Using the Mainz Multipole Fitter `PWA`

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Abstract

This document describes details and usage of the Mainz `PWA` tool used to determine electromagnetic multipoles for pseudoscalar meson photoproduction from experimental results for cross sections and various polarisation observables. `PWA` performs constrained single energy (SE) fits based on a χ^2 minimisation scheme with additional penalty terms.

1 Introduction

`PWA` is a MINUIT-based single energy (SE) multipole fitting tool, used to determine electromagnetic multipoles for pseudoscalar meson photoproduction (π, η, K, ...) from experimental cross sections (polarised and unpolarised) and/or asymmetry observables. Multipoles are extracted using a standard χ^2 minimisation scheme with the possibility to add additional constraints imposed by existing partial wave analyses and models for meson photoproduction (MAID, SAID, BnGa, ...). These constraints are implemented using so-called penalty terms, giving an additional contribution in the minimisation process. The maximum multipole order $L_{\max}$ which is considered to contribute to physical observables can be adjusted up to $L_{\max} = 10$. Indvidiual multipoles can either be fitted in real and imaginary parts, with fixed phases but fittable magnitude, or can be fixed to model predictions completely.

2 χ^2 minimisation and multipole extraction

`PWA` determines electromagnetic multipoles as fit parameters in a χ^2 minimisation process with respect to experimental photoproduction results in form of the standard photoproduction observables, which are typically given in four groups

$$
\begin{aligned}
\text{Group } S: & \quad \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \sigma_0, \Sigma, T, P \\
\text{Group } BT: & \quad E, F, G, H \\
\text{Group } BR: & \quad C_{x'}, C_{z'}, O_{x'}, O_{z'} \\
\text{Group } TR: & \quad T_{x'}, T_{z'}, L_{x'}, L_{z'}
\end{aligned}
$$

Right now, `PWA` only supports observable data for groups S, BT, and BR. These observables can be expressed in form of the four CGLN amplitudes F_i according to

$$
\begin{aligned}
\sigma_0 &= \operatorname{Re}\left\{|F_1|^2 + |F_2|^2 - 2\cos\theta F_1^* F_2 + \tfrac{1}{2}\sin^2\theta\left[|F_3|^2 + |F_4|^2 + 2F_2^* F_3 + 2F_1^* F4 + 2\cos\theta F_3^* F_4\right]\right\} \cdot \rho \\
\sigma_0\Sigma &= -\tfrac{1}{2}\sin^2\theta \operatorname{Re}\left\{|F_3|^2 + |F_4|^2 + 2\left[F_2^* F_3 + F_1^* F_4 + \cos\theta F_3^* F_4\right]\right\} \cdot \rho \\
\sigma_0 T &= \sin\theta \operatorname{Im}\left\{F_1^* F_3 - F_2^* F_4 + \cos\theta\left(F_1^* F_4 - F_2^* F_3\right) - \sin^2\theta F_3^* F_4\right\} \cdot \rho \\
\sigma_0 P &= \sin\theta \operatorname{Im}\left\{F_2^* F_4 - 2F_1^* F_2 - F_1 F_3 + \cos\theta\left(F_2^* F_3 - F_1^* F_4\right) + \sin^2\theta F_3^* F_4\right\} \cdot \rho \\
\sigma_0 E &= \operatorname{Re}\left\{|F_1|^2 + |F_2|^2 - 2\cos\theta F_1^* F_2 + \sin^2\theta\left(F_2^* F_3 + F_1^* F_4\right)\right\} \cdot \rho \\
\sigma_0 F &= \sin\theta \operatorname{Re}\left\{F_1^* F_3 - F_2^* F_4 + \cos\theta\left(F_1^* F_4 + F_2^* F_3\right)\right\} \cdot \rho \\
\sigma_0 G &= \sin^2\theta \operatorname{Im}\left\{F_2^* F_3 + F_1^* F_4\right\} \cdot \rho \\
\sigma_0 H &= \sin\theta \operatorname{Im}\left\{2F_1^* F_2 + F_1^* F_3 - F_2^* F_4 - \cos\theta\left(F_2^* F_3 - F_1^* F_4\right)\right\} \cdot \rho
\end{aligned}
$$

$$\sigma_0 O_{x'} = -\sin\theta \, \text{Im} \left\{ F_1^* F_4 - F_2^* F_3 + \cos\theta \left(F_1^* F_3 - F_2^* F_4 \right) \right\} \cdot \rho$$

$$\sigma_0 O_{z'} = -\sin^2\theta \, \text{Im} \left\{ F_1^* F_3 + F_2^* F_4 \right\} \cdot \rho$$

$$\sigma_0 C_{x'} = \sin\theta \, \text{Re} \left\{ |F_1|^2 - |F_2|^2 + F_1^* F_3 - F_2^* F_3 + \cos\theta \left(F_1^* F_3 - F_2^* F_4 \right) \right\} \cdot \rho$$

$$\sigma_0 C_{z'} = \text{Re} \left\{ 2 F_1^* F_2 + \sin^2\theta \left(F_1^* F_3 + F_2^* F_4 \right) - \cos\theta \left(|F_1|^2 + |F_2|^2 \right) \right\} \cdot \rho$$

with a phase space factor $\rho = \frac{q}{k}$ given by pion and photon momenta q and k. The CGLN amplitudes depend on the electromagnetic multipoles $E_{L\pm}$, $M_{L\pm}$ for multipole orders L up to $L_{\max}$

$$F_1 = \sum_{L \geq 0}^{L_{\max}} \left\{ (L \cdot M_{L+} + E_{L+}) P'_{L+1} + [(L+1) \cdot M_{L-} + E_{L-} \,] P'_{L-1} \right\}$$

$$F_2 = \sum_{L \geq 1}^{L_{\max}} \left[(L+1) \cdot M_{L+} + L \cdot M_{L-} \, \right] P'_L$$

$$F_3 = \sum_{L \geq 1}^{L_{\max}} \left[(E_{L+} - M_{L+}) P''_{L+1} + (E_{L-} + M_{L-}) P''_{L-1} \right]$$

$$F_4 = \sum_{L \geq 2}^{L_{\max}} (M_{L+} - E_{L+} - M_{L-} - E_{L-}) P''_L$$

and derivatives of the Legendre polynoms P_L describing the angular dependencies. Using these relations between observables and electromagnetic multipoles, it is possible to create a χ^2 function having multipoles as fit parameters and physical observables as experimental input

