Bayesian constraints and analytic continuation of scattering amplitudes from lattice QCD

Miguel Salg

In collaboration with Fernando Romero-López and William Jay

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Background

Hadron spectroscopy

- Goal: obtain masses and decay widths of hadronic resonances from QCD

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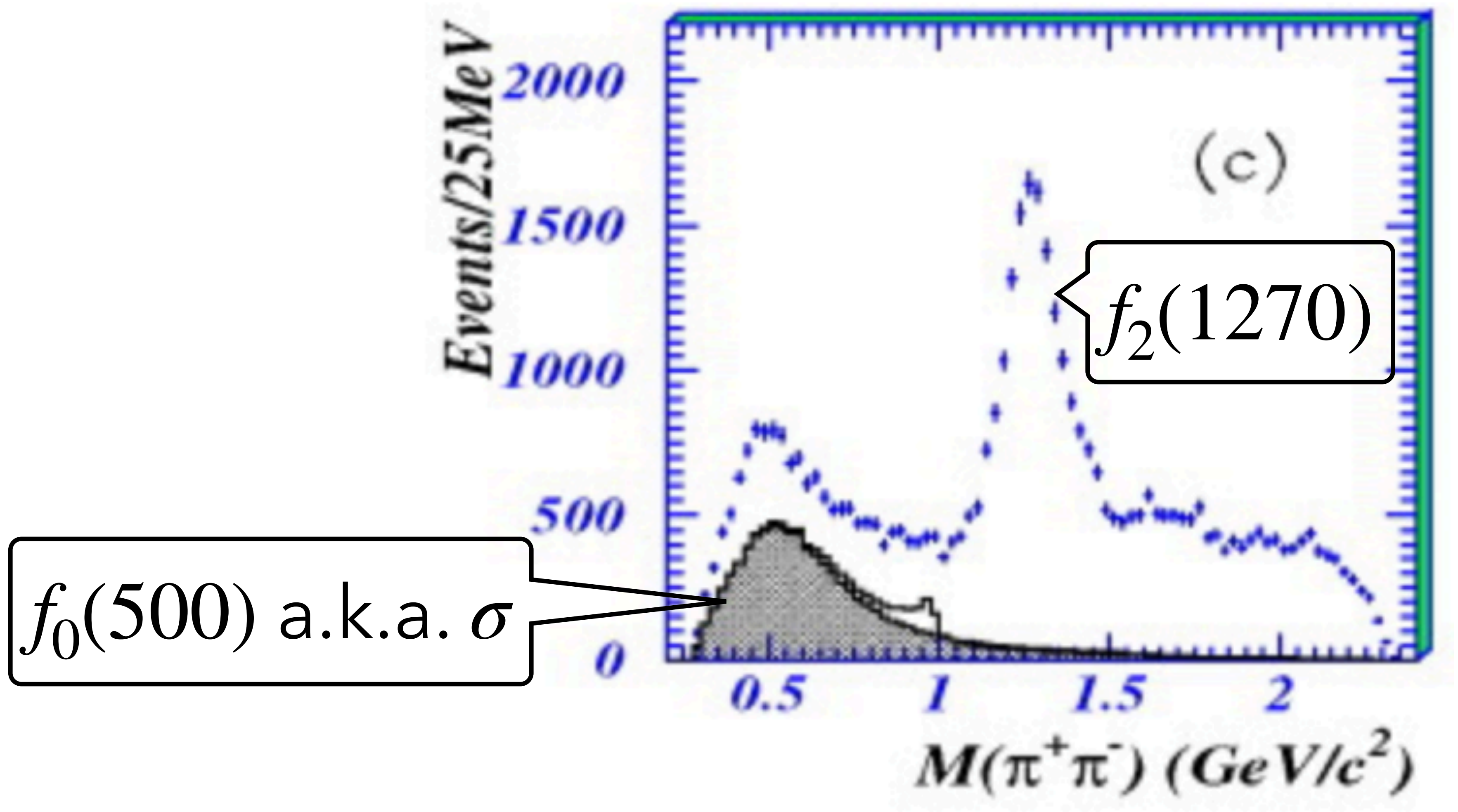
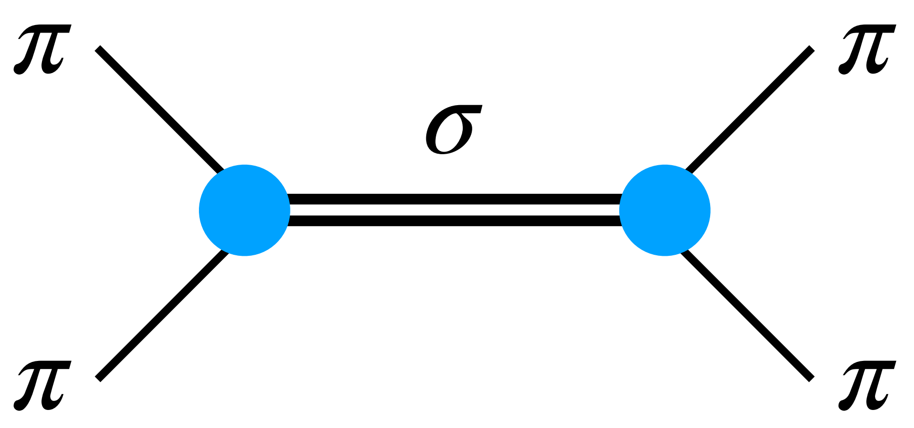
$J/\psi \to \omega\pi^+\pi^-$



Ablikim et al. (BES) 2004 [Phys. Lett. B 598, 149]



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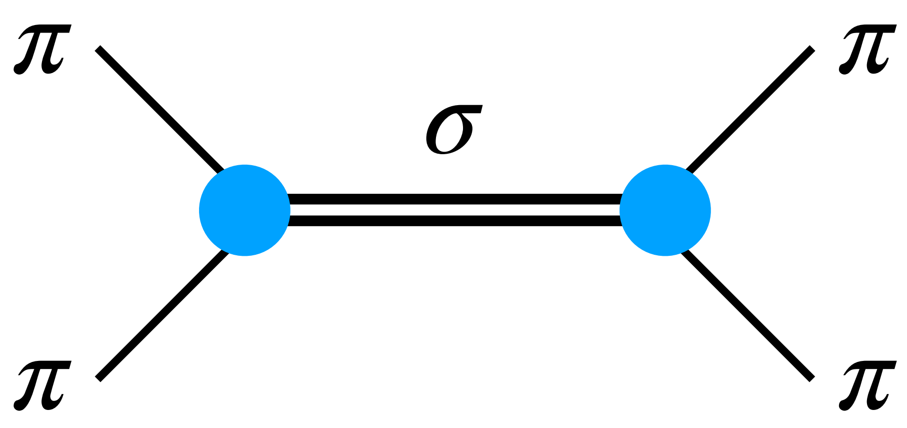

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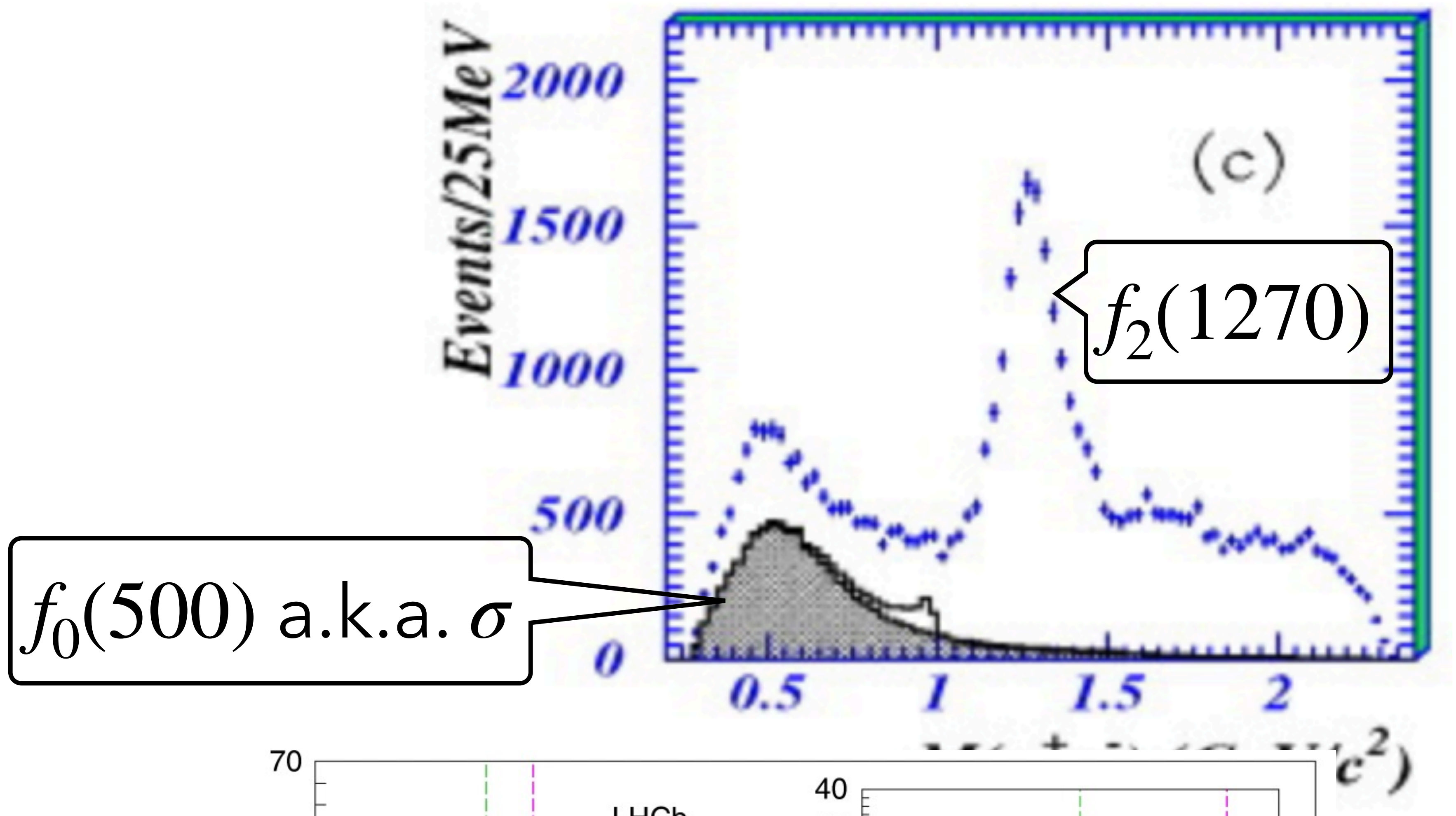

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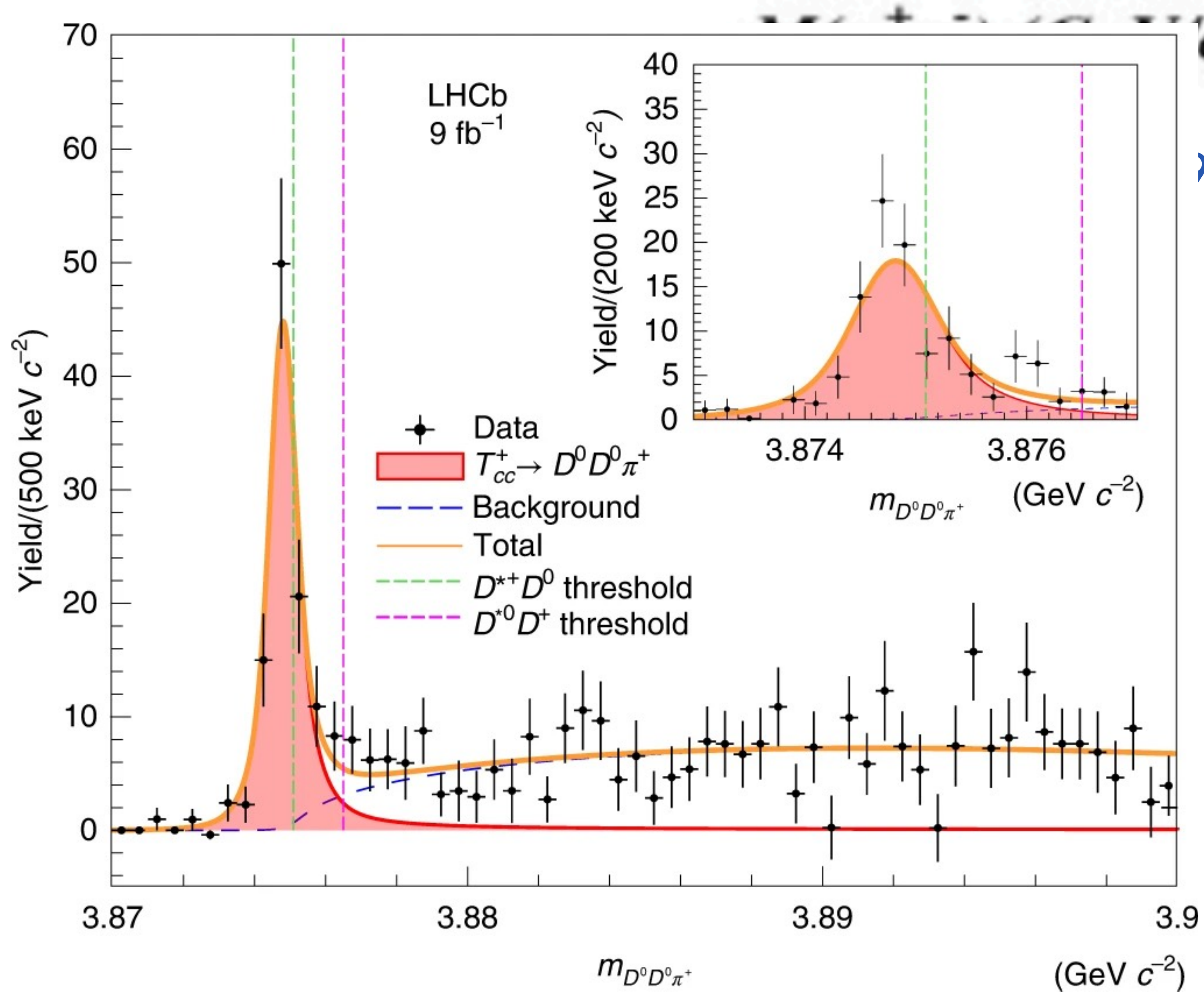

Aaij et al. (LHCb) 2022 [Nature Phys. 18, 751]

