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TITLE: THEORETICAL CALCULATIONS OF THE $^{6}Li(n,t)$ CROSS SECTION

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THEORETICAL CALCULATIONS OF THE ^{6}Li(n,t) CROSS SECTION

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ABSTRACT

The origin of the 1/v cross section for the ^{6}Li(n,t) reaction and the behavior of its angular distribution are discussed in the context of (1) conventional R-matrix analyses, (2) PWBA calculations of deuteron exchange, and (3) consistent R-matrix analyses. Results of a comprehensive, conventional R-matrix analysis of reactions in the ^{7}Li system are presented, and the possible interpretation of some of its parameters in terms of the deuteron exchange mechanism is discussed. An extension of the usual PWBA calculation to include internal bound-state effects in a simple model is shown to introduce additional poles into the T matrix and broaden the energy range over which particle exchange may be important. A consistent R-matrix treatment of the scattering equations in the internal and external regions leads to channel overlap terms that appear to include particle-exchange effects automatically with the resonances in an unitary fashion.

I. INTRODUCTION

The ^{6}Li(n,t) cross section has been an interesting and sometimes controversial subject for the past several years. Although measurements and theoretical descriptions of the reaction have been converging in recent years, questions of interpreting the theoretical results in terms of reaction mechanisms have remained open. The major questions to be answered are (a) What is the origin of 1/v behavior of the cross section at low energies? and (b) How does one account for the rather complicated behavior of the angular distribution at higher energies? These questions will be discussed in the context of three different descriptions: (1) conventional R-matrix approach; (2) deuteron exchange in plane-wave Born approximation; and (3) consistent R-matrix approach.

II. CONVENTIONAL R-MATRIX APPROACH

In conventional R-matrix analyses, the 1/v cross section comes from poles in the R matrix located either above or below the n-^{6}Li threshold. At low energies, about 80% of the cross section comes from the J = ½ S-wave transition.[1] Early attempts[2,3] to explain the n-^{6}Li reactions put a pole in the J = ½ S-wave just below the n-^{6}Li threshold. Our comprehensive study[4] of reactions in the ^{7}Li system, including t-α scattering, from which the ENDF-V cross sections for ^{6}Li were obtained, found that such a pole was inconsistent with t-α scattering data, a result that was later reinforced by a study[5] of low-energy n-^{6}Li elastic scattering done in the Soviet Union. Distant levels both above and below the n-^{6}Li threshold were tentatively ascribed in Ref. 4 to a direct-reaction mechanism for the $\frac{1}{2}^+$ transition. Knox and Lane[6] recently reported an R-matrix analysis of the n-^{6}Li reactions in which the 1/v cross section in the J = ½ state is attributed to a level above the n-^{6}Li threshold that they associate with a compound nuclear state.

All of these R-matrix analyses appear to agree, however, that the J = 3/2 component that accounts for the remaining 20% of the low-energy 1/v cross section comes from a $3/2^+$ level in ^{7}Li that occurs at $E_x \sim 9.5$ MeV. Therefore, the pole positions and associated reaction mechanisms seem to be least clear for the J = ½ transition, which accounts for most of the 1/v cross section at low energies.

Recently we extended the analysis that was used for ENDF-V ^{6}Li cross sections to include more data and higher energies so that it is the most comprehensive R-matrix study of reactions in the ^{7}Li system that has been done. This analysis will provide Li(n,t) cross sections for the combined ENDF-VI standards file, as described by Carlson[7] at this conference, as well as the other neutron cross sections at energies below 4 MeV for the ENDF-VI ^{6}Li evaluation. The table below lists the channel configuration and the types of data for the various reactions that were included in the analysis.

TABLE I

CHANNELS AND DATA TYPES INCLUDED IN ^{7}Li R-MATRIX ANALYSIS

Arrangement	Channel Radius (fm)	ℓ_{max}
t-^{4}He	4.02	5
n-^{6}Li	4.50	2
n-$^{6}Li^{*}$	4.50	1

	Energy Range (MeV)	Integrated Cross Section	Differential Cross Section	Polarization	Number Data Points
e	3.1-14.2	σ_R	x	x	2063
i	8.7-14.4		x		39
i*	12.9		x		4
i	0-4	σ_T, σ_{Elas}	x	x	761
e	0-3.5	x	x	x	734

e 1 shows the types of fits obtained to the t-α elastic scattering ion and analyzing-power measurements of Jarmie et al.[8] One sees le structure in these observables as functions of both energy and :responding to relatively narrow resonances in ^{7}Li. Fits to n-^{6}Li :attering cross sections[9,10] and polarizations[11,12] are shown in Fig. s 3 and 4 show calculated neutron total and elastic scattering cross :ompared to some of the measurements.[13-16] Calculated $^{6}Li(n,t)$ cross plotted at low energies as $\sigma_{n,t}E_n^{\frac{1}{2}}$ to show deviations from 1/v behav- shown compared with some of the measurements[17-19] in Fig. 5. These ogether with the comparisons of thermal cross sections given in Table rate that the analysis gives generally very good representations of ated cross sections in the standards region.

TABLE II

THERMAL n-^{6}Li CROSS SECTIONS

	Recommended[a]	Calculated from R-Matrix Analysis
$\sigma_{n,t}$ (b)	940 ± 4	939.46
$\sigma_{n,n}$ (b)	.75 ± .02	0.74

en from Neutron Cross Sections, Vol. 1, Part A, by S. F. habghab, M. Divadenam, and N. E. Holden, Academic Press (1981).