$$
\begin{aligned}
\chi^2 = & \sum_i \left(\frac{\sigma_0^{\exp}(\theta_i) - \sigma_0^{\text{fit}}(\theta_i)}{\Delta \sigma_0^{\exp}(\theta_i)} \right)^2 \\
& + \sum_i \left(\frac{\Sigma^{\exp}(\theta_i) - \Sigma^{\text{fit}}(\theta_i)}{\Delta \Sigma^{\exp}(\theta_i)} \right)^2 + \sum_i \left(\frac{\sigma_\Sigma^{\exp}(\theta_i) - \sigma_\Sigma^{\text{fit}}(\theta_i)}{\Delta \sigma_\Sigma^{\exp}(\theta_i)} \right)^2 \\
& + \sum_i \left(\frac{T^{\exp}(\theta_i) - T^{\text{fit}}(\theta_i)}{\Delta T^{\exp}(\theta_i)} \right)^2 + \sum_i \left(\frac{\sigma_T^{\exp}(\theta_i) - \sigma_T^{\text{fit}}(\theta_i)}{\Delta \sigma_T^{\exp}(\theta_i)} \right)^2 \\
& + \sum_i \left(\frac{P^{\exp}(\theta_i) - P^{\text{fit}}(\theta_i)}{\Delta P^{\exp}(\theta_i)} \right)^2 + \sum_i \left(\frac{\sigma_P^{\exp}(\theta_i) - \sigma_P^{\text{fit}}(\theta_i)}{\Delta \sigma_P^{\exp}(\theta_i)} \right)^2 \\
& + \sum_i \left(\frac{E^{\exp}(\theta_i) - E^{\text{fit}}(\theta_i)}{\Delta E^{\exp}(\theta_i)} \right)^2 + \sum_i \left(\frac{\sigma_E^{\exp}(\theta_i) - \sigma_E^{\text{fit}}(\theta_i)}{\Delta \sigma_E^{\exp}(\theta_i)} \right)^2 \\
& + \sum_i \left(\frac{F^{\exp}(\theta_i) - F^{\text{fit}}(\theta_i)}{\Delta F^{\exp}(\theta_i)} \right)^2 + \sum_i \left(\frac{\sigma_F^{\exp}(\theta_i) - \sigma_F^{\text{fit}}(\theta_i)}{\Delta \sigma_F^{\exp}(\theta_i)} \right)^2 \\
& + \sum_i \left(\frac{G^{\exp}(\theta_i) - G^{\text{fit}}(\theta_i)}{\Delta G^{\exp}(\theta_i)} \right)^2 + \sum_i \left(\frac{\sigma_G^{\exp}(\theta_i) - \sigma_G^{\text{fit}}(\theta_i)}{\Delta \sigma_G^{\exp}(\theta_i)} \right)^2 \\
& + \sum_i \left(\frac{H^{\exp}(\theta_i) - H^{\text{fit}}(\theta_i)}{\Delta H^{\exp}(\theta_i)} \right)^2 + \sum_i \left(\frac{\sigma_H^{\exp}(\theta_i) - \sigma_H^{\text{fit}}(\theta_i)}{\Delta \sigma_H^{\exp}(\theta_i)} \right)^2
\end{aligned}
$$

where $\sigma_X^{\exp}(\theta_i)$, $X^{\exp}(\theta_i)$ describe experimental cross sections and asymmetries at their polar angle positions θ_i, while $\sigma_X^{\text{fit}}(\theta_i)$, $X^{\text{fit}}(\theta_i)$ are cross sections and asymmetries as calculated from multipole parameters $E_{L\pm}$, $M_{L\pm}$. Minimisation of the above χ^2 function will therefore adjust electromagnetic multipole values in order for the best description of available data. `PWA` will use asymmetries X as well as polarised cross sections $\sigma_X = \sigma_0 \cdot X$ as experimental input, so there is no need to transform one type of experimental information to another beforehand.

3 Penalty terms

Penalty terms act as an additional contribution to the function to be minimised during the fit process, i.e. fitting with penalty no longer mminimises the 'pure' χ^2 but instead

$$f_{\text{FCN}} = \chi^2 + Q$$

where Q is typically designed in a way that it gets larger if current fit parameters deviate from a given model solution. Hence any deviation from the used model is 'penalised' in the fitting. The found solution for fit parameters is therefore a compromise between the best description of the available data (contributing to χ^2) and an agreement with a given model calculation (contributing to Q). Penalty terms in the f_{FCN} function are useful to ensure that results of SE fits at different energies fulfill constraints like a smooth energy dependence and can help to get reasonable fit results if experimental data is too scarce (in terms of the number of observables or angular coverage) or has limited precision. If however the penalty terms dominate the f_{FCN} function, the found solutions will mainly try to reproduce the initial model calculation. Therefore a penalty-supported fit is

never a fully model-independent solution but will always show some bias caused by the used model calculation. Proper adjustment of penalty and χ^2 constributions is crucial in order to get meaningful fit results. `PWA` supports a variety of different penalty implementations that either evaluate model multipoles directly or with an intermediate step of meson photoproduction amplitudes.

3.1 Penalty mode *MLP1*

The *MLP1* penalty calculation evaluates a penalty term Q_1 from the squared sum of all absolute deviations between fitted ($E_{L\pm}^{\text{fit}}$, $M_{L\pm}^{\text{fit}}$) and model ($E_{L\pm}^{\text{sol}}$, $M_{L\pm}^{\text{sol}}$) multipoles, according to

$$
\begin{aligned}
Q_1 \;=\; & \frac{q_1}{|\mathcal{M}^{\text{sol}}|^2} \cdot \frac{N_{\text{pts}}}{N_{\text{par}}} \cdot \Bigg[\sum_{L}^{L_{\max}} \big(\mathrm{Re}E_{L-}^{\text{fit}} - \mathrm{Re}E_{L-}^{\text{sol}}\big)^2 + \sum_{L}^{L_{\max}} \big(\mathrm{Im}E_{L-}^{\text{fit}} - \mathrm{Im}E_{L-}^{\text{sol}}\big)^2 \\
& + \sum_{L}^{L_{\max}} \big(\mathrm{Re}E_{L+}^{\text{fit}} - \mathrm{Re}E_{L+}^{\text{sol}}\big)^2 + \sum_{L}^{L_{\max}} \big(\mathrm{Im}E_{L+}^{\text{fit}} - \mathrm{Im}E_{L+}^{\text{sol}}\big)^2 \\
& + \sum_{L}^{L_{\max}} \big(\mathrm{Re}M_{L-}^{\text{fit}} - \mathrm{Re}M_{L-}^{\text{sol}}\big)^2 + \sum_{L}^{L_{\max}} \big(\mathrm{Im}M_{L-}^{\text{fit}} - \mathrm{Im}M_{L-}^{\text{sol}}\big)^2 \\
& + \sum_{L}^{L_{\max}} \big(\mathrm{Re}M_{L+}^{\text{fit}} - \mathrm{Re}M_{L+}^{\text{sol}}\big)^2 + \sum_{L}^{L_{\max}} \big(\mathrm{Im}M_{L+}^{\text{fit}} - \mathrm{Im}M_{L+}^{\text{sol}}\big)^2 \Bigg]
\end{aligned}
$$

where

$$
|\mathcal{M}^{\text{sol}}|^2 = \sum_{L}^{L_{\max}} \big(|E_{L-}^{\text{sol}}|^2 + |E_{L+}^{\text{sol}}|^2 + |M_{L-}^{\text{sol}}|^2 + |M_{L+}^{\text{sol}}|^2 \big)
$$

is used as a normalisation value which makes Q_1 dimensionless and independent from the absolute magnitude of the multipoles. This ensures that the penalty contribution Q_1 will not vary significantly even when there are large changes in the size of contributing multipoles (e.g. within or beyond the $\Delta(1232)$ region). Q_1 is also normalised to the number of fit parameters N_{par}, as the squared sum over real and imaginary parts up to $L_{\max}$ is proportional to the number of fitted multipoles (fixed multipoles always stay at their model values and hence do not contribute to Q_1). Dividing out N_{par} and multiplying with the number of experimental data points N_{pts} results in a Q_1 with the same scaling behaviour as χ^2 (which is also proportional to N_{pts}) independent from the number of fit parameters. The weight factor q_1 is globally adjustable and used to fine-tune the strength of the penalty contribution. Typical values are around $q_1 = 1...2$. As *MLP1* considers the absolute deviations of multipoles it will mainly try to keep large multipoles close to their model values, while small multipoles will be able to accumulate rather large relative deviations. So, when using *MLP1* the constraining is somewhat proportional to the size of the multipole. This may be not the best approach in cases where a single multipole is vastly dominating, e.g. the E_{0+} wave for η production in the $S_{11}(1535)$ region.

