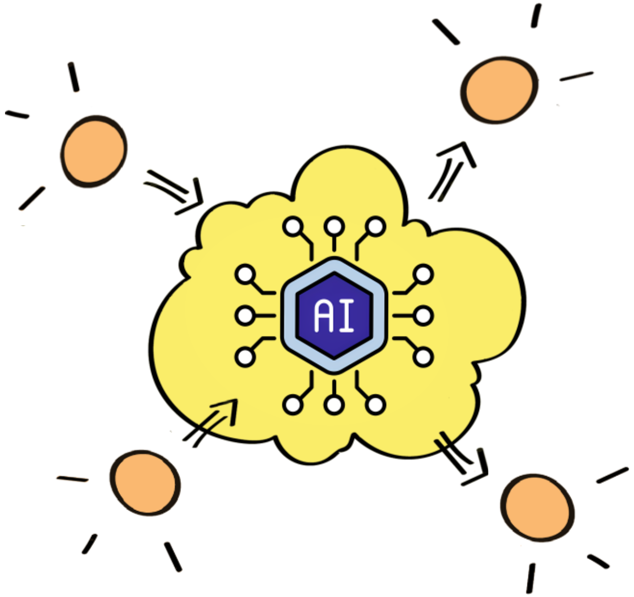
Reconstructing scattering amplitudes with physics-informed generative models

Glòria Montaña
University of Barcelona & ICCUB

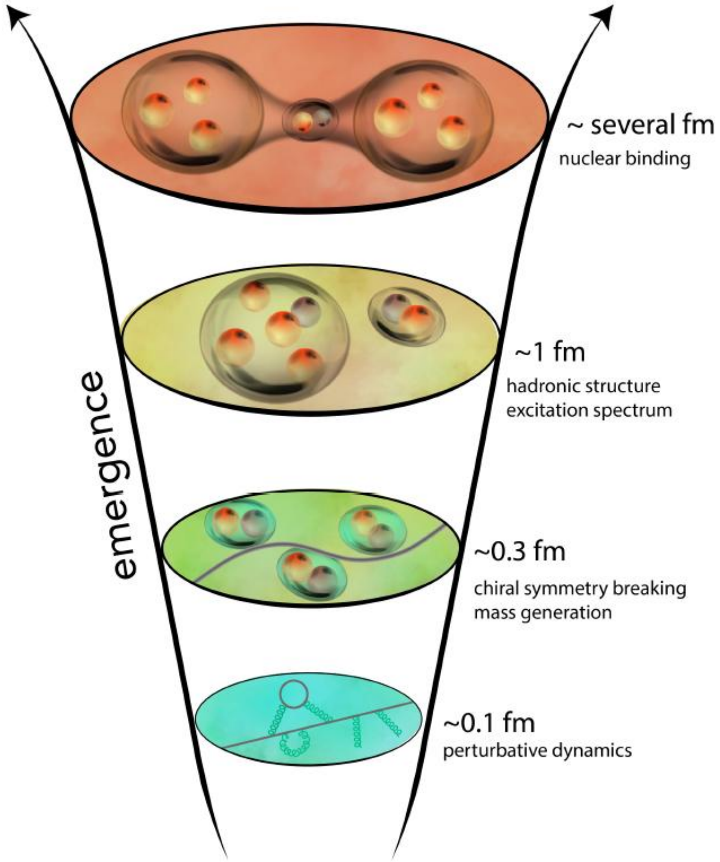
In collaboration with J. Xu, Y. Li,
A. Pilloni, M. Battaglieri and others



Progress in algorithms and numerical tools for QCD
Orsay, 9-10 June 2026

The hadron spectrum

* Hadrons are an emergent phenomenon of QCD at low energies (non-perturbative regime)



Eur.Phys.J.A 60, 173 (2024)

The hadron spectrum

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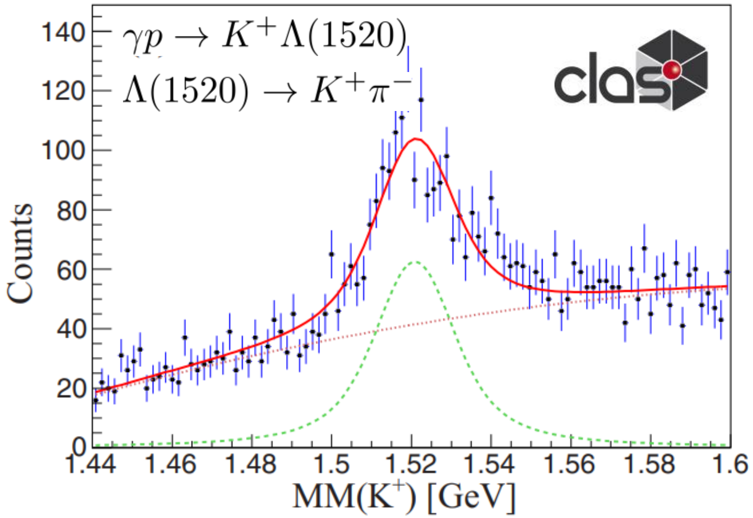
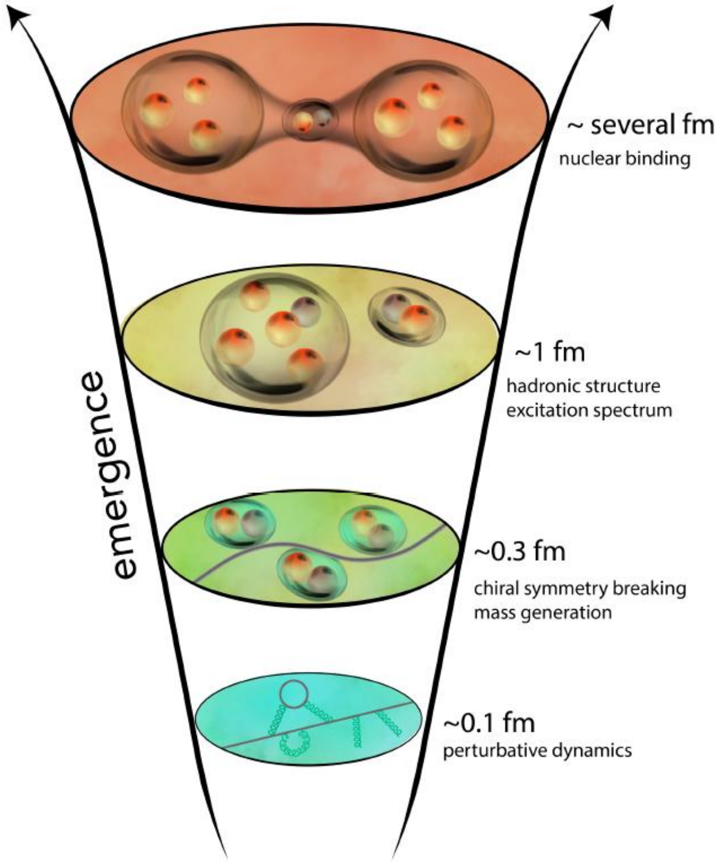
* Most hadrons are short-lived **resonances**

Phys.Rev.C 103, 025206 (2021)





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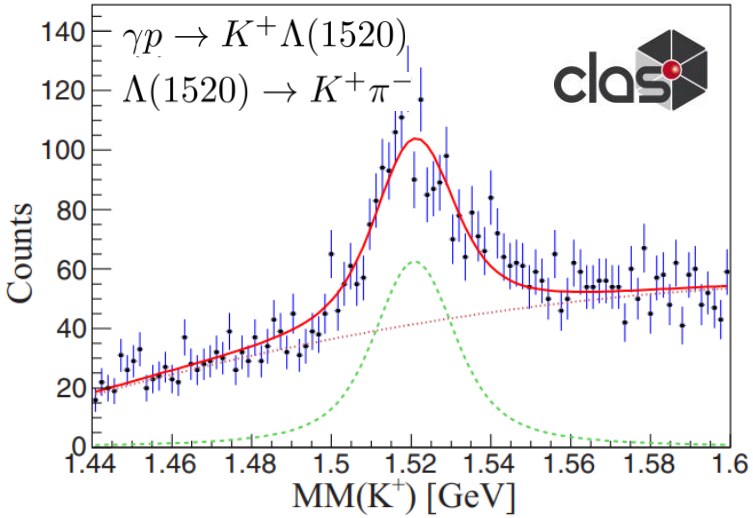
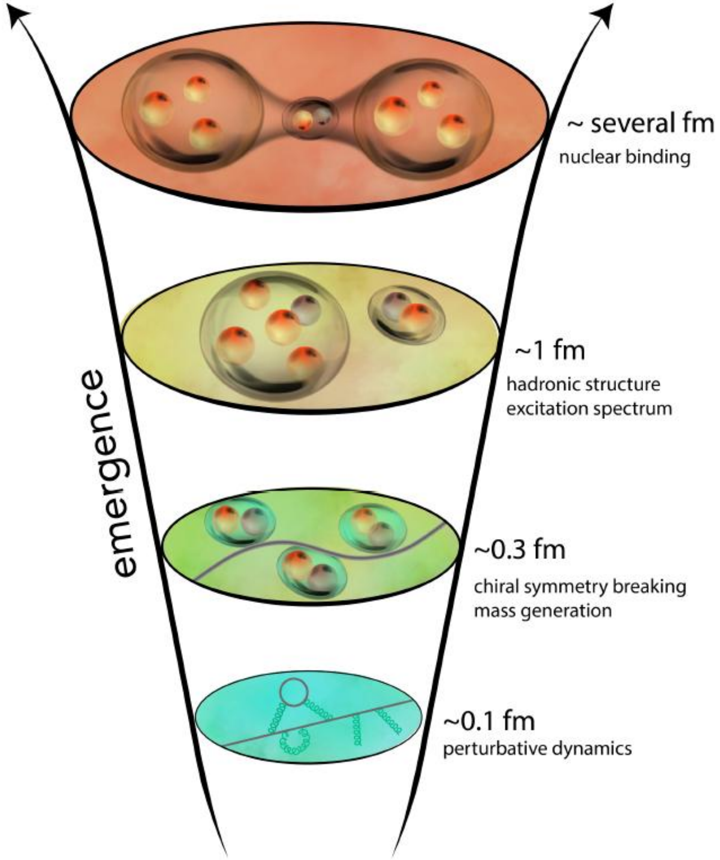


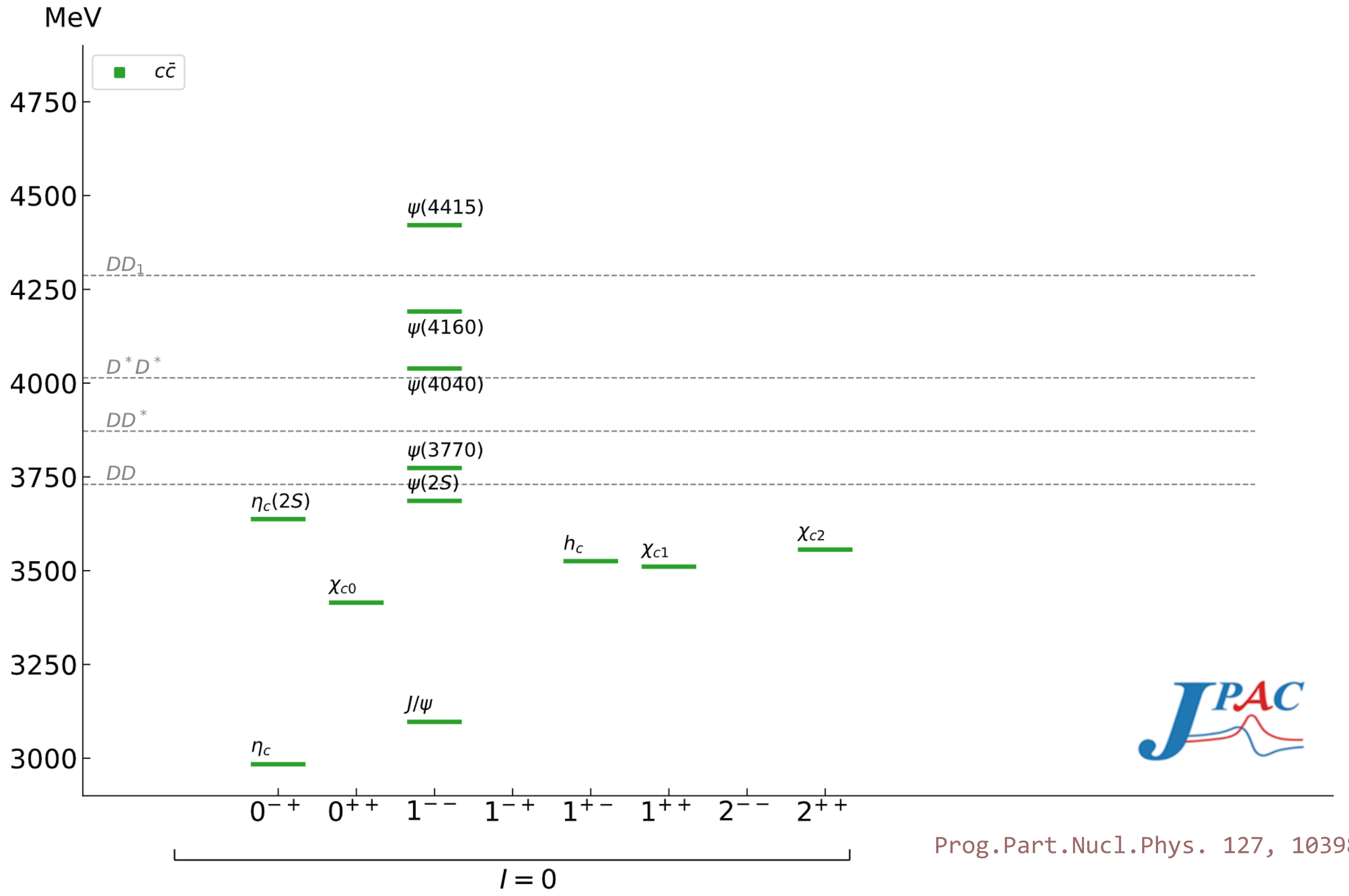


Eur.Phys.J.A 60, 173 (2024)

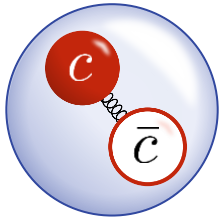
→ Ultimate goals: Understand in terms of quarks and gluons

