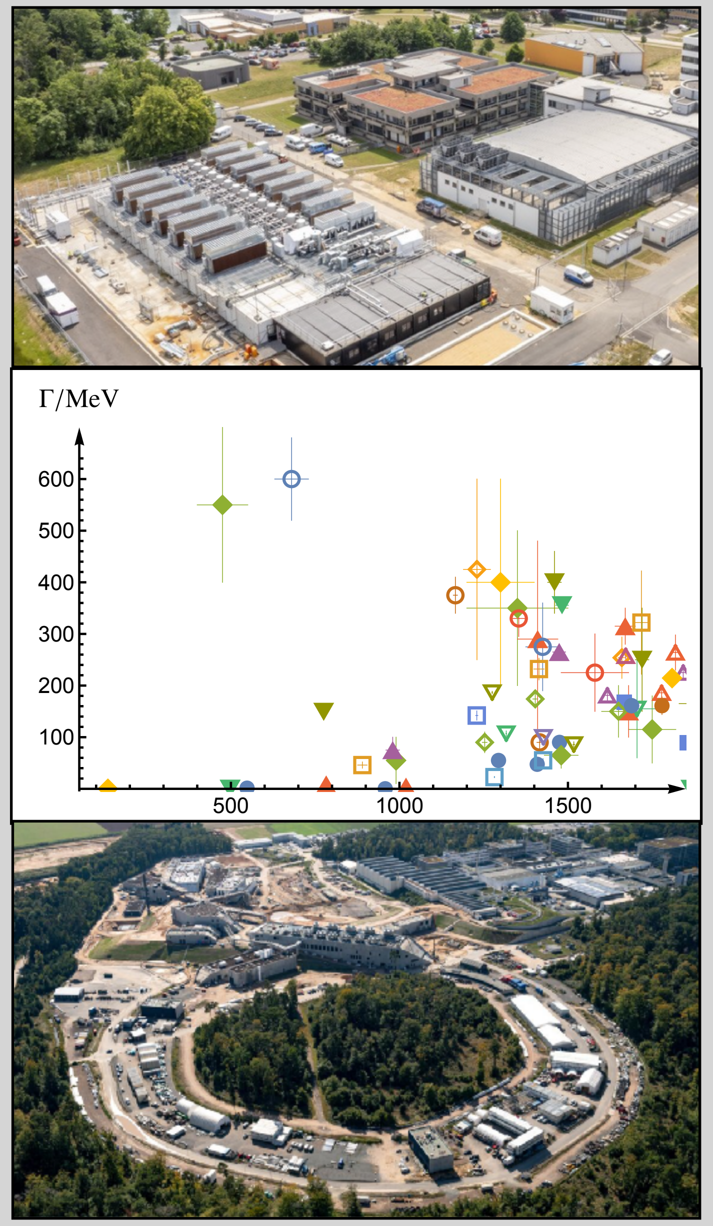
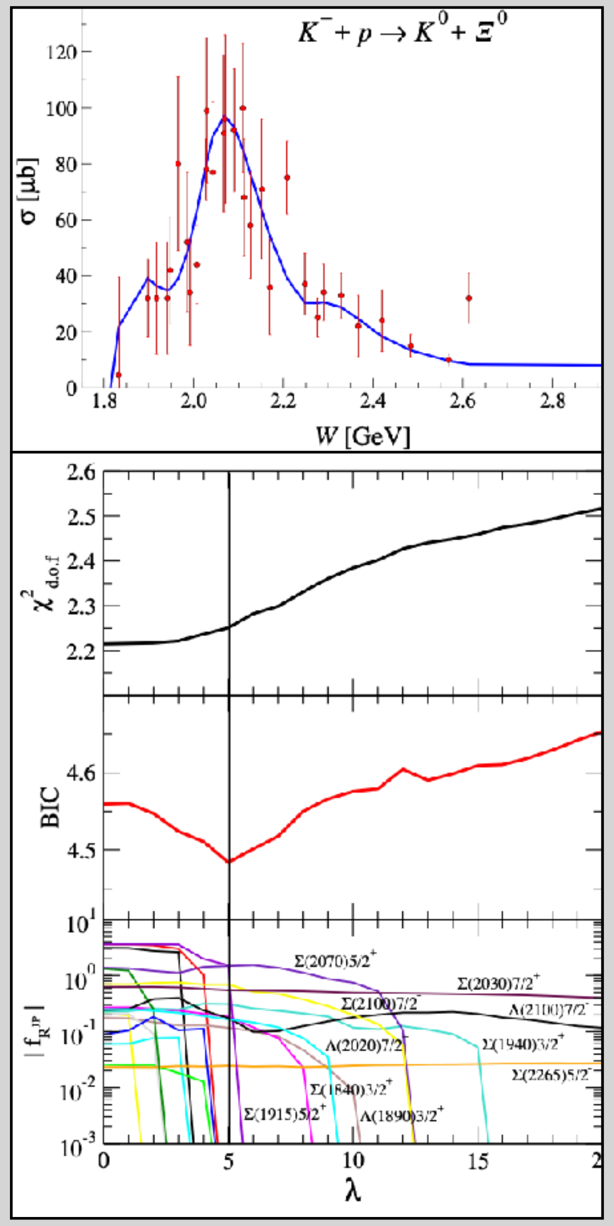
maxim-mai.github.io/talks.html

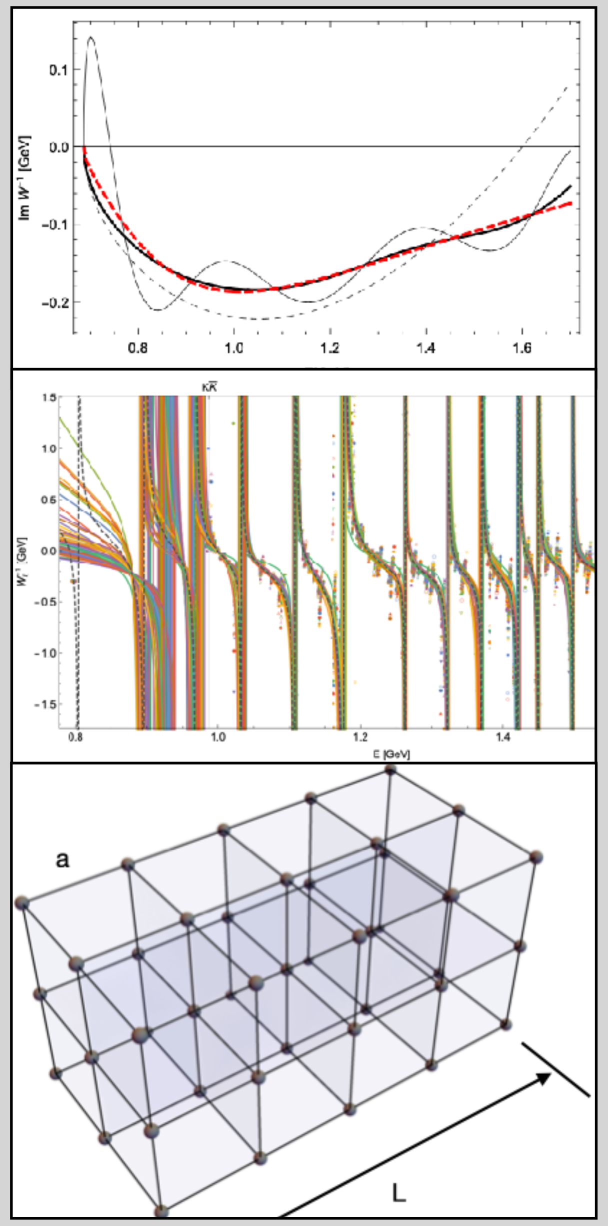
DENOISING AND SHARPENING THE HADRON SPECTRUM THROUGH MACHINE LEARNING



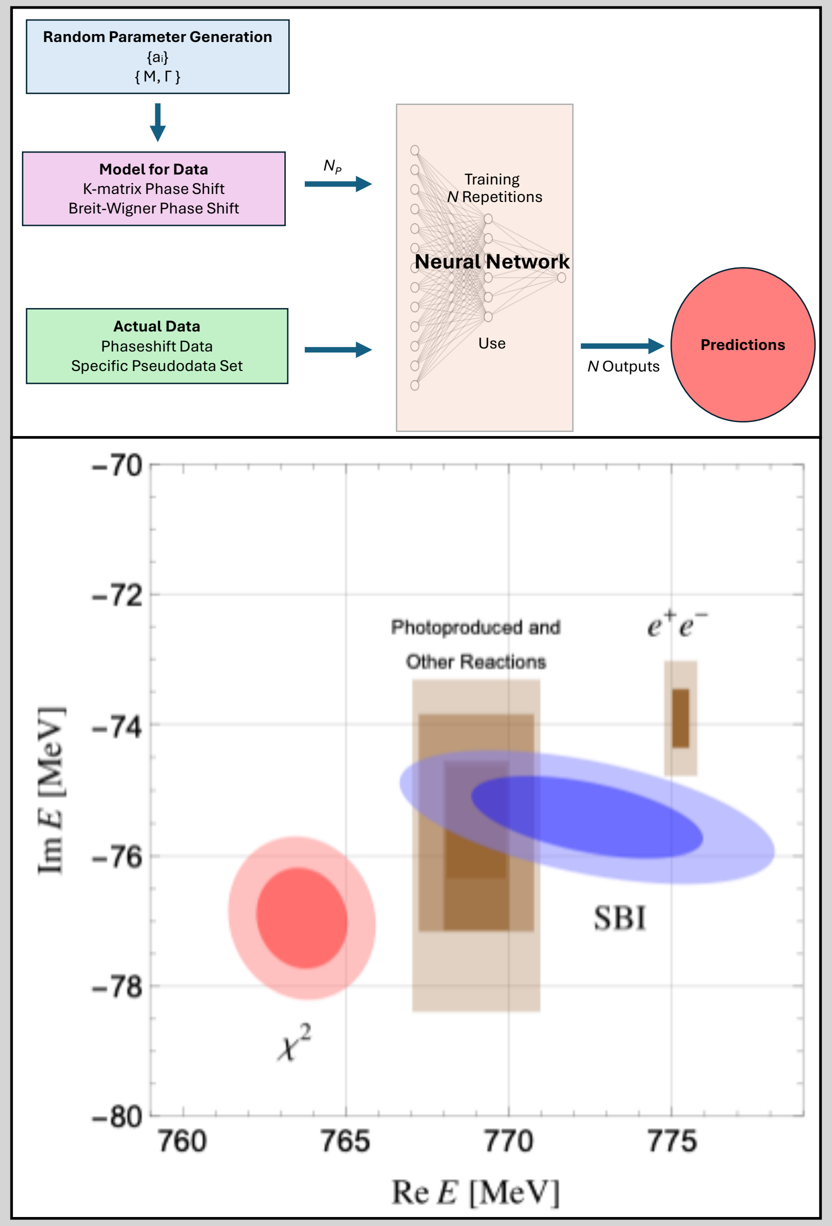
introduction



application 1



application 2



application 3

✔ ! ? ✔ ! ?

summary/outlook/questions

MAXIM MAI (U. BERN & GWU)

M-L-H-N-P May 27 - 29, 2026 Aristotle University of Thessaloniki

HADRON SPECTRUM

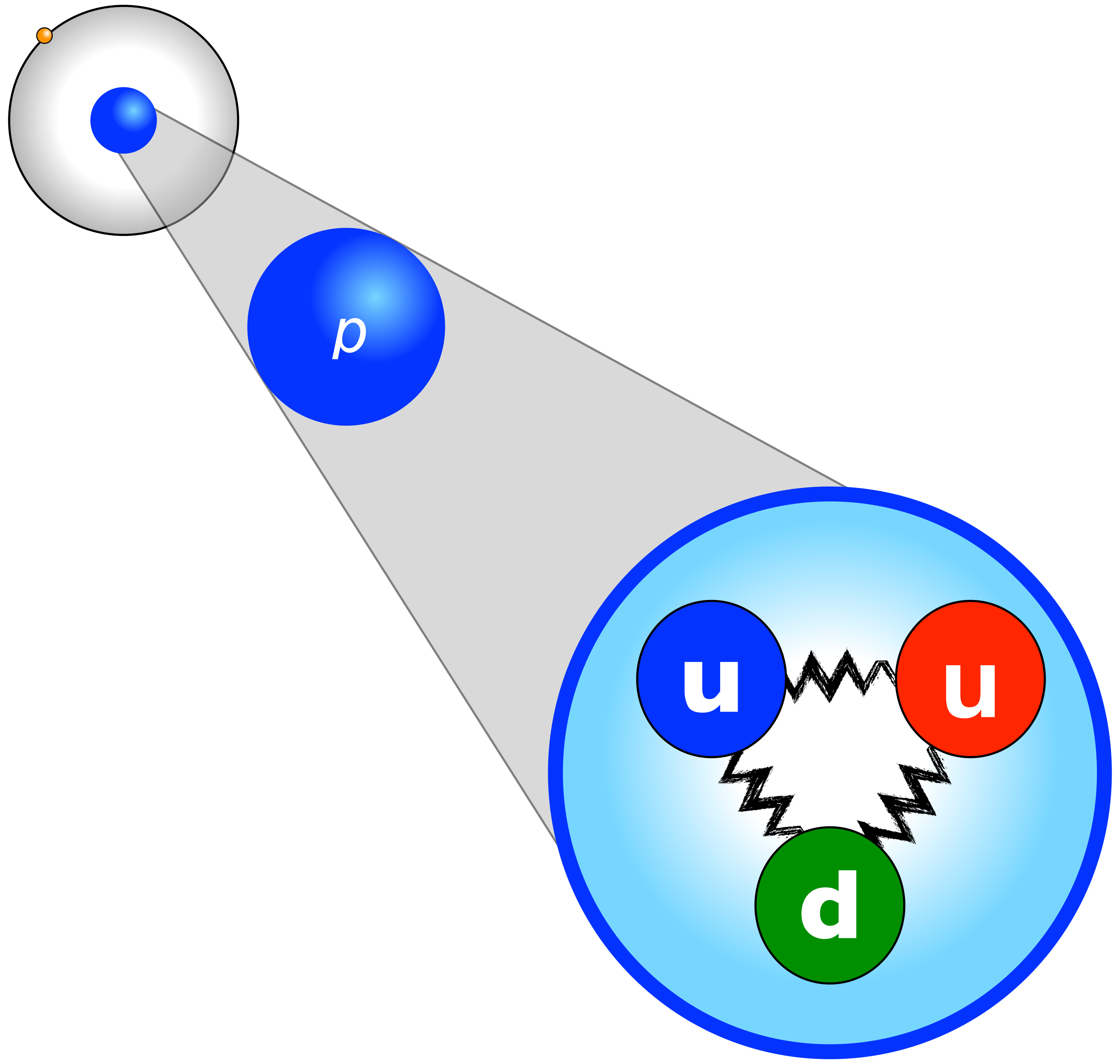
BOUNDARY OF UNDERSTANDING

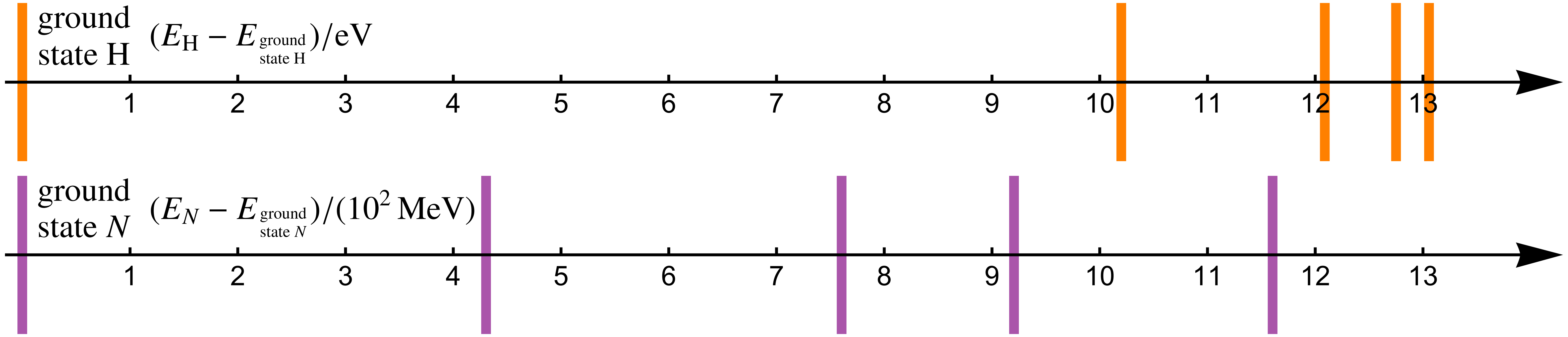
BIG PICTURE

MM Theory of resonances [Encyclopedia of Particle Physics] — (simple introduction)
https://doi.org/10.1016/B978-0-443-26598-3.00001-8 e-Print: 2502.02654 [hep-ph]

Protons/neutrons

- 99% of the mass of visible matter in the universe
- Building blocks: **quarks & gluons (strong force)**
- Part of a large class of particles: **hadrons**





Hydrogen spectrum **(✓)**

Proton spectrum **(?)**

HADRON SPECTRUM

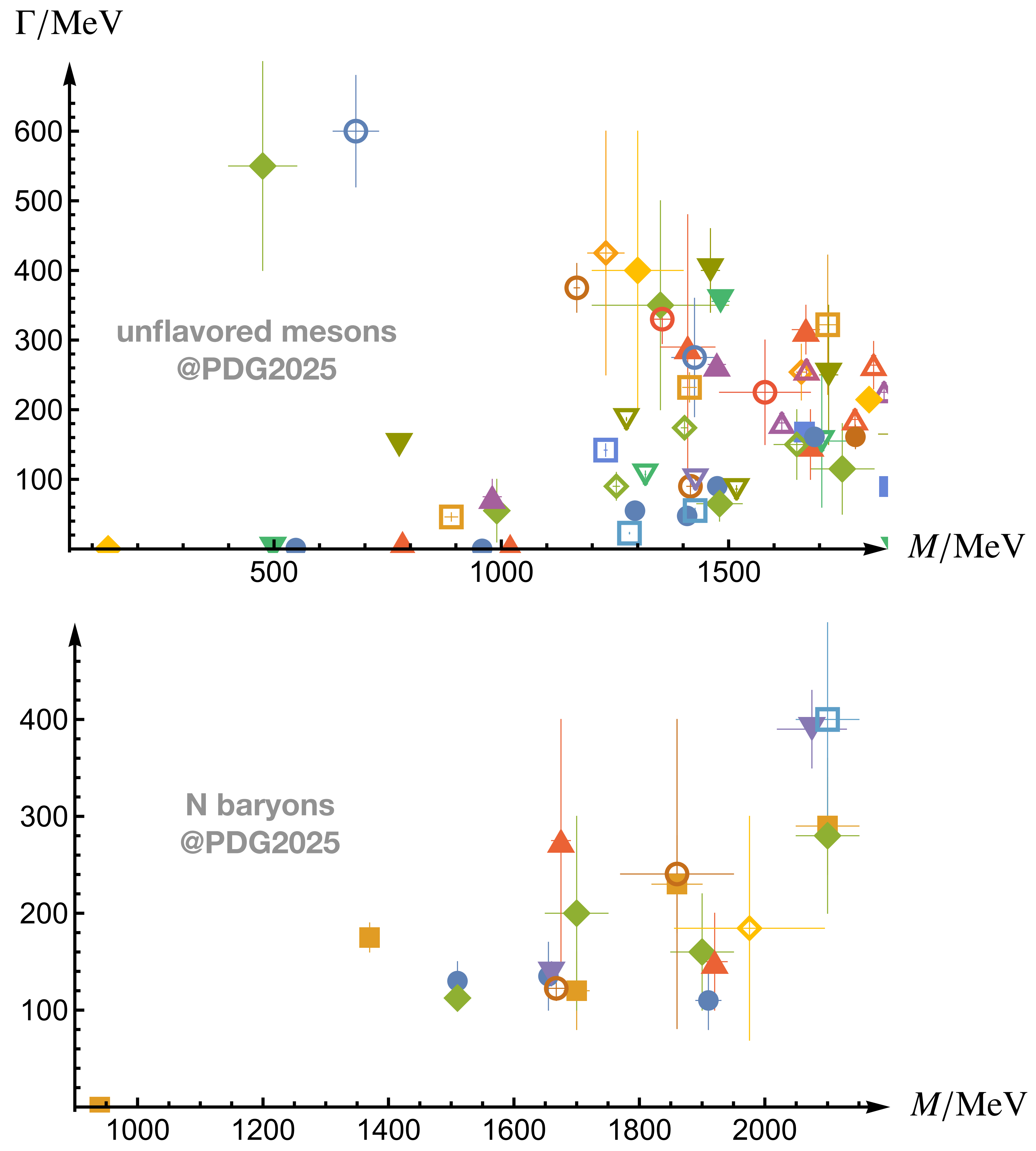
Experimental progress

- 70y research ($\Delta(1232), \rho(770), \omega(782), \ldots$)
- mostly excited states

