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R-MATRIX ANALYSIS OF THE ^7Li SYSTEM*

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ABSTRACT

We describe a multichannel, multilevel, R-matrix analysis of reactions in the ^7Li system which was used to provide the ENDF/B-V neutron cross sections for ^6Li at low energies. Resonance parameters obtained from the R-matrix levels are presented. Various features of the data are interpreted in terms of these resonances.

(^7Li System; $^6\text{Li}(n,t)$; R-Matrix; resonance parameters; standard)

Introduction

Discrepant measurements is a problem one almost always faces in the evaluation of neutron cross sections, but in the case of a standard cross section, the problem intensifies the difficulty of obtaining evaluated cross-section values of the desired accuracy. However, one knows from general considerations of nuclear reaction theory that the standard cross section is linked by unitarity to data for other reactions in the same compound system, and thus one has the prospect of reducing the uncertainty of the evaluated standard cross section by analyzing it simultaneously with these other data in a unitary framework. R-matrix theory¹ is a particularly appropriate unitary framework for such analyses, as was discussed in Ref. 2.

We have used multichannel, multilevel R-matrix analyses of reactions in the ^7Li system to provide evaluated cross sections for the neutron-induced reactions on ^6Li at low energies for versions IV and V of the Evaluated Nuclear Data File (ENDF/B). At the time of the version IV analysis,^{2,3} the data set dominating the fit was the neutron total cross section measurement from Harwell,⁴ both because of its quoted precision and number of points. The resulting $^6\text{Li}(n,t)$ cross section (the "standard" in this system) was not much different from that obtained in Version III, which has been largely based on the Harwell measurement.

The value of the calculated $^6\text{Li}(n,t)$ cross section at the peak of the 240 keV resonance was 3.5 b, some 16% higher than the value indicated by a contemporary group of direct measurements.⁵⁻⁷ However, we noticed, as had the Harwell group, that unitary constraints forced the total section unacceptably high above Dimont's measurements in the peak when the (n,t) cross section was lowered to better agree with the direct measurements. It is emphasized that this discrepancy between the cross section measurements was indicated by attempts to fit them unitarily. The common practice of evaluating the total and (n,t) cross sections separately, then obtaining the elastic cross section by subtraction, would not necessarily have signaled a problem.

We noticed in performing the Version IV analysis that in addition to this strong unitary link to the total cross section in the region of the resonance, the (n,t) cross section was also quite sensitive to the differential cross section for $t + \alpha$ elastic scattering. At that time, however, measurements of this cross section⁸ had not been made with accuracy comparable to that of the Harwell total cross section measurements. Precise measurements of the $t + \alpha$ differential cross section⁹ were later made at Los Alamos, and these were incorporated in the analysis, along with new measurements of the total cross section from Oak Ridge.¹⁰ Preliminary results of this analysis, reported at the Confer-

ence on Nuclear Cross Sections and Technology² two years ago, indicated the effect of the new data was to lower the calculated (n,t) cross section in the peak of the resonance (to 3.4 b) and raise the calculated peak total cross section (to 11.1 b). This trend has continued in subsequent analyses, including that used recently to provide ENDF/B-V neutron cross sections for ^6Li at energies below 2 MeV.

The Version V analysis will be described briefly in the following section, indicating the types of data included, and the fits obtained to representative data sets from each reaction. The third section presents resonance parameters corresponding to R-matrix levels required for the fit, and the concluding section discusses the interpretation of specific features in the data for reactions in the ^7Li system in terms of these resonances.

Version V Analysis

The 3 arrangement channels considered in this analysis were $t + ^4\text{He}$, $n + ^6\text{Li}$, and $n + ^6\text{Li}^*$ (2.18). Various quantities specifying the channel configuration are given in Table I.

TABLE I
Channel Configuration for ^7Li Analysis

Arrangement	Channel Radius	ℓ_{max}	Channel Spins(s)
$t + ^4\text{He}$	4.02 fm	5	1/2
$n + ^6\text{Li}$	4.20 fm	1	3/2, 1/2
$n + ^6\text{Li}^*$	4.50 fm	1	7/2, 5/2

Data for all possible reactions were considered at triton energies below 14 MeV, and at neutron energies below 2 MeV. Although specific references to all the data included will not be given, the different types of data analyzed for each reaction are listed in Table II.