The ^{6}Li(n,t) angular distribution changes markedly in the region $E_n \lesssim 4$ MeV, but there does not yet seem to be an experimental concensus on the details of the changes. Calculations from the R-matrix analysis of the zero-degree and 180-degree differential cross sections are compared in Fig. 6 with recent measurements[20,21] at neutron energies below 400 keV. The relative Legendre coefficients of Knitter et al.[20], which were derived from rather complete angular distributions at energies between 0.035 and 325 keV, have been converted to zero- and 180-degree cross sections whose normalizations are determined by the fitting process. Also shown are absolute measurements at zero and 180 degrees by Brown et al.,[21] which appear to be energy-shifted with respect to the Knitter data.

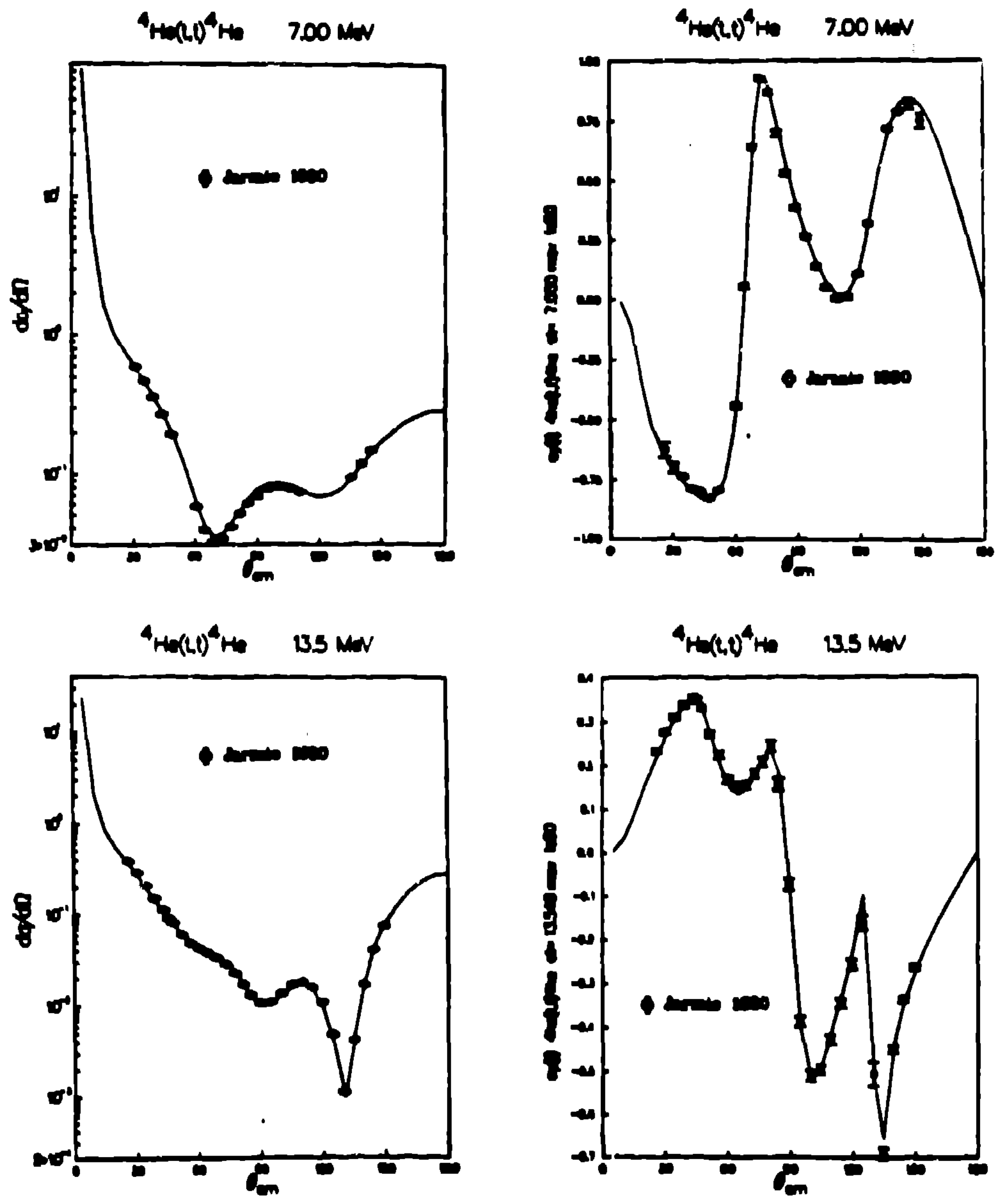
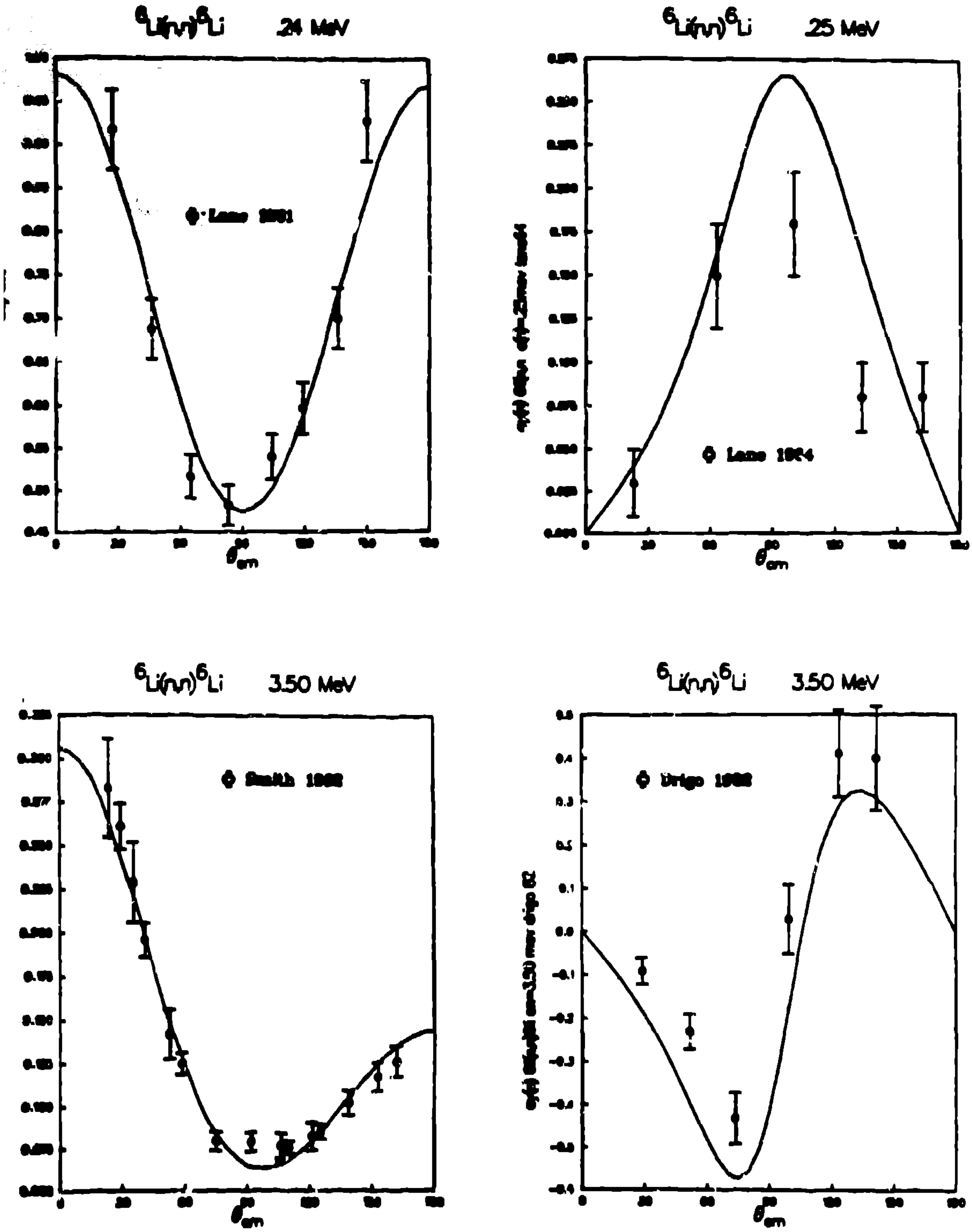