  $\approx$ 100 mesons + 50 baryons (****)
- ongoing experiments @CERN, GSI, JLAB, BES…

New techniques

- Lattice QCD
- Effective Field Theories
- Machine Learning



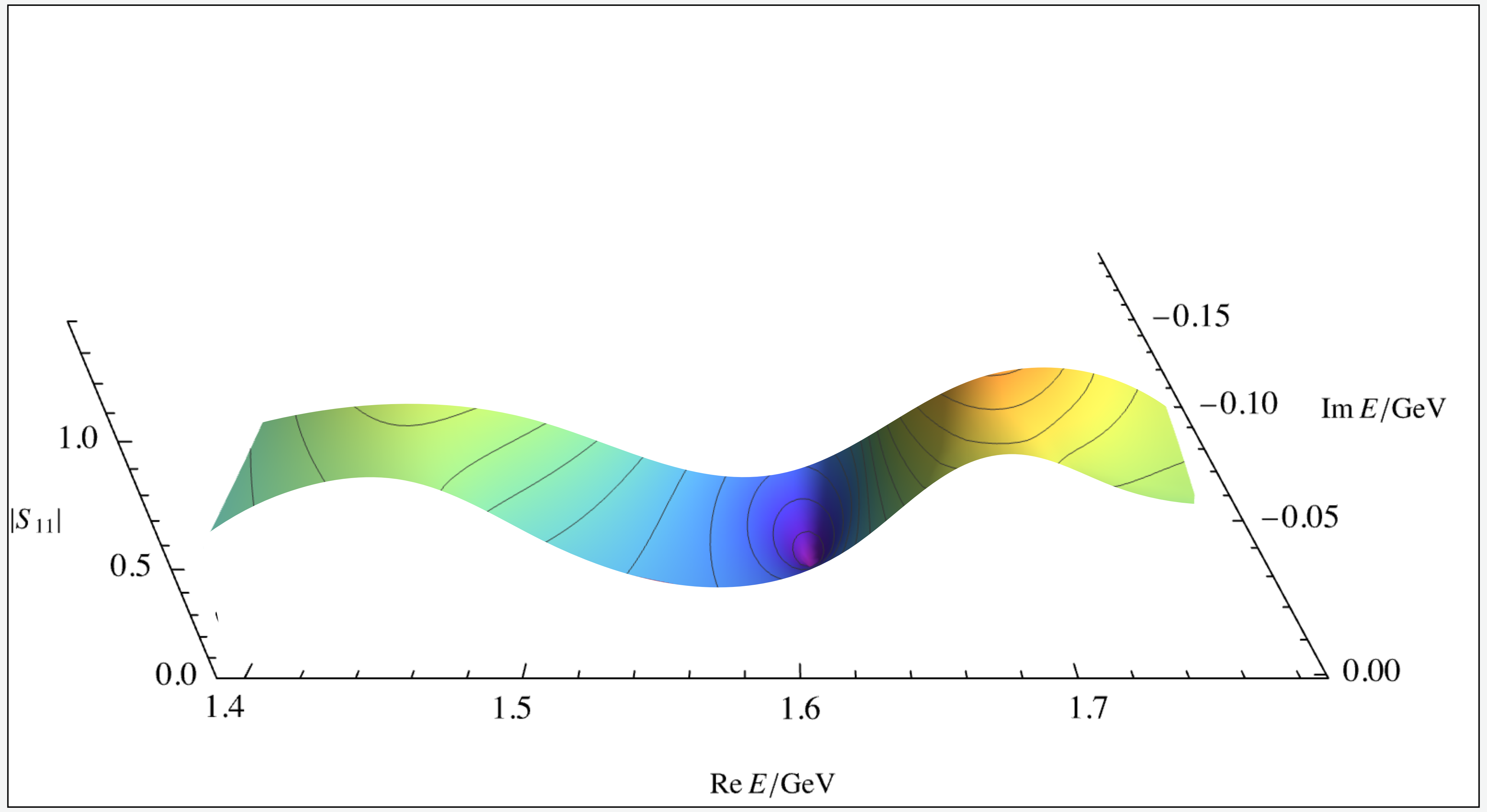
Review: MM/Meißner/Urbach Phys.Rept. 1001 (2023) 1-6

BROADER IMPACT

Review: MM/Meißner/Urbach Phys.Rept. 1001 (2023) 1-6

S-MATRIX

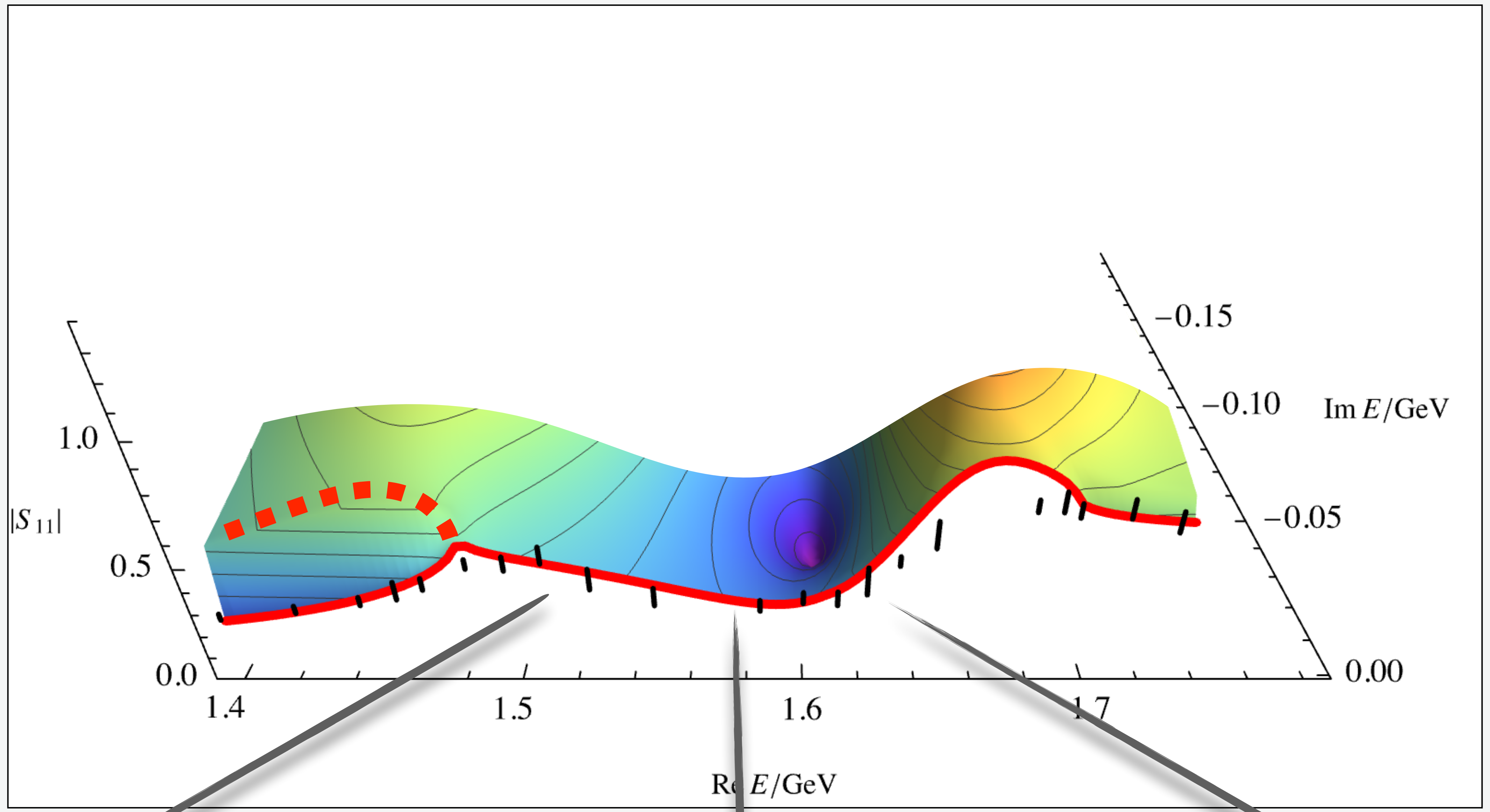
- Crossing symmetry (particle/antiparticle)
- Unitarity (probability conservation)
- Analyticity (causality)



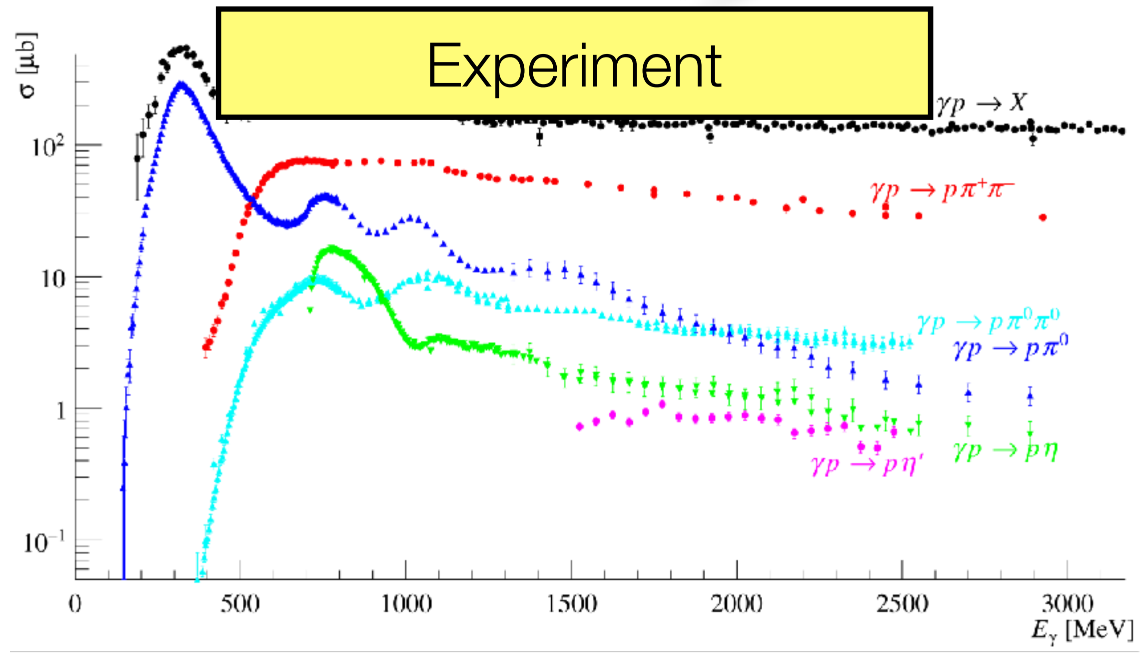
- MM Theory of resonances [Encyclopedia of Particle Physics] — (simple introduction) https://doi.org/10.1016/B978-0-443-26598-3.00001-8 e-Print: 2502.02654 [hep-ph]
- Scott Willenbrock *Eur.Phys.J.Plus* 139 (2024) 6, 523
- …

S-MATRIX

- ✴ *Crossing symmetry (particle/antiparticle)*
- ✴ *Unitarity (probability conservation)*
- ✴ *Analyticity (causality)*

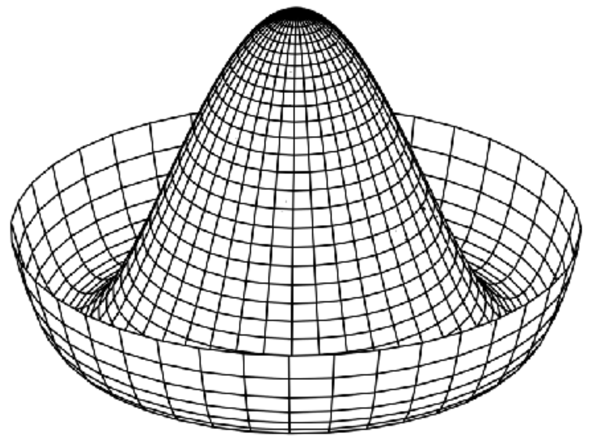


Experiment



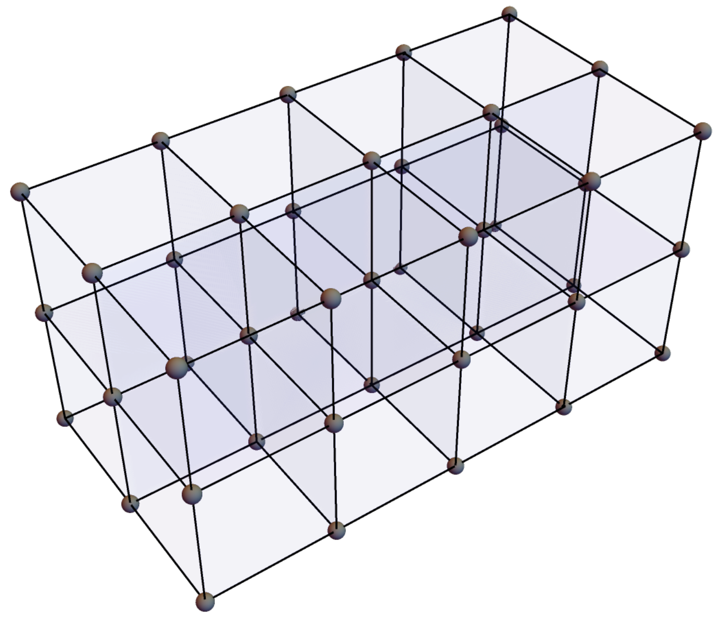
Data: JLAB, ELSA, MAMI CLAS12, GlueX, …
Plot: Thiel+ PPNP 125 (2022) 103949

Effective field theories



Data: SAID: PRC 74 (2006) 045205
Model: MM+ PRD 86 (2012) 094033

Lattice QCD



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- …

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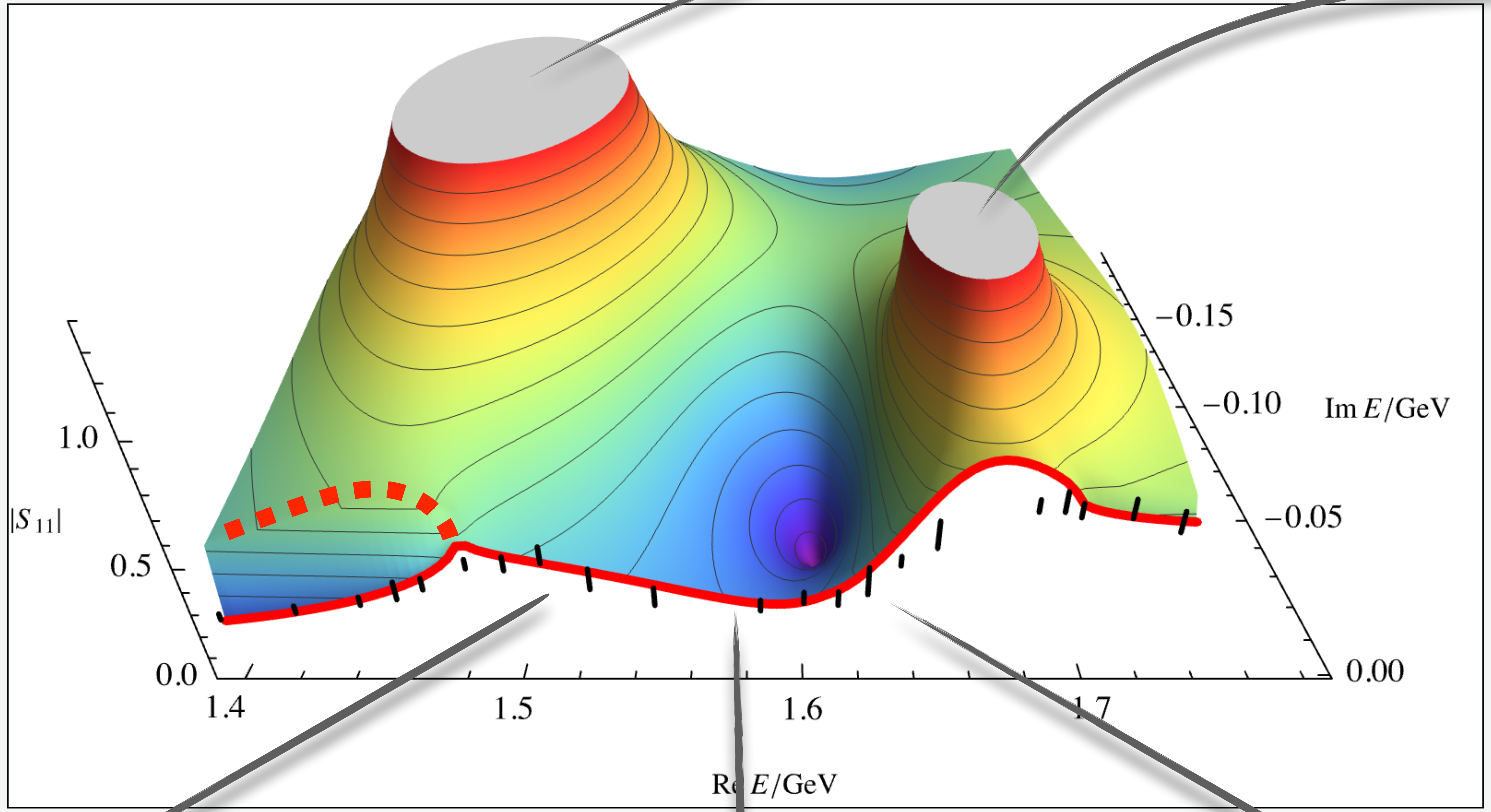
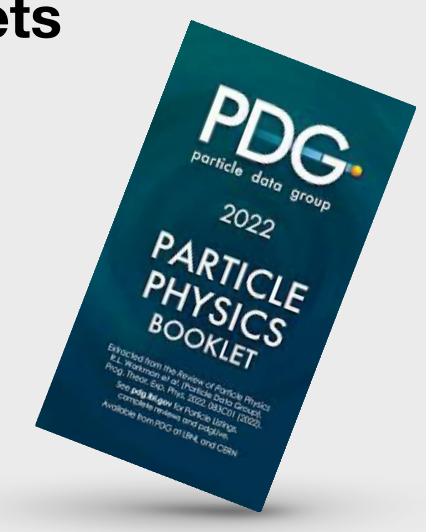


Poles on unphysical Riemann Sheets

- Universal resonance parameter
- Singularities (cuts, …) included
- **Hadron mass** $M = \mathrm{Re}\, E_{\mathrm{pole}}$
- **Decay width** $\Gamma = -2\,\mathrm{Im}\, E_{\mathrm{pole}}$



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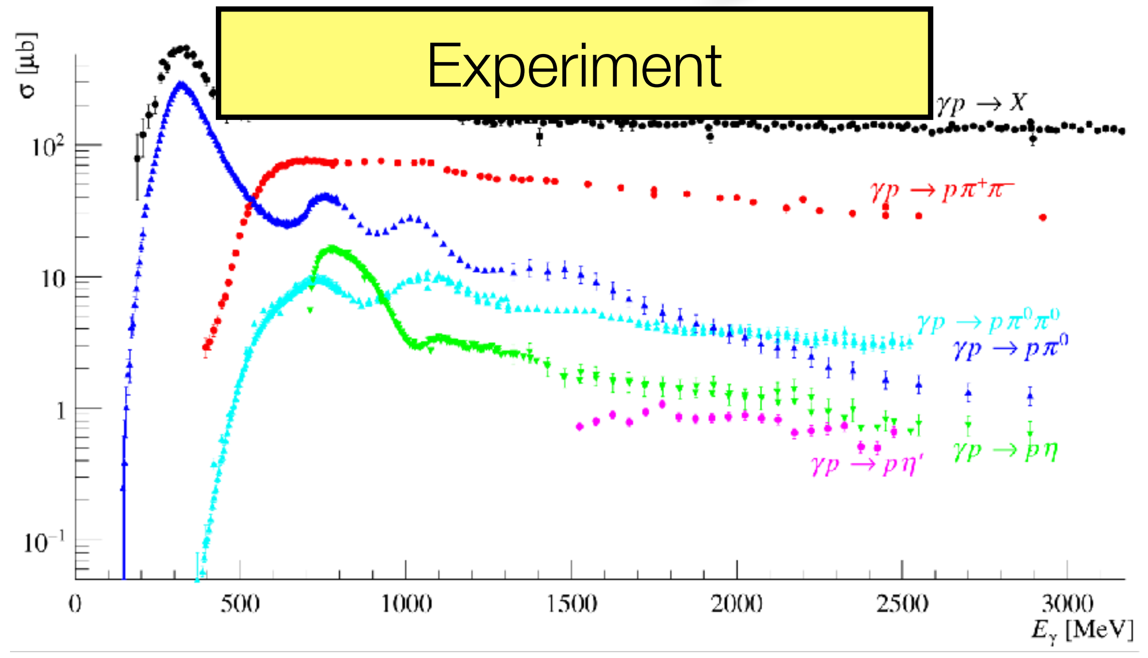
- Scott Willenbrock *Eur.Phys.J.Plus* 139 (2024) 6, 523
- …