3.2 Penalty mode *MLP2*

The *MLP2* penalty calculation evaluates a penalty term Q_2 from the squared sum of all relative deviations between fitted ($E_{L\pm}^{\text{fit}}$, $M_{L\pm}^{\text{fit}}$) and model ($E_{L\pm}^{\text{sol}}$, $M_{L\pm}^{\text{sol}}$) multipoles, according to

$$
\begin{aligned}
Q_2 \;=\; & q_2 \cdot \frac{N_{\text{pts}}}{N_{\text{par}}} \cdot \Bigg[\sum_{L}^{L_{\max}} \frac{\big(\mathrm{Re}E_{L-}^{\text{fit}} - \mathrm{Re}E_{L-}^{\text{sol}}\big)^2}{\big(\mathrm{Re}E_{L-}^{\text{sol}}\big)^2 + \varepsilon^2} + \sum_{L}^{L_{\max}} \frac{\big(\mathrm{Im}E_{L-}^{\text{fit}} - \mathrm{Im}E_{L-}^{\text{sol}}\big)^2}{\big(\mathrm{Im}E_{L-}^{\text{sol}}\big)^2 + \varepsilon^2} \\
& + \sum_{L}^{L_{\max}} \frac{\big(\mathrm{Re}E_{L+}^{\text{fit}} - \mathrm{Re}E_{L+}^{\text{sol}}\big)^2}{\big(\mathrm{Re}E_{L+}^{\text{sol}}\big)^2 + \varepsilon^2} + \sum_{L}^{L_{\max}} \frac{\big(\mathrm{Im}E_{L+}^{\text{fit}} - \mathrm{Im}E_{L+}^{\text{sol}}\big)^2}{\big(\mathrm{Im}E_{L+}^{\text{sol}}\big)^2 + \varepsilon^2} \\
& + \sum_{L}^{L_{\max}} \frac{\big(\mathrm{Re}M_{L-}^{\text{fit}} - \mathrm{Re}M_{L-}^{\text{sol}}\big)^2}{\big(\mathrm{Re}M_{L-}^{\text{sol}}\big)^2 + \varepsilon^2} + \sum_{L}^{L_{\max}} \frac{\big(\mathrm{Im}M_{L-}^{\text{fit}} - \mathrm{Im}M_{L-}^{\text{sol}}\big)^2}{\big(\mathrm{Im}M_{L-}^{\text{sol}}\big)^2 + \varepsilon^2} \\
& + \sum_{L}^{L_{\max}} \frac{\big(\mathrm{Re}M_{L+}^{\text{fit}} - \mathrm{Re}M_{L+}^{\text{sol}}\big)^2}{\big(\mathrm{Re}M_{L+}^{\text{sol}}\big)^2 + \varepsilon^2} + \sum_{L}^{L_{\max}} \frac{\big(\mathrm{Im}M_{L+}^{\text{fit}} - \mathrm{Im}M_{L+}^{\text{sol}}\big)^2}{\big(\mathrm{Im}M_{L+}^{\text{sol}}\big)^2 + \varepsilon^2} \Bigg]
\end{aligned}
$$

with $\varepsilon = $ half the magnitude of the smallest non-zero real or imaginary part of all multipoles, which basically represents the numerical precision of the used model values and is applied here to ensure non-zero denominators even in cases of vanishing multipoles. Q_2 is also normalised to the number of fit parameters N_{par}, as the squared sum over real and imaginary parts up to $L_{\max}$ is proportional to the number of fitted multipoles (fixed multipoles always stay at their model values and hence do not contribute to Q_2). Dividing out N_{par} and multiplying with the number of experimental data points N_{pts} results in a Q_2 with the same scaling behaviour as χ^2 (which is also proportional to N_{pts}) independent from the number of fit parameters. The weight factor q_2 is globally adjustable and used to fine-tune the strength of the penalty contribution. Values for q_2 should be significantly smaller than for q_1 in the *MLP1* mode, a typical number would be $q_2 \simeq 0.5$. As *MLP2* considers relative deviations, large multipoles will be much less constrained compared to *MLP1*. This might be difficult if small multipoles that are not very well described by the used model will contribute significantly to the penalty and affect larger, well-known multipoles.

3.3 Penalty mode *MLP3*

The *MLP3* penalty calculation is a combination of *MLP1* and *MLP2* modes and combines both penalties based on absolute and relative deviations. Consequently, the *MLP3* penalty is calculated according to

$$Q_3 = Q_1 + Q_2$$

The individual weight factors q_1 and q_2 will be used here to adjust the balance between absolute and relative constraints to the fitted multipoles. A careful selection of q_1 and q_2 could therefore mitigate the dominance effects of very large and very small multipoles for *MLP1* and *MLP2* modes.

3.4 Penalty mode *CGLN*

The *CGLN* mode calculates a penalty term from the difference between the four CGLN amplitudes F_i^{fit} obtained from current fit parameters and the model values F_i^{sol}, according to

$$Q_4 = \frac{1}{|\mathcal{F}^{\text{sol}}|^2} \sum_{i=1}^{4} \sum_{j=1}^{N_{\text{pts}}} \frac{|F_i(x_j)^{\text{fit}} - F_i(x_j)^{\text{sol}}|^2}{f_i^2}$$

where

$$|\mathcal{F}^{\text{sol}}|^2 = \sum_{i=1}^{4} \sum_{j=1}^{N_{\text{pts}}} |F_i(x_j)^{\text{sol}}|^2$$

is used as a normalisation value which makes Q_4 dimensionless and independent from the absolute magnitude of the amplitudes. This ensures that the penalty contribution Q_4 will not vary significantly even when there are large changes in the size of the amplitudes (e.g. within or beyond the $\Delta(1232)$ region). CGLN amplitudes are evaluated at N_{pts} (the number of experimental data points from all available observables) positions for $x_j = \cos\theta_j$ which are distributed equidistant in the range $x = [-1, 1]$. Evaluating the CGLN amplitudes at N_{pts} polar angle positions makes sure that Q_4 has the same scaling behaviour as χ^2 (which is also proportional to N_{pts}). For each CGLN amplitude F_i an individual weight f_i is applied in the squared sum of deviations. These weights are used to adjust the size of the penalty contribution Q_4 relative to χ^2. Note that the penalty term Q_4 depends on four external parameters which allows a high level of flexibility.

3.5 Penalty mode *HELI*

The *HELI* mode is basically very similar to the *CGLN* mode, with the only difference being the usage of helicity amplitudes H_i instead of CGLN amplitudes F_i. For the calculation of helicity amplitudes the transformation relations

$$H_1 = -\frac{1}{\sqrt{2}} \sin\theta \cos\frac{\theta}{2} (F_3 + F_4)$$
$$H_2 = \sqrt{2} \cos\frac{\theta}{2} \left[(F_2 - F_1) + \frac{1-\cos\theta}{2} (F_3 - F_4) \right]$$
$$H_3 = \frac{1}{\sqrt{2}} \sin\theta \sin\frac{\theta}{2} (F_3 - F_4)$$
$$H_4 = \sqrt{2} \sin\frac{\theta}{2} \left[(F_1 + F_1) + \frac{1+\cos\theta}{2} (F_3 + F_4) \right]$$

between H_i and F_i are used and the penalty term is given by

$$Q_5 = \frac{1}{|\mathcal{H}^{\text{sol}}|^2} \sum_{i=1}^{4} \sum_{j=1}^{N_{\text{pts}}} \frac{|H_i(x_j)^{\text{fit}} - H_i(x_j)^{\text{sol}}|^2}{h_i^2}$$

with a normalisation value

$$|\mathcal{H}^{\text{sol}}|^2 = \sum_{i=1}^{4} \sum_{j=1}^{N_{\text{pts}}} |H_i(x_j)^{\text{sol}}|^2$$

making Q_5 dimensionless and independent from the absolute magnitude of the amplitudes. Also in this mode amplitudes are evaluated at equidistant x_j positions covering the full angular range. Similar to *CGLN* mode the penalty contribution is adjusted by individual weights h_i for each helicity amplitude H_i.

