Approaching the Inverse Problem

William I. Jay

Lattice 2024

Liverpool, England

29 July 2024







Approaching Spectral Densities

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Hii



Outline

- Connections to the conference
- Motivation and Context
- Spectral Densities and Lattice QCD
 - Role of smearing
 - Analytic continuation

Not a comprehensive review.

Impossible to review all the exciting work in this area in the time allotted.

My topical presentation reflects my interests (and probably biases).

Apologies for all the excellent work not mentioned.



Recent adjacent discussion

Recent plenary talks at Lattice conference series

- J. Bulava's plenary talk at Lattice 2022
 - Spectral Reconstruction of Inclusive Rates [link]
 - PoS LATTICE2022 (2023) 231 [arXiv:2301.04072]
- J. Liang's plenary talk at Lattice 2019
 - Hadronic Tensor and Neutrino-Nucleon Scattering [link]
 - PoS LATTICE2019 (2020) 046 [arXiv:2008.12389]

Lattice@CERN 2024: Inverse Problems 8-12 July 2024 [Indico Link]

• Week of talks/discussion about this topic. Check out the workshop webpage!



Neighboring talks at this conference

More than a dozen presentations related to spectral densities

Monday

Tuesday

Shear viscosity from quenched to full lattice QCD	Pavan Pavan	Virtual radiative Leptonic decays of charged Kaons	Roberto Di Palma
	11:55 - 12:15		11:15 - 11:35
Thermal photon production rate from lattice QCD	Dibyendu Bala	Inclusive semileptonic \$D_s\mapsto X \ell \nu\$ decay from lattice QCD	Dr Alessandro De Santis
	12:15 - 12:35		15:05 - 15:25
Sparse modeling study to extract spectral functions from lattice QCD data	Junichi Takahashi	Semileptonic Inclusive Decay of the \$D_s\$ Meson	Christiane Groß
	15:35 - 15:55		15:25 - 15:45
Pseudo-scalar meson spectral properties from spatial hadron correlators	Tristan Ueding	The Cabibbo Angle from Inclusive \$\tau\$ Decays	Giuseppe Gagliardi
	15:55 - 16:15		16:55 - 17:15

Wednesday

Spectroscopy of lattice gauge theories from spectral densities	Niccolo Forzano
	11:35 - 11:55
Quarkonia Spectral Functions from (2+1)-flavor QCD	Dr Sajid Ali
using Non-perturbative Thermal Potential	12:35 - 12:55
NRQCD Bottomonium spectrum at non-zero temperatures	Antonio Smecca
using Backus-Gilbert regularisations	11:15 - 11:35
NRQCD Bottomonium at non-zero temperature using	Rachel Horohan D'arcy
using time-derivative moments	11:35 - 11:55

Friday

Spectral densities from Euclidean-time lattice correlation functions	Matteo Saccardi	
	15:15 - 15:35	
Progress in Reconstructing the Hadronic Tensor	Douglas Stewart	
from Euclidean Correlators	15:15 - 15:35	



Motivation and Context





 $G(\tau) = \int \frac{d\omega}{2\pi} \rho(\omega) e^{-\omega\tau}$ Evaluate with Lattice QCD $G(\tau) = \int \frac{d\omega}{2\pi} \rho(\omega) e^{-\omega\tau}$ Spectral density
Compute from $G(\tau)$?



Spectral functions for inclusive observables

The R-ratio: $e^+e^- \rightarrow$ hadrons



QCD correlation function

 $\int d^4x \, e^{iq \cdot x} \langle \emptyset \, | \, [j_{\mu}^{\text{EM}}(x), j_{\nu}^{\text{EM}}(0)] \, | \, \emptyset \rangle$ $= (q_{\mu}q_{\nu} - q^2 g_{\mu\nu})\rho(q^2)$

Connection via the optical theorem

$$\rho(s) = \frac{R(s)}{12\pi^2}$$



Figure: arXiv:1908.00921 Davier, Hoecker, Malaescu, Zhang

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Spectral functions for inclusive observables Other high-impact observables



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 $G(\tau) = \int \frac{d\omega}{2\pi} \rho(\omega) e^{-\omega\tau}$ Euclidean correlation function Evaluate with Lattice QCD
Spectral density Compute from $G(\tau)$?



$$G(\tau) = \int \frac{d\omega}{2\pi} \rho(\omega) e^{-\omega\tau}$$

Intertwined conceptual/technical challenges:

- 1. Calculation in finite volume deforms the spectrum.
- 2. Euclidean data is available at a finite set of points.
- 3. Statistical uncertainty is present.