Experiment



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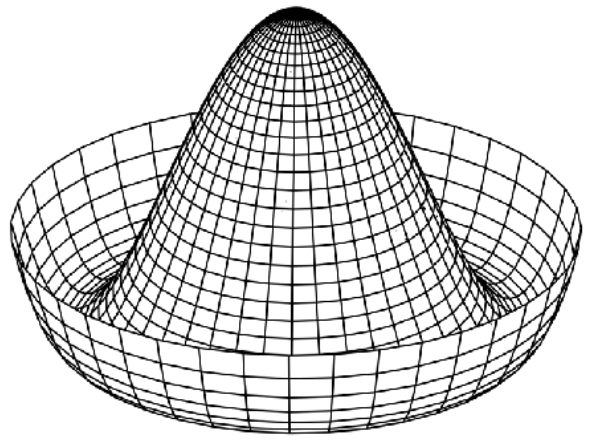

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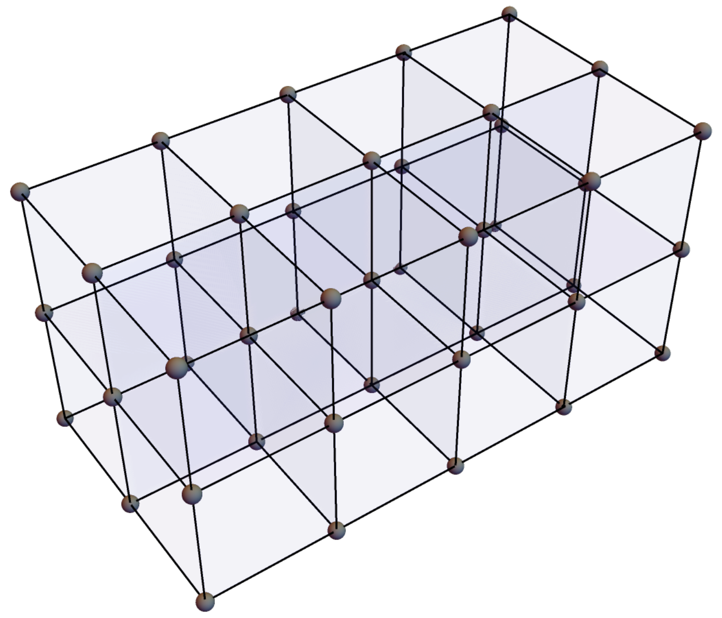


APPLICATION 1

MINIMAL HADRON SPECTRUM

Justin Landay
Maxim Mai
Michael Döring
Helmut Haberzettl
Kanzo Nakayama

Towards the minimal spectrum of excited baryons

PHYSICAL REVIEW D 99, 016001 (2019)

FAKE RESONANCE PROBLEM

Big data models (data driven models)

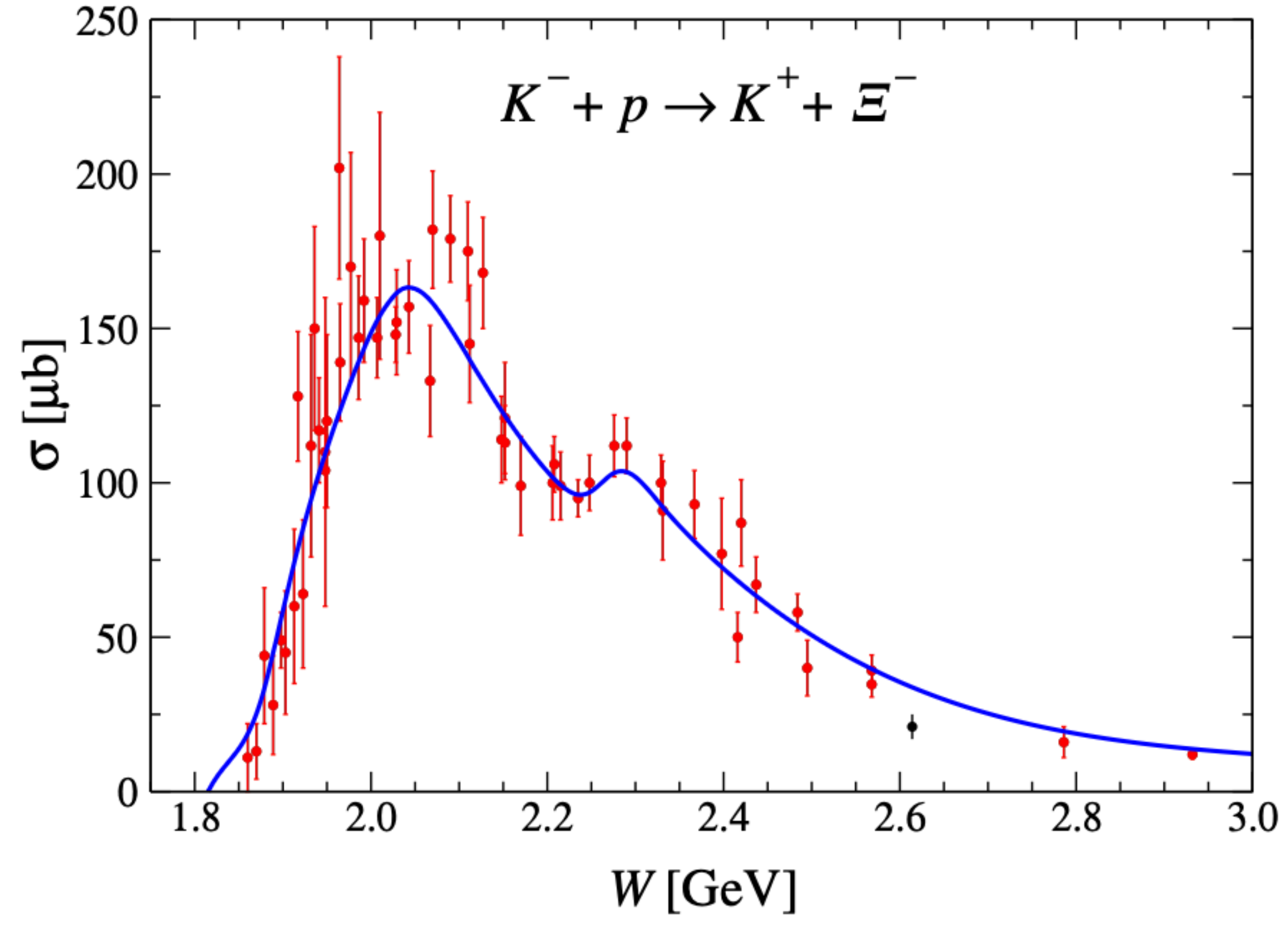
- e.g. Dynamical coupled-channel models, …

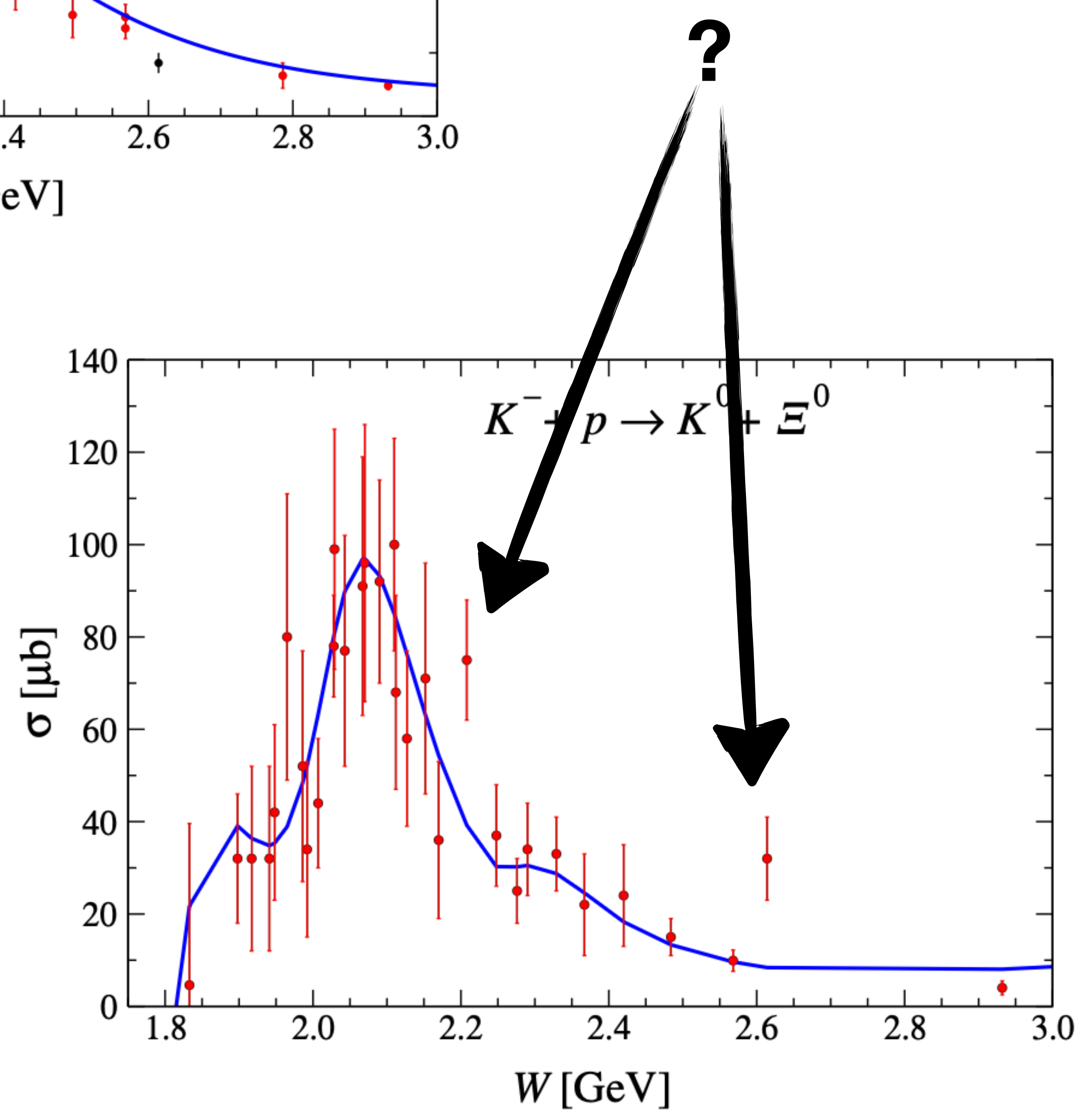
Review: Döring, Haidenbauer, MM, Sato PPNP2025

- $N_{\text{data}} \sim \mathcal{O}(10^5)$
- Very flexible parameterizations $N_{\text{par}} \sim \mathcal{O}(10^3)$
- χ^2 minimization criterion

Possible issue

- adding new resonances improves data description
- Resonances are "seen"





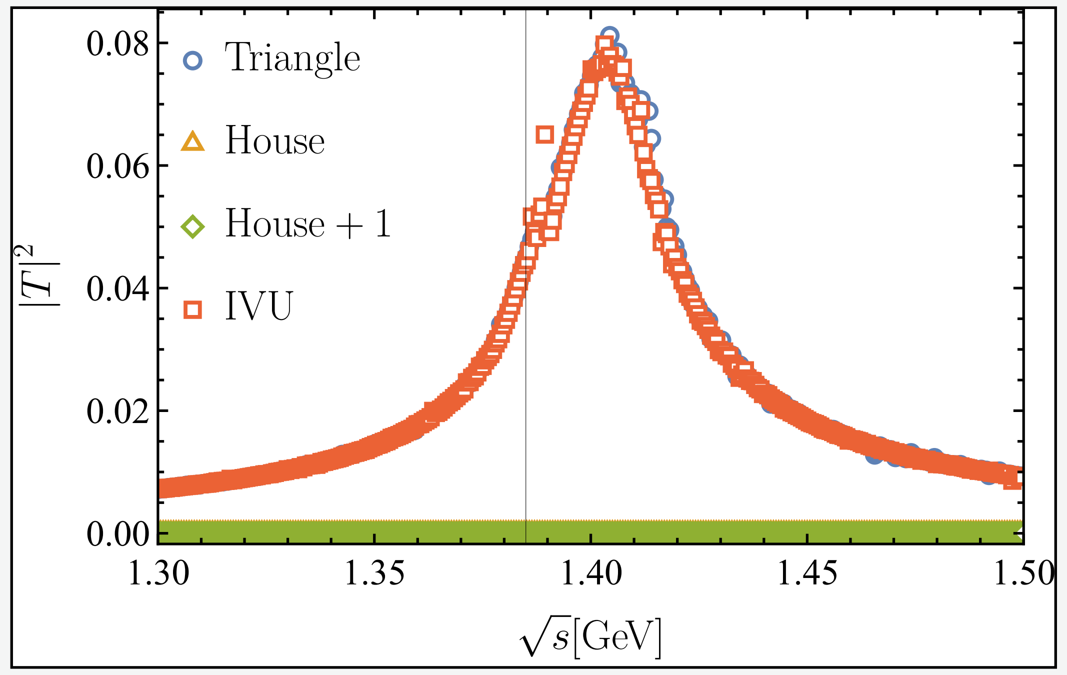
POSSIBLE SOLUTIONS

Better physical constraints

- S-matrix constraints: Thresholds, Triangle singularities, …

Triangle singularity a1(1420)

GUO+ PPNP 112 (2020) 103757 [arXiv:1912.07030]



Sakthivasan/MM/… *JHEP* 10 (2024) 246

- Effective Lagrangian (QCD symmetries)
  - Controlled hadron-hadron dynamics
  - $\Lambda(1405), \Lambda(1380), \ldots$

Review: Eur.Phys.J.ST 230 (2021) 6, 1593-1607

Statistics/MachineLearning/Data-driven tools

- Bayesian criteria
- Least Absolute Shrinkage and Selection Operator (LASSO)
  - minimal spectrum to describe a hadronic reaction

R. Tibshirani, J. R. Stat. Soc. 73, 273 (2011).
T. Hastie, R. Tibshirani, and J. Friedman, The Elements of Statistical Learning
G. James, D. Witten, T. Hastie, and R. Tibshirani, An Introduction to Statistical Learning

- **Main idea:** penalize the appearance of new resonances

$$\chi_T^2 := \chi^2 + P(\lambda)$$

- How to define penalty function $P(\lambda)$?
- How to determine optimal penalty factor λ?

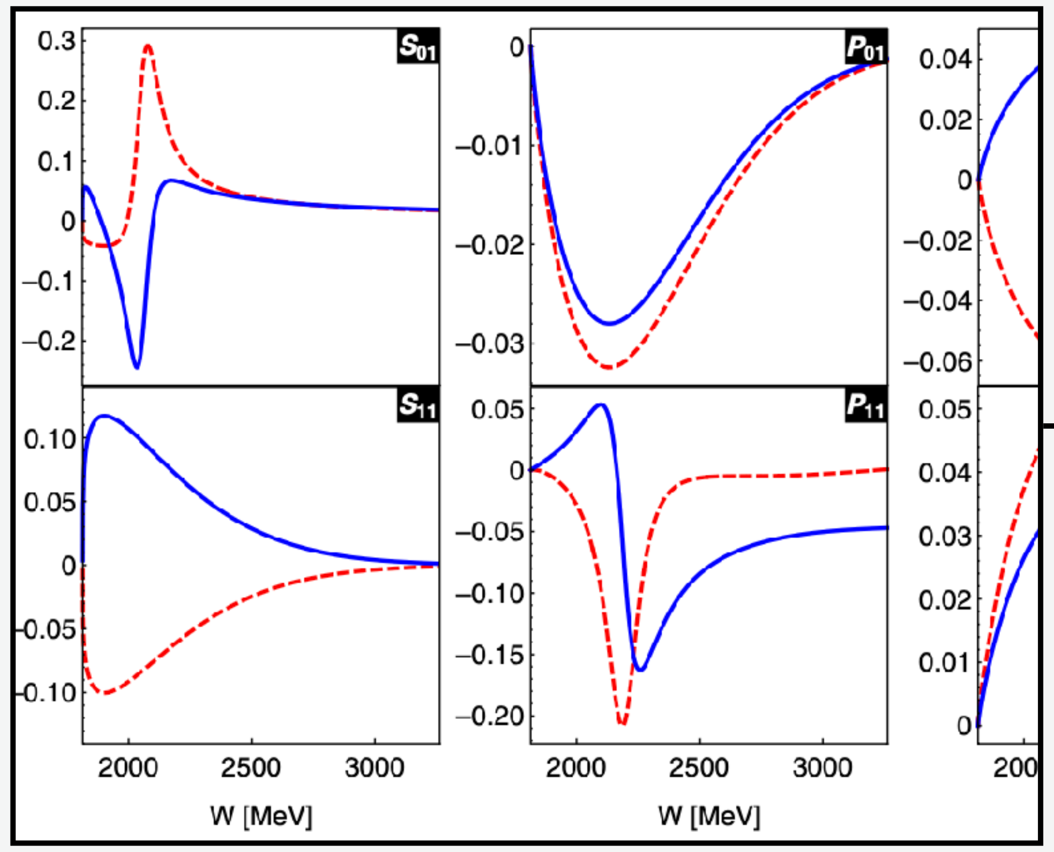
SYNTHETIC DATA TESTS

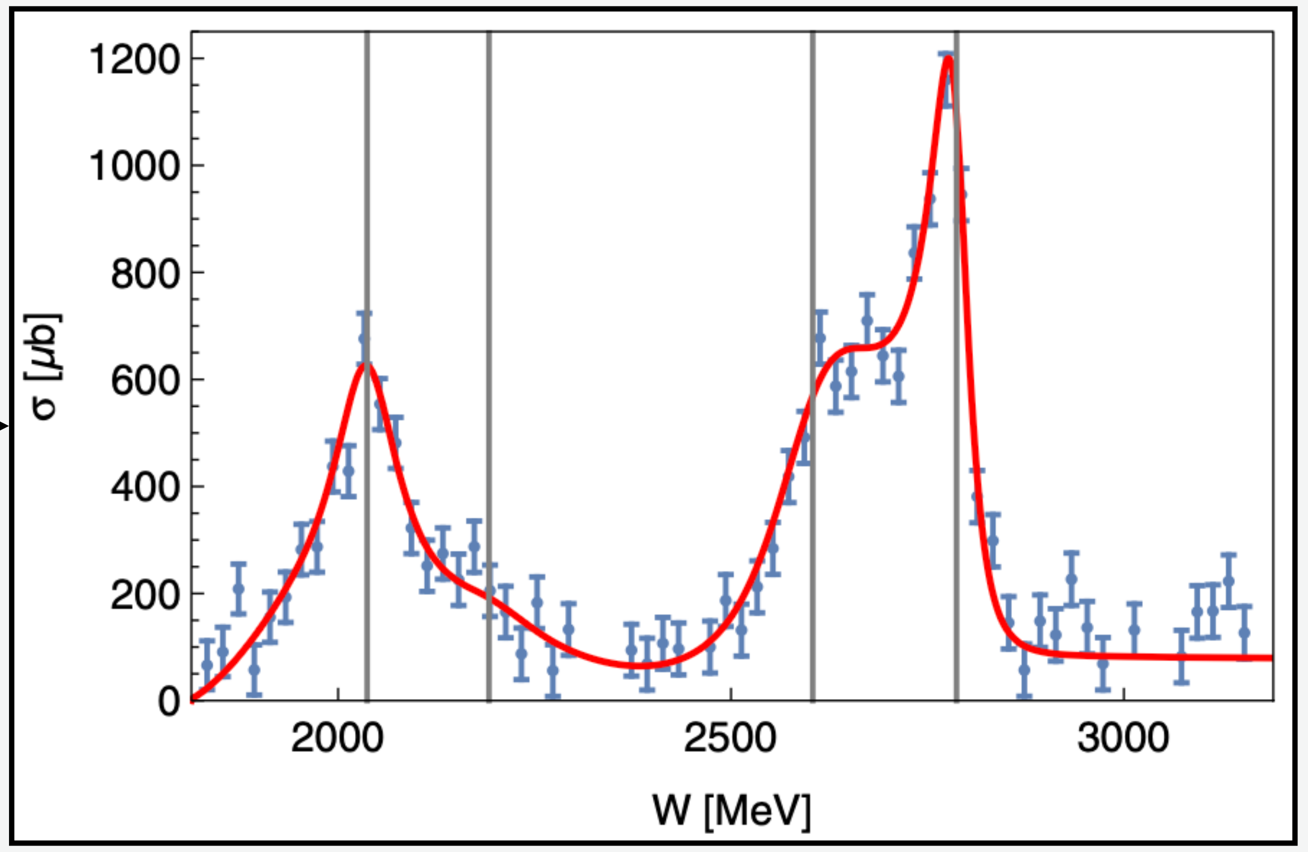
Controlled environment

- 10 partial waves/10 resonance candidates

$$\tau(W) = e^{i\phi}\left(\frac{k_f(W)}{\Lambda}\right)^{L+\frac{1}{2}} \times \left(a\, e^{-\alpha^2\left(\frac{k_f(W)}{\Lambda}\right)^2} - x\, e^{i\Phi}\frac{\Gamma/2}{W-M+i\Gamma/2}\right)$$

