Truncated partial-wave analysis using Bayesian statistics

work done in collaboration with:

Philipp Kroenert, Farah Afzal and Annika Thiel

[Phys. Rev. C **109**, no.4, 045206 (2024)]

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May 31st, 2024

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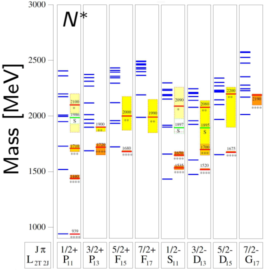
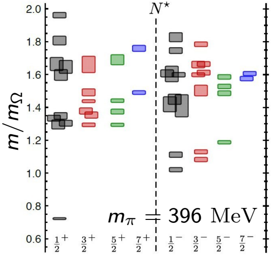
Introduction: Why baryon spectroscopy?

Quark models



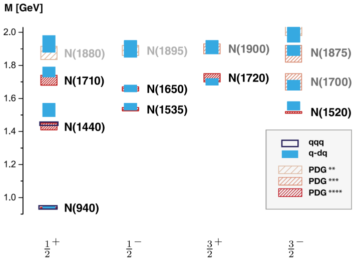
[U. Löring et al., EPJ A **10**, 395 (2001)]

Lattice QCD



[R. Edwards et al., Phys. Rev. D **84**, 07450 (2011)]

DSE-/BSE framework



[G. Eichmann and Ch. S. Fischer, Few Body Syst. **60** (2019) 1, 2]

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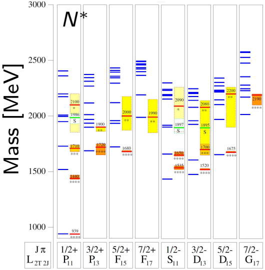

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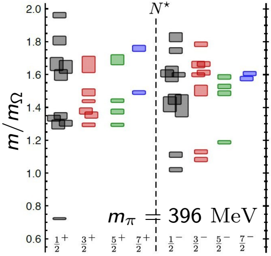

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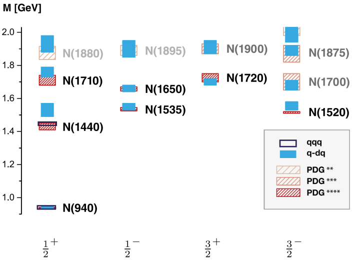

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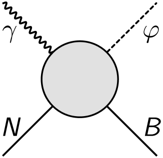
Extract resonances from scattering-data via partial-wave analysis (PWA)

- $*$) Energy-dependent PWA: Reaction theoretic models; extract resonance poles in complex energy-plane; [BnGa], [JüBo], ...
- $*$) Single-energy PWA: Extract partial waves themselves at discrete energies on the real energy-axis $\hookrightarrow$ This work (!): η photoproduction $\gamma N \longrightarrow \eta N$

Photoproduction amplitudes

Photoproduction amplitude in the CMS (e.g. $\gamma N \longrightarrow \eta N$):



$$= \mathcal{T}_{fi} = \mathcal{C}\chi^{\dagger}_{m_{s_f}} \Big[i\vec{\sigma}\cdot\hat{\epsilon}F_1 + \vec{\sigma}\cdot\hat{q}\vec{\sigma}\cdot\left(\hat{k}\times\hat{\epsilon}\right)F_2 + i\vec{\sigma}\cdot\hat{k}\hat{q}\cdot\hat{\epsilon}F_3 + i\vec{\sigma}\cdot\hat{q}\hat{q}\cdot\hat{\epsilon}F_4 \Big]\chi_{m_{s_i}}$$

[Chew, Goldberger, Low & Nambu (1957)]

$\rightarrow$ Process fully described by 4 complex amplitudes $F_i\left(W,\theta\right)$.

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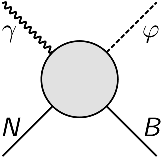

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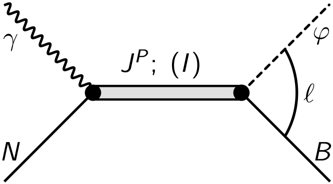
→ Process fully described by 4 complex amplitudes $F_i\left(W,\theta\right)$.

