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R-Matrix Codes for Charged-Particle Induced Reactions in the Resolved Resonance Region (3)

Summary Report of an IAEA Consultants' Meeting
IAEA Headquarters, Vienna, Austria
28-30 June 2017

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ABSTRACT

A Consultants Meeting was held at the IAEA Headquarters, from 28 to 30 June 2017, to discuss the results of a test exercise that had been defined and assigned to all participants of the previous meeting held in December 2016. Five codes were used in this exercise: AMUR, AZURE2, RAC, SFRESCO and SAMMY. The results obtained from these codes were compared and further actions were proposed. Participants′ presentations and technical discussions, as well as proposed additional actions have been summarized in this report.

September 2017

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1. Introduction

The IAEA Nuclear Data Section is coordinating an international effort to (i) evaluate charged-particle cross sections in the resolved resonance region, (ii) produce evaluated nuclear data files for further processing and finally (iii) disseminate the evaluated data through general purpose evaluated nuclear data libraries.

The kick-off meeting of this development project was held on 7-9 December 2015 at the IAEA in Vienna. The focus of the first meeting was on the specific capabilities of the existing R-matrix codes and the translatability of R-matrix calculations produced by the various codes. R-matrix theory and the various approximations that are made when implementing it in the codes were the subjects that were discussed in detail. A summary report of the meeting has been published [1].

A second meeting was held on 5-7 December 2016 at the IAEA in Vienna, with the aim of defining a common exercise for all the R-matrix codes used in the project, in order to assess the R-matrix algorithms implemented in the codes, as well as the minimization techniques and statistical error analysis. The exercise involved fitting the two channels ^{3}He+^{4}He and p+^{6}Li forming the ^{7}Be compound system at sufficiently low excitation energies to exclude other reaction channels. The details of the exercise (Test case 1: ^{7}Be system) are available in the summary report of the meeting [2].

The third meeting was held from 28 to 30 June 2017 to compare the results of the exercise (Test case 1) obtained by the different codes. Five codes were used in the exercise: AMUR, AZURE2, RAC, SFRESCO and SAMMY. The resonance parameters and cross sections as well as the associated uncertainties obtained from these codes were compared in depth with each other as well as with the results of a previous evaluation of the same compound system performed by the code EDA5.

Seven participants from four countries attended the meeting: Z. Chen (People's Rep. of China), R.J. Deboer (USA), S. Kunieda (Japan), H. Leeb (Austria), M. Pigni (USA), T. Srdinko (Austria), I.J. Thompson (USA), IAEA staff including the scientific secretary P. Dimitriou, A.Trkov and J.-C. Sublet. M. Paris (USA) contributed to the meeting via Skype connection.

The participants were welcomed to the IAEA by the Nuclear Data Section Head, A. Koning. P. Dimitriou briefly addressed the objective and scope of the meeting. I. Thompson was appointed Chairman and H. Leeb rapporteur. After adoption of the Agenda, the meeting continued with participants' presentations (see links to presentations in Annex 3). The meeting agenda and participant's coordinates can be found in Annexes 1 and 2, respectively.

2. Summaries of presentations

2.1. Results with SFRESCO, *Ian Thompson (LLNL)*

The common basis for Test case 1: ^{7}Be, Objectives 1 and 2, are described in detail in Appendix 3 of Ref. [2] and in the Appendix of this report.

Email discussions among participants before the meeting revealed that the specifications in Ref. [2] were not uniformly followed, so more work is necessary to enforce these common conditions throughout all the codes in order to be able to compare all the results.

The work presented here only covers Objective 1. All the specifications [2] were implemented, except for the fact that the background poles were not always constrained to 20 MeV. Furthermore, the data for the (^{4}He,p) reaction were not taken from the database distributed by DeBoer for the exercise, but from a file shared by Paris [3]. This file contained data of Spiger and Tombrello for the ^{4}He(^{3}He,p)^{6}Li reaction transformed in the CM frame. These data are not identical to the EXFOR entry A1094008 [4] used by DeBoer to convert to inverse kinematics in the LAB frame. [Sec. Note: there were some problems with the transformation of the original EXFOR A1094008 [4] for the ^{4}He(^{3}He,p)^{6}Li reaction

to inverse kinematics in the LAB. As a result, some of the participants decided to use the original EXFOR data (Chen, Pigni), while others (deBoer, Kunieda, Thompson) used the LANL data after converting to inverse kinematics in the CM frame].

These are the first comprehensive R-matrix fits obtained with SFRESCO. The code FRESCO was used in the version SFRESCOX for searches with the Minuit-1 χ^2 MIGRAD algorithm. Unfortunately, MIGRAD did not converge in this work: the final first-derivatives were *not* small, and no covariance matrix was obtained. But nevertheless χ^2 gets smaller with successive Minuit iterations, so 'plausible' preliminary results were shown with a final χ^2 /N = 21.87. This is considered to be a good starting point for further improvement.

For the specific data sets, the results are:

1. Barnard elastic α-scattering is reasonable: χ^2/N = 3.76, normalization (norm) = 1.0007
2. Spiger elastic α-scattering: χ^2/N = 61.2, norm = 0.9941
3. Tombrello elastic α-scattering: χ^2/N = 19.8, norm = 1.1503
4. Mohr elastic α-scattering: χ^2/N = 4.74, norm = 0.9392
5. Fasoli elastic p scattering: χ^2/N = 28.07, norm = 1.0475
6. McCray elastic p scattering: χ^2/N = 18.259, norm = 1.249
7. Harrison elastic p scattering: χ^2/N = 62.69,norm = 1.659
8. Lin (p,α): χ^2/N = 29.43, norm = 1.6339
9. Elwyn (p,α): χ^2/N = 43.87, norm = 1.4126
10. Spiger (α,p): χ^2/N = 10.003, norm = 1.329

The poles and widths of the fit were also presented: poles in MeV (in the CM frame of ^{7}Be), widths in the formal ENDF6-style; and also widths and R-matrix parameters in the Brune [5] basis (14 poles, 42 widths). Details are available on request. Adding some of the higher energy channels does not lead to significant improvements. However, as these are preliminary results, this remains to be confirmed.