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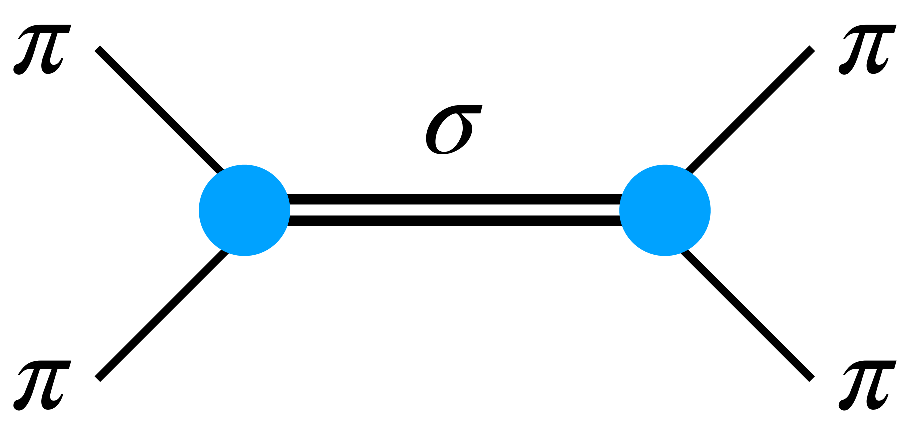
- Goal: obtain masses and decay widths of hadronic resonances from QCD
- Experimentally: resonances as enhancements in scattering cross sections
- Rigorous definition: poles of scattering amplitude $\mathscr{M}$ in complex plane

$$\mathscr{M} \sim -\frac{g^2}{E^2 - E^2_{\text{pole}}}$$



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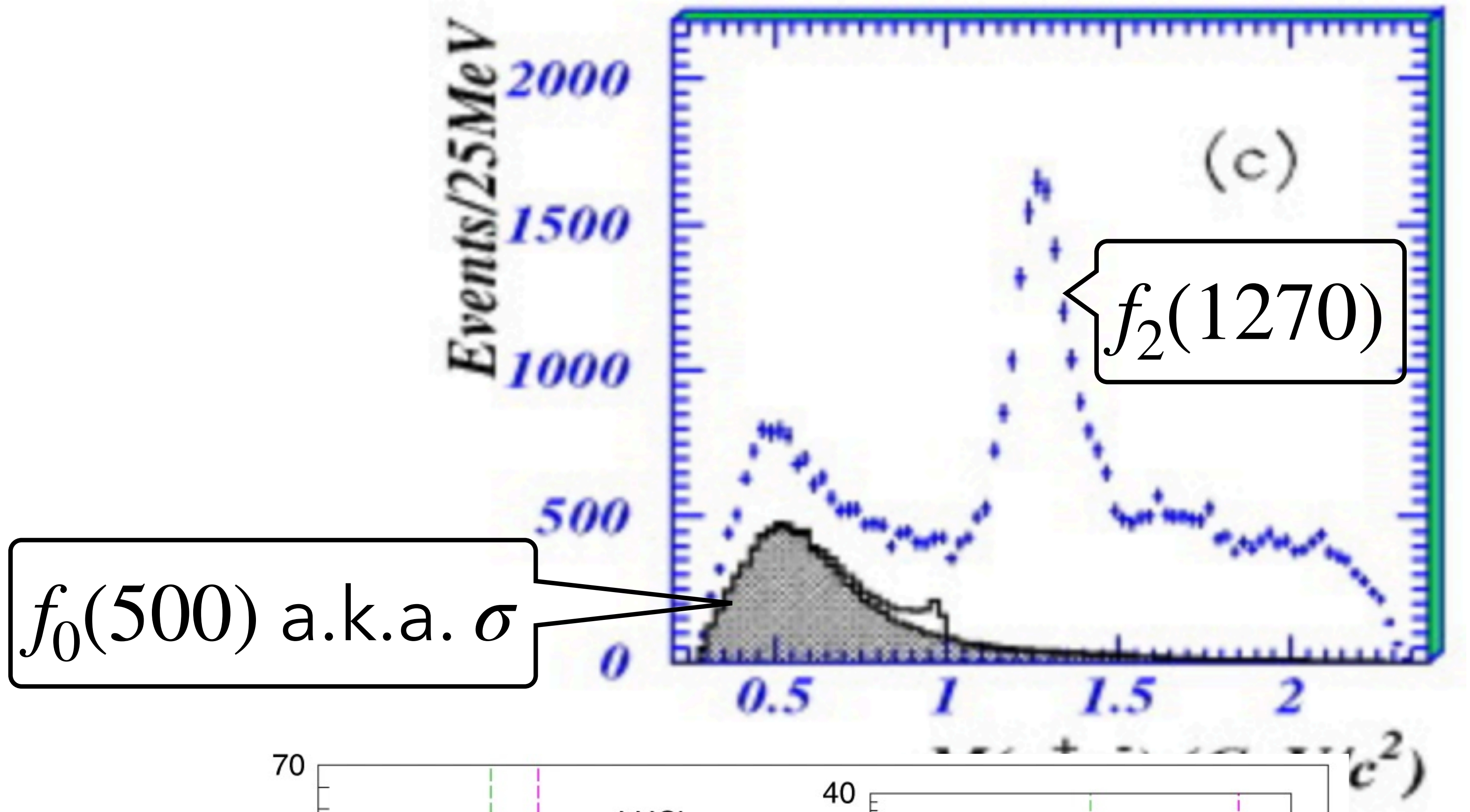

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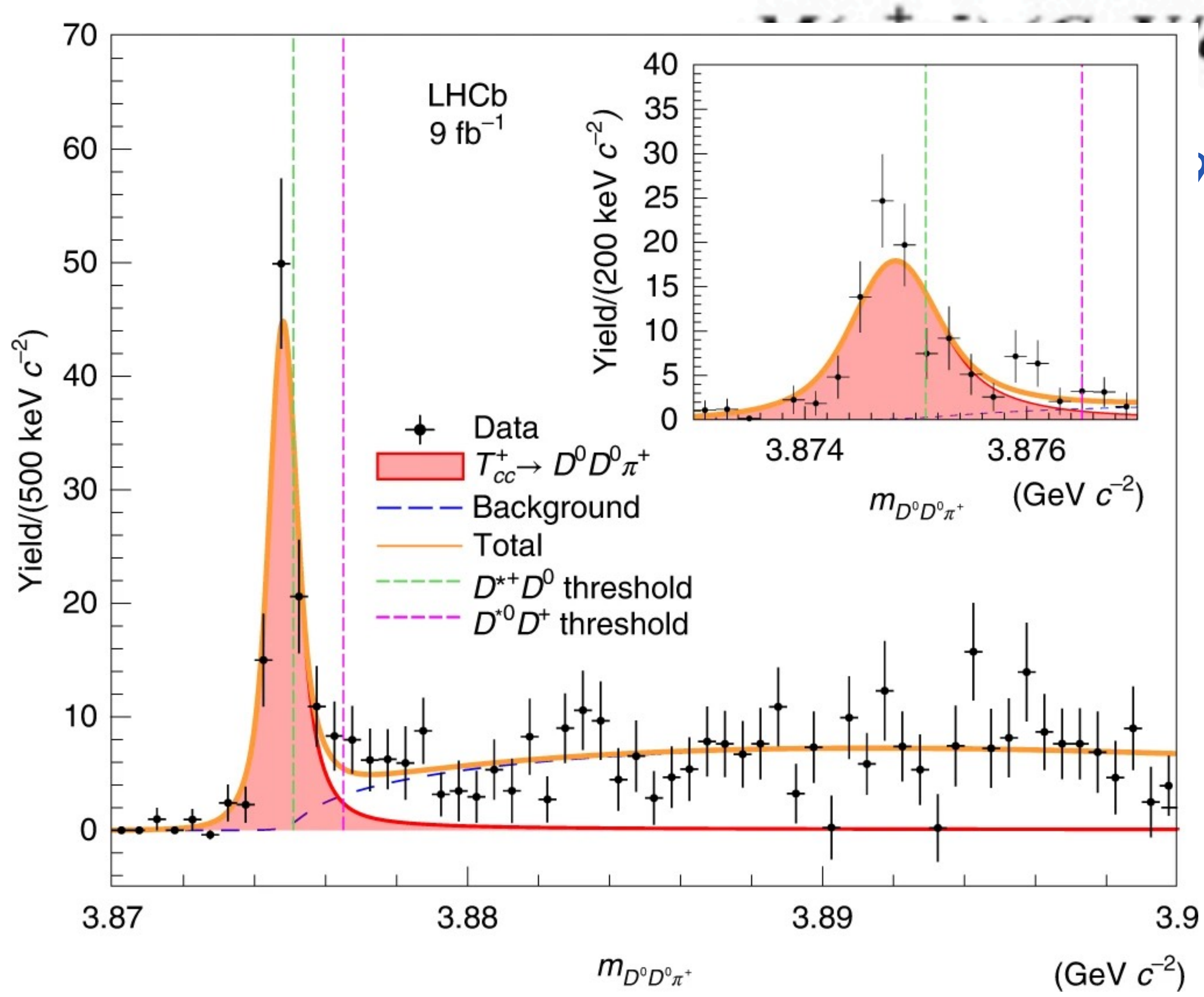

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  - Real energies above threshold (unitarity)
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- No poles allowed:
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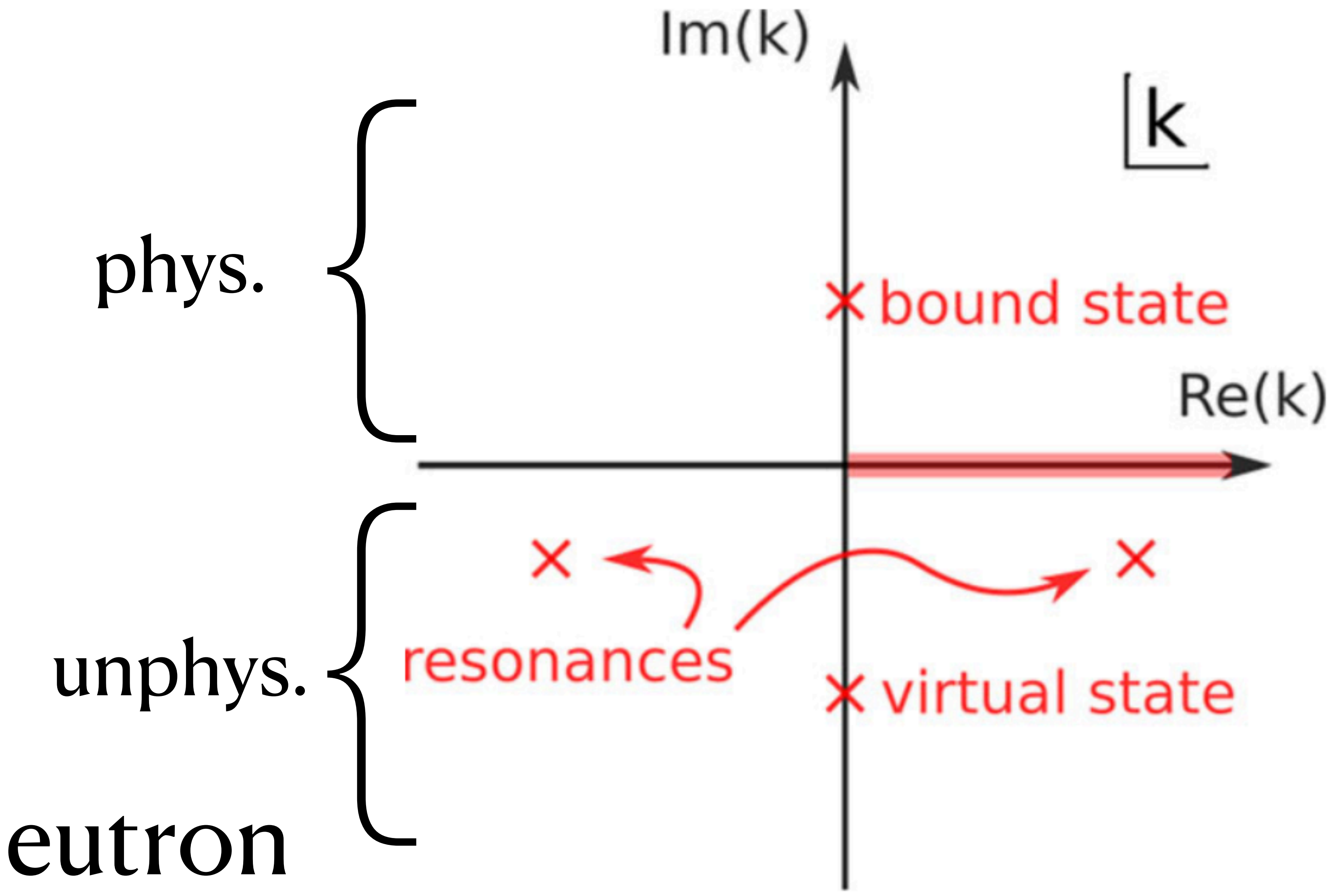
  - Complex energies on the physical sheet (causality)
- Classification of allowed poles
  - Bound states: stable particles, e.g. deuteron
  - Virtual states: „non-normalizable“ QM states, e.g. dineutron
  - Resonances: unstable hadrons, e.g. ρ, σ; $E_{\text{pole}} = M - i\Gamma/2$

Mass

Decay width



Matuschek et al. 2021 [EPJA 57, 101]

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Finite-volume formalism for hadron spectroscopy

$$\langle \mathcal{O}_1(t)\mathcal{O}_2^\dagger(0)\rangle$$

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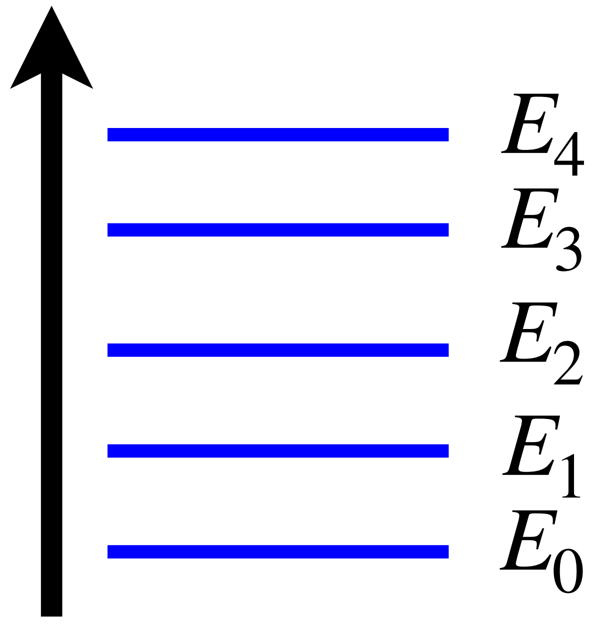
$$\langle \mathcal{O}_1(t)\mathcal{O}_2^\dagger(0)\rangle \longrightarrow$$

Spectrum



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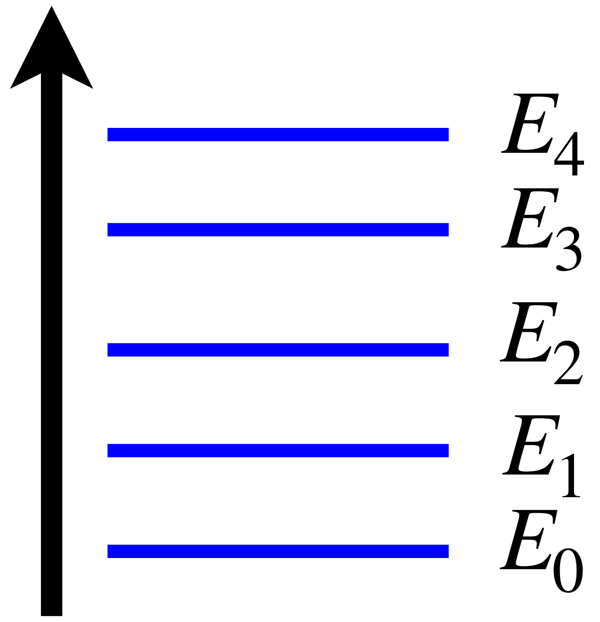

→

Quantisation condition

Lüscher 1986
[Commun. Math. Phys. 105, 153]

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

IV observable, sought

FV function, known

Infinite-volume scattering observables

K-matrix

—> scatt. amplitude, $\mathrm{Re}\,\mathcal{M}^{-1} = K^{-1}$

$E \in \mathbb{R}$

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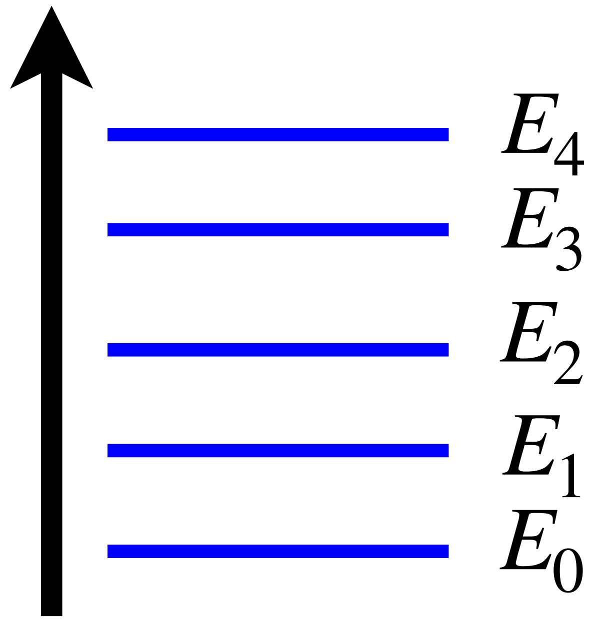

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$E \in \mathbb{R}$

← analytic continuation

Pole positions:

bound states, virtual states, resonances

$\mathcal{M}^{-1}(E_{\mathrm{pole}}) = 0, \quad E_{\mathrm{pole}} \in \mathbb{C}$