Learn about QCD

The heavy hadron spectrum… before 2003



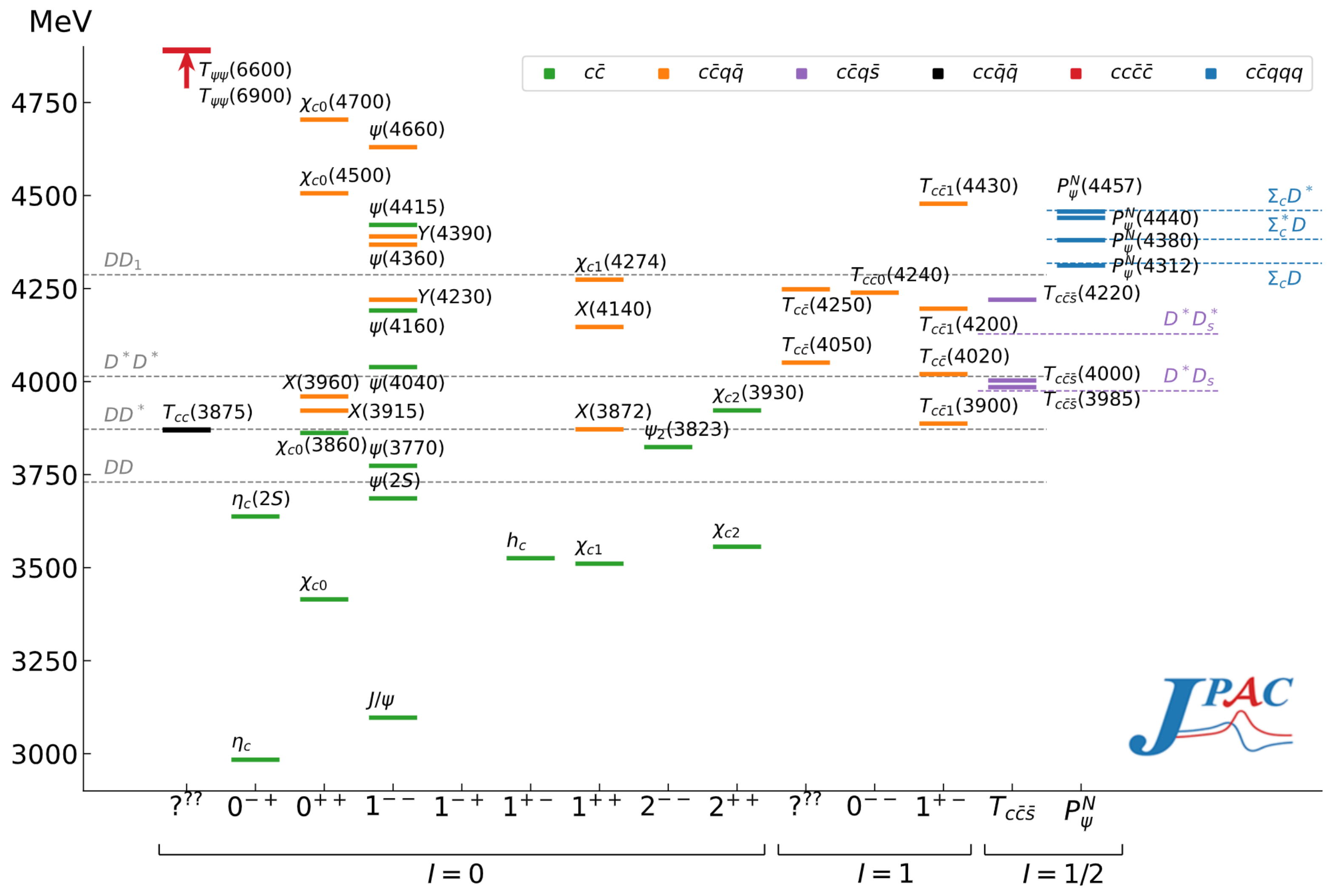
Prog.Part.Nucl.Phys. 127, 103981 (2022)



charmonium

The quark model organizes the spectrum of "conventional" hadrons

The heavy hadron spectrum... after 2003



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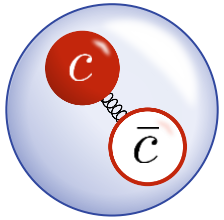
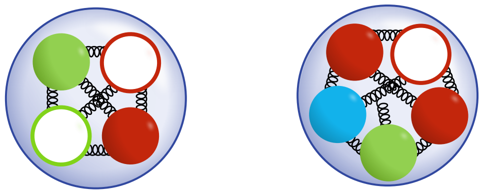


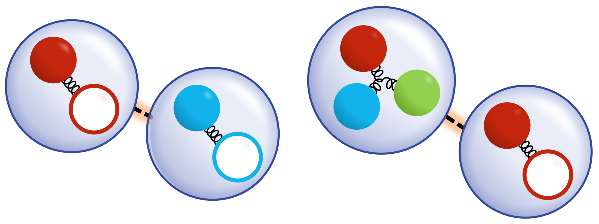
charmonium

Exotic hadrons: don't fit in the "conventional" quark model



tetraquark

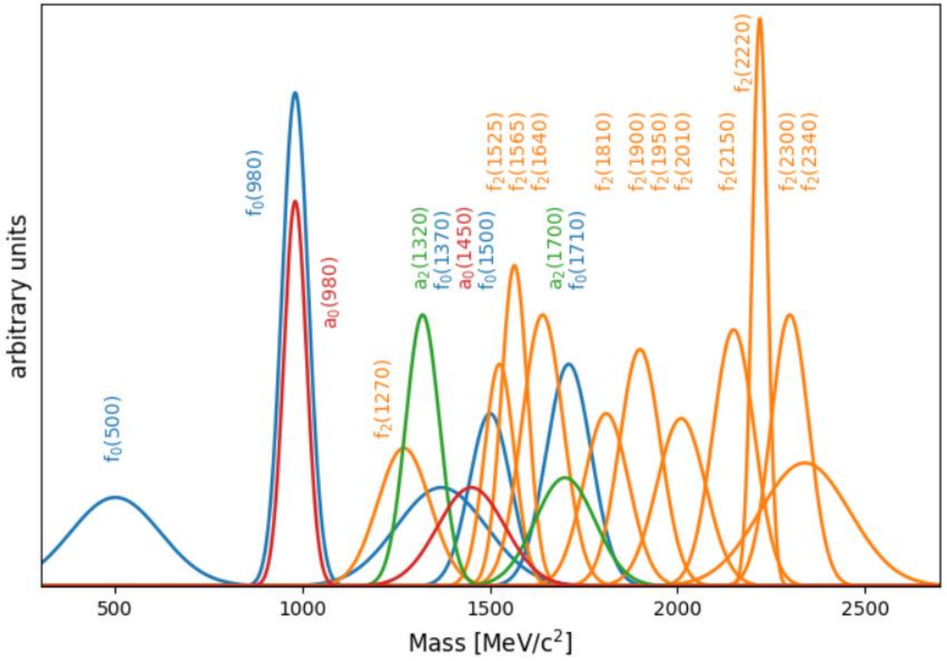
pentaquark



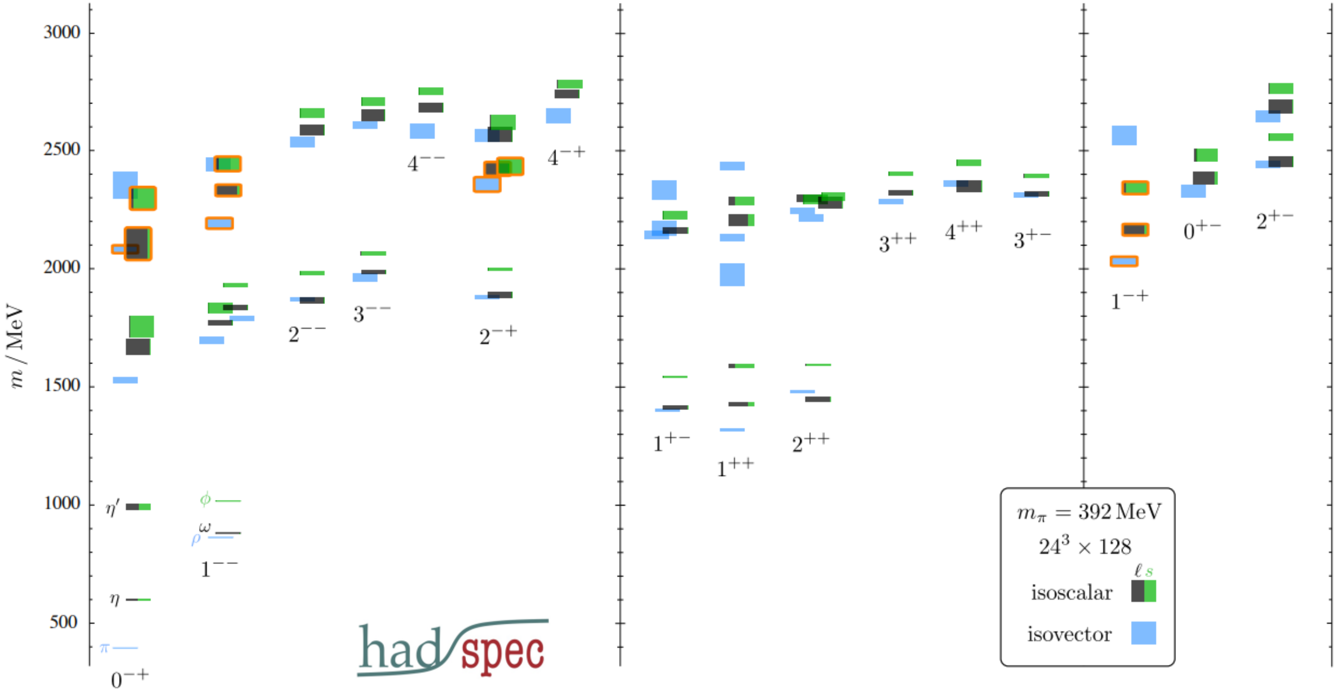
hadronic molecules

Challenges in the light sector

Experimental observations (PDG)



Lattice QCD predictions



J.Dudek et al., Phys.Rev.D 88, 094505 (2013)

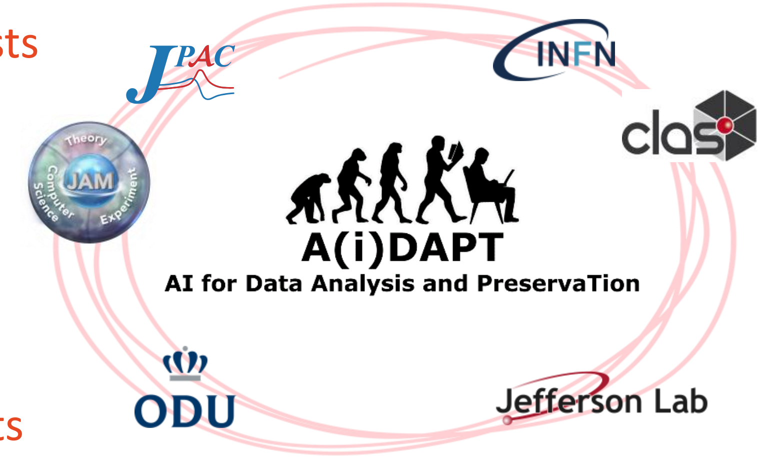
- Wide, overlapping states
- Can’t use simplistic resonance extraction techniques (e.g. Breit Wigner fits)
- Need for amplitude level analyses

The A(i)DAPT collaborative effort

- Experimental data are distorted by detector effects → must be unfolded to extract physics
- Traditional observables may not be adequate in multidimensional space (correlations)
- Modern experiments produce large datasets, which can be difficult to manipulate/preserve

Theorists

Experimentalists



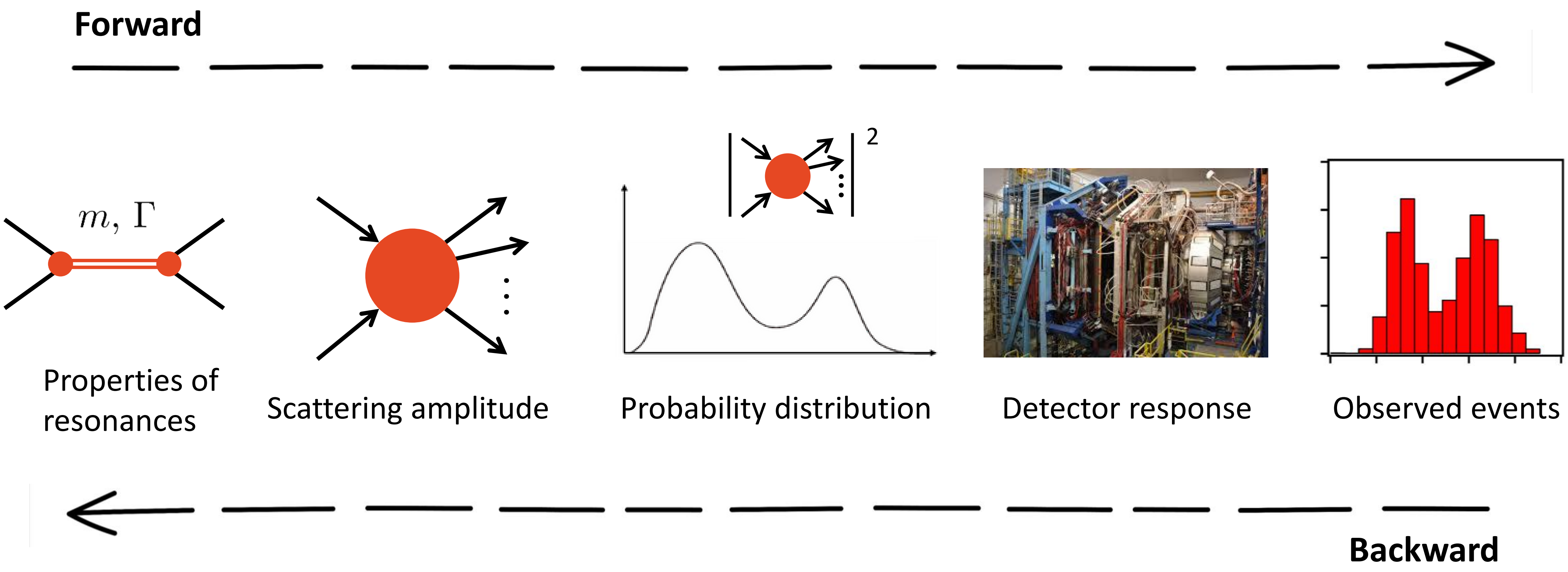
ML experts

M. Battaglieri, Y. Li, A. Pilloni, N. Sato, A. Szczepaniak,
D. Glazier, L. Bibrzycki, G. Montana, G. Foti, J. Xu,
T. Alghamdi, T. Vittorini, and others