2.2. Results with AZURE, *James deBoer (Univ. of Notre Dame)*

The uncertainty analysis is perhaps the most difficult part of any R-matrix analysis. For multi-parameter fits there are well defined ways of calculating uncertainties based on changes in the χ^2 of the fits with respect to the fitting parameters, but these procedures seem to underestimate the uncertainties. The nuclear astrophysics group at the University of Notre Dame has experimented with several types of uncertainty estimation over the years ranging from different $\Delta\chi^2$ prescriptions to Monte Carlo methods. At the moment the favored method is by Monte Carlo, but these procedures are often very computationally expensive.

Another complication is the presence of outlier data points. There are different conventions for first determining the outlier points and then different prescriptions for either inflating the error bars or completely excluding such points from the analysis. An alternative is to reinterpret the meaning of the probability density function of the uncertainties on the data, making them a broader function than the standard Gaussian. This decreases the impact of these points on the fit and is easily implementable. Tests have shown that very similar central values of the fits are often obtained, but that the resulting uncertainties are increased as expected.

Regarding the analysis objectives of the ^{7}Be system, both objectives 1 and 2 were attempted but each was only partially completed. For both objectives, the fitting was performed using the alternate Brune [5] parameterization instead of B = -*l*, which was then transformed to B = -*l* using the Ferdinand code [6].

In objective 1, it was difficult to get a good fit to the data without having very large background pole widths. This problem has not been overcome. When Thompson tried to transform the very large widths of the background poles to B = -*l*, the transformation failed. However, the energies and partial widths of the actual resonances seemed very reasonable as were the normalization factors.

For objective 2 it was possible to transform from the Brune to standard R-matrix parameters. It seems that by adding the higher energy resonance poles into the calculations, the contributions of the background pole were reduced. A preliminary Monte Carlo uncertainty analysis was also performed with reasonable results, although the uncertainties have not been investigated or compared carefully to others yet.

An attempt to calculate the covariance matrix for objective 1 has not been successful, likely because of highly correlated or unphysical parameters that cause the MINOS routine in MINUIT to crash.

It seems that it is very hard to achieve a good fit with the data truncated at the p1 inelastic threshold. A plausible reason for this is that there are several resonances at higher energy that are very broad and therefore have a large impact on the lower energy cross sections. Further, their contributions are likely not flat backgrounds, which makes it very difficult to mimic them with the poles at 20 MeV. However, this still requires some investigation.

2.3. Results with the AMUR code, *Satoshi Kunieda (JAEA)*

An overview of the AMUR code was given. This is a multi-channel, multi-level R-matrix code based on the Wigner-Eisenbud's formalism except for the γ-ray channels which are calculated by the Reich-Moore approximation. The code can be applied to the analysis of cross-sections, differential cross-sections, polarization/analyzing powers for both neutron and charged-particle reactions. All the resonance and experimental parameters can be obtained from fitting experimental data using the generalized least-square method.

The test analysis was performed by following the instructions given in Appendix 3 in Ref [2]. Since the AMUR code uses the analytical formula as in Lane-Thomas [7] (p 292, eq. (2.6)) for the calculation of differential cross-sections, the definition of L_{max} is the maximum order of the Legendre expansion. Therefore, $L_{max} = 7$ for the alpha-particle and 2 for protons in the analysis. It was noted that those values were required for convergence of the differential cross-sections up to the maximum energy of $E_x = 8$ MeV of Objective 1. Re-normalization was assumed only for the data of Mohr et al. [8], Fasoli et al. [9] and Harisson et al. [10] since the systematic uncertainties are already given for the other data files.

Initially, levels 1 – 5 (see Appendix) together with distant levels for each J^{π} were assumed in the test analysis. However, it was difficult to fit all the experimental data simultaneously as the fits would not converge. The problem was attributed to the phase-shifts (ps) of shape-elastic scattering, so additional distant poles independent of the incident particles were introduced to correct the hard-sphere ps. With this approach, an acceptable convergence ($\chi^2/N = 8.33$) was achieved and reasonable agreement with the measured cross-sections was obtained visually. However, it was not possible to reproduce the absolute values of certain data at several energies/angles (e.g., Elwyn et al. [11], $E_{lab} = 2.277–2.575$) due to a plausible systematic uncertainty in the data that is independent of the energies/angles.

The uncertainties of the cross-sections for the $^6Li(p,a_0)^3He$ reaction were estimated with the KALMAN method [12]. The uncertainty was found to be 1–2 % on average, which presumably comes from the systematic uncertainty suggested by Spiger et al. [4]. Preliminary results of the correlation matrix were also shown for the different reactions and scattering angles where the constraint from the theory (unitarity of the S-matrix) is observed around the resonant peaks.

2.4. Results with SAMMY, *Marco Pigni (ORNL)*

The most recent version of the R-matrix code SAMMY [13] allows the study of the ingoing and outgoing charged-particle channels in the low-energy interaction range. This feature makes the code suitable for the resonance analysis of the ^7Be compound system as defined in Test case 1 [2]. However, because the SAMMY R-matrix algorithm is set up to handle only one INCIDENT particle at a time, the two open channel reactions $^3He+^4He$ and $p+^6Li$ forming the ^7Be compound system needed

to be analyzed separately. In this work, specific measured excitation functions of the ^{3}He+^{4}He reaction were analysed in the same kinematics as reported in the EXFOR library (not in the inverse kinematics distributed by deBoer) while the analysis of the p+^{6}Li reaction is still in progress.

In view of the requirements of Test case 1, such as the use of the boundary condition B = -*l* for reaction channels with energy thresholds, it was necessary to make corrections to the SAMMY code algorithm, specifically in the computation of the R-matrix elements and in the calculation of the shift functions for negative energies. Given that the energy-dependent boundary condition B = S is predominantly used in all current evaluations of resonant reactions that are released in the major nuclear data libraries (ENDF/B, JEFF, JENDL), the need for such updates and corrections in the R-matrix algorithms was not apparent. In fact, these updates guarantee full consistency in the conversion between "formal" and "alternative" R-matrix parameters developed by Brune [5] and are therefore important.