- Synthetic data with 4 active resonances





Penalty function

- Residua

$$P(\lambda) = \lambda^4 \sum_{i=1}^{i_{\max}} |x_i|$$

- Second derivative

$$P(\lambda) = \lambda^5 \sum_{i=1}^{10} \frac{\int_{m_K+m_\Xi}^{W_{\max}} \left|\frac{\partial^2}{\partial W^2}\tau_i(W)\right|^2 dW}{\int_{m_K+m_\Xi}^{W_{\max}} |\tau_i(W)|^2\, dW}$$

physically informed

Procedure

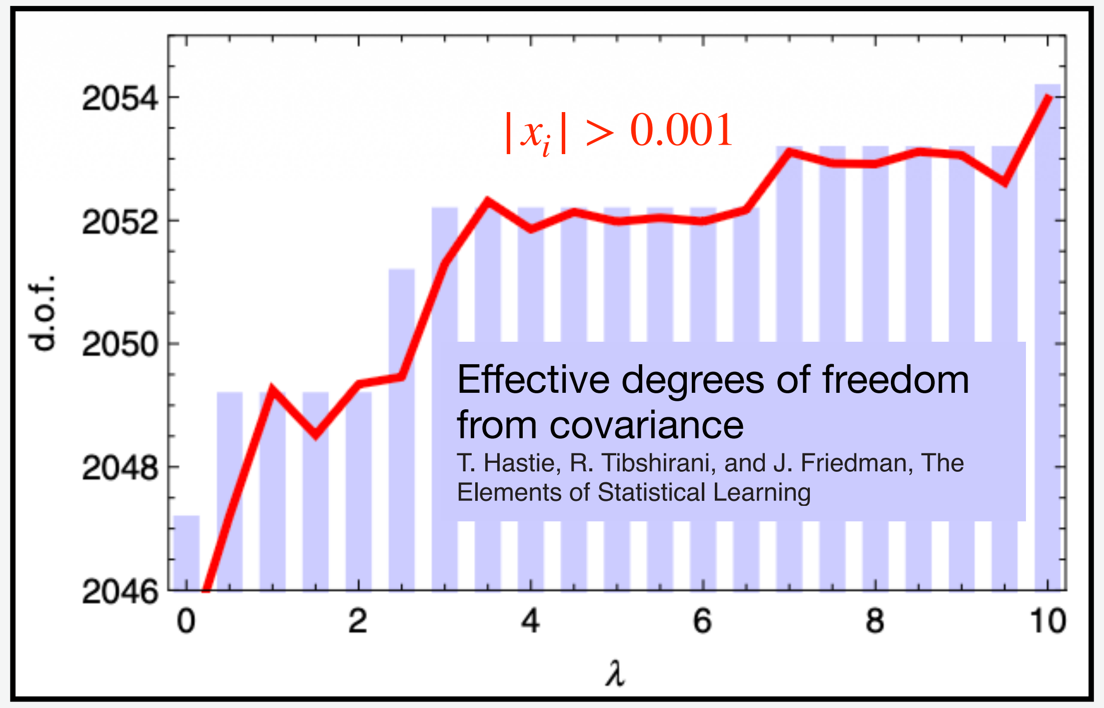
Minimize $\chi^2_T := \chi^2 + P(\lambda)$ stepwise as

- $(\lambda = 10) \to (\lambda = 0)$ forward LASSO
- $(\lambda = 0) \to (\lambda = 10)$ backward LASSO (automatic shutoff)
- …

Optimal penalty factor

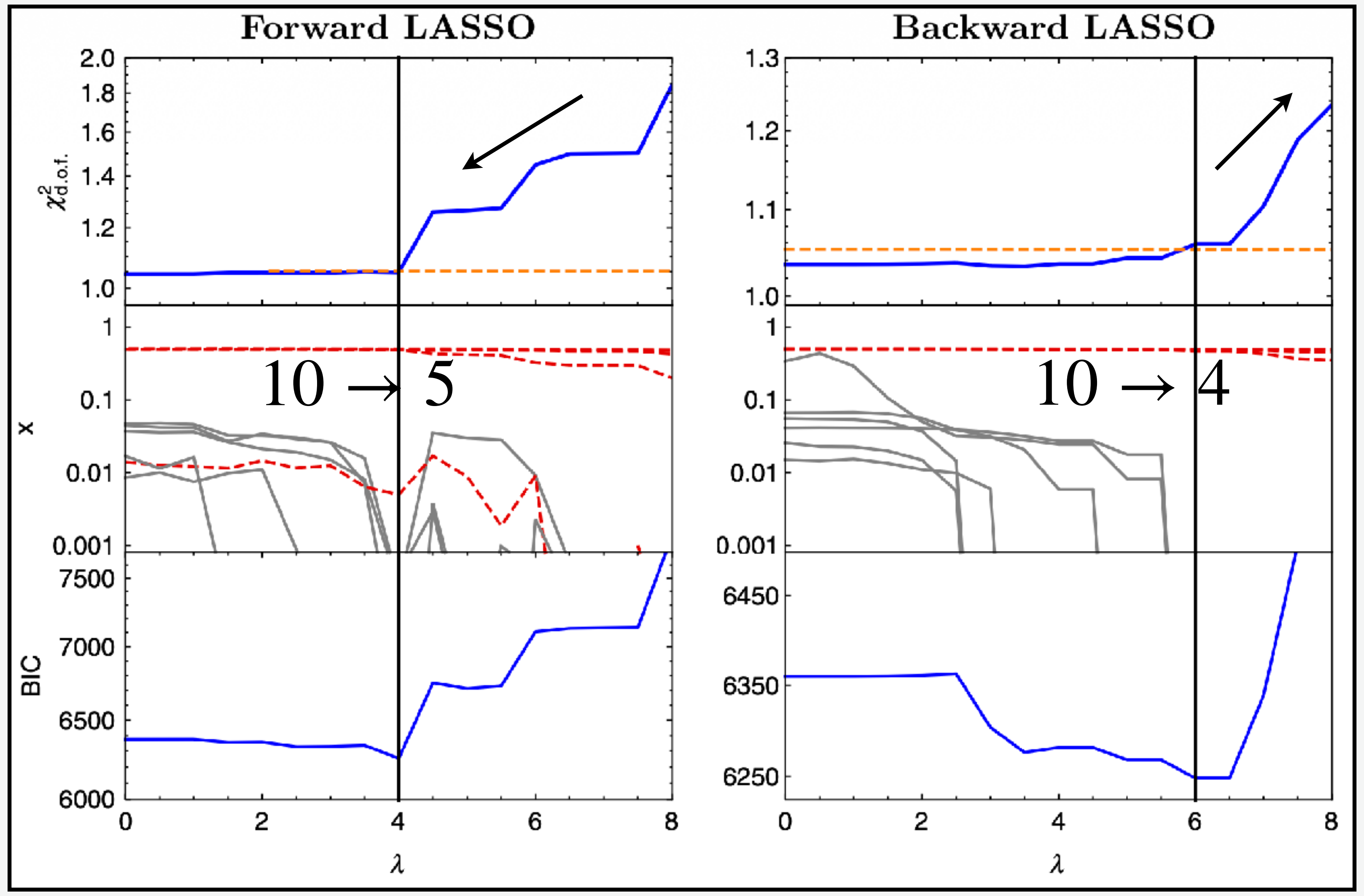
- Bayesian information criterion

$$BIC = k_{\text{eff}} \log(n) + \chi^2 + c$$



RESULTS

Parametric penalty



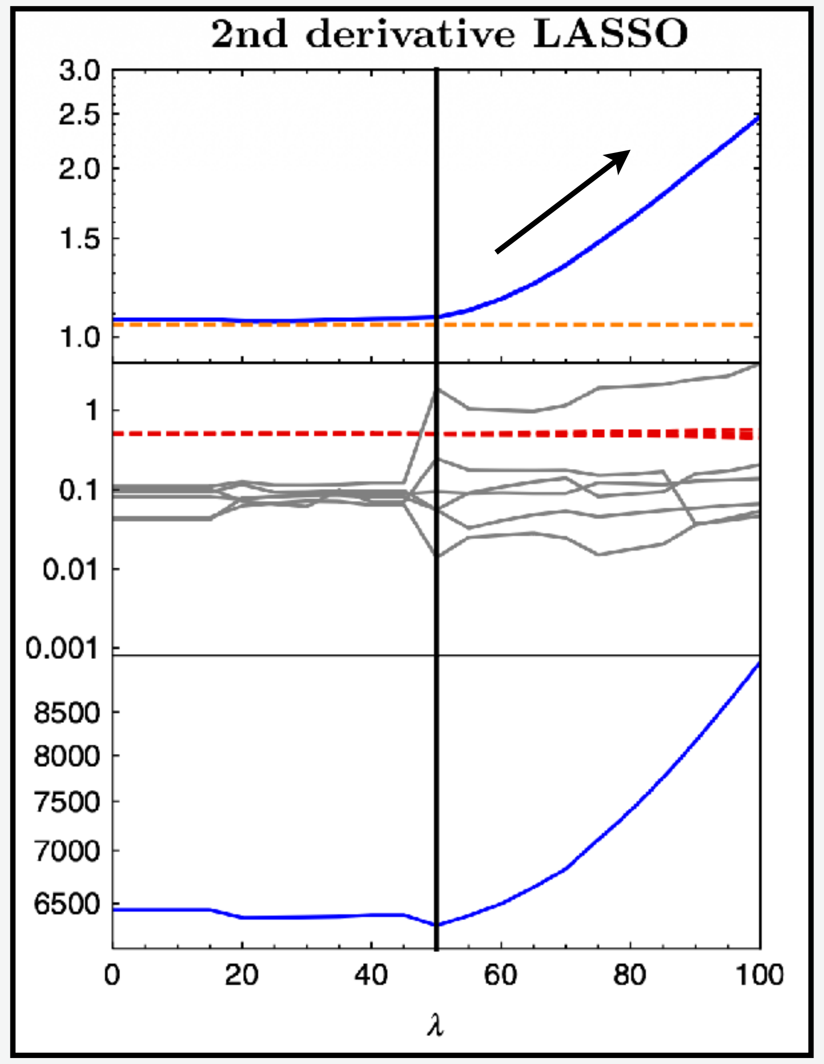
➡ Resonance content reduced

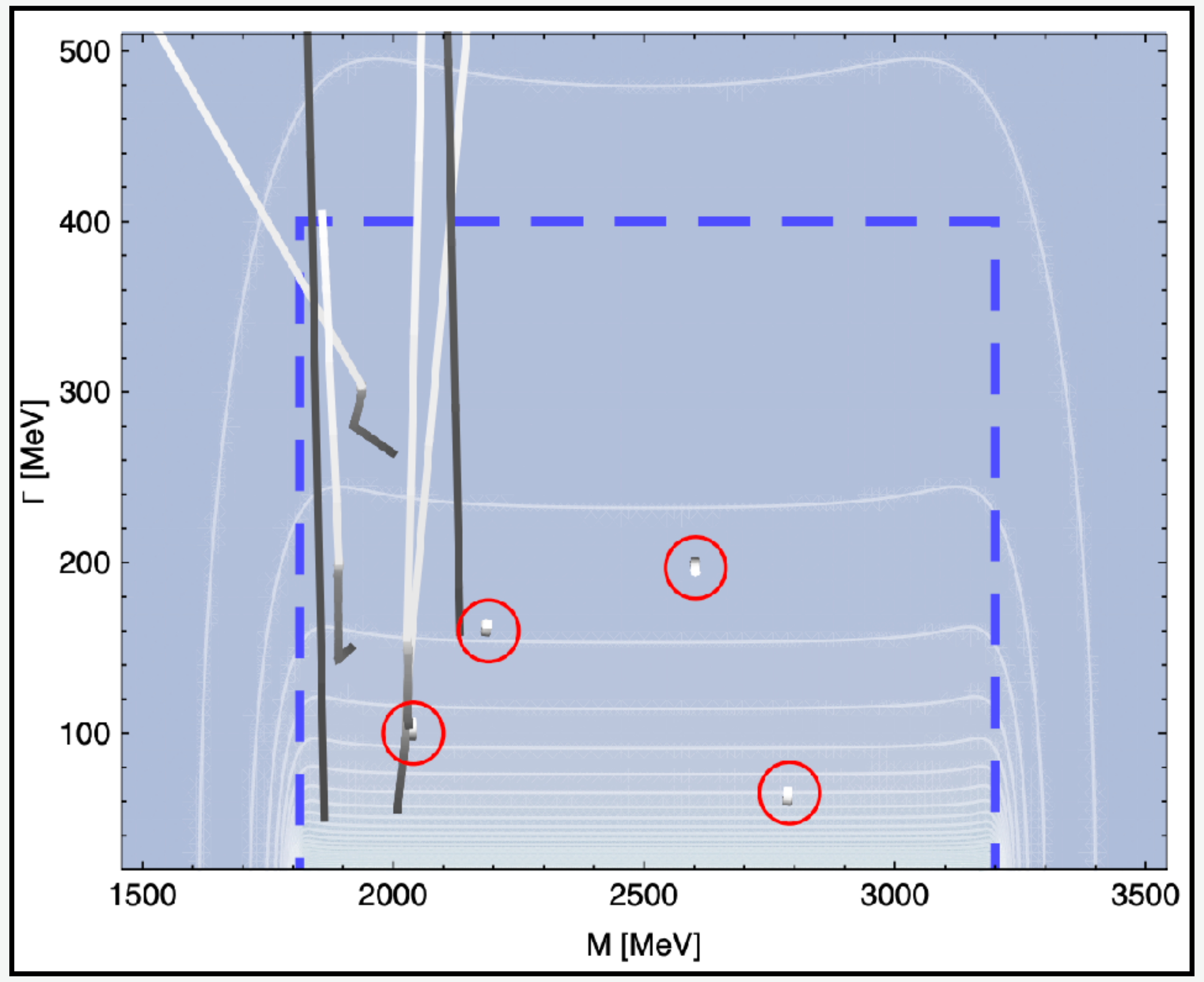
➡ good local minima

➡ background flexibility dependence

M. Williams, J. Instrum. 12, P09034 (2017).

Second derivative penalty





- backward LASSO (second derivative)
  - ➡ picks the $10 \rightarrow 4$ correct resonances
  - ➡ Inactive resonances driven into the complex plane
  - ➡ BIC minimum is less pronounced
- for real data ($K^- p \rightarrow K\Xi$) + data pruning
  - ➡ $21 \rightarrow 10$ resonances

APPLICATION 2

LATTICE QCD — PHENOMENOLOGY

Dimitri Agadjanov
Michael Doring
Maxim Mai
Ulf-G. Meißner
Akaki Rusetsky

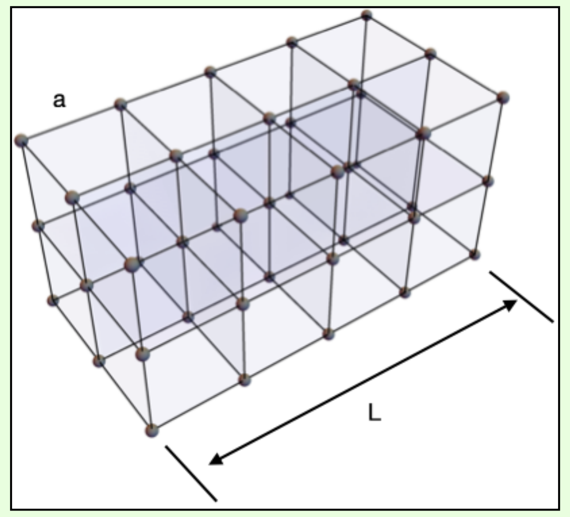
The Optical Potential on the Lattice

JHEP 06 (2016) 043 • e-Print: 1603.07205 [hep-lat]

BACK TO QCD

Lattice Gauge Theory (LQCD)

Wilson, Phys. Rev. D10 (1974) 2445 , …



$$Z[J] = \int [DU] e^{-S_E} \det[M[U]]$$

[+] QCD degrees of freedom

[+/-] unphysical quark masses

[+] non-perturbative access to QCD Green's functions

[-] discretized space-time

[-] Euclidean metric

[-] finite-volume (no S-matrix!)

2-hadron systems

- ρ(770), $f0$(500), K^*(700), K^*(892), . . .

ETMC/GWQCD/HadSpec/CLQCD/…

- Meson-baryon, 2-baryon systems are harder (noise etc..)

BaSC/ETMC/HadSpec/NPLQCD/HALQCD/…

3-hadron systems

- new formalisms

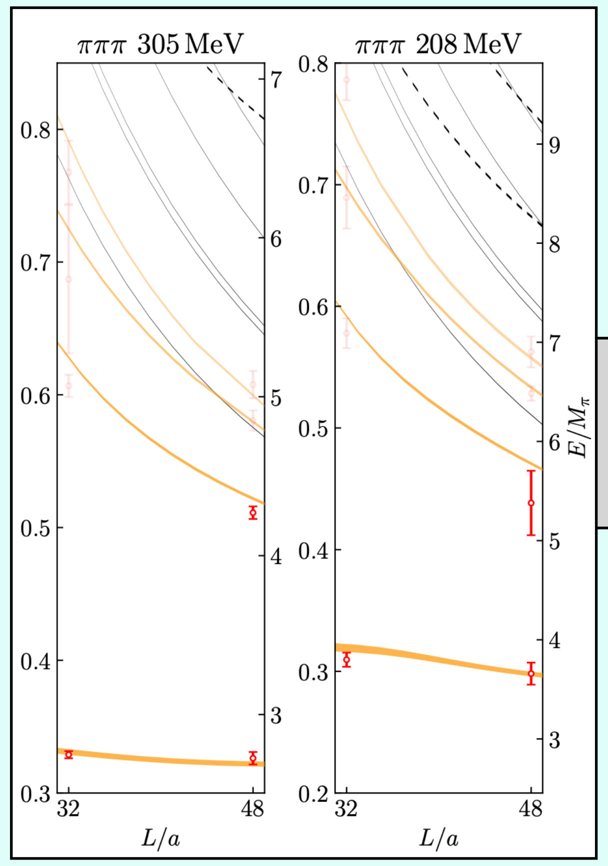
Rusetsky/Döring/Hansen/Davoudi/Sharpe/Guo/MM…