Fig. 1. Differential cross sections (left) and analyzing powers (right) for t-α elastic scattering at E_t = 7 and 13.5 MeV. The solid curves are the R-matrix calculations and the data are those of Jarmie et al.[8]



. 2. Differential cross sections (left) and polarizations (right) for n-^{6}Li stic scattering at E_n = 0.25 and 3.5 MeV. The solid curves are the R-matrix culations and the data are those of Lane,[9,10] Smith,[11] and Drigo.[12]

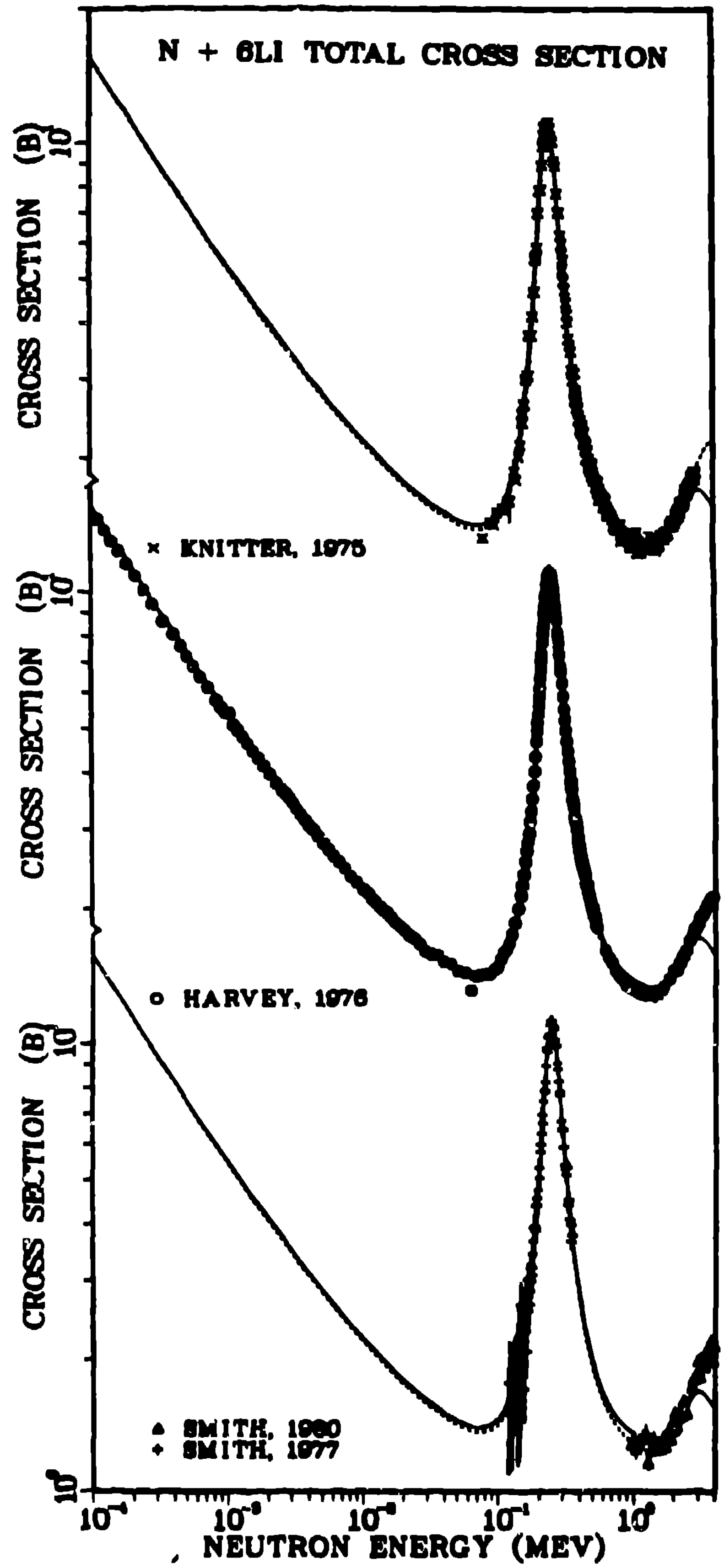
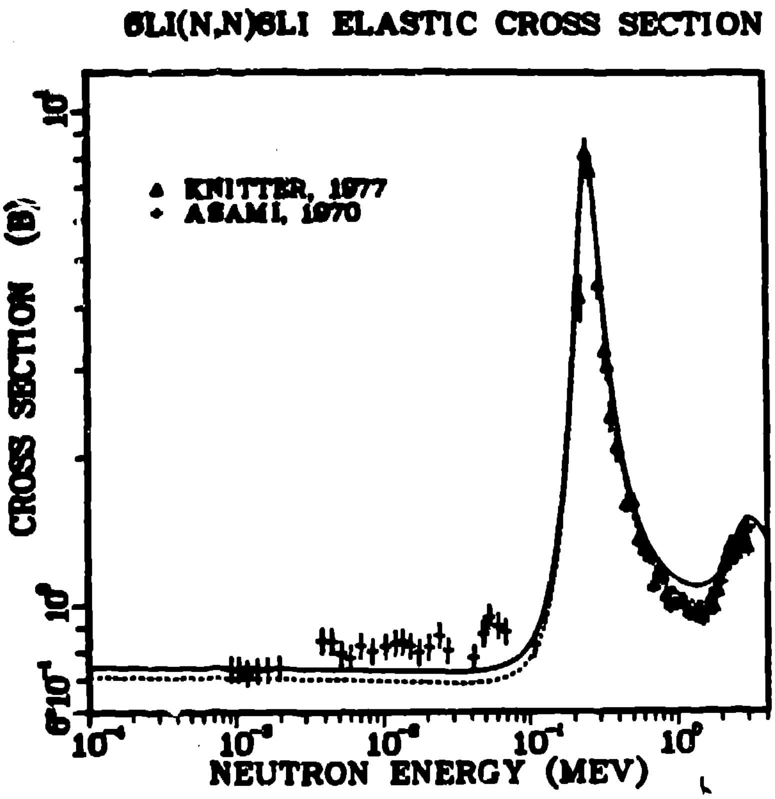
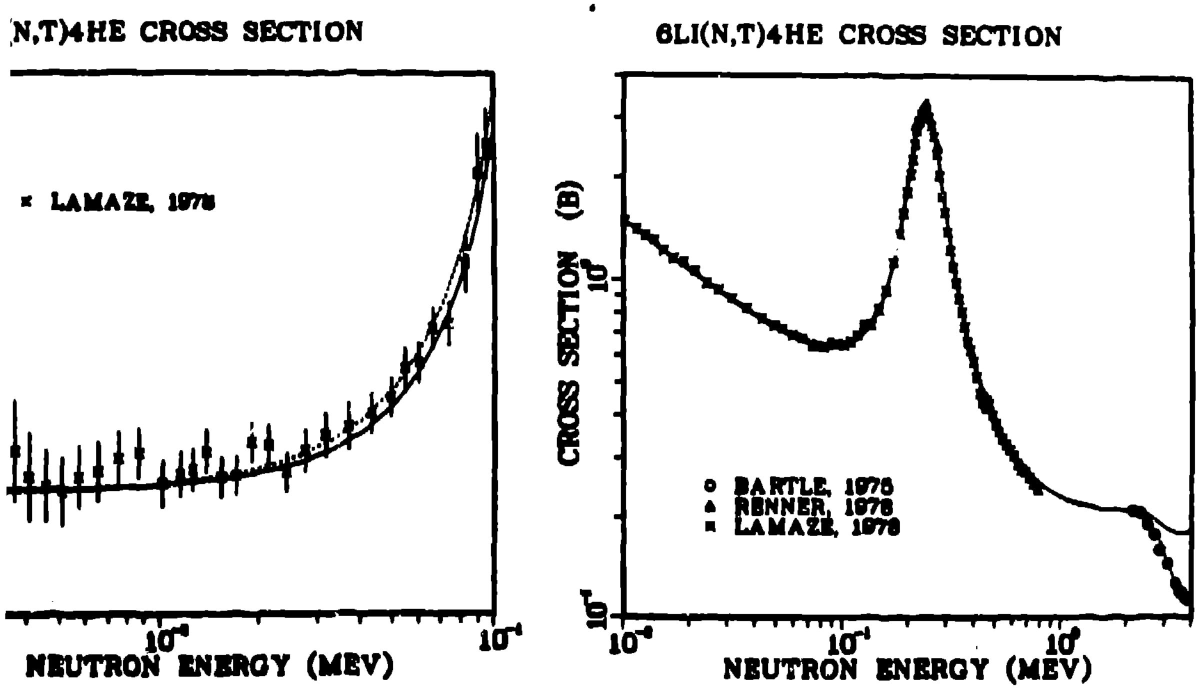


Fig. 3. Comparison of the R-matrix calculation (solid line) to the n+^{6}Li total cross-section measurements of Knitter,[14] Harvey,[15] Guenther,[16] and to the ENDF-V cross section (dashed line). The scales for the three parts of the figure are offset by a factor of 10.