2.5. Results with the RAC code, *Zhenpeng Chen (Tsinghua University)*

Eight different fitting schemes were completed in the period from 2017-01-10 to 2017-06-22.

The first scheme aimed at Objective 1 and included the original data distributed with the Test 1 exercise [2] (deBoer data in LAB frame and inverse kinematics). The fit did not converge nicely and the final chi-square was not so good: $\chi^2 = 5.94$.

In the second scheme, the data sets as well as the level frame were modified leading to significant improvement in the fit with a $\chi^2 = 1.98$, but still there were some problems.

In order to get even better results, a third scheme was analysed, in which the data were taken directly from the EXFOR database, and some additional new data were also included. When normalizing the 4 groups of absolute data, a value of $\chi^2 = 1.67$ was obtained, while without normalization a value of $\chi^2 = 1.98$ was obtained (fourth scheme).

Based on the results of the third and fourth schemes for Objective 1, it was then possible to move on to Objective 2, and the fifth scheme which includes the reaction channel ^{6}Li(p,p$_1$)^{6}Li*. The results obtained look very good with a value of $\chi^2 = 1.55$.

Then, starting from the results obtained for the fifth scheme, the analysis was further extended to include the reaction channels ^{6}Li(p,p$_2$)^{6}Li**, ^{6}Li(p,γ_0)^{7}Be and ^{6}Li(p,γ_1)^{7}Be*. For this sixth scheme, when the 4 sets of absolute data are normalized the obtained results are very good ($\chi^2 = 1.71$); without normalization of these absolute datasets (N = 1) (seventh scheme), the results do not change much ($\chi^2 = 1.89$). This can be explained by the fact that when the database is complete and the data are of good quality, the normalization is not a key problem.

In all the schemes described above, the**'Conventional Least Square'**(CLS) fitting method was used.

For the seventh scheme mentioned above, an analysis using the **'General Least Square'** method has been completed and the results give a value of $\chi^2 = 2.66$ (eighth scheme).

The fitting procedure is objective and well-established. With the original database and the primary level-frame defined in Test 1 [2], the automated search for the best parameter set requires more than 1000 iterations. The suitable levels or parameters will be kept, the unsuitable levels or parameters will be rejected. After getting a rather good fit with the iterative procedure, one can then check if some of the absolute datasets need to be normalized, and/or if an additional level or parameter needs to be added, before making a new iterative search until a perfect fit is obtained.

So far, a series of very good fits for Test 1 and 2 [2] (8 schemes) have been obtained. The next step will be to replace the limited EXFOR entry for the Spiger ^{3}He-elastic scattering and (^{3}He,p) data with a more complete set from his thesis, and also add some other datasets which have not been used so far (e.g. polarization data, (^{3}He,γ)).

Some more general ideas should be emphasized or recommended here:

A. This evaluation of charged-particle resonant reactions requires 'global fitting', i.e. it needs to consider a complete basis of quantum states and all the experimental data that are available for the compound system.

B. The 'Reduced R-Matrix formula' ([7] Chapter X) has to be used to get a good fit at higher energies where several channels contribute. This implies the use of imaginary widths in the denominator of the R-Matrix formula. This approach has been used in the neutron standards for energies above 4 MeV.

C. The '**General Least Square'** method has to be used finally to get accurate covariance matrices for the evaluation data. This is because the '**CLS'** cannot produce accurate covariance matrix, since the pure experimental data evaluation with 'archaeology skill' only considers the correlation of experimental data, while the pure 'model evaluation' (e.g., Monto Carlo method) only considers the correlation of parameters. The '**General Least Square' method** considers both correlation of data and correlation of parameters simultaneously.

If within this coordinated project, we develop several R-matrix codes which have the evaluation ability mentioned above, then we will have the possibility to obtain new information about nuclear structure, accurate evaluated nuclear data, accurate covariance matrices for corresponding nuclear evaluated data, at energies extending from the resolved-resonance range to the un-resolved range.

2.6. EDA5 results for evaluation of ^{7}Be system, *Mark Paris (LANL)* (Presentation via Skype)

In the remote presentation, an existing evaluation of the ^{7}Be system using EDA5 was shown (LA-UR-17-25143). in this evaluation, R-matrix theory was used to fit the data and then the T-matrix theory was used to extract physical resonances from the T-matrix poles. This approach gave an additional 'unobserved' resonance at an +3/2 state at 2.5 MeV. The latter is probably the result of fitting to one particular set of gamma capture data. It would be interesting to check if this state can be predicted by ab initio calculations. Overall, the fit gave a $\chi^2/N = 1.9$ for the entire data set.

Normalization: data sets were treated with independent normalizations depending on how they were measured, if they were angular distribution measurements using the same detector system or excitation functions.

Background poles: several were needed and some at very large energies, ± 100 MeV.

All available data were considered: unpolarised cross sections, reaction cross sections and polarization data.

Ferdinand code: Paris and Thompson were able to feed the EDA parameters + specific boundary conditions into the Ferdinand code, and then use the Barker-Brune transformation to convert them to the B = -*l* boundary condition. The latter parameters were then fed into EDA5 again, and this time using the B = -*l* boundary conditions reproduced the original EDA5 cross sections with remarkable accuracy. This exercise worked well with the elastic scattering and reaction cross sections, but it failed with the polarization data. Several reasons were discussed and one possible cause is the existence of degenerate poles.

Spiger (^{3}He,p) data provided by LANL [3]: they most likely come from private communication. M. Paris will verify the the source.

3. Discussions

Based on the questions and discussions that were triggered by the results presented by the participants, the following issues were raised leading to a revision of Test case 1 and a further splitting into three parts (1a, 1b and 1c) which are detailed in the Appendix.