4 SE fits and observable energies

`PWA` performs multipole fits on fixed energy positions which are (with rare exceptions) given by the energy information of unpolarised cross section σ_0 data. Such σ_0 measurements have typically the finest energy binning as well as the highest statistic precision, while polarisation observable data mostly is only available in much wider energy bins and with lower statistics. Up to now `PWA` does not perform any adjustments of energy positions or interpolation schemes for any observables but determines multipoles at the **exact** energies of the σ_0 dataset, while data points for polarisation observables are considered in the fit, if the current σ_0 energy position is covered by the respective polarisation observable energy bin. This means that a single value for asymmetry observables like Σ, T, P, E, F, G, H which are given in energy bins of typically 20...100 MeV will be used for fits at multiple σ_0 energy positions. The rationale for this scheme is that any energy mismatch between the SE fit energy and the σ_0 energy will have a large impact on the fit quality due to the high precision of cross section data, while the larger uncertainties for polarisation observables provide some insensitivity to such energy deviations. Also keep in mind that a polarisation observable determined for a $\sim$50 MeV bin always represents an average value of all energies within that bin, which justifies the repeated use of such data points for multiple cross section energies that are compatible with the polarisation observable bin. In the long term a more advanced handling of observable energy mismatches might be desirable, however such interpolation schemes are still a rather open question and several different approaches are currently discussed.

5 Fits with variation of start parameters

Multipole fits with high orders L_{max} operate in a high-dimensional parameter space and any found minimum in the f_{FCN} funktion is not necessarily the global minimum representing the physically correct solution. In order to search for possible multiple solutions for an SE fit `PWA` can be configured in a way that it repeats the fit process with slight variations in the start parameters. Such start parameters for the fitting process are typically taken from any existing photoproduction model or partial wave analysis. `PWA` changes these start parameters for all fittable parameters by random numbers from within an adjustable band around the model solution (fixed multipoles that are parametrised in the fit process always stay at their exact model values) and repeats every SE fit several times. Unique solutions are identified using their f_{FCN} value and a configurable number of found solutions is stored. At the moment `PWA` does **no** further processing on these different solutions, like selecting solutions which have a smooth energy dependence with respect to their neighbouring energy points.

6 Observable rescaling

During fits `PWA` has the possibility to rescale observable datasets (that is all data points for a given energy) within given systematic uncertainties to achieve a better agreement between different datasets. Technically this is done by additional fit parameters s_X for scaling each observable and a penalty term, which penalises any deviation from the nominal values. This penalty term and the modified χ^2 contribution (including the scaling parameter) for an observable X (cross sections and asymmetries) are given by

$$Q_s = q_s \cdot \sum_X \left[N_{\mathrm{pts},X} \cdot \left(\frac{s_X - 1}{\delta_X} \right)^2 \right]$$

and

$$\chi_X^2 = \sum_i \left(\frac{s_X X^{\mathrm{exp}}(\theta_i) - X^{\mathrm{fit}}(\theta_i)}{s_X \Delta X^{\mathrm{exp}}(\theta_i)} \right)^2$$

The relative systematic uncertainty (e.g. $5\% = 0.05$) is given by δ_X, while $N_{\mathrm{pts},X}$ is the number of data points for observable X. Making the individual contributions proportional to $N_{\mathrm{pts},X}$ ensures that rescaling observables with many data points gets more 'expensive' than observables with only very few points, and provides a similar scaling behaviour for Q_s as for χ^2 (which is proportional to $N_{\mathrm{pts}} = \sum N_{\mathrm{pts},X}$). The additional global weight factor q_s can be used to adjust the strength of the rescaling. Small values for q_s decrease the penalty contribution and hence give the fitting process more freedom to rescale observables.

7 `PWA` installation

The current version of the Mainz `PWA` package can be obtained from its GitHub repository available under
`https://github.com/MainzPWA/PWA`
`PWA` will run under Linux, FreeBSD, and OS X systems and can be compiled on respective systems using the

provided scripts `build.linux`, `build.freebsd`, and `build.macosx`. `PWA` requires a (recent) `ROOT` installation. For successful compilation it might be necessary to adjust the variables `$ROOT_LIB` and `$ROOT_INC` in the build scripts to match the directories with libraries and header files of your `ROOT` installation. In addition, a `CMakeLists.txt` file for use with the `cmake` build system is provided.

8   Setting up a work directory for `PWA`

It is recommended to set up a special work directory for your `PWA` SE fits. This directory should contain all necessary experimental data, model inputs used for the fits, and a configuration file for `PWA`. A typical work directory consists of the follwing entries:

- A directory `model` containing model values for electromagnetic multipoles, which are used as start parameters and for penalty calculations during the fitting process. It is recommended to have a `model` directory as a symbolic link to one of the models that `PWA` provides within its package, e.g. use the command
  `ln -s /home/`*username*`/PWA/model/ppi0/MAID model`
  to use MAID calculations for your $p\pi^0$ SE fits. As the model path has to be given in the `PWA` configuration file, it is not required to have a dedicated `model` directory, but not having absolute paths in the `PWA` configuration file can simplify things.

- A directory `data` containing experimental datasets for observables you want to use in your fit. It is recommended to have a `data` directory as a symbolic link to the datasets that `PWA` provides within its package, e.g. use the command
  `ln -s /home/`*username*`/PWA/data/ppi0 data`
  This will make various $p\pi^0$ datasets accessible to your work directory. As filenames for all datasets you want to use for fits have to be given in the `PWA` configuration file, it is not required to have a dedicated `data` directory, but not having absolute paths in the `PWA` configuration file can simplify things.

- A `PWA.cfg` file, holding various configuration options (see section 9). `PWA` by default tries to read its configuration from `PWA.cfg` in the current directory, but a different filename can be passed as command-line parameter, e.g.
  `PWA /home/`*username*`/cfg/fit.cfg`

- The `PWA` executable. Here it is recommended to either create a (symbolic) link to the actual `PWA` binary which normally can be found under `build/bin/PWA` or to include `PWA` in your search path.

During the fits `PWA` will create additional `plots.`*n* directories holding the fit results. The number of `plots.`*n* directories depends on the amount of solutions you want `PWA` to store. An example of such a work directory for $p\pi^0$ data and fits based on MAID can be found in `work/ppi0/MAID` in the main directory of the `PWA` package.

9   Configuration options

The following sections describe the various configuration options for fits with `PWA` . Options are generally read from the configuration file `PWA.cfg` in your `PWA` work directory, if `PWA` is invoked without additional command-line parameters. However, a different configuration file may be passed as parameter, e.g.
`PWA fit.cfg`
All following configuration keywords are case-sensitive, which makes `OPTION` different from `option`, where all keywords have to be upper case. Any non-existing keyword will be ignored, therefore no explicit markup for comments is required.

9.1   Kinematic parameters

- `MASS_MESON` *mass*
  Sets the mass of the produced final state meson (π^0, $\pi^\pm$, η, η', $K^\pm$, ...) to the given value (in MeV). This parameter is mandatory for correct calculation of kinematic factors during the fitting process. Examples are

  π^0 134.9766

  π^+ 139.5702

  η 547.8530

  `MASS_INITIAL` *mass*
  Sets the mass of the inital state baryon (p, n) to the given value (in MeV). This parameter is mandatory for correct calculation of kinematic factors during the fitting process. Examples are

   p 938.2720

   n 939.5654

MASS_FINAL *mass*

Sets the mass of the produced final state baryon (p, n, Λ, Σ, ...) to the given value (in MeV). This parameter is mandatory for correct calculation of kinematic factors during the fitting process. Examples are

   p 938.2720

   n 939.5654

   Λ 1115.6830

9.2 Fitted multipoles

- **L_MAX** *n*

  This sets the maximum multipole order $L_{\max}$ (which is considered in the calculation of CGLN amplitudes and observables) to the given value n. Note that this does **not** set the maximum multipole order which is actually fitted, as the fittable multipoles can be selected indiviually later on. Any multipole with $L \leq L_{\max}$ that is not fitted will enter the calculation of CGLN amplitudes and observables as a parametrisation using the current model values.

- **FIX_E*l*P 0/1**
  FIX_M*l*P 0/1
  FIX_E*l*M 0/1
  FIX_M*l*M 0/1

  Any E_{l+}, M_{l+}, E_{l-}, M_{l-} multipole can either be fixed (**1**) to their model values or be used as fit parameters (**0**). Fixing a multipole here fixes both magnitude and phase (or real and imaginary values). Hence any fittable multipole will add two parameters to the fitting process.

