Light Elements R-matrix Analyses with the SAMMY Code towards the Foundation of Charged-particle Nuclear Data Libraries

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OUTLINE

- Newly developed SAMMY module for inverse channel transformation
- R-matrix analysis of ^{7}Be compound nucleus
- R-matrix analysis of ^{17}O compound nucleus
- Evaluated Nuclear Data File generation and processing with the AMPX code
- Future evaluation work and tests on light nuclei
- Conclusions

FORMALISM OF THE INVERSE CHANNEL TRANSFORMATION

SAMMY code[1] was designed to perform calculations for a fixed incident channel c[2]. However, its R-matrix solver can be conveniently used to include multiple incident channels by a simple transformation in the resonance parameters as well as in the Q-values for energetically possible outgoing channels c' such as inelastic and charged-particle emissions

For the ground state targets the Q-value is

$$Q_{cc'} = m_c + M_c - m_{c'} - M_{c'}\,, \tag{1}$$

where, by definition, $Q_{cc} = 0$ and $Q_{c'c} = -Q_{cc'}$. For outgoing channels in the target or residual nucleus, one has

$$q_c = Q_{cc'} + q_{c'}\,, \qquad q_{c'} = Q_{c'c} + q_c \text{ (inverse)}\,, \tag{2}$$

where $q_{c(c')}$ are obtained from the corresponding excited level thresholds $e_{c(c')}$. The relation between c and c' for resonance levels and reduced-width amplitudes (in the laboratory system) is

$$E_{c'} = (E_c/\mu_c + Q_{cc'})\ \mu_{c'} \qquad \text{and} \qquad \gamma_{c(c')} = \gamma_{c(c')}\sqrt{\mu_{c'}/\mu_c}\,, \tag{3}$$

where $\mu_c = (m_c + M_c)/M_c$ and $\mu_{c'} = (m_{c'} + M_{c'})/M_{c'}$ and the relation on the amplitudes can be derived from the R-matrix function as

$$R_{cc'} = \sum_\lambda \frac{\gamma_{c\lambda}\gamma_{c'\lambda}}{E_{\lambda c} - E_c}\delta_{JJ'} \quad (cc' \to c'c) \quad R_{c'c} = \sum_\lambda \frac{(\sqrt{\mu_{c'}/\mu_c}\gamma_{c\lambda})(\sqrt{\mu_{c'}/\mu_c}\gamma_{c'\lambda})}{E_{\lambda c'} - E_{c'}}\delta_{JJ'} \tag{4}$$

[1] Link to SAMMY repository: https://code.ornl.gov/RNSD/SAMMY

[2] For instance, neutron induced reactions on a stationary target nucleus.