Develop AI tools to:

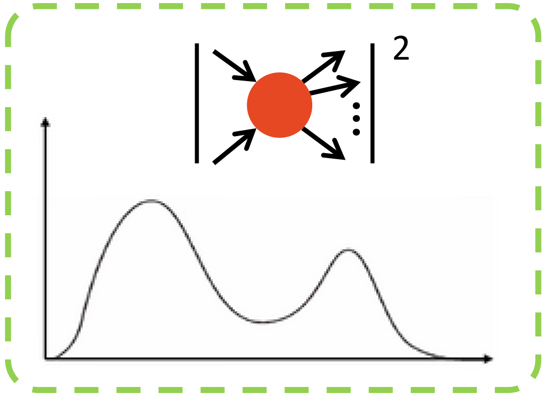
* Accurately fit data in multiD space
* Unfold detector effects
* Quantify the uncertainties
* **Move from cross sections to amplitudes**

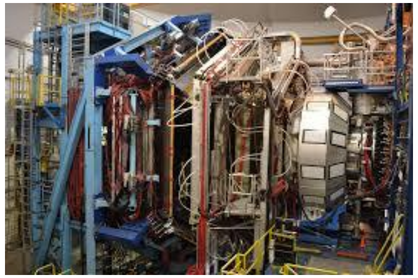
From data to amplitudes and resonance properties

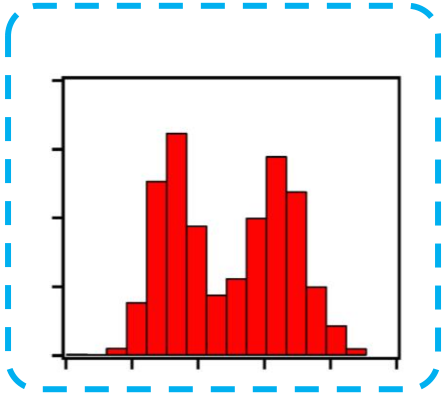


Unfolding of detector effects

Unfold
detector effects







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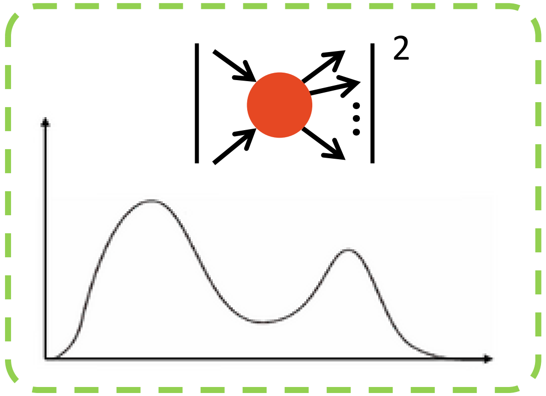

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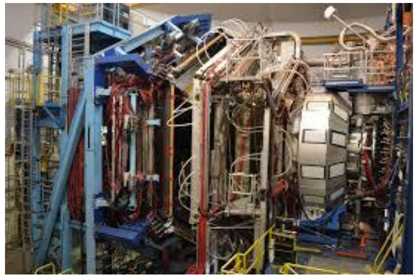
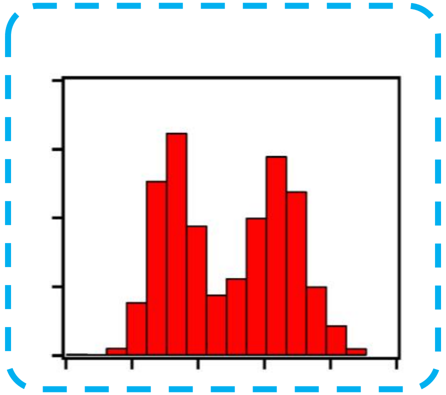


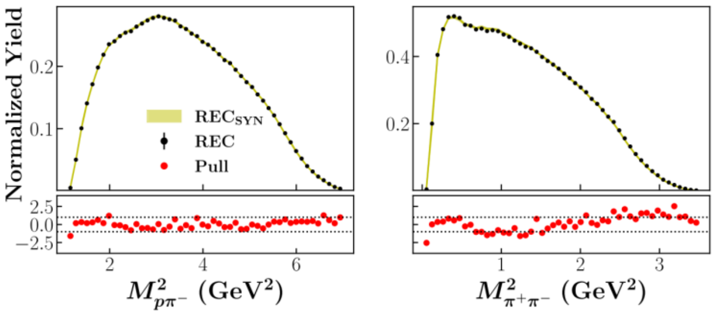


* Smearing (finite detector resolution)

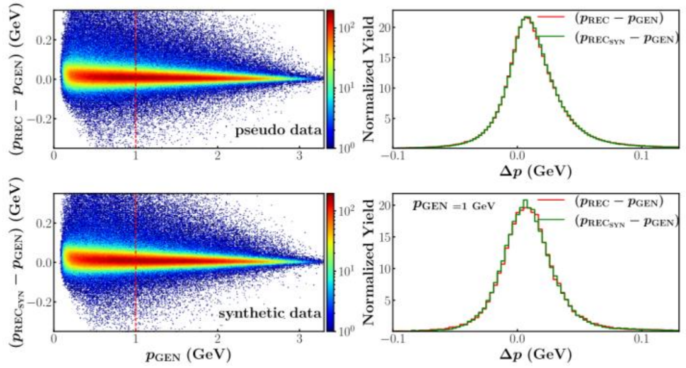
Closure test on pseudodata of CLAS exclusive 2π photoproduction

Alghamdi et al., Phys.Rev.D 108, 094030 (2023)

MC REC pseudodata vs DS-GAN synthetic data



CLAS resolution



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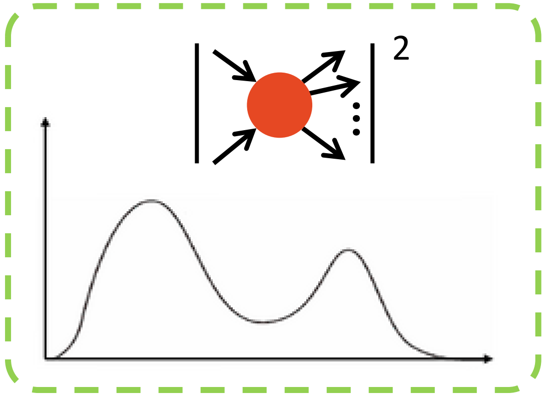
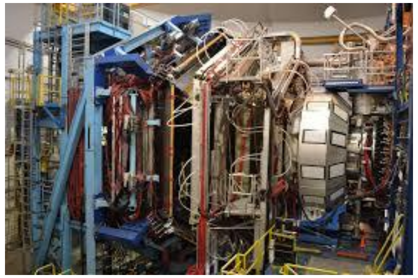
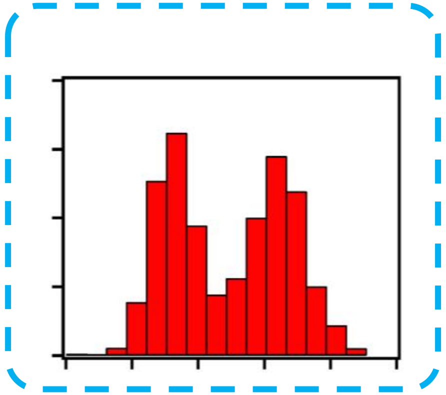






- Smearing (finite detector resolution)
- Acceptance (detector coverage)
- Inefficiency (missed events within acceptance)

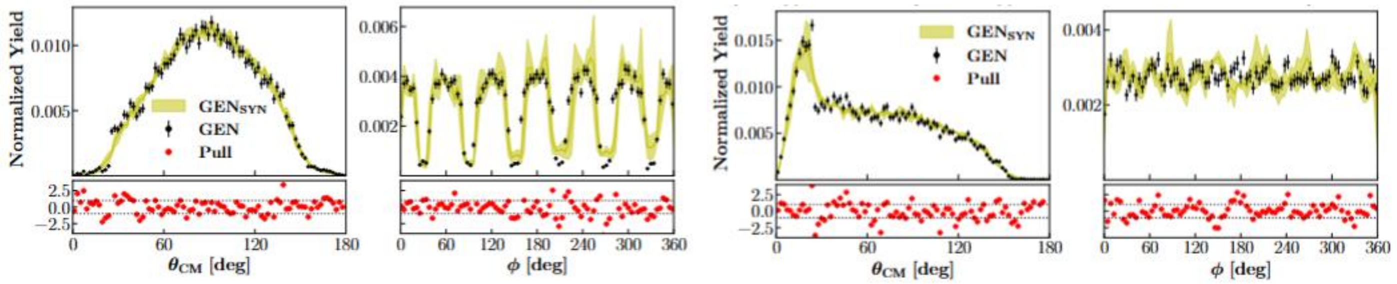
Unfolding of CLAS detector in π^0 photoproduction

Alghamdi et al., (in prepartation)

MC REC pseudodata vs UNF-GAN synthetic data

Phase space

Control model



Unfolding of detector effects

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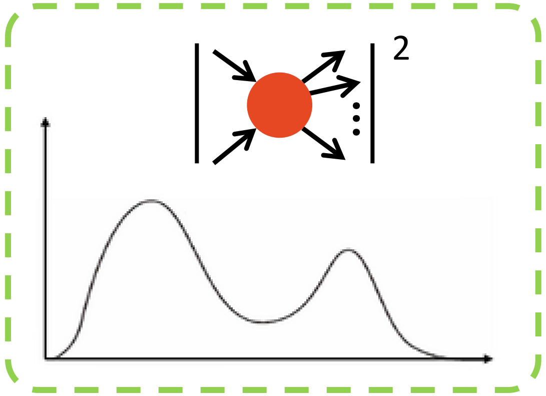

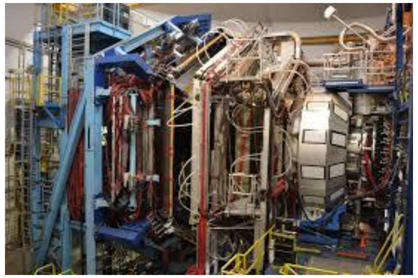

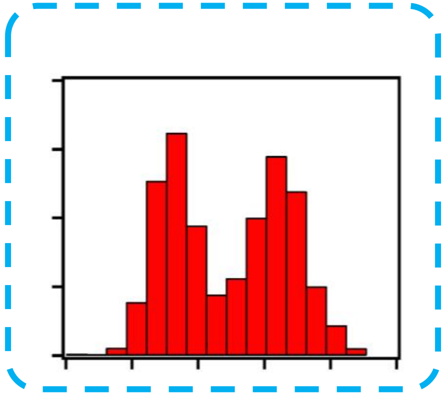

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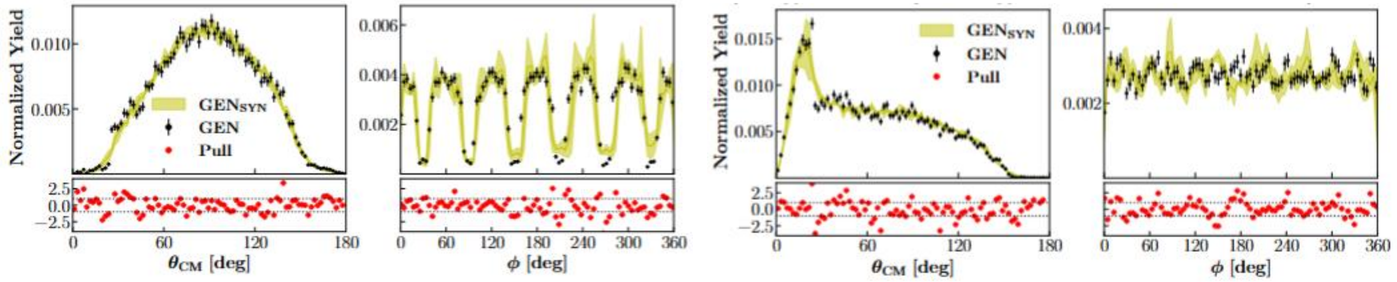
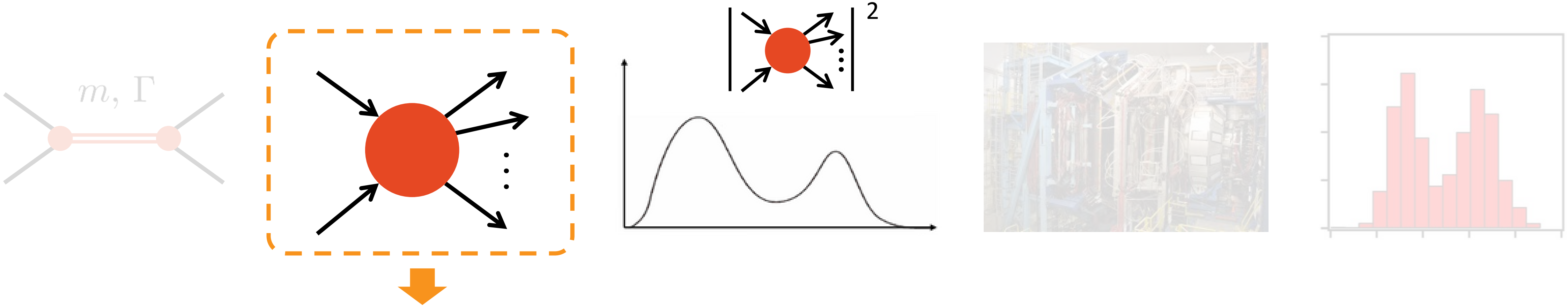


Diffusion Model for CLAS detector unfolding in photoproduction of $\pi^+\pi^-$ G. Foti