- **FIX_E*l*P_PHASE 0/1**
  FIX_E*l*M_PHASE 0/1
  FIX_M*l*P_PHASE 0/1
  FIX_M*l*M_PHASE 0/1

  For any E_{l+}, M_{l+}, E_{l-}, M_{l-} multipole that was previously set as fittable the individual phase can be either fixed (**1**) to its model value or be used as fit parameter (**0**). Fixing a phase will reduce the number of fit parameters by one and only fit the magnitude for the given multipole.

9.3 Penalty options

- **PENALTY_MODE** *n*

  Selects a penalty mode for use during the minimisation process. Possible values for n are

    0 No penalty contribution

    1 *MLP1* penalty mode

    2 *MLP2* penalty mode

    3 *MLP3* penalty mode

    4 *CGLN* penalty mode

    5 *HELI* penalty mode

- **PENALTY_MLP1** *value*

  Sets the weight factor q_1 to the given value. This value will be used for for *MLP1* and *MLP3* penalty modes. Typical values are around $q_1 = 2.0$.

- **PENALTY_MLP2** *value*

  Sets the weight factor q_2 to the given value. This value will be used for for *MLP2* and *MLP3* penalty modes. Typical values are around $q_2 = 0.5$.

- **WEIGHT_A*n*** *value*

  Sets the individual weight factors for CGLN or helicity amplitude $n = 1...4$ to the given value. These values will be used in CGLN or HELI penalty mode only. Typical values are around $f_n = 1.0$.

- **PRINT_PENALTY 0/1**

  When enabled (**1**) an additional line will be printed out for each fit giving the individual contributions of χ^2 and penalty Q for the found solution.

9.4   Error calculation

- `ERROR_MODE` *n*
  Selects a minimisation function for error calculation through MINUIT. Possible options for *n* are

  1. Use only χ^2 function for error determination. This is the mathematically most sound approach, as the definition of parameter error ranges is based on the variation of $\chi^2 \to \chi^2 + 1$. However, for a minimisation with penalty contributions, the minima for χ^2 only and $\chi^2 + Q$ are not necessarily identical and the behaviour of χ^2 only around the chosen minimum might result in ill-defined parameter errors.

  2. Use sum of χ^2 and current penalty Q for error determination. This might in general overestimate parameter errors but will always produce well-defined results.

  3. Use an adaptive mode that prefers the χ^2 only calculation but falls back to the sum of χ^2 and current penalty Q if this produces smaller errors. This is the recommended mode.

9.5   Multiple fit solutions

- `ITERATIONS` *n*
  Indiviual SE fits will be repeated *n* times with small variatons in the starting parameters to find possible additional minima in the parameter space. When the given number of iterations has been processed the best solution(s), i.e. with lowest $\chi^2 + Q$, are selected. Computimg time for the fitting process increases linear with the number of iterations. For reasonable performance, *n* should not exceed values of 50...100.

- `SOLUTIONS` *n*
  Up to *n* unique solutions that have been found during the iterations for each SE fit will be stored (with decreasing fit quality). The number of maximum solutions to store may not exceed the number of iterations for the fit process.

- `VARIATION_REL` *value*
  This will define a **relative** variation of start parameters for each iteration equally distributed in a band around its current model value. The relative size of this band is given by $\pm$***value***. A typical value is 0.2 which will result in parameter variations by $\pm 20\%$. Note that relative and absolute variations will be added.

- `VARIATION_ABS` *value*
  This will define an **absolute** variation of start parameters for each iteration equally distributed in a band around its current model value. The size of this band is given by $\pm$***value*** in units of $10^{-3}/m_{\pi^+}$. This option is useful to define an absolute minimum of the variation band, which will be effective for very small multipoles (where a relative variation would have only a small effect). Note that relative and absolute variations will be added.

9.6   Energy range for fits

- `MIN_ENERGY` *value*
  `MAX_ENERGY` *value*
  These options define the range of photon beam energies ω (in MeV) for which fits are performed.

9.7   Observable rescaling

- `FIX_SCALES` 1/0
  Experimental observables can be fixed to ther actual values (`1`) or scaled within their given systematic uncertainty ranges (`0`) during the fit process. This will introduce one additional fit parameter (scaling value) for each observable. Note that X and σ_X are considered here as different observables.

- `SCALING` *value*
  This is an additional weight factor that is applied to the penalty contribution imposed by the scaling factor variation. A small ***value*** (e.g. 0.1) will decrease this contribution and therefore give the fitter more freedom to rescale experimental values.

9.8 Configuration of experimental data

- `SGO_FILE  Path/Filename  weight  scale`
  `SGS_FILE  Path/Filename  weight  scale`
  `SGT_FILE  Path/Filename  weight  scale`
  `SGP_FILE  Path/Filename  weight  scale`
  `SGE_FILE  Path/Filename  weight  scale`
  `SGF_FILE  Path/Filename  weight  scale`
  `SGG_FILE  Path/Filename  weight  scale`
  `SGH_FILE  Path/Filename  weight  scale`
  `SGCX_FILE Path/Filename  weight  scale`
  `SGCZ_FILE Path/Filename  weight  scale`
  `SGOX_FILE Path/Filename  weight  scale`
  `SGOZ_FILE Path/Filename  weight  scale`
  Defines the experimental datasets for cross sections (unpolarised σ_0 and polarised σ_X). The additional parameter *weight* is applied to any χ^2 contributions from the corresponding dataset. The additional parameter *scale* defines an overall scaling factor to the corresponding data and errors, i.e. a value of *scale* = 1.05 will increase the data by 5%. Multiple lines for observables with more than one dataset are possible (with individual values for *weight* and *scale*). The parameters *weight* and *scale* must not be omitted.

- `S_FILE   Path/Filename  weight  scale`
  `T_FILE   Path/Filename  weight  scale`
  `P_FILE   Path/Filename  weight  scale`
  `E_FILE   Path/Filename  weight  scale`
  `F_FILE   Path/Filename  weight  scale`
  `G_FILE   Path/Filename  weight  scale`
  `H_FILE   Path/Filename  weight  scale`
  `CX_FILE  Path/Filename  weight  scale`
  `CZ_FILE  Path/Filename  weight  scale`
  `OX_FILE  Path/Filename  weight  scale`
  `OZ_FILE  Path/Filename  weight  scale`
  Defines the experimental datasets for asymmetry observables. The additional parameter *weight* is applied to any χ^2 contributions from the corresponding dataset. The additional parameter *scale* defines an overall scaling factor to the corresponding data and errors, i.e. a value of *scale* = 0.95 will decrease the data by 5%. Multiple lines for observables with more than one dataset are possible (with individual values for *weight* and *scale*). The parameters *weight* and *scale* must not be omitted.

- `USE_PRELIMINARY 0/1`
  Defines whether datasets tagged as 'preliminary' in their respective files should be used (1) or not (0). With this option preliminary datasets need not be removed from the `SGX_FILE` and `X_FILE` lists but their data will be ignored.

9.9 Configuration of model values

- `MODEL_PATH Path`
  Defines the directory containing theoretical values for multipoles. The given directory must hold text files following the naming scheme `E`l`p.txt`, `E`l`m.txt` for electric multipoles, and `M`l`p.txt`, `M`l`m.txt` for magnetic multipoles, with angular momentum l, and parity $+$ (p) or $-$ (m).

9.10 Special options for π^0 threshold fits

- `ONLY_CROSS_S 1/0`
  `ONLY_CROSS_F 1/0`
  These options restrict the data used for fitting to $\{\sigma_0, \sigma_\Sigma, \Sigma\}$ or $\{\sigma_0, \sigma_F, F\}$. Any other observables are ignored. These options are mutually exclusive. Also `FIX_E`n`P_PHASE` must be set to 0 for all s and p wave multipoles.

  `FIX_RE_EOP 1/0`
  The real part of the E_{0+} multipole can either be fixed (1) to its model value or be used as a fit parameter (0). In order to use this option, both `FIX_EOP` and `FIX_EOP_PHASE` must be set to 0.