^{7}Be COMPOUND NUCLEUS: THREE INCIDENT CHANNELS

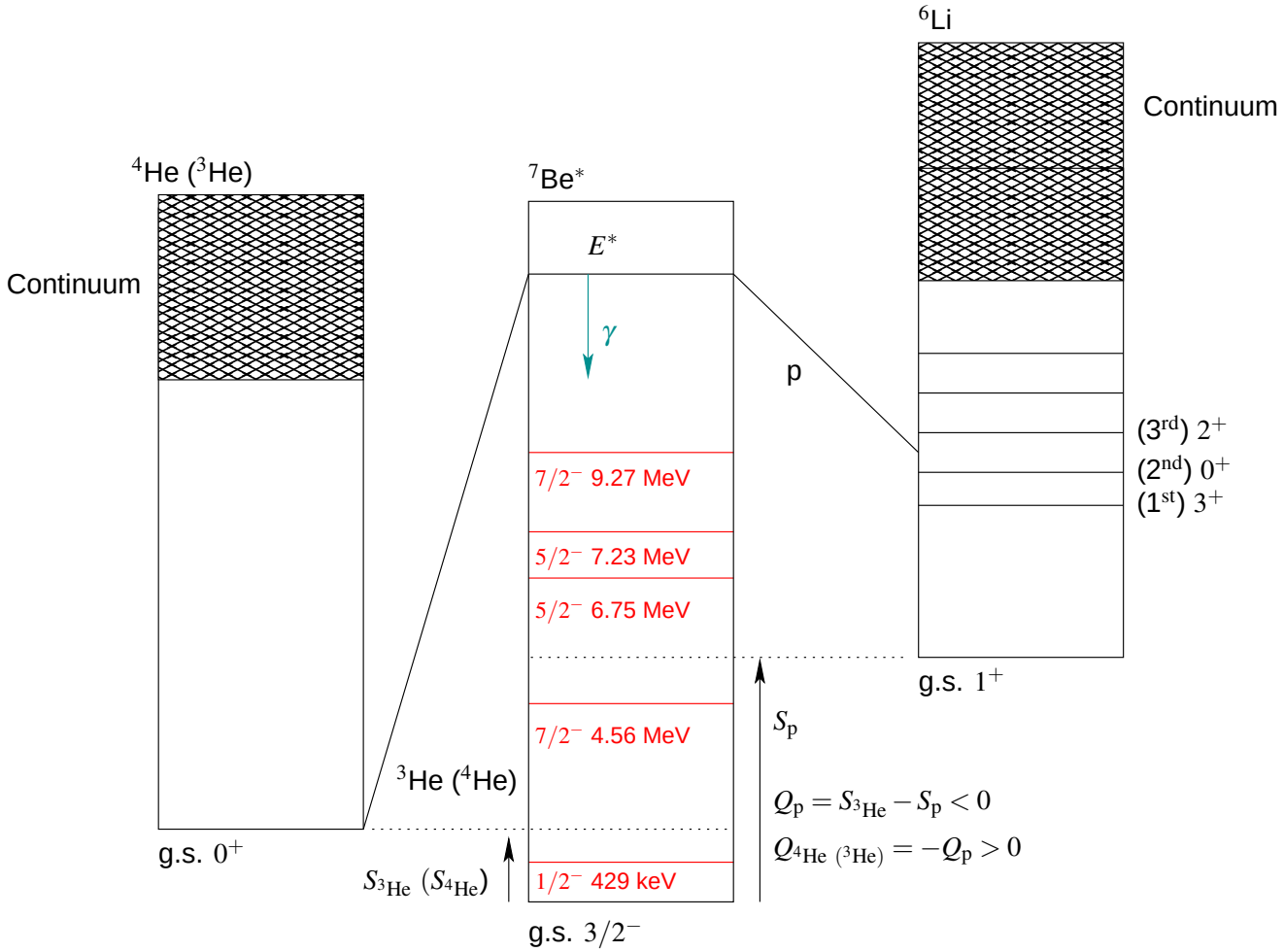


Figure 1: The level diagram of ^{7}Be compound nucleus formed by the reaction ^{3}He (projectile) + ^{4}He (target) or ^{4}He (projectile) + ^{3}He (target) from the left and by p (projectile) + ^{6}Li (target) from the right. The ^{7}Be excitation energies are plotted in red and the ^{3}He (^{4}He) and proton separation energies are shown by $B_{^3He\ (^4He)}$=1.59 MeV and B_p=5.61 MeV, respectively. All quantities are intended in center of mass frame.

INVERSE CHANNEL IMPLEMENTATION IN THE SAMMY CODE

The new SAMMY module developed to perform the inverse channel transformation $T_{cc' \to c'c}$ is called by the alphanumeric card, `NEW INCIDENT = name, Ma`, from the main input SAMMY file

Performed in the sections of `SAMMY.PAR`, $T_{cc' \to c'c}$ starts from the `PARTICLE PAIR DEFINITIONS` defining the complete set of particle-pair information (mass and charge values, spin and parity), Q-values, and penetrability factor and shift function types. Here, everything remains unchanged except for the Q-values accordingly transformed as in Eqs. (1)-(2)