. Comparison of the R-matrix calculation (solid curve) of the n-^{6}Li ated cross section with data of Asami[13] and of Knitter,[14] and with DF-V cross section (dashed curve).



. Comparison of the R-matrix calculation of the ^{6}Li(n,t)^{4}He integrated section (solid curve) with the data of Lamaze,[17] Renner,[18] and Bartle,[19] th ENDF-V (dashed curve). In the righthand figure, $\sigma\sqrt{E}$ is plotted to deviations from 1/v behavior at energies below 100 keV.

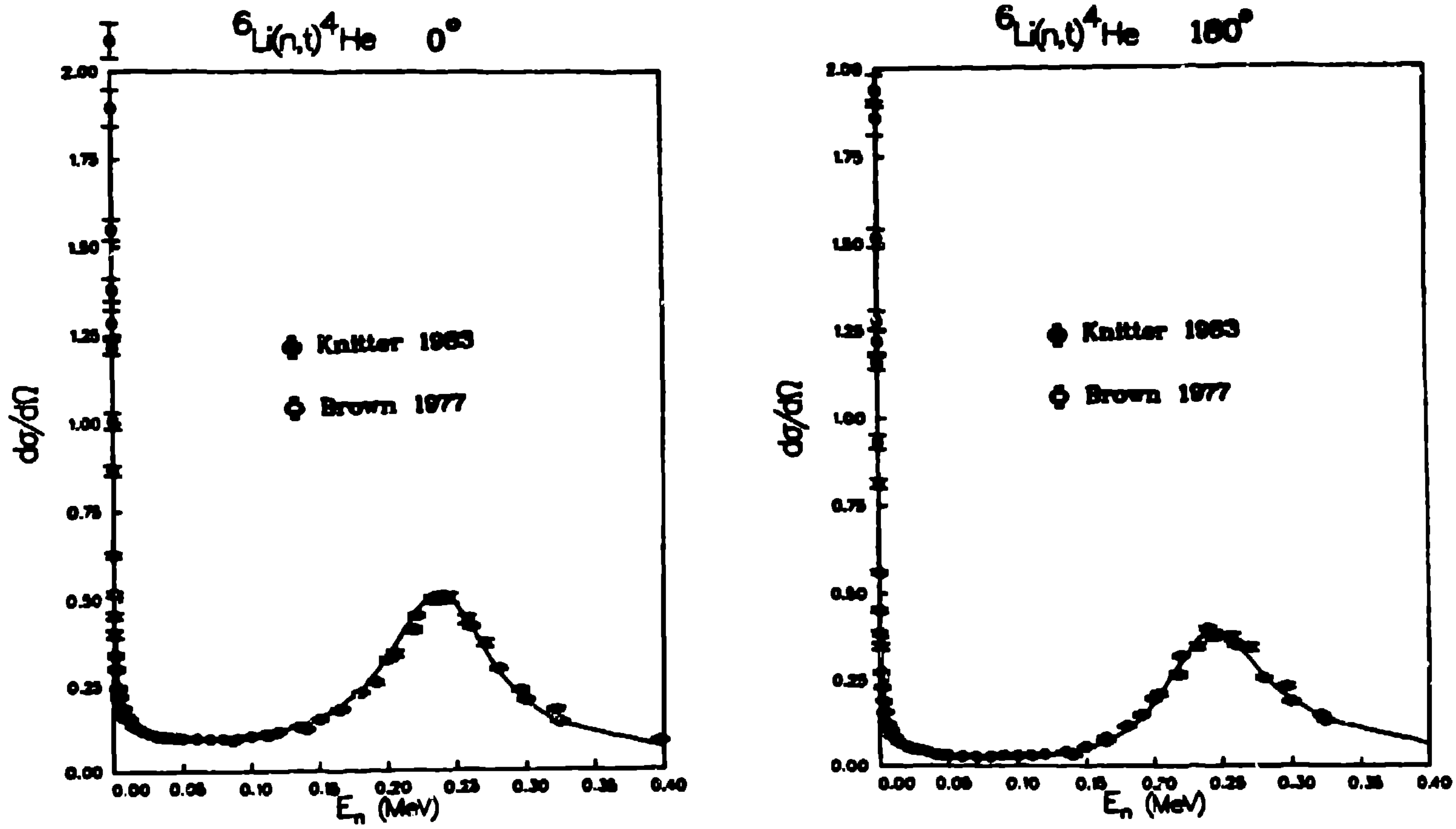


Fig. 6. R-matrix calculations (solid curves) compared to the measurements of Knitter[20] and Brown[21] of the ^{6}Li(n,t)^{4}He differential cross section at 0° (left) and 180° (right).

Absolute ^{4}He(t,n)^{6}Li zero-degree differential cross-section measurements by Drosg[22] are compared with the calculations in Fig. 7. The calculation lies ~ 16% below the data in the region $9 \lesssim E_t \lesssim 13.5$ MeV. In a comparison with Overley's[23] ^{6}Li(n,t) differential cross-section measurement in Fig. 8, one sees again the tendency of the calculation to be low at forward angles in the range $0.4 \lesssim E_n \lesssim 1$ MeV, although the overall shape agreement is fairly good.