  `FIX_IM_EOP`
  The imaginary part of the E_{0+} multipole can either be fixed (1) or be used as a fit parameter (0). If

$\mathrm{Im}E_{0+}$ is fixed, a parametrisation according to $\mathrm{Im}E_{0+} = \beta \cdot \frac{q_{\pi+}}{m_{\pi+}}$ is used. Note that `FIX_IM_EOP` can only be used in combination with `ONLY_CROSS_S` or `ONLY_CROSS_F`. Also both `FIX_EOP` and `FIX_EOP_PHASE` must be set to `0`.

- `BETA` *value*
  This option sets the value for β used in the parametrisation of $\mathrm{Im}E_{0+}$. Typical values are $\beta = 3.43$ (with isospin symmetry) or $\beta = 3.35$ (with isospin breaking).

- `D_WAVES` *n*
  Selects which contributions for d waves is used (if supported by the current model). Possible options are

    1 Full model calculation

    2 Born terms only

    3 Born terms and ρ/ω exchange

  Right now, only MAID and DMT provide these three different d wave contributions.

- `SGT_ENERGIES 1/0`
  With this option enabled (`1`) SE fits are performed at energies given by σ_T data instead of σ_0.

10 Data formats

The following sections describe the different text data formats used by PWA for experimental observable data and model multipole values.

10.1 Experimental observable data

Experimental data is organised in separate files for each observable (asymmetries X and polarised cross sections σ_X are considered here as different observables) **and** for each individual measurement. A file for such an individual experiment however can contain data for more than one energy. Such an entry for an energy bin consists of general information on the current data as well as of the actual observable data for different polar angle positions. A typical file looks like the following:

```
E = 683.50 MeV, E_lo = 667.24 MeV, E_hi = 699.76 MeV
Systematic = 0.0248, Preliminary = 0, CBELSA_2014_Hartmann_PRL113-062001
163.335   -0.2596   0.0976   0.0080
151.045   -0.3346   0.0543   0.0086
142.373   -0.4980   0.0408   0.0129
135.072   -0.6306   0.0347   0.0154
128.682   -0.6693   0.0316   0.0168
122.820   -0.7317   0.0286   0.0170
117.258   -0.8295   0.0338   0.0261
112.024   -0.7583   0.0291   0.0170
106.978   -0.7793   0.0267   0.0180
102.005   -0.7629   0.0263   0.0189
 97.181   -0.7808   0.0249   0.0179
 92.407   -0.7951   0.0247   0.0193
 87.593   -0.7840   0.0251   0.0190
 82.819   -0.7738   0.0260   0.0179
 77.995   -0.7537   0.0269   0.0188
 73.022   -0.7071   0.0278   0.0162
 67.976   -0.6379   0.0285   0.0140
 62.742   -0.4937   0.0408   0.0125
------------------------------------
E = 715.61 MeV, E_lo = 699.76 MeV, E_hi = 731.45 MeV
Systematic = 0.0249, Preliminary = 0, CBELSA_2014_Hartmann_PRL113-062001
163.335   -0.1684   0.1025   0.0038
151.045   -0.1793   0.0599   0.0053
142.373   -0.2888   0.0447   0.0078
135.072   -0.3406   0.0414   0.0081
128.682   -0.5064   0.0369   0.0130
122.820   -0.5747   0.0335   0.0136
```

```
117.258    -0.6330    0.0405    0.0199
112.024    -0.6199    0.0360    0.0147
106.978    -0.6730    0.0335    0.0148
102.005    -0.6214    0.0312    0.0149
 97.181    -0.6742    0.0300    0.0156
 92.407    -0.6291    0.0289    0.0149
 87.593    -0.6920    0.0289    0.0163
 82.819    -0.6456    0.0301    0.0152
 77.995    -0.5926    0.0305    0.0143
 73.022    -0.5031    0.0321    0.0117
 67.976    -0.4865    0.0342    0.0113
 62.742    -0.3185    0.0396    0.0073
 57.180    -0.2622    0.0765    0.0084
-----------------------------------
```

The first header line carries energy information for the current dataset: The central (E) photon beam energy in lab frame and the lower (E_lo) and upper (E_hi) beam energy bounds of the current bin. Energies must be in MeV and the units must be present in the header lines. The second line gives a value for the relative systematic uncertainty (Systematic) which should be an average number valid for all polar angle positions within this energy bin. This systematic uncertainty is used for the observable rescaling option (see FIX_SCALES configuration option). A value of Systematic = 0.05 would correspond to 5% systematic uncertainty. The Preliminary field indicates whether this dataset is preliminary and/or unpublished and may not be used for publications yet. Any data with Preliminary = 1 will be ignored in fits if the configuration option USE_PRELIMINARY is not enabled. The final entry in the second header line is a comment that can carry references or other identification data for the current dataset. This commment may be up to 255 characters long and must not contain any spaces (use '_' instead).

The following lines contain the actual observable data. Each line can hold up to four values which are

theta angle   observable value   statistical error   [systematic error]

Polar angle positions have to be given in degrees, observable values[1] for cross sections in μb/sr. Statistical and systematic errors must be absolute values, e.g. in μb/sr for cross sections. Systematic errors for each data point are optional and individual systematic uncertainties at each polar angle position are not used by PWA during the fit procedure. Each energy bin entry must be terminated by a sparator line like '---------------' (do not use blank lines to separate entries). Such a separator however may not be present at the very first line of an observable file, but must be on the end of the file (terminating the last entry). Polar angle positions within an energy bin may be in increasing or decreasing order (or no order at all). Multiple energy bins within an observable file are possible, also here the ordering in energy is not important. Experimental data files reside in the folders data/ppi0, data/npip, data/peta, ... (depending on the reaction $p\pi^0$, $n\pi^+$, $p\eta$, ...) of your PWA installation. You can add or create additional files in any folder, as data files will be referenced through the PWA.cfg file for your fit settings.

10.2 Model multipoles

PWA needs model calculations for electromagnetic multipoles for use as start parameters and (if applicable) in penalty calculations. These multipole files must reside in a directory model in your PWA work directory, where model may be a link to one of the existing model directories in the model repository of the PWA package. Typical multipole files look like the following:

```
  W         M1-(p pi0)
(MeV)      Re          Im
1074.0    -0.389350    -0.038572
1075.0    -0.427039    -0.042104
1076.0    -0.464727    -0.045635
1077.0    -0.502415    -0.049167
1078.0    -0.540103    -0.052699
1079.0    -0.577792    -0.056231
1080.0    -0.615480    -0.059763
1081.0    -0.653168    -0.063294
1082.0    -0.690856    -0.066826
1083.0    -0.728545    -0.070358
```

---

[1]Asymmetry values must be within a range of $[-1, +1]$.

```
1084.0    -0.766233    -0.073890
```

PWA ignores the first two lines of each multipole file, so these lines can carry column headers or further descriptions. Starting with the third line the actual multipole information has to be present in the form

center-of-mass energy   real part   imaginary part

where the center-of-mass energy W is related to the lab photon beam energy ω according to

$$W^2 = 2M\omega + M^2$$

with the mass M of the target nucleon. Real and imaginary parts of the multipole must be given in units of $10^{-3}/m_{\pi^+}$. If any model provides multipoles in units of 10^{-3} fm a conversion factor of

$$\frac{m_{\pi^+}}{\alpha_{\text{em}}} = \frac{139.5702\,\text{MeV}}{197.3270\,\text{MeV}\cdot\text{fm}} \approx \sqrt{\frac{1}{2}}\,\text{fm}^{-1}$$

has to be applied before using these model calculations with PWA. Multipole files have to follow the naming scheme Elp.txt, Elm.txt for electric multipoles, and Mlp.txt, Mlm.txt for magnetic multipoles, with angular momentum l, and parity + (p) or − (m). PWA supports multipoles up to order $L = 9$. The energy steps in multipole files can be arbitrary, however a rather fine step size (~1 MeV) is recommended in order to have reasonably precise multipole information for any SE fit energy available (up to now, no interpolation on model values is performed). For d wave multipoles additional model values may be provided, carrying only Born term contributions or Bern terms as well as ρ/ω exchange mechanisms (see configuration option D_WAVES). These files must be named E2p_Born.txt, E2m_Born.txt, M2p_Born.txt, M2m_Born.txt, and E2p_BornRhoOmega.txt, E2m_BornRhoOmega.txt, M2p_BornRhoOmega.txt, M2m_BornRhoOmega.txt, respectively. All filenames are case-sensitive.