The following section `SPIN GROUP` section with quantum numbers for each spin group linked to the corresponding particle-pairs defined in the `PARTICLE PAIR DEFINITIONS` is rearranged in the particle pair-definition[3] from "`a+13C 0`" incident channel to "`n+16O 0`" incident channel

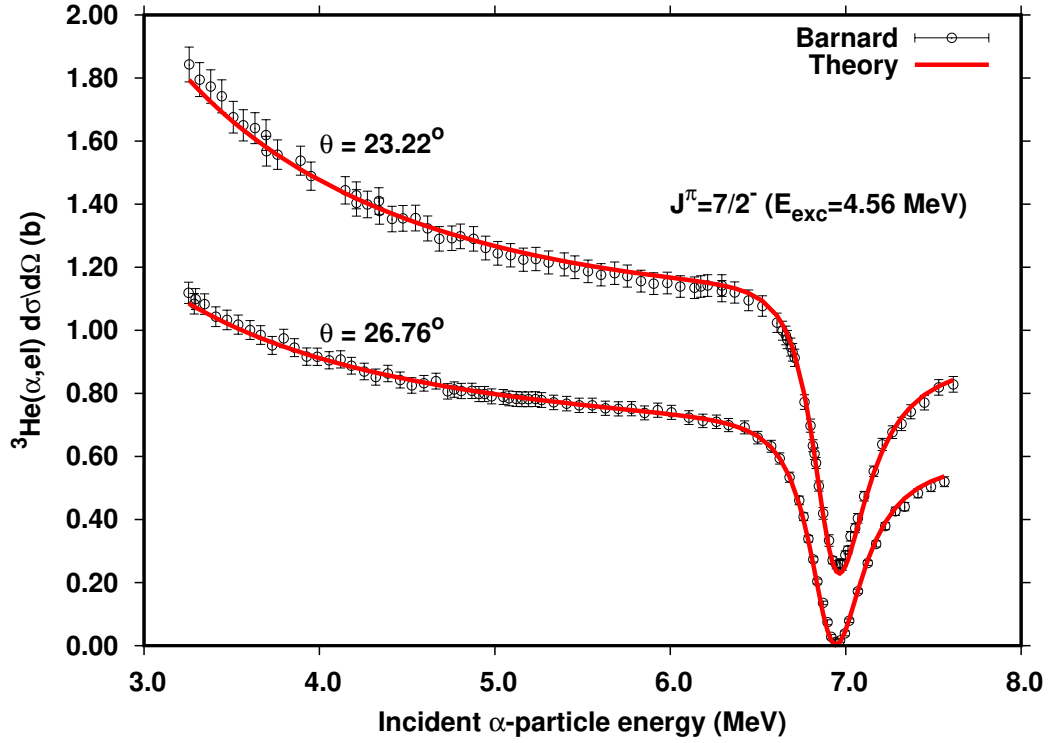
```
 1  1     1     -0.5          |  1  1     1     -0.5
    1  a+13C 0    0    -0.5   |     1  n+16O 0    1    +0.5
    2  n+16O 0    1    +0.5   |     2  a+13C 0    0    -0.5
```

In the section `RESONANCES` the simple parameter conversion of Eqs. 3–4 is performed and followed by the rearrangement of channel radii in the section `RADIUS PARAMETER`

[3] Subjected to change in the future.

^{7}Be COMPOUND NUCLEUS

Part of the verification study within IAEA INDEN light element meetings, the spectroscopic information of ^{7}Be compound nucleus system can be studied by the interaction of several particle pairs, for instance, p+^{6}Li, α+^{3}He, and ^{3}He+α. Here, we consider the p+^{6}Li and α+^{3}He being α-particle the incident particle