Important concept: expansion of full amplitudes into partial waves:

$$F_1\left(W,\theta\right) = \sum_{\ell=0}^{\infty} \Big\{ \left[\ell M_{\ell+} + E_{\ell+}\right] P^{'}_{\ell+1}\left(\cos\left(\theta\right)\right) + \left[\left(\ell+1\right)M_{\ell-} + E_{\ell-}\right] P^{'}_{\ell-1}\left(\cos\left(\theta\right)\right) \Big\}$$

$$F_2\left(W,\theta\right) = \ldots$$



∗) $J = |\ell \pm 1/2|$, $P = (-)^{\ell+1}$.

∗) s-chn. resonance $J^P;\ (I)$

↕

multipole $E^{(I)}_{\ell\pm},\ M^{(I)}_{\ell\pm}$

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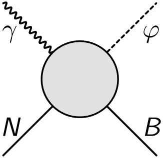

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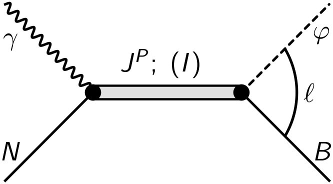

In practice:

Truncate at some finite $\ell_{\max}$
$\rightarrow$ Try to extract the $4\ell_{\max}$ complex multipoles in a fit to the data.

Photoproduction amplitudes - II

The multipole-series fully written out ($x = \cos\theta$):

$$F_1(W,\theta) = \sum_{\ell=0}^{\not\infty\,\ell_{\max}} \left[\ell M_{\ell+}(W) + E_{\ell+}(W)\right] P^{'}_{\ell+1}(x) + \left[(\ell+1) M_{\ell-}(W) + E_{\ell-}(W)\right] P^{'}_{\ell-1}(x)\,,$$

$$F_2(W,\theta) = \sum_{\ell=1}^{\not\infty\,\ell_{\max}} \left[(\ell+1) M_{\ell+}(W) + \ell M_{\ell-}(W)\right] P^{'}_{\ell}(x)\,,$$

$$F_3(W,\theta) = \sum_{\ell=1}^{\not\infty\,\ell_{\max}} \Big\{ \left[E_{\ell+}(W) - M_{\ell+}(W)\right] P^{''}_{\ell+1}(x) + \left[E_{\ell-}(W) + M_{\ell-}(W)\right] P^{''}_{\ell-1}(x) \Big\},$$

$$F_4(W,\theta) = \sum_{\ell=2}^{\not\infty\,\ell_{\max}} \left[M_{\ell+}(W) - E_{\ell+}(W) - M_{\ell-}(W) - E_{\ell-}(W)\right] P^{''}_{\ell}(x)\,,$$

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- $*)$ $4\ell_{\max}$ complex multipoles present in every truncation-order $\ell_{\max} \geq 1$:

$$\{E_{0+}, E_{1+}, M_{1+}, M_{1-}, E_{2+}, E_{2-}, \ldots, M_{\ell_{\max}-}\}.$$

- $*)$ Multipoles determined up to 1 overall phase (!):

$$\Rightarrow 2 \times 4\ell_{\max} - 1 = \underline{8\ell_{\max} - 1} \text{ parameters in the TPWA.}$$