TABLE II
Types of Data Included in ^7Li Analysis

Total Cross Reaction	Integrat-		Differ-
Cross Section	Reaction Cross Section	Cross Section	Polarization
$^4\text{He}(t,t)^4\text{He}$			X X
$^6\text{Li}(n,t)^6\text{Li}$		X	X
$^6\text{Li}(n,n)^6\text{Li}$		X	X X
$\alpha + \gamma$		X	
$n + ^6\text{Li}$	X		

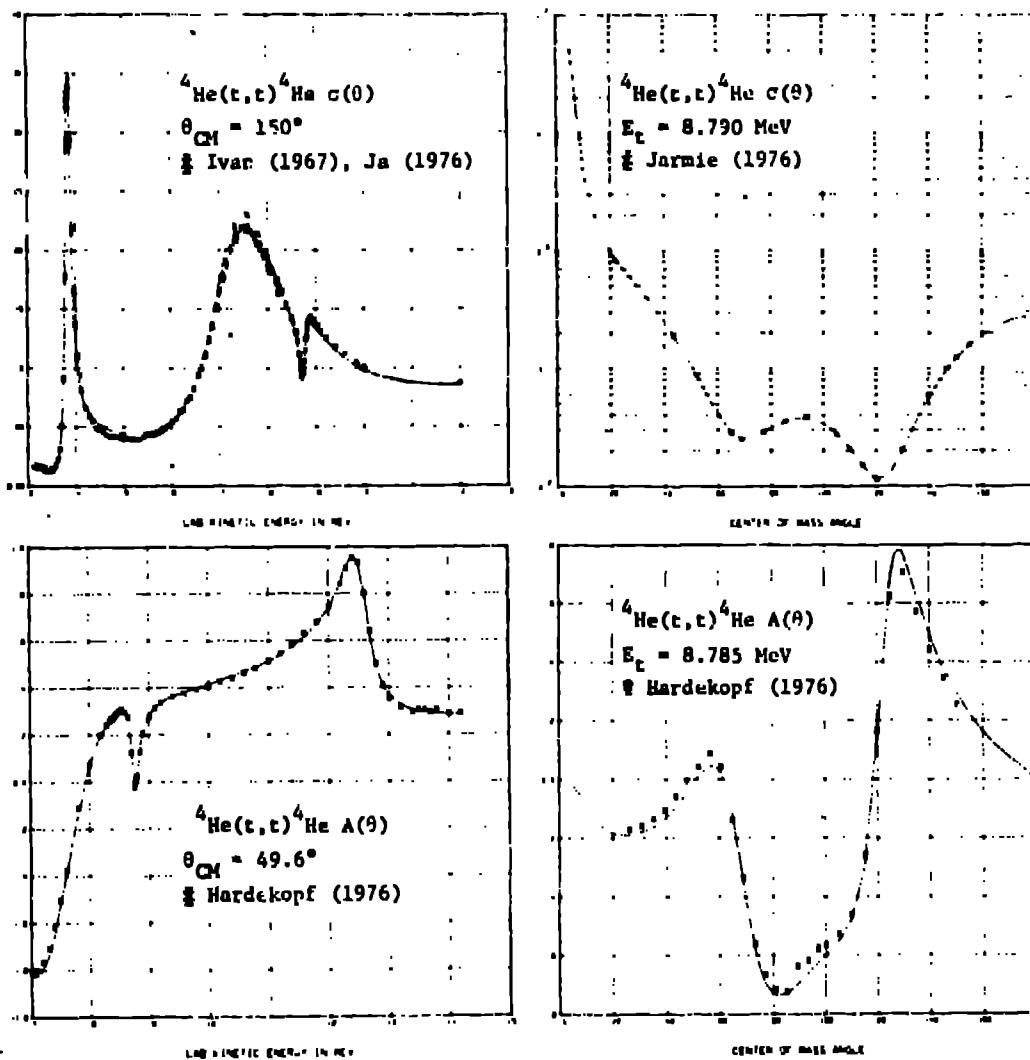


Fig. 1. Calculated and measured observables for ${}^4\text{He}(t,t){}^4\text{He}$. The cross section data are from Refs. 9 and 12; the analyzing power data are from Ref. 13.

The data were fitted in the usual least-squares sense by the R-matrix analysis code ERA.¹¹ Renormalizations and energy shifts were allowed for some of the data sets; in these cases, the deviations from the original experimental scales contributed to the overall χ^2 of the fit.