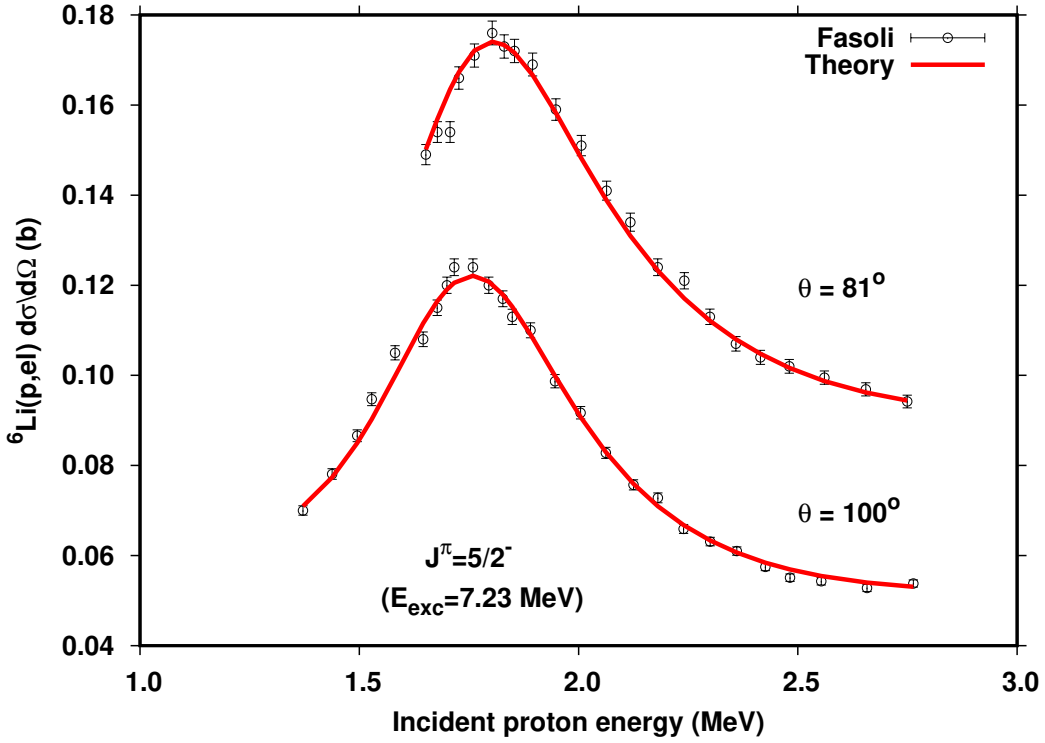
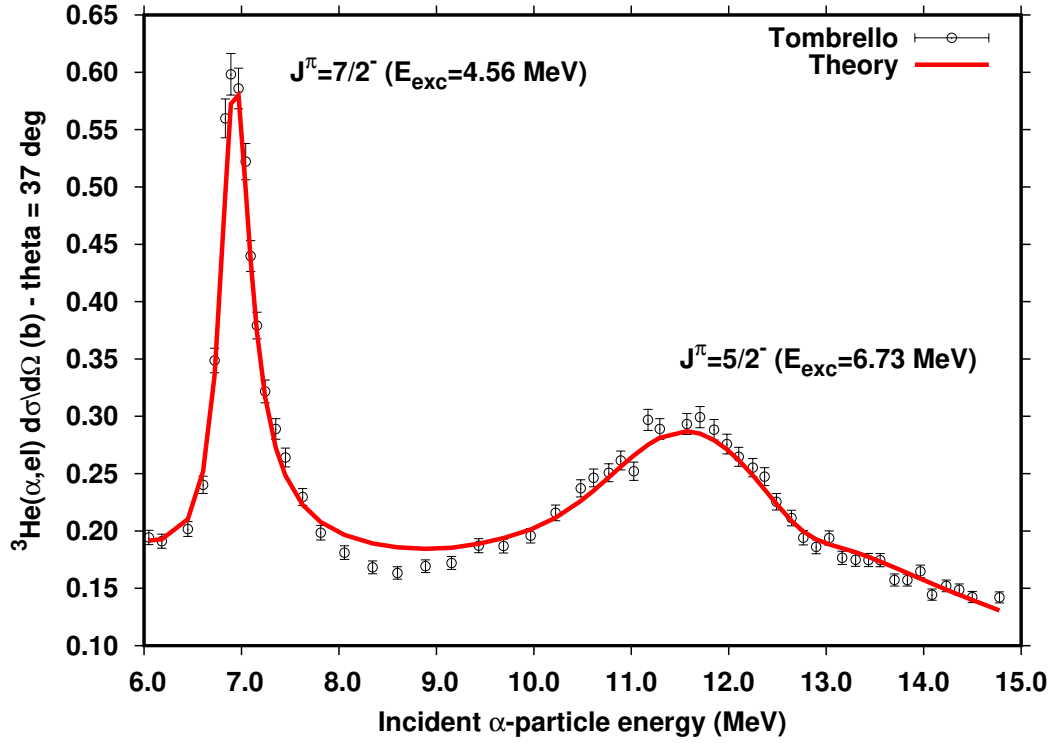