Polarization observables

Observable	Transversity representation	Type
σ_0	$\frac{1}{2}\left(\lvert b_1\rvert^2 + \lvert b_2\rvert^2 + \lvert b_3\rvert^2 + \lvert b_4\rvert^2\right)$	
$\check{\Sigma}$	$\frac{1}{2}\left(-\lvert b_1\rvert^2 - \lvert b_2\rvert^2 + \lvert b_3\rvert^2 + \lvert b_4\rvert^2\right)$	$\mathcal{S}$
$\check{T}$	$\frac{1}{2}\left(\lvert b_1\rvert^2 - \lvert b_2\rvert^2 - \lvert b_3\rvert^2 + \lvert b_4\rvert^2\right)$	
$\check{P}$	$\frac{1}{2}\left(-\lvert b_1\rvert^2 + \lvert b_2\rvert^2 - \lvert b_3\rvert^2 + \lvert b_4\rvert^2\right)$	
$\check{G}$	$\mathrm{Im}\left[-b_1 b_3^* - b_2 b_4^*\right]$	
$\check{H}$	$-\mathrm{Re}\left[b_1 b_3^* - b_2 b_4^*\right]$	$\mathcal{BT}$
$\check{E}$	$-\mathrm{Re}\left[b_1 b_3^* + b_2 b_4^*\right]$	
$\check{F}$	$\mathrm{Im}\left[b_1 b_3^* - b_2 b_4^*\right]$	
$\check{O}_{x'}$	$-\mathrm{Re}\left[-b_1 b_4^* + b_2 b_3^*\right]$	
$\check{O}_{z'}$	$\mathrm{Im}\left[-b_1 b_4^* - b_2 b_3^*\right]$	$\mathcal{BR}$
$\check{C}_{x'}$	$\mathrm{Im}\left[b_1 b_4^* - b_2 b_3^*\right]$	
$\check{C}_{z'}$	$\mathrm{Re}\left[b_1 b_4^* + b_2 b_3^*\right]$	
$\check{T}_{x'}$	$-\mathrm{Re}\left[-b_1 b_2^* + b_3 b_4^*\right]$	
$\check{T}_{z'}$	$-\mathrm{Im}\left[b_1 b_2^* - b_3 b_4^*\right]$	$\mathcal{TR}$
$\check{L}_{x'}$	$-\mathrm{Im}\left[-b_1 b_2^* - b_3 b_4^*\right]$	
$\check{L}_{z'}$	$\mathrm{Re}\left[-b_1 b_2^* - b_3 b_4^*\right]$	

$*$) Transversity amplitudes: $b_i = \sum_j M_{ij} F_j$.
(Different scheme of spin-quantization)

$*$) Observables simplify:

$$\check{\Omega}^{\alpha} = \frac{1}{2} \sum_{i,j} b_i^* \tilde{\Gamma}^{\alpha}_{ij} b_j .$$

Ambiguities of the TPWA problem

$*)$ Consider $\left\{\sigma_0, \check{\Sigma}, \check{T}, \check{P}\right\}$, i.e. $\check{\Omega}^{\alpha s} \propto \pm \left|b_1\right|^2 \pm \left|b_2\right|^2 \pm \left|b_3\right|^2 + \left|b_4\right|^2$.

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*) <u>Instead:</u> Use $t := \tan\left(\frac{\theta}{2}\right)$ and write linear factorizations (for finite ℓ_{max}):

$$b_1(\theta) \propto \frac{\exp\left(-i\frac{\theta}{2}\right)}{\left(1+t^2\right)^{\ell_{\mathrm{max}}}} \prod_{j=1}^{2\ell_{\mathrm{max}}} (t+\beta_j), \; b_2(\theta) \propto \frac{\exp\left(i\frac{\theta}{2}\right)}{\left(1+t^2\right)^{\ell_{\mathrm{max}}}} \prod_{j=1}^{2\ell_{\mathrm{max}}} (t-\beta_j),$$

$$b_3(\theta) \propto \frac{\exp\left(-i\frac{\theta}{2}\right)}{\left(1+t^2\right)^{\ell_{\mathrm{max}}}} \prod_{k=1}^{2\ell_{\mathrm{max}}} (t+\alpha_k), \; b_4(\theta) \propto \frac{\exp\left(i\frac{\theta}{2}\right)}{\left(1+t^2\right)^{\ell_{\mathrm{max}}}} \prod_{k=1}^{2\ell_{\mathrm{max}}} (t-\alpha_k),$$

with $4\ell_{\mathrm{max}}$ complex roots $\{\alpha_k, \beta_j\}$ equivalent to multipoles, i.e.

$$\{E_{\ell\pm}, M_{\ell\pm}\} \Leftrightarrow \{\alpha_k, \beta_j\},$$

if and only if the <u>constraint</u>: $\prod_{k=1}^{2\ell_{\mathrm{max}}} \alpha_k = \prod_{j=1}^{2\ell_{\mathrm{max}}} \beta_j$ is satisfied.