- finite-volume unitarity

MM/Döring Eur.Phys.J.A 53 (2017) 12, 240

- new results of resonant systems

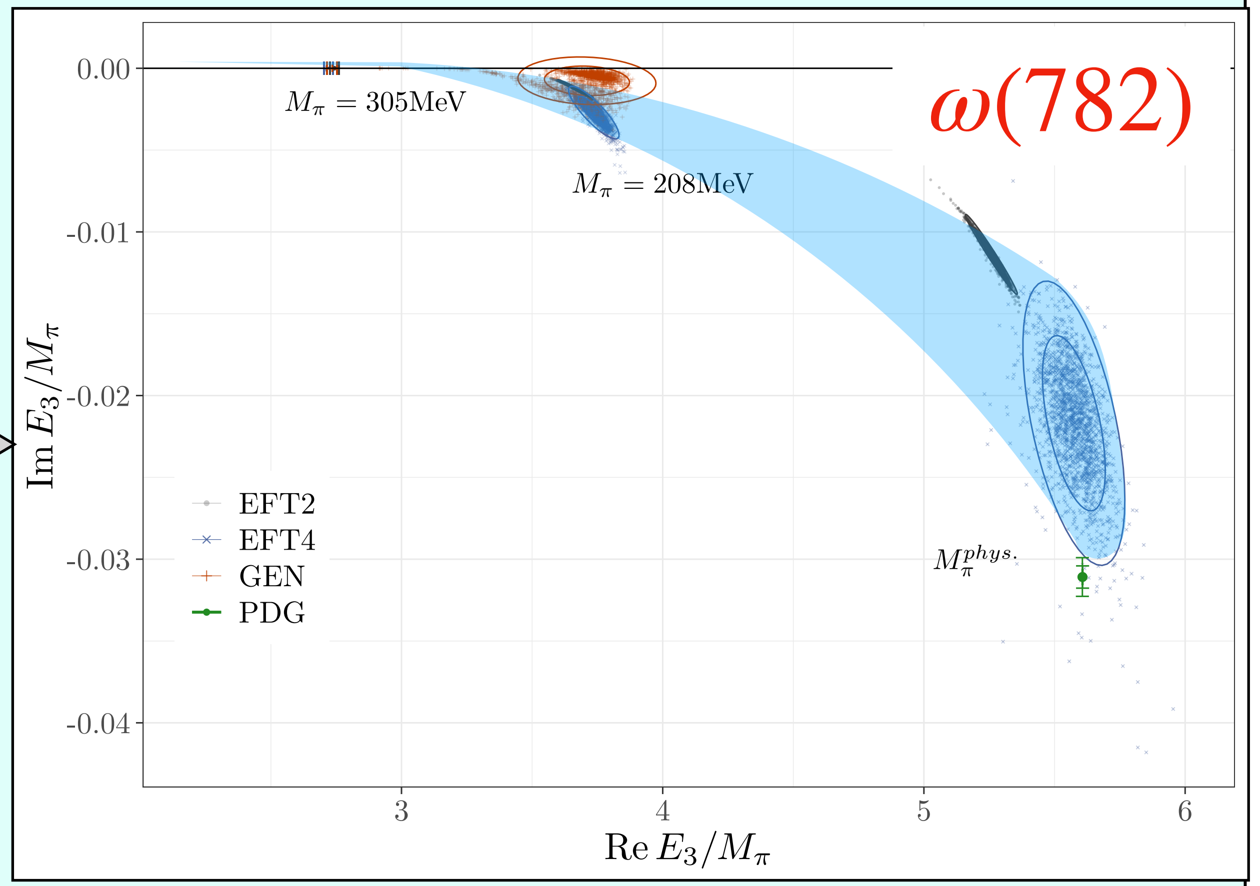
$\pi(1300)$ Phys.Rev.Lett. 136 (2026) 14
$\omega(782)$ Phys.Rev.Lett. 133 (2024) 21



FVU

$$\det\left[2L^3 E_{\mathbf{p}}\left(\tilde{K}^{-1} - \Sigma^L\right) - B - C\right]^{\Lambda} \equiv 0$$

MM/Döring
Eur.Phys.J.A 53 (2017) 12, 240



hep-lat/9807028 [hep-lat] Rev.Mod.Phys. 90 (2018)
Rept.Prog.Phys. 86 (2023)

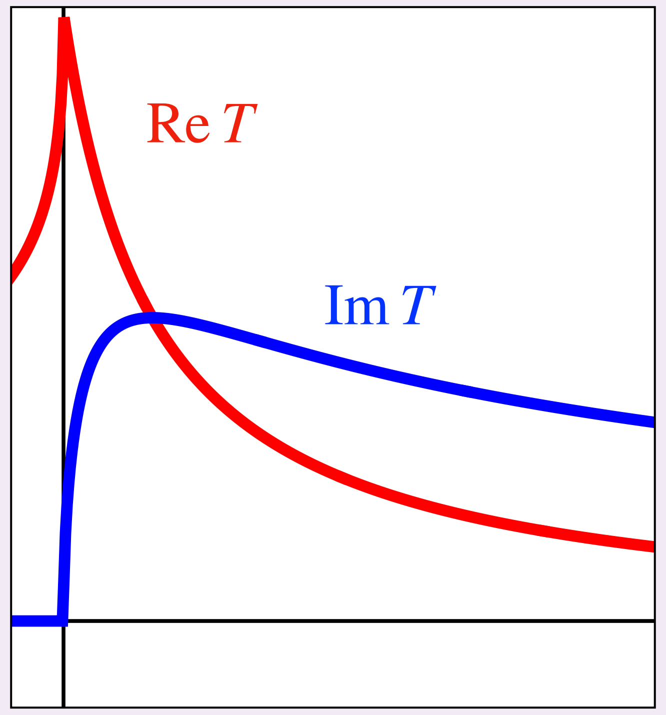
Multi-particle systems on the lattice and chiral extrapolations: a brief review
MM, Michael Döring Akaki Rusetsky Eur.Phys.J.ST 230 (2021) 6, 1623-1643 • e-Print: 2103.00577 [hep-lat]

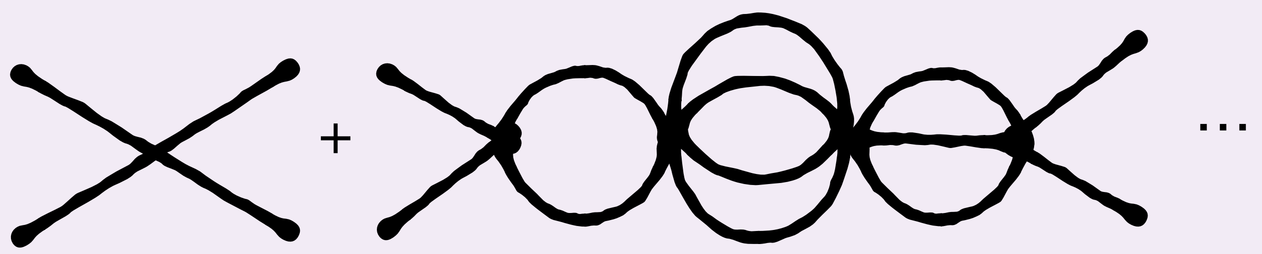
QUANTIZATION CONDITIONS

Continuum QFT

- Asymptotic states at $t \to \pm\infty$
- underlying quantity: $(\sigma \sim |S|^2, \dots)$

$$S = 1 + iT \in \mathbb{C}$$





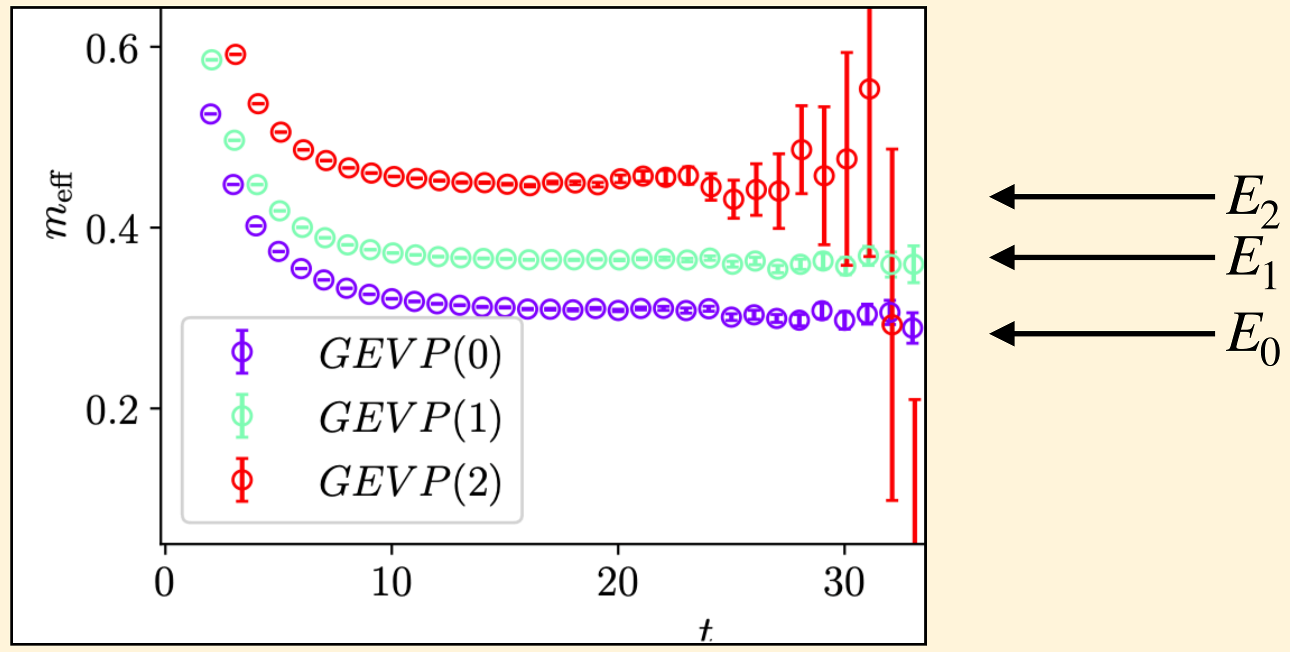
$\mathrm{disc}\, T \sim |T|^2 \quad \sqrt{s} < 3m$

unitarity condition (on-shell-ness)

$$T^{-1} = K^{-1} - \int_l \frac{1}{2E_l} \frac{1}{(s - 4E_l^2 + i\epsilon)} = p \cot\delta - \left(\int \dots - Re \int \dots\right)$$

Finite-volume setup

- Input: energy eigenvalues $\{E_0, \dots\} \in \mathbb{R}$



- 2-body case

$$p \cot\delta(E_i) = Z_{00}(E_i) + \mathcal{O}(e^{-ML})$$

M. Lüscher, Nucl. Phys. B 354, 531 (1991)

- 3-body case

$$\det\left[2L^3 E_{\mathbf{p}}\left(\tilde{K}^{-1} - \Sigma^L\right) - B - C\right]^{\Lambda} \equiv 0$$

MM/Döring Eur.Phys.J.A 53 (2017) 12, 240

- n-body case?

Multi-particle systems on the lattice and chiral extrapolations: a brief review
MM, Michael Döring Akaki Rusetsky Eur.Phys.J.ST 230 (2021) 6, 1623-1643 • e-Print: 2103.00577 [hep-lat]

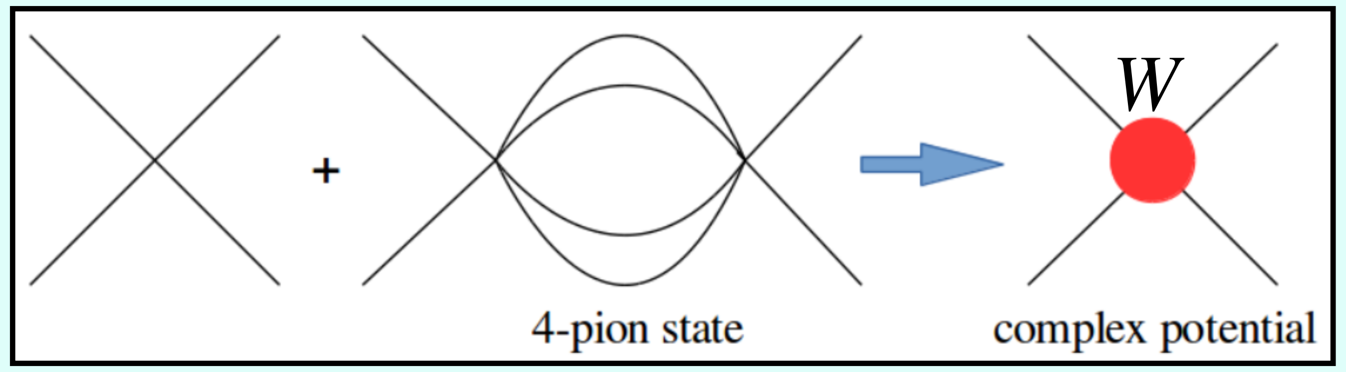
BULK PROPERTIES OF FV SPECTRA

Agadjanov/MM/Doring *JHEP* 06 (2016)

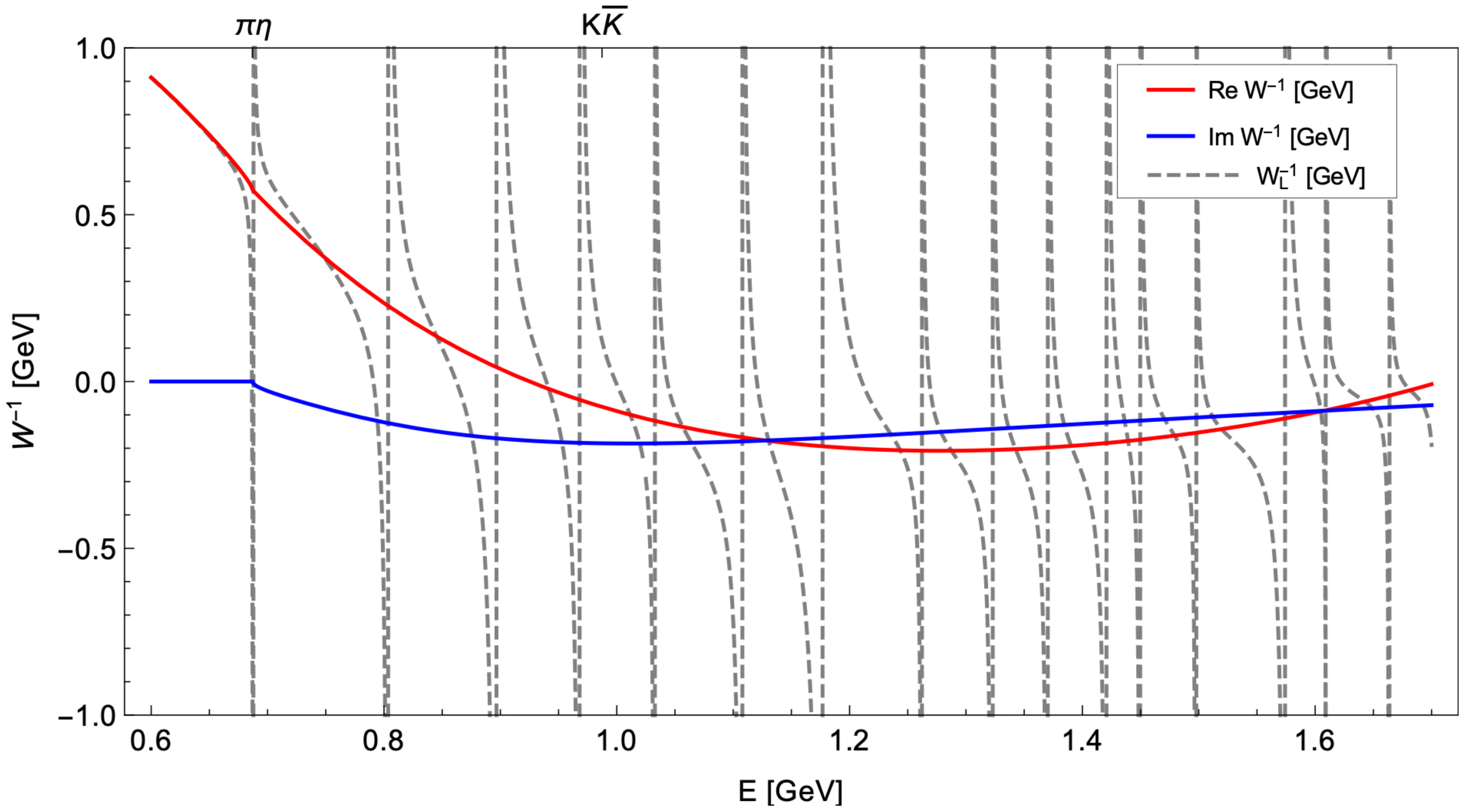
- It is not always necessary to explicitly parameterize complicated intermediate states

  “uninteresting” dynamics in a optical potential $W \in \mathbb{C}$

- How to reconstruct true OP (complex) from finite-volume OP (real)?

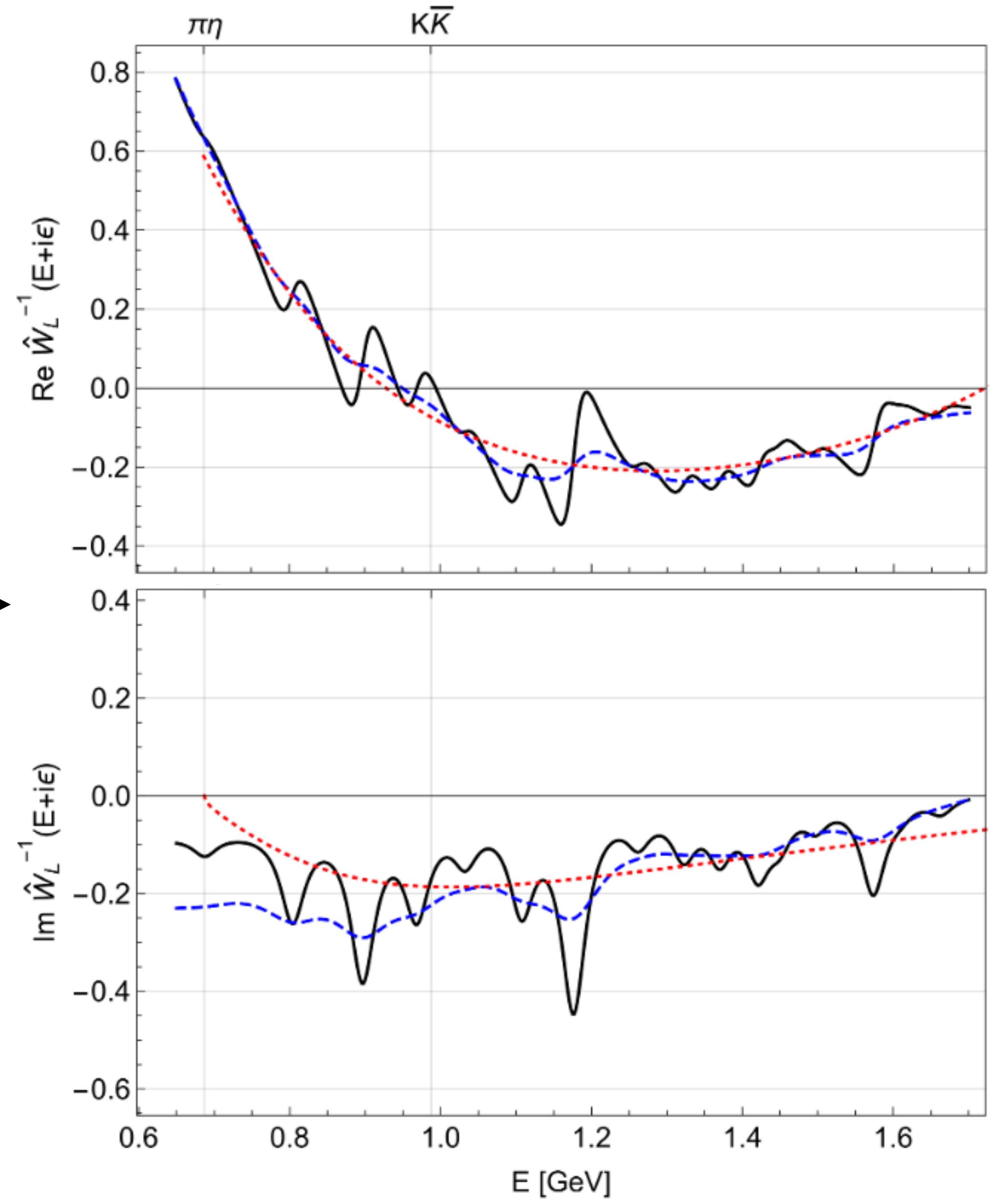


$$\hat{W}_L^{-1}(E) = \sum_i \frac{Z_i}{E - Y_i} + D_0 + D_1 E +$$



$$W^{-1}(E) = \lim_{\epsilon \to 0} \lim_{L \to \infty} W_L^{-1}(E + i\epsilon)$$

double limit



BULK PROPERTIES OF FV SPECTRA

Agadjanov/MM/Doring *JHEP* 06 (2016)

