
Differential Proton-Proton Scattering Cross Section for energies between 1.9 MeV and 50 MeV

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ABSTRACT

We present a phase shift analysis of differential elastic proton-proton scattering cross sections $(d\sigma/d\Omega)_{pp}$ in the energy range from 1.9 MeV to 50 MeV and laboratory scattering angles $\theta_{lab} = 15 \dots 75$. It results in an accurate representation of the experimental data by an analytical function for $(d\sigma/d\Omega)_{pp}(E, \theta)$. The average statistical error of the resulting data fit is 0.2%. For a fast evaluation we extract an $[\mathbf{E}, \theta]$ -matrix for $(d\sigma/d\Omega)_{pp}$ with a negligible interpolation error smaller than 0.02%. This data may be relevant for data evaluation for hydrogen analysis when using proton-proton scattering.

Chapter 1

INTRODUCTION

Elastic proton-proton scattering (pp-scattering) at MeV energies has proven to be the most sensitive method for hydrogen depth profiling at micrometer depth resolution. Even a detection limit as low as 0.08 ppm was achieved in diamond material utilizing a detector setup covering $\Omega = 2.4$ sr of solid angle (1). In particular, the high sensitivity allows this method to be applied to proton microprobes in order to image hydrogen distributions with micrometer or better lateral resolution, resulting in a 3D hydrogen microscopy tool (1). Beside the high sensitivity there is another main advantage compared to other methods for hydrogen imaging like IR-microscopy or imaging SIMS (secondary ion mass spectrometry): There is no need of reference standards to calibrate the detection cross section or absorption coefficient for matrix or other material/sample dependent effects. This universal application potential is due to the high proton energy that is 5-6 orders of magnitudes larger than the binding energy of the hydrogen atoms and hence the chemical and structural environment has negligible influence on the differential proton-proton scattering cross section and thus the detection rate. The hydrogen areal density $n_{\text{H}}\Delta z$ in at/cm², which is the product of the hydrogen density n_{H} and the sample thickness Δz in a certain depth z of the sample,

can be calculated by (2)

$$n_{\text{H}}\Delta z = \frac{N_{\text{pp}}}{N_0 \cdot \sigma_{\text{pp}}} \quad \text{with} \quad \sigma_{\text{pp}} = \int_{\Omega_{\text{pp}}} \int_{\Delta z} \left(\frac{d\sigma}{d\Omega} \right)_{\text{pp}} \varepsilon_{\text{pp}}(z) dz d\Omega \quad (1.1)$$

with N_{pp} being the number of detected pp-scattering events, N_0 is the number of incident protons, $\varepsilon_{\text{pp}}(z)$ accounts for the detection efficiency within the solid angle of detection Ω_{pp} and $(d\sigma/d\Omega)_{\text{pp}}$ is the differential pp-scattering cross section. It varies with depth z due to the change of the proton energy E from energy loss in the sample before the scattering event happens. The accuracy of incident beam current measurement (N_0) is mainly affecting the total accuracy and is a critical experimental task, but as long as particle statistics is good enough and the solid angle is well defined the accuracy in hydrogen analysis is mainly given by the accuracy of $(d\sigma/d\Omega)_{\text{pp}}$. The aim of this paper is to extract $(d\sigma/d\Omega)_{\text{pp}}$ from experimental data found in literature for a wide range of scattering angles θ and incident proton energies E with optimum accuracy.

Existing databases (see Section 3.1) give data sets in discrete steps. With the aim of a closed nuclear potential theory, partial-wave analyses of this data have been performed for a broad energy range up to $E = 450 \text{ MeV}$ (e.g.(3; 4; 5)). These analyses result in a parameterization of the nuclear potential with many parameters additionally to nuclear phase shifts. We found this to be a too complex evaluation method for $(d\sigma/d\Omega)_{\text{pp}}$ for applied nuclear physics in the range of usable energies from $1.9 \dots 50 \text{ MeV}$. We focus here on this energy range and an angular range of $\theta_{\text{lab}} = 15^\circ \dots 75^\circ$ that is the maximum reasonable range used for hydrogen analysis by proton-proton scattering. Lower energies or steeper angles reduce the analysable sample thickness to uncomfortably low values and higher energies are difficult to analyse with reasonable detector effort. With this restriction, we have developed two new kinds of parameterizations of $(d\sigma/d\Omega)_{\text{pp}}$:

(A) A simple exponential approximation with an analytical formula that can

be applied without numerical calculations, but with errors up to 4%, and hence slightly larger than the experimental errors at large angles and some particular data sets. Errors are within the experimental uncertainties ($\sim 1\%$) for a limited range of angles and energies. This parameterization is already published in (2), but for completeness and some critical typos in the book chapter we summarize the results of the parameterization with the revision of the former publication and we additionally present the validation of the fit.

(B) An approximation using physical functions, which describes a series expansion of $(d\sigma/d\Omega)_{pp}$ in the angular momenta with nuclear phase shifts as parameters, similar to the above mentioned theoretical nuclear potential analyses, but with as low as possible parameters. The statistical error of this fit is even less than the given experimental errors due to the large number of simultaneously fitted data.

Chapter 2

THEORY

2.1 NUCLEON-NUCLEON SCATTERING

Proton-proton scattering is scattering of two identical particles (e. g. (6; 7)). Due to indistinguishability of two scattered protons at angles θ_{CM} and $\pi - \theta_{\text{CM}}$ in the center-of-mass (CM) system, it comes to an interference phenomenon. The scattering amplitudes $f(\theta_{\text{CM}})$ and $f(\pi - \theta_{\text{CM}})$ have to be added for both particles when considering the exchange symmetry (8)

$$f_J(\theta) = f(\theta_{\text{CM}}) + (-1)^J f(\pi - \theta_{\text{CM}}) \quad (2.1)$$

for each state of total spin J . If scattering is independent of the spin s of the particles (no spin flip), and no spin polarization occurs, Eq. (2.1) has to be weighted with the statistical spin states in order to obtain the differential pp-scattering cross section

$$\frac{d\sigma}{d\Omega} = \sum_{J=0}^{2s} \frac{2J+1}{(2s+1)^2} |f_J(\theta_{\text{CM}})|^2 \quad (2.2)$$

with the spin s for the particle.

For scattering on the Coulomb potential only, Eq. (2.2) results in the well known

Mott scattering cross section (8) that is given for the CM system by

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Mott}} = \frac{\eta^2}{4k^2} \left[\sin^{-4} \frac{\theta_{\text{CM}}}{2} + \cos^{-4} \frac{\theta_{\text{CM}}}{2} + \frac{(-1)^{2s}}{2s+1} \frac{2 \cos(\eta \ln(\tan^2 \frac{\theta_{\text{CM}}}{2}))}{\sin^2 \frac{\theta_{\text{CM}}}{2} \cos^2 \frac{\theta_{\text{CM}}}{2}} \right] \quad (2.3)$$

$$\begin{aligned} \text{with } k &= \frac{m_p v}{2\hbar} \\ \eta &= \frac{e^2}{4\pi\epsilon_0 v \hbar} \text{ Sommerfeld - parameter} \end{aligned}$$

with m_p being the proton mass, v the relative velocity, e the electronic charge, $\hbar = \frac{h}{2\pi}$ the Planck constant divided 2π and ϵ_0 the dielectric constant. The first coefficient can be written for the calculations in the CM-system

$$\frac{\eta^2}{4k^2} = \left(\frac{e^2}{4\pi\epsilon_0 m_p v^2} \right)^2 = \left(\frac{e^2}{4\pi\epsilon_0 2m_p^* v^2} \right)^2 = \left(\frac{e^2}{4\pi\epsilon_0 4E_{\text{CM}}} \right)^2 \quad (2.4)$$

with $m_p^* = m_p/2$ the reduced proton mass and E_{CM} for the kinetic energy in the CM-system.

For the relativistic transformation of the kinetic energy E_{CM} from the CM-system in the lab system¹ \mathbf{E} and vice versa the following relationship is used:

$$E_{\text{CM}} = \frac{\mathbf{E}}{1 + \gamma_{\text{CM}}} \quad (2.5)$$

with γ_{CM} as the Lorentz-factor for both protons in the CM-system, which is given by

$$\gamma_{\text{CM}} = \sqrt{\frac{\mathbf{E}}{2m_p c^2} + 1} \quad (2.6)$$

¹if not stated otherwise, a bold \mathbf{E} marks the kinetic energy of the incident proton in the lab system.

In case of unpolarized pp-scattering, the spin dependence term $\frac{(-1)^{2s}}{2s+1}$ of Eq. (2.3) results in $-\frac{1}{2}$.

Considering nuclear contributions one can efficiently analyse the scattering amplitudes by a partial wave expansion. With respect to this, one has to fulfil the Pauli's exclusion principle. The wave function of the two protons has to be antisymmetric under their exchange. Hence, a symmetric space wave function (S, D, G, \dots -states) can only be associated with an antisymmetric spin wave function (even J , i. e. pp-singlet), whereas an antisymmetric space wave function (P, F, \dots -states) requires a symmetric spin wave function (odd J , i. e. pp-triplet). At 10 MeV the cross section is dominated more than 99% by S -wave scattering (3; 4). The contribution of the P -states increases with energy but still is a minor fraction below 30 MeV. In all cases, the P -wave scattering cross section is zero at $\theta_{\text{lab}} = 45^\circ$ in the lab frame, due to the interference in the identical particle system. In the interesting energy range, higher order states (like D -states) have an even lower scattering amplitude than the P -states.

In the present analysis, a partial wave expansion for the angular momentum is used that is restricted to the angular momentum $L = 0, 1, 2$, respectively, the S , P and D -states (9; 10):

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{CM}} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{Mott}} + \left(\frac{d\sigma}{d\Omega}\right)_{\text{V}} + \sum_{i=0}^2 \left(\frac{d\sigma}{d\Omega}\right)_{L=i} \quad (2.7)$$

with $\left(\frac{d\sigma}{d\Omega}\right)_{\text{V}}$ being a correction of the Mott cross section for the vacuum polarization effects and $\sum_{i=0}^2 \left(\frac{d\sigma}{d\Omega}\right)_{L=i}$ is the contribution of the different partial waves.

The nuclear interaction terms from phase shift analysis are written as

$$\left(\frac{d\sigma}{d\Omega}\right)_{L=0}^S = \frac{\eta^2}{4k^2} \left[-\frac{2X_0}{\eta} \sin(\delta_0) \cos(\delta_0) + \left(\frac{2Y_0}{\eta} + \frac{4}{\eta^2}\right) \sin^2(\delta_0) \right] \quad (2.8)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{L=1}^P = \frac{\eta^2}{4k^2} \left[-\frac{2X_1 P_1}{\eta} Z_2 + \left(\frac{2Y_1 P_1}{\eta} + \frac{4}{\eta^2}\right) Z_1 + \frac{4P_2}{\eta^2} Z_3 \right] \quad (2.9)$$

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega}\right)_{L=2}^D &= \frac{\eta^2}{4k^2} \left[-\frac{10X_2 P_2}{\eta} \sin(\delta_d) \cos(\delta_d) \right. \\ &\quad + \left. \left(\frac{10Y_2 P_2}{\eta} + \frac{100P_2^2}{\eta^2}\right) \sin^2(\delta_d) \right. \\ &\quad \left. + \frac{40P_2}{\eta^2} \sin(\delta_0) \sin(\delta_d) \cos(\delta_d - \delta_0 + \zeta) \right] \end{aligned} \quad (2.10)$$

These terms depend on the phase shifts δ_0 for S-wave scattering, $\delta_P^{(0)}, \delta_P^{(1)}, \delta_P^{(2)}$ for the P-wave scattering and on an effective D-wave phase shift δ_d . The representation of the P-wave scattering is transformed using coupling parameters Z_1, Z_2 and Z_3 :

$$Z_1 = \sin^2(\delta_P^{(0)}) + 3 \sin^2(\delta_P^{(1)}) + 5 \sin^2(\delta_P^{(2)}) \quad (2.11)$$

$$\begin{aligned} Z_2 &= \sin(\delta_P^{(0)}) \cos(\delta_P^{(0)}) + 3 \sin(\delta_P^{(1)}) \cos(\delta_P^{(1)}) \\ &\quad + 5 \sin(\delta_P^{(2)}) \cos(\delta_P^{(2)}) \end{aligned} \quad (2.12)$$

$$\begin{aligned} Z_3 &= \frac{3}{2} \sin^2(\delta_P^{(1)}) + \frac{7}{2} \sin^2(\delta_P^{(2)}) \\ &\quad + 4 \sin(\delta_P^{(2)}) \sin(\delta_P^{(0)}) \cos(\delta_P^{(2)} - \delta_P^{(0)}) \\ &\quad + 9 \sin(\delta_P^{(2)}) \sin(\delta_P^{(1)}) \cos(\delta_P^{(2)} - \delta_P^{(1)}) \end{aligned} \quad (2.13)$$

