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A STATISTICAL FRAMEWORK FOR AUTOMATING RESONANCE DETECTION: MODELLING PION PROTON COLLISION ACTIVITY

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Abstract

In this paper, we analyze $\pi^- + p$ elastic collision data from the Particle Data Group (PDG), by creating a general framework to study resonance activity: automating peak detection, extrapolating, parametrizing thresholds, filtering resonances and further comparing and extracting characteristics, to identify Delta ($\Delta$) baryons. We then analyse experimental Energy vs Phase-Shift ($\delta$) data for the collision $\pi^+ + \pi^- \rightarrow \pi^- + \pi^+$, model the $T$ matrix from a curve fitted polynomial representation of the $K^{-1}$ matrix, simulate its Riemann sheets and analyse it to identify the characteristics of $\rho^0(770)$ meson, as well as estimate their uncertainties. These methodologies offer a foundation for similar analyses in different systems and events.

1 INTRODUCTION

A priceless example of where studying scattering has contributed in changing our understanding of the world is the Geiger-Marsden experiments [1], led by Rutherford between 1908 and 1913, where a beam of $\alpha$ particles was scattered against a thin gold foil and the scattering angles were then measured. Studying the results led to understanding that most of the atom mass is concentrated in the nucleus and has a positive charge, a pivotal result at the time.

To further aid in scattering research, the scattering matrix, or $S$-matrix [2], was introduced by John Archibald Wheeler in 1937, later developed by Werner Heisenberg in the 40s [3]. In the context of QFT, the $S$-matrix is defined as the unitary matrix connecting sets of asymptotically free particle states (the in-states and the out-states) in the Hilbert space of physical states.

While the $S$-matrix may be defined for any background (space-time) that is asymptotically solvable and has no event horizons, it has a simple form in the case of Minkowski space. We take the 1-D case where $S$-matrix is 2-dimensional. Consider a localized one-dimensional potential barrier $V(x)$, subjected to a beam of quantum particles with energy $E$, incident on the potential barrier from left to right.

The solutions of Schrödinger’s equation outside the potential barrier are plane waves given by

$$\psi_L(x) = Ae^{ikx} + Be^{-ikx}$$

for the region to the left of the potential barrier, and

$$\psi_R(x) = Ce^{ikx} + De^{-ikx}$$

for the region to the right of the potential barrier, where

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

is the wave vector.

The “scattering amplitude,” i.e., the transition overlap of the outgoing waves with the incoming waves, is a linear relation defining the $S$-matrix,

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}.$$
where
\[ \Psi_{\text{out}} = \left( \begin{array}{c} B \\ C \end{array} \right), \quad \Psi_{\text{in}} = \left( \begin{array}{c} A \\ D \end{array} \right), \quad S = \left( \begin{array}{cc} S_{11} & S_{12} \\ S_{21} & S_{22} \end{array} \right). \]

The elements of \( S \) completely characterize the scattering properties of the potential barrier \( V(x) \).

This \( S \)-matrix formulation lays the foundation to our study of resonance phenomena, emerging as features within scattering data signifying the presence of quasi-stable states [3]. Resonances are characterized by sharp changes in the phase shift as a function of energy, indicating the presence of intermediate states that significantly affect the scattering process [5].

A widely used theoretical framework for analyzing resonance behavior in scattering processes is the Breit-Wigner formula [6], describing the energy dependence of phase shift in the vicinity of a resonance,

\[ \delta(E) = \arctan \left( \frac{\Gamma_{\rho}}{2} \frac{1}{E - m_{\rho}} \right), \tag{1} \]

where \( \delta(E) \) is the phase shift at energy \( E \), \( m_{\rho} \) is the resonance mass, and \( \Gamma_{\rho} \) is the total width of the resonance. The phase shift exhibits a characteristic behavior with a maximum/minimum value corresponding to the resonant peak position \((E_{\text{peak}} = m_{\rho})\) [5]. Additionally, the width of the resonance in the data \((\Delta E_{\text{FWHM}})\) is related to the total width by \( \Delta E_{\text{FWHM}} \approx \Gamma_{\rho} \).

## 2 METHODOLOGY

### 2.1 Energy vs Cross-Section

We first consider the simpler case of analysing **Energy vs Probabilistic Cross-Section** in the \( \pi^- - p \) collision scenario from the **Particle Data Group** [7] (PDG), where resonances may appear as localized enhancements or peaks in the cross-section measurements, indicating a higher likelihood of interaction at particular energy values. This will lay the foundation to build on to higher dimensional model-fits and parametrizations.