Figure 2: Results of excitation functions of ^{3}He(α, el) and ^{6}Li(p, el) calculated from the resonance parameter converted from the incident particle pair p+^{6}Li to α+^{3}He.

^{7}Be COMPOUND NUCLEUS (continued)

Part of the verification study within IAEA INDEN light element meetings, the spectroscopic information of ^{7}Be compound nucleus system can be studied by the interaction of several particle pairs, for instance, p+^{6}Li, α+^{3}He, and ^{3}He+α. Here, we consider the p+^{6}Li and α+^{3}He being α-particle the incident particle



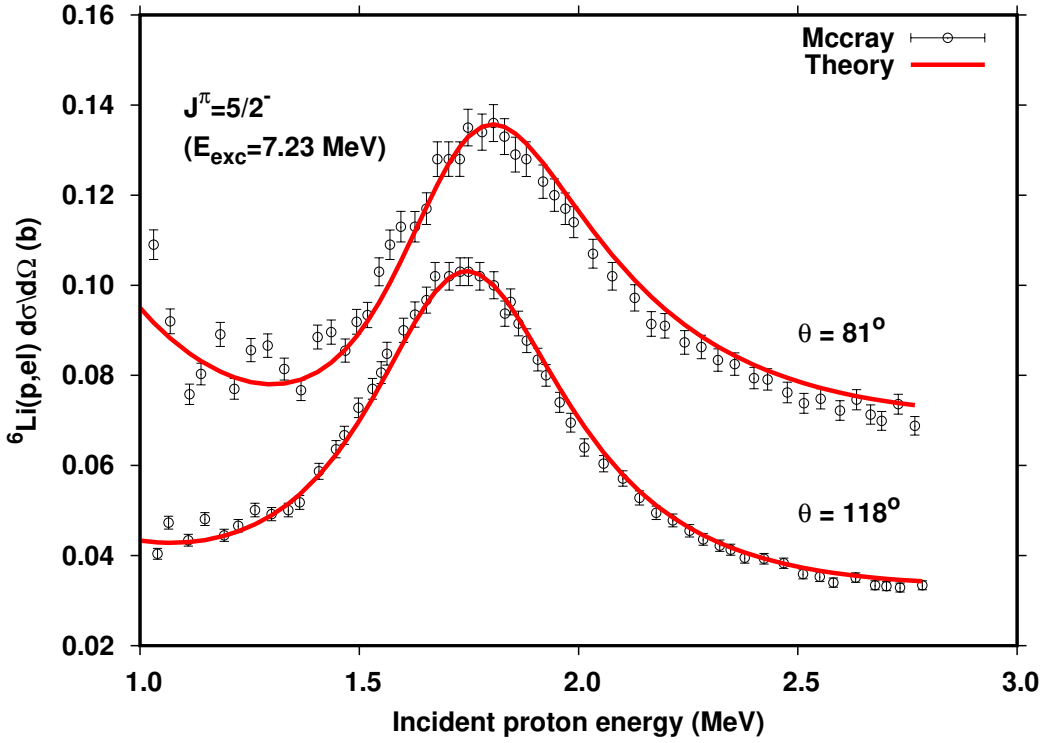
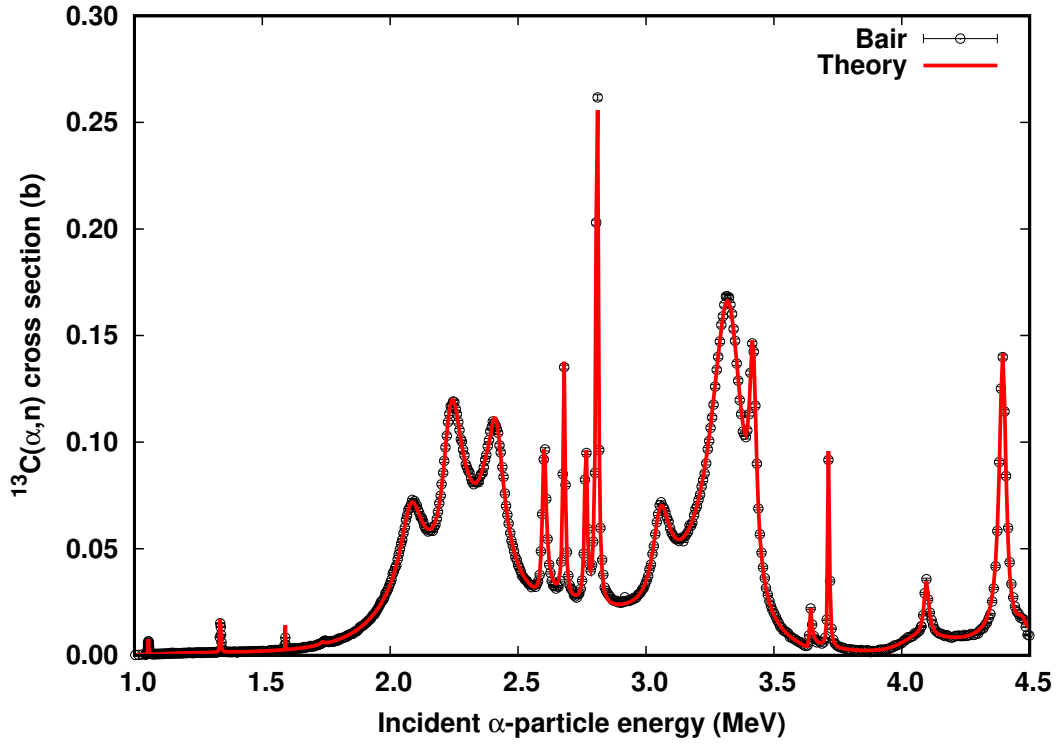


Figure 3: Results of excitation functions of ^{3}He(α, el) and ^{6}Li(p, el) calculated from the resonance parameter converted from the incident particle pair p+^{6}Li to α+^{3}He.

^{17}O COMPOUND NUCLEUS

Important for criticality applications n+^{16}O evaluation include α-particle emission for incident neutron energy $E > 2.35$ MeV. However, measured data are available for the inverse reaction α+^{13}C