The main issues raised are:

- Experimental data: transforming from CM to LAB and vice versa, or from forward to inverse kinematics can be dangerous and therefore, to the extent it is possible, we should use the original data and avoid these manipulations.
  Recommendation: all participants should report problems in EXFOR files [14] to the IAEA (Otsuka: n.otsuka@iaea.org)

  The problem with the (^{3}He,p) data of Spiger et al. [4] included in the database is still not entirely clarified: The EXFOR data entry has no clear definition whether the cross sections are in the LAB or CM frame. If nothing is specified in the published article, then neither is it in EXFOR, but it is assumed that the cross section is given in the same frame as the angles, i.e. in this particular case they are given in the LAB frame. More Spiger data at several angles were provided by Paris from the EDA database [3] (angles and cross sections in CM frame). However, the source of these data still needs to be verified, whether they are from the thesis of Spiger [15] or another source.

  Action on M. Paris to provide more information. In the remaining exercises/tests the Spiger data of EDA in the CM frame will be used.

  Chen also claims that there is a problem with the (α,α) data of Mohr [8] as provided in the deBoer database. **Action on P. Dimitriou to investigate this.**

- Systematic uncertainties: how are they treated? Thompson and deBoer treat them with normalization factors and then add a term in the χ^2. Kunieda, Chen and Pigni include them in the data covariance matrix.

- Normalization: in some analyses (EDA) some of the data sets are treated with independent normalizations depending on how they were measured, whether they were angular distribution measurements using the same detector system or excitation functions. It was decided that a more thorough review of the experimental papers was required to make sure whether the data could be grouped in sub-groups with the same normalization in energy or angular distributions.
  An Action was placed on all participants to review at least one of the experimental articles and on P. Dimitriou to collect all the reviews by 31 July 2017.

  The reviews were collected and the following normalizations were adopted for the Test cases 1a-c:

  Articles for Review

  [1] ^{3}He(α,α)^{3}He, dσ/dΩ: A. Barnard et al., [16] Nucl. Phys. 50 (1964) 629-640. →
  H. Leeb: In this paper there is a mixture between measurements of excitation functions and angular distributions which has been considered simultaneously in the analysis. **Hence a unique normalization constant for both quantities might be the appropriate choice**.

  [2] ^{6}Li(p,α)^{3}He, dσ/dΩ: L. Chia-Shou et al., [17] Nucl. Phys. A 275(1) (1977) 93-99. →
  R.J. deBoer: two detectors were used in a scattering chamber with a solid transmission target for simultaneous measurements, but these were always used in tandem for coincidence

between the outgoing ^{3}He and ^{4}He in order to remove background contributions from the always present ^{19}F(p,a) reaction (at least in solid targets in forward kinematics). No monitor detector is reported.
According to the text "The cross sections were measured from 1.0 to 2.6 MeV proton energy at angles from 20 to 90 degrees in the lab system in steps of 10 degrees. The energy steps used were from 50 keV to ... 200 keV ...". The language makes it a bit difficult to determine exactly how the experiment was performed, but since the data are presented mostly in the form of **angular distributions** it seems reasonable to treat them as such.
It should be noted that the point-to-point error bars include all of the uncertainties, not just the statistical ones. **Different normalization per angular distribution should be applied.**

[3] ^{6}Li(p,α)^{3}He, dσ/dΩ: A. J. Elwyn et al., [11] Phys. Rev. C 20 (1979), 1984-1992. →
H. Leeb: In this case it is suggested to follow the analysis and to use **a normalization constant on the θ_{lab} = 50° excitation function and normalize the differential cross sections correspondingly**.

[4] ^{6}Li(p,p)^{6}Li, dσ/dΩ: U. Fasoli et al., [9] Il Nuovo Cimento 34(6) (1964) 1832-1836. →
P. Dimitriou: it is not clear whether the authors measured excitation curves at each angle, or moved the detector to different angles for each fixed beam energy. However, since they mention 'Fig.1 shows the excitation curves obtained...' it is reasonable to assume they measured **excitation curves**. On the other hand, their measurements are relative so **they should be treated as shape data only, using separate normalization per angle**.

[5] ^{6}Li(p,p)^{6}Li, dσ/dΩ: W. D. Harrison and A. B. Whitehead, [10] Phys. Rev. 132 (1963) 2607-2613. →
M. Pigni: The **angular distributions** were measured simultaneously with three independent detectors. In EXFOR, the statistical error (1% up to 12%) is reported for each angle at a given energy. In addition a 5% absolute error for the normalization is reported. This value was based on McCray's differential cross sections to which the entire set of Harrison's data was normalized. **Therefore, for Harrison's set of data, a unique normalization constant should be used for all angular distributions**.

[6] ^{6}Li(p,p)^{6}Li, dσ/dΩ: J. A. McCray et al., [18] Phys. Rev. 130 (1963) 2034-2042. →
I. Thompson: excitation functions were measured at small energy increments, therefore all the energies in a given excitation function should have the same systematic error.
It is not clear how much the detector configuration varied between excitation functions, and so whether or not the different excitation functions have common systematic errors. Since a single magnetic spectrometer was moved to the different angles, **different normalizations should be given to the separate excitation functions**.
Specifically, from the paper:

I. The error bars indicate relative errors which are 3% for the backward angles and 4% for the 70 and 90 deg data.
II. The probable error in the absolute values of the measured scattering cross sections was estimated to be about 5%.

[7] ^{3}He(α,α)^{3}He, dσ/dΩ: P. Mohr et al., [8] Phys. Rev. C 48 (1993) 1420-1427. →
R.J. DeBoer: it is stated that there were "...ten surface-barrier detectors mounted at fixed positions." around the gas jet target and that scattering cross sections were measured at "...20 energies in the range from 1 to 3.3 MeV...". This indicates that the differential cross sections were measured simultaneously. Therefore, for these cross sections, it is recommended that they be treated as **angular distributions**. No information is given in the text regarding the systematic uncertainties of the data, **so separate normalizations can be used per angular distribution**.

