCD}}, \mathbf{u}_0) = p(\mathbf{E}_{\text{LQCD}} | \mathbf{u}) \times p(\mathbf{u} | \mathbf{u}_0)$

• Expectation values (mean, errors) defined with respect to the posterior, as usual:

$$\langle \mathbf{u} \rangle_{\text{post}} = \frac{1}{Z} \int d^d u \, \mathbf{u} \, p(\mathbf{u} \,|\, \mathbf{E}_{\text{LQCD}}, \mathbf{u}_0)$$

Solving the quantization condition - a Bayesian approach

Goal: non-parametric model for K-matrix at nodes on the real line



Benefit: no Markov chain, so no autocorrelations.

Challenge: Sampling can be inefficient when prior and posterior dissimilar

Solving the quantization condition - a Bayesian approach

Goal: non-parametric model for K-matrix at nodes on the real line

Posterior Sampling: Monte Carlo

- 1. Linearize quantization condition
- 2. Sample from resulting Gaussian approximation to (Likelihood) \times (Prior)

3. Apply reweighting to recover exact result

- Benefit: Easy to compute normalization (Bayesian evidence) for model comparison
- Challenge: Sampling can still be inefficient when prior and posterior dissimilar

Approach #2

Solving the quantization condition - a Bayesian approach

Goal: non-parametric model for K-matrix at nodes on the real line

Posterior Sampling: Monte Carlo

Approach #3

1. Generate samples using Hybrid Monte Carlo algorithm

- Benefit: Robust sampling method
- Challenge: Introduces familiar complications like autocorrelations
- Challenge: Accessing normalization Z for model comparison is more cumbersome

Solving the quantization condition - a Bayesian approach

Goal: non-parametric model for K-matrix at nodes on the real line

• Upshot: sampling furnishes $\langle \mathbf{u} \rangle_{\text{post}} = K^{-1}(\mathbf{E})$



Analytic continuation to locate poles in the complex plane



with robust quantification of uncertainty

Analytic continuation to locate poles in the complex plane



Analytic continuation to locate poles in the complex plane

The natural setting for complex analysis is the unit disk.



Analytic continuation to locate poles in the complex plane

Nota bena: Such a mapping is required for both domain and codomain.



Analytic continuation to locate poles in the complex plane

Nota bena: Such a mapping is required for both domain and codomain.



- The Riemann mapping theorem guarantees existence of required conformal maps
 - Use physics knowledge to guide the choice of domain and codomain and maps
 - Ex: Locations of poles and zeros, range of possible values, etc...
- These maps implicitly contain strong theoretical assumptions. Be careful.

Analytic continuation to locate poles in the complex plane

One appealing choice: Schwarz-Christoffel mapping



Numerical Analytic Continuation

The sharp technical problem

• Given data for real energies $\{E_n\}, \{\mathcal{M}^{-1}(E_n)\}$

$$\{E_n\} \to \zeta_n \subset \mathbb{D},$$

$$\{\mathscr{M}^{-1}(E_n)\} \mapsto w_n \subset \mathbb{D},$$

construct an analytic function $f(\zeta)$

on the disk that interpolates these points: $f(\zeta_n) = w_n$.

• Locate zero by extrapolation to the interior of the disk



Nevanlinna-Pick Interpolation The big idea: "factor out what you know"

• Basic fact (maximum modulus principle \Longrightarrow):

Let $g(\zeta) : \mathbb{D} \to \mathbb{D}$ be an analytic function.

Suppose $g(\zeta)$ has a zero at $\mathbf{a} \in \mathbb{D}$: $g(\mathbf{a}) = 0$.





Nevanlinna-Pick Interpolation The big idea: "factor out what you know"

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Let $g(\zeta) : \mathbb{D} \to \mathbb{D}$ be an analytic function.

Suppose $g(\zeta)$ has a zero at $\mathbf{a} \in \mathbb{D}$: $g(\mathbf{a}) = 0$.

Then $g(\zeta) = b_a(\zeta)\tilde{g}(\zeta)$.

- Note: Setup familiar in quark-flavor physics from *z*-expansion of form factors
 - Blaschke factors "factor out" known analytic structure, e.g., sub-threshold poles.