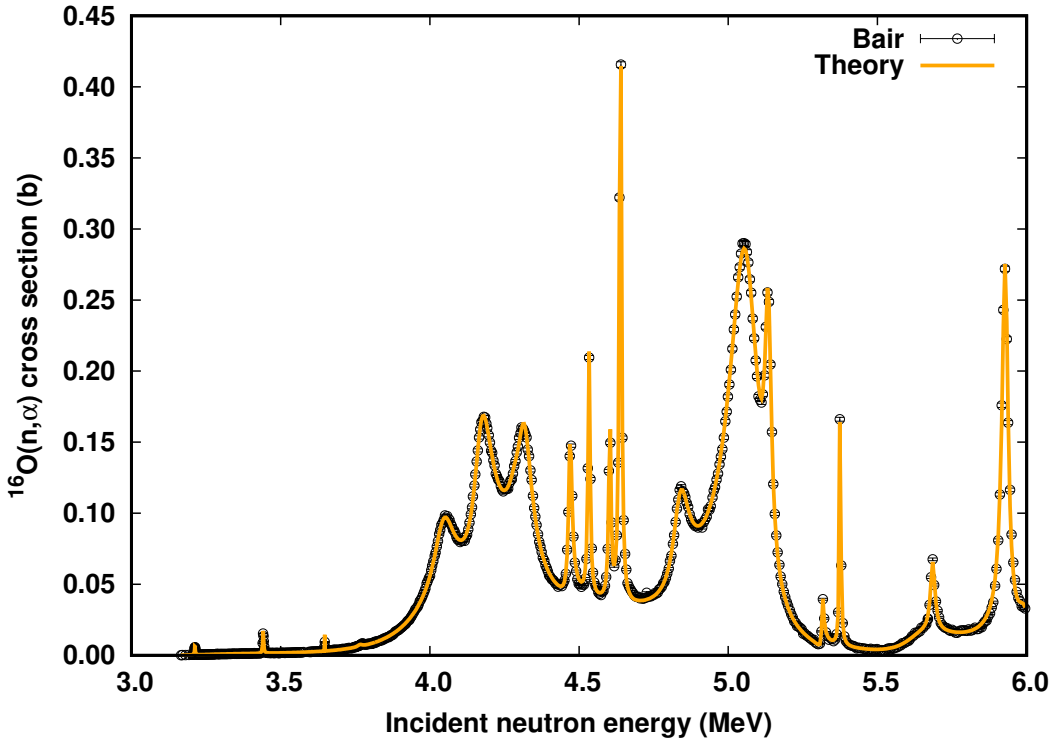


Figure 4: Results of the ^{13}C(α, n) cross sections calculated from the resonance parameter converted from the incident particle pair n+^{16}O to α+^{13}C (left). Results of the ^{16}O(n, α) cross sections compared to Bair's measured data converted from α-particle to neutron induced reactions (right). Incident energies are in the laboratory system.

EVALUATED NUCLEAR DATA FILE GENERATION

To fully test the development of R-matrix analysis of light nuclei within nuclear data libraries, the ENDF generation and related verification of the processing capabilities must be routinely performed.

For the ^{7}Be compound nucleus, three ENDFs can be generated from the same set of resonance parameters, i.e. (1) ^{4}He+^{3}He, (2) ^{4}He+^{3}He, (3) ^{1}H+^{6}Li.

Defining the structure of ENDFs for charged-particle evaluations

- File MF=2 and MF=32 can be reported as complementary information (not to be used)
- Legendre Polynomials can be reported in File 4 for the elastic scattering
  - However, File MF=34 should be defined but it is an open problem
- File MF=3 and MF=33 can be repeated for any reaction cross sections
- **Best solution is to report evaluated data in File MF=6 coupled to File MF=3**
  - However, some work is needed for the covariance information

Tests in processing resonance parameters, cross sections, and covariance information, for three ENDFs are currently in progress using the AMPX code

FUTURE EVALUATION WORK AND TESTS ON LIGHT NUCLEI

- R-matrix analysis of ^{7}Be compound nucleus (three incident channels)
  - Finalizing IAEA “Test2” and extension of the evaluation to 30 MeV
- R-matrix analysis of ^{9}Be compound nucleus for testing purposes
- R-matrix analysis of ^{17}O compound nucleus (two incident channels)
  - Including measured data for α+^{13}C and possible extension up to 8 MeV (neutron channel)
- Auxiliary tool for automatic generation of File MF=6 for outgoing particles couple to a File MF=3 distributions from resonance parameters (File MF=2) is needed
  - SAMMY has already the capability to generate Legendre Polynomials (File MF=4)
  - More discussion on covariance information generation, eventually from File MF=32 and/or MF=33, is needed
  - Preservation of File MF=2 and MF=32 after conversion to File MF=3 and MF=6 is recommended

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Thank you!