The problems with shape disagreements among recent measurements in regions where the angular distribution is changing rapidly are illustrated in Figs. 9 and 10. The top panel of Fig. 9 shows relative measurements of Condé[24] compared with Overley's[23] absolute measurements (bottom panel) at nearly the same energies, and with the calculations. One sees that, with the exception of a few isolated Condé points, the measurements are generally consistent with each other and with the calculations at these energies. The situation is not so clear in Fig. 10 where the Condé data (top) are compared with ^{4}He(t,n)^{6}Li ntial cross-section measurements by Drosg[22] (bottom) at nearly equiva- energies. In this case, the fit has assumed a shape intermediate between two measurements, but clearly more data are required to better define the lar distributions in the 2-4 MeV region.

Of particular interest in this analysis is the level structure affecting spin-$\frac{1}{2}$ transitions (of which the $\frac{1}{2}^+$ is one). In the S- and P-waves, there levels a few MeV below the t-α threshold (in the P-waves, they are bound es), positive-energy levels at $E_x \sim 12.0$ MeV, and higher-lying background es. The reduced-width products, $\gamma_n\gamma_t$, in the negative-energy (relative to levels have the opposite sign from those in the ~ 12 MeV positive-energy ls. A possible interpretation of such structure comes from considering the eron exchange contribution to the ^{6}Li(n,t) reaction in plane-wave Born ap- imation (PWBA).

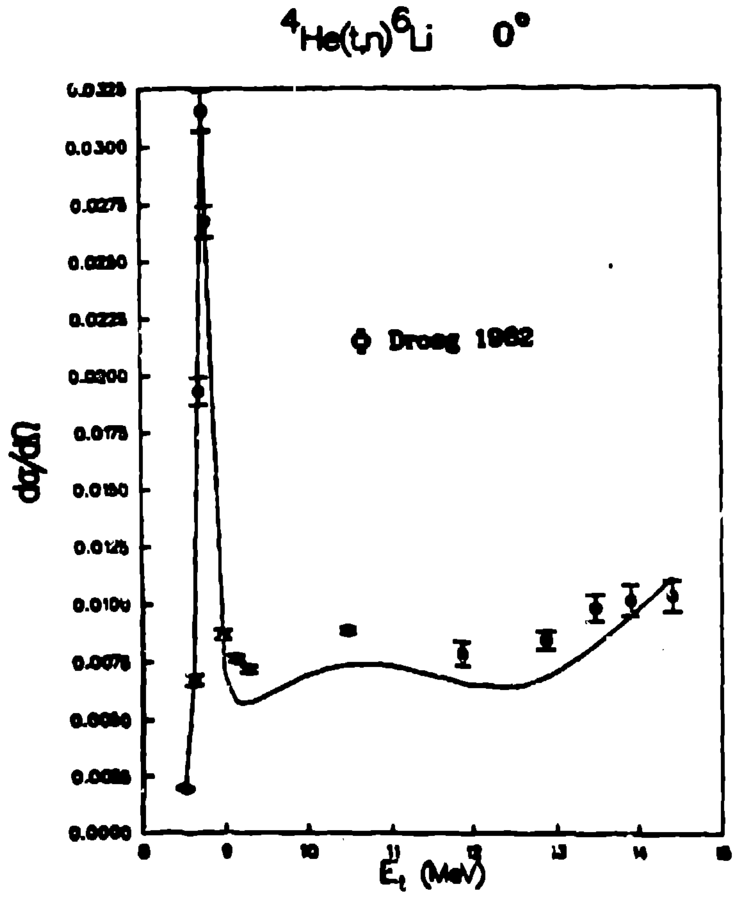


Fig. 7. R-matrix calculation of the ^{4}He(t,n)^{6}Li differential cross section at zero degrees compared with the measurement of Drosg.[22]