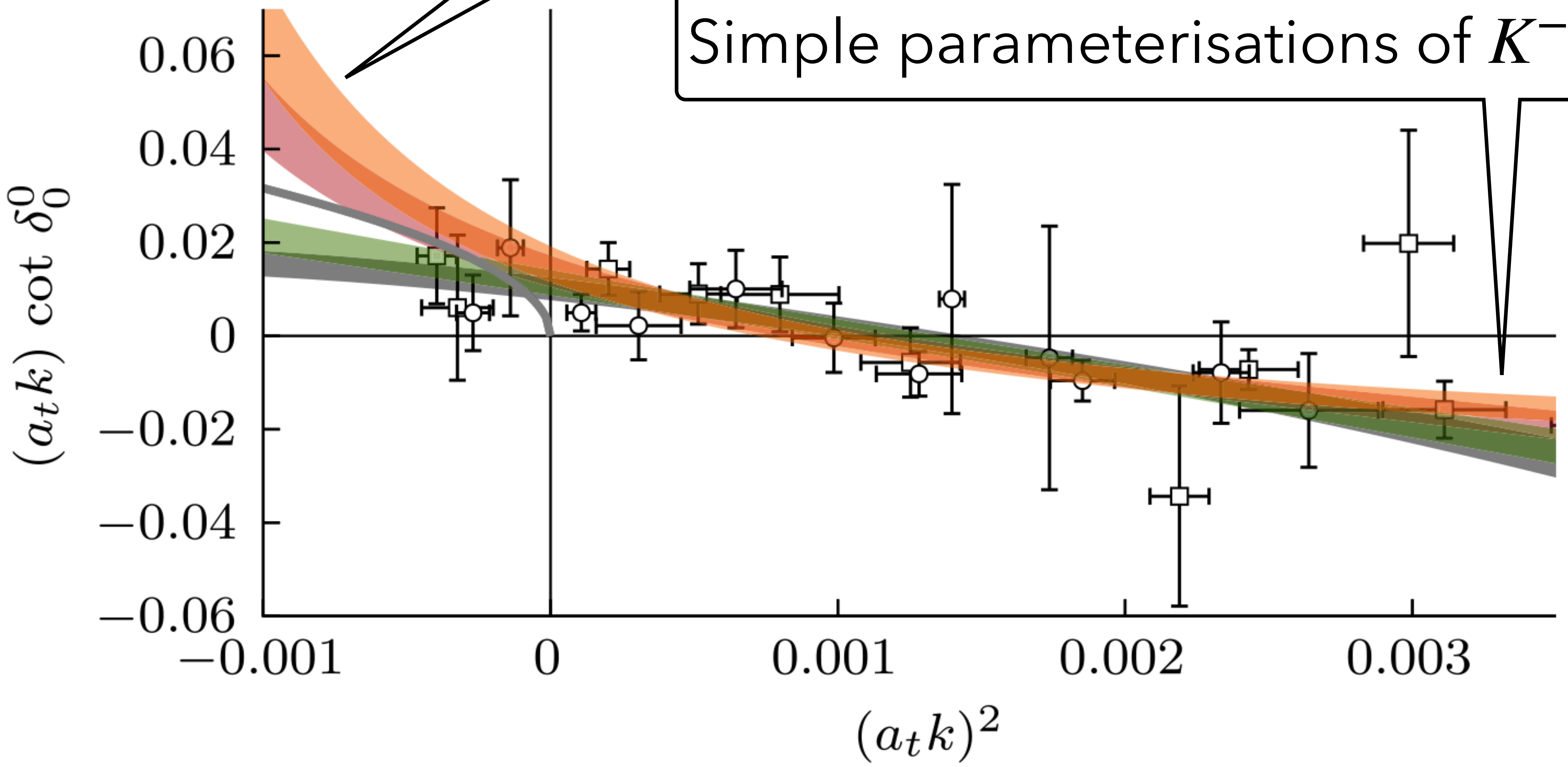
Motivation

- Conventional approach: spectrum fits

Phase shift, $K^{-1} \propto k \cot \delta$ for 1 channel and 1 ℓ

Model dependence

Simple parameterisations of $K^{-1}(E)$



Rodas, Dudek, and Edwards (HadSpec) 2023 [PRD 108, 034513]

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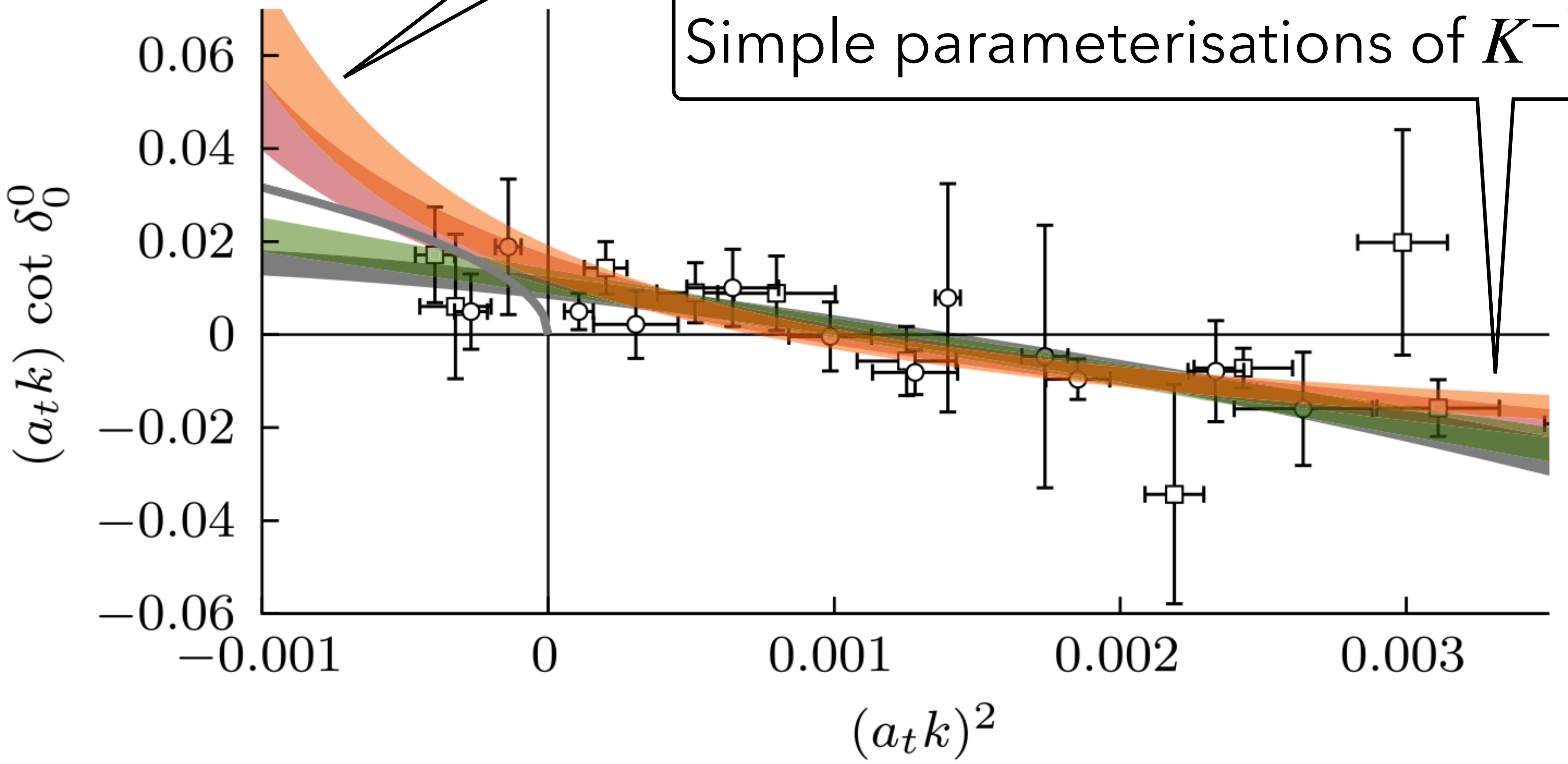

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- Our approach: avoid explicit model dependence
  - Bayesian analysis of FV spectrum to constrain K-matrix for real energies (inspired by Gaussian processes)
  - Nevanlinna-Pick interpolation for analytic continuation to complex energies with strict uncertainty quantification —> Wertevorrat

Outline of our method

Bayesian analysis

General framework

Evaluate K^{-1} at n_p discrete „nodes" $\mathbf{E}$ —> values $\mathbf{u} = K^{-1}(\mathbf{E})$

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Prior central values

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Likelihood

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Covariance of $\mathbf{E}_\mathrm{d}$

Solution of QC (nonlinear!)

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LQCD data

Covariance of $\mathbf{E}_\mathrm{d}$

Solution of QC (nonlinear!)

Posterior (Bayes' theorem)

$$p(\mathbf{u}\,|\,\mathbf{E}_\mathrm{d},\mathbf{u}_0) = p(\mathbf{E}_\mathrm{d}\,|\,\mathbf{u})\,p(\mathbf{u}\,|\,\mathbf{u}_0)$$

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Computing expectation values and errors

- Expectation values given by Bayesian integrals, e.g. $\langle \mathbf{u} \rangle_{\text{post}} = \frac{1}{Z} \int d^{n_p}u\, \mathbf{u}\, p(\mathbf{u} \,|\, \mathbf{E}_{\text{d}}, \mathbf{u}_0)$
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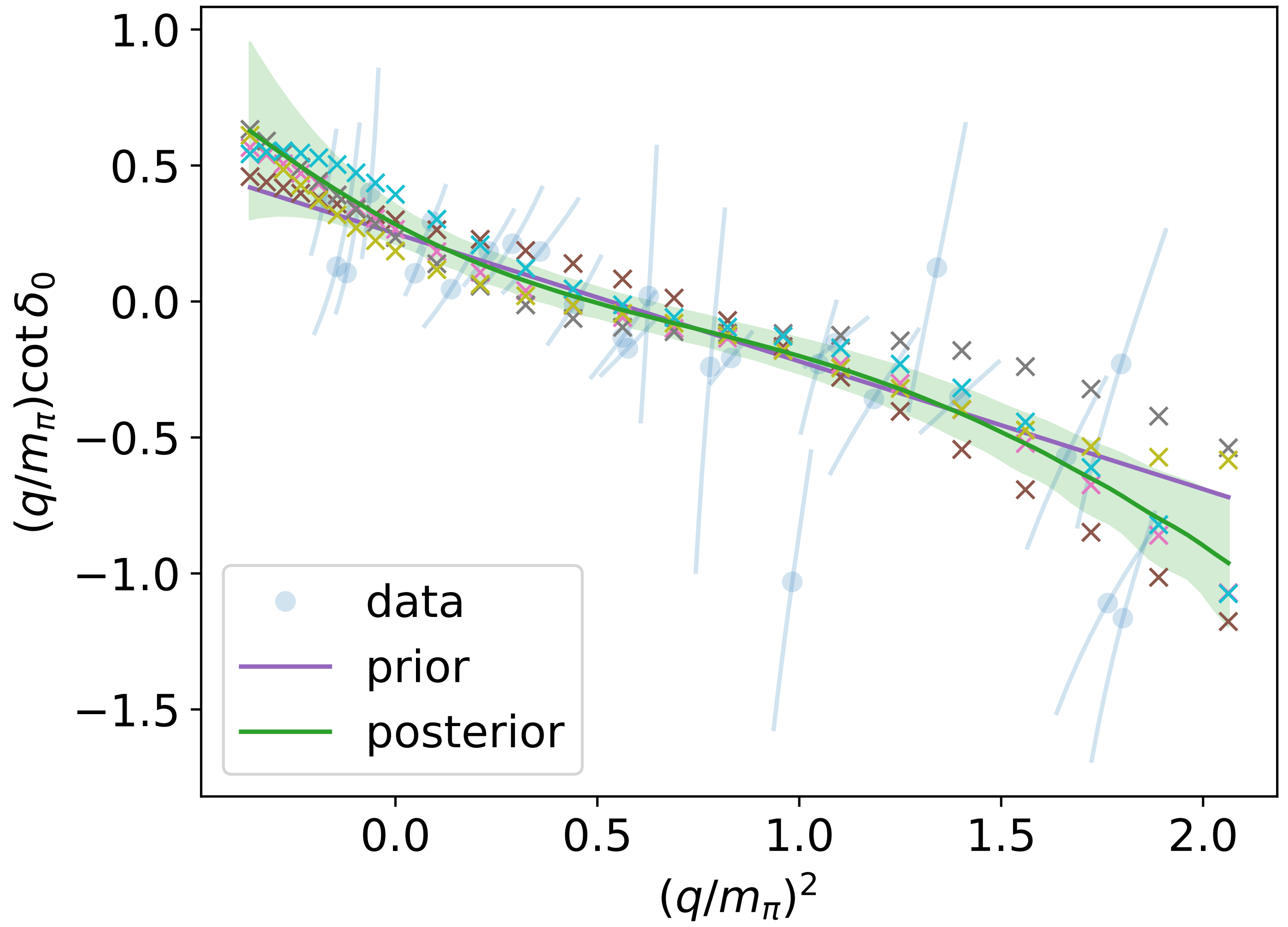

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- Quantify prior dependence by Bayes factor, $B_{12} = \frac{p(\mathbf{E}_{\text{d}} \,|\, M^{(1)})}{p(\mathbf{E}_{\text{d}} \,|\, M^{(2)})} = \frac{Z_{\text{post}}^{(1)}}{Z_{\text{post}}^{(2)}}$

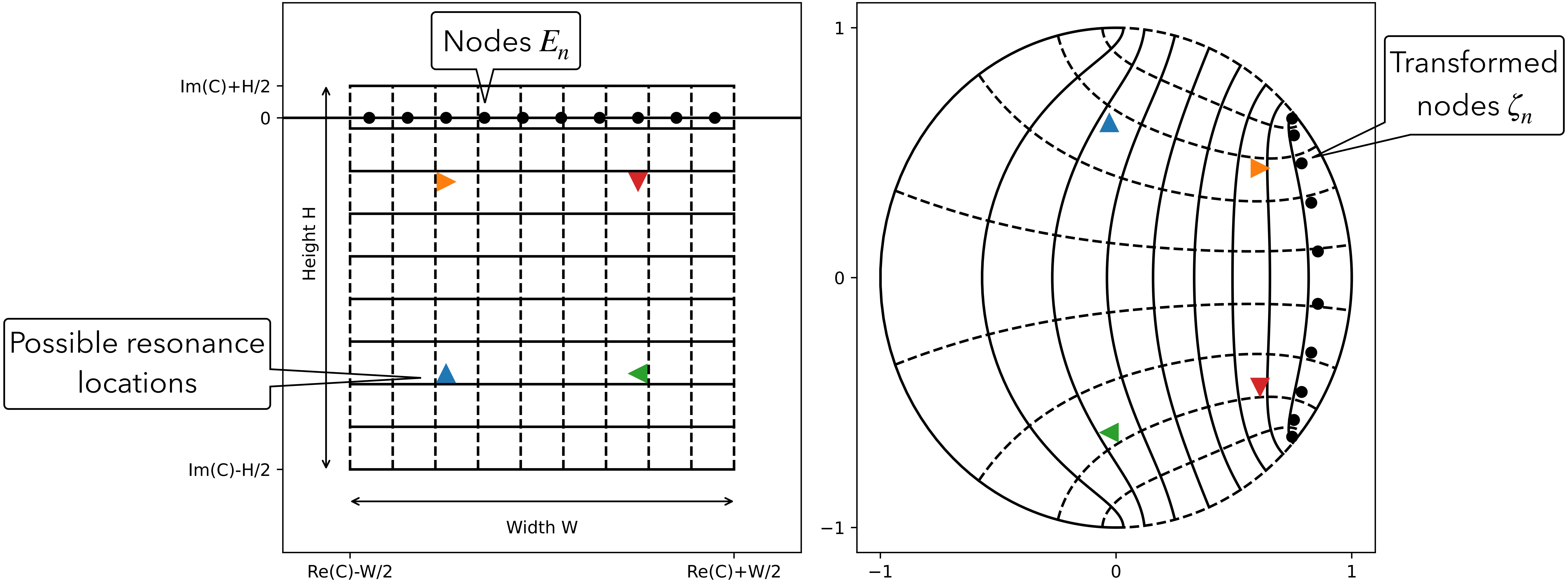
  —> ratio of average reweighting factors

Model $M^{(2)}$ with prior $\mathbf{u}_0^{(2)}$

Jeffreys 1935 [Math. Proc. Cambridge Philos. Soc. 31, 203]
Kass and Raftery 1995 [J. Am. Stat. Assoc. 90, 773]