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$\hookrightarrow$ The complex conjugation of roots leaves the group $\mathcal{S}$ invariant:

$$(t-\alpha^*)(t-\alpha) \xrightarrow{\alpha\to\alpha^*} \left(t-[\alpha^*]^*\right)(t-\alpha^*) = (t-\alpha^*)(t-\alpha).$$

$\Rightarrow$ Mechanism can result in *multiple 'solutions' (or 'modes')* of single-energy fit!

Bayes' Theorem and Bayesian inference

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$*$) Obtain *parametric version* by making the 'choice': $\begin{cases} A = \boldsymbol{\theta} (\text{parameters}), \\ B = \boldsymbol{y} (\text{data}), \end{cases}$

$$\Rightarrow \quad \underbrace{p(\boldsymbol{\theta}|\boldsymbol{y})}_{\text{'posterior'}} = \frac{\overbrace{p(\boldsymbol{y}|\boldsymbol{\theta})}^{\text{'likelihood'}} \overbrace{p(\boldsymbol{\theta})}^{\text{'prior'}}}{\underbrace{\int d^D\theta \, p(\boldsymbol{y}|\boldsymbol{\theta}) \, p(\boldsymbol{\theta})}_{\text{'Bayesian evidence'}}}.$$

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∗) In our case, i.e. for the TPWA:

- $\boldsymbol{\theta} = \{E_{\ell\pm}, M_{\ell\pm}\}$ (option: *nuisance parameters* to model syst. errors),
- $\boldsymbol{y} = [\boldsymbol{y}^{\sigma_0}, \boldsymbol{y}^{\check{G}}, \ldots, \boldsymbol{y}^{\check{F}}]^T$: values of measured observables,
- Likelihood has 'exp$[-\frac{1}{2}\chi^2]$-form', with a *correlated chisquare*:
  $p(\boldsymbol{y}|\boldsymbol{\theta}) = \frac{1}{\sqrt{(2\pi)^N |\boldsymbol{\Lambda}|}} \exp\left[-\frac{1}{2}\left(\boldsymbol{y} - \boldsymbol{\mu}\right)^T \boldsymbol{\Lambda}^{-1} \left(\boldsymbol{y} - \boldsymbol{\mu}\right)\right]$, $\{\boldsymbol{\Lambda}$: cov.-matrix$\}$
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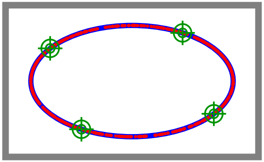
⇒ We want to obtain individual distribution for each parameter θ_i from the *un*normalized posterior

→ *Marginalize*: $p(\theta_i|y) = \int \ldots \int d\theta_1 \ldots d\theta_{i-1} d\theta_{i+1} \ldots d\theta_D\, p(\theta_1 \ldots \theta_D|\boldsymbol{y})$,

→ Complicated integrals! Use (Markov chain) Monte Carlo methods ...

Solution strategy for multimodal posteriors

I. Monte Carlo maximum a posteriori estimation:
minimize the function $\chi^2(\boldsymbol{\theta}) + P(\boldsymbol{\theta})$ ('P': contains possible penalty-terms for nuisance parameters).
Employ Monte Carlo sampling, with N_{MC} initial conditions and equally many fits ($N_{MC} \simeq 10000$).
$\Rightarrow$ Filter non-redundant sol.'s via clustering-algorithm



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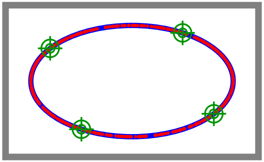
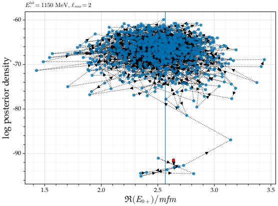
II. Sampling the posterior:
Each solution found in step 'I.' is used as initial condition for the *Hamilton Monte Carlo (HMC)* algorithm as implemented in `Stan`.
For each solution, use $N_c \simeq 10$ Markov chains and $S \simeq 100000$ sampling points (50000 'warmup'-pts).