Amplitude level unfolding



The **scattering amplitude** $\mathcal{A}$ is the fundamental quantity of interest in hadron reactions:

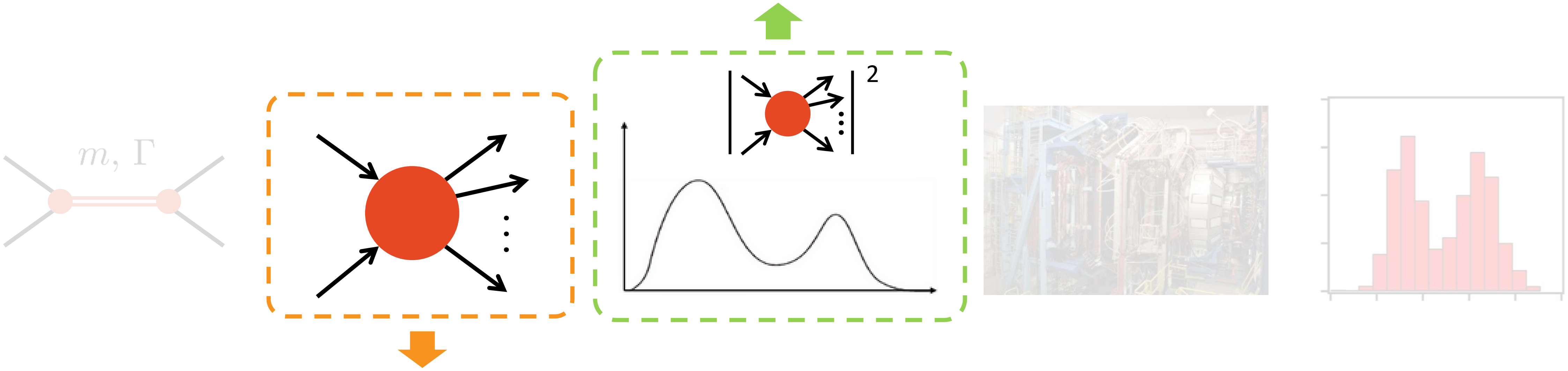
▻ Encodes the underlying dynamics of the interaction

▻ Is a complex quantity: magnitude + phase

Amplitude level unfolding

The **cross section** σ is an experimentally observable quantity:

⊳ Related to $|\mathcal{A}|^2$ (phase information is lost)



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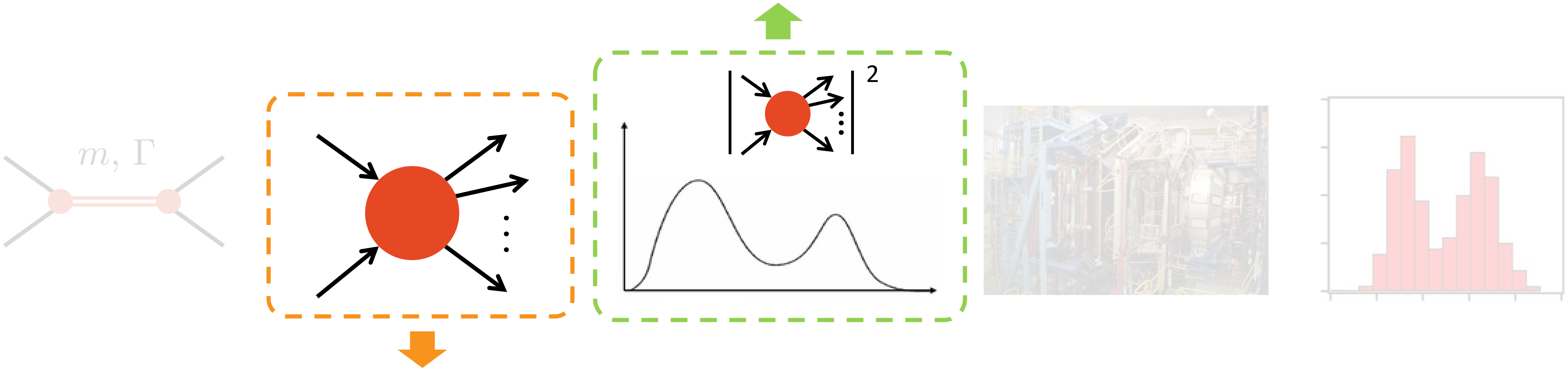

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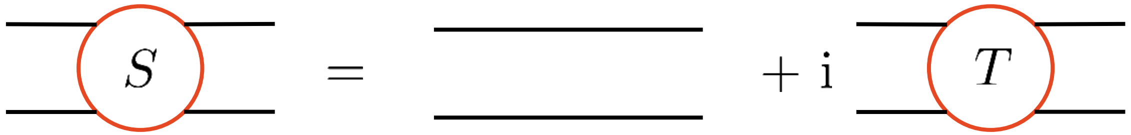
→ **Ill-posed inverse problem**

Properties of scattering amplitudes

S-matrix theory

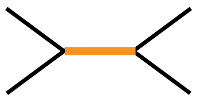


Properties of scattering amplitudes

S-matrix theory $\longrightarrow$ Fundamental principles of scattering

* Rotational invariance → **Partial wave expansion**

$$\langle \mathrm{out}|T|\mathrm{in}\rangle \equiv A(s,\cos\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(s)P_\ell(\cos\theta)$$

$\sum$ 

$$f_\ell \sim \frac{1}{s-m_R^2}$$

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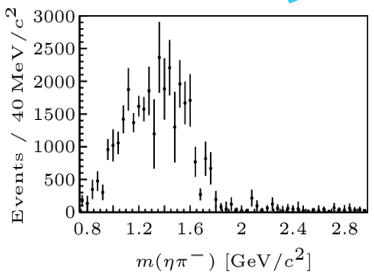
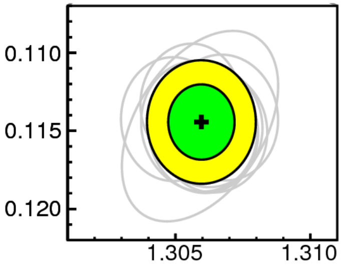
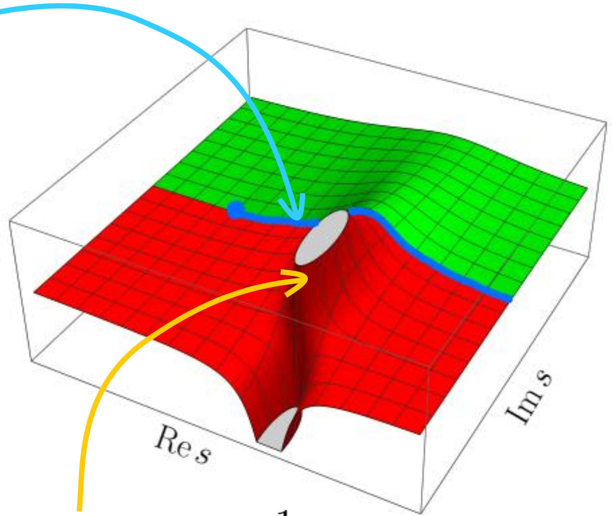
* Causality → **Analyticity**

$$f_\ell(s) = \frac{1}{\pi}\int ds' \frac{\text{Disc}\, f_\ell(s')}{s'-s-i\epsilon}$$

Resonances are characterized by poles in the complex energy plane







$$f_\ell(m_R^2) \sim \frac{1}{s-m_R^2}$$

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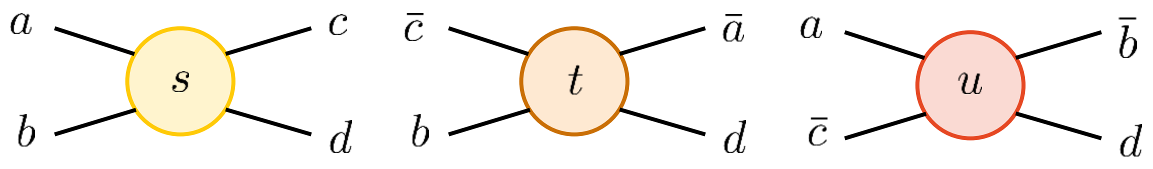
* Existence of antiparticles → **Crossing symmetry**

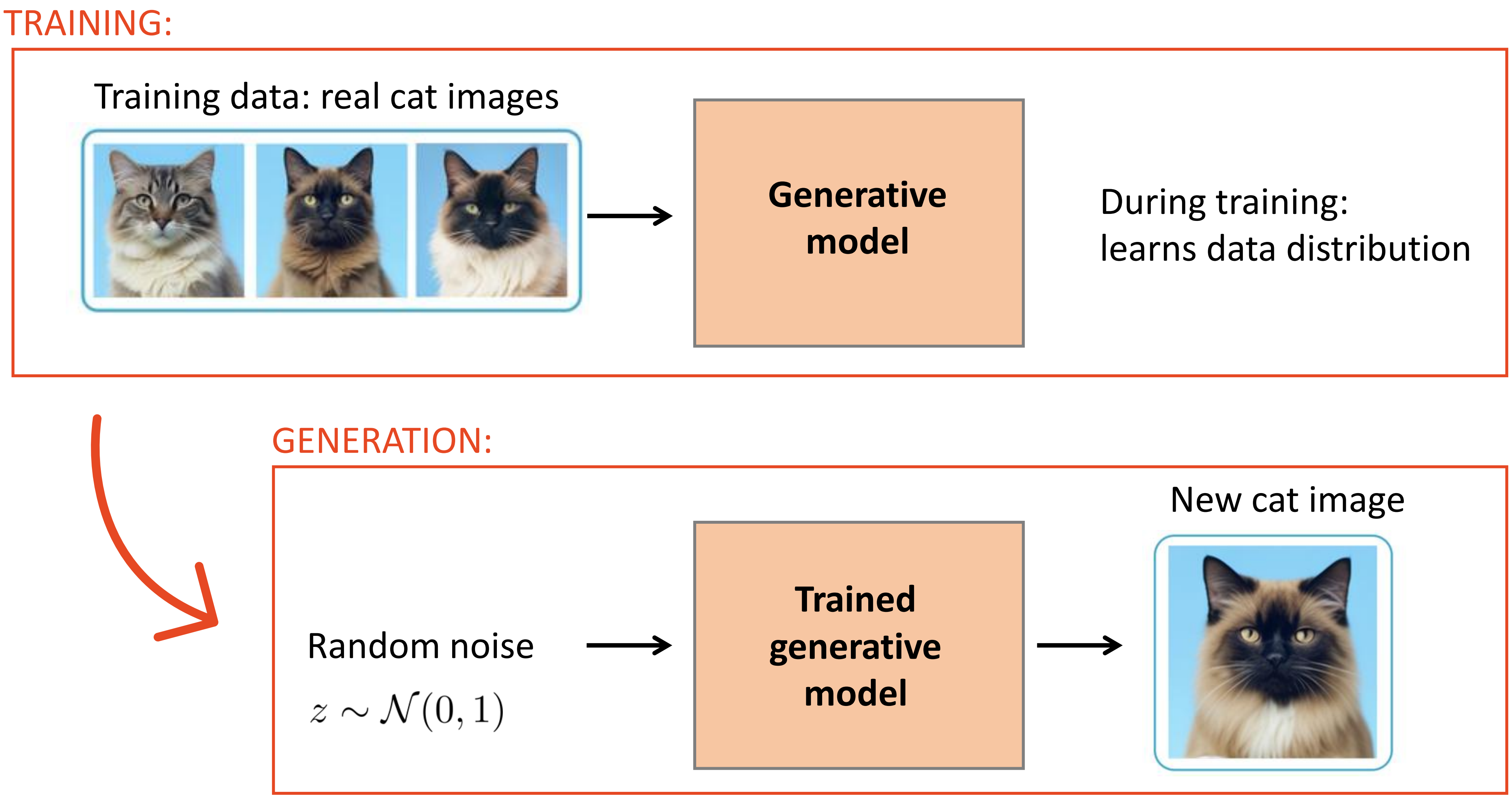


$$A(s,\cos\theta_s) = A(t,\cos\theta_t) = \sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(t)P_\ell(\cos\theta_t)$$

Build a generative approach informed by S-matrix principles to reconstruct scattering amplitudes

* Generative model → **Generative adversarial network (GAN)**
* Physics case → **Pion-pion scattering**

Generative models



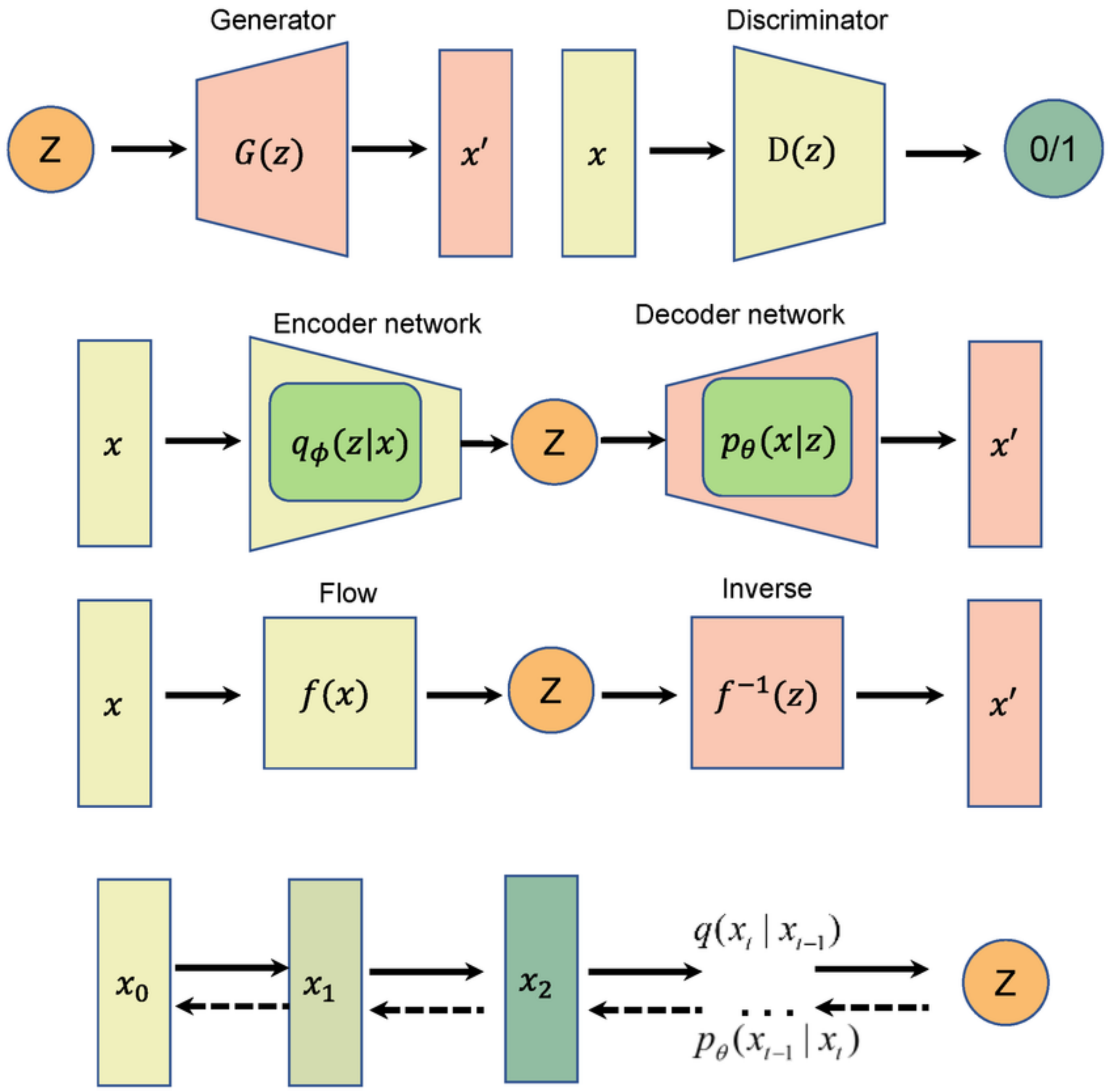
Generative models

Generative adversarial network (GAN)