Nevanlinna-Pick interpolation

Mapping to the unit disk



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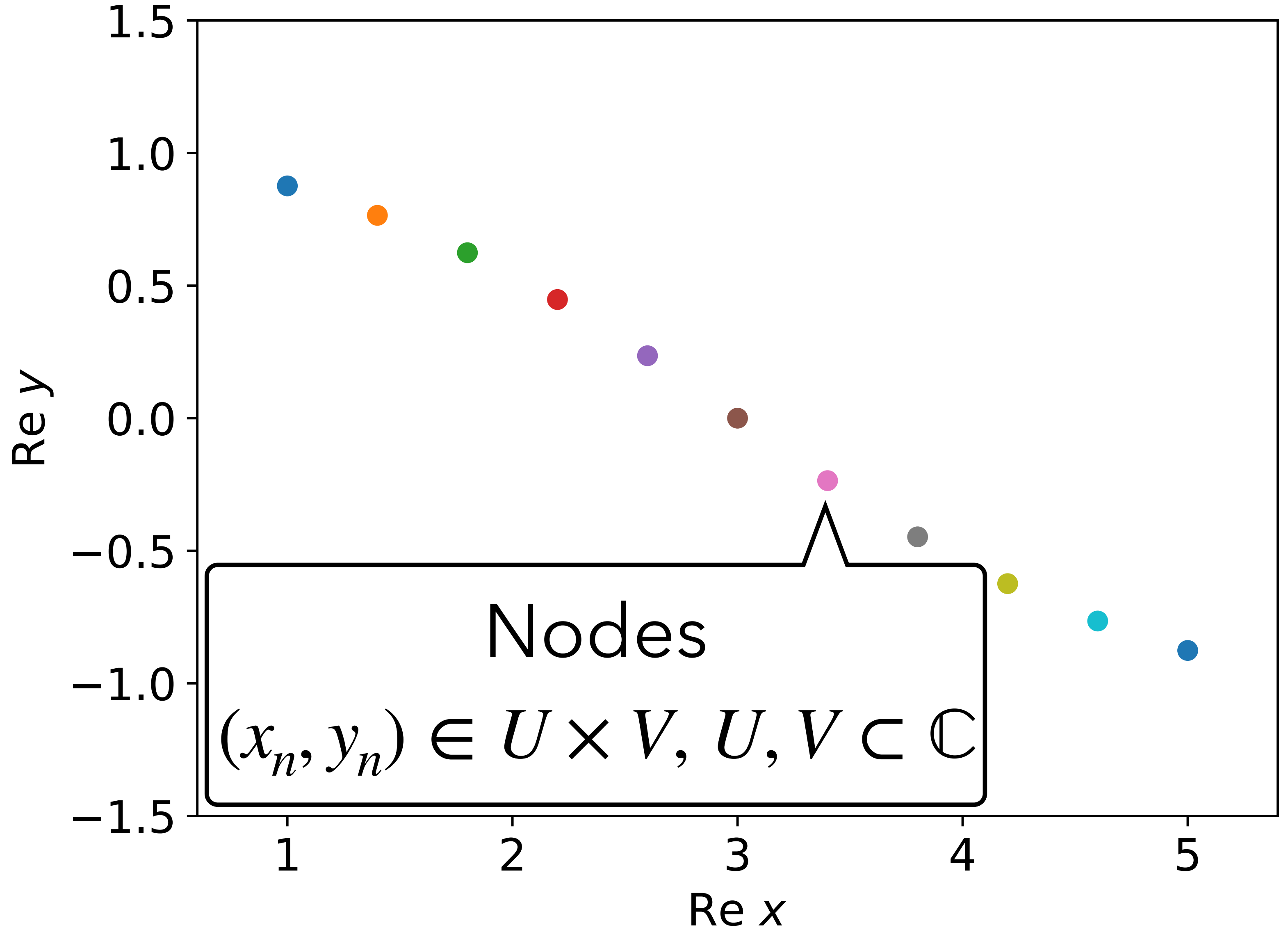

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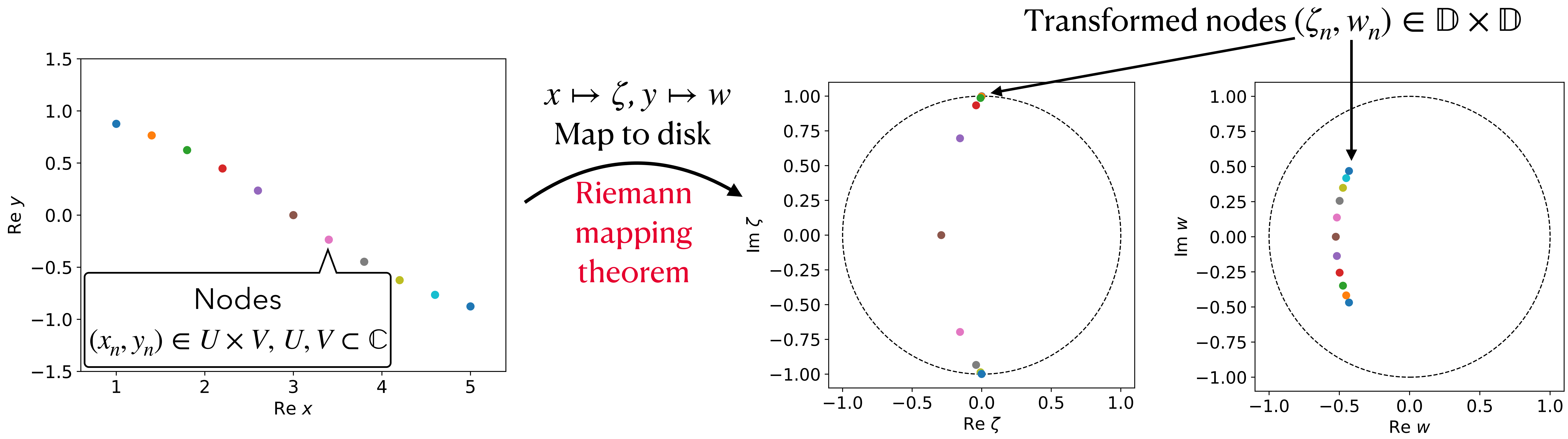

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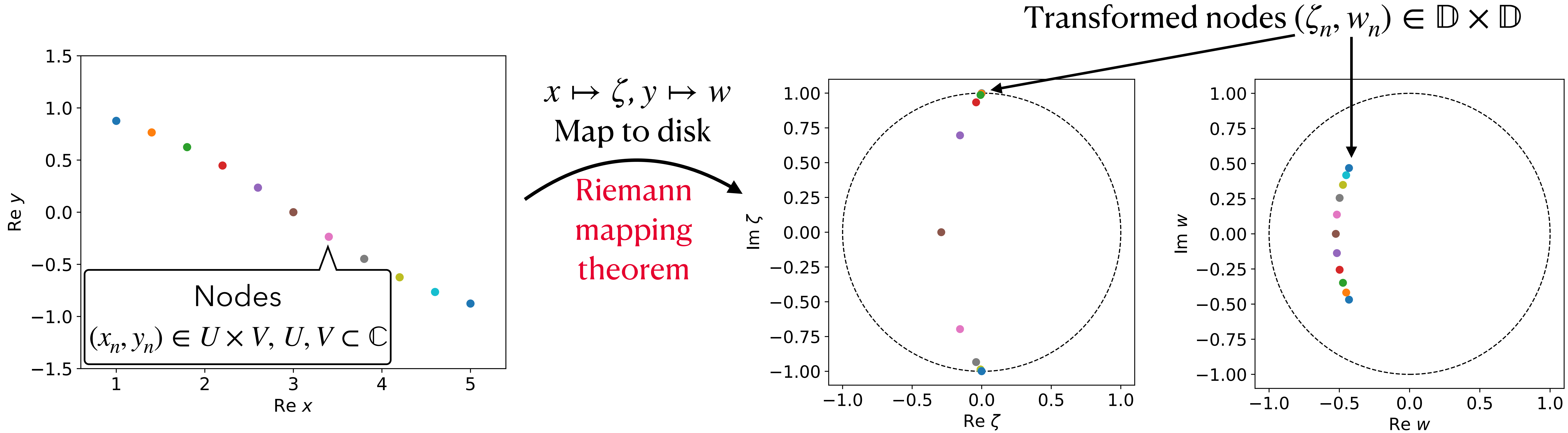

- Any solution can be written as $f(\zeta) = \dfrac{P(\zeta)g(\zeta) + Q(\zeta)}{R(\zeta)g(\zeta) + S(\zeta)}$ with $g : \mathbb{D} \to \mathbb{D}$ analytic, but arb.

  Recursively calculable coefficients

- For fixed ζ, all possible solutions fall within a disk $\Delta(\zeta) \subset \mathbb{D}$ —> Wertevorrat (WV)

Pick 1915 [Math. Ann. 77, 7]; Nevanlinna 1919 [Ann. Acad. Sci. Fenn. Ser. A 13]; Nevanlinna 1929 [Ann. Acad. Sci. Fenn. Ser. A 32]
Bergamaschi, Jay, and Oare 2023 [PRD 108, 074516]

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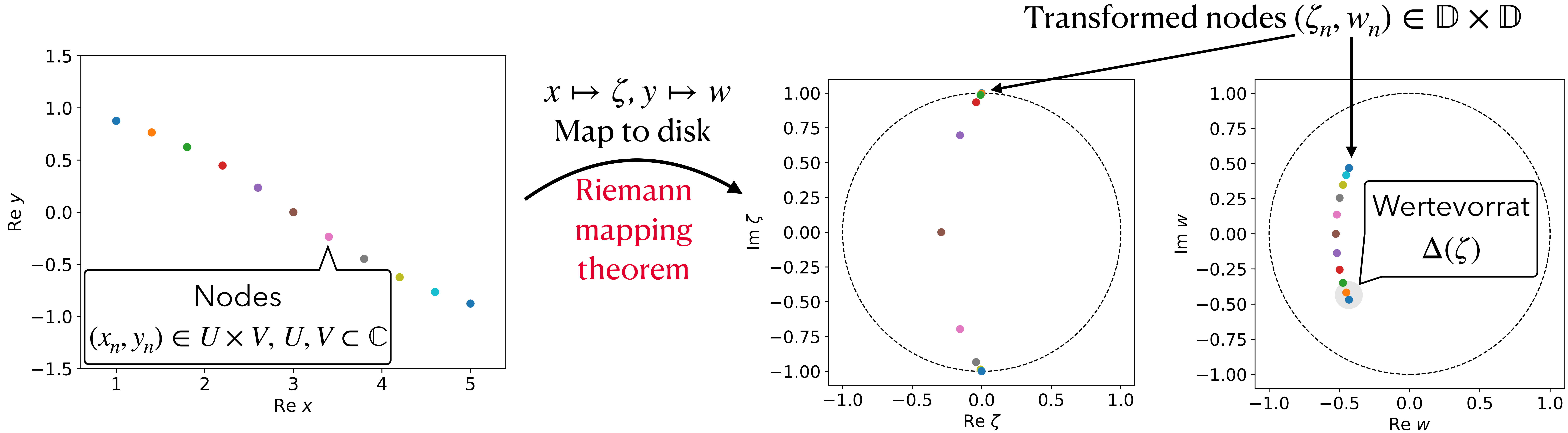

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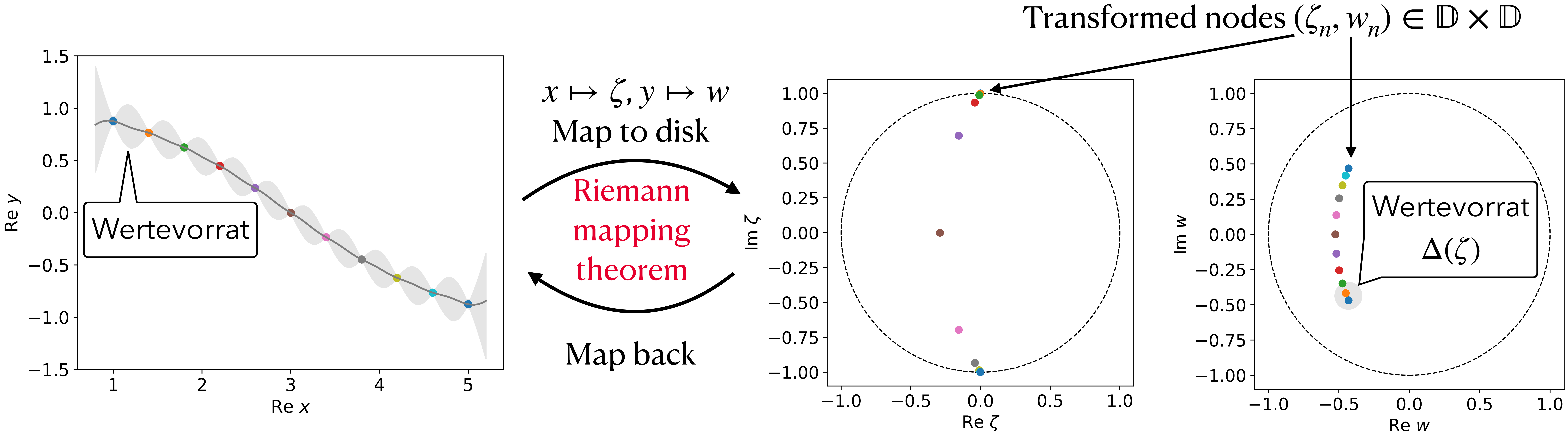

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Application to analytic continuation of scattering amplitudes

1. Transform domain (energies $\mathbf{E}$) and codomain (values $\mathbf{u}$) of K^{-1} to unit disk using Schwarz-Christoffel mapping of a rectangle to the disk Liu, Chen, and Karageorghis 2017 [J. Sci. Comput. 71, 1035]

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2. For each sample from posterior:

   2.1. Compute Nevanlinna coefficients P, Q, R, S

   2.2. Evaluation of interpolating function + uncertainty (Wertevorrat) for complex energies furnishes desired analytic continuation (after mapping back)

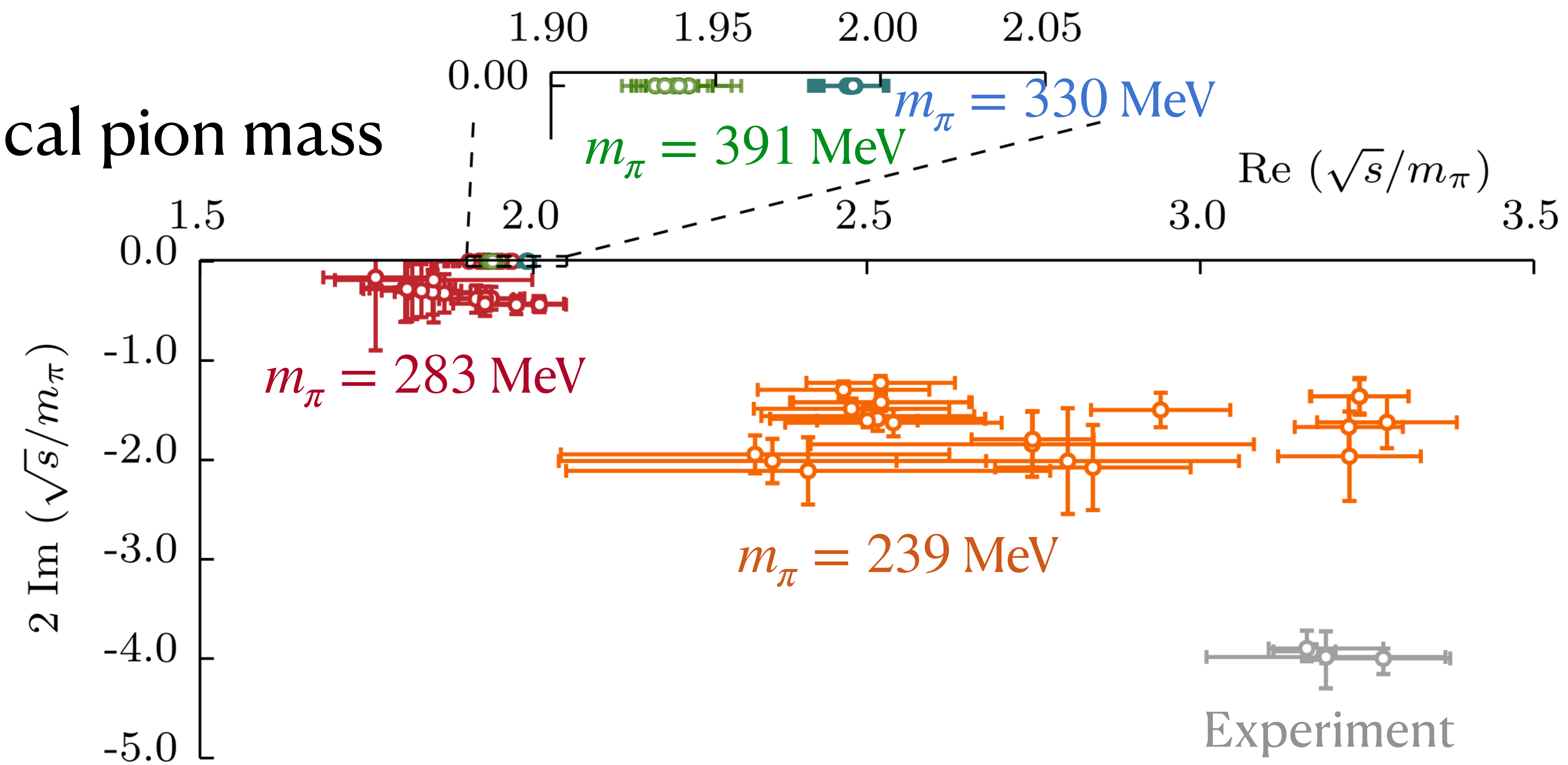
   2.3. Solve for zeros of $\mathcal{M}^{-1}(E)$ in the complex energy plane, incorporating WV uncertainty („sampling from WV“) —> resonances