Currently, for $p\pi^0$ the following models are provided:

model/ppi0/BG2011-01	Bonn-Gatchina PWA (solution 2011-01) [2]
model/ppi0/BG2011-02	Bonn-Gatchina PWA (solution 2011-02) [2]
model/ppi0/DMT	DMT model [3]
model/ppi0/MAID	MAID 2007 [4]
model/ppi0/SAID	SAID CM12 [5]
model/ppi0/ThrFit	Empirical fit to π^0 threshold data [1]
model/ppi0/ThrChPT4	χPT (4$^{\text{th}}$ order) [6]
model/ppi0/ThrHBChPT4	Heavy-baryon χPT (4$^{\text{th}}$ order) [6]
model/ppi0/ThrHDT97	Hanstein, Drechsel, Tiator solution [7]
model/ppi0/ThrLG	Lutz, Gasparyan calculation [8]

Any models prefixed with Thr are only supposed to be used within the π threshold region up to $\omega \sim 180\text{MeV}$.

For $n\pi^+$ the following models are provided:

model/ppi0/BG2011-01	Bonn-Gatchina PWA (solution 2011-01) [2]
model/ppi0/BG2011-02	Bonn-Gatchina PWA (solution 2011-02) [2]
model/ppi0/DMT	DMT model [3]
model/ppi0/MAID	MAID 2007 [4]
model/ppi0/SAID	SAID CM12 [5]

For $p\eta$ the following models are provided:

model/ppi0/BG2011-01	Bonn-Gatchina PWA (solution 2011-01) [2]
model/ppi0/BG2011-02	Bonn-Gatchina PWA (solution 2011-02) [2]
model/ppi0/MAID	ηMAID 2000 [9]
model/ppi0/SAID	SAID [10]

10.3 PWA output files

PWA will create .root files of TCanvas objects with TGraph representations of fitted multipoles and the model parameters used as start parameters during the fit. For each real and imaginary part of all multipoles up to L_{max} individual files are created in the directories plots.n for the different found solutions. Files are named according to the scheme ReElp.root, ImElp.root, ReElm.root, ImElm.root, ReMlp.root, ImMlp.root, ReMlm.root, and ImMlm.rootfor electric and magnetic multipoles of order l and + (p) or − (m) parity. These files can be displayed directly from within a .root TBrowser. Further processing (e.g. generating plain text files with multipole results) is possible using the provided macros (see section 11).

11 Macros

`PWA` provides different `ROOT` macros for further processing of fit results. This includes macros for generating plain text files with multipole data as well as tools for drawing fitted multipoles and model calculations.

11.1 Macro functions in `macros/Extract.cpp`

- `Extract(Char_t* REACT, Int_t L_MAX, Int_t SOLUTIONS=1, Double_t MASS_INITIAL=938.2720)`

  Converts `.root` files from `PWA` output to plain text files. `Extract()` will create text files for all multipoles up to multipole order `L_MAX` from fit results in directories `plots.0` up to `plots.{`$SOLUTIONS$`-1}`. `REACT` is an (arbitrary) reaction identifier that will be written in the header lines of output files, e.g. ''p pi0''. `MASS_INITIAL` (in MeV) is used for calculating the center-of-mass energy W. This parameter is optional, if it is omitted the proton mass is assumed. Output files will be named `E`l`p.txt`, `E`l`m.txt` for electric multipoles, and `M`l`p.txt`, `M`l`m.txt` for magnetic multipoles, with angular momentum l, and parity $+$ (p) or $-$ (m). These files will be created in the corresponding `plots.`n directories and have the following format:

  ```
       W              E0+(p pi0)
     (MeV)     Re     DRe      Im      DIm
   1074.018  -0.837   0.107   -0.028   0.195
   1075.131  -0.793   0.063   -0.253   0.325
   1076.242  -1.670   0.801   -0.905   1.106
   1077.351  -2.188   0.243   -0.112   4.192
   1078.460  -0.541   0.027    0.408   0.243
  ```

  Each line consists of the center-of-mass energy W of an SE fit as well as values and errors for real and imaginary parts obtained from the fit. **Note:** After execution of `Extract()` it is recommended to restart `ROOT` to avoid problems when drawing `TCanvas` objects. `Extract()` must be executed from your work directory (having subdirectories `plots.`n).

- `Multipole(Char_t* Mlp, Int_t SolLo=0, Int_t SolHi=0, Bool_t W=true,`
  `          Bool_t SAVE=false, Double_t Lo=0.0, Double_t Hi=0.0,`
  `          Double_t MASS_INITIAL=938.2720, Int_t D_WAVES=MODEL)`

  Plots the given multipole (real and imaginary part) `Mlp` for solutions between `SolLo` and `SolHi`. `Mlp` must be given in the form ''E`$l$`p'', ''E`$l$`m'' for electric multipoles, and ''M`$l$`p'', ''M`$l$`m'' for magnetic multipoles, with angular momentum l, and parity $+$ (p) or $-$ (m). The plot will contain SE fit results as well as model predictions from the current values in the directory `model`. if `SAVE` is true, a `.pdf` file of the plot is created. `Lo` and `Hi` denote the plot range on the y-axis, if ommitted or equal 0, the range is automatically adjusted. `MASS_INITIAL` (in MeV) is used for calculating the center-of-mass energy W. This parameter is optional, if it is omitted the proton mass is assumed. `D_WAVES` indicates, which d wave contributions are used for plotting model multipoles (if supported by the current model). **Note:** For successful operation of `Multipole()` it is necessary to have produced fitted multipole text files with `Extract()` beforehand once. `Multipole()` must be executed from your work directory (having subdirectories `plots.`n and `model`).

- `Magnitude(Char_t* Mlp, Int_t SolLo=0, Int_t SolHi=0, Bool_t W=true,`
  `          Bool_t SAVE=false, Double_t Lo=0.0, Double_t Hi=0.0,`
  `          Double_t MASS_INITIAL=938.2720, Int_t D_WAVES=MODEL)`

  Plots the magnitude of the given multipole `Mlp` for solutions between `SolLo` and `SolHi`. `Mlp` must be given in the form ''E`$l$`p'', ''E`$l$`m'' for electric multipoles, and ''M`$l$`p'', ''M`$l$`m'' for magnetic multipoles, with angular momentum l, and parity $+$ (p) or $-$ (m). The plot will contain SE fit results as well as model predictions from the current values in the directory `model`. if `SAVE` is true, a PDF file of the plot is created. `Lo` and `Hi` denote the plot range on the y-axis, if ommitted or equal 0, the range is automatically adjusted. `MASS_INITIAL` (in MeV) is used for calculating the center-of-mass energy W. This parameter is optional, if it is omitted the proton mass is assumed. `D_WAVES` indicates, which d wave contributions are used for plotting model multipoles (if supported by the current model). **Note:** For successful operation of `Magnitude()` it is necessary to have produced fitted multipole text files with `Extract()` beforehand once. `Magnitude()` must be executed from your work directory (having subdirectories `plots.`n and `model`).