Boyd, Grinstein, Lebed *Nucl.Phys.B* 461 (1996) 493-511 *Phys.Rev.D* 56 (1997) 6895-6911 Caprini, Lellouch, Neubert Nucl.Phys.B 530 (1998) 153-181

Analytic Continuation

Repeated application of "factoring"

Theorem (Nevanlinna, 1919/1929):

 Any solution to the interpolation problem with N points can be written in the form

 $f(\zeta) = \frac{P_N(\zeta)f_N(\zeta) + Q_N(\zeta)}{R_N(\zeta)f_N(\zeta) + S_N(\zeta)}.$

• "Nevanlinna coefficients" P_N , Q_N , R_N , S_N

 \Leftrightarrow Known / calculable from input data

• Arbitrary function analytic function $f_N(\zeta) : \mathbb{D} \to \mathbb{D}$

 \iff Freedom to specify further data to constrain the interpolating function

 \iff Plays role of the "remainder" function on the previous slide

R. Nevanlinna Ann. Acad. Sci. Fenn. Ser. A 13 (1919) Ann. Acad. Sci. Fenn. Ser. A 32 (1929)

A. Nicolau Proc. Summer School in Complex and Harmonic analysis... (2016) [LINK]

> First application in QFT (Condensed Matter Physics) J. Fei, C.-N. Yeh, E. Gull, *PRL* 126, 056402 (2021) arXiv:2010.04572

> > Bergamaschi, WJ, Oare PRD 108 (2023) 7, 074516 arXiv:2305.16190



Patrick Oare MIT \rightarrow BNL

Analytic Continuation The full space of solutions

- Key point: The freedom and influence of the "remainder" is constrained, since $f_N(\zeta) \in \mathbb{D}$.
- Question: What possible values can the interpolating function $f(\zeta)$ can take when extrapolated to arbitrary points " \star "?
 - Remarkably, this set can be parameterized explicitly for each N and each point " \star ".
 - Size of this set ⇐⇒ ambiguity in the analytic continuation

Bergamaschi, WJ, Oare PRD 108 (2023) 7, 074516 arXiv:2305.16190



= given

Analytic Continuation The full space of solutions

• **Answer**: The space of possible values is a disk of radius $r_N(\zeta)$ centered at $c_N(\zeta)$. This disk called the *Wertevorrat* $\Delta_N(\zeta)$.

$$c_{N} = \frac{P_{N}(-R_{N}/S_{N}) + Q_{N}}{R_{N}(-R_{N}/S_{N}) + S_{N}} \qquad r_{N} = \frac{|P_{N}S_{N} - Q_{N}R_{N}|}{|S_{N}|^{2} - |R_{N}|^{2}}$$

- Given N interpolation points, the Wertevorrat $\Delta_N(\zeta)$ rigorously contains all possible analytic continuations at each extrapolation point $\zeta \in \mathbb{D}$.
- Complete characterization of systematic uncertainty
- No model assumptions just analyticity!

Bergamaschi, WJ, Oare PRD 108 (2023) 7, 074516 arXiv:2305.16190



Analytic continuation to locate poles in the complex plane

Searching for zeros in $\mathcal{M}^{-1}(E)$ with the Wertevorrat

- Use a random point in $\Delta_N(\zeta)$ as the function estimator.
 - Sampling trivial with formulae for radius and center

 $w(\zeta) = c_N(\zeta) + rr_N(\zeta)e^{i\theta}$

- Map the $w(\zeta)$ back to original energy coordinates to find zero
- Fix random numbers (r, θ) on each posterior sample
 - Can sample additional values for (r, θ) on each sample for "improved estimator"
 - Similar in spirit to using many point sources on a given gauge-field configuration when solving the Dirac equation in lattice QCD.



Analytic continuation to locate poles in the complex plane

2.) Solve quantization condition for $K^{-1}(E_n)$ 3.) Locate poles using analytic continuation $det \left[K^{-1}(E) + F(E, \mathbf{P}, L) \right] \Big|_{E=E_n} = 0$ $\mathscr{M}^{-1}(E) \to \mathscr{M}^{-1}(Z)$

Our method:

2.) Solve quantization condition with Bayesian analysis

3.) Locate poles using Nevanlinna interpolation

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 $\Lambda(1405)$ and $\Lambda(1380)$ resonances

Lattice QCD calculation

Single ensemble

- $a \approx 0.06 \text{ fm}$
- $M_{\pi} \approx 200 \text{ MeV}$

 $M_K \approx 487 \text{ MeV}$



Energy levels E_n

 $\langle \hat{\mathcal{O}}(\tau) \hat{\mathcal{O}}(0) \rangle$

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 $\Lambda(1405)$ and $\Lambda(1380)$ resonances



Energy w.r.t. $\pi\Sigma$ threshold

 $\Lambda(1405)$ and $\Lambda(1380)$ resonances

How do results look with the new method?