1. **Fit general form of the OP**

$$\hat{W}_L^{-1}(E) = \sum_i \frac{Z_i}{E - Y_i} + D_0 + D_1 E +$$

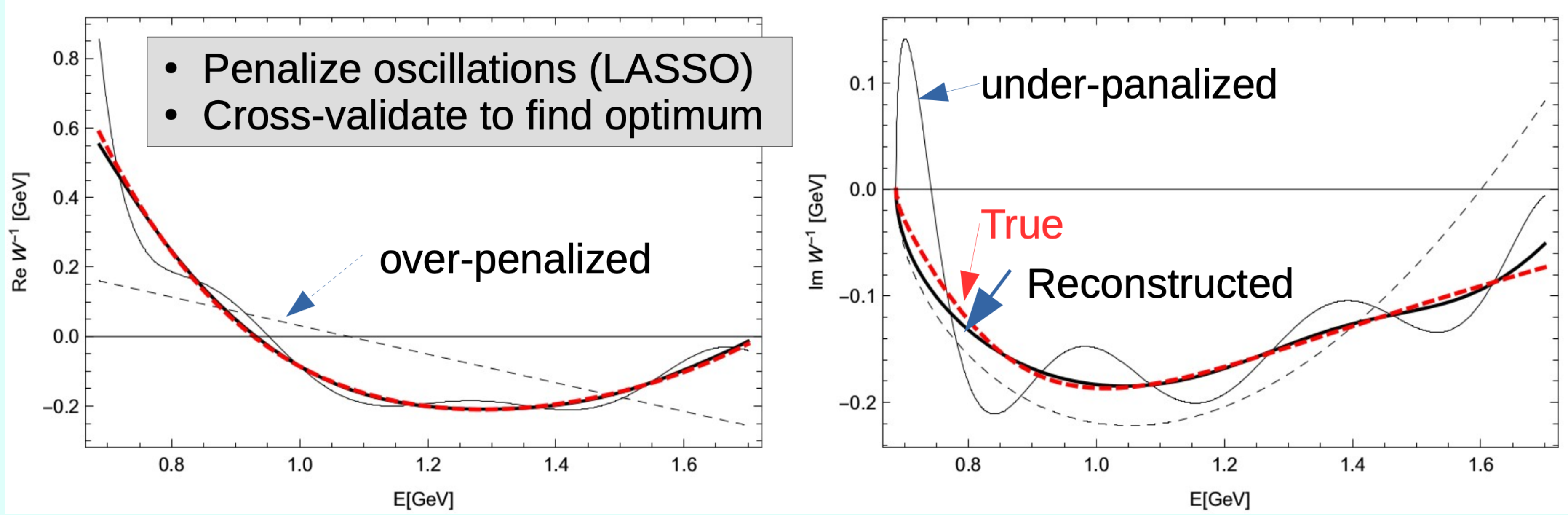
2. **Extrapolate to complex plane** $W_L(E + i\epsilon)$

3. **Smoothing oscillations**

… = infinite-volume limit

LASSO + cross validation

- fit at finite a ϵ
- validate at a different ϵ'



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Agadjanov/MM/Doring *JHEP* 06 (2016)

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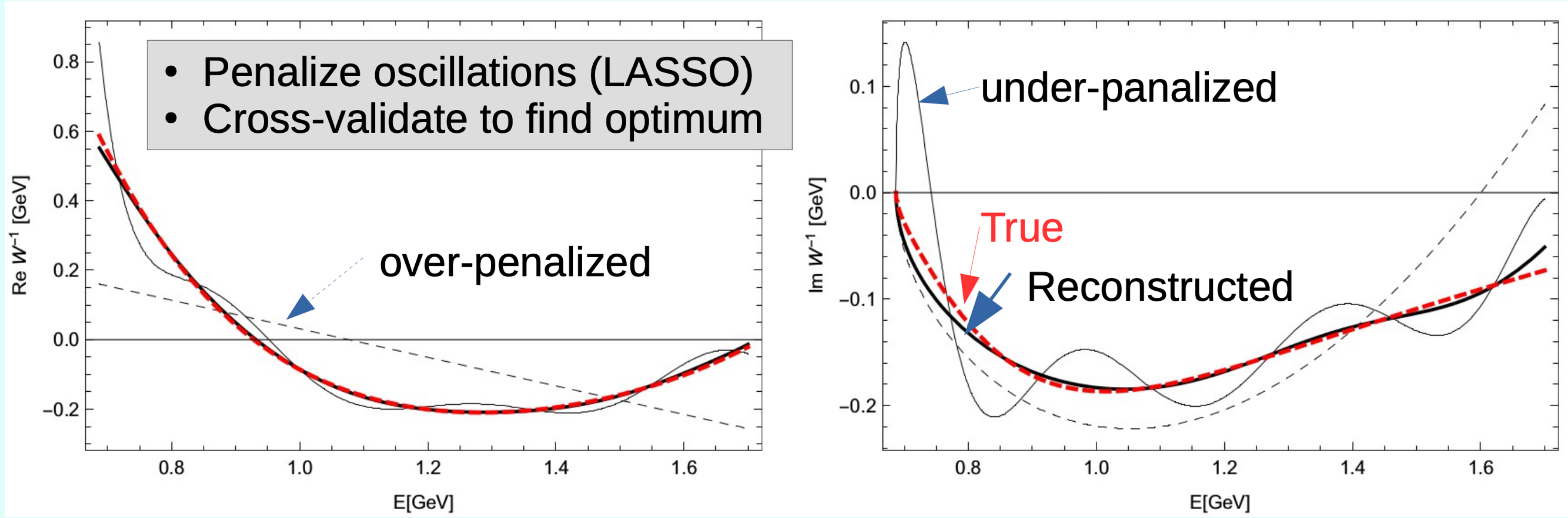
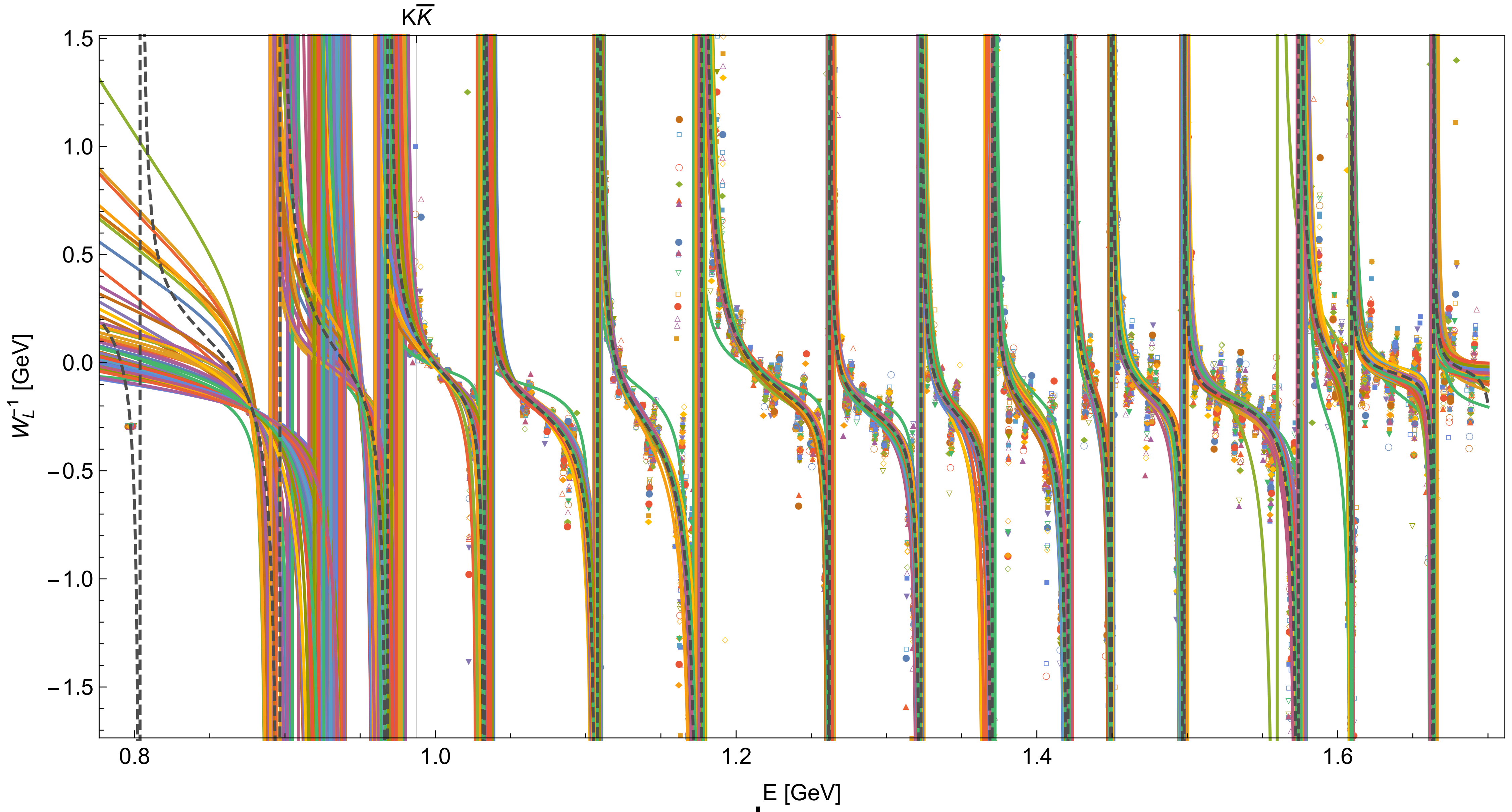
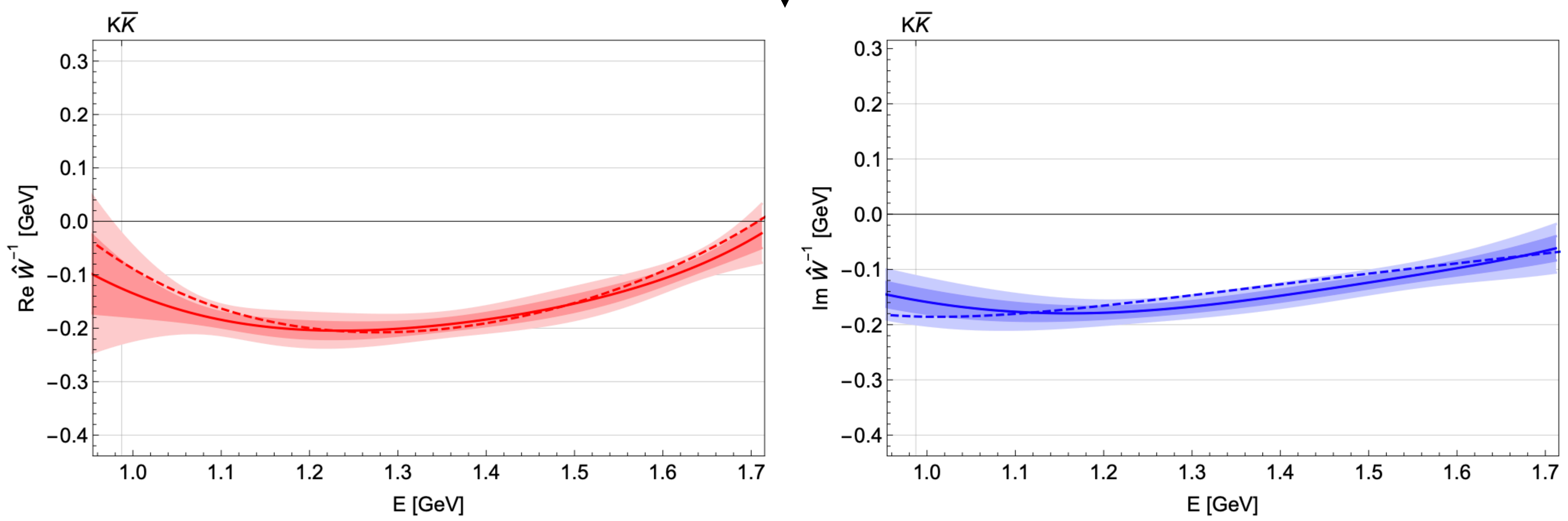






APPLICATION 3

SIMULATION-BASED INFERENCE

Daniel Sadasivan
Isaac Cordero
Andrew Graham
Cecilia Marsh
Daniel Kupcho
Melana Mourad
Maxim Mai

Deep Neural Network Driven Simulation Based Inference Method for Pole Position Estimation under Model Misspecification

e-Print: 2507.18824 [hep-ph]

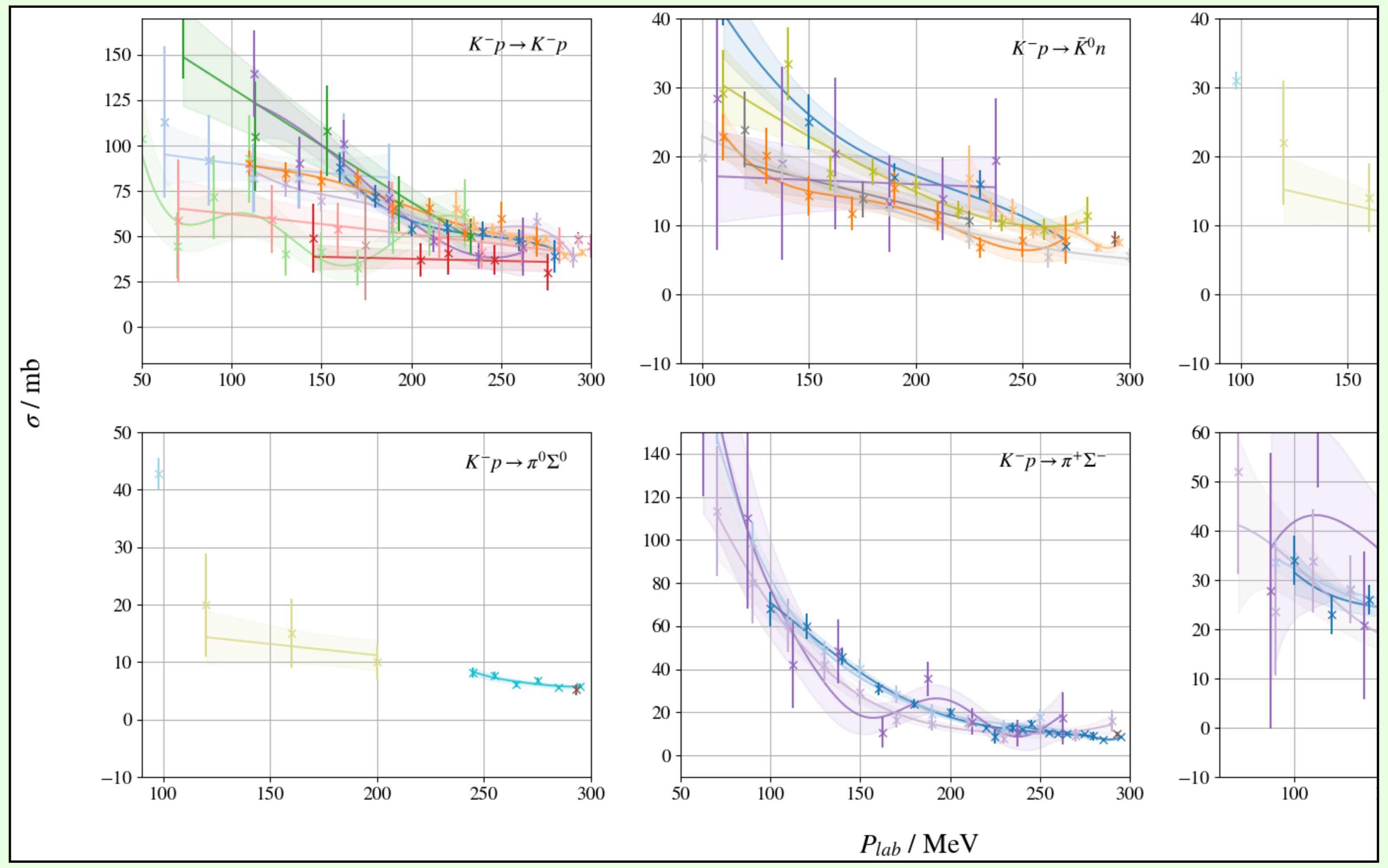
FROM DATA TO POLES

Hadron physics relevant experimental data

- often old (1950's+)
- sometimes low/wrong statistics
- barely any correlations
- unknown systematics/bias

G. D'Agostini Nucl.Instrum.Meth.A 346 (1994), 306-311, …

Ball et al. JHEP05(2010)075



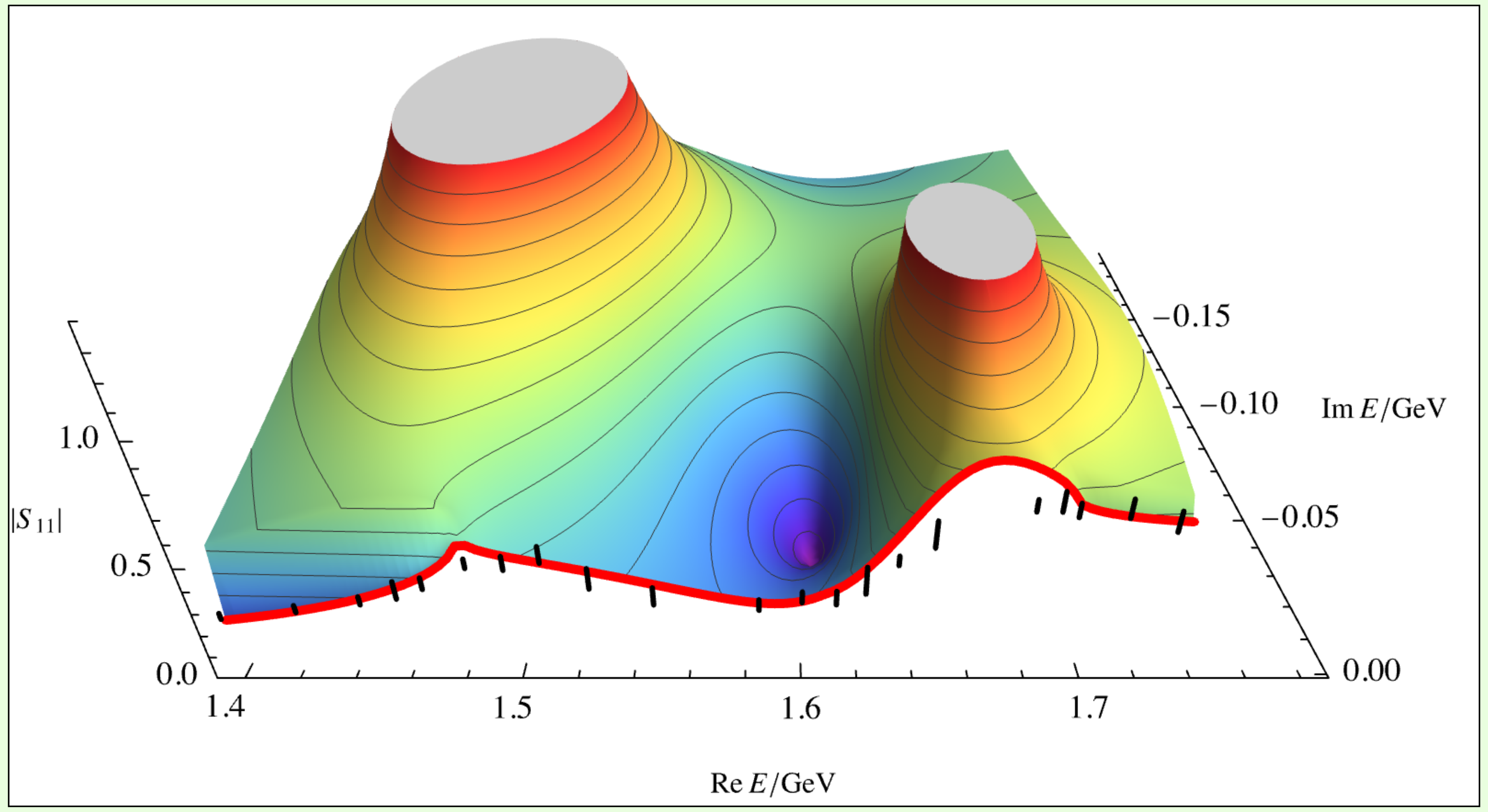
Review: MM *Eur.Phys.J.ST* 230 (2021) 6, 1593-1607

Resonance parameter

- full solution from QCD does not exist
- model parameters $T(x\,|\,\vec{a}) \in \mathbb{C}$ from

$$\chi^2 = \sum_i \left(\frac{|T(x_i, \vec{a})| - y_i}{\Delta y_i} \right)^2$$

- Analytic continuation of the amplitude $x \in \mathbb{C}$



MODEL MISSPECIFICATION

χ^2 statistic

*most probable parameters a given the measured data yi under the assumption that the **data are normally distributed** about the function for some values of a, and the **prior uniform probability distribution** of fit parameters.*