[Fig. courtesy of P. Kroenert] [YW, arXiv:2008.00514]

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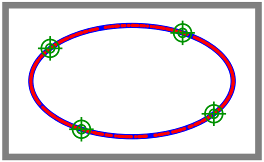

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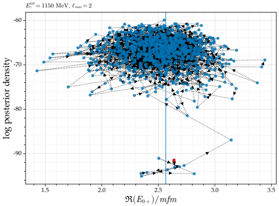


[Fig. courtesy of P. Kroenert] [YW, arXiv:2008.00514]

III. **Monte Carlo convergence diagnostics:**

- Cluster the chains into groups according to their sampled parameter space (calculate vector of quantiles for each chain $\rightarrow$ evaluate distance-matrix among quantile-vectors $\rightarrow$ input to `DBSCAN`-algorithm),

$\rightarrow$ Apply MC convergence diagnostics ($\hat{R}$-statistic, MC standard error) to *each group individually*.

Solution strategy for multimodal posteriors

I. Monte Carlo maximum a posteriori estimation,

II. Sampling the posterior,

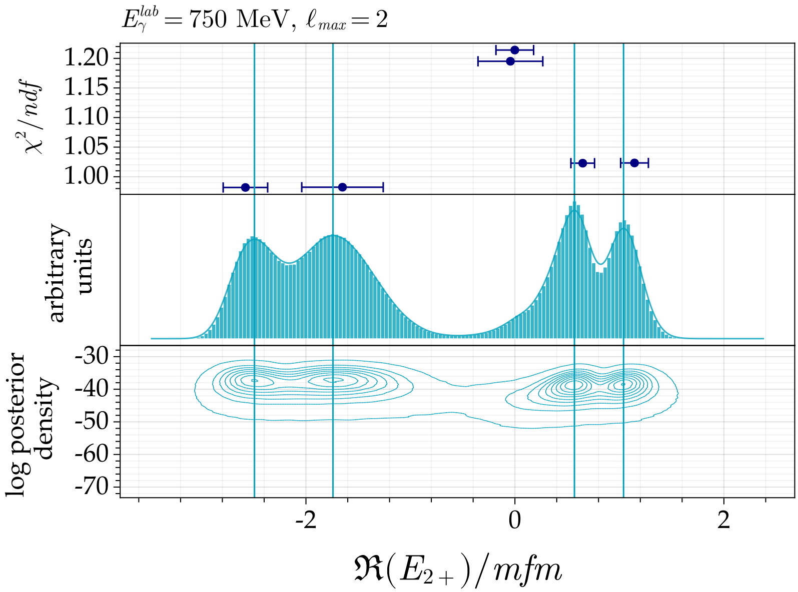
III. Monte Carlo convergence diagnostics,

$\hookrightarrow$ Apply the above-described procedure to a selected set of 6 polarization observables for the process $\gamma p \longrightarrow \eta p$:

Observable	No. of datapoints	Exp. facility	References
σ_0	5736	MAMI	[Kashevarov et al., PRL **118**, 212001 (2017)]
T, F	144	MAMI	[Akondi et al., PRL **113**, 102001 (2014)]
Σ	140	GRAAL	[Bartalini et al., EPJ A **33**, 169 (2007)]
E	84	MAMI	[F. Afzal, PhD thesis, ULB Bonn (2019)]
G	47	CBELSA/TAPS	[Müller et al., Phys. Lett. B **803**, 135323 (2020)]

[cf.: P. Kroenert, YW, F. Afzal and A. Thiel, Phys. Rev. C **109**, no.4, 045206 (2024)]

Example: full results for one 'fit-parameter'



