INDEN-LE Online Meeting on Evaluation of ^{7}Be system

13-16 Feb 2023, 15:00-18:00 CET, WEBEX

Monday, 13 Feb 2023:

Chairs: Helmut Leeb, Ian Thompson
Rapporteurs: James deBoer, Vivian Dimitriou, Marco Pigni

Present: Goran Arbanas, Zhenpeng Chen, James deber, Vivian Dimitriou, Gerry Hale, Satoshi Kunieda, Helmut Leeb, Jie Liu, Mark Paris, Marco Pigni, Thomas Srdinko, Ye Tao, Pierre Tamagno, Ian Thompson

1. Introduction, Vivian Dimitriou

The evaluation of 7Be system was first introduced as test case for the INDEN-LE group at the INDEN-LE 2018 meeting (INDC(NDS)-0726). After having tested the R-matrix algorithms and the fitting and minimization methods adopted in the different R-matrix codes in exercises Test 1 and 2, the purpose of this final exercise Test3 was to compare the evaluation methods adopted by the different evaluators. An important part of this exercise was to determine an experimental database of thoroughly assessed and certified experimental data to be used in the R-matrix analysis.

Since 2018, two new evaluations of 7Be have been submitted: by Zhenpeng Chen using RAC at the 2019 INDEN-LE meeting (details are given in INDC(NDS)-0791) and by Ian Thompson (submitted to CSEWG Nov. 2022 meeting).

As more evaluations are completed and presented for discussion, the following questions need to be addressed:

i. Is the sole purpose of performing Test 3 the submission of an evaluation to CSEWG for consideration in the next ENDF/B-VIII.1 release?
ii. How do we determine a joint evaluation?
iii. Is the file that is to be submitted to CSEWG going to be an individual evaluation or a joint evaluation?

2. Evaluation of 7Be submitted to CSEWG 2022, Ian Thompson

The evaluation of 7Be submitted to CSEWG (2022) was up to 11.5 MeV excitation energy. It should be considered as a preliminary evaluation that needs to be extended to much higher energies (up to 20 MeV projectile energy in the lab instead of the 3 MeV currently) and resubmitted by May 2023.

In this evaluation, the sequence of particles in the incident channel has been kept identical to the EXFOR ordering: light particle on heavier or equal. This approach should be followed in all evaluations.

In the process of the evaluation, errors were found in the EXFOR data files for Elwyn's higher energy angular distributions. The EXFOR compilers were notified and EXFOR is expected to be corrected accordingly. Need to follow up with EXFOR compilers.

Discrepancies are observed between Elwyn and Lin $^{6}Li(p, ^{3}He)^{4}He$ data.

Scaling/normalization factors for the different experimental data sets are an important result of the evaluation. Where can they be stored in the ENDF-6 file?

The evaluation tends to show discrepancies with increasing energies, it is therefore essential that the R-matrix fit is extended to higher energies including all the available data in those energies to get a better fit.

Ian plans to use his evaluated R-matrix parameters to reproduce the cross sections and compare with the original EXFOR data. In such a case, it would be useful to compare the evaluated data with both the original and normalized data.

Comment from Helmut: you used different normalizations for excitation functions at different angles (for the same measurement). In some cases, these differ significantly.

Ian: This has been discussed at previous meetings and it was agreed that it was reasonable to split the normalizations across energies or angles for angular distributions and excitation functions, respectively. This is justified by the experimental conditions such as efficiencies that vary with energy, etc.

Ian has developed a template for storing metadata useful for the evaluator. This template should be used by all the evaluators ideally.

Reaction data in inverse kinematics can be derived in principle from forward kinematics data and vice versa. If the experimental data do not agree, then that is most likely due to an issue with the data.

Discussion
Goran Arbanas: what about the uncertainties and covariances of the evaluated data? Are they small?

Ian Thompson: they have not been plotted but they are small. Charged-particle data in ENDF/B do not have any associated uncertainties.