Model misspecification

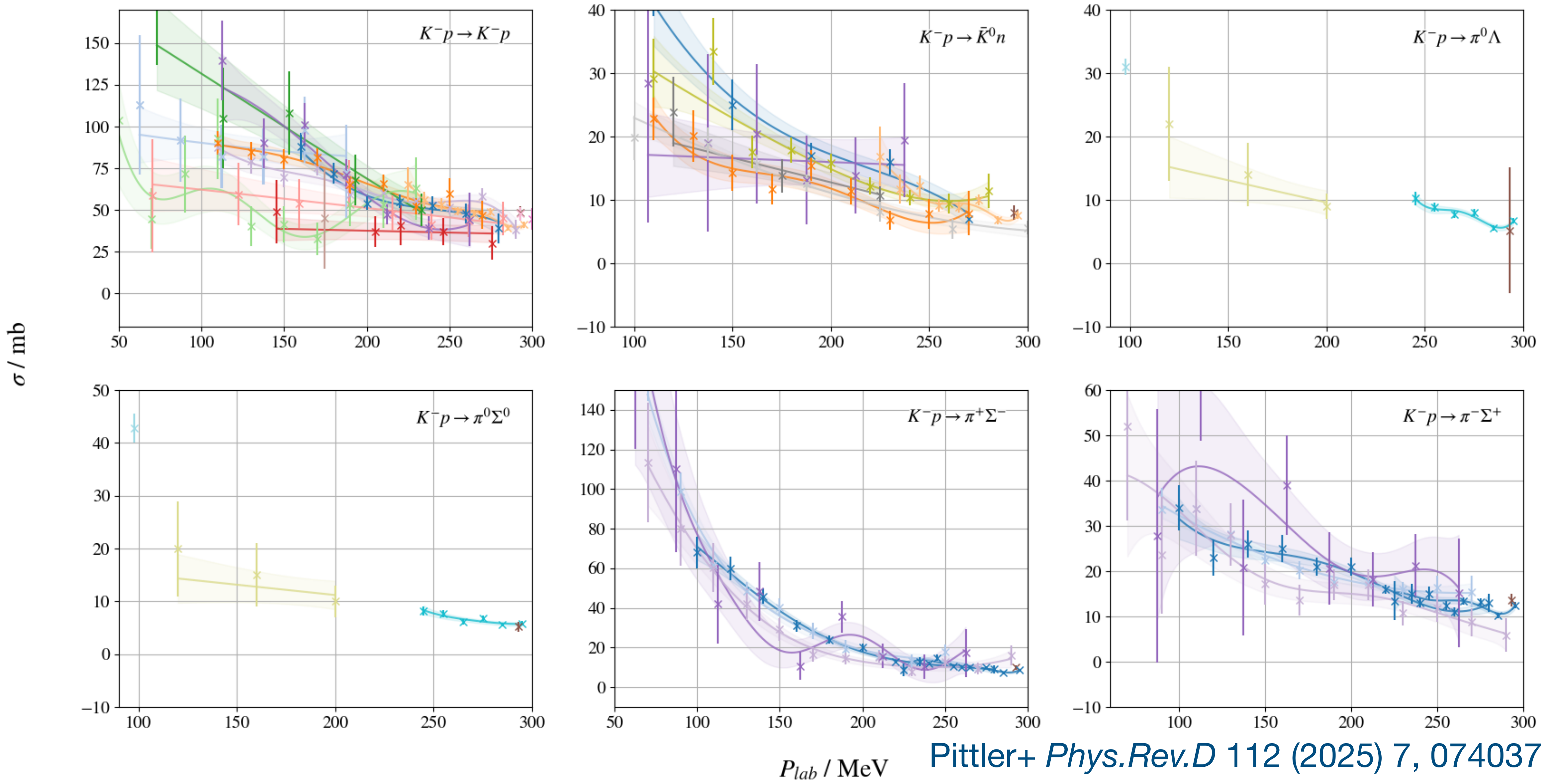
no values of a exist for which the data are normally distributed about the function

- outliers
- non-gaussian (systematic) uncertainties
- …

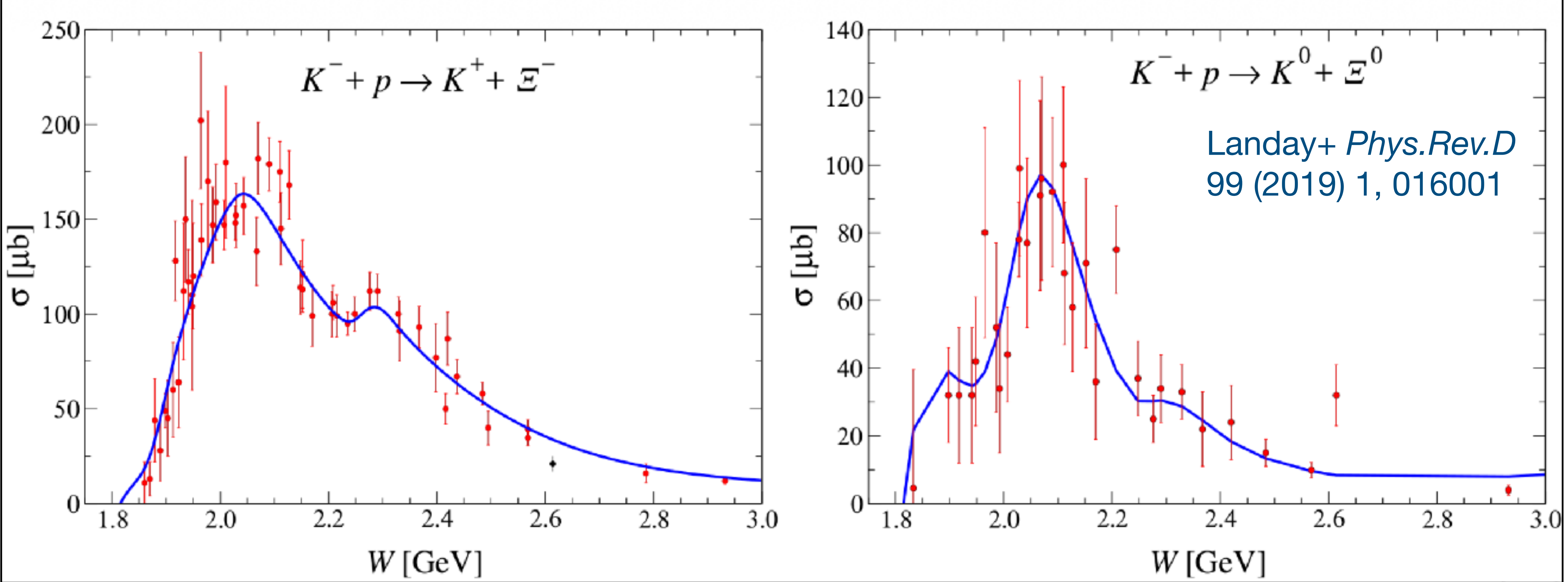
Solutions:

- ➡ **Data pruning**
- ➡ **LASSO**
- ➡ **…**
- ➡ **Simulation-Based Inference**

Tavare+ Genetics 145, 505–518 (1997)
Astro Automata, "A tutorial on simulation-based inference," (2020)
Johann Brehmer, Cranmer 2010.06439 [hep-ph]
…

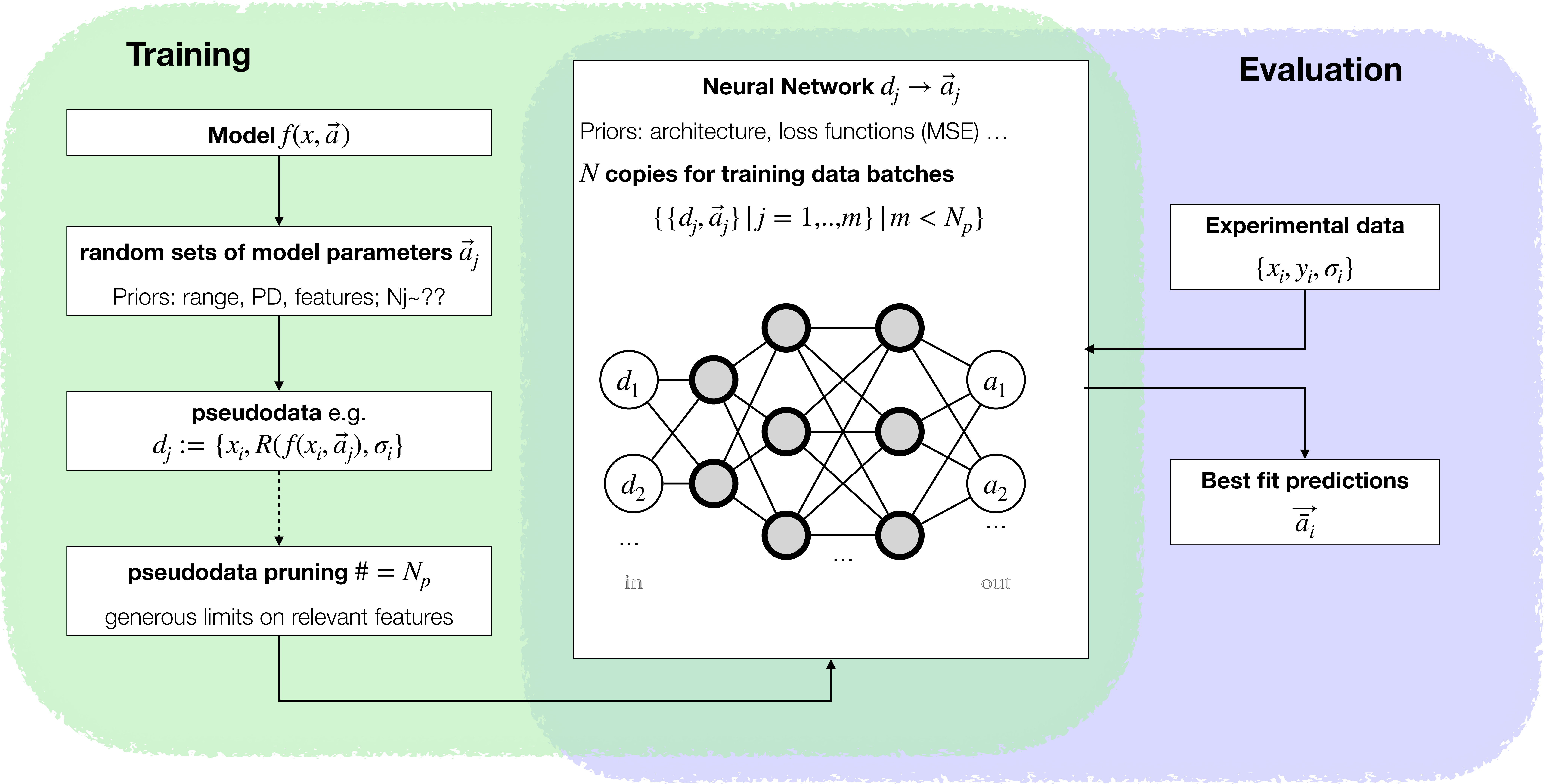


Pittler+ *Phys.Rev.D* 112 (2025) 7, 074037



Landay+ *Phys.Rev.D* 99 (2019) 1, 016001

SIMULATION-BASED INFERENCE



TOY EXAMPLES

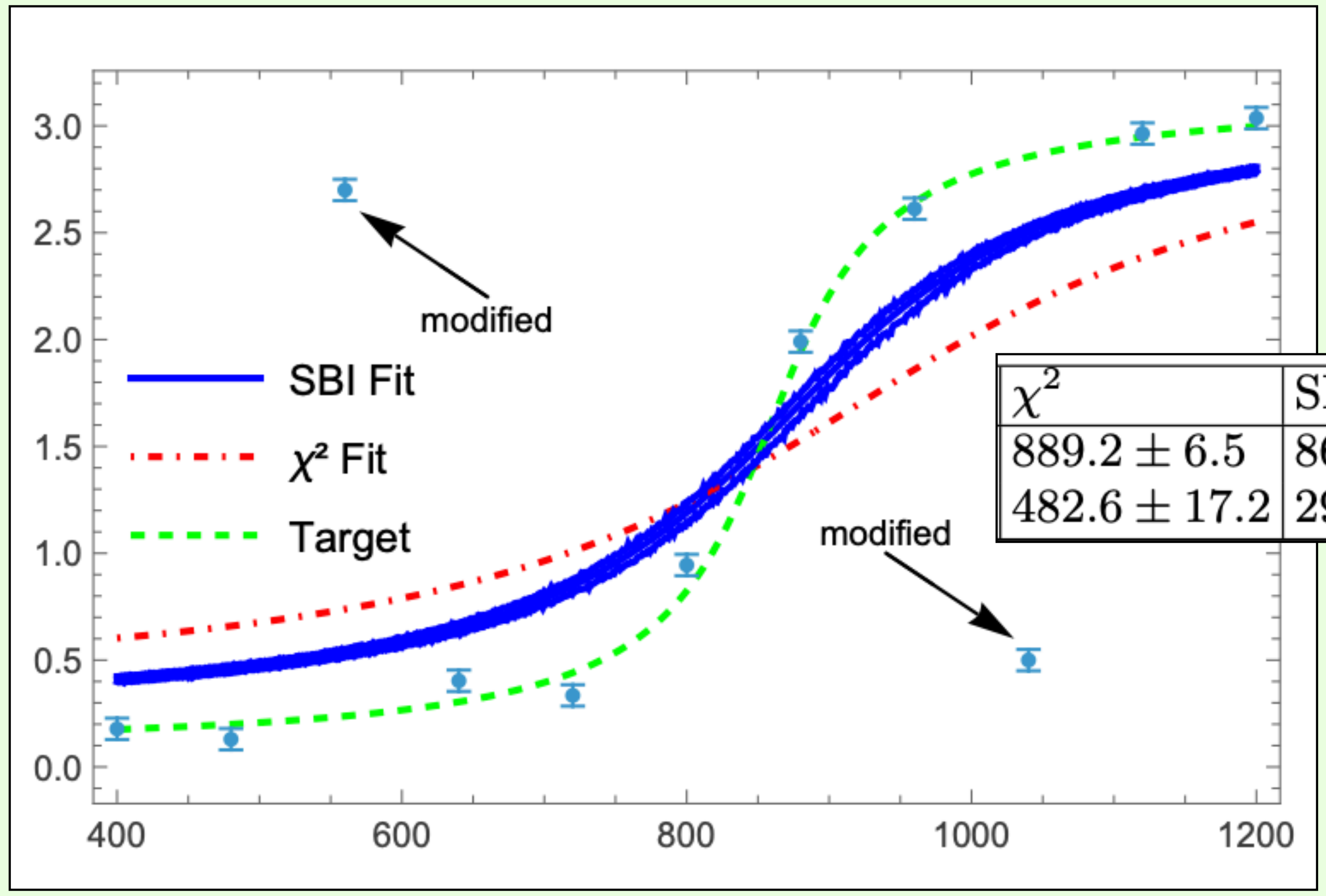
Toy example 1

- target function

$$T(E) = \frac{\sqrt{k}}{(E^2 - M^2) - iM\Gamma}$$

Modified	Generating
M [MeV]	857.0
Γ [MeV]	119.0

- add visible outliers



χ^2	SBI
889.2 ± 6.5	861.3 ± 5.0
482.6 ± 17.2	293.5 ± 6.5

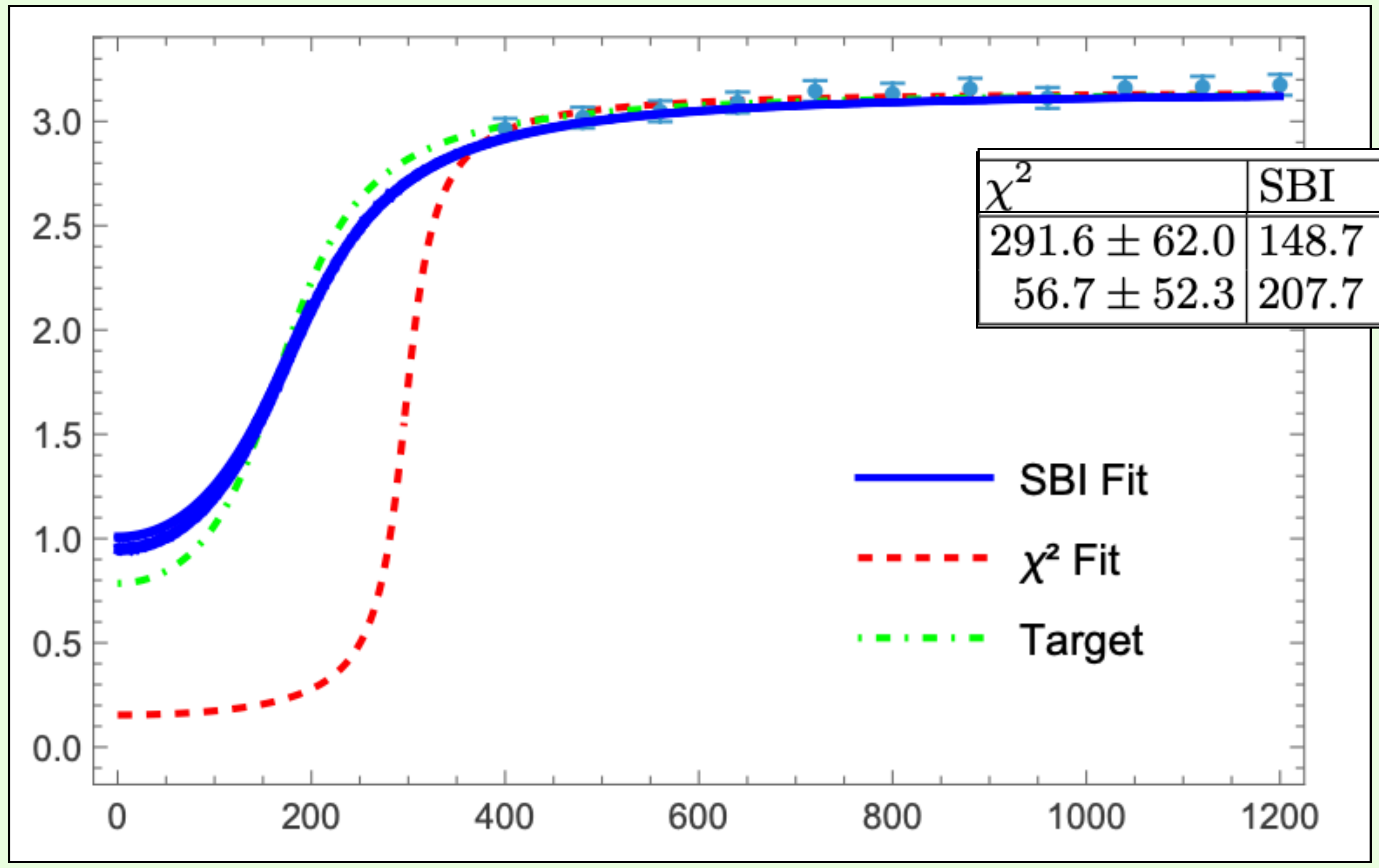
Toy example 2

- target function

$$T(E) = \frac{\sqrt{k}}{(E^2 - M^2) - iM\Gamma}$$

Non-gaussian	
M [MeV]	150.0
Γ [MeV]	150.0

- data outside the resonance region
- non-Gaussian noise



χ^2	SBI
291.6 ± 62.0	148.7 ± 1.2
56.7 ± 52.3	207.7 ± 2.8

$\pi\pi$ SCATTERING

Model

- generic K-matrix form

$$T(E) = \tilde{v}(k_{\rm cm})\frac{1}{K_n^{-1}(E) - \Sigma(E)}\tilde{v}(k_{\rm cm})\,,$$

$$K_n^{-1}(E) = M_\pi^2 \sum_{i=0}^{n-1} a_i \left(\frac{E^2}{M_\pi^2}\right)^i\,,$$

$$\Sigma(E) = \int_0^\infty \frac{dk\,k^2}{(2\pi)^3}\frac{1}{2E_k}\left(\frac{E^2}{4E_k^2}\right)^n \frac{\tilde{v}^2(k)}{\sigma - 4E_k^2 + i\epsilon}\,,$$