The resulting fits to some of the $t + \alpha$ elastic scattering measurements are shown in Fig. 1. Anomalies occurring in the differential cross section and analyzing power excitation curves (left side of the figure) at triton energies of approximately 3.9, 7.3, 8.8, and 12.4 MeV correspond to the first 4 resonances in ${}^7\text{Li}$ above the $t + \alpha$ threshold. Parameters for these resonances, which have total angular momentum and parity (J^P) assignments of $7/2^+$, $5/2^+$, $5/2^+$, and $7/2^+$, respectively, are given in the next section. The third resonance is the $J^P = 5/2^+$ level which shows up prominently in the neutron cross sections at $E_n = 250$ keV. Angular distributions of the cross section and analyzing power are shown on the right side of the figure at triton energies close to this resonance. The low-energy measurements of the cross-section excitation are those of Ivanovich,¹² while those at overlapping energies and higher are of Jarmie.⁹ The calculated curve follows the newer, more precise Jarmie data in the region of the overlap. The differential cross section data shown are also those

of Jarmie,^{9,13} while the analyzing power excitation and angular distributions were measured by Hardekopf.¹¹

Figure 2 compares the R-matrix calculation with selected data for the ${}^6\text{Li}(n,t){}^4\text{He}$ reaction. On the left are shown recent measurements¹⁴ of the ${}^6\text{Li}(n,t)$ cross section over the $5/2^+$ resonance at center-of-mass angles of 0 and 180° . These measurements became available after the Version V analysis was completed, so that the curves represent a prediction, rather than a fit. The right side of the figure shows the fits to Overlev's measurements¹⁵ of the ${}^6\text{Li}(n,t)$ angular distributions at $E_n = 1$ and 1.0 MeV. The pronounced asymmetry in the cross section evident at 100 keV persists down to energies as low as 25 keV.¹⁶ These low-energy asymmetry effects in the cross section are well reproduced by the calculations, and can be explained in terms of resonance interference, as discussed in the concluding section.

Representative fits to the ${}^6\text{Li}(n,n){}^6\text{Li}$ angular distributions measured by Lane¹⁷ and Knitter¹⁸ are shown in Fig. 3. The Lane angular distributions required substantial renormalizations at energies near the peak of the 240 keV resonance, with the result that our calculated integrated elastic cross section lies somewhat above Lane's points over the peak. This agrees with recent results of Knitter¹⁹ for the elastic cross sec-