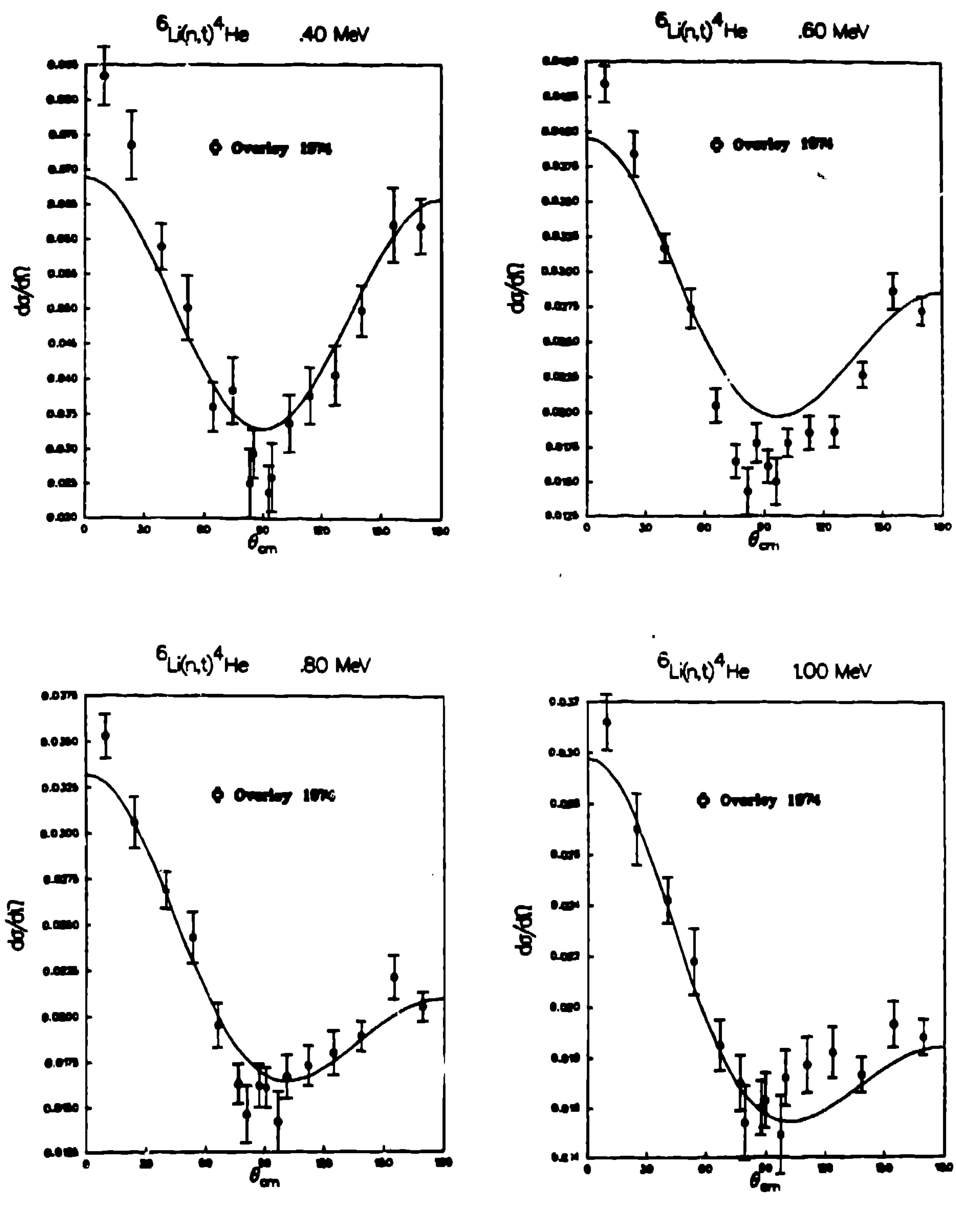


Fig. 8. Calculated $^{6}Li(n,t)^{4}He$ differential cross sections compared with the measurements of Overley[23] at neutron energies between 0.4 and 1 MeV.

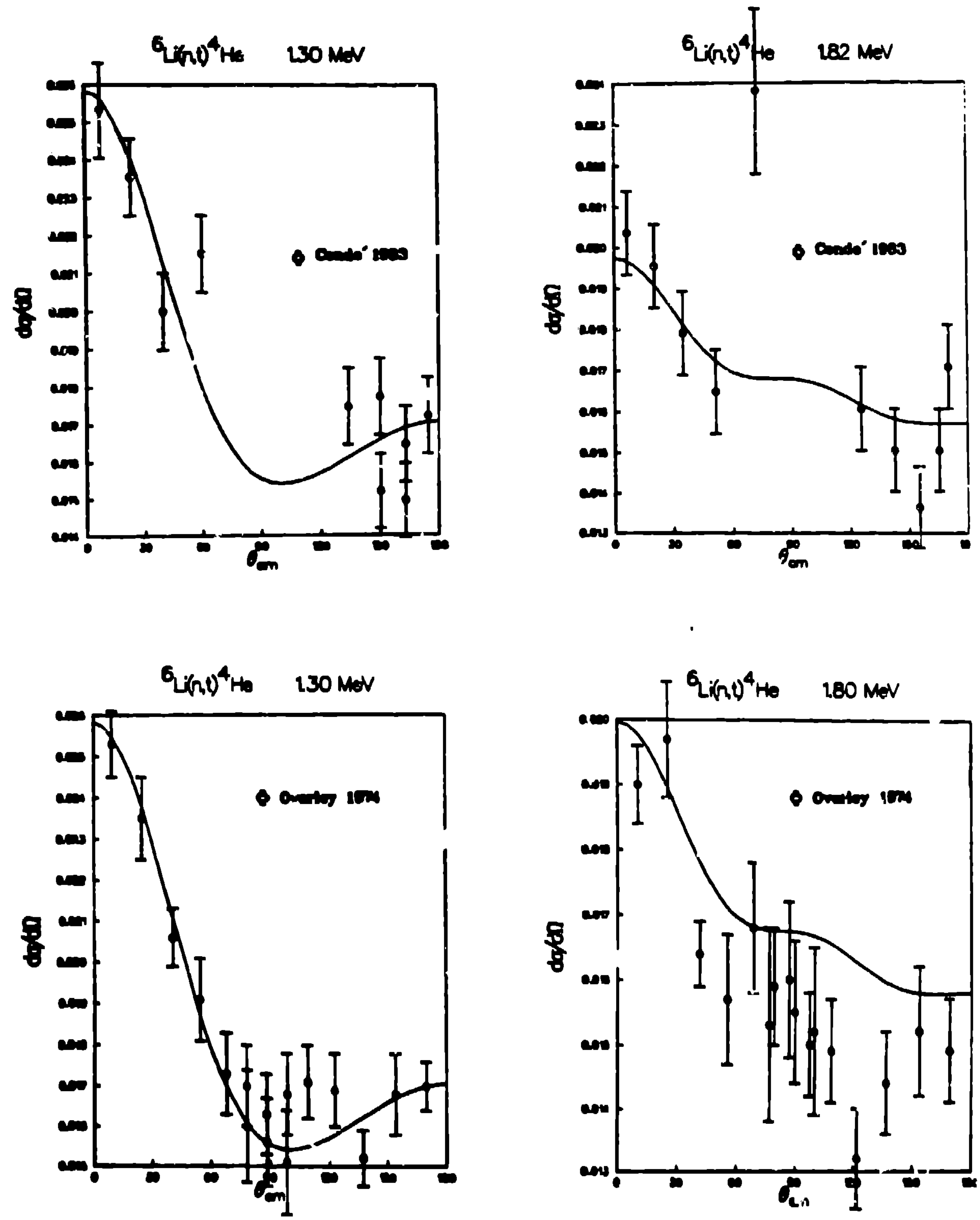


Fig. 9. R-matrix calculations (solid curves) of $^{6}Li(n,t)$ differential cross sections compared with measurements of Condé[24] (top) and of Overley[23] (bottom) at energies near E_n = 1.3 and 1.8 MeV.