3. Progress towards an evaluation of the 7Be system with AZURE2, James deBoer

Starting from Ian's compilation of EXFOR data, and using his tables of metadata, James went through the data and selected 13 out of the existing 50 to start his evaluation.

In the process he identified some outliers: Spiger and Tombrello data for …at … have very small systematic uncertainties of 1.5% which does not seem reasonable.

Also found inconsistencies in Jeronymo (p,alpha) angular distributions and Mohr's (p,p) angular distributions.

The decision to fit data as excitation functions or angular distributions depends on the conditions of the experiment, i.e. calibration, etc.

Apart from the chi2 minimization performed by AZURE2 using MINUIT, he also performed a MC uncertainty analysis using the MCMC package developed by D. Odell (BRICK) for AZURE2. He used this mainly to check the sensitivity of the fit to certain parameters.

The main difficulty in this evaluation is determine the level structure at excitation energies about 9 MeV, where our knowledge of levels, spins and parities, is incomplete.

Goran Arbanas: could the MCMC method be affecting the fitting procedure and inadvertently giving misleading results for the minimum and posterior values? This could happen for example if the number of MC samples is smaller than the number of data and can be solved by renormalizing the chi2 calculated by MCMC.

James deBoer: MCMC is used only to check the sensitivity of the fit to the parameter space. He uses MINUIT for the chi2 minimization.

4. Small progress in evaluation of 7Be system with AMUR, Satoshi Kunieda

Two more levels were added to the level scheme in AMUR.

Introduced single-channel distant poles, one for p elastic and one for 3He elastic, at 30 MeV.

Used the same normalization constants at all energies for angular distributions and at all angles for excitation functions.

Did not include inelastic channels or capture channels.

Ian Thompson: it would be interesting to see the resonance parameters that you obtained as a result of the fit. Could you send them to us? [Sec. note: Satoshi send the file with resonance parameters before Tuesday's session]

James deBoer: a simultaneous evaluation of elastic scattering and capture data in the case of 3He+4He has allowed for a complete analysis of the 3He,3He scattering data from very low energies up to the higher energies [which data??]. The analysis revealed interferences between the two channels. In this case, the capture channel was described as direct capture consisting of E1 multipoles mainly.

So far, LANL and Chen have used both capture and polarization data in their evaluations.

Tuesday, 14 Feb 2023:

1. Some notes on the adoption of RAC, Zhenpeng Chen and Jie Liu

For the presentation contents, please refer to the MS word document sent by Zhenpeng Chen (ZP) which was faithfully read by Jie Liu.

Questions and comments

Mark Paris: Mark think ZC raised serious points to be considered. The problem Mark is having is there is no systematic approach to determine cross-experiment data covariances or correlations as well as experimental covariances defining correlation between different energies. It seems to Mark (together with Gerry, Mark believes) that ZP is trading one set of unknowns for another. This is because ZP is not including cross-experiment and experiment correlations, RAC methodology is trying to include those in a different way. Due to the lack of information reported in the historical data, to generate experimental correlations may be difficult.

Vivian Dimitriou: ZP mentioned data are first normalized per energy as angular distributions, and then, per angle as an excitation function. So, are these the same datasets? Can be treated both as angular distribution and excitation function? Ian Thompson is not sure because the normalized data sometime are not uniformly normalized.

2. LANL evaluation of 7Be, Gerry Hale

Slide 2: reminder of chi-squared expression used in EDA that, Gerry thinks, refers to the approximate chi-squared expression in RAC. Although EDA expression is what most people are using, it is slightly different in the chi-squared definition because the normalization factors are applied to the theoretical calculations rather than to the experimental data. Algebraically, it is the same thing, but mathematically it is convenient because the normalization appears only in the numerator, and it makes it easier to handle. In fact, one can calculate the first and second derivatives with respect to the normalization factor analytically in a straightforward manner. The scaling factor S shown in the slide is usually one but there is the option to allow for a value different from one because of the quoted experimental work. Taylor's series expansion shown on the slide gives the minimum value of the chi-squared plus a quadratic term showing the deviation of the chi-squared. As you move towards their solution values, the second term goes to zero because the gradient of chi-squared with respect to the parameters goes to zero. This is checked numerically. This is to make sure the gradient is very small, and it leaves only the quadratic third term (second derivative of the chi-squared with respect to the parameters, namely G in the equation). The first derivative is computed analytically, and the second derivatives are built up out of rank one variable metric algorithm mentioned at the bottom of the slide. This algorithm is simple to generate. As the second derivative is defined, it is an exact algorithm in the approximation that chi-squared function is quadratic. This worked with every problem we have tried except for cases when you are away from the solution region for which it is possible higher order terms of the Taylor's series are needed.