![Figure 1: Raw Data](image1)

![Figure 2: Detected resonances at energy band (1,4)](image2)

Initially, peak indices in the dataset are identified and corresponding energy and cross-section values extracted. Using interpolation techniques, we translate these peak indices into energy values. Additionally, we ascertain peak widths and locate inflection points and incorporate adjustable parameters for peak height, width and threshold to filter these peaks and identify important resonance classes. Error bars associated with each data point is not explicitly a part of the method.

The width of the resonance \( (\Gamma) \) is related to the mean lifetime \( (\tau) \) of the particle (or its excited state) by the relation

\[ \Gamma = \frac{\hbar}{\tau}, \tag{2} \]

where \( \hbar \) is the reduced Planck constant [8] given by \( \hbar = \frac{h}{2\pi} \), and \( h \) is the Planck constant. These identified peak widths and masses with very high thresholds can be matched and referenced for discovering prominent particles.

### 2.2 Energy vs Phase-Shift \((\delta)\)

We first fit the theoretical model represented by the Breit-Wigner formula to the experimental data for the phase shift \( (\delta) \) and energy \((E)\). The fitting process aims to determine the best-fit values of \( M, \Gamma, \) and a constant that provide the closest agreement between the theoretical model and the experimental observations using non-linear least squares [9]. We then calculate the pole position of the resonance state using the fitted parameters \( M \) and \( \Gamma \), and extract its mass \((M)\), width \((\Gamma)\) from the pole position.
When dealing with strong interactions and resonances, the $K$-matrix [10] representation can efficiently describe resonant states and scattering amplitudes in a model-independent way. We utilise the methodology proposed by [11] for extracting resonance parameters defined as $K$-matrix mass and width, exactly at the energies of the $K$-matrix poles, in our method. The $S$-matrix is related to the $K$-matrix through

$$S = \eta - \frac{iK}{1+iK},$$

where $\eta$ is a diagonal matrix representing the relative phase between the different scattering channels.

The $K$-matrix is a complex symmetric matrix whose poles correspond to resonant states [11], containing information about their masses, widths, and couplings without assuming a specific Breit-Wigner resonance form. The $K$-matrix form of the $T$-matrix simplifies our calculation for certain scattering processes, which can be expressed as follows,

$$T_l(s) = \frac{\sqrt{s}}{K_l^{-1}(s) - ip_{\text{cms}}}.$$  \hspace{1cm} (4)

for the $l$th partial wave where $s$ is the center-of-mass energy squared, $p_{\text{cms}}$ is the center-of-mass momentum. And

$$p_{\text{cms}} = \sqrt{\frac{s}{4} - m^2},$$ \hspace{1cm} (5)

where $m$ is the mass of the pion.

In scattering theory, the function $K_l^{-1}(s)$ is the inverse of the $K$-matrix and is related to the scattering phase shift $\delta_l(s)$ for the partial wave $l$ by

$$K_l^{-1}(s) = p_{\text{cms}} \cot \delta_l(s),$$ \hspace{1cm} (6)

where $\delta_l(s)$ is the phase shift for the $l$-th partial wave at the given energy $\sqrt{s}$.

Our first task is to formulate a representation for $K^{-1}$ in terms of $s$ or $E$, for this we make use of the phase-shift ($\delta$) data provided. We assume $K^{-1}$ has a polynomial representation:

$$K^{-1} = \sum_{i=1}^{n} a_i (\sqrt{s})^i.$$ 

To identify coefficients $a_i$, we perform curve fitting with respect to known data ($\sqrt{s}$ vs $p_{\text{cms}} \cot(\delta)$) by minimizing error through Ordinary Least Squares (OLS), or finding the coefficients $a_i$ that minimize the sum of squared differences between the observed and predicted $K^{-1}$ values:

$$\text{minimize} \sum_{i=1}^{n} \left( \frac{y_i - \sum_{i=1}^{k} a_i (\sqrt{s})^i}{\sigma_i} \right)^2.$$ \hspace{1cm} (7)

Here, $n$ is the number of data points, $k$ is the number of powers considered and $\sigma_i$ is the standard error associated with the $i$th data point. Once the optimal parameters ($a_i$ and $n$) are determined, the model $K^{-1}$ can be used for predicting $p \cot(\delta)$ at new energy values. We then obtain the final form of $T$:

$$T(s, a_i) = \frac{\sqrt{s}}{\sum_{i=1}^{n} a_i (\sqrt{s})^i - i \sqrt{\frac{s}{4} - m^2}},$$ \hspace{1cm} (8)

where $a_i'$s are obtained from parameter tuning using OLS, $n$ is the number of terms considered, $s$ is the centre-of-mass energy squared, and $m$ corresponds to mass of the pion. We obtain the optimal parameters that best "fit" the experimental data, and then identify the presence of where poles occur in subsequent Energy-$|T|$ complex $3-D$ plots.