Applications to lattice QCD analyses

Isospin-0 $\pi\pi$ system on HadSpec ensembles

Pion-mass dependence of the σ pole position

Broad σ meson resonance at physical pion mass



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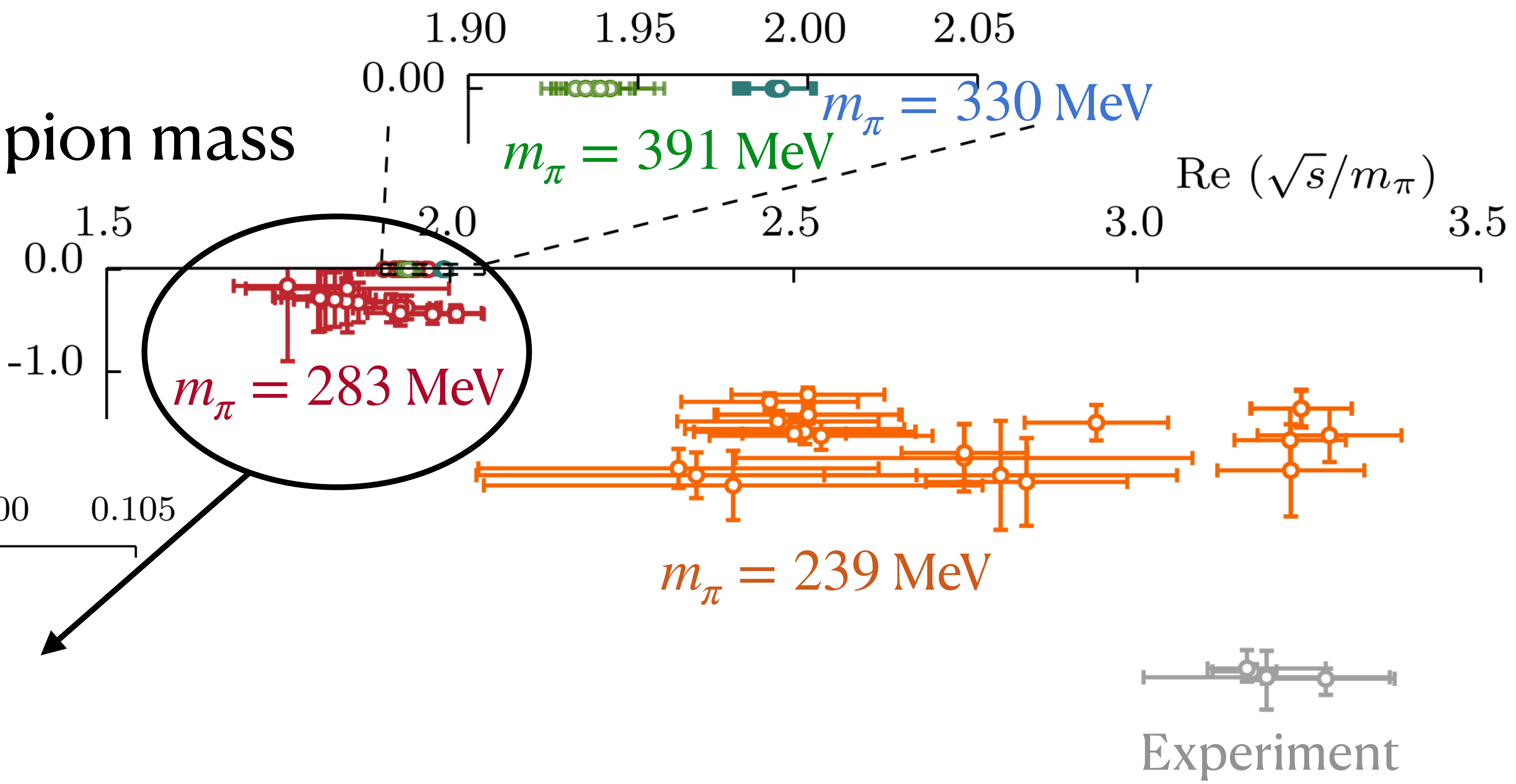
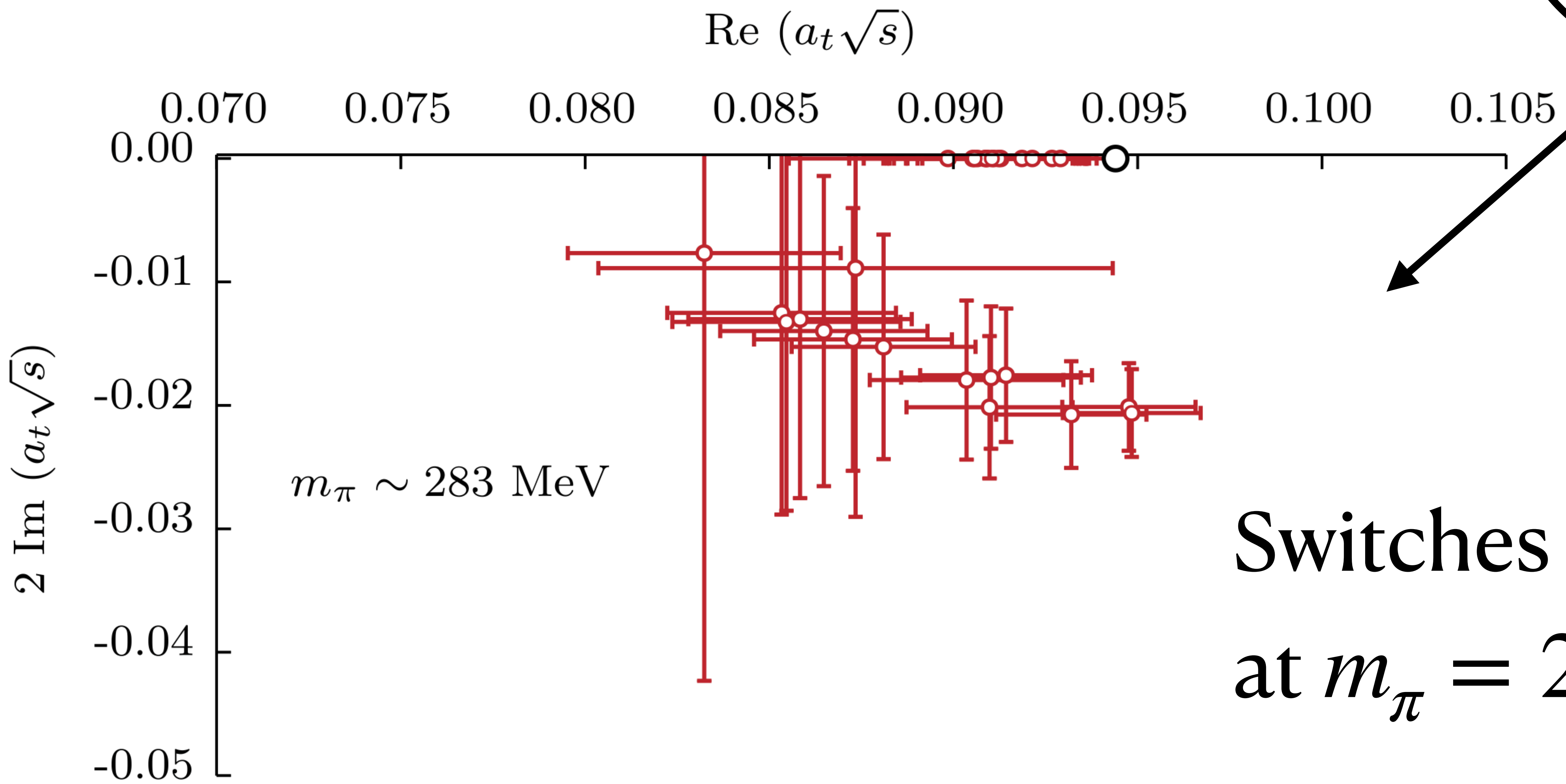
Pole position hard to pin down





Switches from being a resonance to a virtual bound state at $m_\pi = 283$ MeV

Rodas, Dudek, and Edwards (HadSpec) 2023 [PRD 108, 034513]

Big thanks for sharing data!

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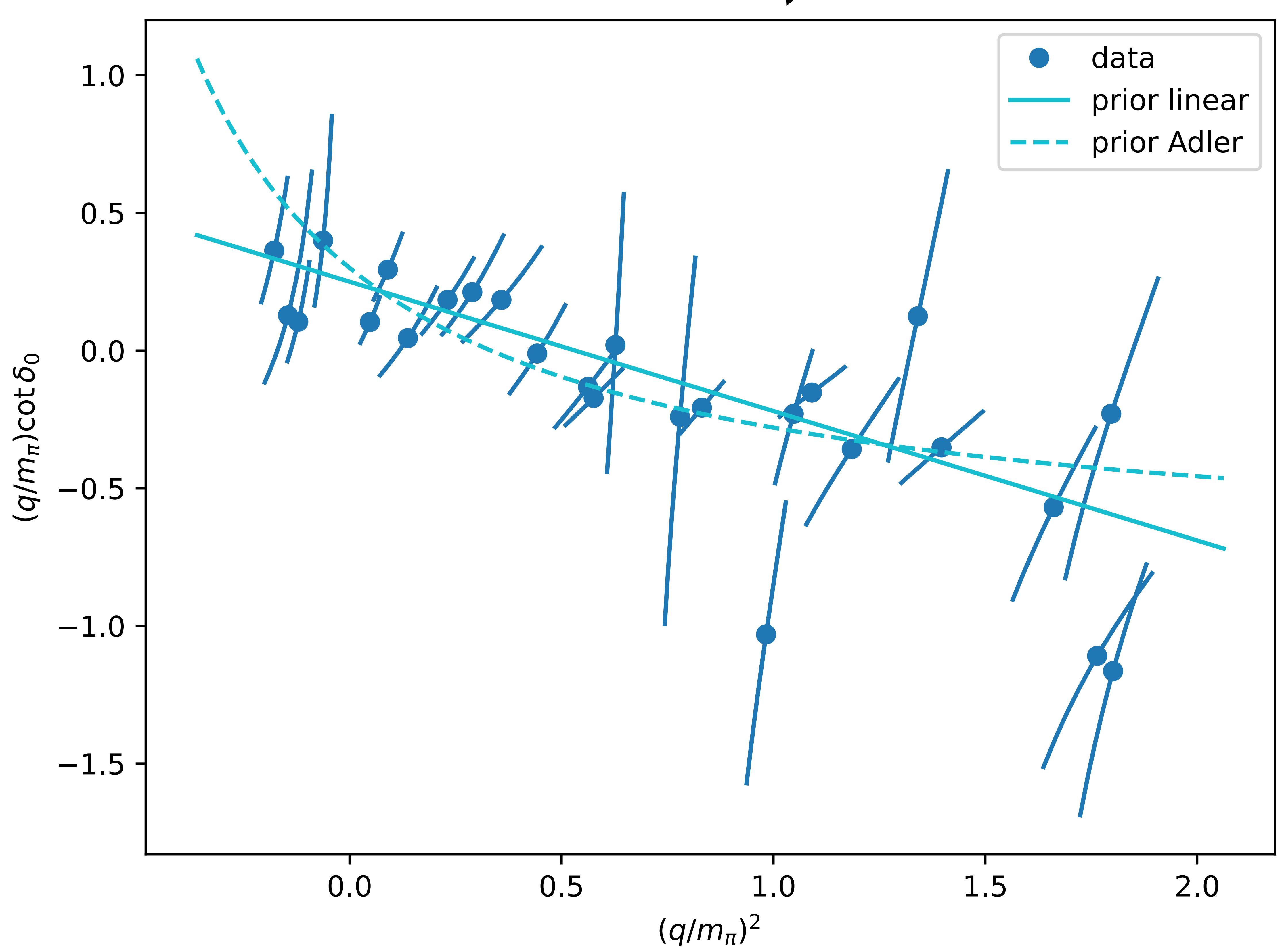
Priors and posteriors on the real energy line



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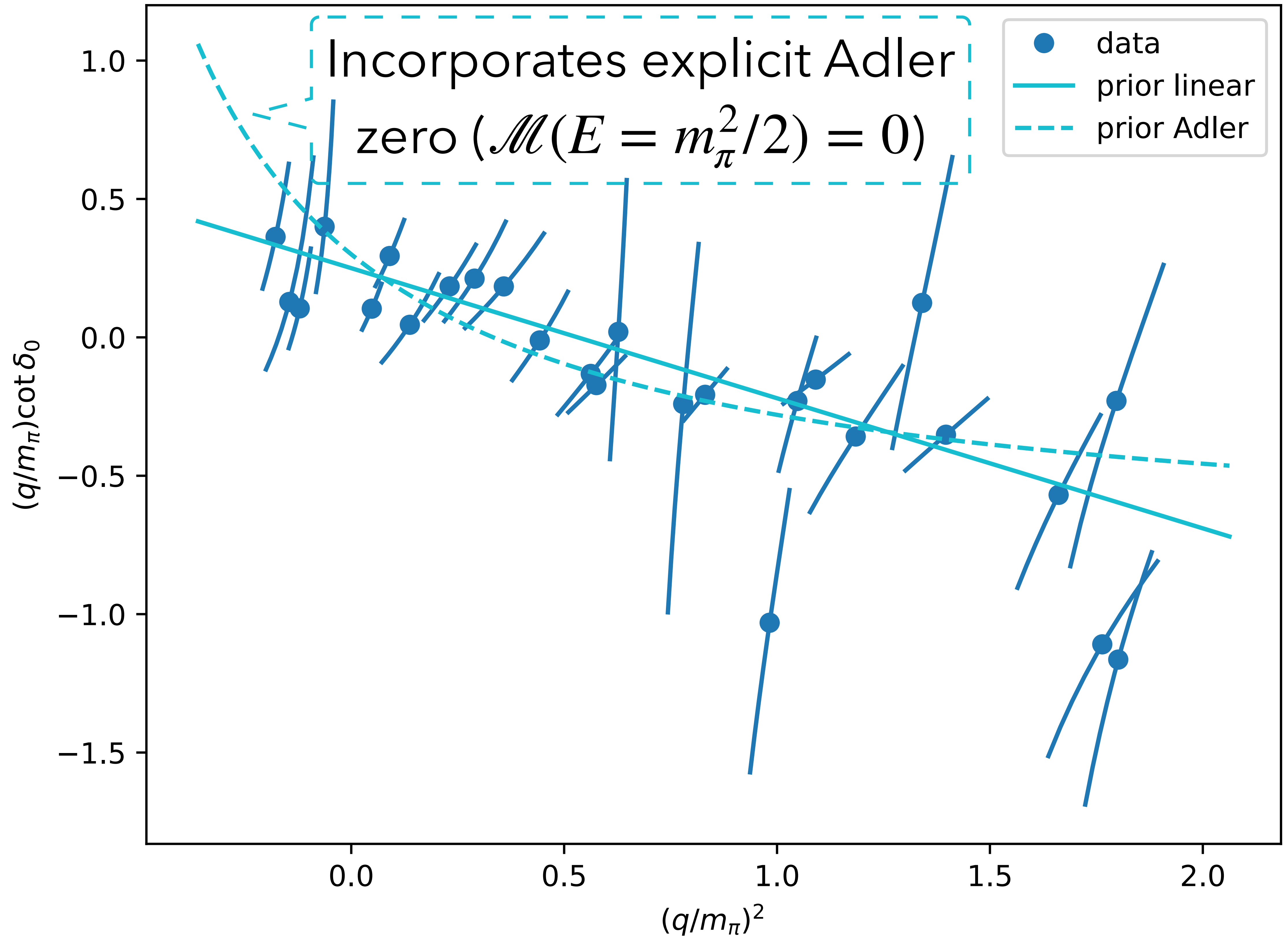