Slide 3--21: 7Be system is not the highest priority at LANL. More focus has been given to 16O and 7Li. However, the extension of 7Be system to higher energies has similarities to the extension of 7Li because the same levels are involved. They are just in different positions relative to the thresholds of the various channels which, of course, causes differences in the cross sections.

Discussion on the table shown on slide 3. Energies are in laboratory system.

Discussion of the plotted measured and calculated data 4-21. The results are plotted including normalization factor when applied. The fit included analyzing power data that change shape quite dramatically. This is a different kind of information, and it is helpful to have these data together with the cross-section data as a confirmation the two types of data are compatible with the same parameters.

Slide 23: The slide shows the 6li(p,a)3He integrated cross section in both lin-lin and log-log scale. As many other evaluations, the peak at between 1.7 and 2 MeV is well described. However, it is not clear why the pronounced valley visible at 2.8 MeV. Gerry is not sure, but this shape can be linked to some interference effect from levels above 3 MeV. This has been a feature of LANL evaluation for a while. By extending the evaluation at higher energies, the nature of that effect may become clearer.

Slide 24: integrated capture cross sections. Cluster of points from Singh measured at a single energy. This maybe because Singh used different target thicknesses. The upper point of Singh measured data overlaps with Osborne measurement.

Summary and Conclusions: Gerry emphasized the prescription used in EDA for the photon channels is based on R.G. Newton's semiclassical treatment (no reference given): In Newton's description the electric multipoles are a combination of multipoles. Since EDA adopted Newton formalism, EDA parameters are not comparable to other data sets. The only thing comparable could be what Lane and Thomas call the "Capital Gamma" for the photon channels since this is more closely related to the experiments.

James DeBoer: Comment on alpha gamma reactions. There are many nice measurements performed in the last twenty years. A big success for the astrophysics community. They have all very consistent evaluations and uncertainty coming out in 3% or 4%.

Ian Thompson: Did you include background terms? Yes, for all Jpi. Sometimes there are both positive and negative background terms with large width. Discussion on testing Satoshi's approach with separate background poles for each channel.
Is the treatment of the gamma channel from Newton equivalent to have current operators? No. With that theory Newton describes only electric and magnetic fields. However, the connection that we make to quantum mechanics is that we define the electric field directly proportional to the vector potential and the vector potential is a kind of wave function (this is what is done in field theory). Ian, so you are still using the Siegert's theorem to transform the current operator into special operators.

James DeBoer: did you (Gerry) show a level diagram? The level structure presented in this energy region is known except for the background levels. There is nothing new we are doing from the standpoint. In other words, we have not found any new levels.

Marco Pigni: How many iterations to reach convergence? It depends on how close your starting values are to the minimum but usually it takes hundreds up to a few thousands of iterations.

Vivian Dimitriou: Are all you measured data taken from EXFOR? I do not know; we must make sure of it with James. Gerry thinks that once LANL sent all data they were using.

Pierre Tamagno: what is impact of polarization data. In regions where the level structure is not well known, it is important to include this kind of information because polarization data are different as the give a linear combination of scattered amplitudes from the cross sections. Especially where one does not know the level structure this data are extremely useful. Since in this case we know the level structure, this serves as confirmation.

Wednesday, 15 February 2023:

1. Measurements of ^{3}He(α,γ) at higher energies, Tamás Szücs

Using the activation technique to measure the total capture cross section.