Spectral Densities The deformation of finite volume

Consider inclusive electron-proton scattering

Elastic scattering: $\rho(\omega) \sim \delta(\omega - E_p) \times (\text{form factor})^2$

Inelastic scattering: $\rho(\omega) \sim \Theta\left(\omega - M_N - M_{\pi}\right) \times (\text{phase space}) \times |\mathcal{M}|^2$



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But... a QM system in a box has a discrete spectrum.

See plenary talks by Felix Erben — Tues 9:00 Nilmani Mathur — Sat 9:00

Finite-volume formalism in elastic region

M. Lüscher (1986) L. Lellouch and M. Lüscher (2001)

...and many, many other contributors!

Spectral Densities The deformation of finite volume

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The deformation of finite volume

How to reconcile these two pictures?



The deformation of finite volume

How to reconcile these two pictures? Smearing.

Choose a smearing kernel $\delta_{\epsilon}(\omega) =$

Define a smeared spectral function $\rho_{\epsilon}(\omega, L)$

Hansen, Meyer, and Robaina PRD 96 (2017) 9, 094513 [arXiv:1704.08993]

Poggio, Quinn, and Weinberg PRD 13 (1976) 1958

Hansen, Meyer, and Robaina PRD 96 (2017) 9, 094513 [arXiv:1704.08993]

The deformation of finite volume

How to reconcile these two pictures? Smearing.

 $\rho(\omega) = \lim_{\epsilon \to 0} \lim_{L \to \infty} \rho_{\epsilon}(\omega, L)$



The HLT Algorithm State of the art for practical reconstructions

Hansen, Lupo, and Tantalo PRD 99 (2019) 9, 094508 arXiv:1903.06476

• Write linear Ansatz for solution:

$$\rho_{\epsilon}(\omega) = \sum_{t} q_{t}(\omega)C(t) = \int d\omega' \rho(\omega')\hat{\delta}_{\epsilon}(\omega',\omega)$$

• Determine coefficients $g_t(\omega)$ by minimizing distance to smearing kernel—which can be chosen freely.

$$A[q] = \int d\omega' \left\{ \delta_{\epsilon}(\omega' - \omega) - \hat{\delta}_{\epsilon}(\omega', \omega) \right\}^{2}$$

$$Tune \lambda \text{ for tradeoff between bias/variance}$$

- Minimize the convex sum: $\mathscr{F}_{\lambda}[q] = (1 \lambda)A[q] + \lambda B[q]$
- Elegant connection to Bayesian methods / Gaussian processes
 - Del Debbio *et al.* arXiv:2311.18125

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Open-source implementation

github.com/LupoA/lsdensities

Probing the energy-smeared R-ratio

ETMC PRL 130 (2023) 24, 241901 arXiv: 2212.08467

Spectral reconstruction of $\langle VV \rangle$ correlators with HLT



E [GeV]

- Gaussian smearing kernel used with the reconstruction using HLT algorithm
- Results presented in continuum limit
- Explicit check of systematic effect of finite volume (B64/B96)
- Same $\langle VV\rangle$ correlators as used in recent ETMC work on μ (g-2) [arXiv:2206.15084]. No QED/SIB corrections.

ID	$L^3 \times T$	$a~{ m fm}$	$aL~{ m fm}$	$m_{\pi}~{ m GeV}$
B64	$64^3 \cdot 128$	0.07957(13)	5.09	0.1352(2)
B96	$96^3 \cdot 192$	0.07957(13)	7.64	0.1352(2)
C80	$80^3 \cdot 160$	0.06821(13)	5.46	0.1349(3)
D96	$96^3 \cdot 192$	0.05692(12)	5.46	0.1351(3)



As a matter of principle, how differential could one go?

How much analytic information is contained in, say, O(100) points?





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

Patrick Oare MIT \rightarrow BNL



Another perspective on smearing

Consider a Green function $G(z) = 1/(z - E_0)$ with $E_0 = \frac{1}{2}$.



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Another perspective on smearing

Consider a Green function $G(z) = 1/(z - E_0)$ with $E_0 = \frac{1}{2}$.

Look at $\text{Im}G(\omega + i\epsilon)$ for various distances ϵ above real line.

