Theoretical calculations and analysis for n + ^{6}Li reaction

Xi Tao[a], Jimin Wang, Guochang Chen, and Qingbiao Shen

China Nuclear Data Center, China Institute of Atomic Energy, PO Box 275-41, Beijing 102413, China

Abstract. R-matrix theory is an important methodology for applications on light, medium and heavy mass nuclides nuclear reaction in the resonance energy range. Full R-matrix formalism contains the diagonal elements of the energy levels matrix and it is a rigorous theory. Because of different assumptions and approximations, many kinds of R-matrix derived methods are obtained. The new R-matrix code FDRR is presented and includes 4 kinds of R-matrix applications. It can be used for calculating integral cross sections and angular distributions of 2-bodies reactions. The cross sections and angular distributions of n+^{6}Li reaction are calculated and analyzed by FDRR code. The results are in good agreement with experimental data below 20 MeV.

1. Introduction

R-matrix theory is an important tool for applications on light, medium and heavy mass nuclides nuclear reaction in the resonance energy range. Statistical theory cannot describe the resonance. In 1947, the R-matrix theory was introduced by E.P. Wigner and L. Eisenbud [1]. In 1958, A.M. Lane and R.G. Thomas [2] published the paper named "R-Matrix Theory of Nuclear Reactions", and this paper is the classic work in R-matrix theory. Based on different assumptions, many R-matrix calculation methods have been developed, such as full R-matrix formalism, Multilevel Breit-Wigner R-matrix formalism, Adler-Adler R-matrix formalism, Eliminated channel R-matrix formalism, Reich-Moore R-matrix method, etc. Many nuclear data evaluations have been done by R-matrix methods. G.M. Hale [3], and R.E. Azuma [4], S. Kunieda [5], Chengjiu Zhu [6], Zhenpeng Chen [7], Qingbiao Shen [8] et al., did a lot of work on R-matrix theory and calculations. SAMMY, REFIT, CONRAD, EDA, AZURE, AMUR and RAC, etc, are R-matrix codes for theoretical calculations and nuclear data evaluations. EDA, AZURE, AMUR and RAC are used in light nuclides reactions.

Lithium is widely used in reactor design and analysis. Neutron inducing ^{6}Li can produce tritium, and the cross section of ^{6}Li(n,t) below 1.7 MeV is a standard cross section.

2. Introduction of FDRR code

FDRR is short for Full and Diagonal Reduced R-matrix. It is a new theoretical code, which is based on R-matrix theory and compiled by FORTRAN language. It is developed by the China Nuclear Data Center (CNDC) and Nankai University.

2.1. Formulas

The cross section can be calculated by the S-matrix elements as

$$S_{c'c} = e^{-i(\phi_{c'}+\phi_c)} W_{c'c} \qquad (1)$$

Where ϕ_c is the phase shift, F_c and G_c are the regular and irregular Coulomb wave functions

$$\phi_c = \arctan\left(\frac{F_c}{G_c}\right) \qquad (2)$$

$$W_{c'c} = \delta_{c'c} + 2i\, p_{c'}^{\frac{1}{2}} (\Sigma_{\lambda\mu}\gamma_{\lambda c'}\,\gamma_{\mu c}A_{\lambda\mu})\, p_c^{\frac{1}{2}} \qquad (3)$$

$$P_c(E) = \frac{\rho_c}{G_c^2 + F_c^2} \qquad (4)$$

P_c is the penetration factor, $\gamma_{\lambda c}$ is the reduced width of λ energy level and c reaction channel.