and the other used notations are

$$\begin{aligned}
X_0 &= \frac{\cos\left(\eta \ln\left(\sin^2 \frac{\theta_{\text{CM}}}{2}\right)\right)}{\sin^2 \frac{\theta_{\text{CM}}}{2}} + \frac{\cos\left(\eta \ln\left(\cos^2 \frac{\theta_{\text{CM}}}{2}\right)\right)}{\cos^2 \frac{\theta_{\text{CM}}}{2}} \\
Y_0 &= \frac{\sin\left(\eta \ln\left(\sin^2 \frac{\theta_{\text{CM}}}{2}\right)\right)}{\sin^2 \frac{\theta_{\text{CM}}}{2}} + \frac{\sin\left(\eta \ln\left(\cos^2 \frac{\theta_{\text{CM}}}{2}\right)\right)}{\cos^2 \frac{\theta_{\text{CM}}}{2}} \\
X_1 &= \frac{\cos\left(\eta \ln\left(\sin^2 \frac{\theta_{\text{CM}}}{2}\right) + \xi\right)}{\sin^2 \frac{\theta_{\text{CM}}}{2}} - \frac{\cos\left(\eta \ln\left(\cos^2 \frac{\theta_{\text{CM}}}{2}\right) + \xi\right)}{\cos^2 \frac{\theta_{\text{CM}}}{2}} \\
Y_1 &= \frac{\sin\left(\eta \ln\left(\sin^2 \frac{\theta_{\text{CM}}}{2}\right) + \xi\right)}{\sin^2 \frac{\theta_{\text{CM}}}{2}} - \frac{\sin\left(\eta \ln\left(\cos^2 \frac{\theta_{\text{CM}}}{2}\right) + \xi\right)}{\cos^2 \frac{\theta_{\text{CM}}}{2}} \\
X_2 &= \frac{\cos\left(\eta \ln\left(\sin^2 \frac{\theta_{\text{CM}}}{2}\right) + \zeta\right)}{\sin^2 \frac{\theta_{\text{CM}}}{2}} + \frac{\cos\left(\eta \ln\left(\cos^2 \frac{\theta_{\text{CM}}}{2}\right) + \zeta\right)}{\cos^2 \frac{\theta_{\text{CM}}}{2}} \\
Y_2 &= \frac{\sin\left(\eta \ln\left(\sin^2 \frac{\theta_{\text{CM}}}{2}\right) + \zeta\right)}{\sin^2 \frac{\theta_{\text{CM}}}{2}} + \frac{\sin\left(\eta \ln\left(\cos^2 \frac{\theta_{\text{CM}}}{2}\right) + \zeta\right)}{\cos^2 \frac{\theta_{\text{CM}}}{2}} \\
\xi &= 2 \arctan(\eta) \\
\zeta &= 2 \arctan(\eta) + 2 \arctan\left(\frac{1}{2}\eta\right) \\
P_1 &= P_{L=1}(\cos(\theta_{\text{CM}})) = \cos(\theta_{\text{CM}}) \text{ 1st Legendre polynomial} \\
P_2 &= P_{L=2}(\cos(\theta_{\text{CM}})) = -\frac{1}{2} + \frac{3}{2} \cos(\theta_{\text{CM}})^2 \text{ 2nd Legendre polynomial}
\end{aligned} \tag{2.14}$$

Chapter 3

PARAMETERIZATION

3.1 EXPERIMENTAL DATA

There are several experimental data pools for differential pp-scattering cross section $(d\sigma/d\Omega)_{pp}(\theta, E)$ like (11) and EXFOR/CSISRS (12; 13). Experimental data have been pooled to parameterize the data between $\mathbf{E} = 1.855 \dots 50.1$ MeV and scattering angles $\theta_{CM} > 20^\circ$ in (2). The experimental data of $(d\sigma/d\Omega)_{pp}(\theta)$ with references are shown for the lab system in Fig. 3.1.

3.2 EXPONENTIAL APPROXIMATION

This section gives a short overview on the 3-parameter exponential approximation as discussed in (2), where a detailed documentation of this approximation is given. The approximation is given by:

$$\frac{d\sigma}{d\Omega}(\mathbf{E}, \theta_{CM}) = \left(\frac{d\sigma}{d\Omega} \right)_{Mott} + A(\mathbf{E}) \cdot (1 - e^{C(\mathbf{E})(B(\mathbf{E}) + \theta_{CM})}) \quad (3.1)$$

where $(d\sigma/d\Omega)_{Mott}$ is taken from Eq. (2.3) and $A(\mathbf{E})$, $B(\mathbf{E})$ and $C(\mathbf{E})$ are the least square fit parameters¹. The parameters are parameterized depending on

¹The Eq. (3.2)-(3.3) in (2) contains some typos, which are corrected here.

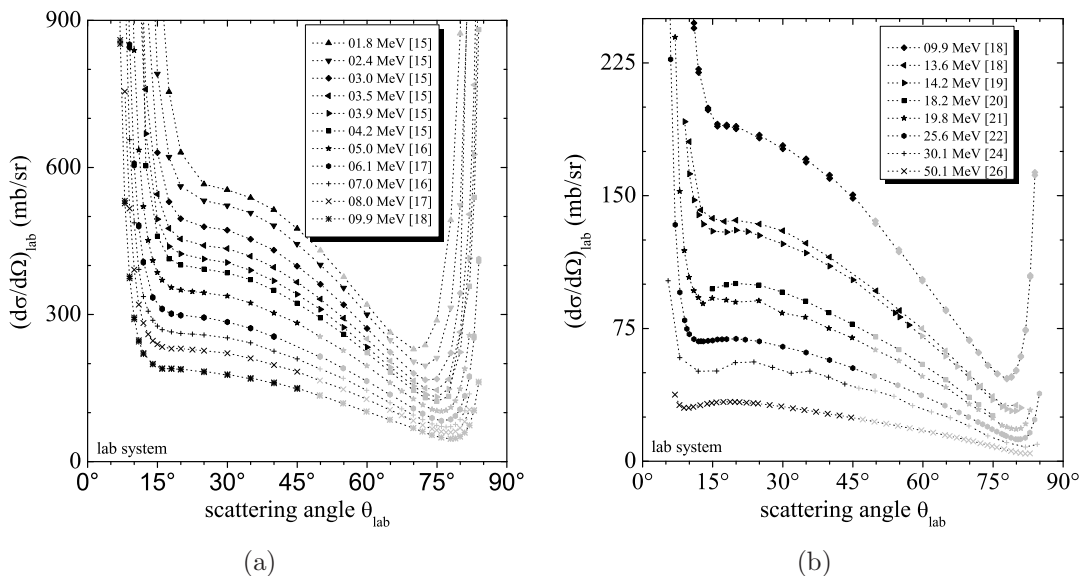


Figure 3.1: Elastic pp-scattering cross section data (lab system) (from (2)). Data points are connected for better visibility. Reported relative errors are smaller than 1% for $\theta_{\text{lab}} = 20^\circ \dots 70^\circ$. This data and further data including inelastic scattering data are available in collection (11) or databases like EXFOR/CSISRS (12; 13). Grey data points are calculated from symmetrical angles. Note that the differential cross section is symmetrical to 90° in the CM system, but not in the lab system due to $d\Omega$ transformation!

the kinetic energy in the lab system \mathbf{E} with:

$$A(\mathbf{E}) = a_0 (1 + a_1 \mathbf{E})^{-a_2} \quad (3.2)$$

$$B(\mathbf{E}) = b_0 + b_1 e^{b_2 \mathbf{E}} \quad (3.3)$$

$$C(\mathbf{E}) = c_0 + c_1 \mathbf{E} \quad (3.4)$$

The obtained values using in total 8 parameters a_i , b_i and c_i are listed in Table 3.1. Thus, we obtain pp-scattering cross sections in the CM-system as an analytical function of the CM-scattering angle $\theta_{\text{CM}} = 20^\circ \dots 90^\circ$ and kinetic energy $\mathbf{E} = 1.4 \text{ MeV} \dots 50.1 \text{ MeV}$ using Eq. (3.1) - (3.4). However, note that the accuracy of this fit is limited. For energies below 3 MeV, the fit does not represent the

data well. At higher energies, the deviations exceed 3% only for few single data points, in particular at small scattering angles.

Table 3.1: Fit parameters for regression analysis of parameters $A(\mathbf{E})$, $B(\mathbf{E})$ and $C(\mathbf{E})$ with Eqs. (3.2)-(3.4). The Table is also an erratum of Table in (2).

Parameter	Value	χ_{red}^2	R_{corr}^2
a_0 (mb/sr)	365 ± 23		
a_1 (1/MeV)	0.37 ± 0.04	32.6	0.9988
a_2	1.267 ± 0.024		
b_0 ($^\circ$)	-14.92 ± 0.14		
b_1 ($^\circ$)	-36.6 ± 1.9	17.8	0.9838
b_2 (1/MeV)	-0.368 ± 0.020		
c_0 (1/ $^\circ$)	$(-78.6 \pm 2.4) \cdot 10^{-3}$	8.4	0.888
c_1 (1/ $^\circ$ MeV)	$(-1.68 \pm 0.13) \cdot 10^{-3}$		

3.3 EVALUATION OF THE EXPONENTIAL APPROXIMATION

For quantification of the goodness of the regression formula of Eq. (3.1) - (3.4) we have calculated the reduced least square function

$$\chi_{\text{red}}^2 = \frac{1}{N_{\text{df}}} \sum_{j=1}^n \frac{\left(\frac{d\sigma}{d\Omega_{\text{pp}}}(\mathbf{E}_j, \theta_j) - X(\mathbf{E}_j, \theta_j) \right)^2}{\Delta_{\text{exp}}^2(\mathbf{E}_j, \theta_j)} \quad (3.5)$$

with the experimental data X_j including its experimental errors $\Delta_{\text{exp},j}$. The value N_{df} is the reduced number of degrees of freedom that is given by $N_{\text{df}} = n - p$ with $n = 566$ data points and $p = 8$ parameters. As a second parameter for the goodness of the fit we calculated the correlation parameter:

$$R_{\text{corr}}^2 = 1 - \frac{\frac{1}{n-p-1} \sum_{j=1}^n \left(X(\mathbf{E}_j, \theta_j) - \frac{d\sigma}{d\Omega_{\text{pp}}}(\mathbf{E}_j, \theta_j) \right)}{\frac{1}{n-1} \sum_{j=1}^n (X_j - \bar{X})} \quad (3.6)$$

with \bar{X} for an averaged value of the data. The goodness of fit coefficient χ_{red}^2 describes the mean square deviation relative to the experimental error Δ_{exp} . For $\chi_{\text{red}}^2 = 1$ the deviation of the fit function could be explained by the experimental errors, otherwise the value is > 1 . The R_{corr}^2 coefficient can get values between $0 \dots 1$. For $R_{\text{corr}}^2 = 1$ the function is correlated with the dataset and for $R_{\text{corr}}^2 = 0$ uncorrelated. The calculated values of χ_{red}^2 and R_{corr}^2 for the fitted parameters are listed in Table 3.1. The $R_{\text{corr}}^2 = 0.9988$ shows a good correlation of the fit with the data. The χ_{red}^2 , however, has an value of 32.6 for the parameter $A(\mathbf{E})$ which indicates an inefficient fitting function. This could be problematical for interpolations and extrapolations.

For hydrogen analysis, angles $\theta_{\text{CM}} > 50^\circ$ are used in general. Here, the data are fitted with deviations better than 1 %, which is in the range of the reported experimental errors and hence the fit is suitable for many quantification pur-

poses. Also, note that the fit function is only to be used for $\theta_{\text{CM}} \leq 90^\circ$, but the scattering cross section is symmetrical to 90° in the CM-system anyway. The parameterization of Eq. (3.1) - (3.4) using the parameters from Table 3.1 are shown exemplarily for selected energies in Fig. 3.5 (tagged as EV2).

3.4 REGRESSION BY PHASE SHIFT ANALYSIS

In order to obtain a fit of $(d\sigma/d\Omega)_{\text{pp}}$ with a higher accuracy we utilize the phase shift analysis of Section 2 according to Eq. (2.7) - (2.14). In a first step, the phase shifts δ_0 , δ_d and the three coupling parameters Z_1 , Z_2 and Z_3 are fitted for each energy where a complete data set of $(d\sigma/d\Omega)_{\text{pp}}(\theta)$ existed. The fitting of the three coupling parameters Z_i was introduced instead of fitting $\delta_P^{(i)}$ because of a better convergence behavior. Initial values for the phase shifts δ_0 , $\delta_P^{(0)}$, $\delta_P^{(1)}$, $\delta_P^{(2)}$ were taken from (10) in the energy range of 1.855 . . . 3.037 MeV in order to obtain a stable fit behavior. For further regression computations at higher energies, the set of parameters at one energy was used as the initial values of the fit at the next higher energy. In (10) or other physical phase shift calculations the data are corrected by the vacuum polarization contribution $(\frac{d\sigma}{d\Omega})_{\text{V}}$. In first calculations we saw, that a fit without considering explicitly the vacuum polarisation contribution has the same significance than including the vacuum polarisation contribution. However, parameter fluctuations are larger when the vacuum polarisation was included. Hence we performed the fit without the term $(\frac{d\sigma}{d\Omega})_{\text{V}}$ accepting that the physical meaning of the phase shift values for nuclear physics theory gets lost. Fig. 3.2 - 3.3 shows the phase shifts for S, P and D-state scattering resulting from the least square fits depending on the incident proton energy E (\square). For comparison the computations from (5) are plotted therein as well (small (\triangleright)-data points with chain line). Due to successive restriction of the angular range to scattering

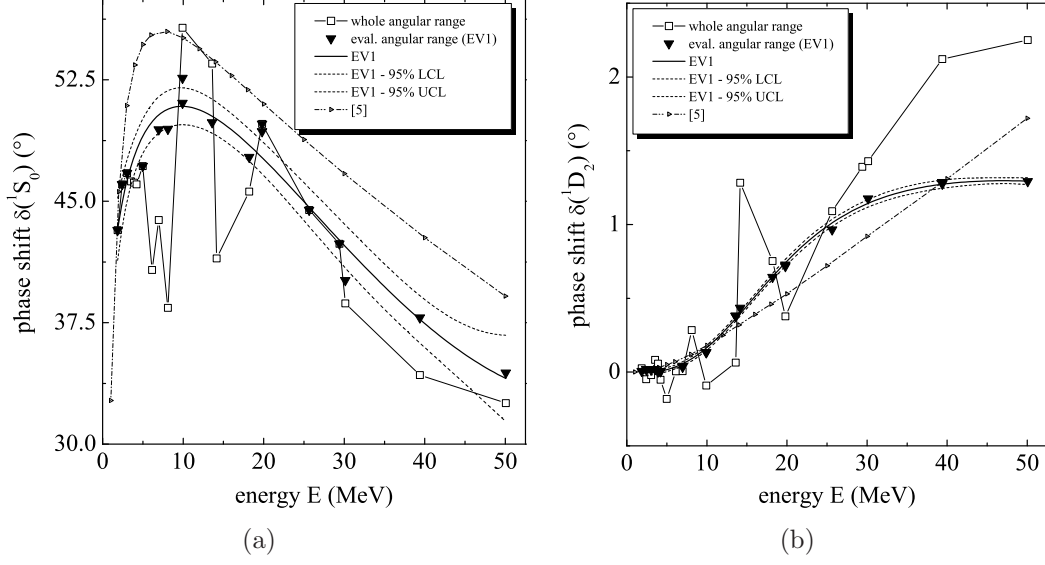


Figure 3.2: Calculated 1S_0 phase shift δ_0 (a) and 1D_2 phase shift δ_d (b) in degrees vs particle energy E . The data points (\square) (connected for better visibility) represent the calculations with full angular range compared to the (\blacktriangledown)-points in which the calculations are done by successive reduction of the angular range. For comparison, the connected smaller (\blacktriangleright)-data points (chain line) are from other phase shift calculations (5). The solid line shows calculated parameterizations $\delta_{0,d}(E)$ of these phase shifts (EV1) as explained in Section 3.5 with 95% confidential intervals (dashed lines).

angles where mainly the nuclear part contributes to $(d\sigma/d\Omega)_{pp}$ we obtain stable fits with a smooth energy dependence of the parameters (\blacktriangledown).