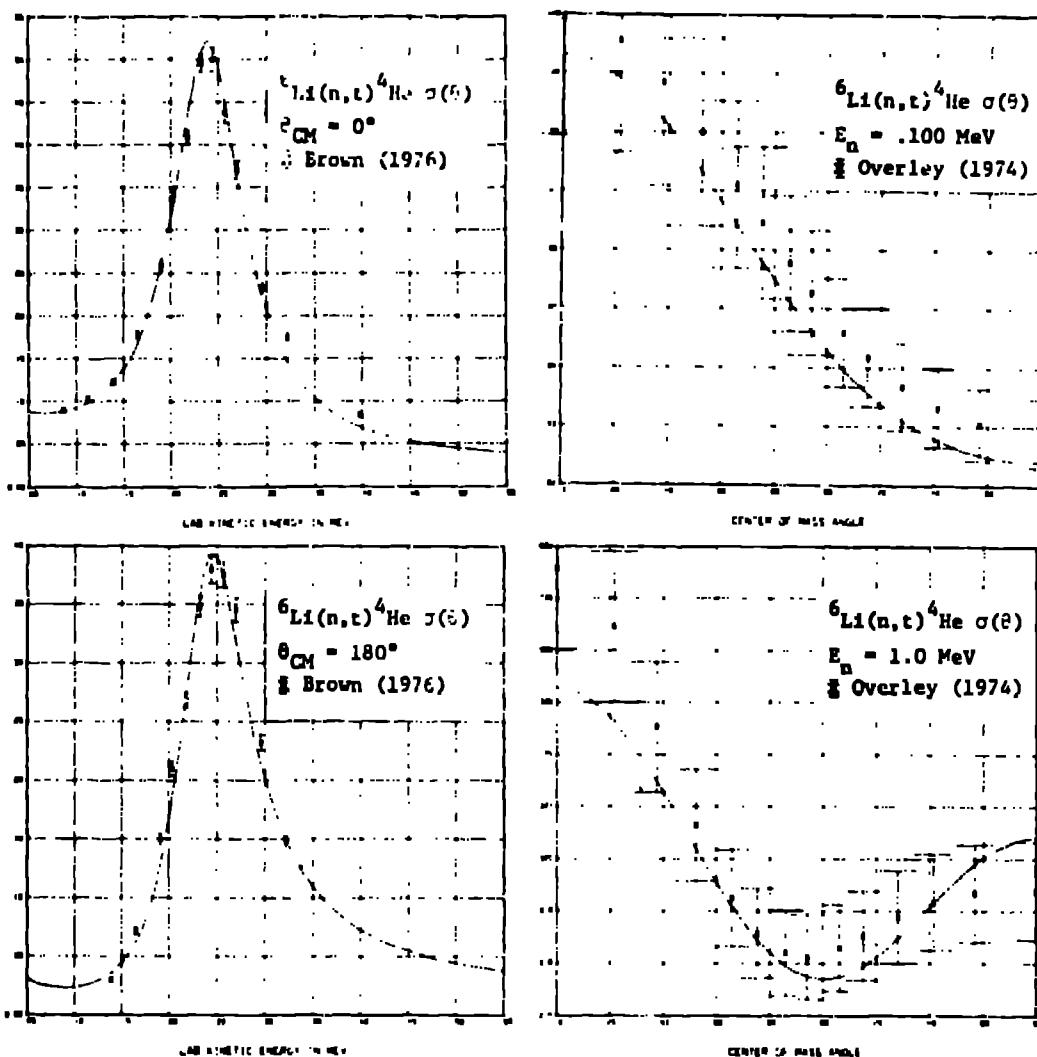


Fig. 2. Calculated and measured observables for ${}^6\text{Li}(n,t){}^4\text{He}$. Data for the excitation curves are from Ref. 14. Data for the angular distributions are from Ref. 15.

tion over the resonance. Calculated values of the polarization (not shown) for elastically scattered neutrons also agree well with measurements by Lane.²⁰

Figure 4 shows the fits to the total cross sections of primary interest in this discussion, the neutron total and ${}^6\text{Li}(n,t)$ integrated cross section. Of course, the latter cross section is the standard and is, at that, only recommended for use at energies below the 240 keV resonance. But because of the strong influence of the resonance on the ${}^6\text{Li}(n,t)$ cross section as it begins to deviate from $1/v$ behavior (at about 20 keV), and because of the close unitary connection, already mentioned, it has with the neutron total cross section, an isolated discussion of the standard cross section would not suffice.

We see that the calculated ${}^6\text{Li}(n,t)$ cross section is generally in very good agreement with recent measurements made at the National Bureau of Standards²¹ (NBS) up to 600 keV. In the region of the resonance, the calculated cross section has come down by roughly half the difference between the Version IV results and the earlier direct measurements,^{5,7} and still exceeds the NBS data by about 2.5% in the peak of the resonance. The data shown are those that were used in the analysis. Corrections to the data since that time have raised the experimental values in the minimum around 90 keV to agree

even better with the calculation, but have reduced somewhat the experimental values in the peak. The largest uncertainty of the calculated cross section in the standard region (below 150 keV) occurs in the vicinity of the 90 keV minimum. At lower energies, the thermal value of 35.9 b is in excellent agreement with Meadows' value,²² and the cross section is quite consistent with Soverby's ratio measurements,²³ below 80 keV, when considered in conjunction with the Version V ${}^7\text{B}(n,\alpha)$ cross section.

The calculated total cross section agrees well with measurements of Diment²⁴ and Harvey,¹⁹ except for a systematic tendency to overshoot the experimental values in the peak of the resonance and undershoot them in the preceding minimum. These differences are of the order of 2-6%, and may be within the bounds of realistic uncertainties on the total cross sections in these regions, if not within the stated errors. The energy scale of these total cross section measurements^{24,19} essentially determined the position of the $5/2^+$ resonance, with the calculated peak total cross section occurring at 244 keV, and the calculated peak (n,t) cross section at 340 keV, in agreement with most of the measurements using time-of-flight neutron energy determination.