- `Phase(Char_t* Mlp, Int_t SolLo=0, Int_t SolHi=0, Bool_t W=true,`
  `      Bool_t SAVE=false, Double_t Lo=0.0, Double_t Hi=0.0,`
  `      Double_t MASS_INITIAL=938.2720, Int_t D_WAVES=MODEL)`

Plots the phase (in radians) of the given multipole `Mlp` for solutions between `SolLo` and `SolHi`. `Mlp` must be given in the form ''Elp'', ''Elm'' for electric multipoles, and ''Mlp'', ''Mlm'' for magnetic multipoles, with angular momentum l, and parity $+$ (p) or $-$ (m). The plot will contain SE fit results as well as model predictions from the current values in the directory `model`. if `SAVE` is true, a PDF file of the plot is created. `Lo` and `Hi` denote the plot range on the y-axis, if omitted or equal 0, the range is automatically adjusted. `MASS_INITIAL` (in MeV) is used for calculating the center-of-mass energy W. This parameter is optional, if it is omitted the proton mass is assumed. `D_WAVES` indicates, which d wave contributions are used for plotting model multipoles (if supported by the current model). **Note:** For successful operation of `Phase()` it is necessary to have produced fitted multipole text files with `Extract()` beforehand once. `Phase()` must be executed from your work directory (having subdirectories `plots.`*n* and `model`).

- `Model(Char_t* Mlp, Bool_t W=true, Bool_t SAVE=false, Double_t Lo=0.0, Double_t Hi=0.0, Double_t MASS_INITIAL=938.2720, Int_t D_WAVES=MODEL)`

  Plots model predictions for the given multipole (real and imaginary part) `Mlp`. `Mlp` must be given in the form ''Elp'', ''Elm'' for electric multipoles, and ''Mlp'', ''Mlm'' for magnetic multipoles, with angular momentum l, and parity $+$ (p) or $-$ (m). The plot will contain only model predictions from the current values in the directory `model`. if `SAVE` is true, a PDF file of the plot is created. `Lo` and `Hi` denote the plot range on the y-axis, if ommitted or equal 0, the range is automatically adjusted. `MASS_INITIAL` (in MeV) is used for calculating the center-of-mass energy W. This parameter is optional, if it is omitted the proton mass is assumed. `D_WAVES` indicates, which d wave contributions are used for plotting model multipoles (if supported by the current model). **Note:** `Model()` must be executed from your work directory (having a subdirectory `model`).

- `Chi2(Int_t SOLUTION=0, Double_t MASS_INITIAL=938.2720)`

  Draws the χ^2 values for the given `SOLUTION` depending on the center-of-mass energy W. `MASS_INITIAL` (in MeV) is used for calculating W. This parameter is optional, if it is omitted the proton mass is assumed. `Chi2()` must be executed from your work directory (having subdirectories `plots.`*n*).

- `Penalty(Int_t SOLUTION=0, Double_t MASS_INITIAL=938.2720)`

  Draws the penalty contributions for the given `SOLUTION` depending on the center-of-mass energy W. `MASS_INITIAL` (in MeV) is used for calculating W. This parameter is optional, if it is omitted the proton mass is assumed. `Penalty()` must be executed from your work directory (having subdirectories `plots.`*n*).

12 Isospin multipoles

13 Datasets included in `PWA` package

The `PWA` package comes with a selection of different experimental datasets for cross sections and polarisation observables for π^0, π^+, and η photoproduction. These datasets consist of recent Mainz, Bonn, and JLabmeasurements as well as some additional older results that are also present in the SAID database.

13.1 π^0 data

Datasets for π^0 photoproduction observables can be found in the directory `data/ppi0` of the `PWA` package. The following datasets for cross sections are provided:

σ_0: `sg0_CBMAMI_2008_Prakhov_PRL111-062004.txt`
    `sg0_CBMAMI_2014_Prakhov.txt`

σ_T: `sgT_CBMAMI_2014_Schumann-Otte.txt`

σ_E: `sgE_DAPHNE_2001_Preobrajenski.txt`

σ_F: `sgF_CBMAMI_2014_Schumann-Otte.txt`

The following datasets on polarisation asymmetries are provided:

Σ: `S_CBMAMI_2008_Prakhov_PRL111-062004.txt`
    `S_TAPSA2_2001_Leukel.txt`
    `S_GRAAL_2005_Bartalini_EPJA26-399.txt`

T: `T_CBMAMI_2014_Kashevarov.txt`
    `T_CBELSA_2014_Hartmann_PRL113-062001.txt`

P: P_CBELSA_2014_Hartmann_PRL113-062001.txt
   P_DNPL_1972_Prentice_NPB41-353.txt
   P_DNPL_1979_Bussey_NPB154-492.txt
   P_KHARKOV_1976_Derebchinski_JETP43-218.txt
   P_KHARKOV_1978_Zybalov_SJNP28-52.txt
   P_KHARKOV_1980_Bratashevski_NPB166-525.txt
   P_KHARKOV_1983_Belyaev_NPB213-201.txt

E: E_CBELSA_2014_Gottschall_PRL112-012003.txt

F: F_CBMAMI_2014_Kashevarov.txt

G: G_DAPHNE_2005_Ahrens_EJPA26-135.txt
   G_CBELSA_2012_Thiel_PRL109-102001.txt

H: H_CBELSA_2014_Hartmann_PRL113-062001.txt

13.2 π^+ data

Datasets for π^+ photoproduction observables can be found in the directory `data/npip` of the `PWA` package. The following datasets for cross sections are provided:

σ_0: sg0_JLAB_2009_Dugger_PRC79-065206.txt
   sg0_DAPHNE_2004_Ahrens_EPJA21-323.txt
   sg0_DAPHNE_2000_Beck_PRC61-034604.txt
   sg0_MAMI_1999_Branford_PRC61-014603.txt
   sg0_SAL_1996_Fisum_PRC53-1278.txt
   sg0_SAL_1999_Korkmaz_PRL83-3609.txt
   sg0_PHOENICS_1994_Buechler_NPA570-580.txt
   sg0_TOKYO_1979_Fujii_NPB120-395.txt
   sg0_BONN_1972_Fischer_ZP253-38.txt
   sg0_ORSAY_1968_Betourne_PR172-1343.txt
   sg0_ORSAY_1962_Walker_PRL8-37.txt
   sg0_CALTECH_1967_Ecklund_PR159-1195.txt
   sg0_GLASGOW_1964_Leith_PL8-355.txt

σ_E: sgE_DAPHNE_2001_Preobrajenski.txt

The following datasets on polarisation asymmetries are provided:

Σ: S_JLAB_2013_Dugger_PRC88-065203.txt
   S_DAPHNE_2000_Beck_PRC61-034604.txt
   S_GRAAL_2000_Ajaka_PLB475-372.txt
   S_GRAAL_2002_Bartalini_PLB544-113.txt
   S_LEGS_2001_Blanpied_PRC64-025203.txt
   S_KHARKOV_1989_Getman_VANT8-3.txt
   S_KHARKOV_1976_Ganenko_SJNP23-52.txt
   S_DNPL_1979_Bussey_NPB154-205.txt
   S_STANFORD_1963_Smith_PR130-2429.txt

T: T_PHOENICS_1996_Dutz_NPA601-319.txt
   T_KHARKOV_1981_Getman_NPB188-397.txt
   T_DNPL_1979_Bussey_NPB154-205.txt

P: P_KHARKOV_1981_Getman_NPB188-397.txt
   P_DNPL_1979_Bussey_NPB154-205.txt

G: G_DAPHNE_2005_Ahrens_EJPA26-135.txt
   G_KHARKOV_1984_Belyaev_SJNP40-83.txt
   G_DNPL_1980_Bussey_NPB169-403.txt

H: H_KHARKOV_1986_Belyaev_SNJP43-947.txt
   H_DNPL_1980_Bussey_NPB169-403.txt

13.3 η data

Datasets for η photoproduction observables can be found in the directory `data/peta` of the `PWA` package. The following datasets for cross sections are provided:

σ_0: `sg0_CBMAMI_2010_McNicoll_PRC82-035208.txt`

The following datasets on polarisation asymmetries are provided:

Σ: `S_GRAAL_2007_Bartalini_EPJA33-169.txt`

T: `T_CBMAMI_2014_Kashevarov_PRL113-102001.txt`

F: `F_CBMAMI_2014_Kashevarov_PRL113-102001.txt`

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