[8] $^{3}He(\alpha,\alpha)^{3}He$, dσ/dΩ: R. J. Spiger and T. A. Tombrello, [4] Phys. Rev. 163 (1967) 964-984. →

R.J. deBoer: The setup in figure 2 of that work shows two detectors in the setup. This is also stated in a paragraph in the text where it also explains that each detector itself consists of two detectors, one a thin transmission detector and the other a thick detector capable of stopping the particles, to form a E-deltaE detector configuration. Later under the ^{3}He-^{4}He scattering section, it is stated that "excitation curves of the differential elastic-scattering cross sections were obtained...", which indicates that the detectors were probably held at a constant angle and the energy of the beam was then changed.

Zh. Chen: **Excitation curves** of the differential elastic-scattering cross section were obtained at 14 center-of-mass angles between bombarding energies of 4.6 and 14.75 MeV. From 14.75- to 18 MeV, data were obtained at ten center-of-mass angles. Figure 7 of the paper shows three of the excitation curves obtained. The EXFOR data are from a digitization of these three curves.

The systematic errors for the curves in figure 7 were from 1.1 to 1.5% which may be a gross underestimation. Typical relative errors were: 2% (54.7'), 3% (90.0'), and 3% (125.2'). **Different normalizations for each excitation curve.**

[9] $^{4}He(^{3}He,p)^{6}Li$, dσ/dΩ: R. J. Spiger, [3] source tbc →

M. Paris: **in EDA5 different normalizations were used for each angular distribution curve.**

[10] $^{3}He(\alpha,\alpha)^{3}He$, dσ/dΩ: T. A. Tombrello and P. D. Parker, [19] Phys. Rev. 130 (1963) 1112-1119. →

S. Kunieda: there are no reasons to give a separate re-normalization for each scattering angle. Looking through a related paper [20], we draw the same conclusion.

The authors used the same detectors for all scattering angles:
„The scattered He-3 particles and recoiled alpha particles were detected with two collimated counters. The angular position of one counter was varied while the other was fixed at a laboratory angle of 30 deg as a monitor."

Therefore, it is recommended that we assume only **one unique normalization (or dSyst = 5%) to this measurement as an initial approach**.

- Processing codes are currently unable to handle angular distributions of charged-particles. This is an important gap in processing capabilities which unless it is solved will mean that these new evaluations will not be incorporated properly into the libraries used in transport codes for some of the applications. A more detailed discussion with A. Trkov and J.-C. Sublet is described Section 3.3.
- Finally, it became obvious that certain conditions of the test case had not been defined so explicitly before, therefore, a more detailed list of conditions was prepared. Specifically, the test case was split into three sub-cases: one to compare R-matrix calculations without fitting, one to compare the minimization methods used for fitting, one to compare the effect of fitting data in different kinematics. The details are described in the following section and in the Appendix.

3.1. Definite Benchmark Test

A detailed write-up of the conditions is included in the Appendix. A short summary is given below.

3.1.1. Conditions of the benchmark 1a (R-matrix calculations using same parameters – no fit) – end of August, 2017

Since Kunieda's R-matrix fits described in Section 2.3 gave reasonable results while respecting most of the specifications of Test 1, it was decided that the whole group would use his resonance parameters to perform R-matrix calculations with the different codes and compare the results.

The parameters to be used in these calculations are given in the Appendix. They include using one multi-channel pole in each partial wave up to $J^{\pi} = 4.5$; B = -*l*; Channel radius $r_c = 1.4 \cdot [A_1^{(1/3)+} A_2^{(1/3)}]$.

Calculations will be performed for the (α,α) elastic scattering data of Barnard [16], the (α,p) data of Spiger (Los Alamos) [3], the (p,p) data of McCray [18], and the (p,α) data of Elwyn [11].

The calculated cross sections should be in the same frame as the experimental data (to define energy grid and kinematics).

J. deBoer will collect the cross sections by 31 August 2017 and plot them for comparison at a few angles.

3.1.2. Conditions of the benchmark 1b (to compare minimization method and treatment of uncertainties in the different codes)

This is a more detailed definition of the previous Test 1 case (Objective 1) [2]. The aim is to produce fits and corresponding uncertainty covariance matrix using

- Same input cross section data defined in Tables 3 and 4 of write-up (Appendix)
- Background poles at fixed energy of 20 MeV in the energy scale of excitation energy of ^{7}Be
- Five resonance poles with fixed energy (see level scheme of Appendix)
- One background pole per J^{π} included up to $J^{\pi} = 4.5+$ and 4.5-
- $B = -l_c$
- same channel radii as before
- comparison will include resonance parameters, normalization and cross sections, including uncertainties and covariances of parameters
- normalizations according to Table 4 of the Appendix should be adopted.

Chen insists that there should be a 0.5+ pole in the fit in order to improve the data. An attempt to verify this is mentioned in Sect. 3.2.

Recommendation (not obligatory): use initial resonance parameters of Test 1a as starting values for the fit.

All results of Test 1b will be collected by **I. Thompson by 30 November 2017.** All resonance parameters, normalizations, variances and covariances, eigenvalues of the matrix on the parameters are requested.

3.1.3. Benchmark 1c: Compare effect of kinematics frame

Calculate with the same parameters obtained in Test 1b the EXFOR cross sections in original kinematics and compare the χ^2. Results will be sent to **I. Thompson by 22 December 2017**.

3.2. Comparison of the resonance parameters of Z .Chen

Thompson compared the resonance data that Chen used to obtain the good fits for benchmark Test 1 (see Sect. 2.5). In the case of the third scheme where he obtained $\chi^2 = 1.67$, he has 13 poles, among which several with very large widths. The comparison was possible by using Ferdinand to convert the parameters in an energy scale of g.s. of compound nucleus: the results showed a huge background pole at zero energy (b.s.), and strong amplitudes for sub-threshold proton poles as well. The 5/2- and 7/2- poles are described well. However there is only one 5/2- pole in contrast with the level scheme of the Appendix.

When using these parameters in SFRESCO to calculate cross sections, the following results were obtained: there is a missing resonance at 7 MeV, the cross sections below proton threshold are wrong, possibly due to the 7/2- pole which is the sub-threshold for the proton channel. Also, the monstrous background pole at $J^{\pi} = 3/2-$, 114 MeV with a width of 13708 GeV apparently has no effect whatsoever on the cross sections so that it may as well be removed.