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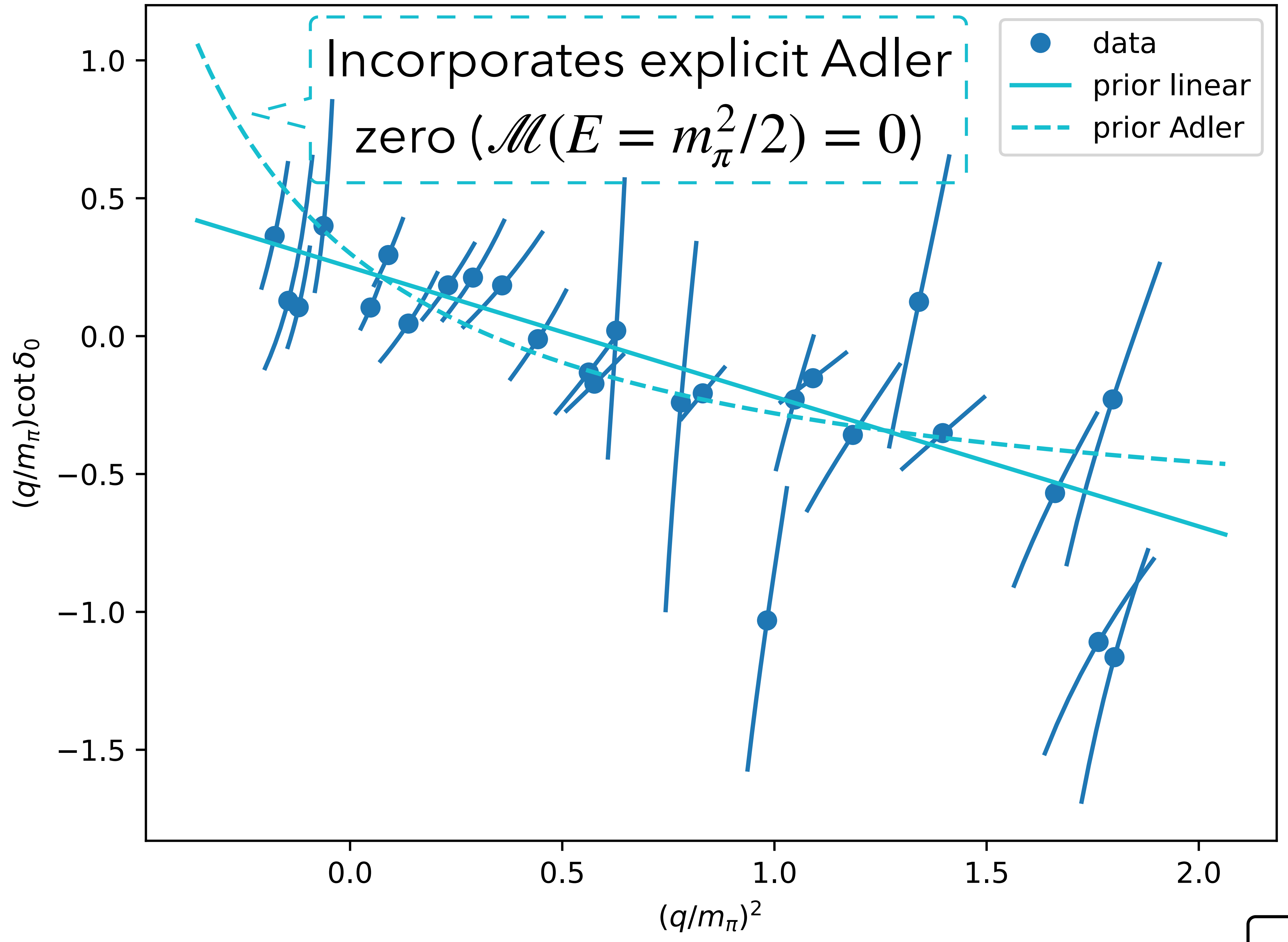
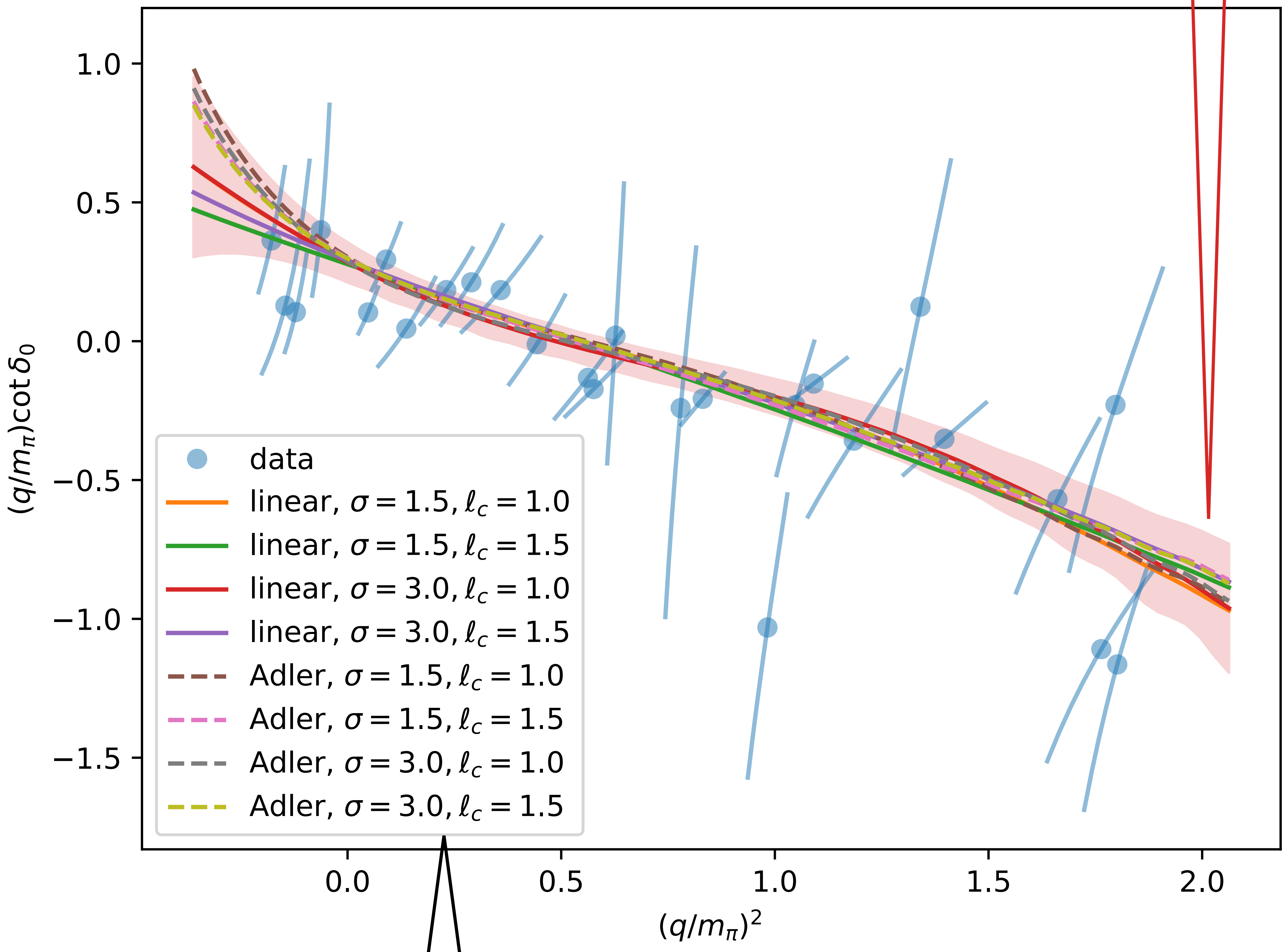


Width of posterior



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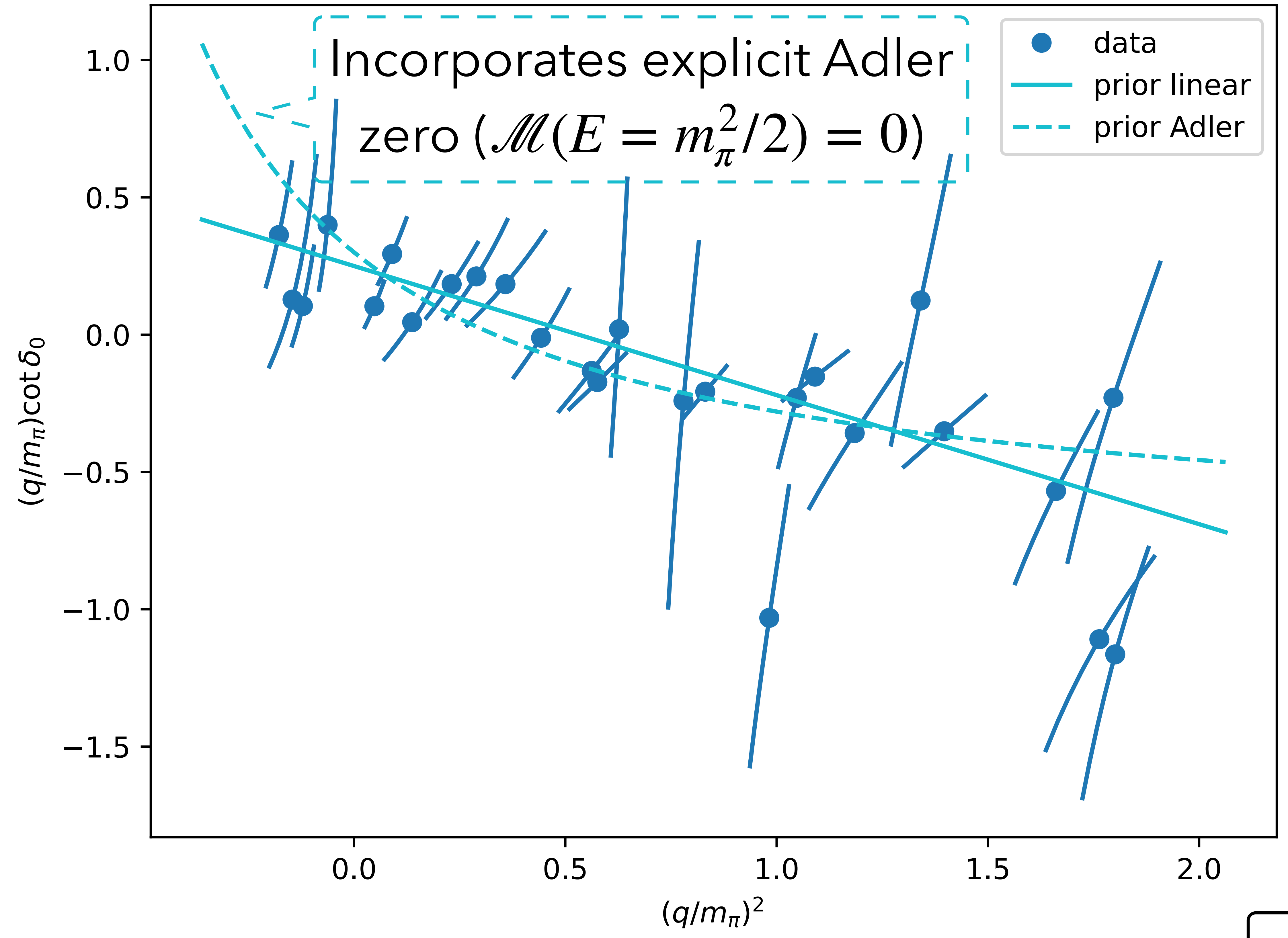

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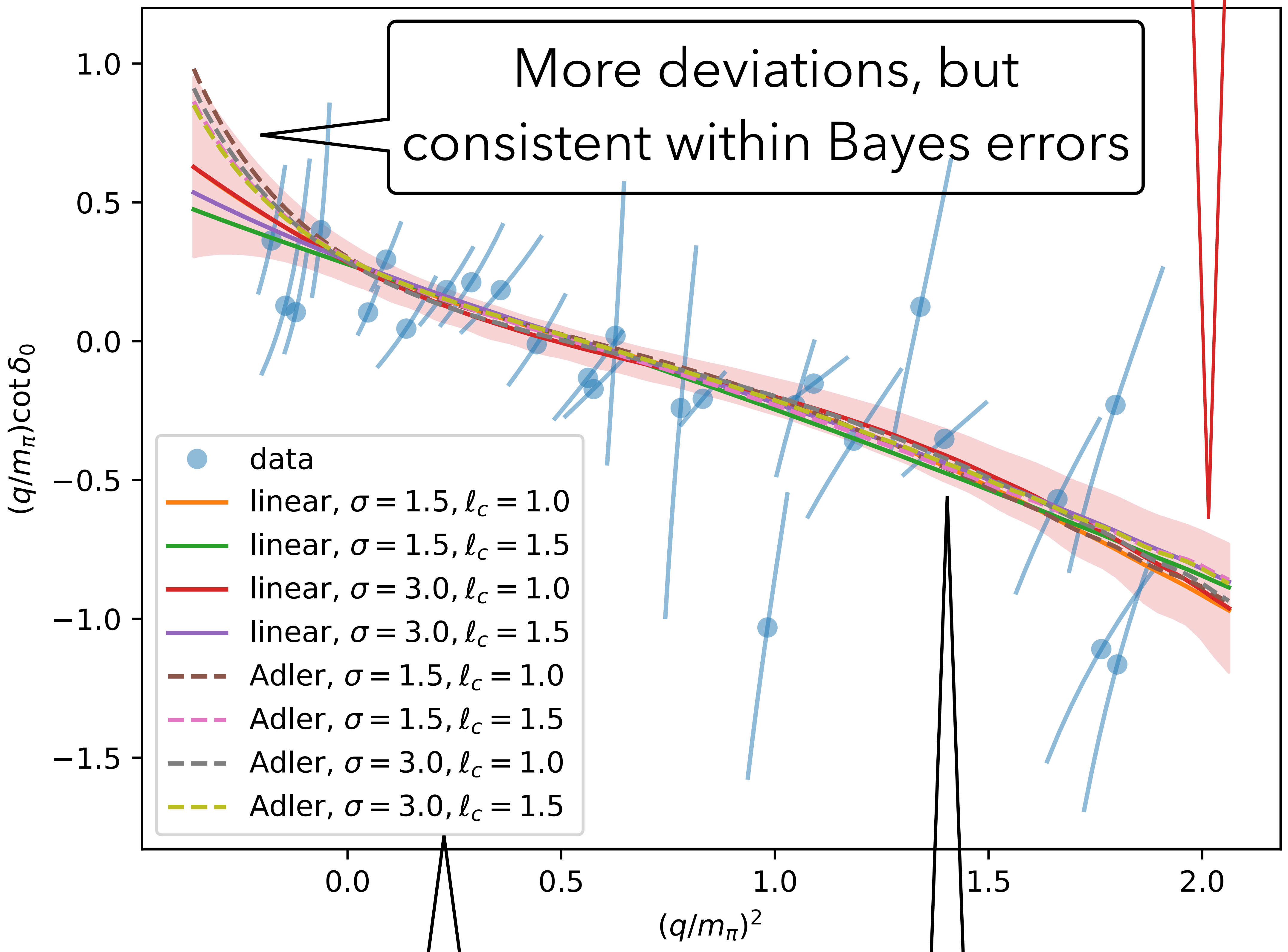

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Little variation above threshold

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σ pole location

Pole position under assumption of...