It is difficult to calculate the inverse matrix of R-matrix. $A_{\lambda\mu}$ energy matrix has been introduced to solve this problem. C is the inverse matrix of $A_{\lambda\mu}$

$$A_{\lambda\mu} = C_{\lambda\mu}^{-1} \qquad (5)$$

The inverse matrix of full R-matrix method is

$$C_{\lambda\mu} = (E_\lambda - E)\delta_{\lambda\mu} + \Delta_{\lambda\mu} - \frac{i}{2}\Gamma_{\lambda\mu} \qquad (6)$$

Diagonalizing the matrix, Breit-Wigner method is given as

$$C_{\lambda\mu} = \left(E_\lambda - E + \Delta_{\lambda\mu} - \frac{i}{2}\Gamma_{\lambda\mu}\right)\delta_{\lambda\mu} \qquad (7)$$

E_λ is the resonance energy level, $\Delta_{\lambda\mu}$ is the energy shift, $\Gamma_{\lambda\mu}$ is the resonance width.

If the capture cross section is considered, the matrix is written like

$$C_{\lambda\mu} = \left(E_\lambda - E - \frac{i}{2}\Gamma_{\lambda\gamma}\right)\delta_{\lambda\mu} + \Delta_{\lambda\mu} - \frac{i}{2}\Gamma_{\lambda\mu} \qquad (8)$$

[a] e-mail: `taoxixishi@ciae.ac.cn`

When R-matrix is used for evaluation, lots of experimental data is required. Reduced reaction channel is introduced to describe the channel, which lacks experimental data. Full reduced r-matrix method is

$$C_{\lambda\mu} = \left(E_\lambda - E + \Delta_{\lambda e} - \frac{i}{2}\Gamma_{\lambda e}\right)\delta_{\lambda\mu} + \Delta_{\lambda\mu} - \frac{i}{2}\Gamma_{\lambda\mu}$$

(9)

$\Delta_{\lambda e}$ is the energy shift of reduced channel, $\Gamma_{\lambda e}$ is the resonance width of reduced channel.

The width of reserved channel and the energy shift of reduced channel are assumed no contribution. Diagonal energy shift reduced R-matrix method is obtained

$$C_{\lambda\mu} = \left(E_\lambda - E - \frac{i}{2}\Gamma_{\lambda e}\right)\delta_{\lambda\mu} + \Delta_{\lambda\mu}$$

(10)

The contribution of the energy shift to the non-diagonal element is zero, diagonal energy shift reduced R-matrix method is

$$C_{\lambda\mu} = \left(E_\lambda - E + \Delta_\lambda - \frac{i}{2}\Gamma_{\lambda e}\right)\delta_{\lambda\mu}$$

(11)

The capture reaction is defined as the reduced channel, and is called the Reich-Moore method given as

$$C_{\lambda\mu} = \left(E_\lambda - E - \frac{i}{2}\Gamma_{\lambda e}\right)\delta_{\lambda\mu}.$$

(12)

2.2. Functions

Based on Eqs. ((6), (7), (10), (11)), four R-matrix applications are compiled in FDRR code. They are MLBW and reduced R-matrix method, diagonal energy shift reduced R-matrix method, full R-matrix method, and un-diagonal energy shift reduced R-matrix method.

There are two input files for FDRR code. FDRRi.dat contains the adjusted parameters, including resonance energy levels, reduced resonance widths, channel radius, and boundary conditions. Nuclear structure parameters and experimental data are put into the FDRRk.dat file.

FDRR code can be used for calculating cross sections, angular distributions, and polarization Data of 2-bodys reactions. Reaction channels can be defined by the user.

3. Calculation and analysis of n+6Li reaction

3.1. Analysis of reaction channels

The process of n+6Li reaction is very complicated. Considering the same residual nucleus, the reaction channels are simplified as

$$n + {}^6\text{Li} \rightarrow {}^7\text{Li}^* \begin{cases} \gamma + {}^7\text{Li} \\ n + {}^6\text{Li} \\ p + {}^6\text{He} \\ 2n + {}^5\text{Li} \\ t + \alpha \\ n + d + \alpha \end{cases}$$