Variational autoencoder (VAE)

Normalizing flow (NF)

Diffusion model (DM)



$\pi^+\pi^-$ elastic scattering

Simplest physics case: elastic $2 \longrightarrow 2$ of spinless particles

⊳ Dominated by $f_0(500)$ and $\rho(770)$ resonances

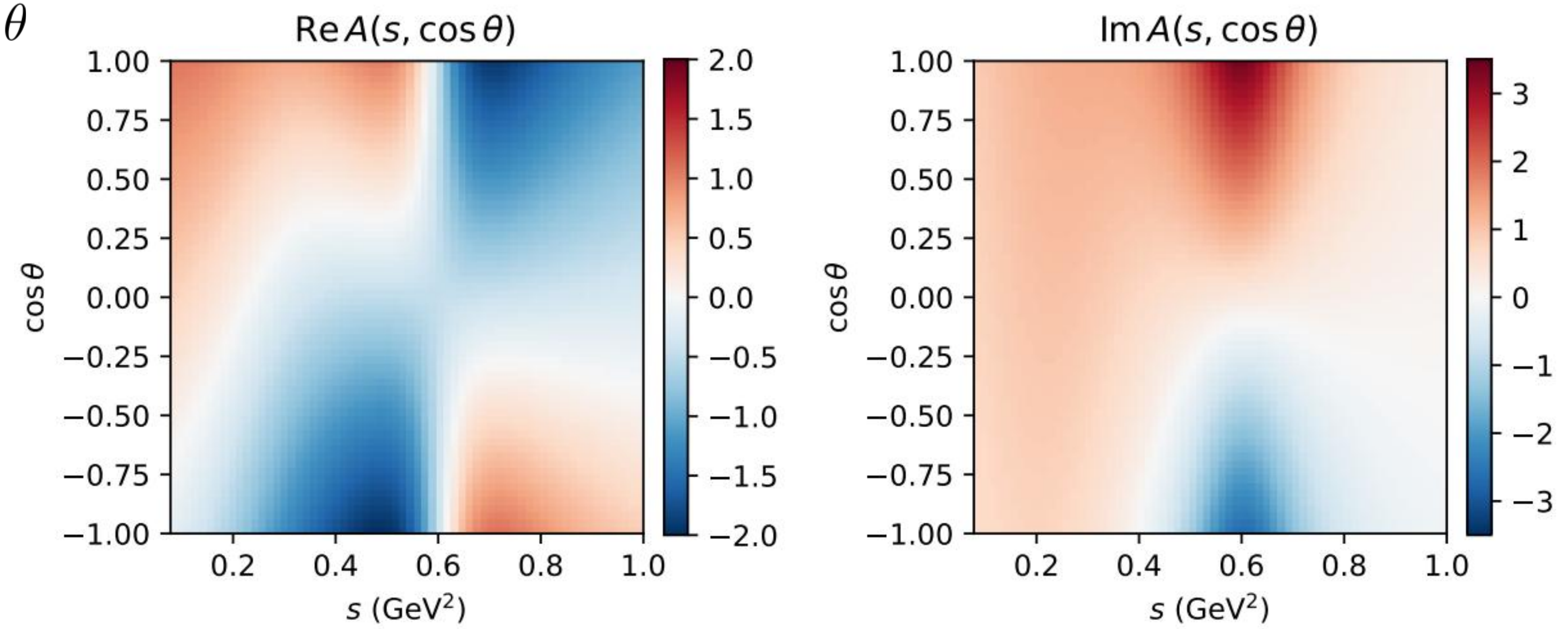
Model:

Partial-wave decomposition of the **amplitude** truncated to $n = 1$

$$\mathcal{A}(s, \cos\theta) = \sum_{\ell=0}^{n=1} (2\ell + 1) f_\ell(s) P_\ell(\cos\theta)$$

and Breit-Wigner type partial waves: $f_\ell = \dfrac{m_\ell \Gamma_\ell}{m_\ell^2 - s - i m_\ell \Gamma_\ell}$

$$\mathcal{A}(s, \cos\theta) = f_0(s) + 3 f_1(s) \cos\theta$$



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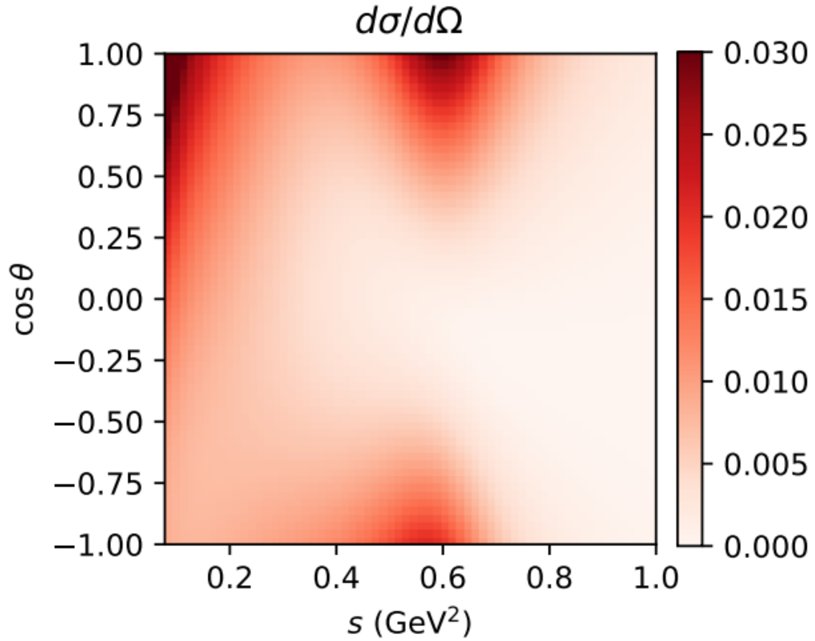
Differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{1}{64\pi^2} \frac{1}{s} |\mathcal{A}(s, \cos\theta)|^2$$



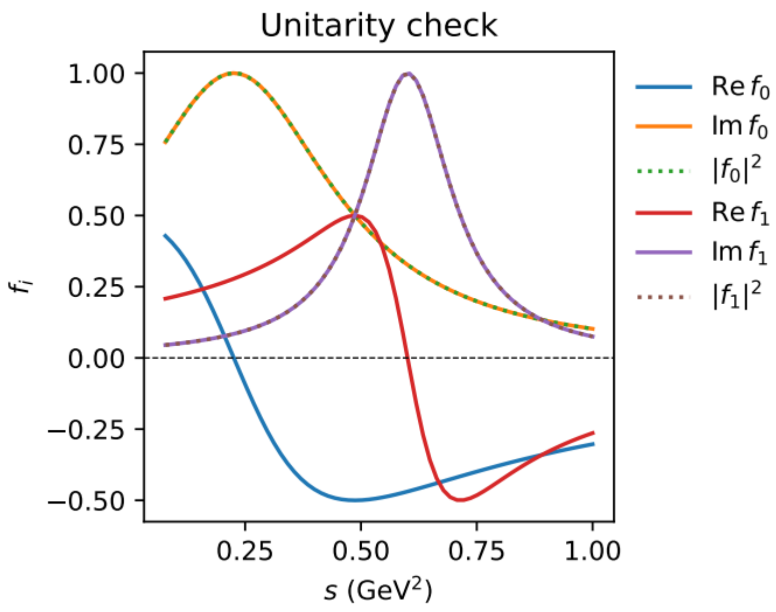
Amplitudes and cross sections as images (discretized functions)

$\pi^+\pi^-$ elastic scattering

Unitarity relation

For the partial waves: $\text{Im}\ f_\ell(s) = |f_\ell(s)|^2$

$$f_\ell(s) = \frac{1}{2}\int_{-1}^{+1} dz P_\ell(z)\mathcal{A}(s,z)$$



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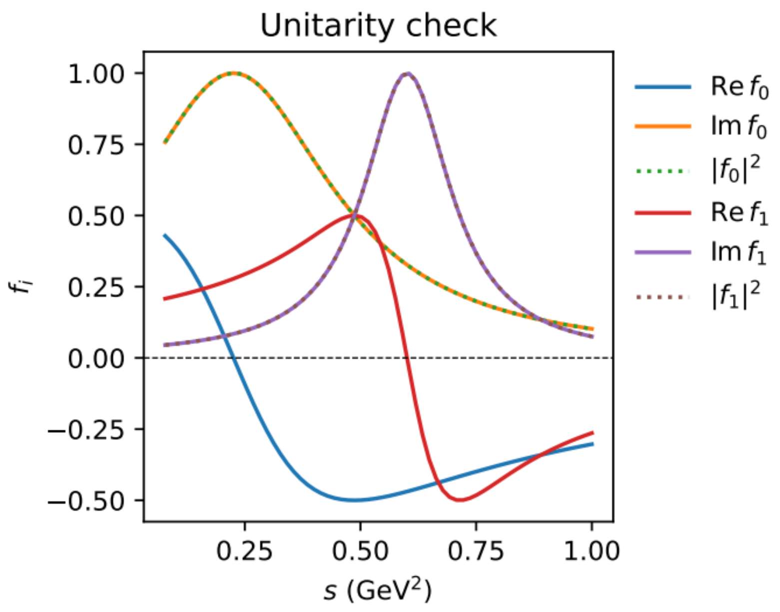

Integral relation for the full amplitude:

$$\text{Im}\ \mathcal{A}(s,z) = \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_{-1}^{+1} dz' \mathcal{A}(s,z')\mathcal{A}^*(s,z'')$$

$$z'' = zz' + \sqrt{1-z^2}\sqrt{1-z'^{\,2}}\cos\phi$$

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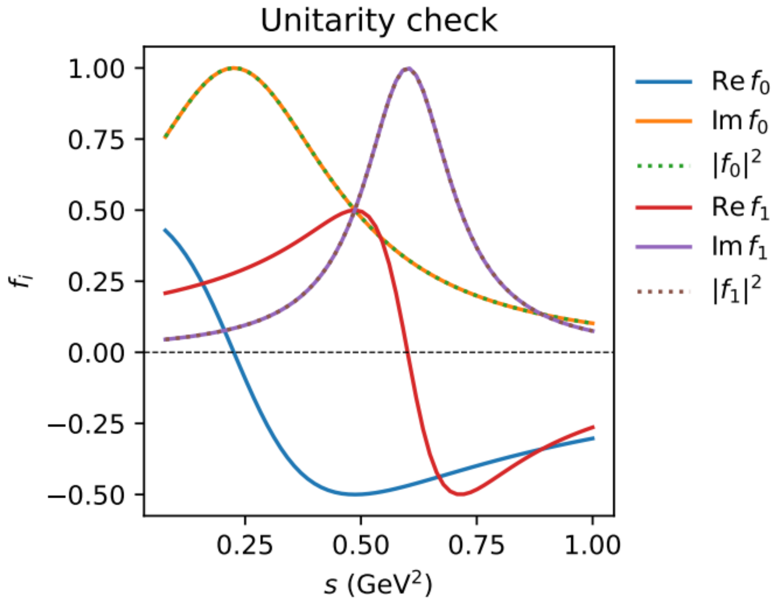

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Phase ambiguity: $\mathcal{A}(s,z) \to -\mathcal{A}^*(s,z)$

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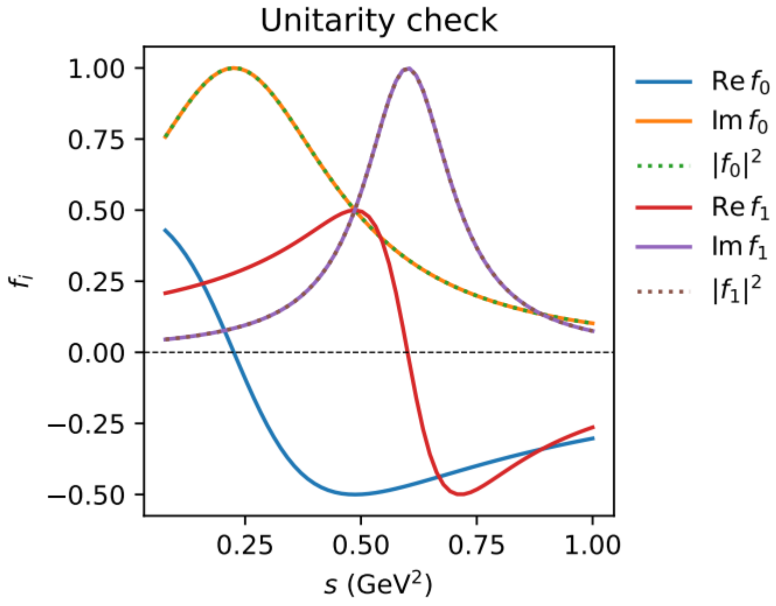
For the partial waves: $\text{Im}\ f_\ell(s) = |f_\ell(s)|^2$

$$f_\ell(s) = \frac{1}{2}\int_{-1}^{+1} dz P_\ell(z)\mathcal{A}(s,z)$$



Integral relation for the full amplitude:

$$\text{Im}\ \mathcal{A}(s,z) = \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_{-1}^{+1} dz' \mathcal{A}(s,z')\mathcal{A}^*(s,z'')$$