Prior	Probability of v.b.s.	E_0/m_π	E_0/m_π (v.b.s.)	E_0/m_π (res.)
Linear	$0.502(57)$	$1.890(90) - 0.08(10)i$	$1.88(10)$	$1.904(77) - 0.164(86)i$
Adler-zero	$0.328(52)$	$1.901(97) - 0.099(91)i$	$1.86(11)$	$1.921(82) - 0.147(73)i$

$(\sigma = 3, \ell_c = 1)$

Full error: integration + Bayes + Wertevorrat

- Pole locations consistent within errors between different priors
- Adler-zero prior prefers resonance

Isospin-0 $\pi\pi$ system on HadSpec ensembles

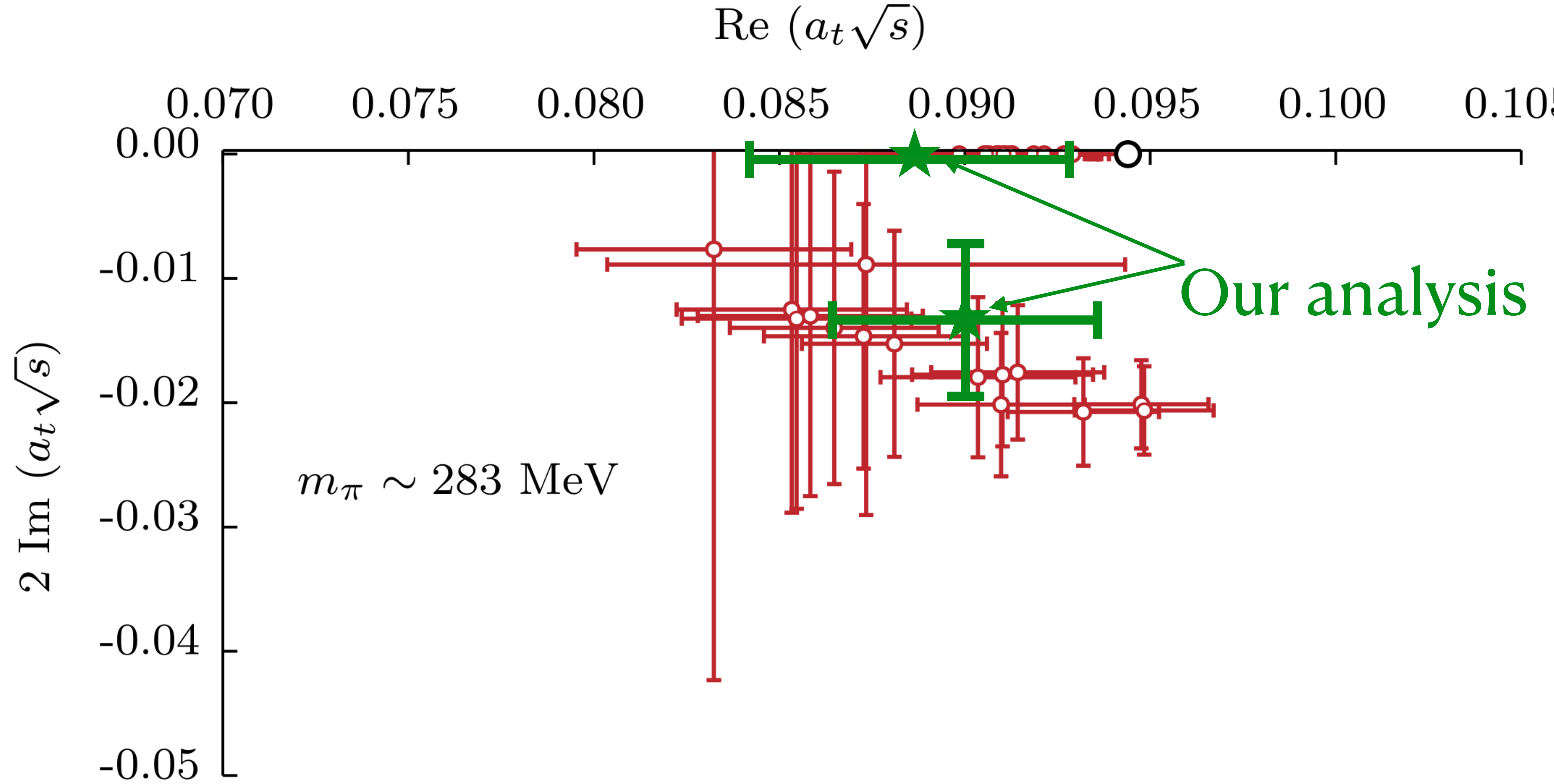
σ pole location

Pole position under assumption of…

Prior	Probability of v.b.s.	E_0/m_π	E_0/m_π (v.b.s.)	E_0/m_π (res.)
Linear	0.502(57)	$1.890(90) - 0.08(10)i$	1.88(10)	$1.904(77) - 0.164(86)i$
Adler-zero	0.328(52)	$1.901(97) - 0.099(91)i$	1.86(11)	$1.921(82) - 0.147(73)i$

$(\sigma = 3, \ell_c = 1)$

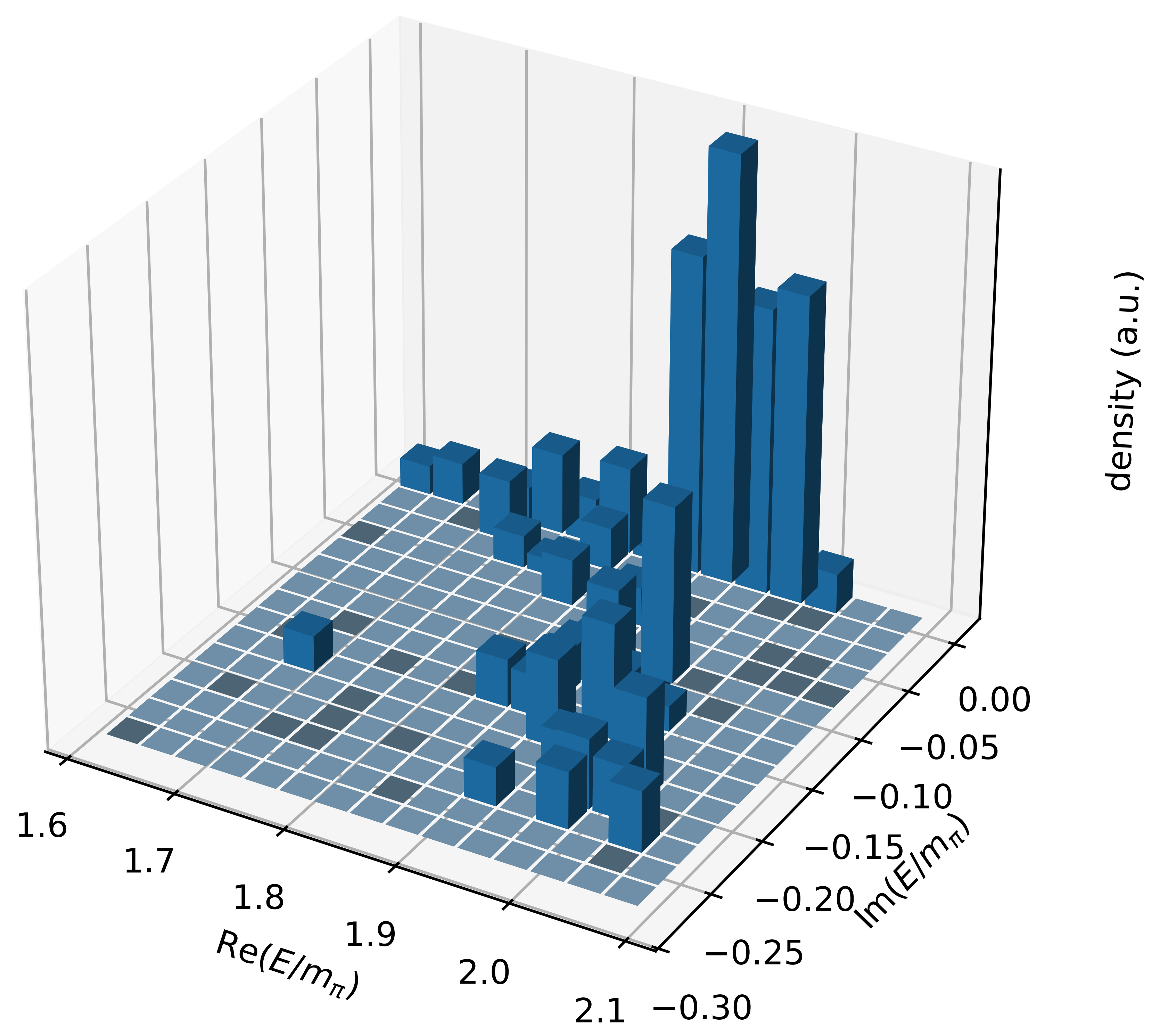
- Pole locations consistent within errors between different priors
- Adler-zero prior prefers resonance
- Compares well with original analysis, but quantifies model dependence



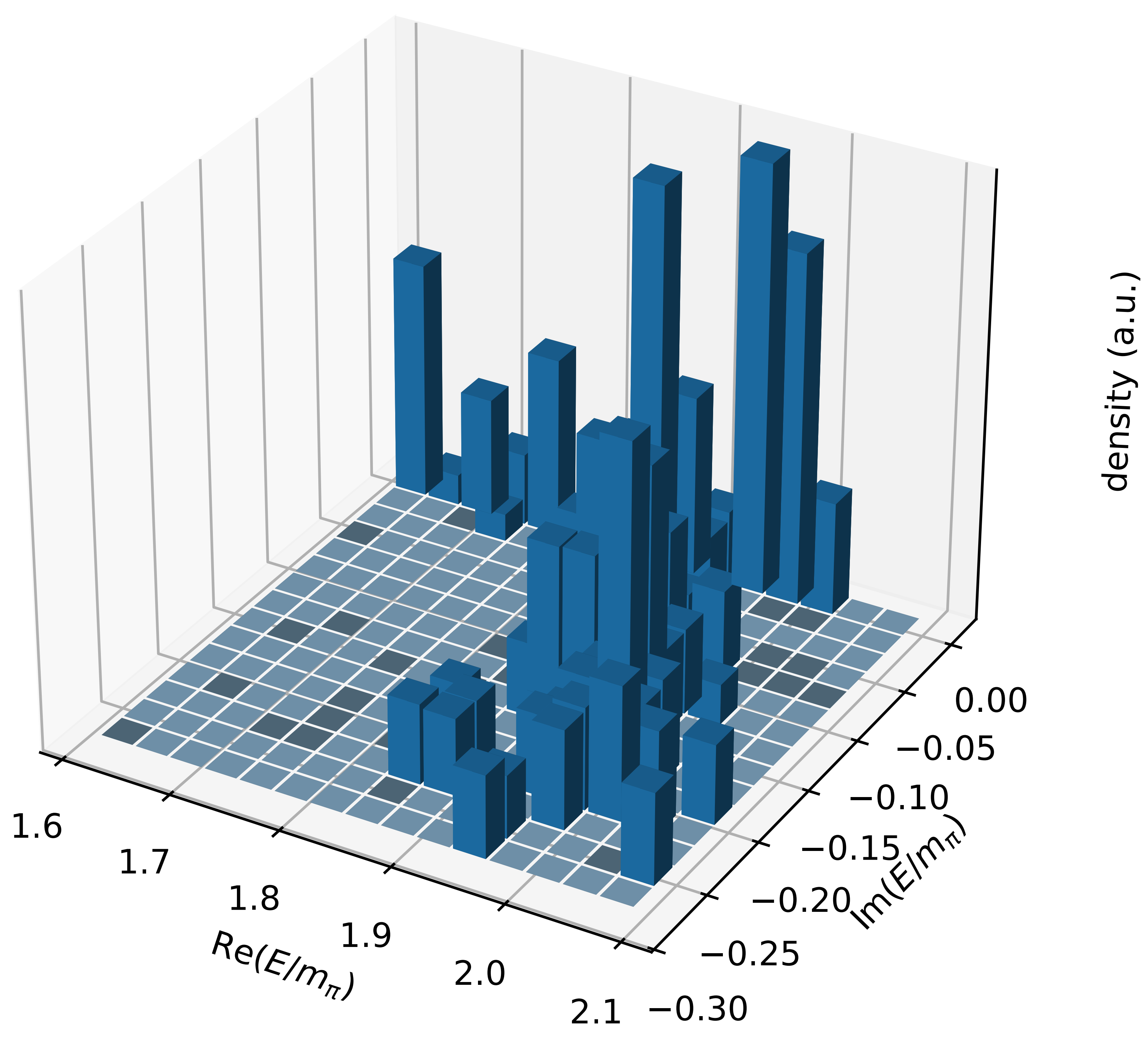
Rodas, Dudek, and Edwards (HadSpec) 2023 [PRD 108, 034513]

Isospin-0 $\pi\pi$ system on HadSpec ensembles

σ pole location



Linear prior



Adler-zero prior

Coupled-channel $\pi\Sigma - \bar{K}N$ scattering on D200

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

$M_\pi = 200$ MeV

- One or two poles?

Dalitz and Tuan 1959 [Annals Phys. 8, 100]
Oller and Meißner 2001 [Phys. Lett. B 500, 263]
Anisovich et al. 2020 [EPJA 56, 139]
Mai 2021 [EPJ Spec. Top. 230, 1593]

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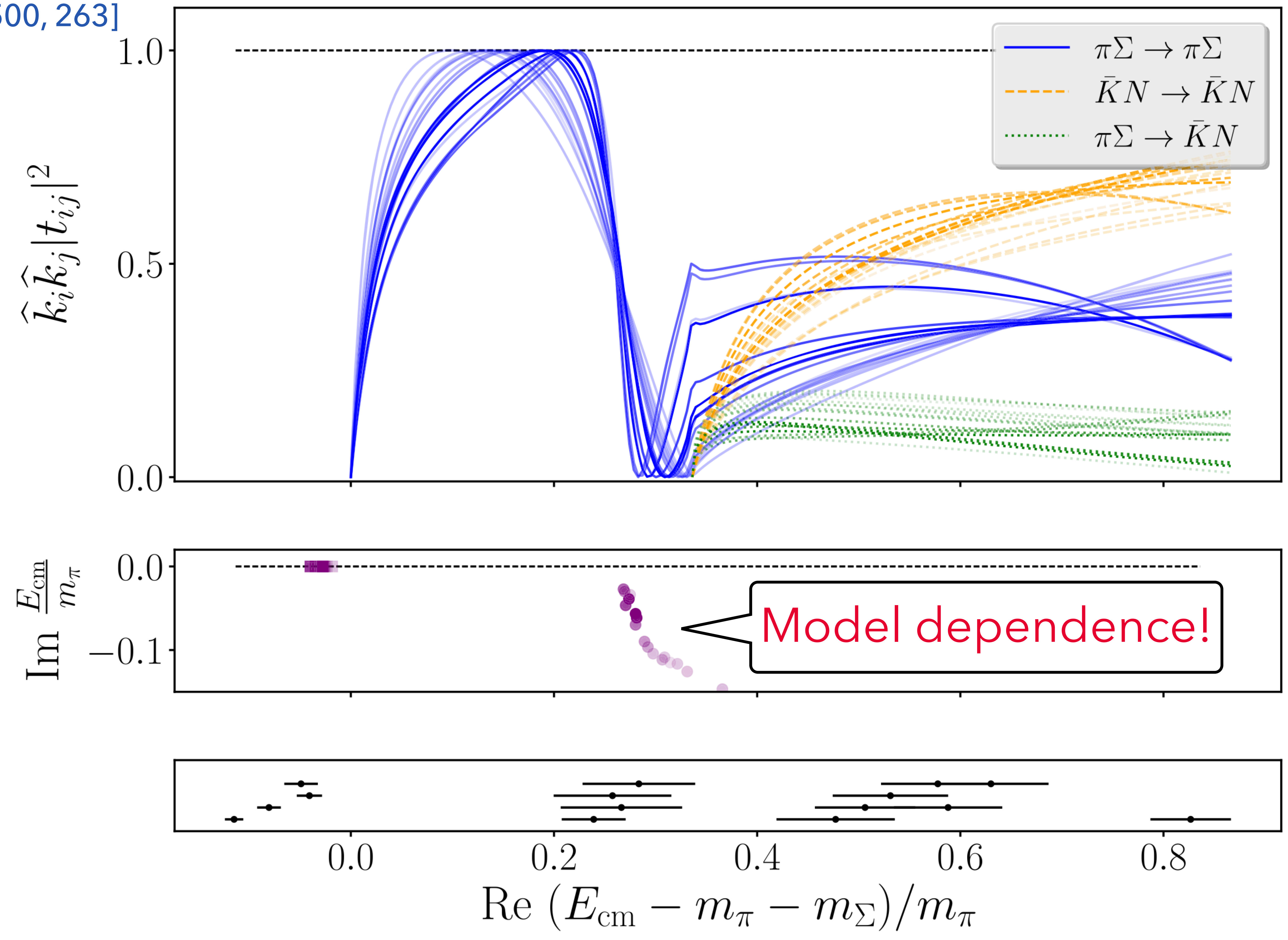

Bulava et al. (BaSc) 2024 [PRD 109, 014511]