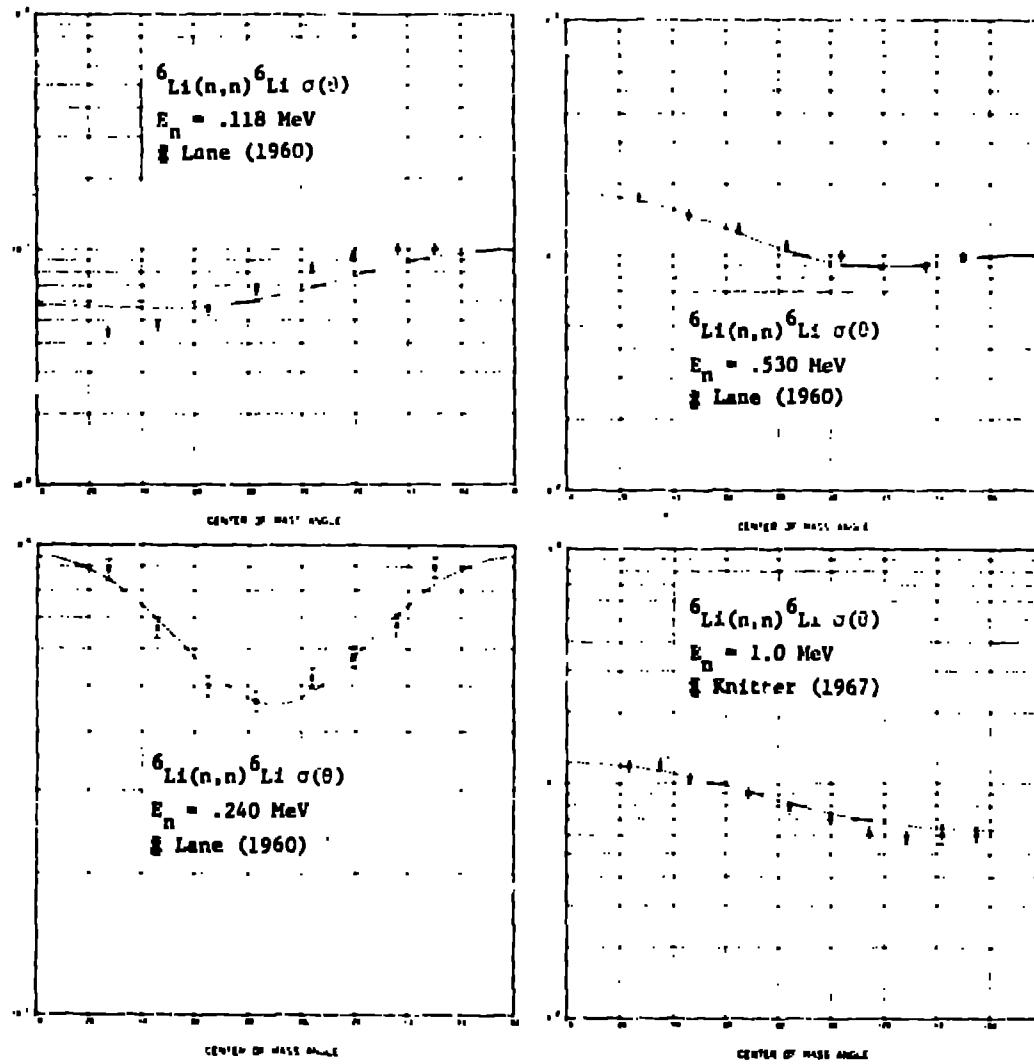


Fig. 3. Calculated and measured angular distributions for ${}^6\text{Li}(n,n){}^6\text{Li}$. The data are from Refs. 17 and 18.

Resonance Parameters

Since experimental data for nuclear reactions are most directly related to matrices (such as the S-matrix) of amplitude ratios for asymptotic wavefunctions, it is appropriate that resonance parameters for asymptotic measurements be related to the poles and residues of such matrices. The R-matrix is not, of course, an asymptotic quantity, and its poles and residues depend on the boundary conditions imposed at the nuclear surface to define the R-matrix, and upon the channel radii which define the nuclear surface. However, one can always transform the R-matrix to an asymptotic form having poles and residues which, although energy-dependent, no longer depend on boundary conditions at the nuclear surface, or upon radial distances outside that surface.²⁴