3.2. Calculation results of n+6Li

Assuming that the energy levels are not related, MLBW and reduced R-matrix method is used for calculating n+6Li reaction below 20 MeV.
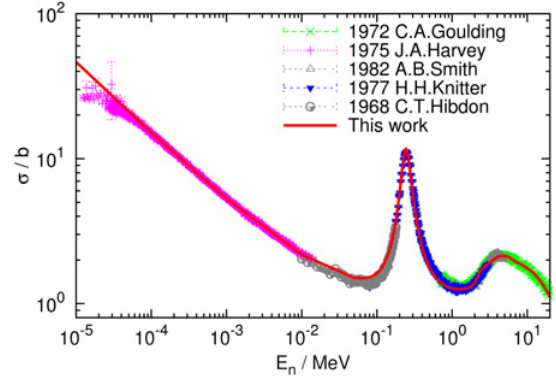

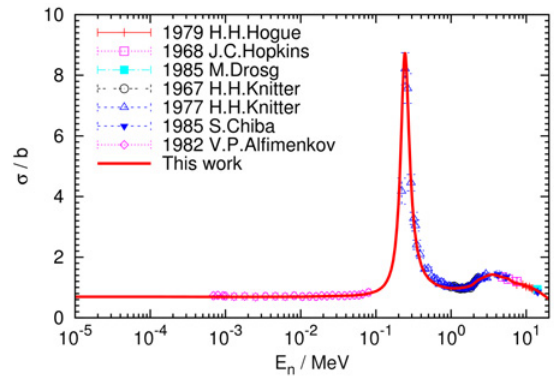**Figure 1.** Total cross section of n+6Li reaction.

Figure 2. Elastic scattering cross section of n+6Li reaction.
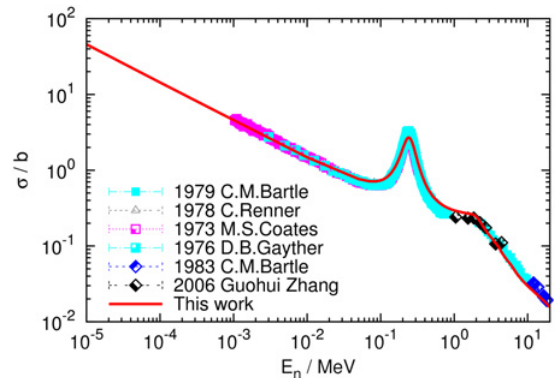

Figure 3. The cross section of 6Li(n,t) reaction.

Figure 1 shows that the total cross section of n+6Li compared with the experimental data [9–13]. The calculation result is in good agreement with the experimental data from 10 eV to 20 MeV.

Below 0.1 MeV, the calculation of hard sphere scattering agrees with the measure of V. P. Alfimentkov [19]. The result of the resonance peak is also in good agreement with the experimental data [12, 14–19] in Fig. 2.

The shape of 6Li(n,t) cross section is almost the same with the experimental data [20–25]. The peak of the calculation is not very good, and need to be improved.

Figure 4 is the inelastic scattering result of the first excited state. The theoretical calculation is a little higher than experiment data [11, 26–29]. The threshold of 6Li(n,nd) is lower than the first excited energy level, the first excited state is unstable. The accuracy of measurement is not high. The result of the second excited state is shown
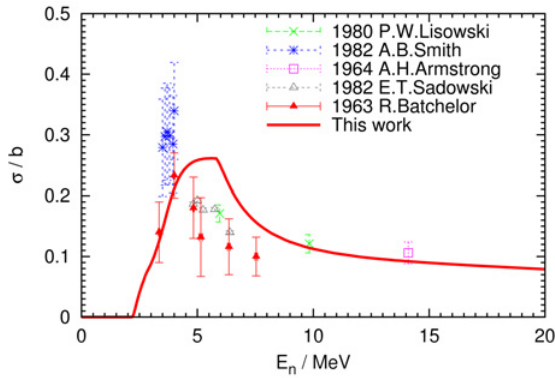
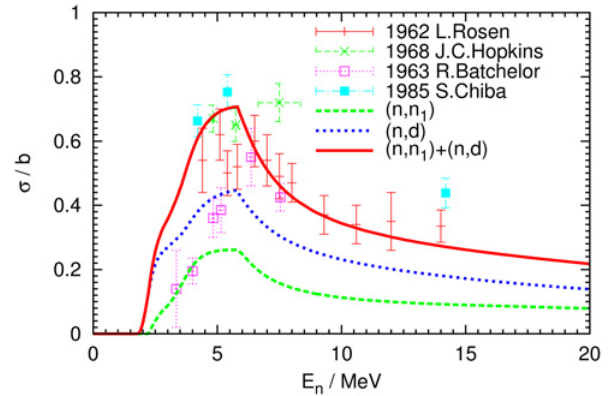**Figure 4.** The cross section of ^{6}Li(n,n$_1$) reaction.