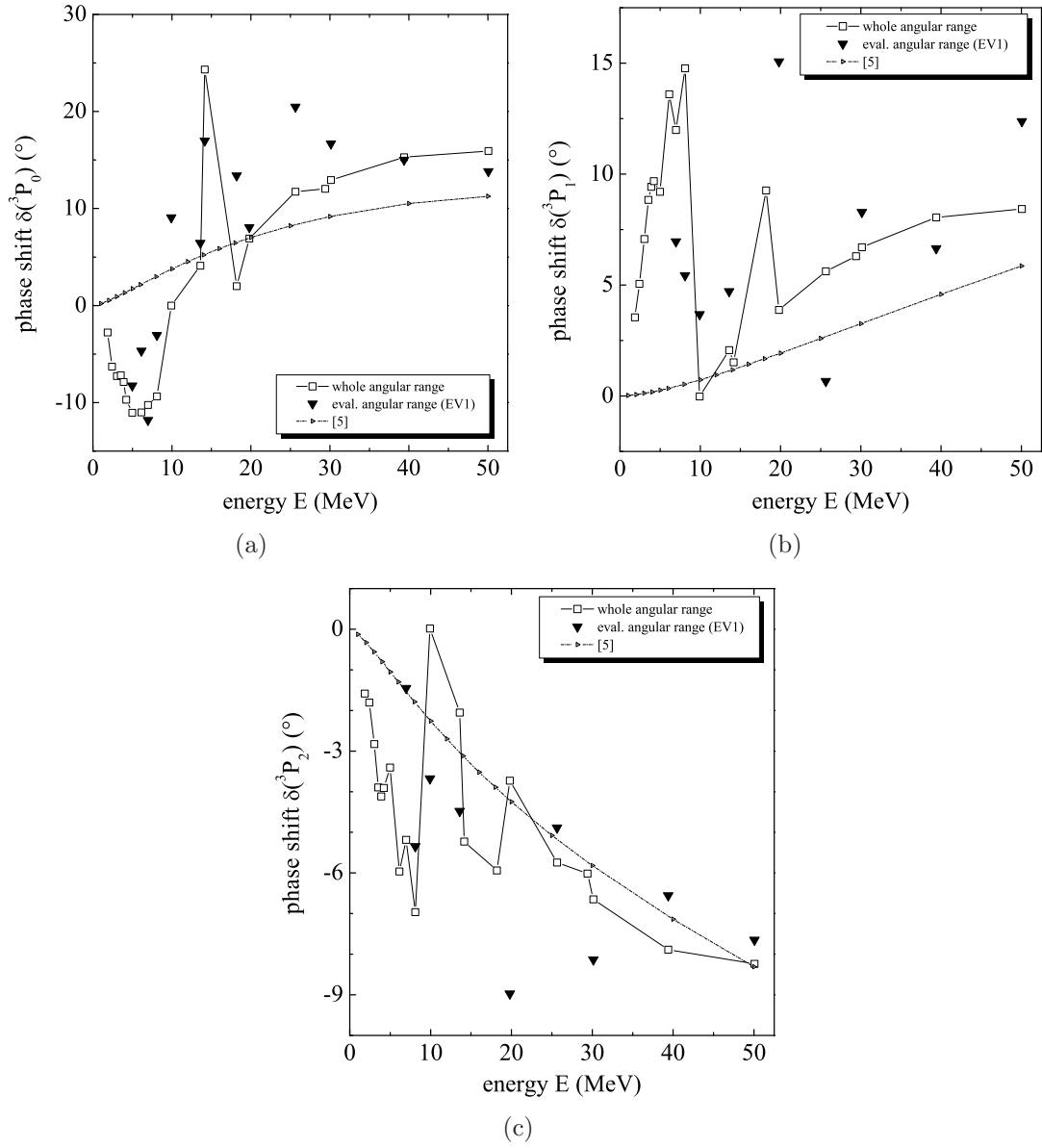


Figure 3.3: Calculated P-wave phase shifts $\delta_P^{(0)}$ (a), $\delta_P^{(1)}$ (b) and $\delta_P^{(2)}$ (c) in degrees vs particle energy E . The data points (\square) (connected for better visibility) represent the calculations with full angular range compared to the (\blacktriangledown)-points in which the calculations are done by successive reduction of the angular range. For comparison, the connected smaller (\triangleright)-data points (chain line) are from other phase shift calculations (5).

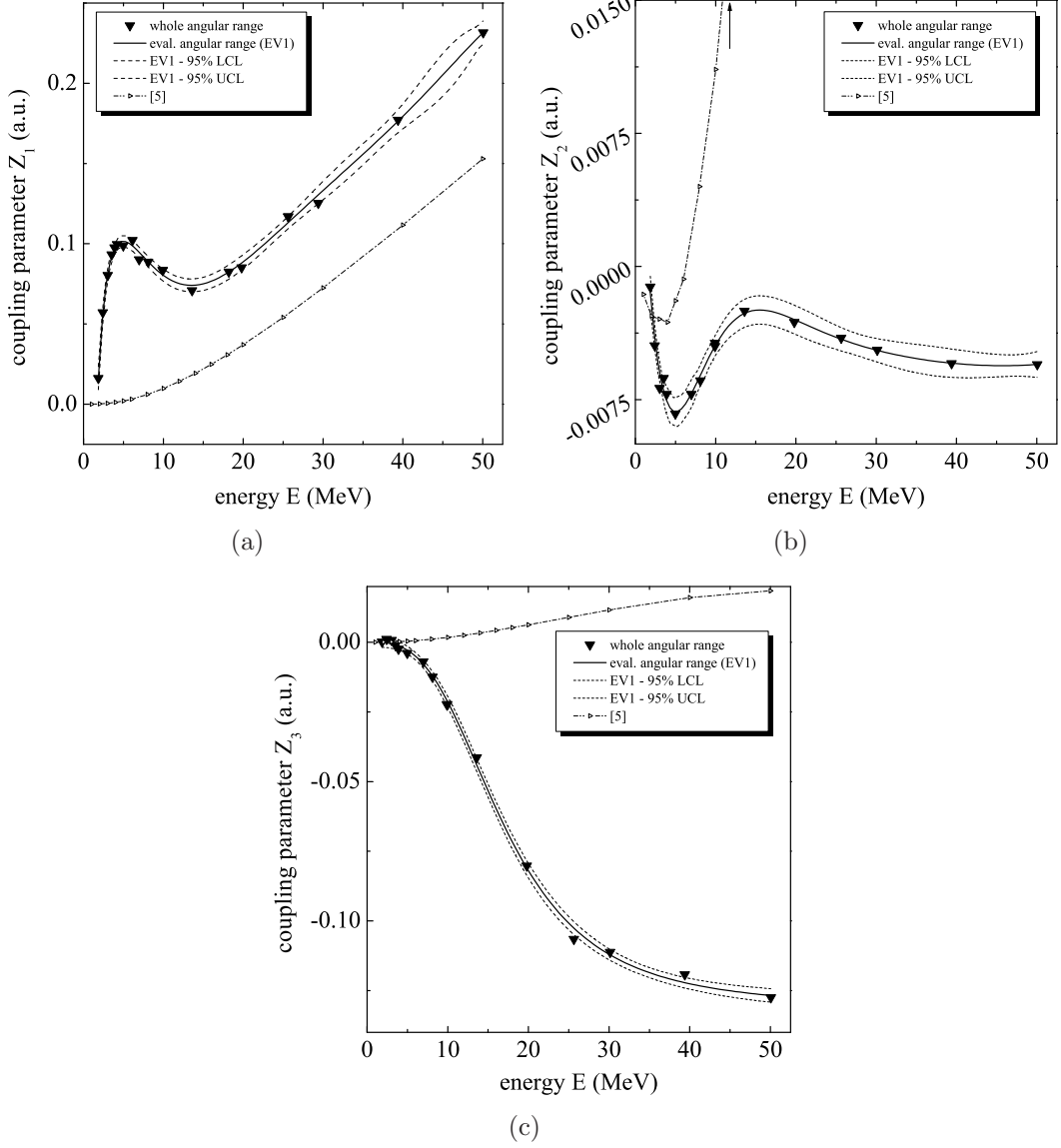


Figure 3.4: Calculated $Z_{1,2,3}$ coupling parameter for the P-wave phase shifts $\delta_P^{(i)}$ vs particle energy E . The (\blacktriangledown)-points are calculated for the reduced angular range $\theta_{\text{CM}} = 30^\circ \dots 150^\circ$ of the angle range. For comparison, the connected smaller (\blacktriangleright)-data points (chain line) are from other phase shift calculations (5). The solid line shows calculated parameterizations $Z_{1,2,3}(E)$ of these parameters as explained in Section 3.5 with 95% confidential intervals (dashed line).

3.5 PARAMETERIZATION OF THE PHASE SHIFT FUNCTION

In a second step, we fitted the energy dependent phase shifts as shown in Fig. 3.2 by the following functions.

$$\delta(^1S_0) = \delta_0(\mathbf{E}) = A_{\delta_0} + B_{\delta_0} \cdot \mathbf{E} + C_{\delta_0} \cdot \mathbf{E}^{\frac{1}{2}} + D_{\delta_0} \cdot \mathbf{E}^2 \quad (3.7)$$

$$\delta(^1D_2) = \delta_d(\mathbf{E}) = B_{\delta_d} + \frac{A_{\delta_d} - B_{\delta_d}}{1 + \left(\frac{\mathbf{E}}{C_{\delta_d}}\right)^{D_{\delta_d}}} + E_{\delta_d} \cdot \mathbf{E}^2 \quad (3.8)$$

In Fig. 3.2 we show the results of the calculated δ_0 and δ_d phase shifts, with their computed regression parameters (Table 3.2).

First parameterization attempts of the P-state phase shifts $\delta_P^{(i)}$ (Fig. 3.3) showed a unstable behavior on the entire energy range. Oscillations occur due to a strong dependence of the parameterized $\delta_P^{(i)}$ phase shifts on each other. A direct fit of the coupling parameter Z_i results in a much smoother behavior (Fig. 3.4) of the regression analysis for optimization of the fit functions of Eq. (3.9) - (3.11). In Fig. 3.4 the results of the calculated Z_i parameter are presented, with their computed regression parameters (Table 3.2).

$$\begin{aligned} Z_1(\mathbf{E}) = & A_{Z_1} + B_{Z_1} \cdot \mathbf{E} + C_{Z_1} \cdot \mathbf{E}^2 + D_{Z_1} \cdot \mathbf{E}^3 \\ & + E_{Z_1} \cdot \mathbf{E}^4 + F_{Z_1} \cdot \mathbf{E}^5 + G_{Z_1} \cdot \mathbf{E}^{-1} + H_{Z_1} \cdot \mathbf{E}^{-2} \end{aligned} \quad (3.9)$$

$$\begin{aligned} Z_2(\mathbf{E}) = & A_{Z_2} + B_{Z_2} \cdot \mathbf{E} + C_{Z_2} \cdot \mathbf{E}^2 \\ & + (1 - D_{Z_2})e^{-E_{Z_2} \cdot \mathbf{E} + F_{Z_2}} \sin(G_{Z_2} \cdot \mathbf{E} + H_{Z_2}) \end{aligned} \quad (3.10)$$

$$Z_3(\mathbf{E}) = B_{Z_3} + \frac{A_{Z_3} - B_{Z_3}}{1 + \left(\frac{\mathbf{E}}{C_{Z_3}}\right)^{D_{Z_3}}} \quad (3.11)$$

Table 3.2: Calculated fit parameters for regression analysis of parameter δ_0 , δ_d , Z_1, Z_2 and Z_3 with Eqs. (3.7) - (3.11).