3 RESULTS

3.1 Resonance Detection by Automated Peak Selection

The collision $\pi^- + p \rightarrow p + \pi^-$ is studied with Beam Mass, or mass of the incoming particle ($\pi^-$), 0.139570 GeV/$c^2$ and the Target Mass, or mass of the target particle ($p$), being 0.938270 GeV/$c^2$. The threshold energy for the reaction to occur is 0, or the reaction is possible at all energies. The Final State Multiplicity is 2 and the number of data points available for the reaction is 277.
In our initial analysis of Energy vs Cross-Section Data of the studied system, we observe the resonance at around Energy 1270 MeV showing up at several very different parameter threshold settings. For example, at entirely different thresholds of energy band (0,30), prominence 10 and height 1 and energy band (1, 1.5), prominence 4 and height 1, peak index 13 shows up.

Table 1: B:(0,30) P:10 H:1

<table>
<thead>
<tr>
<th>Peak Index</th>
<th>Mass (MeV/c²)</th>
<th>Width (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>1287.8412</td>
<td>127.1235</td>
</tr>
<tr>
<td>76</td>
<td>1843.2671</td>
<td>114.5381</td>
</tr>
<tr>
<td>89</td>
<td>1964.8420</td>
<td>131.5981</td>
</tr>
</tbody>
</table>

Table 2: B:(1,1.5) P:4 H:1

<table>
<thead>
<tr>
<th>Peak Index</th>
<th>Mass (MeV/c²)</th>
<th>Width (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1242.8413</td>
<td>121.0759</td>
</tr>
<tr>
<td>10</td>
<td>1262.8410</td>
<td>121.0759</td>
</tr>
<tr>
<td>13</td>
<td>1287.8412</td>
<td>127.1235</td>
</tr>
<tr>
<td>18</td>
<td>1316.8375</td>
<td>113.7291</td>
</tr>
</tbody>
</table>

This possibly indicates the presence of a prominent resonance particle, the Delta (Δ) baryon. We calculate the mass (in GeV/c²) and mean-lifetime (s) of selected peaks and the error relative to true Δ Baryon values, obtained from Particle Listings of PDG [7]. The error ranges of both lifetime and mass are well within the statistical bounds relative to their respective orders.

Table 3: Particle Properties & error

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Identified Mass (GeV/c²)</td>
<td>1.287</td>
</tr>
<tr>
<td>Identified Mean Lifetime (s)</td>
<td>5.47 ± 0.14 × 10⁻²⁴</td>
</tr>
<tr>
<td>True Mass (GeV/c²)</td>
<td>1.232</td>
</tr>
<tr>
<td>True Mean Lifetime (s)</td>
<td>5.63 ± 0.14 × 10⁻²⁴</td>
</tr>
<tr>
<td>Error in Lifetime (s)</td>
<td>2.84±2.55 %</td>
</tr>
<tr>
<td>Error in Mass (GeV/c²)</td>
<td>4.46 %</td>
</tr>
</tbody>
</table>

3.2 Resonance Detection by T-Matrix Modelling & Optimisation

We observe the following pole position from the fitted parameters $M$ and $\Gamma$ using Breit-Weigner formula. The extracted parametric information about resonance state, like its mass ($M$), width ($\Gamma$) are identified.

This Mass and Width corresponds closely to a $\rho$ (770) meson [7], a short-lived hadronic particle forming an isospin triplet, with its three states $\rho^+$, $\rho^0$, and $\rho^-$, all with a mass of 775.45 ± 0.04 MeV.

They exhibit a very brief lifetime [12], and their decay width is approximately 145 MeV. As we can observe, with an error percent ~20, the decay widths ($\Gamma$) deviate well from a standard Breit–Wigner form.