Motivates defining

$$\rho_{\epsilon}(\omega) \equiv \frac{1}{\pi} \text{Im}G(\omega + i\epsilon)$$
$$\int d\omega' \delta_{\epsilon}(\omega - \omega')\rho(\omega')$$

Poggio, Quinn, and Weinberg PRD 13 (1976) 1958

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PHYSICAL REVIEW D

VOLUME 13, NUMBER 7

1 APRIL 1976

Smearing method in the quark model*

E. C. Poggio, H. R. Quinn,[†] and S. Weinberg Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138 (Received 8 December 1975)

We propose that perturbation theory in a gauge field theory of quarks and gluons can be used to calculate physical mass-shell processes, provided that both the data and the theory are smeared over a suitable energy range. This procedure is explored in detail for the process of electron-positron annihilation into hadrons. We show that a smearing range of 3 GeV^2 in the squared center-of-mass energy should be adequate to allow the use of lowest-order perturbation theory. The smeared data are compared with theory for a variety of models. It appears to be difficult to fit the present data with theory, unless there is a new charged lepton or quark with mass in the region 2 to 3 GeV.

The smeared ratio is defined as

$$\overline{R}(s,\Delta) = \frac{\Delta}{\pi} \int_0^\infty \frac{ds' R(s')}{(s'-s)^2 + \Delta^2}.$$
 (3)

$$2i\overline{R}(s,\Delta) = \Pi(s+i\Delta) - \Pi(s-i\Delta).$$
(5)

Another perspective on smearing

Consider a Green function $G(z) = 1/(z - E_0)$ with $E_0 = \frac{1}{2}$.

Look at $\text{Im}G(\omega + i\epsilon)$ for various distances ϵ above real line.

Motivates defining

HLT framing of problem: this is a "Cauchy" kernel:

$$\rho_{\epsilon}(\omega) \equiv \frac{1}{\pi} \operatorname{Im} G(\omega + i\epsilon) \\ \int d\omega' \delta_{\epsilon}(\omega - \omega') \rho(\omega')$$

$$\delta_{\epsilon}(\omega - \omega') \equiv \frac{1}{\pi} \frac{\epsilon}{(\omega - \omega')^2 + \epsilon^2}$$

✓ Becomes delta-function as $\epsilon \to 0$



$$G(\tau) = \int \frac{d\omega}{2\pi} \rho(\omega) e^{-\omega\tau}$$

Intertwined conceptual/technical challenges:

- ✓ Calculation in finite volume deforms the spectrum. $\rho(\omega) = \lim_{\epsilon \to 0} \lim_{L \to \infty} \rho_{\epsilon}(\omega, L)$
- 2. Euclidean data is available at a finite set of points.
- 3. Statistical uncertainty is present.

"How much analytic information is contained in this set of points?"

The Inverse Problem Analytic continuation from a finite set of points

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

Lattice QCD calculations furnish data in Euclidean time \bullet $G(\tau) = \sum \left| \langle 0 | \mathcal{O} | n \rangle \right|^2 \left(e^{-E_n \tau} + e^{-E_n(\beta - \tau)} \right)$ Euclidean data at Matsubara frequencies iω₂ In frequency space (take $a \ll 1$): $G(i\omega_{\ell}) = \int d\tau \, e^{i\omega_{\ell}\tau} G(\tau)$ Finite-volume energy levels $=\sum_{n}\left|\langle 0 | \mathcal{O} | n \rangle\right|^{2} \left(\frac{1}{E_{n} + i\omega_{\ell}} + \frac{1}{E_{n} - i\omega_{\ell}}\right)$ Spectral weight \iff Residue of pole(s)

Analytic continuation from a finite set of points



Analytic continuation from a finite set of points



The Inverse Problem The role of 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



The Inverse Problem The role of conformal maps

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

- 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!



The sharp technical problem

• Given Euclidean data $\{\zeta_l\}, \{w_l\}$

 $\{i\omega_{\ell}\} \to \zeta_{\ell} \subset \mathbb{D},$

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

construct an analytic function $f(\zeta)$

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



on the disk that interpolates these points: $f(\zeta_{\ell}) = w_l$.

• Evaluating this function near the boundary gives $\rho_{\epsilon}(\omega)$

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

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

• 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 $\mathbf{a} \in \mathbb{D}$: $g(\mathbf{a}) = 0$.





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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

↔Known / calculable from input data

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

 \iff Freedom to specify further Euclidean 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

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 " \blacklozenge "?
 - Remarkably, this set can be parameterized explicitly for each N and each point "
 ".
 - Size of this set ⇐⇒ ambiguity in the analytic continuation

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 $\mathbf{X} = given$



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* $\Delta_N(\zeta)$,.

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

- 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 "regularization" beyond smearing
 - No model assumptions just analyticity!