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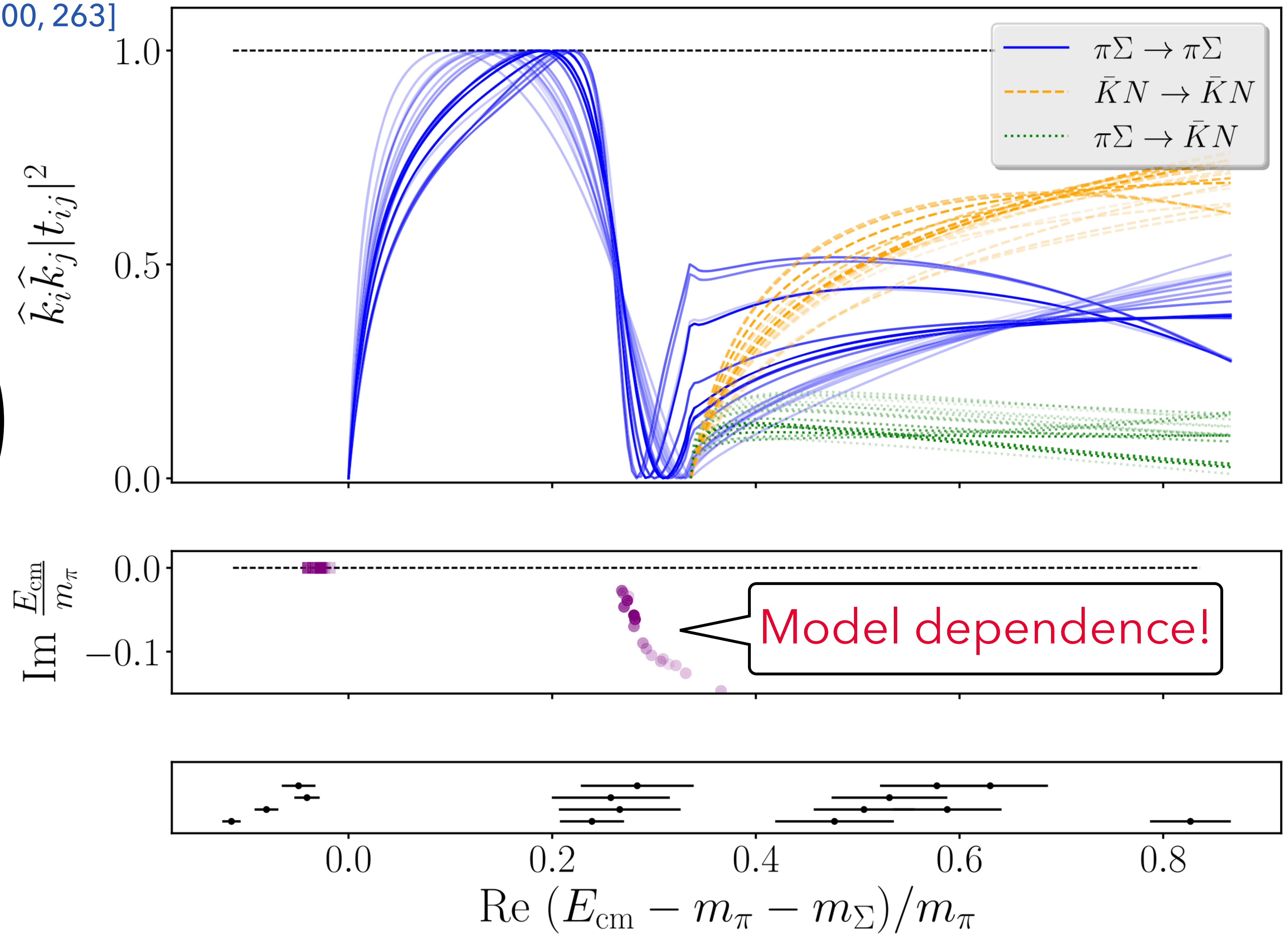
- Coupled-channel scattering:

$$K^{-1} = \begin{pmatrix} K^{-1}(\pi\Sigma \to \pi\Sigma) & K^{-1}(\pi\Sigma \to \bar{K}N) \\ K^{-1}(\bar{K}N \to \pi\Sigma) & K^{-1}(\bar{K}N \to \bar{K}N) \end{pmatrix}$$



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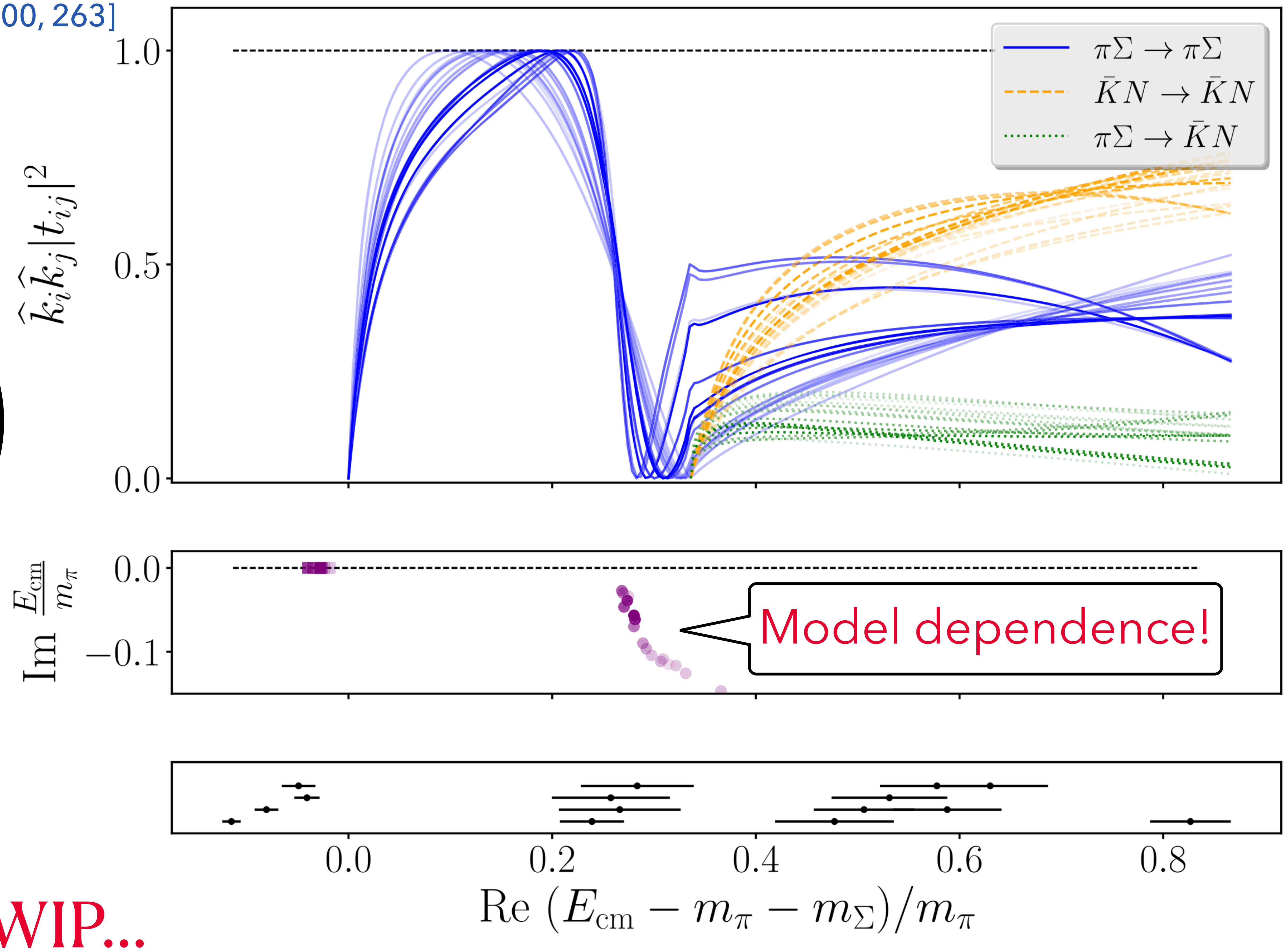
- Symmetries:
  - $(K^{-1})^T = K^{-1}$ —> K_{00}, K_{01}, K_{11}
  - $K_{01} \to -K_{01}$ at each E separately



WIP...

Bulava et al. (BaSc) 2024 [PRD 109, 014511]

Summary and outlook

Summary and outlook

- Novel analysis procedure for hadron spectroscopy from LQCD using FV formalism —> incorporate systematic error without need for explicit choice of parametrisation
- Key ingredients
  - Bayesian analysis of FV spectrum
  - Nevanlinna-Pick interpolation for analytic continuation
- Single-channel case works very well —> promising results in analysing σ resonance
- Coupled-channel analysis ongoing —> $\Lambda(1405)$
- Future directions: three-hadron systems —> parameterise K_3 in addition to K_2

Hansen and Sharpe 2014 [PRD 90, 116003], 2015 [PRD 92, 114509]
Mai and Döring 2017 [EPJA 53, 240]

Backup

Bayesian analysis

Sampling from posterior distribution

- Linearisation of QC around $\mathbf{u}_l$: $\mathbf{E}_{\mathrm{QC}}(\mathbf{u}) - \mathbf{E}_l \simeq J(\mathbf{u} - \mathbf{u}_l)$
- Approximate posterior distribution:
$$p^*(\mathbf{u}) = \frac{1}{\sqrt{(2\pi)^{n_p} \det \Sigma^*}} \exp\left[-\frac{1}{2}(\mathbf{u} - \mathbf{u}^*)(\Sigma^*)^{-1}(\mathbf{u} - \mathbf{u}^*)\right] \text{ with}$$
$$(\Sigma^*)^{-1} = J^T \Sigma_{\mathrm{d}}^{-1} J + \Sigma_p^{-1} \text{ and } \mathbf{u}^* = \Sigma^* \left[\Sigma_p^{-1}\mathbf{u}_0 + J^T \Sigma_{\mathrm{d}}^{-1}(\mathbf{E}_d - \mathbf{E}_l + J\mathbf{u}_l)\right]$$
- Reweighting factors: $w_* = p(\mathbf{u} \,|\, \mathbf{E}_{\mathrm{d}}, \mathbf{u}_0) \big/ p^*(\mathbf{u} \,|\, \mathbf{E}_{\mathrm{d}}, \mathbf{u}_0)$
- Probabilities entering Bayes factors:
$$p(\mathbf{E}_{\mathrm{d}} \,|\, M^{(k)}) = \int d^{n_p}u\, p(\mathbf{E}_{\mathrm{d}} \,|\, \mathbf{u}) p(\mathbf{u} \,|\, \mathbf{u}_0^{(k)}) = \int d^{n_p}u\, p(\mathbf{u} \,|\, \mathbf{E}_{\mathrm{d}}, \mathbf{u}_0^{(k)}) = \langle w_*^{(k)} \rangle_*^{(k)}$$

Nevanlinna-Pick interpolation

General framework and employed mappings

- Schwarz-Christoffel mapping from rectangle to unit disk: $\zeta = \dfrac{s-i}{s+i}$ with

$$s = \mathrm{sn}\left[\left(z - C + i\frac{H}{2}\right)\frac{2K(k)}{W}, k\right], \text{ where } K(k)/K(\sqrt{1-k^2}) = W/2H$$

Rectangle height ($\in \mathbb{R}$)

Jacobi elliptic function

Complete elliptic integral, 1st kind

Rectangle width ($\in \mathbb{R}$)

- Inverse mapping: $z = F\left[\arcsin\left(i\frac{1+\zeta}{1-\zeta}\right), k\right]\frac{W}{2K(k)} - i\frac{H}{2} + C$

Incomplete elliptic integral, 1st kind

Rectangle center ($\in \mathbb{C}$)

- WV center (in disk coords.): $c(\zeta) = \left(Q(\zeta)\bar{S}(\zeta) - P(\zeta)\bar{R}(\zeta)\right) \Big/ \left(|S(\zeta)|^2 - |R(\zeta)|^2\right)$

- WV radius (in disk coords.): $r(\zeta) = |P(\zeta)S(\zeta) - Q(\zeta)R(\zeta)| \Big/ \left(|S(\zeta)|^2 - |R(\zeta)|^2\right)$

Nevanlinna-Pick interpolation

Uncertainty analysis for pole positions

- Use randomly chosen point within WV as function estimator, $w(\zeta) = c(\zeta) + \rho\, r(\zeta)\, e^{i\theta}$ with uniform random numbers $\rho \in [0,1)$ and $\theta \in [0,2\pi)$
- Use independent random point(s) for each sample from the posterior (cf. source positions in lattice QCD)
- Effectively, the expectation value of the pole location takes the form $$\langle E_0 \rangle = \frac{1}{\pi Z} \int d^{n_p}u \int_0^1 dr\, r \int_0^{2\pi} d\theta\, E_0(\mathbf{u}, r, \theta) p(\mathbf{u} \,|\, \mathbf{E}_\mathrm{d}, \mathbf{u}_0)$$
- Uncertainty: $(\delta E_0)^2 = \langle E_0^2 \rangle - \langle E_0 \rangle^2$

Isospin-0 $\pi\pi$ system on X252

$M_\pi = 280$ MeV

Setup and preliminary results

- Exact distillation with 48 eigenvecs, all source times, 1050 configs
- Site-local operators included so far: $\sigma, \phi, \pi\pi, \eta_l\eta_l, \eta_s\eta_s, \eta_l\eta_s, K\bar{K}$
- Outlook
  - Singly-displaced operators
  - Moving frames
  - More ensembles: X253, D251, J250

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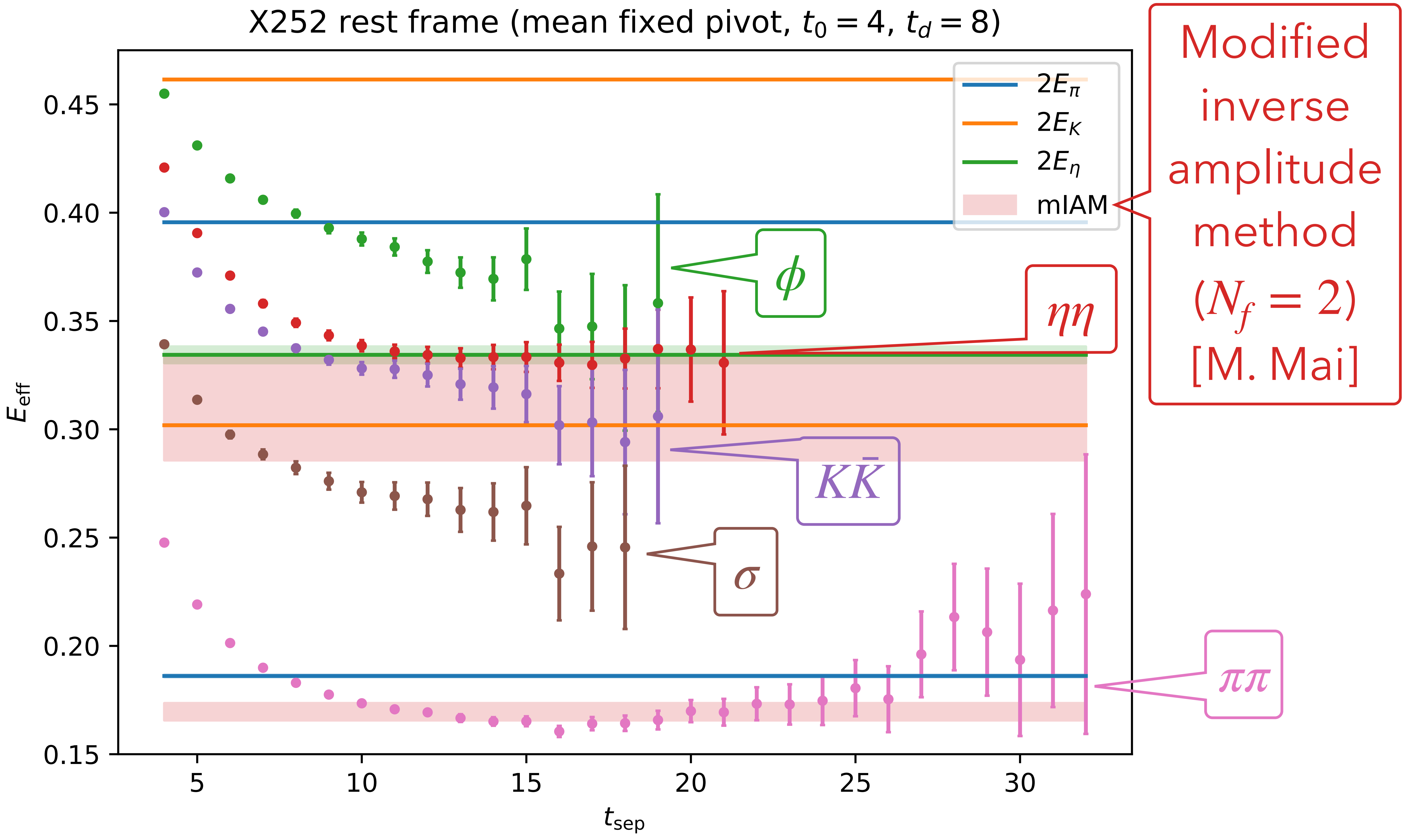

WIP in collaboration with H. Alharazin, J. Bulava, F. Romero-López, and the BaSc collaboration