Action on J. deBoer, S. Kunieda, M. Pigni: use same resonance parameters of Chen sent by Thompson to verify results from SFRESCO, especially the impact of sub-threshold poles and how they are calculated by the several codes.

3.3. Discussion on Possible Processing Codes (with A. Trkov and J-C. Sublet)

Processing codes are needed to verify the cross sections produced from ENDF resonance parameter files [21] and then use them to produce libraries for transport codes.

Processing codes start with ENDF files. PREPRO [22] does not deal with charged-particle differential data. It can use resonance parameters but with neither Coulomb term nor the B = -*l* boundary condition. The same is true for NJOY [23]. Therefore, these codes can currently not process charged-particle elastic cross section data. NJOY uses the SAMRML subroutine from SAMMY [13] and therefore has the same limitations for treating boundary conditions for threshold reactions as SAMMY according to M. Pigni.

A Meeting on Processing Codes will take place at IAEA in December 2017. One question might be "Which of the codes has the capability to process charged-particle data" (MF = 3 contains integrated cross sections and MF = 6 contains angular distribution Legendre distributions).

The best solution would be to have a stand-alone program which would produce angular cross sections from an ENDF resonance parameter file at a given dense angular grid and adaptable energy grid so as not to lose the resonance structure.

In principle, any of the R-matrix codes can be adapted to do this point-wise reconstruction of the Coulomb + nuclear elastic scattering.

FUDGE [24] is in development phase and SAMMY can already do this. However both are heavy codes that include many other capabilities such as fitting algorithms. Therefore, one way would be to produce a lighter and limited version of FUDGE and SAMMY that do only the point-wise reconstruction of angular distributions starting from a resonance parameter file. To make things even simpler, a regular energy grid could be implemented in the beginning.

The RAC code can also reconstruct cross sections from resonance parameters and a test case will be sent for verification. Chen and Thompson will collaborate on this.

Another code that could be considered for reconstruction of angular distributions from resonance parameter representation is GRUKON [25].

To help with starting up the code, an example of an ENDF file produced from the SigmaCalc online calculator [26] was downloaded from the ENDF IBA-EVAL library (https://www-nds.iaea.org/public/download-endf/IBA-Eval/).

Recommendation: I. Thompson uses his FRESCO code to reconstruct angular distributions at a fixed angle and energy grid starting from resonance parameters, for charged particle reactions in the RRR. This code will be further discussed at the next R-matrix codes meeting.

3.4. Perspectives

Participants agreed to publish and disseminate the results of Tests 1a, 1b and 1c as follows:

- Write a paper with all the comparisons from Tests 1a-c that would include:
  - Physics insight
  - Specifications of the different R-matrix codes
  - Comparison of fitted cross sections and covariance matrices
- Work on an evaluation of ^{7}Be: this will be the subject of the next R-matrix meeting in 2018.
  - Include all available data and open channels in the resolved-resonance region
  - Comparison of the fit with existing evaluations and covariance matrices
  - Publish evaluation
  - Contribute evaluation to CSEWG
- Produce 2-dimensional grid of reconstructed cross sections from resonances for processing and dissemination through the ENDF databases

4. Conclusions

Benchmark tests need to be defined more precisely. Tests 1a-c have been re-defined in order to avoid ambiguities and allow a straightforward comparison between the different codes.

The ultimate goal of this project is to reach a consensus on R-matrix calculations, minimization methods and treatment of uncertainties, and finally an evaluation methodology that would allow the production of evaluated charged-particle reaction cross sections in the resolved-resonance region for adoption by the evaluated libraries.

The dates of the next meeting in 2018 will be decided after submission of the results of Tests 1a-c and a preliminary evaluation of the comparisons.

Participation should be limited to those who contribute to all of the above test cases (1a-c).

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Test case: ^{7}Be compound

James deBoer

1 Objective 1a

Calculate cross sections for the data of Barnard et al. [1], McCray [6], Elwyn et al. [3] and Spiger and Tombrello [8] from the level parameters (energies and reduced width amplitudes) given in Table 1 provided by Satoshi Kuniuda. [Note: To avoid any confusion, Table 1 contains the poles that have non-zero reduced width amplitudes in at least one channel. Additional poles, with reduced width amplitudes that are zero for all channels, may be required by some codes for angular momentum and spin conservation reasons, so code developers will also share their input files when performing this and other similar exercises.]

Cross sections must be given in the frame of reference of the data (^{3}He$(\alpha,\alpha)^3$He, ^{6}Li$(p,\alpha)^3$He, and ^{6}Li$(p,p)^6$Li in the laboratory frame and ^{3}He$(\alpha,p)^6$Li in the center-of-mass frame of reference).

The calculations should be made using $B_c = -l_c$ (orbital angular momentum) and maximum orbital angular momentum needed to produce all the channels up to $J^\pi = 9/2^\pm$ (see note above). Channel radii should be determined as $a_c = 1.4$ [fm] ($A_1^{1/3}+A_2^{1/3}$) and should be the same for all channels within a particle pair.

Calculations should be completed by August 31, 2017 and the cross section data files sent via email to James deBoer.

Table 1: R-matrix parameters in the $B = -l$ basis
Pole energies in the centre-of-mass frame of the elastic channel.
Reduced width amplitudes are given in MeV$^{1/2}$.