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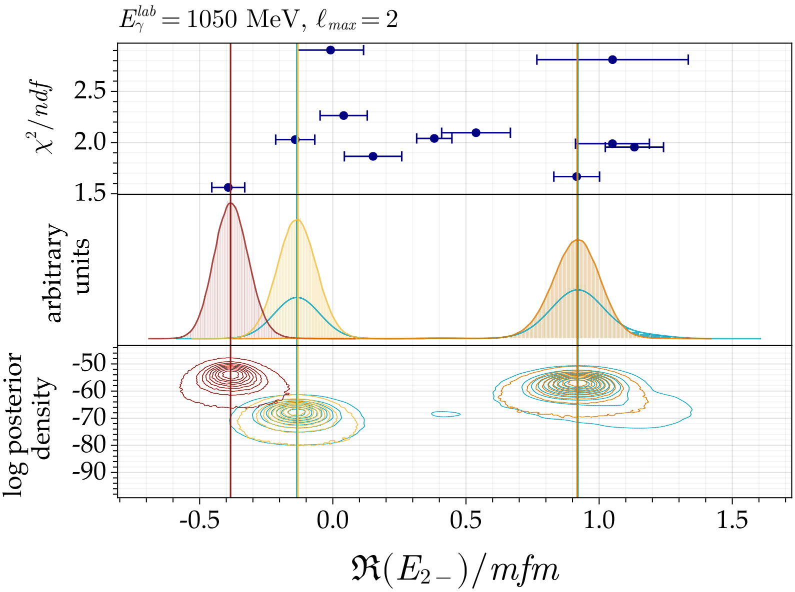
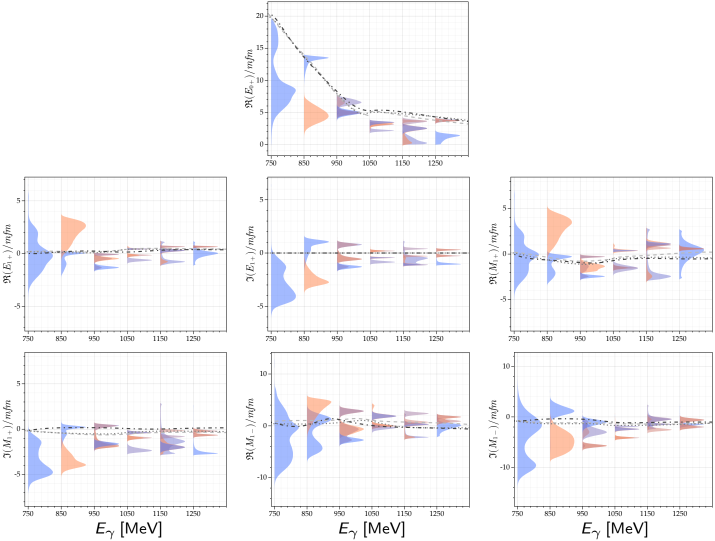


$\ell_{\max} = 2$: results for multipoles



<u>PWA-curves:</u>

EtaMAID2018 (dashed); BnGa-2019 (dotted); Jülich-Bonn-2022 (dash-dotted);

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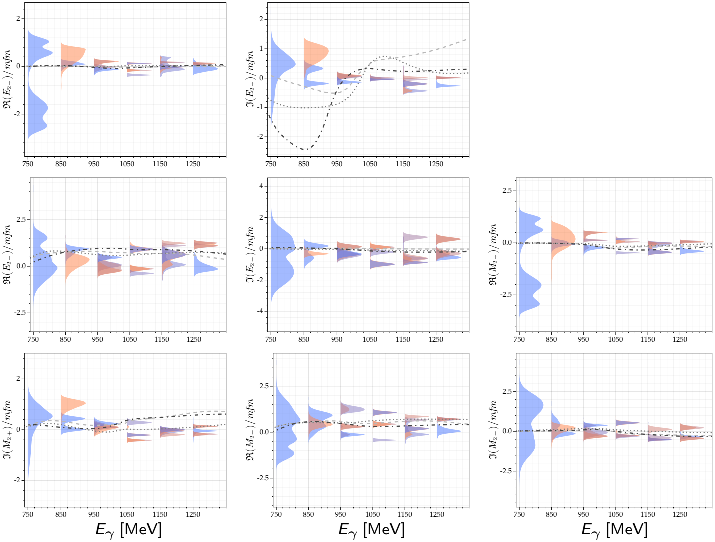