Function	Parameter	i	Value	χ_{red}^2	R_{corr}^2
$\delta_0(\mathbf{E})$	A_{δ_0} ($^\circ$)	1	25.5 ± 3.0	1.72	0.9306
	B_{δ_0} ($^\circ/\text{MeV}$)	2	-3.06 ± 0.6		
	C_{δ_0} ($^\circ/\sqrt{\text{MeV}}$)	3	17.2 ± 2.9		
	D_{δ_0} ($^\circ/\text{MeV}^2$)	4	$(16 \pm 4.3) \cdot 10^{-3}$		
$\delta_d(\mathbf{E})$	A_{δ_d} ($^\circ$)	5	$(-7.94 \pm 50) \cdot 10^{-3}$	$5.28 \cdot 10^{-4}$	0.9979
	B_{δ_d} ($^\circ$)	6	1.58 ± 0.15		
	C_{δ_d} (MeV)	7	20.1 ± 1.9		
	D_{δ_d} ($^\circ$)	8	2.94 ± 0.50		
	E_{δ_d} ($^\circ/\text{MeV}^2$)	9	$(-7.37 \pm 2.44) \cdot 10^{-5}$		
$Z_1(\mathbf{E})$	A_{Z_1} ($^\circ$)	10	0.459 ± 0.028	$1.11 \cdot 10^{-5}$	0.9942
	B_{Z_1} (1/MeV)	11	$(-56.06 \pm 3.79) \cdot 10^{-3}$		
	C_{Z_1} (1/MeV ²)	12	$(3.5 \pm 0.4) \cdot 10^{-3}$		
	D_{Z_1} (1/MeV ³)	13	$(-10.225 \pm 1.731) \cdot 10^{-5}$		
	E_{Z_1} (1/MeV ⁴)	14	$(1.4792 \pm 0.3190) \cdot 10^{-6}$		
	F_{Z_1} (1/MeV ⁵)	15	$(-8.3876 \pm 2.2719) \cdot 10^{-9}$		
	G_{Z_1} (MeV)	16	$(-829.8 \pm 82.3) \cdot 10^{-3}$		
	H_{Z_1} (MeV ²)	17	$(334.9 \pm 59.5) \cdot 10^{-3}$		
$Z_2(\mathbf{E})$	A_{Z_2} ($^\circ$)	18	$(1.8 \pm 5.6) \cdot 10^{-3}$	$2.1 \cdot 10^{-7}$	0.9386
	B_{Z_2} (1/MeV)	19	$(-3.23 \pm 9.59) \cdot 10^{-4}$		
	C_{Z_2} (1/MeV ²)	20	$(3.54 \pm 18.59) \cdot 10^{-6}$		
	D_{Z_2}	21	99.091 ± 0.371		
	E_{Z_2} (1/MeV)	22	$(24.8 \pm 14.7) \cdot 10^{-2}$		
	F_{Z_2}	23	1.52 ± 0.32		
	G_{Z_2} (rad/MeV)	24	$(21.5 \pm 4.2) \cdot 10^{-2}$		
	H_{Z_2} (rad)	25	2.85 ± 0.30		
$Z_3(\mathbf{E})$	A_{Z_3}	26	$(1.18 \pm 44.62) \cdot 10^{-4}$	$3.48 \cdot 10^{-6}$	0.9987
	B_{Z_3}	27	$(-13.1 \pm 0.3) \cdot 10^{-2}$		
	C_{Z_3} (MeV)	28	16.95 ± 1.02		
	D_{Z_3}	29	3.08 ± 0.41		

3.6 COMPARISON TO EXPERIMENTAL DATA

The result of this work is a closed analytical function for $(d\sigma/d\Omega)_{\text{pp}}(\mathbf{E}, \theta)$ when using Eq. (2.7) and its energy dependent parameterizations of Eqs. (3.7) - (3.11) with the parameters of Table 3.2:

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega}\right)_{\text{CM}} &= \left(\frac{d\sigma}{d\Omega}\right)_{\text{Mott}}(\mathbf{E}, \theta_{\text{CM}}) + \left(\frac{d\sigma}{d\Omega}\right)_{L=0}^S(\delta_0(\mathbf{E}), \theta_{\text{CM}}) \\ &+ \left(\frac{d\sigma}{d\Omega}\right)_{L=1}^P(Z_{1,2,3}(\mathbf{E}), \theta_{\text{CM}}) \\ &+ \left(\frac{d\sigma}{d\Omega}\right)_{L=2}^D(\delta_d(\mathbf{E}), \theta_{\text{CM}}) \end{aligned} \quad (3.12)$$

In the following, we tag this evaluation as EV1 and the exponential evaluation from (2) as EV2. For a quantification of the goodness of the fits we calculated the residua Δ_{res} between fit function and experimental data as shown in Fig. 3.5 exemplarily for selected data sets. As a main result, the residua Δ_{res} are not larger than the experimental errors Δ_{exp} . For validation of the complete fit, we calculate the averaged residua and experimental errors $\bar{\Delta}_{\text{res,exp}} = \frac{1}{N} \sum_{i=1}^N \Delta_{\text{res,exp}}$ in the angular range $\theta_{\text{CM}} = 30^\circ \dots 150^\circ$ and energy range $\mathbf{E} = 1.855 \dots 50.1$ MeV for each data set, respectively.

In Fig. 3.6 we show the averaged residua $\bar{\Delta}_{\text{res}}$ (\blacktriangle, \square), the averaged experimental errors $\bar{\Delta}_{\text{exp}}$ (\bullet -points) of the data depending on the energy.

As a result, the averaged residua of the fit $\bar{\Delta}_{\text{res}}$ are always in the range of the experimental error $\bar{\Delta}_{\text{exp}}$. We calculated a $(\chi_{\text{red}}^2)^\dagger$ using Eq. (3.5) for the single data fits and the correlation parameter R^2 using Eq. (3.6). The number p of independent fit parameters is small compared to the number of data and thus, $p = 0$ is used for simplification. These values are tabulated in Table 3.3. Only few data sets with large variation of the data points (19.8 MeV, 30.1 MeV) show low R^2 values.

For the entire fits over 566 data points (fd = full data set) in the energy

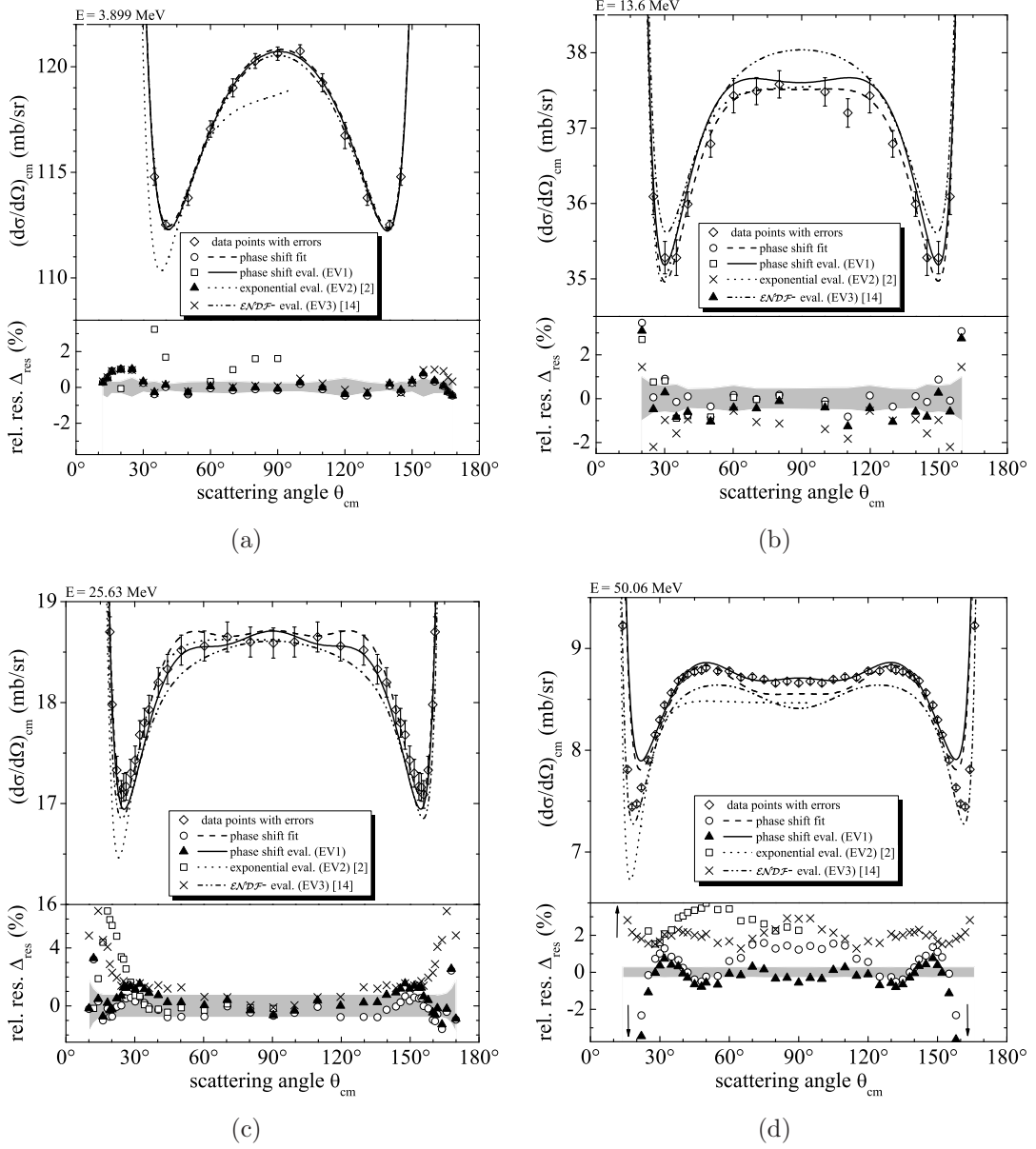


Figure 3.5: Elastic pp-scattering cross section data $(d\sigma/d\Omega)_{pp}$ (\diamond) for some selected energies with its experimental uncertainties (absolute: error bars; relative: gray band). Calculated regression curves from Eqs. (2.7) - (2.10) (dash line) and its relative residua Δ_{res} (\circ) are shown. In addition, the parameterized function (EV1) from Eqs. (3.7) - (3.11) (solid line) and its relative residua Δ_{res} (\blacktriangle) are plotted. For comparison, the simple exponential regression (EV2) from (2) (dotted line) from Eq. (3.1) and the $\epsilon\mathcal{NDF}$ evaluation (EV3) from (14) (chain line) and their relative residua Δ_{res} (\square , \times) are also plotted, respectively.

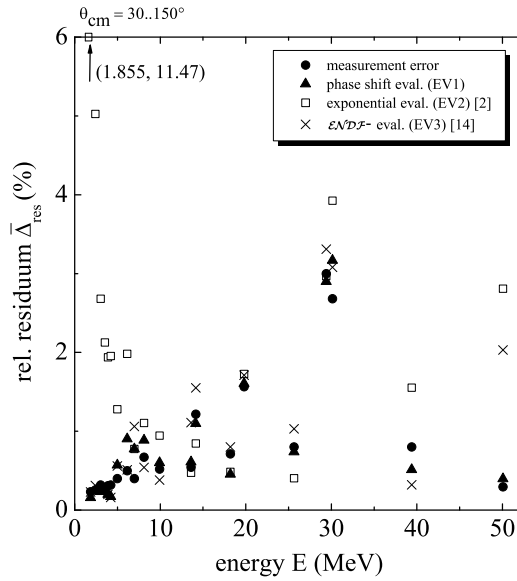


Figure 3.6: Calculated averaged relative residua $\bar{\Delta}_{\text{res}}$ (\blacktriangle , \square , \times), averaged experimental relative error $\bar{\Delta}_{\text{exp}}$ (\bullet) of the fit function $(d\sigma/d\Omega)_{\text{pp}}(E, \theta)$ for the angle range $\theta_{\text{CM}} = 30^\circ \dots 150^\circ$ and energy range $E = 1.855 \dots 50.1$ MeV, respectively.

range of 1.855...50.1 MeV the fit procedure reached a $(\chi_{\text{red}}^2)_{\text{fd}} = 7.03$. We see a discrepancy in the fit mainly at small angles where the Mott scattering cross section dominates and $(d\sigma/d\Omega)_{\text{pp}}$ strongly varies with θ_{CM} . We speculate, whether the data may obtain larger errors or even systematic deviations in the measured scattering angles than cited, e.g. a misinterpreted mean scattering angle due to non-negligible detector aperture. However, we are only interested in $(d\sigma/d\Omega)_{\text{pp}}$ for hydrogen analysis. Therefore we limited the angular range for fitting to $\theta_{\text{CM}} \approx 30^\circ \dots 150^\circ$. Thus the number of data is reduced to 354 data points and we obtain $\chi_{\text{red}}^2 = 1.95$ and $R_{\text{corr}}^2 = 0.99992$. Also, the calculated $(\chi_{\text{red}}^2)^\dagger$ is mostly between 1...3 coupled with a R^2 value of mostly 0.8...0.9 that promised a good agreement to the experimental data. In Fig. 3.5 we show exemplarily for selected energies the results of the fitted functions compared to the parameterized function from Eq. 3.12 and the simple approximation from (2).

At energies below the last used data set of $E = 1.855$ MeV, we exemplarily determined for the data set of $E = 1.397$ MeV an averaged residue of $\bar{\Delta}_{\text{res}} \sim 3.5\%$

with a $\chi_{\text{red}}^2 = 105$. The latter number is $\gg 1$ which indicates an inadequate extrapolation of the existing parameterization, but this is mainly caused by the stated low experimental errors. As another reason we see in the single data set fit that the vacuum polarization contribution $\left(\frac{d\sigma}{d\Omega}\right)_V$ becomes significant and cannot be compensated with our function where the physical effect of the vacuum polarization contribution is not included. Therefore, it would be the next step to implement such effects on this parameterization for calculations in the low energy range of 0.5 MeV . . . 1.855 MeV, as this has been done partly already in (10).

Table 3.3: Tabulated goodness parameters $(\chi_{\text{red}}^2)^\dagger$ and R^2 see Eq. (3.6) and Eq. (3.5) of the single data fits with the fit restricted to a limited angular range. fd: full data set; NoP: number of points.