$J^\pi = 1.5^-$				
E	H1+Li6	H1+Li6	H1+Li6	He4+He3
(MeV)	LS: 1, 1/2	LS: 1, 3/2	LS: 3, 3/2	LS: 1, 1/2
-1.586097	−1.34077	−0.41816	0.00000	1.05725
$J^\pi = 2.5^-$				
E	H1+Li6	H1+Li6	He4+He3	
(MeV)	LS: 1, 3/2	LS: 3, 1/2	LS: 3, 1/2	
5.746671	0.94880	0.00000	0.18770	
7.088367	−0.34947	0.00000	1.18381	
$J^\pi = 3.5^-$				
E	H1+Li6	H1+Li6	H1+Li6	He4+He3
(MeV)	LS: 3, 1/2	LS: 3, 3/2	LS: 5, 3/2	LS: 3, 1/2
3.483949	0.00000	0.00000	0.00000	0.79362

2 Objective 1b

With the data listed in Table 3 (available on Box) by James deBoer, obtain an R-matrix fit up to $E_x = 8.0$ MeV using only the ^{3}He+α and ^{6}Li+p_0 partitions as given in Table 2. Data sets have been truncated in incoming laboratory energies at $E_{\rm proton} = 2.79$ and $E_\alpha = 15.0$ MeV, corresponding to the excitation energy limit of $E_x = 8.0$ MeV. Background levels should be fixed at an excitation

energy in the ^{7}Be compound nucleus of 20 MeV. One background level is allowed for each J^π. Free parameters for the fit are: energies of unbound levels (excluding background pole energies), reduced width amplitudes of bound and unbound levels, reduced width amplitudes of the background poles and the normalization factors for each data set as detailed in Table 4.

Data sets are given in AZURE2 format files except for those of Spiger and Tombrello [8] ^{3}He$(\alpha,p)^6$Li, which are given in a labeled spreadsheet taken from the EDA (Los Alamos) data file. All AZURE2 data quantities are in the laboratory frame, while those of Spiger and Tombrello [8] are given in the center-of-mass frame. AZURE2 data are arranged in four space or tab separated columns in the following format:

E(MeV), Angle (degrees), $\frac{d\sigma}{d\Omega}$(b/sr), $\Delta\frac{d\sigma}{d\Omega}$(b/sr).

Note that if the data are of the angle integrated type, the angle column is still included but becomes a dummy value (usually set to 0). For this example, the adopted kinematics has the ^{3}He or ^{6}Li nucleus as the target, and the α particle or proton as the projectile.

Details of the normalization procedures for the data will be reviewed by the members of the group by July 31, 2017. Results should be sent to P. Dimitriou who will update this document in Table 4.

Fits should be completed by November 30, 2017 and the results, including all R-matrix parameters, normalizations, and parameter covariance matrix should be sent to Ian Thompson. [Note: the original deadline of 31 October 2017 has been extended on account of the detailed comparisons of the results of Test1a. The latter exercise is expected to be completed by the end of October.]

3 Objective 1c

Take data directly from EXFOR using the original kinematics and perform a calculation using the best fit parameters and normalizations obtained in Objective 1b and compare the χ^2 of the two calculations. The results of objective 1c are due at the next workshop meeting.

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Table 2: Particle pair information for ^{7}Be compound system. Masses are in amu, separation and excitation energies in MeV, and channel radii in fm.

particle pair 1		
light particle:	^{4}He	
	J =	0
	π =	+
	M =	4.0026
	Z =	2
heavy particle:	^{3}He	
	J =	0.5
	π =	+
	M =	3.01603
	Z =	2
Excitation Energy =	0	
Separation Energy =	1.587	
particle pair 2		
light particle:	^{1}H	
	J =	0.5
	π =	+
	M =	1.0078
	Z =	1
heavy particle:	^{6}Li	
	J =	1
	π =	+
	M =	6.0151
	Z =	3
Excitation Energy =	0	
Separation Energy =	5.6068	

Table 3: Summary of data. For the absolute normalization, a "?" symbol indicates that the published work does not give an overall systematic uncertainty. A "-" indicates that the data have been normalized to other data. Both of these data sets should be treated as shape data only. Data in the second half of the table are for objective 2 only. Thanks to Mark Paris and Gerry Hale for giving more detailed (α, p_0) cross section data for the experiment reported in Ref. [8].

Ref.	data type	file name	source
[1]	^{3}He$(\alpha,\alpha)^{3}$He, $\frac{d\sigma}{d\Omega}$	Barnard_aa.dat	EXFOR (A1269002)
[7]	^{3}He$(\alpha,\alpha)^{3}$He, $\frac{d\sigma}{d\Omega}$	Mohr_aa.dat	EXFOR (D0147002)
[9]	^{3}He$(\alpha,\alpha)^{3}$He, $\frac{d\sigma}{d\Omega}$	Tombrello_aa.dat	EXFOR (A1039002, A1039003)
[8]	^{3}He$(\alpha,\alpha)^{3}$He, $\frac{d\sigma}{d\Omega}$	Spiger_aa.dat	EXFOR (A1094006)
[8]	^{3}He$(\alpha,p_0)^{6}$Li, $\frac{d\sigma}{d\Omega}$	Spiger_ap0.dat	EDA private communication
[6]	^{6}Li$(p,p)^{6}$Li, $\frac{d\sigma}{d\Omega}$	McCray_pp.dat	EXFOR (A1410002)
[4]	^{6}Li$(p,p)^{6}$Li, $\frac{d\sigma}{d\Omega}$	Fasoli_pp.dat	EXFOR (D0135002, D0135003)
[5]	^{6}Li$(p,p)^{6}$Li, $\frac{d\sigma}{d\Omega}$	Harrison_pp.dat	EXFOR (F0018002)
[3]	^{6}Li$(p,\alpha)^{3}$He, $\frac{d\sigma}{d\Omega}$	Elwyn_pa.dat	EXFOR (F0012002), (F0012003)
[2]	^{6}Li$(p,\alpha)^{3}$He, $\frac{d\sigma}{d\Omega}$	Lin_pa.dat	EXFOR (A1539002)

Table 4: Details of the systematic uncertainties of the reference data. Systematic uncertainties are treated based on the experimental measurement type. When excitation functions are measured, each angle is given its own independent systematic uncertainty. When data are measured at different angles simultaneously, the data at each energy are allowed to vary with an independent normalization. * confirmed by responsible participant.