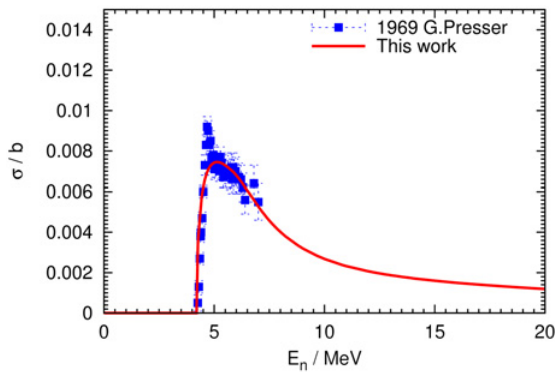**Figure 5.** The cross section of ^{6}Li(n,n$_2$) reaction.

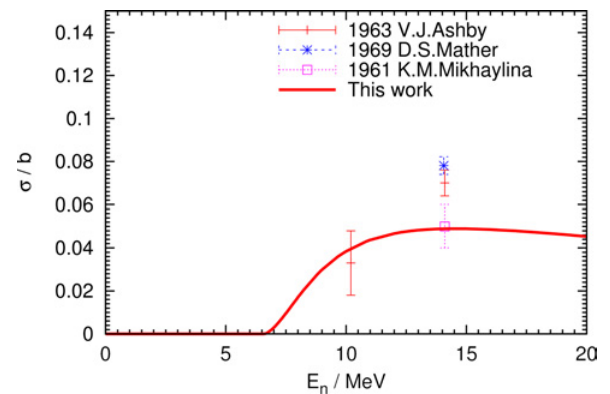**Figure 6.** The cross section of ^{6}Li(n,p) reaction.

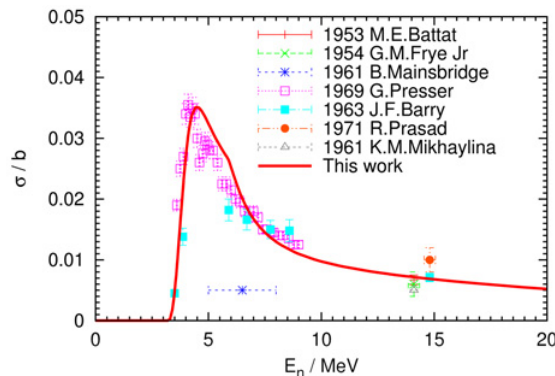**Figure 7.** The cross section of ^{6}Li(n,d) reaction.

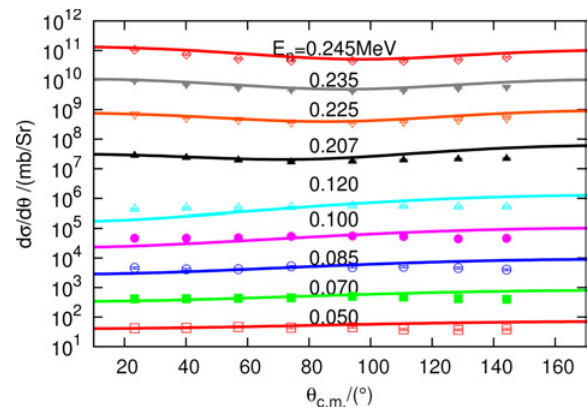**Figure 8.** The cross section of ^{6}Li(n,2n) reaction.

Figure 9. The elastic scattering angular distribution.

in Fig. 5, which is in good agreement with experimental data [30].