Data set	energy E [MeV]	$Range_{\text{fd}}$ [$^\circ$]	NoP_{fd}	$(\chi_{\text{red}}^2)^\dagger_{\text{fd}}$	$Range_{\text{fit}}$ [$^\circ$]	NoP_{fit}	$(\chi_{\text{red}}^2)^\dagger$	R^2
(15)	1.855	14..166	23	2.51	30..150	15	0.75	0.9999
(15)	2.425	12..168	23	2.31	30..150	15	2.44	0.9992
(15)	3.037	12..168	25	2.19	30..150	15	1.12	0.9985
(15)	3.527	12..168	25	1.63	30..150	15	1.60	0.9962
(15)	3.899	12..168	25	1.33	30..150	15	0.66	0.9964
(15)	4.203	12..168	25	0.51	30..150	15	0.48	0.9957
(16)	4.978	16..164	33	2.84	30..150	19	2.57	0.9380
(17)	6.141	12..168	30	7.14	28..152	16	4.01	0.8450
(16)	6.968	16..164	33	5.25	28..152	21	5.23	0.8685
(17)	8.097	12..168	31	8.67	28..152	17	2.23	0.7242
(18)	9.918	20..160	19	7.10	30..150	15	2.34	0.8611
(18)	13.6	20.1..159.9	18	2.42	30..150	14	1.79	0.9249
(19)	14.16	18.1..161.9	29	1.39	30..150	19	1.36	0.7382
(20)	18.2	30..150	15	0.63	30..150	15	0.63	0.9499
(21)	19.8	14..166	29	1.94	30..150	15	2.34	-0.0661
(22)	25.63	10.1..169.9	45	1.27	28..152	23	1.22	0.8875
(23)	29.4	24..156	18	2.07	32..148	16	1.39	0.5416
(24)	30.1	11..169	22	203.39	32..148	16	2.59	0.3332
(25)	39.4	8.1..171.9	53	42.17	27..153	25	0.61	0.9441
(26)	50.06	14..166	47	457.17	30..150	33	2.4	0.9080

3.7 COMPARISON TO \mathcal{ENDF} CALCULATIONS

In order to get the most accurate parameterization for the differential cross section the validation with a closed theoretical calculation is indispensable. The data pool (27) provides the theoretical evaluation with the help of an R-matrix analysis with a maximum nuclear partial wave expansion of $L = 6$ of elastic pp scattering cross sections and polarization data with respect to an angular range $\theta_{\text{CM}} = 0^\circ \dots 180^\circ$ and energy range $E = 0 \dots 150$ MeV, respectively (14). The formula for calculating $(d\sigma/d\Omega)_{\text{pp}}$ and its coefficients are described in the Evaluated Nuclear Data File (\mathcal{ENDF}) (27) and the 21 coefficients given for each energy are listed in the \mathcal{ENDF} -file (14). For this evaluation we use the abbreviation EV3, in contrast to EV1 and EV2.

For the evaluation of the goodness of EV3 we calculated the residua Δ_{res} between EV3 and experimental data as shown in Fig. 3.5 exemplarily for selected data sets. In principal, the residua Δ_{res} (\times -points) are mostly out of the experimental uncertainties (gray-band) and larger than the EV1 residua, especially in the nuclear interaction range in which we are interested. We also calculated the averaged residua $\bar{\Delta}_{\text{res}}$ (\times) and added this to Fig. 3.6 for each data set, respectively. Above ~ 10 MeV $\bar{\Delta}_{\text{res}}$ (\times) is always larger than the experimental uncertainties $\bar{\Delta}_{\text{exp}}$ (\bullet) and the EV1 residua (\blacktriangle), except at 39.4 MeV. For a more detailed analysis of the evaluation EV1 (\blacktriangle) and EV3 (\times) an angular and energy disperse evaluation of the goodness parameter $(\chi_{\text{red}}^2)^\dagger$ is shown in Fig. 3.7 and summarized in Table 3.4. Thus, we made two evaluations, one of the whole evaluated angular range $\theta_{\text{CM}} = 30^\circ \dots 150^\circ$ (see Fig. 3.7a) and one for the detector range $\theta_{\text{lab}} = 25^\circ \dots 65^\circ$ in which we are mainly interested with regard for hydrogen quantification. Due to symmetric behavior in the CM-system the calculation of the angular range $\theta_{\text{CM}} = 50^\circ \dots 130^\circ$ is useful (see Fig. 3.7b).

The differences of $(\chi_{\text{red}}^2)^\dagger$ between EV1 and EV3 below ~ 10 MeV are small, but the $(\chi_{\text{red}}^2)^\dagger$ of EV3 is slightly better in this energy range. We also calculated a

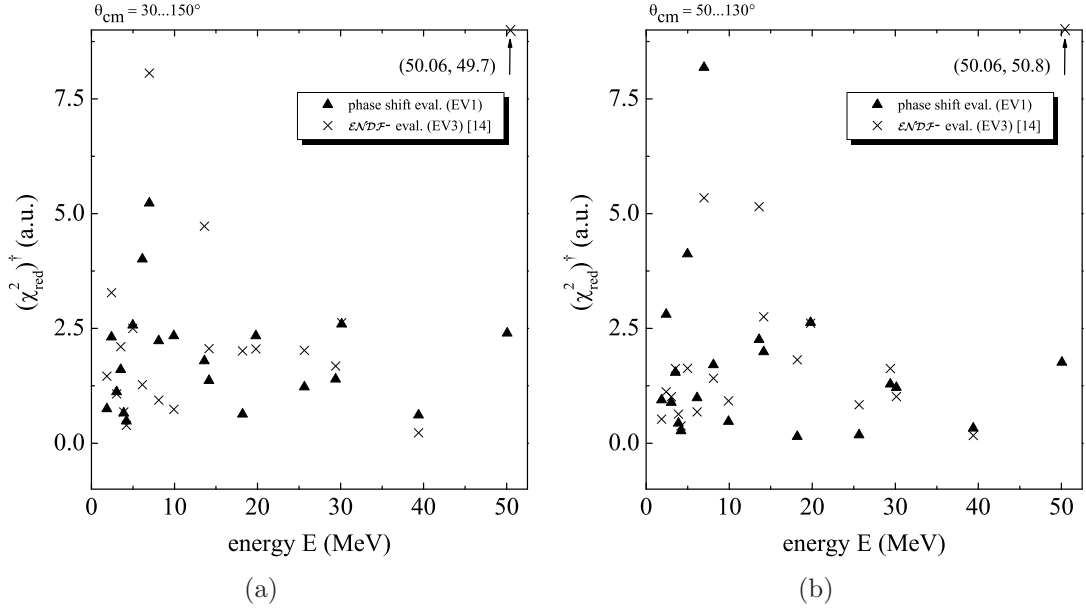


Figure 3.7: Calculated goodness parameters $(\chi_{\text{red}}^2)^\dagger$ see Eq. (3.5) of the single data evaluations with the restriction to a limited angular range in a) for $\theta_{\text{CM}} = 30^\circ \dots 150^\circ$ and b) for $\theta_{\text{CM}} = 50^\circ \dots 130^\circ$. For comparison, both evaluations EV1 (\blacktriangle) and EV3 (\times) are plotted.

$(\chi_{\text{red}}^2)^\dagger$ excluding the 6.968 MeV dataset, where $(\chi_{\text{red}}^2)^\dagger$ shows a too large deviation to be included in an overall data evaluation. For the restricted angular range, at energies below ~ 10 MeV, the $(\chi_{\text{red}}^2)^\dagger$ of EV3 is also slightly smaller (i.e. better) than $(\chi_{\text{red}}^2)^\dagger$ of EV1. This is also conform with the whole data set calculation of $(\chi_{\text{red}}^2)^\dagger$ in Table 3.4 for the energy range 1.9...10.0 MeV. However, for energies above 8.1 MeV the goodness parameter $(\chi_{\text{red}}^2)^\dagger$ for EV3 is significantly larger, i.e. worse, than that of EV1, in particular for the 50.1 MeV dataset. The only exception is at 19.8 MeV and 39.4 MeV, where $(\chi_{\text{red}}^2)^\dagger$ of EV3 is slightly smaller than $(\chi_{\text{red}}^2)^\dagger$ of EV1. This quantification is also conform with the full dataset evaluation in Table 3.4, in which the χ_{red}^2 parameter is calculated and listed for all energy ranges above 8.1 MeV and for the different angular restriction, respectively.

In summary, for the representation of the experimental data below ~ 10 MeV

Table 3.4: Tabulated goodness parameter (χ_{red}^2)[†] for EV1 and EV3 evaluation of the whole dataset with the restriction to a limited angular and energy range. fd: full data set; NoP: number of points n ; *without 6.968 MeV;

<i>Range_{fit}</i>	$\theta_{\text{CM}} = 30^\circ \dots 150^\circ$			$\theta_{\text{CM}} = 50^\circ \dots 130^\circ$		
	NoP	<i>EV1</i>	<i>EV3</i>	NoP	<i>EV1</i>	<i>EV3</i>
	n	$p = 5$	$p = 21$	n	$p = 0$	$p = 0$
1.9 ... 10.0 MeV	178	2.25	2.24	98	2.04	1.40
1.9 ... 10.0 MeV*	157	1.85	1.46	89	1.42	1.00
8.1 ... 50.1 MeV	208	1.71	9.39	120	1.26	8.65
8.1 ... 39.4 MeV	175	1.58	1.80	103	1.18	1.69
	n	$p = 29$	$p = 21$	n	$p = 29$	$p = 21$
1.9 ... 50.1 MeV	354	1.95	6.98	200	1.94	6.45

both evaluations (EV1, EV3) have similar quality. However, EV1 represents the experimental data above 8.1 MeV better than EV3. We speculate, whether this significant discrepancy is caused by too few freedom parameters of EV3 at small angles where the Coulomb interaction dominates (Mott-scattering): There we find a steep gradient in the differential cross section $(d\sigma/d\Omega)_{\text{pp}}(\theta)$. A small scattering angle mismatch $\Delta\theta$ due to misinterpretation of the mean detector angle could cause a "runaway" of the fit parameters and therefore a deviation at larger angles where nuclear scattering dominates. We saw a similar behavior of our fit (EV1) when we included the data at small scattering angles with the consequence that the representation is worse at the larger angles. Thus, a restriction of the angular fit range helps for the convergence of the fit at larger angles.

3.8 QUALITY OF THE PARAMETERIZED FUNCTION

The statistical error for each $(d\sigma/d\Omega)_{\text{pp}}$ - value calculated from EV1 is evaluated at all angles between $\theta_{\text{CM}} = 30^\circ \dots 150^\circ$ and energies in the range of $1.855 \dots 50.1$. We define the least square function

$$\chi^2(A_i) = \sum_{j=1}^n \frac{\left(\frac{d\sigma}{d\Omega}_{\text{pp}}(A_i, \mathbf{E}_j, \theta_j) - X(\mathbf{E}_j, \theta_j) \right)^2}{\Delta_{\text{exp}}^2(\mathbf{E}_j, \theta_j)} \quad (3.13)$$

with A_i for the fit parameters², using the differential cross sections $(d\sigma/d\Omega)_{\text{pp}}(A_i, \mathbf{E}_j, \theta_j)$ that are evaluated for $n = 354$ experimental data points (\mathbf{E}_j, θ_j) and the corresponding experimental data $X(\mathbf{E}_j, \theta_j)$ together with the experimental uncertainties $\Delta_{\text{exp}}(\mathbf{E}_j, \theta_j)$.

From χ^2 one gets, the covariance matrix \mathbf{C}_{ov} for the fitting parameters A_i as

$$\mathbf{C}_{\text{ov}} = 2 \cdot \left[\frac{\partial^2 \chi^2(A_i)}{\partial A_i \partial A_k} \Big|_{\tilde{A}_{i,k}} \right]^{-1} \quad (3.14)$$

with $\tilde{A}_{i,k}$ as the expectancy values of Table 3.2. Since the A_i are not statistically independent non-diagonal elements of the \mathbf{C}_{ov} occur. The statistical error is obtained with the gradient ∇_{A_i} of the function multiplied by the covariance matrix \mathbf{C}_{ov} . The relative experimental uncertainties Δ_{exp} are low ($< 1\%$) compared to the number of free parameter (29) and there is a large number of data points (354). As a consequence, the statistical error $\Delta_{\text{stat}}(\mathbf{E}, \theta)$ of any differential cross section $(d\sigma/d\Omega)_{\text{pp}}$ is given by:

$$\Delta_{\text{stat}}(\mathbf{E}, \theta) = \left[\nabla_{A_i} \left(\frac{d\sigma}{d\Omega}(\mathbf{E}, \theta, A_i) \right) \right]_{\tilde{A}_i}^T \cdot \mathbf{C}_{\text{ov}} \cdot \left[\nabla_{A_i} \left(\frac{d\sigma}{d\Omega}(\mathbf{E}, \theta, A_i) \right) \right]_{\tilde{A}_i} \quad (3.15)$$

The covariance matrix \mathbf{C}_{ov} has a cardinal number of 29×29 and is listed in

²The fit parameters A_k, B_k, C_k from Table 3.2 are reduced to A_i with $i = 1 \dots 29$.

Table A.1. In Fig. 3.8a we show the computed results for $\Delta_{\text{stat}}(\mathbf{E}, \theta)$ with Eq. (3.15) as a normalized 2D-histogram.

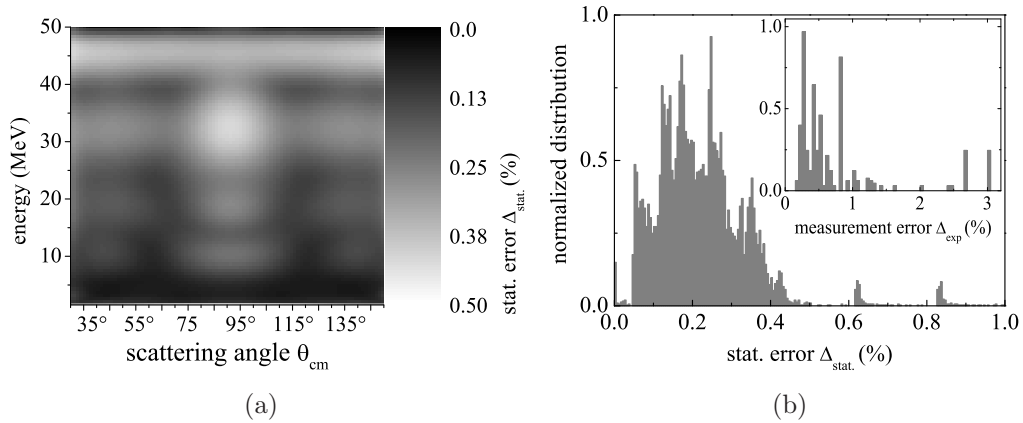


Figure 3.8: Calculated statistical error Δ_{stat} for the $(d\sigma/d\Omega)_{\text{pp}}(\mathbf{E}, \theta, A_i)$ function with the $\Delta_{\text{stat}}(\mathbf{E}, \theta, A_i)$ function in a) a 2D-histogram and in b) as normalized distribution of the errors for the ranges $\theta_{\text{CM}} = 30^\circ \dots 150^\circ$ and $E_{\text{in}} = 1.855 \dots 50.1$ MeV. For comparison, the normalized distribution of the experimental measurement error is also plotted.