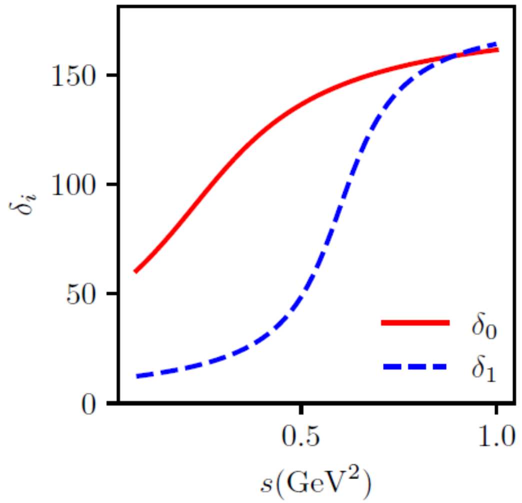
$$z'' = zz' + \sqrt{1-z^2}\sqrt{1-z'^{\,2}}\cos\phi$$

Phase ambiguity: $\mathcal{A}(s,z) \to -\mathcal{A}^*(s,z)$

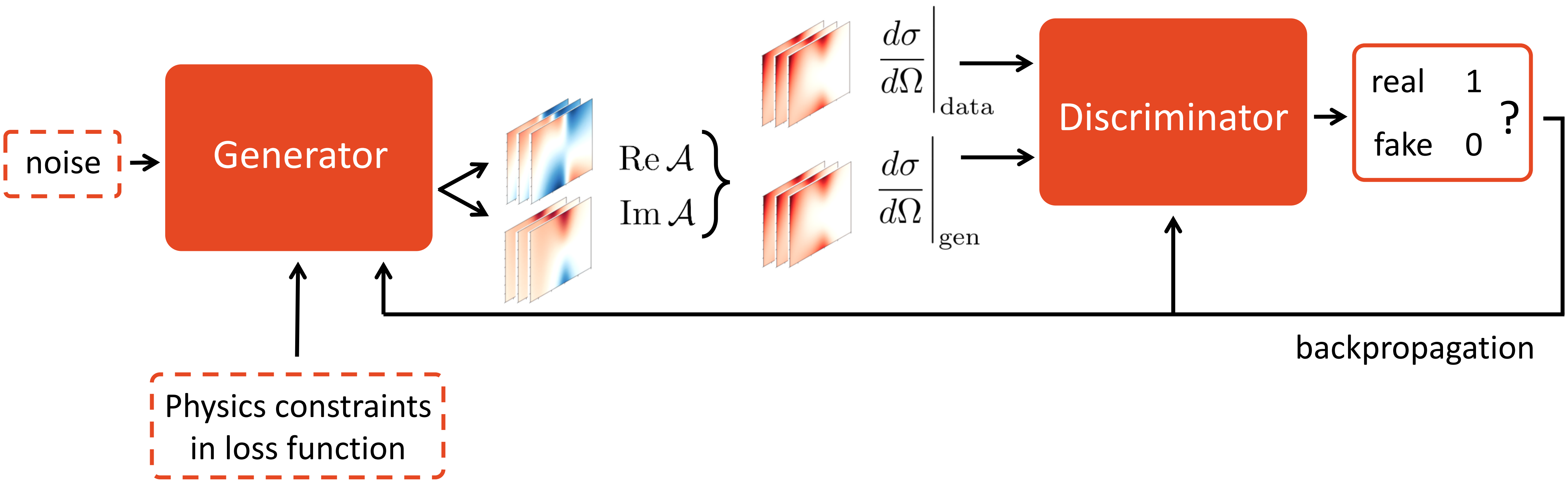
Phase shift monotonicity (**causality**)

$$\delta_\ell = \text{atan}\left(\frac{\text{Im}\ f_\ell(s)}{\text{Re}\ f_\ell(s)}\right)$$

$$\frac{d\delta_\ell(s)}{ds} \geq 0$$



GAN with physics constraints



$$\mathcal{L} = \mathcal{L}_{\text{GAN}} + \lambda_{\text{u}}\mathcal{L}_{\text{u}} + \lambda_{\delta}\mathcal{L}_{\delta}$$

Loss function

Adversarial loss: Mean squared error (LSGAN)

Unitarity loss: Enforce unitarity by comparing the modulus squared of the numerical integral of the scattering amplitude over angular variables to the imaginary part

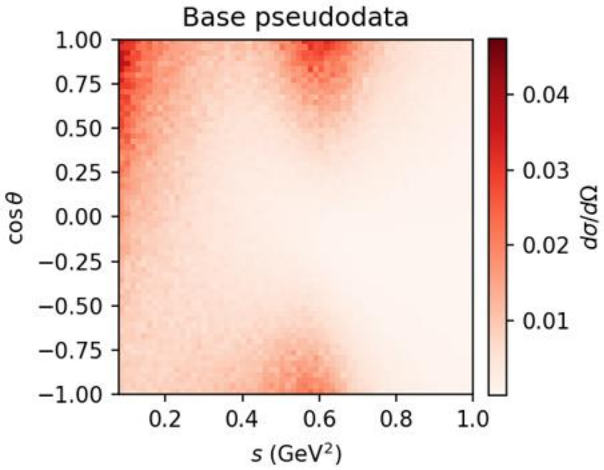
$$\mathcal{L}_{\mathrm{u}} = \frac{1}{N \cdot N_s \cdot N_z} \sum_{i=1}^{N} \sum_{j=1}^{N_s} \sum_{k=1}^{N_z} \left(\left| \mathrm{Im}\, \mathcal{A}(s,z) - \mathrm{Re}\, \mathcal{I}(s,z) \right| + \left| \mathrm{Im}\, \mathcal{I}(s,z) \right| \right)$$

$$\mathcal{I}(s,z) = \frac{1}{4\pi} \int_{-1}^{1} dz' \int_{0}^{2\pi} d\phi \left(\mathcal{A}(s,z') \mathcal{A}(s, z''(z,z',\phi)) \right) \qquad [\cos\theta \times \phi] = 64 \times 10$$

Phase shift loss: Ensure the positive derivative of the phase shift (causality)

$$\mathcal{L}_{D_\ell} = \frac{1}{N} \sum_{i=1}^{N} \log\left(\max\left(0, -\Delta\delta_\ell(s)\right) + 1 \right),$$

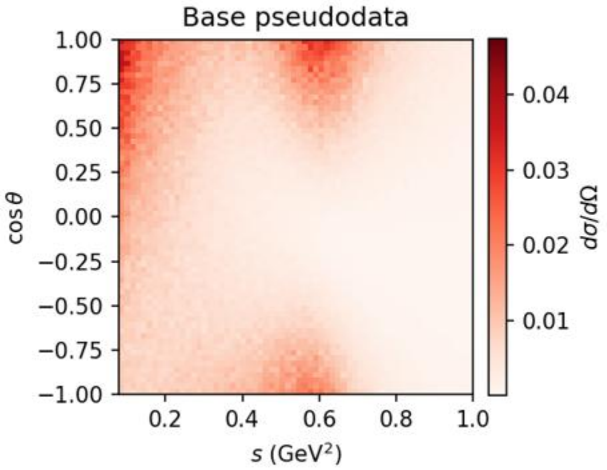
Training pseudodata



Differential cross section from the model
with relative Gaussian noise $\mathcal{N}(0, \sigma_{\text{exp}})$ (mimic experimental data)

- ▻ discretized $64 \times 64,\ s \in [(2m_\pi)^2, 1\ \text{GeV}^2],\ \cos\theta \in [-1, 1]$
- ▻ normalized

Training pseudodata

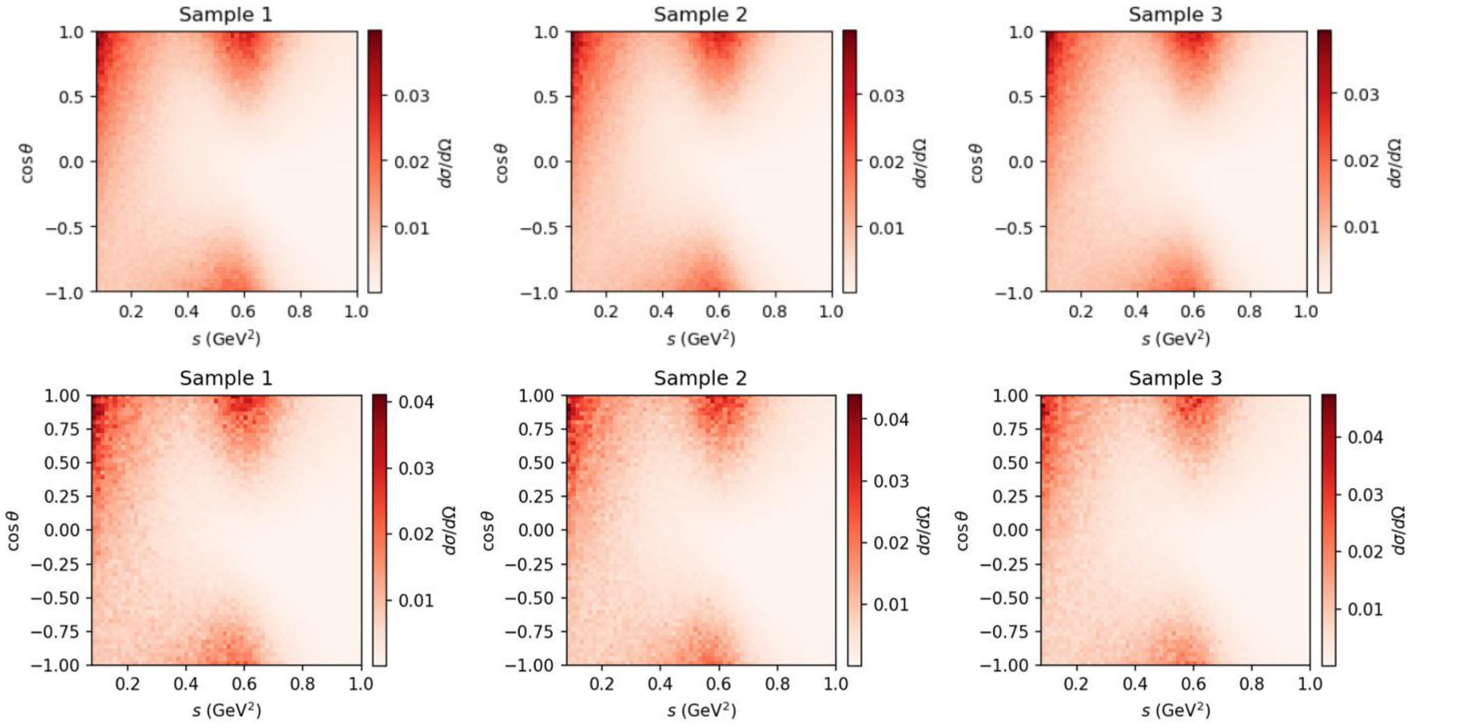


Differential cross section from the model
with relative Gaussian noise $\mathcal{N}(0, \sigma_{\rm exp})$ (mimic experimental data)

- ⊳ discretized $64 \times 64,\ s \in [(2m_\pi)^2, 1\ {\rm GeV}^2],\ \cos\theta \in [-1, 1]$
- ⊳ normalized
- ⊳ with additional noise $\mathcal{N}(0, \sigma_{\rm aug})$ (augment around base image)

$$\sigma_{\rm exp} = \sigma_{\rm aug} = 0.05$$

$$\sigma_{\rm exp} = \sigma_{\rm aug} = 0.10$$



The convergence challenge

Stabilizing the adversarial game

⊳ Spectral normalization to prevent runaway gradients

⊳ Asymmetric learning rates ($\mathrm{LR}_D < \mathrm{LR}_G$) and label smoothing (real = 0.9) to avoid over-confident discriminator

⊳ Dropout in D after each conv block

⊳ LSGAN (MSE) instead of BCE (non-saturating gradients far from the decision boundary)

Multi-loss optimization

⊳ PCGrad gradient surgery: physics gradients are projected onto the ortogonal direction when they conflict before optimization

Convergence detection (based on $\mathcal{L}_{\mathbf{unit}}$)

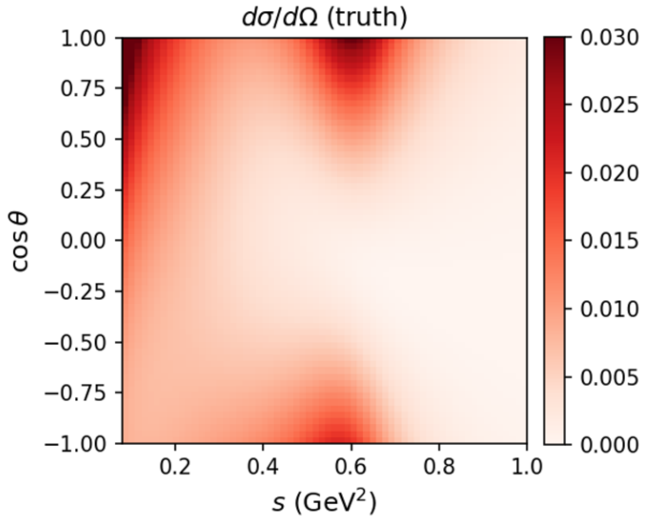
⊳ Early failure detection: abort the trial and restart training (up to 5 restarts before declaring failure)