An up bend in the S-factor has been observed by the ERNA experiment for the first time. The first experimental study at ATOMKI was performed in about 2011 to investigate this. It confirmed the trend.

Measuring to higher energies is challenging because of new background sources and the amount of power deposition.

The solution to this was to use a gas target cell with two windows. A leak can cause problems with the absolute normalization, and some different types of target configurations have been continually developed to improve the setup.

Note: An erratum has been published for the previous measurements that extend just above the proton separation energy. The data need to be scaled down by a factor.

A detailed uncertainty estimation is performed. Gamma peak is clearly visible, and counting is done at various different times.

Background sources: ^{54}Fe(α,2n), ^{129}Xe(α,2n), ^{128}Xe(α,n) at very nearby gamma energies, but they can be resolved with the high resolution HPGe.

Third cell configuration is even more leak tight. Pressure increases observed from beam heating and cell foil de-gassing.

Different thickness catcher foils are used at higher energies. As thin as possible to reduce background, but thick enough to stop the ^{7}Be recoils for the counting.

Target thickness is determined from the ideal gas law.

Entrance and exit foils can bend, changing the volume. This has been investigated using laser measurements, which resulted in an uncertainty of 1 mm in the cell length. The cell length is 43 mm, so this leads to about a 2% uncertainty.

The new data shows a broad structure at high energies. Hard to tell if it is resonant or direct.

General discussion

There is concern about the large normalization factors that are needed for several data sets in the ^{7}Be system.

Marco Pigni: Can the processing codes handle resonance parameter files for charged-particles and can we use the b=-l boundary condition? The problem can be solved by setting the boundary condition equal to the calculated shift parameter for a single resonance.

Ian Thompson recommends that we use Legendre expansions for the reconstructed cross sections and do not include "non R-matrix" background terms.

It is recommended to always use the light particle as the projectile.

Should we submit an ^{6}Li+p evaluation?

Ian Thompson proposes to TRY going up to 20 MeV projectile energy. If the fit looks reasonable, we should submit it to CSEWG. SEQUENTIAL break up channels will be introduced at energies above the break-up threshold. The ^{6}Li+p is of secondary priority, however.

The INDEN-LE evaluations are performed for different applications and are not meant exclusively for ENDF/B 8.1.

LANL will try to work on a charge invariant calculation based on their ^{7}Li system fit. However, they can't commit to the ^{3}He+α evaluation until at least the fall of 2023.

It was agreed that evaluators who have completed an evaluation to higher energies should submit their resonance parameter files to Ian Thompson, who will transform the files using Ferdinand for redistribution among the group. Evaluators should also submit their normalization factors.

Deadline for sending files: 28 February 2023.

LANL will add new LOW ENERGY data to their current low energy fit.

Are damping widths and imaginary channel radii going to be allowed for fits?

These are likely not an option in ENDF, so they are not encouraged.

Riech-Moore eliminated channels are allowed, with only one eliminated channel per spin group.

To answer the questions that were asked at the beginning of the meeting, the main objective of Test 3 is to arrive at an improved evaluation of the 7Be system over an extended energy region through in-depth discussions, exchange of techniques and experiences within the INDEN-LE group.

The plan to submit an evaluation to CSEWG for consideration in ENDF/B-VIII.1 will undoubtedly intensify the efforts and lead to an improved evaluation in the relatively short time that is left till the submission deadline (May 2023). However, the INDEN-LE effort to obtain an evaluation of ^{7}Be to higher energies will continue beyond the ENDF/B-VIII.1 deadlines, as the problems of dealing with an increasing number of open channels and break-up effects within the R-matrix theory are still very much open for discussion and technical development. The ultimate output of the INDEN-LE collaboration on Test 3 could be more than one evaluated file that would be made available to the user community to process, validate, and possibly adopt in an evaluated library. The evaluated data could also be distributed in different formats (other than ENDF-6) depending on the needs of the users in different applications (i.e. R33 format for Ion Beam Analysis applications).

Tentative dates for next IAEA INDEN-LE meeting: 28-31 August 2023.

The meeting will be hybrid however, in person participation is favoured.