The calculated result of ^{6}Li(n,p) cross section is compared with the experimental data [30–36] in Fig. 6.

Because the first excited state is unstable, the experimental data of (n,d) cross section should be the sum of ^{6}Li(n,n1) and ^{6}Li(n,d) cross sections. In Fig. 7, the red curve is the sum of ^{6}Li(n,n1) and ^{6}Li(n,d) cross sections, the theoretical results are in good agreement with the experimental data [15,18,37,38].

A fake channel of ^{6}Li(n,(2n))^{5}Li is defined to take place ^{6}Li(n,2n)^{5}Li channel. The calculated result shown in Fig. 8 is in agreement with the experimental data [36,39,40].

The calculated results of elastic scattering angular distributions are compared and in good agreement with the experimental data [41], which are shown in Fig. 9. The results are offset by factors of 10.

The theoretical results of ^{6}Li(n,t) angular distributions are compared with the experimental data [42] in Fig. 10. The calculations are consistent with the experimental data. The curve lines and points are offset by factors of 10.

3.3. Preliminary result of full R-matrix

Because of the MLBW and reduced R-matrix method only considered the diagonal matrix elements, the peak of ^{6}Li(n,t) cross section is not very good. The subroutine of Full R-matrix method is developed and used for n+^{6}Li reaction, and a preliminary result of n+^{6}Li is obtained in the resonance range. Spin and parity conservations are considered in FDRR code. Shown in Fig. 11, the height and shape of the first resonance peak are better than the result of MLBW method. The spins of neutron and lithium-6 are coupled, and the resonance energy level can be in the states
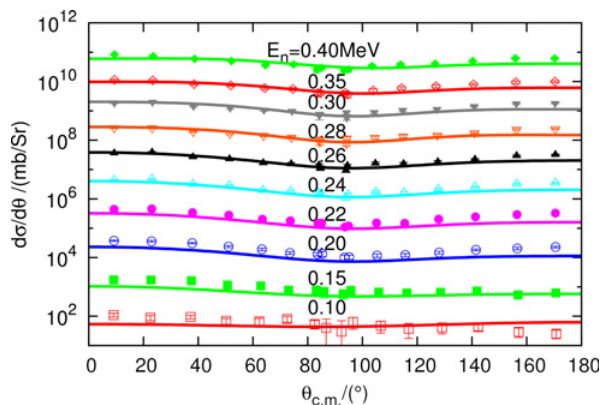
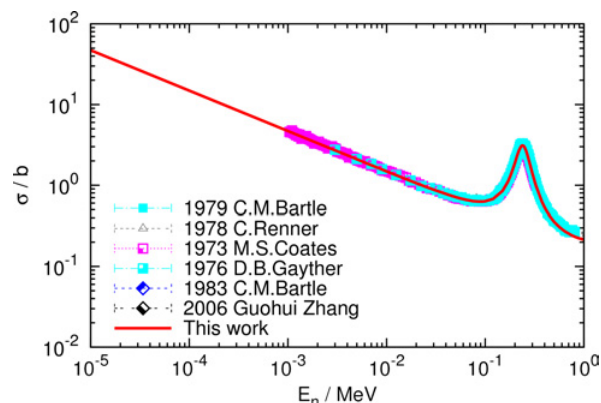**Figure 10.** The angular distribution of ^{6}Li(n,t) reaction.

Figure 11. The full R-matrix result of ^{6}Li(n,t) reaction.

of S=1/2 and S=3/2. Now in FDRR code, the resonance widths of the two states set to the same parameters.

4. Summary and conclusions

FDRR is developed for obtaining light nuclei cross sections and angular distributions. MLBW + reduced R-matrix method is used for analyzing n+^{6}Li reaction below 20 MeV. Full matrix method is still under development. Preliminary result shows that full R-matrix method can improve the calculation results. In future, we will give different reduced resonance width for each state to further improve the calculation results. FDRR will be combined with LUNF [43] code and used for evaluations and updating CENDL.

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