⊳ Early stopping

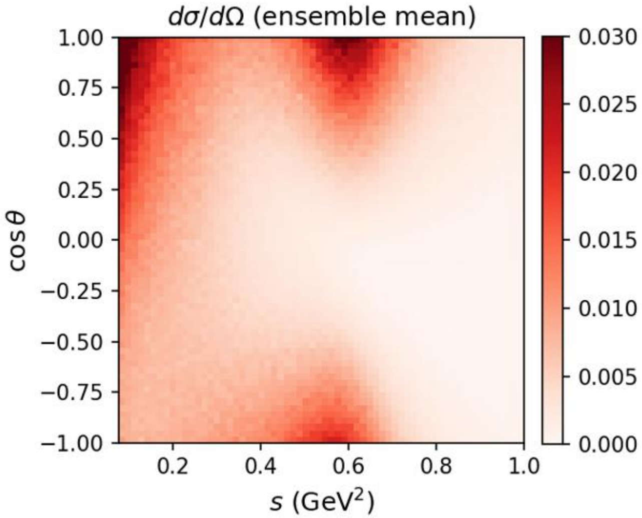
⊳ Learning-rate reduction near the minimum

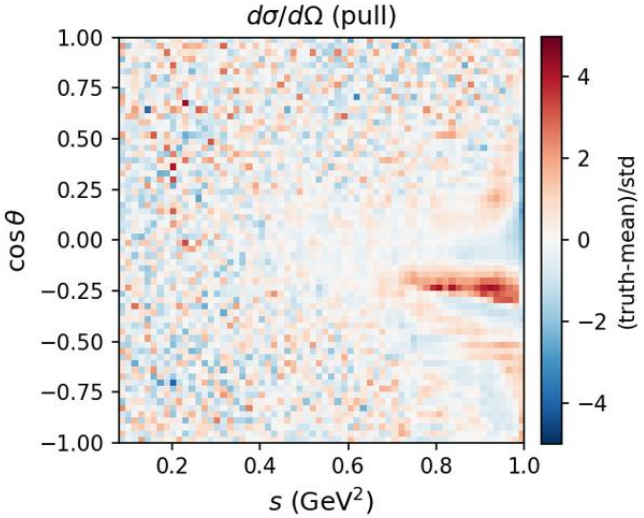
Preliminary results: cross section

Mean over 10 trained GAN, with 10 generated samples per GAN (100 total samples)

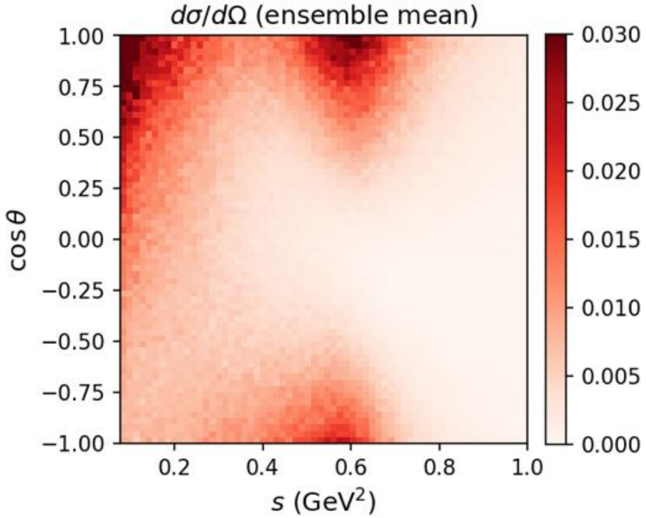


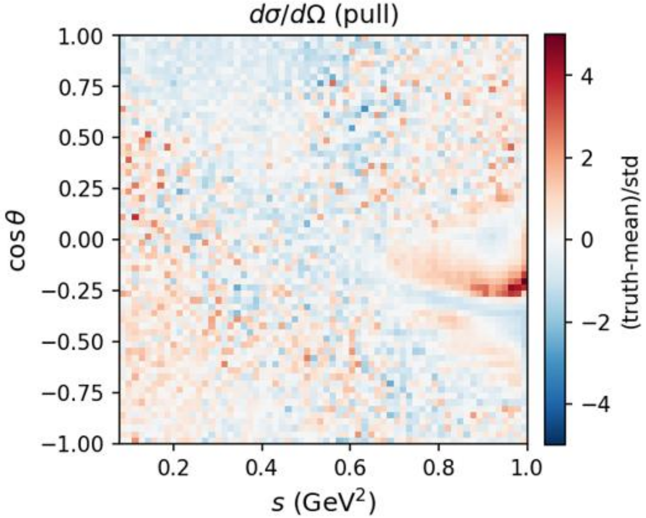
$\sigma = 0.05$





$\sigma = 0.10$

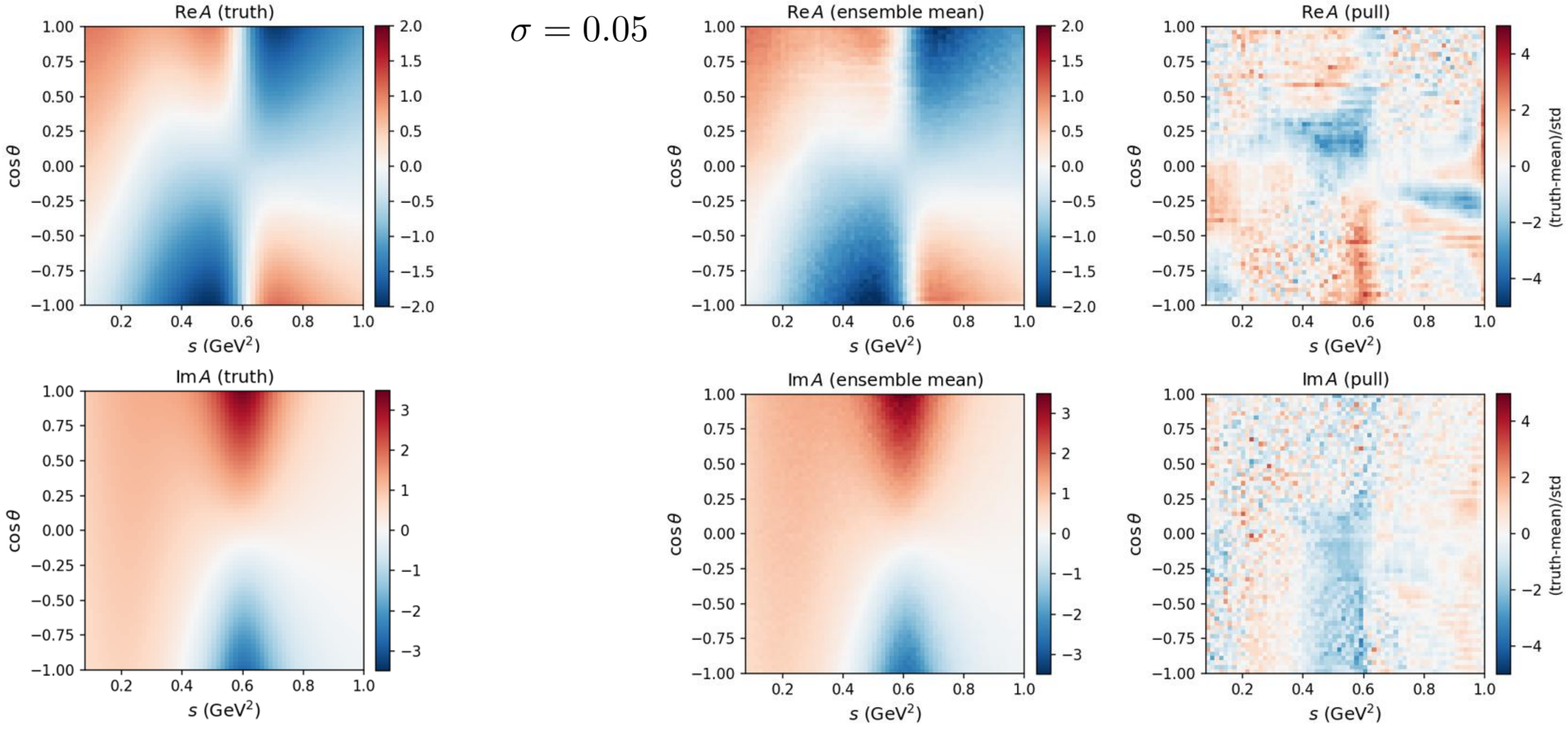




Preliminary results: amplitude

Mean over 10 trained GAN, with 10 generated samples per GAN (100 total samples)

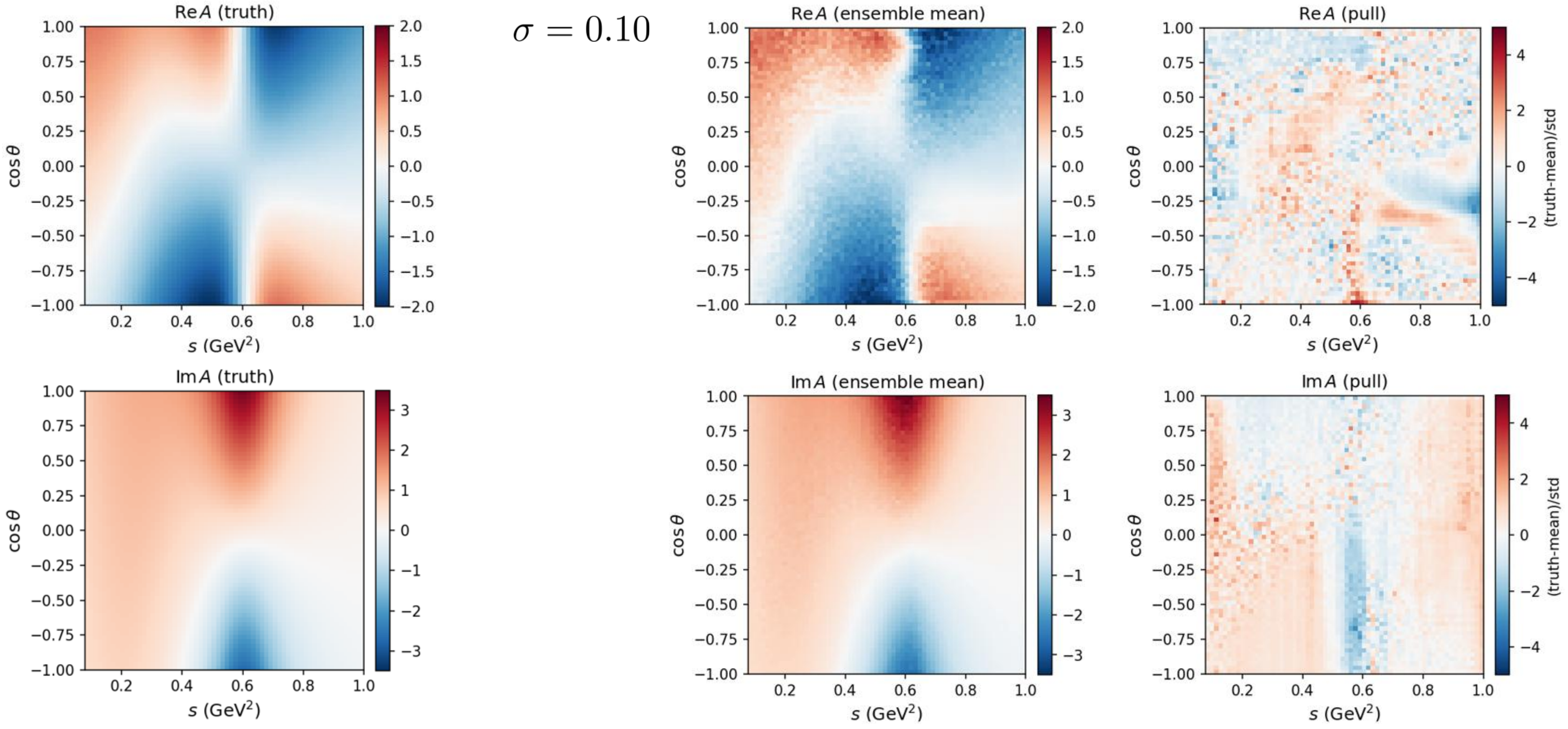
$\sigma = 0.05$



Preliminary results: amplitude

Mean over 10 trained GAN, with 10 generated samples per GAN (100 total samples)