We choose the asymptotic form to be the S-matrix so that our specification of resonance parameters corresponds with the prescription given by Humblet.²⁵ The transformed R-matrix in that case has the form

$$R_L = \sum_{\mu} \frac{R_{\mu}^T R_{\mu}}{E_{\mu} - E} ,$$

where the R_{μ} and E_{μ} are known, complex (energy-dependent) functions of the parameters $\gamma_{\lambda}, E_{\lambda}$ of the original R-matrix. If, for some complex energy E_0 ,

$$E_{\mu}(E_0) - E_0 = 0 ,$$

then E_0 is a pole of R_L and thus, of the S-matrix as well. The resonant energy and total width associated with the pole are

$$E_R = R_{\mu}(E_0)$$

$$\Gamma = -2 \operatorname{Im}(E_0) ,$$

while the partial widths are given by

$$\Gamma_c = \Gamma \frac{|R_{\mu c}(E_0)|^2 p_c(E_0)}{\sum_c |R_{\mu c}(E_0)|^2 p_c(E_0)} .$$

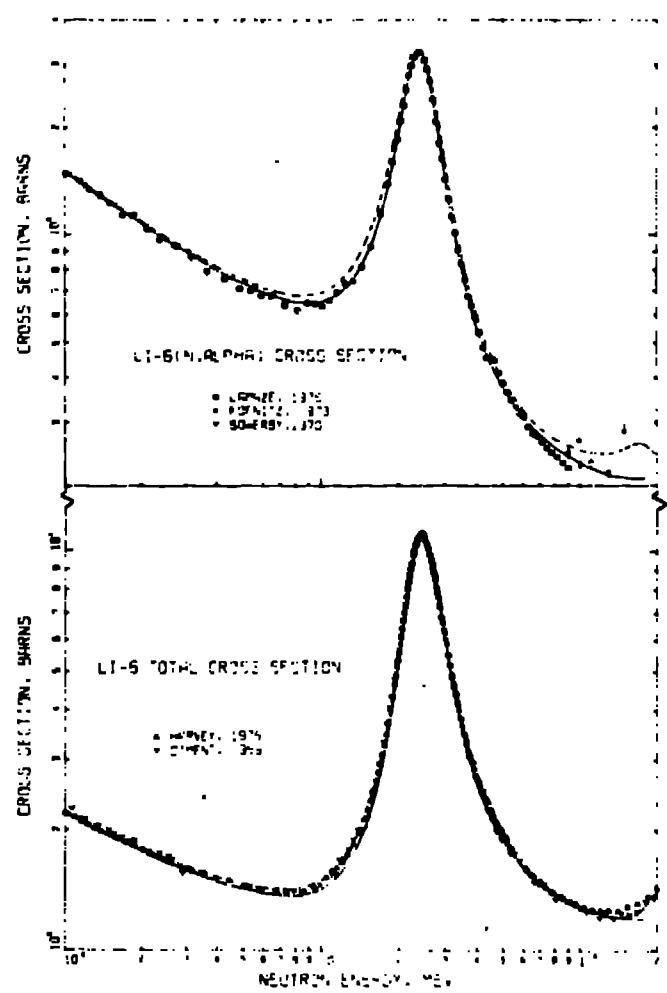


Fig. 4. The ${}^6\text{Li}(n,t){}^4\text{He}$ integrated cross section and $n + {}^6\text{Li}$ total cross section for E_n between .01 and 2 MeV. The solid curves are the ENDF/B-V results, and the dashed curves are ENDF/B-IV. Data for the upper curve are from Refs. 5, 21, and 23; data for the lower curves are from Refs. 4 and 10.

with

$$p_c(E_0) = \frac{\text{Re}(\rho_c)}{|\rho_c|^2}$$

where ρ_c is the product of the channel radius with the channel wave number, and ρ_c is the channel outgoing-spherical-wave function, all evaluated at the complex energy E_0 .

Resonance parameters obtained in this way from the Version V R-matrix parameters are presented in Table III, along with widths and resonance positions from F. Selsove's latest compilation for ${}^7\text{Li}$.²⁶ The first 4 resonances listed are those visible in the excitation curves shown in Fig. 1. The agreement of our calculated parameters for those resonances with values taken from the compilation²⁶ is satisfactory, although not always within the errors assigned by Selsove.

The last two resonances lie above the highest energy at which experimental data were included, and their parameters are therefore quite uncertain. They do correspond roughly with the levels found by Holt et al.²⁷

in their analysis of $n + {}^6\text{Li}$ elastic polarizations at neutron energies between 1 and 5 MeV, except that our calculated widths are somewhat narrower.