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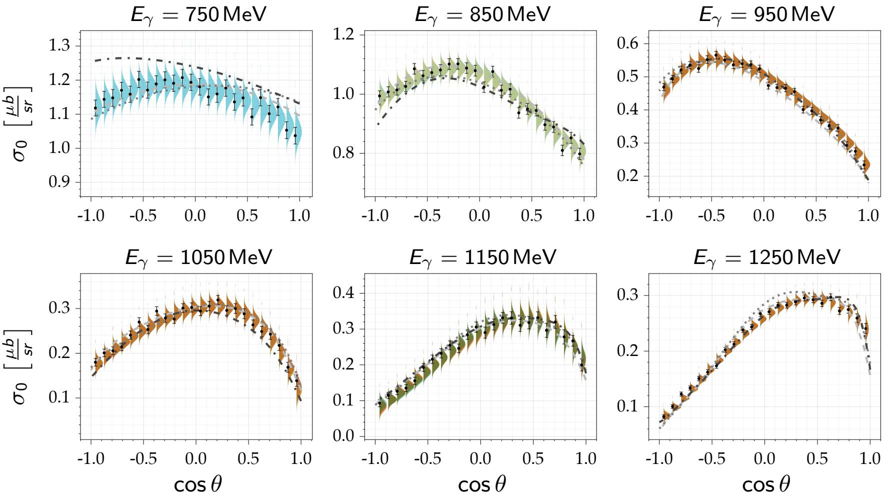
$\ell_{\max} = 2$: reproduced data



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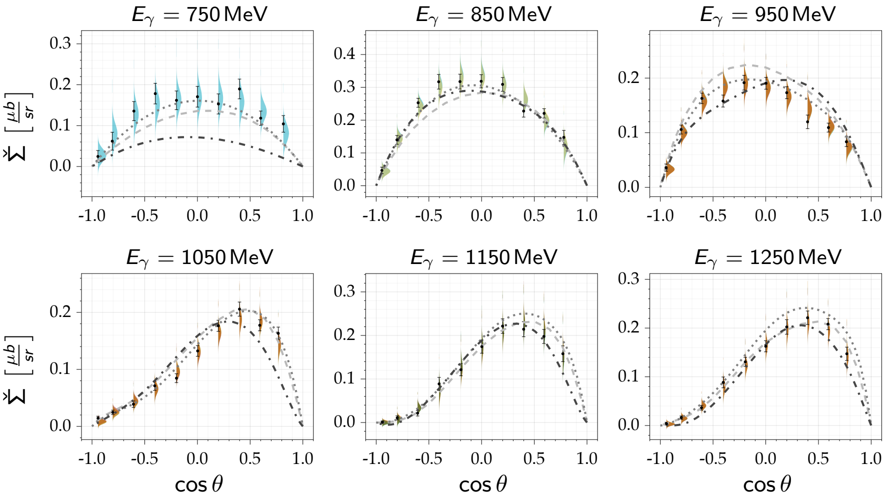

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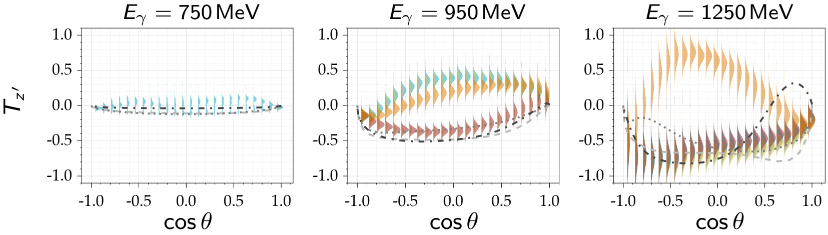
$\ell_{\max} = 2$: predicted data-distributions



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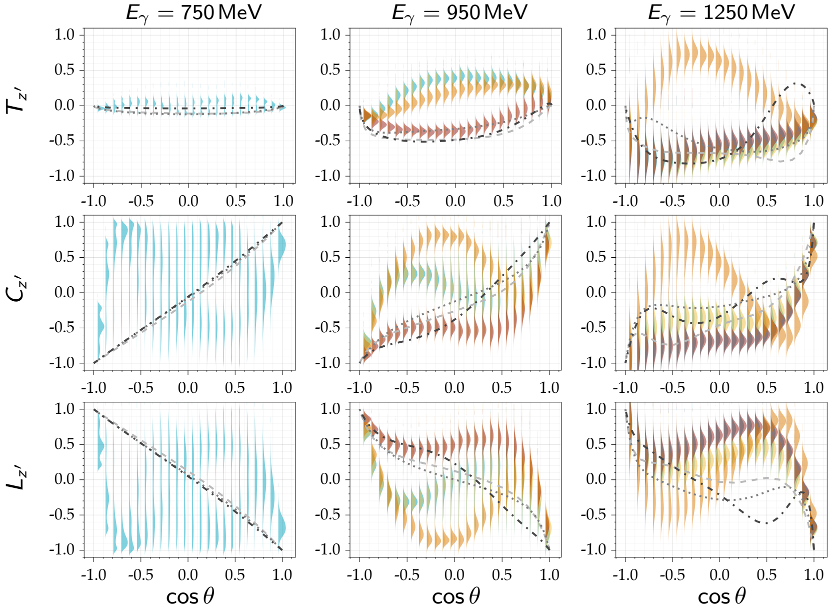