Analytic Continuation Back to the upper half-plane

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• Map the Wertevorrat back to the original coordinates



$$\rho^{\epsilon}(\omega) = \frac{1}{\pi} \operatorname{Im} G(\omega + i\epsilon)$$

$$\delta \rho^{\epsilon}(\omega) = \frac{1}{\pi} \left[\max \operatorname{Im} \partial D_{N}(\omega + i\epsilon) - \min \operatorname{Im} \partial D_{N}(\omega + i\epsilon) \right]$$

Bernecker and Meyer Eur.Phys.J.A 47 (2011) 148 arXiv:<u>1107.4388</u>

The R-ratio — reconstructing a parameterization

- Bernecker and Meyer give a useful parameterization of Rratio 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"



The R-ratio — reconstructing a parameterization

- Euclidean data generated for $\beta = 96$ total points on the imaginary-energy axis
- Run reconstruction for different smearing widths ϵ



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The R-ratio — reconstructing a parameterization

- Euclidean data generated for $\beta = 96$ total points on the imaginary-energy axis
- Run reconstruction for different smearing widths ϵ
- Exact answer is contained within the bounding envelope of the Wertevorrat



Numerical Example The R-ratio — reconstructing a parameterization

- Euclidean data generated for $\beta = 96$ total points on the imaginary-energy axis
- Run reconstruction for different smearing widths $\boldsymbol{\epsilon}$
- \checkmark Exact answer is contained within the bounding envelope of the Wertevorrat
- ✓ Spectral peaks from $\rho(770)/\omega(782)$ and $\phi(1020)$ clearly visible in reconstructions



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The R-ratio — reconstructing a parameterization

- Euclidean data generated for $\beta = 144$ total points on the imaginary-energy axis
- How does the size of the Wertevorrat scale with the number of points?
- Fix reconstruction energy and smearing ϵ . Vary number of points used in reconstruction. ulletSmeared spectral reconstruction 30 Uncertainty scaling Wertevorrat 10% 25 100 Exact result, Fixed $\varepsilon = 0.1$ ⁻ractional uncertainty 1% $\varepsilon = 0.1$ s=0.65 GeV² 0.1% 20 10^{-1} $R(s, \varepsilon)$ 15 10^{-2} 10-10-3 5 10^{-4} 60 20 40 80 100 120 0 Number of points used in reconstruction *s* [GeV²]

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The R-ratio — reconstructing a parameterization

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$$G(\tau) = \int \frac{d\omega}{2\pi} \rho(\omega) e^{-\omega\tau}$$

Intertwined conceptual/technical challenges:

- ✓ Calculation in finite volume deforms the spectrum. $\rho(\omega) = \lim_{\epsilon \to 0} \lim_{L \to \infty} \rho_{\epsilon}(\omega, L)$
- ✓ Euclidean data is available at a finite set of points. $\delta \rho^{\epsilon}(\omega) \sim \operatorname{Im} \partial D_{N}(\omega + i\epsilon)$
- 3. Statistical uncertainty is present.
 - Regularize, e.g., as with HLT or other familiar methods
 - Impose analytic self-consistency conditions on statistical noise.



Summary

- Inclusive quantities contain a wealth of hadronic information
- A fresh look at these observables is timely:
 - Muon (g-2) and the R-ratio
 - $|V_{ud}|$, $|V_{us}|$, and the "Cabibbo anomaly"
 - Inclusive versus exclusive determinations of $|V_{cb}|$ and $|V_{ub}|$
 - Hadronic structure needed for upcoming DUNE and the EIC experiments
- Recent improved practical and formal understanding of the challenges associated with spectral reconstruction
- Exciting calculations have appeared over the past few years. I expect the community to see many more in the coming years.
- Lots of important and exciting work is happening in our field that I haven't had time to discuss!



Backup slides



What about sin(iz) and friends?

- 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 $f: \mathbb{D} \to \mathbb{D}$ 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.

Spectral functions for inclusive observables

Inclusive electron-proton scattering: $ep \rightarrow eX$



Inclusive decay of the τ lepton and $|V_{\mu\nu}|$

ETMC PRL 132 (2024) 26, 261901 arXiv:2403.05404

Spectral reconstruction of $\langle J_{us}J_{us}\rangle$ correlators with HLT

ETMC PRD 108 (2023) 7, 074513 arXiv:2308.03125

$$R_{us}^{(\tau)} = \frac{\Gamma(\tau \mapsto X_{us}\nu_{\tau})}{\Gamma(\tau \mapsto e\bar{\nu}_e\nu_{\tau})}$$

- Results given in continuum limit, with estimate of finite-size effects
- HLT method used, with the step function from kinematic threshold regulated via smearing





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