Additionally, we plotted the distribution of the statistical error Δ_{stat} in Fig. 3.8b. As a result, the average statistical error Δ_{stat} is about 0.2% and most errors are less than 0.4%. This is smaller than the given average experimental uncertainty. The entire fit of $n = 354$ data points obviously enhances the statistical accuracy. Although, the cited experimental uncertainties Δ_{exp} include systematical uncertainties Δ_{sys} ($\Delta_{\text{exp}} = \Delta_{\text{stat,exp}} + \Delta_{\text{sys}}$) the improvement is mainly regarded to the statistical uncertainties Δ_{stat} . As a consequence, quantification of hydrogen contents with an statistical accuracy in the 0.2% range is possible.

3.9 NUMERICAL APPROXIMATIONS

For a fast analysis the analytical function $(d\sigma/d\Omega)_{pp}(\mathbf{E}, \theta)$ is not practicable because of the long analytical expression. Hence, numerical tables that can be interpolated to any desired value are favorable for routine data analysis of hydrogen profiling. We give two $[\mathbf{E}, \theta]$ -matrices for numerical $(d\sigma/d\Omega)_{pp}$ data: one for a quick evaluation in the lab system in Table 3.6). For the transformations from CM to lab system we used the equations as given in (2). The interpolation error Δ_{int} of two points of this table is $< 0.8\%$. For computations a second table is calculated with an interpolation error of $\Delta_{\text{int}} \approx \frac{1}{10}\Delta_{\text{stat}}$. These data will be included on the website SigmaCalc (28) for nuclear cross sections. The tables for a fast analysis could also be found in the internet for free download (29) to be included into data evaluation software. The interpolation errors of both representations are plotted depending on the scattering angle in Fig. 3.9a and depending on the energy in Fig. 3.9b. The entire error for the analysis for the differential scattering cross section is given by

$$\Delta_{d\sigma/d\Omega} = \sqrt{(\Delta_{\text{stat}})^2 + (\Delta_{\text{int}})^2} \quad (3.16)$$

When using the accurate numerical table the error is dominated by the Δ_{stat} and therefore $\Delta_{d\sigma/d\Omega} \approx \Delta_{\text{stat}}$.

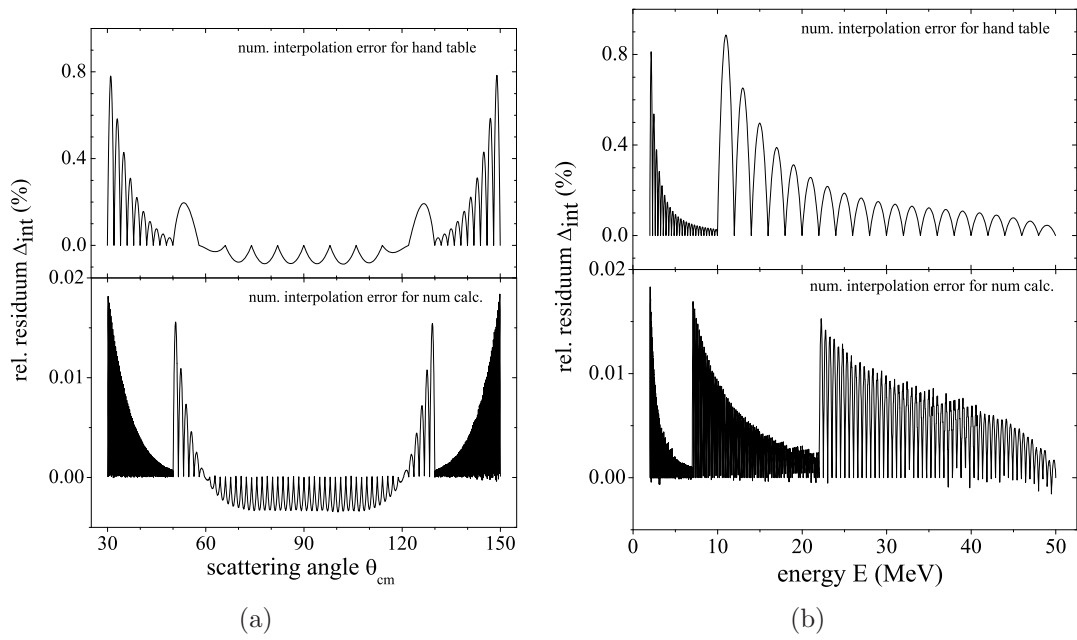


Figure 3.9: Calculated interpolation relative residua Δ_{int} (of two points) for the highest gradient of the angle (CM-system) (a) and for the energy (b).

Table 3.5: Computed cross section data matrix $d\sigma/d\Omega(\theta_{\text{CM}}, \mathbf{E})$ for pp-scattering continued...

E (MeV)	θ_{CM} (deg)																														
	30	32	34	36	38	40	42	44	46	48	50	58	66	74	82	90	98	106	114	122	130	132	134	136	138	140	142	144	146	148	150
12	40.31	40.28	40.41	40.63	40.90	41.18	41.44	41.68	41.91	42.12	42.30	42.78	42.99	43.05	43.07	43.05	43.07	43.07	43.01	42.79	42.29	42.12	41.92	41.68	41.44	41.16	40.91	40.63	40.42	40.26	40.32
14	34.04	34.13	34.33	34.57	34.82	35.07	35.30	35.51	35.70	35.87	36.00	36.35	36.44	36.43	36.40	36.38	36.40	36.43	36.44	36.35	36.00	35.87	35.71	35.51	35.31	35.06	34.80	34.57	34.33	34.13	34.04
16	29.39	29.54	29.76	30.00	30.24	30.47	30.67	30.86	31.03	31.15	31.26	31.51	31.54	31.51	31.46	31.44	31.46	31.51	31.54	31.5	31.26	31.15	31.03	30.86	30.67	30.46	30.24	30.00	29.76	29.54	29.40
18	25.82	26.00	26.21	26.45	26.66	26.87	27.06	27.22	27.36	27.47	27.56	27.74	27.75	27.71	27.68	27.67	27.68	27.71	27.74	27.74	27.56	27.47	27.36	27.22	27.06	26.87	26.67	26.43	26.22	26.00	25.82
20	22.92	23.10	23.32	23.54	23.73	23.92	24.08	24.22	24.35	24.44	24.52	24.67	24.67	24.64	24.64	24.65	24.64	24.64	24.67	24.67	24.52	24.44	24.35	24.22	24.09	23.92	23.73	23.52	23.32	23.10	22.90
22	20.55	20.74	20.94	21.15	21.33	21.49	21.65	21.77	21.87	21.96	22.02	22.13	22.14	22.14	22.18	22.18	22.18	22.14	22.14	22.13	22.02	21.96	21.87	21.77	21.65	21.49	21.33	21.13	20.94	20.74	20.53
24	18.60	18.78	18.97	19.17	19.33	19.48	19.62	19.73	19.83	19.89	19.95	20.04	20.05	20.07	20.13	20.17	20.13	20.07	20.05	20.04	19.95	19.89	19.83	19.73	19.63	19.49	19.33	19.15	18.99	18.78	18.60
26	16.89	17.08	17.27	17.44	17.59	17.73	17.84	17.94	18.03	18.09	18.14	18.22	18.23	18.28	18.35	18.38	18.34	18.28	18.23	18.22	18.14	18.09	18.03	17.94	17.85	17.73	17.59	17.42	17.25	17.07	16.89
28	15.53	15.70	15.88	16.05	16.18	16.31	16.41	16.50	16.58	16.63	16.67	16.74	16.75	16.80	16.89	16.94	16.89	16.8	16.75	16.74	16.67	16.63	16.58	16.51	16.41	16.31	16.18	16.03	15.86	15.69	15.53
30	14.29	14.46	14.62	14.78	14.91	15.02	15.12	15.20	15.26	15.31	15.35	15.41	15.42	15.47	15.57	15.62	15.57	15.47	15.42	15.41	15.35	15.31	15.26	15.20	15.12	15.02	14.91	14.76	14.60	14.46	14.29
32	13.24	13.39	13.54	13.69	13.80	13.91	14.00	14.08	14.13	14.17	14.22	14.25	14.26	14.31	14.40	14.45	14.40	14.31	14.26	14.25	14.22	14.18	14.13	14.08	14.00	13.91	13.81	13.67	13.52	13.38	13.24
34	12.33	12.46	12.62	12.74	12.86	12.96	13.04	13.11	13.17	13.20	13.24	13.26	13.25	13.30	13.40	13.45	13.40	13.30	13.25	13.25	13.23	13.20	13.17	13.11	13.04	12.96	12.86	12.74	12.60	12.46	12.33
36	11.53	11.66	11.81	11.93	12.04	12.13	12.20	12.27	12.32	12.36	12.38	12.40	12.38	12.43	12.52	12.56	12.52	12.43	12.38	12.39	12.38	12.36	12.33	12.27	12.20	12.13	12.04	11.93	11.79	11.67	11.53
38	10.83	10.97	11.11	11.22	11.32	11.41	11.48	11.54	11.59	11.62	11.64	11.63	11.62	11.65	11.73	11.78	11.73	11.65	11.62	11.63	11.64	11.62	11.59	11.54	11.48	11.41	11.33	11.22	11.09	10.97	10.83
40	10.23	10.37	10.49	10.59	10.70	10.77	10.85	10.9	10.94	10.97	10.99	10.98	10.94	10.97	11.04	11.07	11.04	10.97	10.94	10.98	10.99	10.97	10.94	10.90	10.85	10.78	10.70	10.59	10.47	10.36	10.22
42	9.740	9.867	9.983	10.08	10.18	10.26	10.33	10.37	10.42	10.45	10.45	10.44	10.39	10.40	10.46	10.48	10.46	10.40	10.39	10.43	10.45	10.44	10.41	10.37	10.33	10.25	10.18	10.08	9.980	9.861	9.736
44	9.305	9.426	9.539	9.641	9.730	9.806	9.868	9.915	9.950	9.972	9.983	9.954	9.894	9.892	9.936	9.961	9.938	9.895	9.897	9.956	9.983	9.973	9.951	9.914	9.867	9.804	9.729	9.638	9.537	9.423	9.301
46	8.904	9.022	9.132	9.228	9.314	9.386	9.445	9.490	9.522	9.542	9.551	9.512	9.443	9.429	9.463	9.486	9.466	9.432	9.446	9.515	9.550	9.543	9.523	9.489	9.444	9.386	9.313	9.228	9.129	9.017	8.904
48	8.676	8.790	8.895	8.989	9.073	9.142	9.198	9.240	9.270	9.287	9.295	9.249	9.170	9.142	9.164	9.183	9.166	9.145	9.171	9.25	9.295	9.288	9.271	9.240	9.197	9.141	9.071	8.987	8.894	8.786	8.672
50	8.273	8.385	8.488	8.579	8.659	8.726	8.780	8.819	8.847	8.862	8.868	8.813	8.725	8.687	8.698	8.714	8.701	8.688	8.728	8.814	8.868	8.864	8.847	8.818	8.778	8.725	8.657	8.577	8.487	8.381	8.272

Table 3.6: Computed cross section data matrix $d\sigma/d\Omega(\theta_{\text{lab}}, \mathbf{E})$ for pp-scattering continued. . .