Ref.	data type	% syst. unc.	angular dist./excitation function
Barnard_aa [1]	^{3}He$(\alpha,\alpha)^3$He, $\frac{d\sigma}{d\Omega}$	5	excitation functions/same normalization
Mohr_aa [7]	^{3}He$(\alpha,\alpha)^3$He, $\frac{d\sigma}{d\Omega}$	?	angular distributions/separate normalizations
Tombrello_aa [9]	^{3}He$(\alpha,\alpha)^3$He, $\frac{d\sigma}{d\Omega}$	5	excitation functions/same normalization
Spiger_aa [8]	^{3}He$(\alpha,\alpha)^3$He, $\frac{d\sigma}{d\Omega}$	1.5	excitation functions/separate normalizations
Spiger_ap [8]	^{3}He$(\alpha,p_0)^6$Li, $\frac{d\sigma}{d\Omega}$	1.5	angular distributions/separate normalizations
McCray_pp [6]	^{6}Li$(p,p)^6$Li, $\frac{d\sigma}{d\Omega}$	5	excitation functions/separate normalizations
Fasoli_pp [4]	^{6}Li$(p,p)^6$Li, $\frac{d\sigma}{d\Omega}$	-	excitation functions/separate normalizations
Harrison_pp [5]	^{6}Li$(p,p)^6$Li, $\frac{d\sigma}{d\Omega}$	-	angular distributions/same normalization
Elwyn_pa [3]	^{6}Li$(p,\alpha)^3$He, $\frac{d\sigma}{d\Omega}$	9	angular distributions/normalization to excitation curve at 50 deg
Lin_pa [2]	^{6}Li$(p,\alpha)^3$He, $\frac{d\sigma}{d\Omega}$	10	angular distributions/separate normalizations

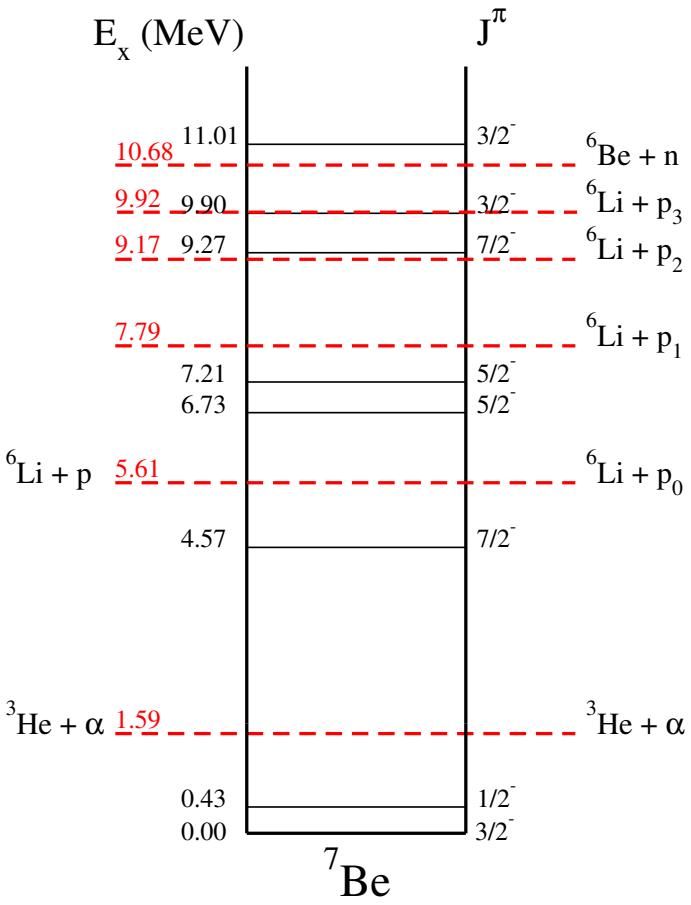

Figure 1: Level diagram of ^{7}Be. The low mass nucleus has only two bound states, the ground state and the level at $E_x = 0.429$ MeV.

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Annex 1

3rd Consultants' Meeting on

R-matrix Codes for Charged-particle Induced Reactions in the Resolved Resonance Region

IAEA, Vienna, Austria
28-30 June 2017 Meeting Room VIC A2311

PROVISIONAL AGENDA

Wednesday, 28 June

08:30 – 09:00 **Registration (IAEA Registration Desk, Gate 1)**

09:00 – 09:30 **Opening Session**
Welcoming address
Administrative matters
Election of Chairman and Rapporteur
Adoption of the Agenda

09:30 – 18:00 **Presentations by participants**
I. Thompson, LLNL
R. DeBoer, Notre-Dame U.
S. Kunieda, JAEA
M. Pigni, ORNL
Z. Chen, Tsinghua Univ.
M. Paris (remote connection) *Coffee break(s) as needed*

(13:00 – 14:00 Lunch break)

19:00 Dinner at a local restaurant (see separate information in folder)

Thursday, 29 June

09:00 – 18:00 **Round Table Discussion**

Results of test case: ^{7}Be

- Resonance parameters and uncertainties
- Cross section fits and uncertainties
- Ferdinand code
- Conclusions

Review of other previous action items (from meetingS 1 and 2)

What next? *Coffee break(s) as needed*

(13:00 – 14:00 Lunch break)

Friday, 30 June

09:00 – 12:30 **Round Table Discussion cont'd –**

Drafting of the Summary Report

Closing of the Meeting *Coffee break as needed*

IAEA
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Atoms for Peace

Consultants' Meeting on

R-Matrix Codes for Charged-Particle Reactions in the Resolved Resonance Region

5-7 December 2016
A24-11, IAEA Headquarters, Vienna, Austria

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Links to Participants' Presentations

#	Author	Title	Link
1	I.J. Thompson	R-matrix fitting of scattering in A=7 system	PDF
2	R.J. deBoer	Uncertainty estimation with AZURE	PDF
3	Z. Chen	Summary report on the evaluation of ^{7}Be system	PDF
4	S. Kunieda	IAEA Test Analysis for the ^{7}Be* system with the AMUR Code	PDF
5	M.T. Pigni	Applications of the R-Matrix SAMMY Code for Induced Charged-particle Reactions for the ^{7}Be Compound System	PDF
6	M. Paris	LANL-EDA5 Analysis of the ^{7}Be System	PDF

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