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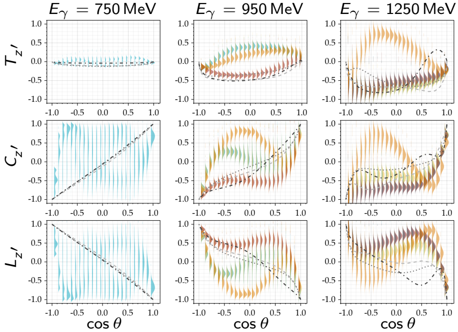

$\hookrightarrow$ Predict promising *candidate observables* for resolving discrete ambiguities:

E_γ^{lab} / MeV	Observables
750	$C_{x'}, C_{z'}, L_{x'}, L_{z'}$
850	$C_{x'}, C_{z'}, L_{x'}, L_{z'}, T_{x'}, T_{z'}$
950	$C_{x'}, C_{z'}, L_{x'}, L_{z'}, T_{z'}$
1050	$C_{x'}, C_{z'}, L_{x'}, O_{z'}, T_{z'}$
1150	$C_{z'}, O_{x'}, T_{x'}, T_{z'}$
1250	$C_{z'}$

cf.:[P. Kroenert, YW, F. Afzal and A. Thiel, Phys. Rev. C **109**, no.4, 045206 (2024)]

$\ell_{\text{max}} = 3$: systematics studies and ambiguities

Analyze data with $\underline{\ell_{\text{max}} = 3}$: (Trial for $E_\gamma = 1250$ MeV)

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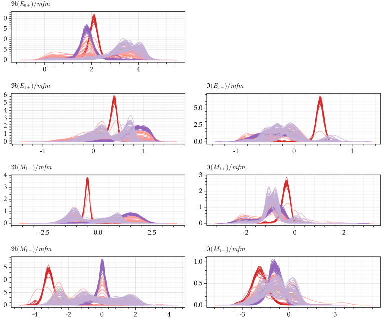
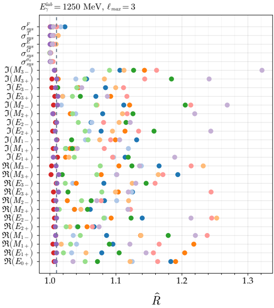
→ *Larger numerical effort* due to larger set of possible initial-conditions ('ambiguities'),

→ Chain-clustering difficult,

→ Hard to reach good/acceptable MCMC convergence-diagnostics:
- More chains needed for each initial config.,
- More iterations for each individual chain.





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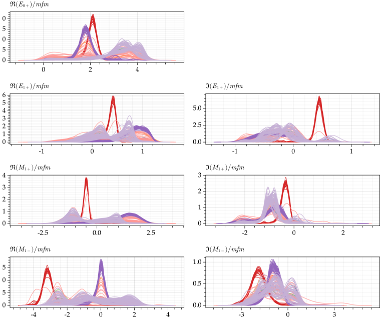

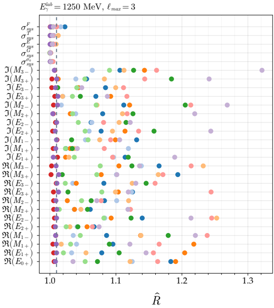

Things to think (/worry) about:

- *In addition* to the usual (discrete) PWA-ambiguities, we have to face the so-called *curse of dimensionality*,
- In particular: in higher dimensions, largest part of posteriors probability-mass concentrates in thin strip *away from the mode* ('typical set'), since:

$$\text{'probability-mass'} = \mathbb{P} \times \text{'parameter-volume'}.$$

Thank You!