E	E_{CM}	θ_{lab} (deg)																														
(MeV)	(MeV)	15	16	17	18	19	20	21	22	23	24	25	29	33	37	41	45	49	53	57	61	65	66	67	68	69	70	71	72	73	74	75
12	5.99	156.7	155.6	155.3	155.4	155.5	155.6	155.6	155.2	155.0	154.5	153.9	150.0	144.6	137.7	130.1	121.7	113.0	103.4	93.52	82.70	71.20	68.20	65.19	62.13	59.08	55.99	52.97	49.96	46.97	44.16	41.52
14	6.987	132.3	132.0	132.2	132.5	132.5	132.7	132.6	132.4	132.1	131.7	131.3	127.8	122.7	116.5	110.0	103.0	95.55	87.52	79.35	70.25	60.62	58.05	55.56	52.93	50.34	47.72	45.11	42.5	39.92	37.41	35.07
16	7.983	114.7	114.7	115.0	115.1	115.5	115.6	115.5	115.4	115.3	114.9	114.2	111.1	106.4	101.1	95.44	89.13	82.56	75.79	68.58	60.90	52.62	50.47	48.31	46.00	43.77	41.42	39.15	36.83	34.57	32.42	30.28
18	8.979	100.8	101.0	101.4	101.7	101.8	102.0	102.0	101.9	101.5	101.4	100.8	97.74	93.63	88.79	83.71	78.33	72.60	66.63	60.28	53.58	46.35	44.42	42.52	40.50	38.56	36.50	34.50	32.43	30.37	28.50	26.54
20	9.973	89.41	89.81	90.24	90.44	90.64	90.91	90.82	90.72	90.45	90.13	89.62	86.76	83.20	78.92	74.58	69.75	64.56	59.18	53.54	47.53	41.16	39.45	37.79	35.99	34.25	32.44	30.64	28.79	26.96	25.18	23.51
22	10.97	80.40	80.79	81.23	81.50	81.72	81.8	81.79	81.76	81.48	81.09	80.62	78.13	74.92	71.20	67.12	62.90	58.18	53.32	48.17	42.74	37.02	35.50	34.00	32.40	30.83	29.18	27.57	25.91	24.26	22.69	21.06
24	11.96	72.95	73.36	73.73	74.05	74.22	74.25	74.12	73.90	73.59	73.19	70.80	68.00	64.48	61.11	57.22	52.89	48.38	43.56	38.74	33.54	32.17	30.77	29.36	27.94	26.45	24.99	23.50	21.98	20.56	19.10	
26	12.96	66.11	66.47	66.93	67.17	67.31	67.31	67.39	67.35	67.09	66.74	66.36	64.28	61.50	58.60	55.57	51.96	48.04	43.78	39.46	35.04	30.38	29.15	27.89	26.59	25.28	23.94	22.63	21.30	19.92	18.58	17.24
28	13.95	60.95	61.35	61.68	61.89	62.05	62.13	62.06	62.06	61.86	61.50	61.07	59.09	56.70	53.98	51.18	47.92	44.27	40.30	36.37	32.25	27.96	26.80	25.65	24.43	23.29	22.07	20.84	19.58	18.29	17.13	15.90
30	14.94	56.05	56.47	56.73	56.98	57.10	57.22	57.07	57.02	56.9	56.59	56.26	54.29	52.06	49.66	47.11	44.17	40.77	37.03	33.39	29.62	25.66	24.62	23.58	22.48	21.41	20.27	19.16	18.00	16.81	15.71	14.56
32	15.93	51.97	52.28	52.63	52.82	52.97	52.99	52.97	52.84	52.65	52.45	52.17	50.32	48.14	45.94	43.57	40.82	37.70	34.28	30.80	27.41	23.77	22.80	21.83	20.81	19.82	18.75	17.73	16.63	15.59	14.53	13.46
34	16.92	48.44	48.68	49.01	49.26	49.32	49.42	49.31	49.22	49.09	48.86	48.52	46.85	44.74	42.70	40.55	37.99	35.10	31.79	28.60	25.45	22.09	21.19	20.31	19.37	18.42	17.45	16.48	15.44	14.48	13.50	12.51
36	17.91	45.36	45.63	45.87	46.04	46.24	46.27	46.21	46.15	46.00	45.72	45.37	43.77	41.85	39.87	37.85	35.42	32.69	29.69	26.75	23.78	20.66	19.81	19.01	18.10	17.23	16.32	15.40	14.46	13.51	12.63	11.69
38	18.9	42.63	42.99	43.18	43.36	43.46	43.56	43.50	43.43	43.19	42.97	42.68	41.04	39.18	37.37	35.47	33.24	30.66	27.79	25.04	22.30	19.39	18.61	17.82	16.99	16.19	15.33	14.47	13.58	12.70	11.85	10.97
40	19.89	40.41	40.76	40.98	41.14	41.34	41.27	41.29	41.20	40.98	40.77	40.51	38.87	37.10	35.37	33.53	31.35	28.92	26.28	23.65	21.13	18.39	17.63	16.89	16.12	15.35	14.51	13.70	12.85	12.05	11.23	10.43
42	20.88	38.51	38.78	39.04	39.23	39.32	39.31	39.27	39.26	39.06	38.83	38.51	36.98	35.23	33.49	31.73	29.71	27.41	24.95	22.48	20.05	17.45	16.77	16.06	15.31	14.57	13.80	13.06	12.25	11.45	10.70	9.891
44	21.87	36.76	37.07	37.32	37.47	37.53	37.59	37.56	37.45	37.32	37.02	36.76	35.27	33.54	31.84	30.19	28.21	26.01	23.71	21.39	19.09	16.64	15.98	15.32	14.62	13.91	13.17	12.44	11.68	10.92	10.15	9.440
46	22.86	35.29	35.55	35.73	35.91	36.01	36.01	36.02	35.92	35.75	35.49	35.15	33.75	32.02	30.32	28.70	26.87	24.76	22.61	20.43	18.23	15.91	15.27	14.63	13.96	13.28	12.59	11.88	11.18	10.44	9.742	9.014
48	23.85	34.39	34.65	34.87	35.02	35.09	35.11	35.02	34.96	34.77	34.56	34.24	32.78	31.08	29.40	27.80	25.98	23.97	21.86	19.82	17.72	15.46	14.85	14.23	13.57	12.92	12.24	11.56	10.86	10.17	9.455	8.757
50	24.84	32.88	33.16	33.36	33.50	33.58	33.61	33.54	33.45	33.26	33.04	32.77	31.29	29.67	28.03	26.44	24.69	22.81	20.80	18.86	16.91	14.77	14.18	13.58	12.97	12.36	11.69	11.06	10.37	9.695	9.038	8.365

Chapter 4

CONCLUSION

Proton-proton scattering at MeV energies has proven to be the most sensitive method for hydrogen depth profiling at micrometer depth resolution without any need for reference standards when the differential scattering cross section $(d\sigma/d\Omega)_{pp}$ is known.

We performed a phase shift analysis of experimental scattering cross section datasets, i.e. by fitting 354 data points in the energy range $1.9 \dots 50$ MeV and laboratory scattering angles $\theta_{\text{lab}} = 15^\circ \dots 75^\circ$, resulting in total uncertainties that are below the measurement error. Thus, the differential cross section can be calculated for any energy and angle in the given intervals. For the parameterizations we determined an average statistical error $\Delta_{\text{stat}}(\mathbf{E}, \theta)$ of the $(d\sigma/d\Omega)_{pp}(\mathbf{E}, \theta)$ function as low as $\bar{\Delta}_{\text{stat}}$ of 0.2% and a maximum error of $\sim 0.4\%$. A comparison with existing \mathcal{ENDF} -files (27) shows a better representation of the experimental data by our analysis ($\chi_{\text{red}}^2 = 1.95(\text{EV1})$), especially for $\mathbf{E} > 8$ MeV, in contrast to the \mathcal{ENDF} -data ($\chi_{\text{red}}^2 = 6.98(\text{EV3})$). For fast numerical calculations we computed two types of $[\mathbf{E}, \theta]$ -matrices, one for quick by hand evaluations with an interpolation error Δ_{int} of $< 0.8\%$, and one for accurate computations with $\Delta_{\text{int}} < 0.02\%$.

Appendix A

APPENDIX

Table A.1: Computed covariance matrix $(\mathcal{C}_{ov})_{i,k}$ (Eq. (3.14)) for the ranges $\theta_{CM} = 30^\circ \dots 150^\circ$ and $E = 1.855 \dots 50.1$ MeV.

k	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
1	8.78	1.78	-8.70	-1.44E-02	-4.04E-02	1.38E-01	1.22	-8.29E-01	-5.68E-06	5.82E-02	6.52E-03	-9.04E-04	3.23E-05	-5.02E-07	3.12E-09	-2.00E-01	1.30E-01	-2.02E-03	7.02E-05	-5.03E-07	6.36E-09	5.44E-04	1.06E-02	4.38E-02	-1.65E-01	4.07E-03	-6.71E-03	1.53E-01	-8.10E-01
2	1.78	3.40E-01	-1.74	-2.59E-03	-9.09E-03	2.31E-02	1.18E-01	-1.42E-01	-1.55E-06	1.14E-02	1.57E-03	-1.85E-04	6.43E-06	-1.00E-07	6.28E-10	-4.04E-02	2.65E-02	-4.15E-04	7.12E-06	4.09E-08	1.28E-09	-2.09E-04	8.90E-04	9.05E-03	-3.41E-02	9.03E-04	-9.47E-04	-6.41E-02	-1.34E-01
3	-8.70	-1.74	8.62	1.39E-02	4.55E-02	-1.26E-01	-9.25E-01	8.04E-01	4.94E-06	-5.80E-02	-6.77E-03	8.98E-04	-3.18E-05	4.95E-07	-3.09E-09	1.99E-01	-1.30E-01	2.05E-03	-6.15E-05	3.22E-07	-6.30E-09	-1.64E-04	-9.08E-03	-4.37E-02	1.65E-01	-4.53E-03	6.02E-03	6.88E-02	7.78E-01
4	-1.44E-02	-2.59E-03	1.39E-02	1.84E-05	7.05E-05	-1.63E-04	-3.14E-04	9.28E-04	1.86E-08	-8.62E-05	-1.46E-05	1.52E-06	-5.14E-08	8.03E-10	-5.06E-12	3.24E-04	-2.14E-04	3.30E-06	1.76E-09	-1.47E-09	-1.03E-11	4.27E-06	3.01E-06	-7.45E-05	2.81E-04	-6.98E-06	4.55E-06	1.00E-03	8.26E-04
5	-4.04E-02	-9.09E-03	4.55E-02	7.05E-05	2.51E-03	1.08E-03	4.68E-02	1.05E-02	-4.57E-07	-4.63E-04	-2.91E-05	4.38E-06	-1.59E-07	2.53E-09	-1.61E-11	1.19E-03	-7.75E-04	2.01E-05	-7.40E-07	6.74E-09	-2.99E-11	-8.14E-05	-3.72E-04	-2.45E-04	9.10E-04	-2.23E-04	-1.99E-05	4.08E-02	8.11E-03
6	1.38E-01	2.31E-02	-1.26E-01	-1.63E-04	1.08E-03	-2.34E-02	-3.95E-01	3.00E-02	4.80E-06	4.19E-04	1.93E-04	-1.89E-05	6.79E-07	-1.12E-08	7.23E-11	-2.43E-03	1.58E-03	-2.13E-05	-7.04E-07	2.31E-08	9.98E-11	-9.90E-05	-2.73E-04	6.86E-04	-2.59E-03	-1.04E-04	5.75E-04	-2.48E-01	3.87E-02
7	1.22	1.18E-01	-9.25E-01	-3.14E-04	4.68E-02	-3.95E-01	-3.46	1.10	7.09E-05	-2.67E-03	2.66E-03	-1.73E-04	5.39E-06	-8.58E-08	5.41E-10	-1.39E-02	9.43E-03	1.20E-05	-3.79E-05	7.44E-07	7.76E-10	-3.14E-03	-1.15E-02	6.02E-03	-2.31E-02	-4.29E-03	1.04E-02	-9.18E-01	9.79E-01
8	-8.29E-01	-1.42E-01	8.04E-01	9.28E-04	1.05E-02	3.00E-02	1.10	2.46E-01	-1.07E-05	-4.94E-03	-1.07E-03	1.04E-04	-3.72E-06	6.33E-08	-4.24E-10	1.86E-02	-1.24E-02	2.23E-04	2.89E-06	-1.47E-07	-5.80E-10	1.27E-04	-2.92E-04	-4.44E-03	1.67E-02	-1.01E-03	-8.88E-04	1.08	1.87E-01
9	-5.68E-06	-1.55E-06	4.94E-06	1.86E-08	-4.57E-07	4.80E-06	7.09E-05	-1.07E-05	-5.97E-10	3.40E-08	-4.77E-09	1.27E-09	-5.45E-11	8.98E-13	-5.56E-15	-9.81E-09	2.06E-08	-1.49E-09	-1.76E-10	3.89E-12	-3.66E-15	4.70E-09	1.61E-08	-1.54E-08	5.95E-08	4.56E-08	-1.94E-07	4.41E-05	-1.32E-05
10	5.82E-02	1.14E-02	-5.80E-02	-8.62E-05	-4.63E-04	4.19E-04	-2.67E-03	-4.94E-03	3.40E-08	7.76E-04	-1.68E-05	-2.84E-07	-3.11E-08	1.44E-09	-1.37E-11	-2.26E-03	1.65E-03	-1.53E-05	3.35E-07	-8.79E-11	4.66E-11	-2.29E-05	-2.76E-05	3.00E-04	-1.14E-03	4.50E-05	-2.34E-05	-6.95E-03	-4.60E-03
11	6.52E-03	1.57E-03	-6.77E-03	-1.46E-05	-2.91E-05	1.93E-04	2.66E-03	-1.07E-03	-4.77E-09	-1.68E-05	1.43E-05	-1.73E-06	7.14E-08	-1.30E-09	9.01E-12	6.91E-06	-3.60E-05	-1.49E-06	1.33E-07	-1.97E-09	4.02E-12	6.88E-06	3.25E-05	3.01E-05	-1.12E-04	2.97E-06	-1.08E-05	1.28E-03	-1.10E-03
12	-9.04E-04	-1.85E-04	8.98E-04	1.52E-06	4.38E-06	-1.89E-05	-1.73E-04	1.04E-04	1.27E-09	-2.84E-07	-1.73E-06	1.90E-07	-7.51E-09	1.35E-10	-9.32E-13	7.10E-06	-2.24E-06	2.07E-07	-7.52E-09	5.73E-11	-5.83E-13	-2.80E-07	-1.89E-06	-4.44E-06	1.66E-05	-4.39E-07	8.52E-07	-3.57E-05	1.01E-04
13	3.23E-05	6.43E-06	-3.18E-05	-5.14E-08	-1.59E-07	6.79E-07	5.39E-06	-3.72E-06	-5.45E-11	-3.11E-08	7.14E-08	-7.51E-09	3.00E-10	-5.47E-12	3.83E-14	-1.73E-07	1.91E-08	-7.33E-09	2.00E-10	-7.14E-13	2.03E-14	7.46E-09	5.69E-08	1.59E-07	-5.97E-07	1.59E-08	-2.77E-08	4.12E-07	-3.57E-06
14	-5.02E-07	-1.00E-07	4.95E-07	8.03E-10	2.53E-09	-1.12E-08	-8.58E-08	6.33E-08	8.98E-13	1.44E-09	-1.30E-09	1.35E-10	-5.47E-12	1.02E-13	-7.22E-16	5.35E-10	1.42E-09	1.13E-10	-3.08E-12	1.08E-14	-3.02E-16	-1.37E-10	-9.56E-10	-2.46E-09	9.21E-09	-2.53E-10	4.49E-10	-3.01E-09	6.06E-08
15	3.12E-09	6.28E-10	-3.09E-09	-5.06E-12	-1.61E-11	7.23E-11	5.41E-10	-4.24E-10	-5.56E-15	-1.37E-11	9.01E-12	-9.32E-13	3.83E-14	-7.22E-16	5.16E-18	7.39E-12	-1.74E-11	-7.06E-13	1.98E-14	-8.14E-17	1.82E-18	9.94E-13	6.43E-12	1.53E-11	-5.69E-11	1.61E-12	-2.90E-12	1.23E-12	-4.06E-10
16	-2.00E-01	-4.04E-02	1.99E-01	3.24E-04	1.19E-03	-2.43E-03	-1.39E-02	1.86E-02	-9.81E-09	-2.26E-03	6.91E-06	7.10E-06	-1.73E-07	5.35E-10	7.39E-12	6.78E-03	-4.85E-03	4.87E-05	-1.63E-06	1.11E-08	-1.56E-10	5.04E-05	-7.52E-06	-1.00E-03	3.79E-03	-1.18E-04	1.30E-04	6.88E-03	1.80E-02
17	1.30E-01	2.65E-02	-1.30E-01	-2.14E-04	-7.75E-04	1.58E-03	9.43E-03	-1.24E-02	2.06E-08	1.65E-03	-3.60E-05	-2.24E-06	1.91E-08	1.42E-09	-1.74E-11	-4.85E-03	3.54E-03	-3.16E-05	1.14E-06	-8.80E-09	1.03E-10	-5.18E-05	-6.89E-05	6.44E-04	-2.44E-03	7.72E-05	-8.72E-05	-4.27E-03	-1.20E-02
18	-2.02E-03	-4.15E-04	2.05E-03	3.30E-06	2.01E-05	-2.13E-05	1.20E-05	2.23E-04	-1.49E-09	-1.53E-05	-1.49E-06	2.07E-07	-7.33E-09	1.13E-10	-7.06E-13	4.87E-05	-3.16E-05	3.19E-05	-4.46E-06	7.94E-08	-1.69E-12	1.88E-04	2.32E-03	-3.86E-04	1.43E-03	-1.93E-06	1.28E-06	1.96E-04	2.13E-04
19	7.02E-05	7.12E-06	-6.15E-05	1.76E-09	-7.40E-07	-7.04E-07	-3.79E-05	2.89E-06	-1.76E-10	3.35E-07	1.33E-07	-7.52E-09	2.00E-10	-3.08E-12	1.98E-14	-1.63E-06	1.14E-06	-4.46E-06	9.20E-07	-1.74E-08	9.74E-14	-5.97E-05	-3.53E-04	4.54E-05	-1.64E-04	6.87E-08	9.19E-08	-3.26E-05	4.61E-06
20	-5.03E-07	4.09E-08	3.22E-07	-1.47E-09	6.74E-09	2.31E-08	7.44E-07	-1.47E-07	3.89E-12	-8.79E-11	-1.97E-09	5.73E-11	-7.14E-13	1.08E-14	-8.14E-17	1.11E-08	-8.80E-09	7.94E-08	-1.74E-08	3.46E-10	-1.24E-15	1.16E-06	6.33E-06	-7.80E-07	2.81E-06	-5.98E-10	-2.44E-09	5.73E-07	-1.78E-07
21	6.36E-09	1.28E-09	-6.30E-09	-1.03E-11	-2.99E-11	9.38E-11	7.76E-10	-5.80E-10	-3.66E-15	4.66E-11	4.02E-12	-5.83E-13	2.03E-14	-3.02E-16	1.82E-18	-1.56E-10	1.03E-10	-1.69E-12	9.74E-14	-1.24E-15	-1.38E-05	-1.76E-11	-1.52E-03	3.09E-11	-1.16E-10	3.00E-12	-4.56E-12	3.63E-11	-5.65E-04
22	5.44E-04	-2.09E-04	-1.64E-04	4.27E-06	-8.14E-05	-9.90E-05	-3.14E-03	1.27E-04	4.70E-09	-2.29E-05	6.88E-06	-2.80E-07	7.46E-09	-1.37E-10	9.94E-13	5.04E-05	-5.18E-05	1.88E-04	-5.97E-05	1.16E-06	-1.76E-11	2.16E-02	7.13E-02	7.43E-03	-1.75E-02	7.22E-06	6.95E-06	-2.49E-03	2.61E-04
23	1.06E-02	8.90E-04	-9.08E-03	3.01E-06	-3.72E-04	-2.73E-04	-1.15E-02	-2.92E-04	1.61E-08	-2.76E-05	3.25E-05	-1.89E-06	5.69E-08	-9.56E-10	6.43E-13	-7.52E-06	-6.89E-05	2.32E-03	-3.53E-04	6.33E-06	-1.52E-03	7.13E-02	1.04E-01	3.50E-02	-2.97E-02	3.35E-05	2.15E-05	-9.83E-03	2.56E-04
24	4.38E-02	9.05E-03	-4.37E-02	-7.45E-05	-2.45E-04	6.86E-04	6.02E-03	-4.44E-03	-1.54E-08	3.00E-04	3.01E-05	-4.44E-06	1.59E-07	-2.46E-09	1.53E-11	-1.00E-03	6.44E-04	-3.86E-04	4.54E-05	-7.80E-07	3.09E-11	7.43E-03	3.50E-02	1.81E-03	-2.04E-02	2.43E-05	-3.57E-05	6.72E-04	-4.35E-03
25	-1.65E-01	-3.41E-02	1.65E-01	2.81E-04	9.10E-04	-2.59E-03	-2.31E-02	1.67E-02	5.95E-08	-1.14E-03	-1.12E-04	1.66E-05	-5.97E-07	9.21E-09	-5.69E-11	3.79E-03	-2.44E-03	1.43E-03	-1.64E-04	2.81E-06	-1.16E-10	-1.75E-02	-2.97E-02	-2.04E-02	9.21E-02	-9.02E-05	1.35E-04	-2.89E-03	1.64E-02
26	4.07E-03	9.03E-04	-4.53E-03	-6.98E-06	-2.23E-04	-1.04E-04	-4.29E-03	-1.01E-03	4.56E-08	4.50E-05	2.97E-06	-4.39E-07	1.59E-08	-2.53E-10	1.61E-12	-1.18E-04	7.72E-05	-1.93E-06	6.87E-08	-5.98E-10	3.00E-12	7.22E-06	3.35E-05	2.43E-05	-9.02E-05	1.99E-05	1.28E-06	-4.75E-03	-8.29E-04
27	-6.71E-03	-9.47E-04	6.02E-03	4.55E-06	-1.99E-05	5.75E-04	1.04E-02	-8.88E-04	-1.94E-07	-2.34E-05	-1.08E-05	8.52E-07	-2.77E-08	4.49E-10	-2.90E-12	1.30E-04	-8.72E-05	1.28E-06	9.19E-08	-2.44E-09	-4.56E-12	6.95E-06	2.15E-05	-3.57E-05	1.35E-04	1.28E-06	8.69E-06	4.75E-03	-6.21E-04
28	1.53E-01	-6.41E-02	6.88E-02	1.00E-03	4.08E-02	-2.48E-01	-9.18E-01	1.08	4.41E-05	-6.95E-03	1.28E-03	-3.57E-05	4.12E-07	-3.01E-09	1.23E-12	6.88E-03	-4.27E-03	1.96E-04	-3.26E-05	5.73E-07	3.63E-11	-2.49E-03	-9.83E-03	6.72E-04	-2.89E-03	-3.75E-03	4.75E-03	1.04	8.53E-01
29	-8.10E-01	-1.34E-01	7.78E-01	8.26E-04	8.11E-03	3.87E-02	9.79E-01	1.87E-01	-1.32E-05	-4.60E-03	-1.10E-03	1.01E-04	-3.57E-06	6.06E-08	-4.06E-10	1.80E-02	-1.20E-02	2.13E-04</											