It should be mentioned in this connection that the prescription we use can result in resonance parameters that are quite different from those obtained from the usual expressions²⁸ relating R-matrix parameters to external widths and resonance positions at real energies. This is particularly true at higher excitation energies, where the complex pole prescription tends to give smaller widths which appear to correspond more closely with the widths of the experimentally observed anomalies. We also note that the complex poles and partial widths defined above are formally radius-independent in the external region, while those resulting from the usual R-matrix relations are not.

Exclusions

This analysis indicates that many of the features observed in the measurements for reactions in the ${}^7\text{Li}$ system can be interpreted in terms of the resonances identified. In addition to the obvious structure in the cross sections and polarizations due to the presence of the first 4 levels above the $t + n$ threshold, one can ascribe the behavior of the low-energy ${}^6\text{Li}(n,t)$ cross section to broader, more distant states. Near-background levels having $J^P = 1/2^+$ (one of which may be associated with the broad structure at $E_n = 16.8$ MeV in ${}^7\text{Li}$), and the broad $3/2^+$ resonance tentatively identified in this analysis seems to be mainly responsible for the large $1/v$ integrated cross sections at low energies. Interference terms, arising from the presence of the prominent $5/2^-$ resonance at 7.46 MeV excitation energy and of the $3/2^+$ level higher up, cause most of the asymmetry in the differential cross sections at low energies, with interference between the $1/2^+$ and negative parity levels having non-zero 2_p^+ widths contributing to a lesser extent. More recent extensions of this analysis to somewhat higher energies²⁹ indicate that the $3/2^-$ level is responsible for the broad structure seen in both the neutron elastic and total cross sections at $E_n \sim 3.5$ MeV, and at the same time, produces a "shoulder" in the ${}^6\text{Li}(n,t)$ integrated cross section at $E_n \sim 2.2$ MeV.

Recent measurements for reactions in this system appear to be approaching unitary consistency. At this stage, however, the precise experimental determination of the total cross section below and over the resonance seems to be most elusive, both in terms of the magnitude of the cross section near the peak, and the energy of the peak. New measurements of the total cross section by Knitter¹⁹ and by Smith³⁰ agree well in magnitude with the Version V calculations, but not in energy scale. Questions about the ${}^6\text{Li}(n,t)$ cross section persist in relation to ratio measurements. While Gayther's³¹ new ratio measurement of ${}^{235}\text{U}(n,f)$ relative to ${}^6\text{Li}(n,t)$ appears quite consistent with the Version V results, Macklin's³² ratio of ${}^{197}\text{Au}(n,\gamma)$ relative to ${}^6\text{Li}(n,t)$ does not. The resolution of these differences will doubtless require further (but hopefully, small) changes in the neutron cross sections for ${}^7\text{Li}$. We feel, however, that the utility of this approach, and the importance of analyzing standard cross sections in a unitarily consistent way with other data from the same system, have been demonstrated by the Version V results.

TABLE III

Resonance Parameters for the ^7Li System

J^P	E_x^a	E_x^b	State	Partial Width ^a	Total Width ^a	Total Width ^b
$7/2^-$	4.622	4.633 \pm .008	$^2\text{F}_1$.071	.071	.093 \pm .008
$5/2^-$	6.596	6.575 \pm .054	$^2\text{F}_1$.944	.945	.875 \pm .2
			$^4\text{P}_n$.001		.1
$3/2^-$	7.455	7.467 \pm .004	$^2\text{F}_1$.023	.077	.089 \pm .007
			$^4\text{P}_n$.054		
$7/2^-$	9.568	9.61 \pm .81	$^2\text{F}_1$.294	.412	---
			$^8\text{P}_n^*$.118		
$3/2^-$	9.853 ^c	10.25 \pm .1	$^2\text{P}_1$.182 ^c	1.171 ^c	1.4 \pm .1
			$^4\text{P}_n$.969 ^c		
			$^2\text{P}_n$.020 ^c		
$3/2^+$	11.279 ^c		$^2\text{P}_1$	1.360 ^c	2.517 ^c	
			$^4\text{S}_n$	1.157 ^c		

^a. Values (in MeV) derived from the Version V R-matrix parameters.^b. Values (in MeV) tabulated in Ref. 26.^c. Values given for resonances above the range of the analysis, which are therefore quite uncertain.Acknowledgments

This analysis is an outgrowth of work begun by D. C. Dodder and K. Witte. The effort still benefits from collaboration with them on many aspects of the problem. I am grateful to N. Jarmie, R. Brown, L. Stewart, and P. Young for their help in collecting and reviewing the experimental data.