- 2.) Solve quantization condition with Bayesian analysis
- 3.) Locate poles using Nevanlinna interpolation

$\Lambda(1405)$ and $\Lambda(1380)$ resonances



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 $\Lambda(1405)$ and $\Lambda(1380)$ resonances



- Two-pole picture consistent with original BaSc analysis
- $\Lambda(1380)$: virtual bound state on second sheet below threshold on real line
- $\Lambda(1405)$: resonance with finite imaginary part
- Results are statistically consistent with previous analysis

* Slight vertical offset for $\Lambda(1380)$ to aid readability

Conclusions

- Lattice QCD calculations of resonance spectroscopy are based on the finite-volume formalism.
- Lattice QCD is reaching the maturity to weigh in on decades-old questions, e.g., the nature of the $\Lambda(1405)$ resonance in $\pi\Sigma \bar{K}p$ scattering.
- Exotic hadrons ("XYZ") discovered over the past 20 years have caused a renaissance in hadron spectroscopy.
- Analysis methods offering improved systematic control are timely.
- Today's talk: proof-of-concept for a new analysis method based on Bayesian reconstruction and Nevanlinna interpolation.



Backup

What about sin(iz) and friends?

Bergamaschi, WJ, Oare PRD 108 (2023) 7, 074516 arXiv:2305.16190

- The context where this is best understood is for Green functions G(z).
- Recall: a green function is a map $G(z) : \mathbb{H} \to \mathbb{H}$ (\mathbb{H} =upper half-plane)
 - Functions with this property are called Nevanlinna functions
 - Roughly speaking, any Nevanlinna function can be written as an integral of a suitable spectral function.
 - Mapping the problem to the disk to invoke Nevanlinna's theorem invokes these properties in an essential way.
 - In other words, the interpolating function f : D → D already and automatically has the correct analytic structure
- The function $\sin(iz)$:
 - Vanishes at infinitely many points, e.g., $z \in i\pi \mathbb{N}$
 - Blows up to $\pm \infty \Longrightarrow \underline{\text{Not}}$ a function $\mathbb{H} \to \mathbb{H}$.
 - Has the wrong singularity structure/asymptotic behavior.
- Constructing an interpolating function $f : \mathbb{D} \to \mathbb{D}$ automatically excludes inconsistent/pathological functions like $\sin(iz)$. This property holds when translated back to $G(z) : \mathbb{H} \to \mathbb{H}$.



What about statistical noise?

The method announces its failure in two ways.

- 1. The Wertevorrat is expected to decrease monotonically as more information is included. If the radius of the Wertevorrat begins to jitter around some "saturation width," numerical precision has become a limiting factor.
- 2. Nevanlinna's theorem assumes the data satisfy an analytic self-consistency condition: the Pick matrix P_{ij} must be positive semi-definite.

$$P_{ij} = \frac{1 - w_i \bar{w}_j}{1 - \zeta_i \bar{\zeta}_j}$$

Possible Solutions

- A. Check this condition and avoid data that violate the hypotheses of the theorem.
- B. Rephrase the difficulty as a statistical pre-denoising problem:

Given a statistical sample of $\mathbf{G} \in \mathbb{R}^N$, project to the closest set of points $\mathbf{G}' \in \mathbb{R}^N$ such that P_{ij} is positive semidefinite. "Closest" is determined by the covariance matrix.

Real vs Virtual Bound State

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- Bound state:
 - Pole in $\mathcal{M}(E)$ on real axis below threshold of physical sheet
 - Corresponds to a bona fide asymptotic state (e.g., I=0 deuteron)

•
$$p = i |p|$$
 so wavefunction $\psi \sim e^{ipr} \sim e^{-|p|r}$

- Virtual bound state:
 - Pole in $\mathcal{M}(E)$ on real axis below threshold of *unphysical* sheet
 - Gives rise to an observable enhancement in the cross section at threshold. No asymptotic state (e.g., I=1 di-neutron)

•
$$p = -i |p|$$
 so wavefunction $\psi \sim e^{ipr} \sim e^{+|p|r}$

- Look for phase-shift curve to intersect the virtualbound-state condition:
 - $\cdot p \cot \delta(p) ip = 0$
 - for purely imaginary and negative p = -i|p|





Analytic continuation to locate poles in the complex plane

What not to do:



Suppose I have point $z \in \mathbb{C}$. Consider some neighborhood around z.

Map this neighborhood to the unit disk.

Analytic continuation to locate poles in the complex plane

What not to do:



Analytic continuation to locate poles in the complex plane

• What **not** to do:



Analytic continuation to locate poles in the complex plane

What not to do:



Analytic continuation to locate poles in the complex plane