- flexibility: 2, 3 subtractions

SBI vs χ^2

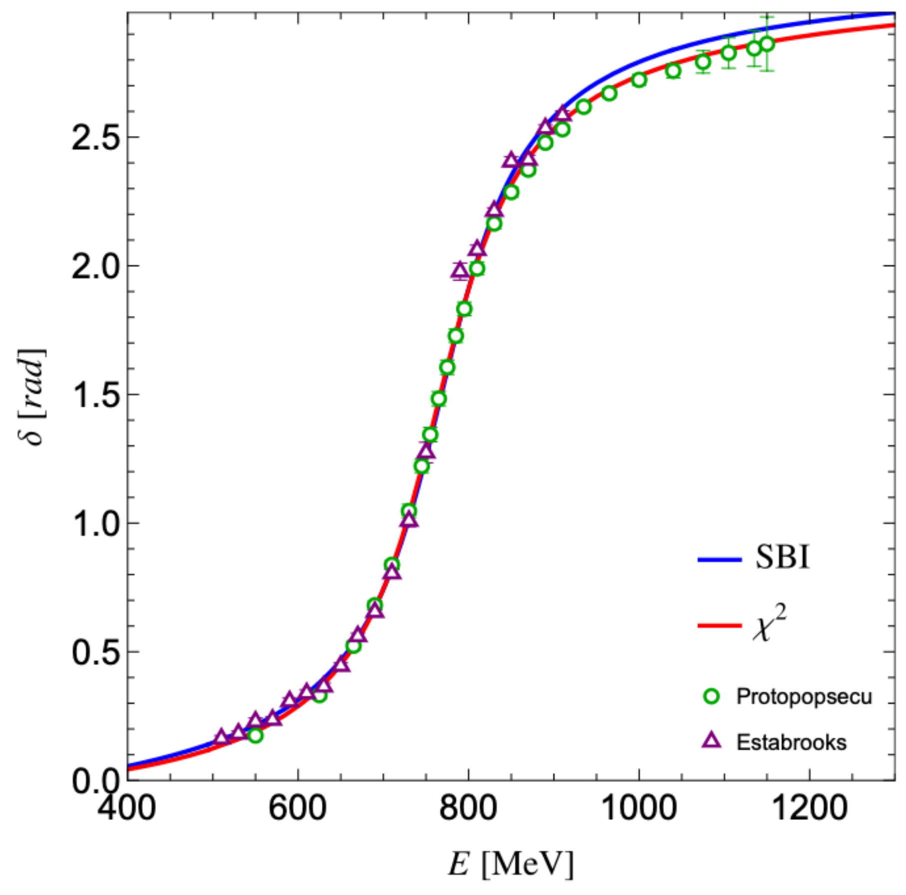
SBI

Data	n	$a_0 \cdot 10^3$	$a_1 \cdot 10^3$	$a_2 \cdot 10^3$	E^*[MeV]
All	3	-187	-3.17	$+0.42$	$772.4(2.3) - i\,75.4(0.4)$

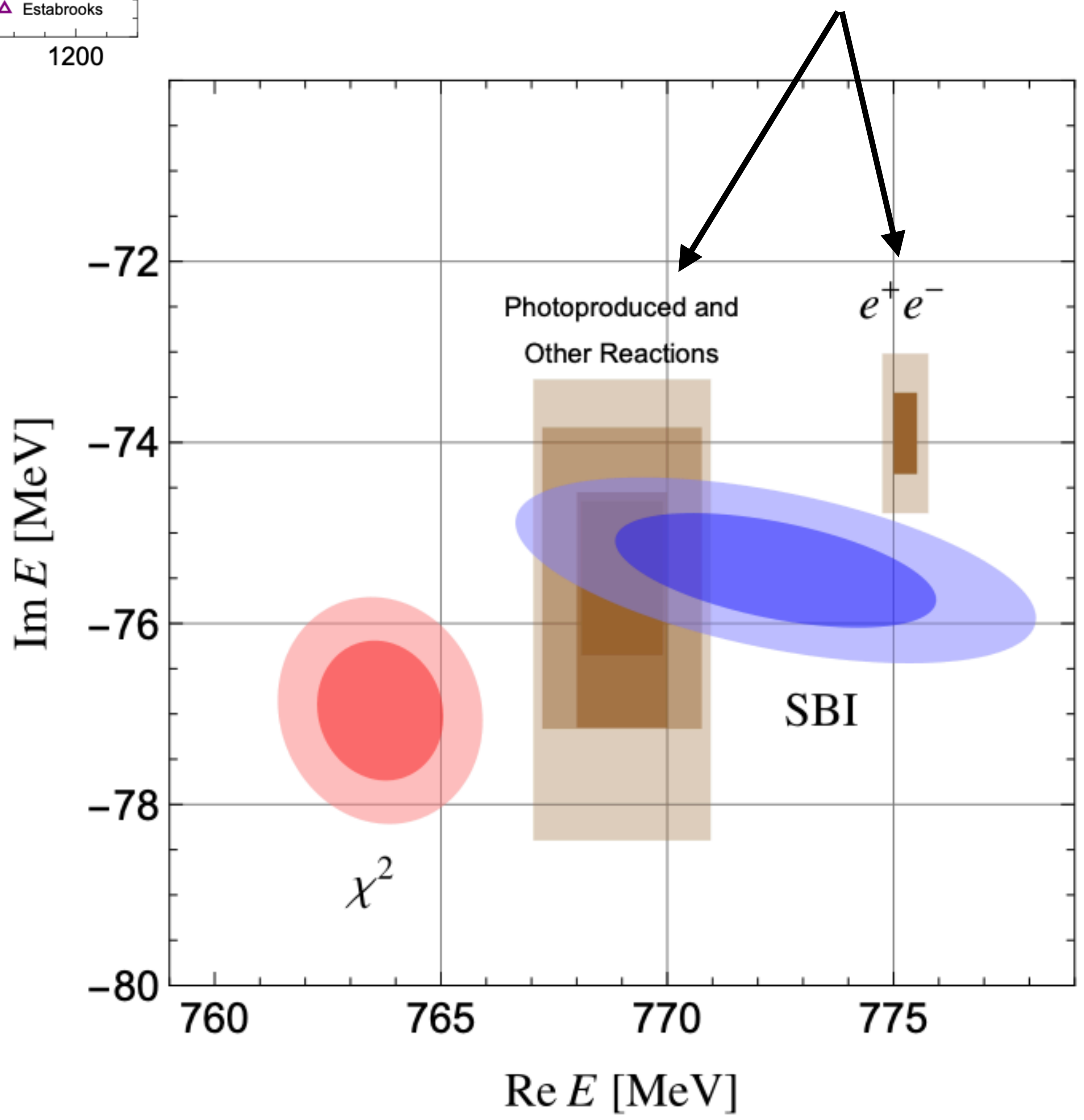
χ^2

$a_0 \cdot 10^3$	$a_1 \cdot 10^3$	$a_2 \cdot 10^3$	$\chi^2_{\rm dof}$	E^*[MeV]
-290	$+4.10$	$+0.29$	3.1	$763.7(0.9) - i\,76.9(0.6)$

- bias through outliers in χ^2 method
- **SBI pole positions overlapping w. higher-data-PDG-result**



reference values from other reactions



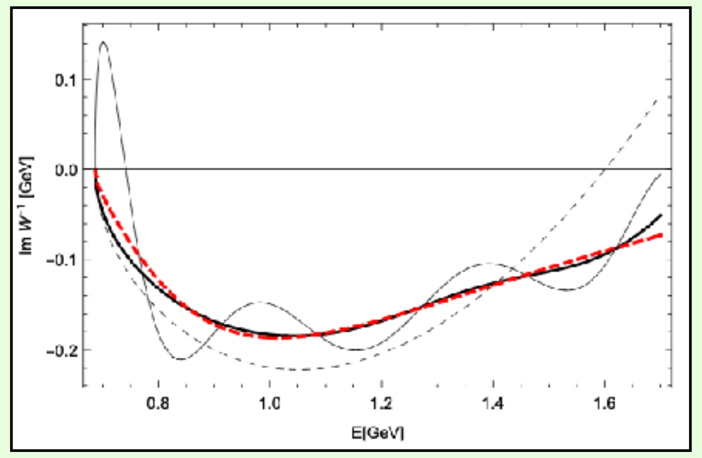
SUMMARY

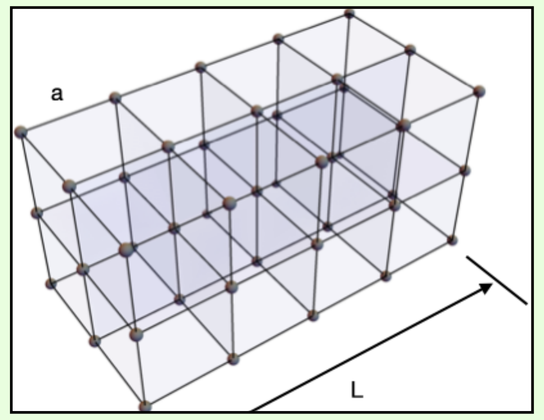
Experiment: Data abundance

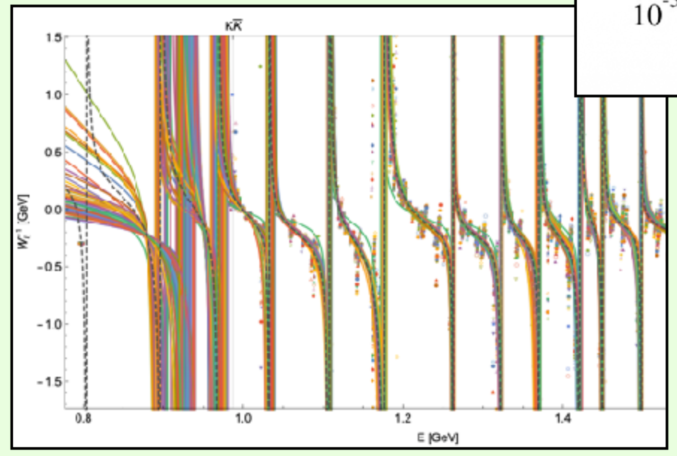
- many new experiments
- new technology

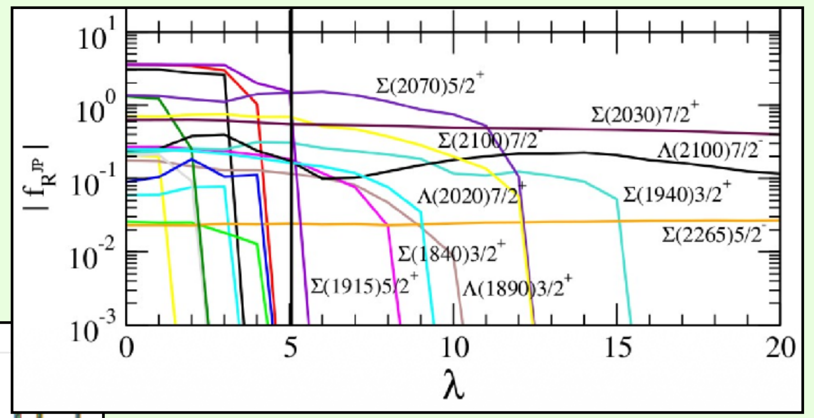
Theory: No surprises in the Standard Model

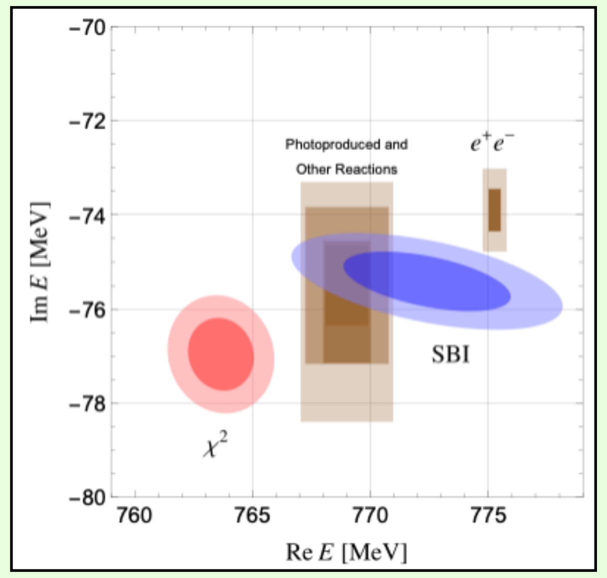
- consistency/precision tests become more important
- new techniques (EFTs, Lattice, Machine learning)











Future directions and open questions

✴ Universality:

convolution networks, spaces, loss functions, …

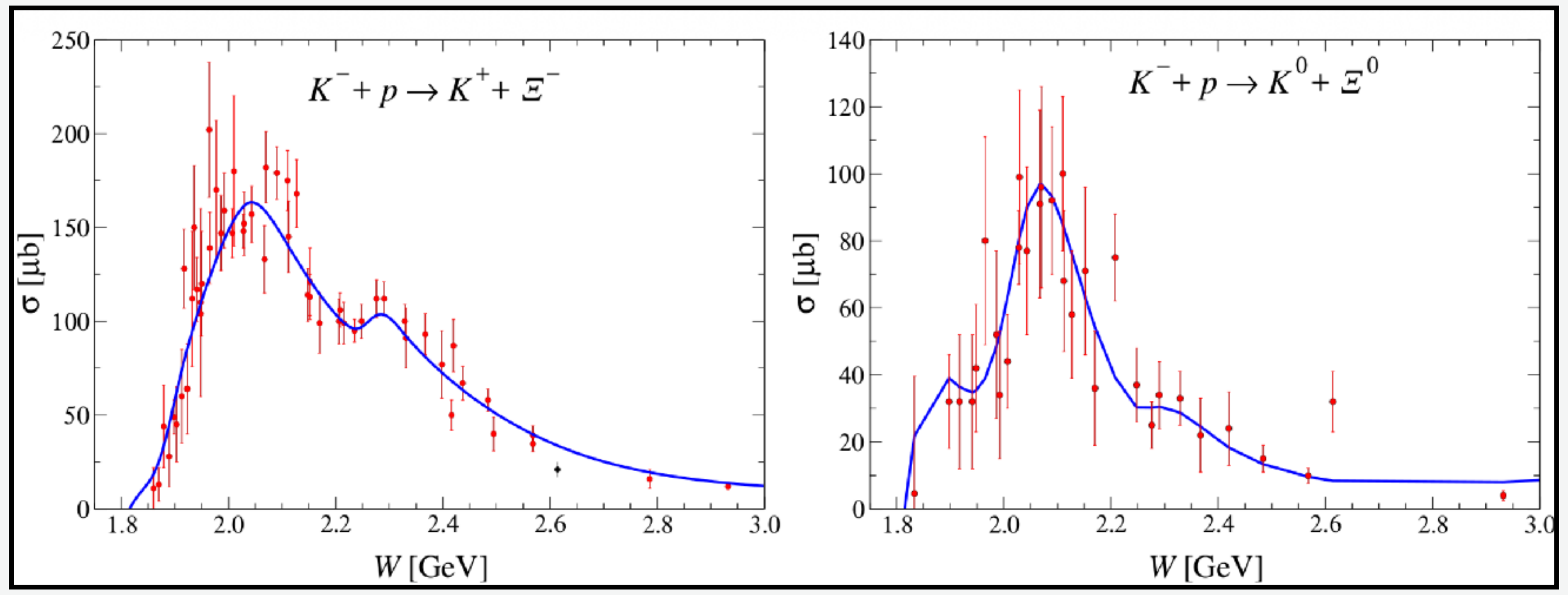
✴ Skepticism: How to filter hype from necessity?

“never trust a statistics you have not faked yourself” (Germany Saying)

✴ Good practice:

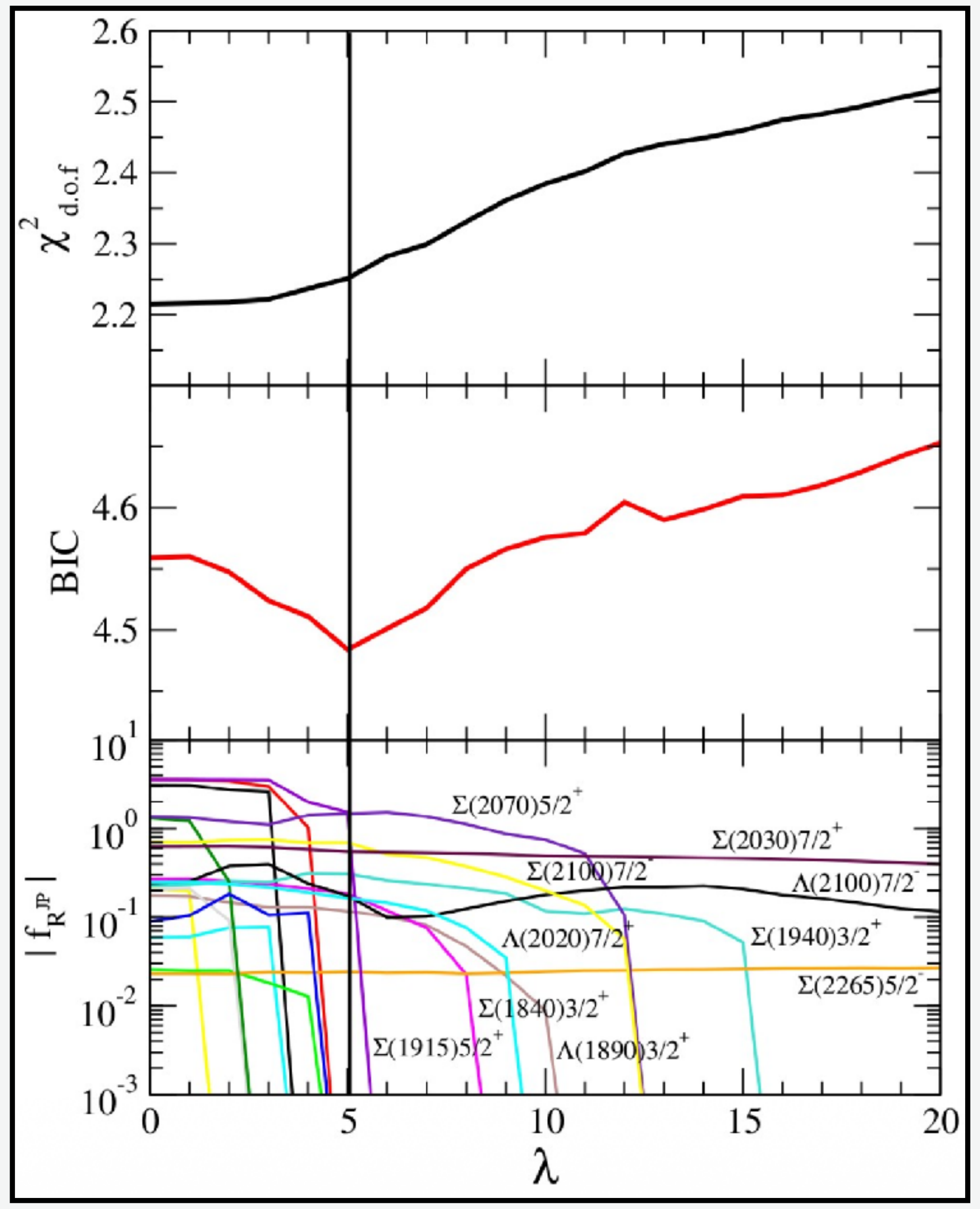
Toy models, Formal proofs?

REAL DATA $K^- p \to K\Xi$



- Data pruning for outliers using smoothness as criterion (self-consistent 3σ criterion) Navarro Perez,+ Phys. Rev. C 88, 064002 (2013);
- d'Agostini bias potentially an issue if rescaling is included

Pjerrou:1962pc,Carmony:1964zza,Berge:1966zz,Haque:1966mda,London:1966zz,Tripp e:1967wat,Trower:1968zz,Merrill:1968zz,Burgun:1969ee,Dauber:1969hg



- LASSO
  - Backward selection (automatic shutoff LASSO)
  - All 21 resonance candidates from PDG
- Masses and widths fixed to PDG values

- Only x fitted
- 10 out of 21 resonances identified

Solving eq. (2.8), one finds an explicit expression of the on-shell T-matrix in terms of the optical potential $W(E)$:

$$T_{K\bar{K}\to K\bar{K}}(E) = \frac{1}{W^{-1}(E) - ip_{K\bar{K}}}\,. \tag{2.10}$$

Note that the form of eq. (2.10) with a complex optical potential W is a completely general expression for the case of the multi-channel and -particle scattering problem.

It is often useful to introduce the so-called M-matrix $M = V^{-1}$, i.e.,

$$M = \frac{1}{\Delta}\begin{pmatrix} V_{\pi\eta\to\pi\eta} & -V_{K\bar{K}\to\pi\eta} \\ -V_{K\bar{K}\to\pi\eta} & V_{K\bar{K}\to K\bar{K}} \end{pmatrix}, \qquad \Delta = V_{K\bar{K}\to K\bar{K}}V_{\pi\eta\to\pi\eta} - V^2_{K\bar{K}\to\pi\eta}\,. \tag{2.11}$$

In terms of this quantity, the above formula can be rewritten in the following form:

$$W^{-1}(E) = M_{K\bar{K}\to K\bar{K}} - \frac{M^2_{K\bar{K}\to\pi\eta}}{M_{\pi\eta\to\pi\eta} - ip_{\pi\eta}}\,. \tag{2.12}$$

$$W_L^{-1}(E) := \frac{2}{\sqrt{\pi}L}\,Z_{00}(1;q^2_{K\bar{K}}) = M_{K\bar{K}\to K\bar{K}} - \frac{M^2_{K\bar{K}\to\pi\eta}}{M_{\pi\eta\to\pi\eta} - \frac{2}{\sqrt{\pi}L}\,Z_{00}(1;q^2_{\pi\eta})}\,. \tag{2.15}$$