References

1. E. P. Wigner and L. Eisenbud, Phys. Rev. 72, 29 (1947), and A. M. Lane and R. G. Thomas, Rev. Mod. Phys. 30, 257 (1958).
2. G. M. Hale, "R-Matrix Analysis of the Light Element Standards," Proceedings of a Conference on Nuclear Cross Sections and Technology, Vol. 1, 302 (1975).
3. G. M. Hale, L. Stewart, and P. G. Young, Los Alamos Scientific Laboratory report LA-6518-MS (1976).
4. K. M. Diment and C. A. Uttley, Harwell report AERE-PR/NP 15, p 12 (1969).
5. W. P. Poenitz, Z. Phys. 268, 359 (1974).
6. W. Fort and J. P. Marquette, "Experimental Methods Used at Cadarache to Determine the $^6\text{Li}(n,\alpha)\text{T}$ Cross Section between 200 keV and 1700 keV," Proceedings of a Panel on Neutron Standard Reference Data, November 20-24 (1972), IAEA, Vienna. Note: Fort expects to renormalize his data upward by ~11%.
7. M. S. Coates, G. J. Hunt, and C. A. Uttley, "Measurements of the Relative $^6\text{Li}(n,\alpha)$ Cross Sections in the Energy Range 1 keV to 7500 keV," Neutron Standards Reference Data, IAEA, Vienna, p. 105 (1974).
8. R. J. Spiger and T. A. Tombrello, Phys. Rev. 163, 964 (1970).
9. N. Jarmie et al., Bull. Am. Phys. Soc. 20, 596 (1975).
10. J. A. Harvey and N. W. Hill, Proc. Conf. on Nuclear Cross Sections and Technology, Vol. I, 244 (1975).
11. D. C. Dodder, K. Witte, and G. M. Hale, "The LASL Energy-Dependent Analysis Code EDA," unpublished.
12. M. Ivanovich, P. G. Young, and G. G. Ohlsen, Nucl. Phys. A110, 441 (1968).
13. R. A. Hardekopf et al., Los Alamos Scientific Laboratory report LA-6188 (1977).
14. R. E. Brown, G. G. Ohlsen, R. F. Haglund, Jr., and N. Jarmie, LA-UR-77-407 (1977) (Submitted to Phys. Rev. C).
15. J. C. Overley, R. M. Sealock, and D. H. Ehlers, Nucl. Phys. A221, 573 (1974).
16. I. G. Schröder, E. D. McGarry, G. de Leeuw-Gierta, and S. de Leeuw, Proc. Conf. on Nuclear Cross Sections and Technology, Vol. I, 240 (1975).

17. R. O. Lane, Ann. Phys. 12, 135 (1961).
18. H. H. Knitter and A. M. Coppola, EANDC report (E) 57(U) (1967).
19. H. H. Knitter, C. Budtz-Jorgensen, M. Mailly, and R. Vogt, CBNM-VG (1970).
20. R. O. Lane, A. J. Elwyn, and A. Langsdorf, Jr., Phys. Rev. 136, B 1710 (1964).
21. G. P. Lamaze, O. A. Wesson, R. A. Schrack, and A. D. Carlson, Proc. International Conference on the Interactions of Neutrons with Nuclei, Vol. 2, 1341 (1976).
22. J. W. Meadows, Neutron Standards and Flux Normalization (AEC23), 129 (1971).
23. M. G. Sowerby, B. H. Patrick, C. A. Uttley, and K. M. Diment, J. Nucl. Energy 24, 323 (1970).
24. G. M. Hale, Nuclear Theory in Neutron Nuclear Data Evaluation, Vol. II (IAEA-190) 1 (1976).
25. J. Humblet and L. Rosenfeld, Nucl. Phys. 26, 529 (1961).
26. F. Seloive and T. Lauritsen, Nucl. Phys. A227, 54 (1974).
28. See, for instance, Lane and Thomas (Ref. 1), p. 295.
29. G. M. Hale and D. C. Dodder, Proc. International Conf. on the Interactions of Neutrons with Nuclei, Vol. 2, 1459 (1976).
30. A. B. Smith, P. Guenther, D. Havel, and J. F. Whalen, ANL/NDM-29 (1977).
31. D. G. Gayther, AERE-R 8556 (1977).
32. R. L. Macklin, J. P. Halperin, and R. R. Winters, Phys. Rev. C11, 1270 (1975).

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