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Bibliography

- [1] P. Reichart, G. Datzmann, A. Hauptner, R. Hertenberger, C. Wild, G. Dollinger, Three-dimensional hydrogen microscopy in diamond, *Science* (306) (2004) 1537–1540.
- [2] P. Reichart, G. Dollinger, Hydrogen analysis by proton proton scattering, in: Y. Wang, M. Nastasi (Eds.), *Handbook of Modern Ion Beam Material Analysis*, 2nd Edition, Materials Research Society, 2009.
- [3] J. R. Bergervoet, P. C. van Campen, W. A. van der Sanden, J. J. de Swart, Phase shift analysis of 0-30 MeV pp scattering data, *Phys. Rev. C* 38 (1) (1988) 15–50. doi:10.1103/PhysRevC.38.15.
- [4] J. R. Bergervoet, P. C. van Campen, R. A. M. Klomp, J.-L. de Kok, T. A. Rijken, V. G. J. Stoks, J. J. de Swart, Phase shift analysis of all proton-proton scattering data below $T_{lab}=350$ MeV, *Phys. Rev. C* 41 (4) (1990) 1435–1452. doi:10.1103/PhysRevC.41.1435.
- [5] M. H. MacGregor, R. A. Arndt, R. M. Wright, Determination of the nucleon-nucleon scattering matrix. x. (p, p) and (n, p) analysis from 1 to 450 MeV, *Phys. Rev.* 182 (5) (1969) 1714–1728. doi:10.1103/PhysRev.182.1714.
- [6] C. J. Joachain, *Quantum collision theory*, Elsevier Science Publishing Company, 1984.

- [7] J. M. Blatt, V. F. Weisskopf, *Theor. Nucl. Phys.*, new Edition, Dover Publications Inc., April 1991.
- [8] N. F. Mott, The collision between two electrons, *Proc. R. Soc. London, Ser. A* 126 (801) (1930) 259–267.
- [9] G. Breit, E. U. Condon, R. D. Present, Theory of scattering of protons by protons, *Phys. Rev.* 50 (9) (1936) 825–845. doi:10.1103/PhysRev.50.825.
- [10] D. J. Knecht, P. F. Dahl, S. Messelt, Proton-proton scattering: Revision and analysis of experimental measurements from 1.4 to 3.0 MeV, *Phys. Rev.* 148 (3) (1966) 1031–1044.
- [11] J. Bystricky, F. Lehar, et al., Numerical data and functional relationships in science and technology, in: K.-H. Hellwege, H. Schopper (Eds.), *Elastic and Charge Exchange Scattering of Elementary Particles*, Vol. 9a of *Landolt-Börnstein (New Series – Group I)*, Springer, Berlin, 1980, p. 110 ff.
- [12] IAEA Nucl. Data Services, int. Atomic Energy Agency, Austria, www.nds.iaea.org (2009).
- [13] NNDC Databases, brookhaven National Laboratory, USA, www.nndc.bnl.gov (2009).
- [14] M. Chadwick, P. G. Young, G. M. Hale, D1a150 documentation of cross sections, heating, and damage, Los Alamos National Laboratory Report LA-UR-99-1222.
- [15] H. R. Worthington, J. N. McGruer, D. E. Findley, Proton-proton scattering from 1.8 MeV to 4.2 MeV, *Phys. Rev.* 90 (5) (1953) 899.
- [16] K. Imai, K. Nisimura, N. Tamura, H. Sato, Measurements of proton-proton differential cross sections at 5, 7 and 8 MeV, *Nucl. Phys. A* 246 (1) (1975) 76–92.

- [17] R. J. Slobodrian, H. E. Conzett, E. Shield, W. F. Tivol, Proton-proton elastic scattering between 6 and 10 MeV, *Phys. Rev.* 174 (4) (1968) 1122.
- [18] N. Jarmie, J. H. Jett, J. L. Detch, R. L. Hutson, Proton-proton scattering at 9.690, 9.918, and 13.600 MeV, *Phys. Rev. Lett.* 25 (1) (1970) 34.
- [19] S. Kikuchi, J. Sanada, S. Suwa, I. Hayashi, K. Nisimura, K. Fukunaga, Elastic scattering of 14 MeV protons by deuterons and by protons, *J. Phys. Soc. Jpn.* 15 (1) (1960) 9–17.
- [20] J. L. Yntema, M. G. White, Scattering of protons by hydrogen near 18 MeV, *Phys. Rev.* 95 (5) (1954) 1226.
- [21] J. W. Burkig, J. R. Richardson, G. E. Schrank, Proton-proton scattering at 19.8 MeV, *Phys. Rev.* 113 (1) (1959) 290.
- [22] T. H. Jeong, L. H. Johnston, D. E. Young, C. N. Waddell, Proton-proton scattering at 25 MeV, *Phys. Rev.* 118 (4) (1960) 1080.
- [23] W. K. H. Panofsky, F. L. Fillmore, The scattering of protons by protons near 30 MeV, photographic method, *Phys. Rev.* 79 (1) (1950) 57.
- [24] F. L. Fillmore, Proton-proton scattering near 30 MeV, *Phys. Rev.* 83 (1951) 1252.
- [25] L. H. Johnston, D. A. Swenson, Proton-proton scattering at 40 MeV, *Phys. Rev.* 111 (1) (1958) 212.
- [26] A. Berdoz, F. Foroughi, C. Nussbaum, The differential cross section of elastic proton-proton scattering at 50 MeV, *J. Phys. G* 12 (6) (1986) L133–L137.
- [27] IAEA Nucl. Data Services, int. Atomic Energy Agency, Austria, www-nds.iaea.org, manual for data evaluation. (2010).

- [28] IAEA Nucl. Data Services, int. Atomic Energy Agency, Austria, <http://www-nds.iaea.org/sigmaCalc/> (2010).
- [29] M. Moser, P. Reichart, C. Greubel, G. Dollinger, tabulated Proton-Proton Scattering Cross Sections, Munich, www.e12.physik.tu-muenchen.de/groups/rim/pp or alternatively www.unibw.de/lrt2/forschung-en/snake/pp (2010).

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Erklärung

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Hiermit erkläre ich, dass ich die Masterarbeit selbstständig verfasst, noch nicht anderweitig für Prüfungszwecke vorgelegt, keine anderen als die angegebenen Quellen oder Hilfsmittel benützt sowie wörtliche und sinngemäße Zitate als solche gekennzeichnet habe.

Ort, Datum

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