We now move to the explicit parametrisation of $T$-matrix based on $K$ matrix form as mentioned. Error minimisation of the polynomial form of $K^{-1}$ with respect to given $\cot(\delta)$ using OLS with number of coefficients, $n = 4$, gives us the following set of values:

<table>
<thead>
<tr>
<th>Power</th>
<th>Coefficient</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>1.22900884 × 10⁻⁷</td>
<td>MeV</td>
</tr>
<tr>
<td>3</td>
<td>-8.80327494 × 10⁻¹¹</td>
<td>MeV</td>
</tr>
<tr>
<td>2</td>
<td>4.08050667 × 10⁻¹⁴</td>
<td>MeV</td>
</tr>
<tr>
<td>1</td>
<td>-1.10636185 × 10⁻¹⁷</td>
<td>MeV</td>
</tr>
<tr>
<td>0</td>
<td>1.33353224 × 10⁻⁻²¹</td>
<td>MeV</td>
</tr>
</tbody>
</table>

Substituting these values, with $n$ increased to 10, into the final form of $K^{-1}$ and plotting it against real data gives us an almost coinciding fit. Using this representation of $K^{-1}$ in the $K$ matrix form of $T$, we simulate the Riemann sheets of $|T|$ against $\Re(E)$ and $\Im(E)$. We then identify the arguments $\Re(E)$ and $\Im(E)$ corresponding to $\max(|T|)$ in our ranges of interest, and extract the pole position to the 4th decimal point. The Mass corresponding to these parameters (772.7273 MeV) align closely with that of $\rho$ (770) meson but the Width (81.8182 MeV) shows significant deviation.
4 DISCUSSION

Our primary analysis of Energy vs Cross-Section data in $\pi^- - p$ collision for identifying resonance states using automated peak identification and threshold filtering techniques reveals the existence, with error within error bounds associated with true values, of Delta ($\Delta$) baryons. This is to be expected in the system as Delta states are created when sufficiently energetic probes like photons, electrons, neutrinos, and pions collide with protons and neutrons [13].

All Delta ($\Delta$) baryons, with masses around 1232 MeV, decay rapidly [12] (within orders of $10^{-23}$ seconds as observed), into nucleons (protons or neutrons) and pions by strong interactions, making it relatively difficult to accurately measure its mass (a 4.46% deviation was found from the true mass). As the baryon decayed into a $\pi^-$ and $p$, it is most possibly the $\Delta^0$ particle composed of one u quark and two d quarks, with isospin number -1/2, angular momentum 3/2 and parity + [14]. This result, i.e, the formation and very fast decay of Delta $\Delta$ baryons agrees with parameters of the collision system, including the particles before and after the collision ($\pi^- + p \rightarrow p + \pi^-$).

Secondly, resonance characteristics extracted from $\pi^-\pi^-$ collision data by 1) fitting of the model represented by Breit-Wigner formula and 2) $T$ matrix modelling correlates well with the behaviour of $\rho(770)$ mesons which can be considered to be an excited state of the pion. Very importantly, the very short mean life-time of $\rho^0(770)$ resonance at $(4.453 \pm 0.027) \times 10^{-24}$ seconds [12] along with the absurd feature of its decay widths not being described by a Breit-Wigner form may explain the deviation in our measurements.

The $\rho(770)$ meson carries the nuclear force within the atomic nucleus and are the lightest strongly interacting particle after the pions and kaons, with a mass of 775.45±0.04 MeV for all three states. Our identified masses of 765 and 772.72 MeV, with errors of 1.34% and 0.35% respectively, correspond closely to previously observed values. It is a short-lived hadronic particle that is an isospin triplet whose three states are denoted as $\rho^+$, $\rho^0$ and $\rho^-$, and commonly decays into $\pi^+$ and $\pi^-$ or $\pi^+/\pi^-$ and $\pi^0$, consistent with our system ($\pi^+ + \pi^- \rightarrow \pi^- + \pi^+$).

5 CONCLUSION

The automated pole detection in our primary Energy vs Cross-Section analysis can be refined further by considering more and better variety of thresholds. The resonance mass identified from extracting pole parameters from $T$ based on selected $K^{-1}$ can be made more accurate by considering higher order powers for the the polynomial approximation.

In synopsis, the paper presents the outline of a statistical methodology in analysing scattering data between different subatomic particles, especially tools to identify characteristics of extremely short-lived resonance states in collisions. These tools in peak detection, matrix modelling, optimisation, parameter selection and pole detection can be used analogously to study various different events. Specifically, the study of resonance states as particles like baryons and mesons reveals ever-evolving insights into strong and weak nuclear forces, quark gluon structures and theoretical models like Quantum Chromodynamics (QCD) [15], to name some.
References