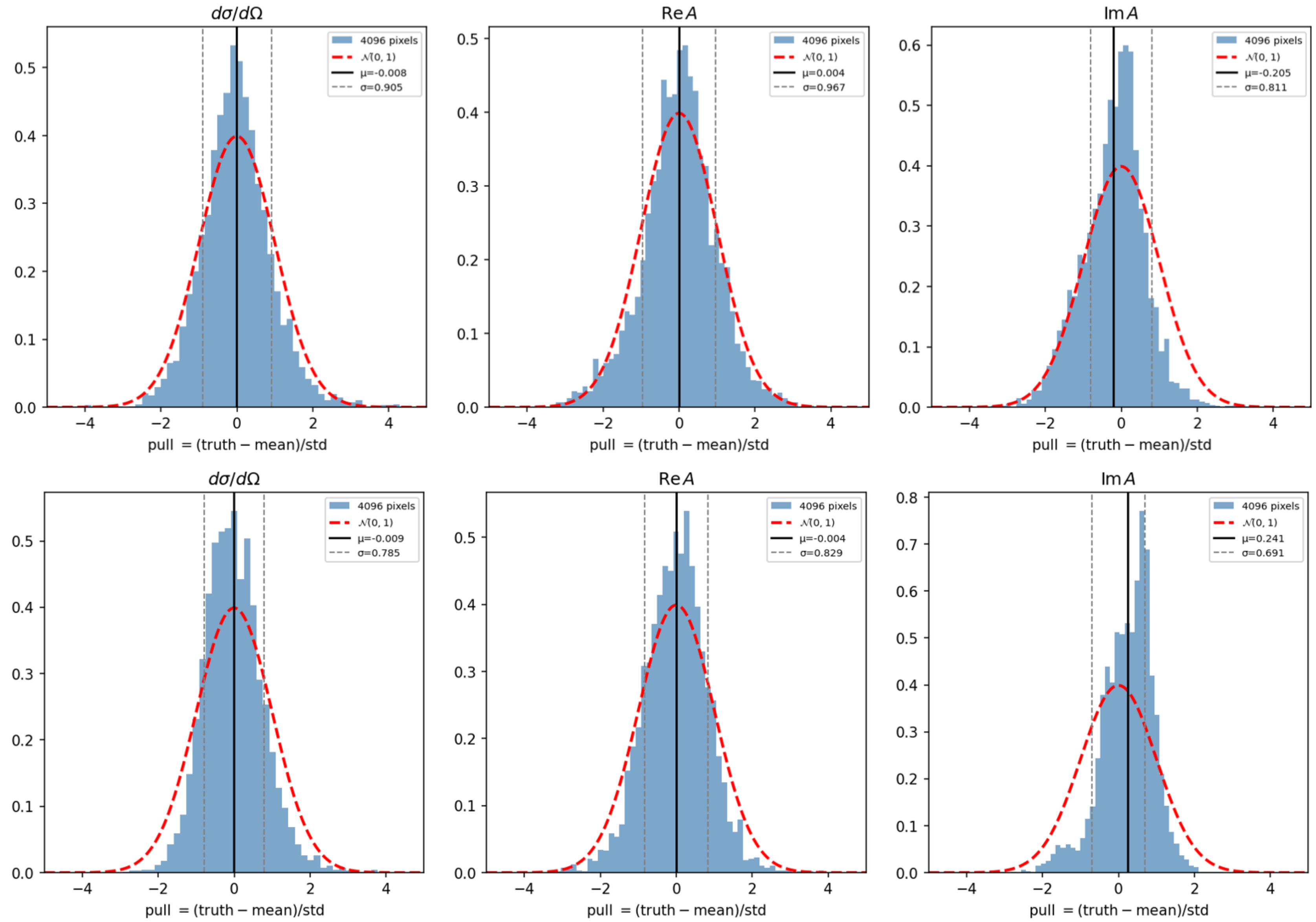
$\sigma = 0.10$



Preliminary results: pull histograms

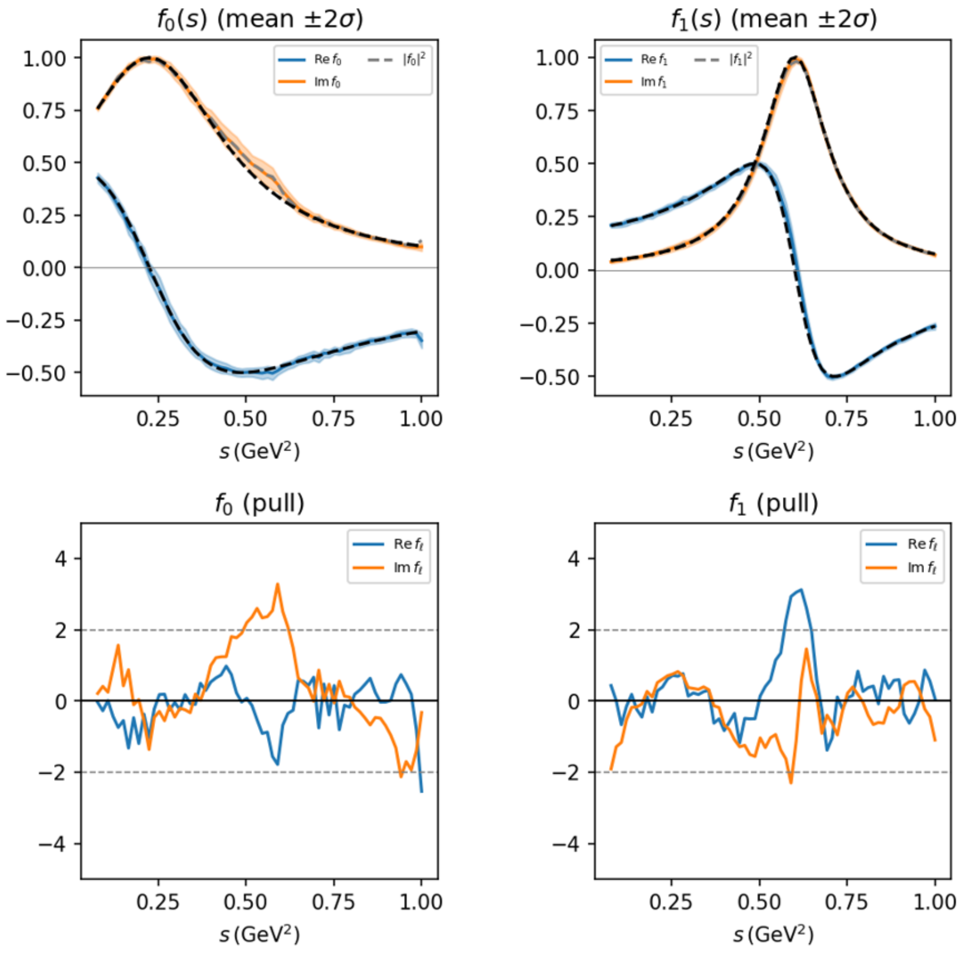
$\sigma = 0.05$

$\sigma = 0.10$

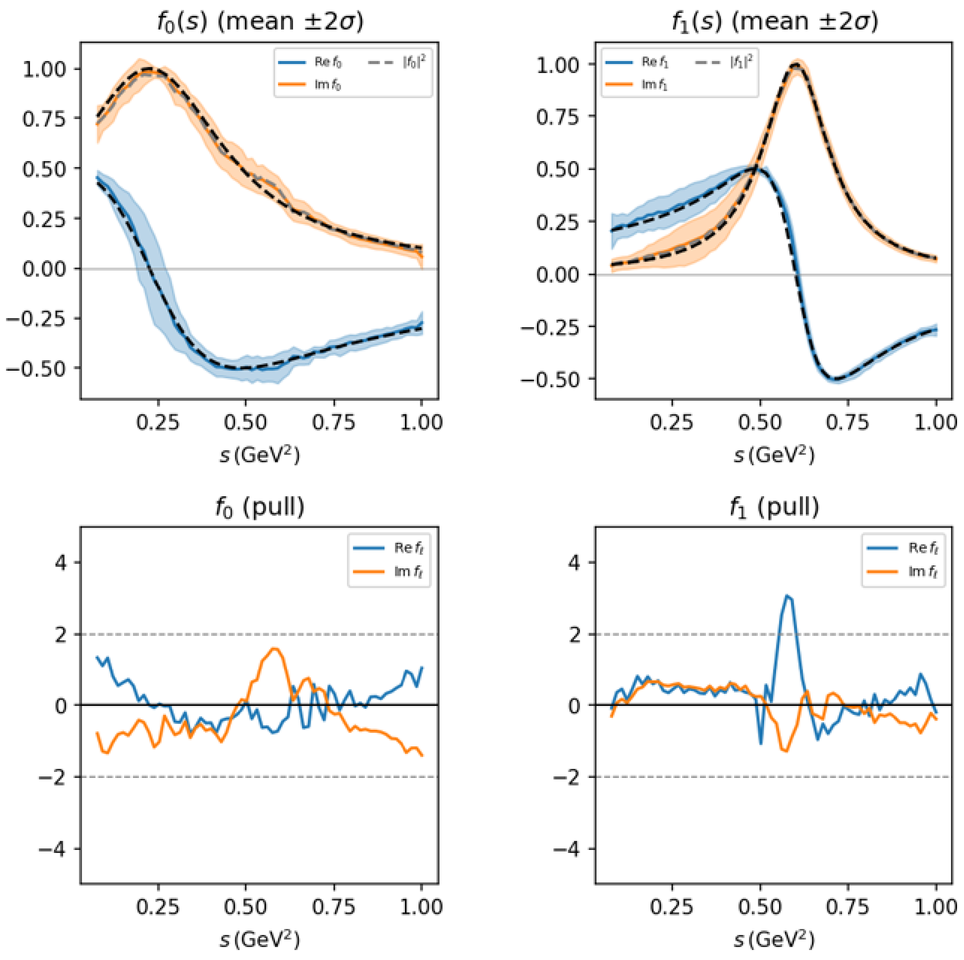


Preliminary results: partial waves $\ell = 0, 1$

$\sigma = 0.05$

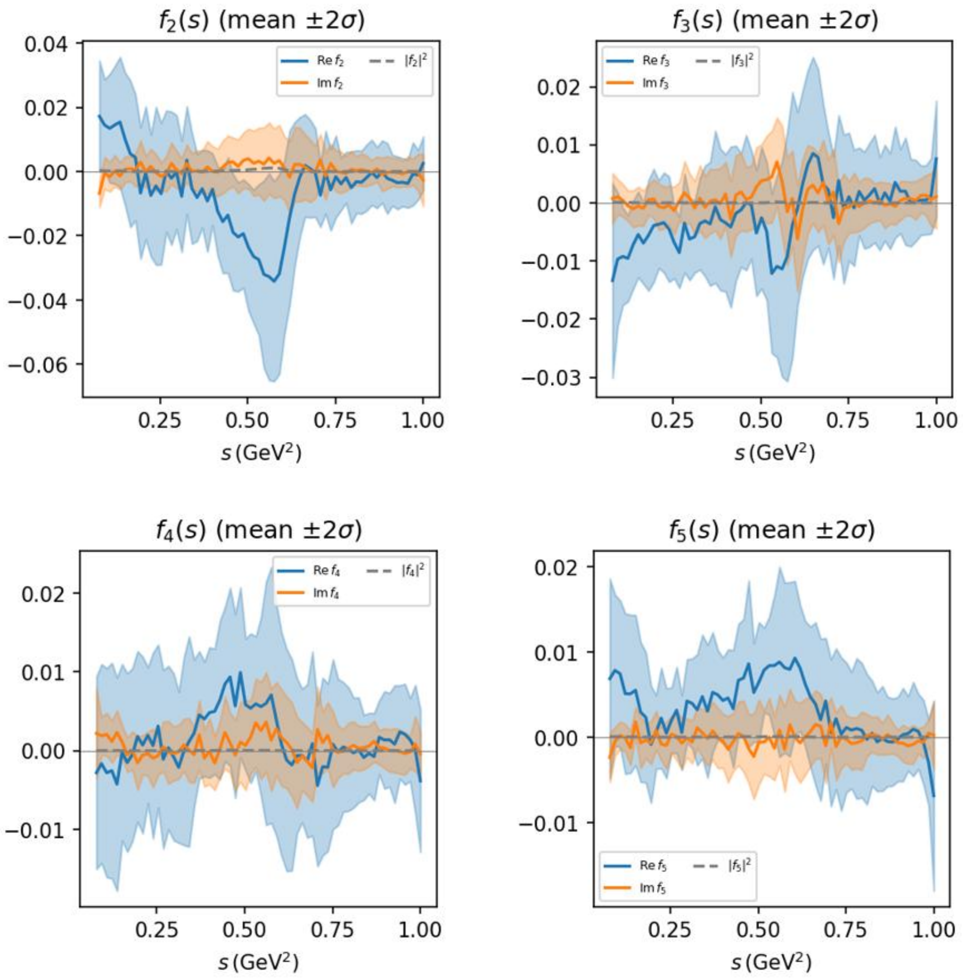


$\sigma = 0.10$

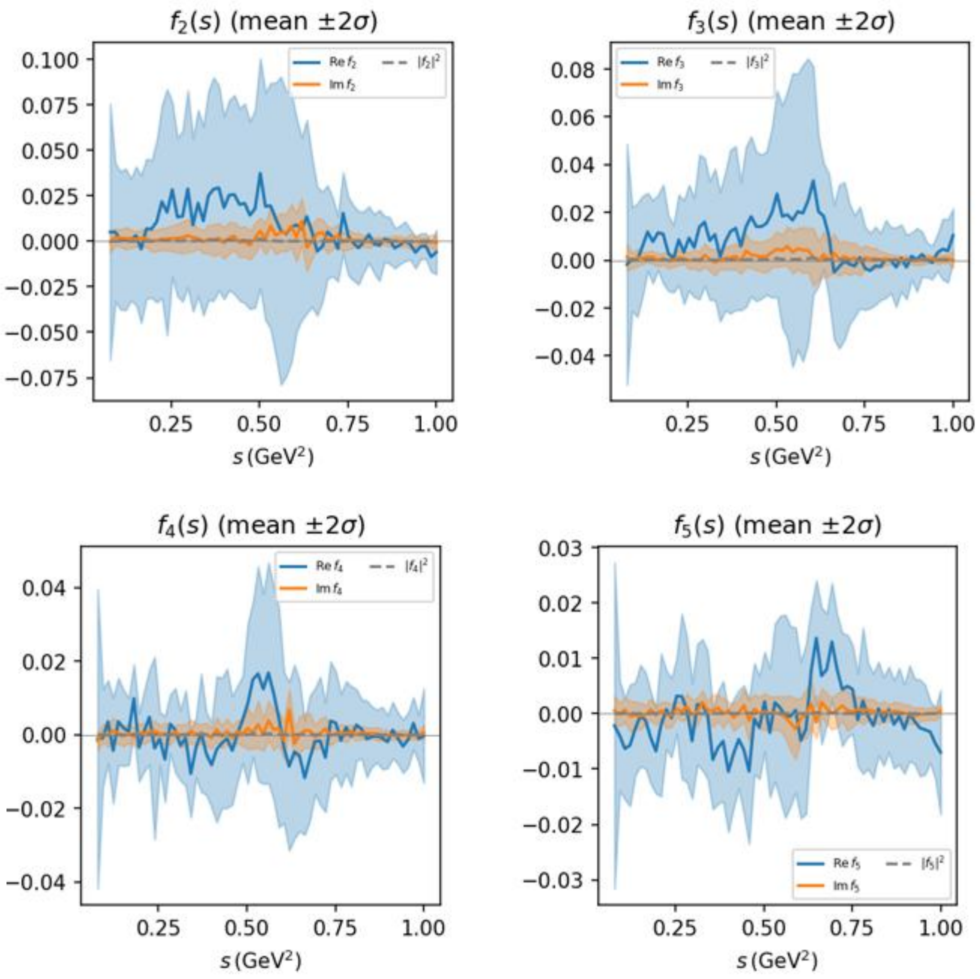


Preliminary results: higher partial waves

$\sigma = 0.05$



$\sigma = 0.10$



Conclusions & outlook

- Amplitude reconstruction from cross section is an ill-posed inverse problem
- Generative models with S-matrix constraints to solve it
- Can handle noisy pseudodata
- Questions:
  - Can we scale to inelastic scattering ($\pi\pi \leftrightarrow K\bar{K}$)?
    channels with spin ($\gamma p \to \pi N$)?
    $2 \to 3$ reactions?
  - Apply to real experimental data from Jefferson Lab

- GANs are difficult to train: consider alternative generative models