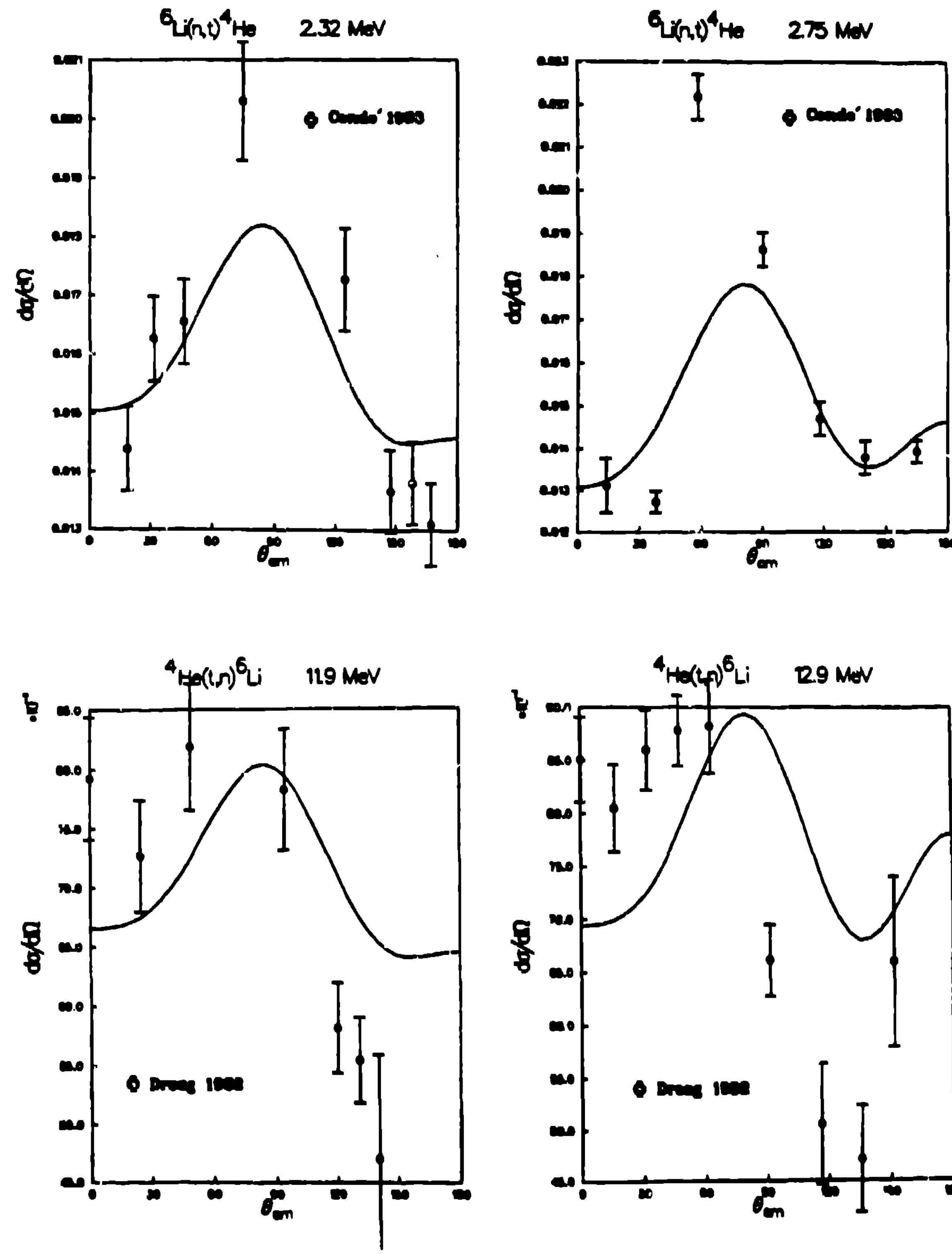


Fig. 10. Calculations of ^{6}Li(n,t)^{4}He differential cross sections compared with data of Condé[24] (top) at E_n = 2.32 and 2.75 MeV, and of ^{4}He(t,n)^{6}Li differential cross sections at approximately corresponding values of E_t (bottom) compared with measurements of Drosg.[22]

III. DEUTERON EXCHANGE IN PWBA

Weigmann and Manakos[25] have suggested that deuteron exchange may account for the $\frac{1}{2}^+$ component of the Li(n,t) 1/v cross section at low energies, and serve as a "background" mechanism at low energies for the resonant behavior of the angular distributions. Their PWBA calculation (which appears to have inherited errors in numerical factors from earlier work) makes the standard assumption that the bound-state wavefunctions for ^{6}Li and ^{3}H have their exponentially decaying asymptotic forms all the way in to zero radius, with the result that the Born-approximate T matrix has only negative-energy poles. A more realistic calculation would take into account the internal behavior of the bound-state wavefunctions, properly matched to the exponentially decaying asymptotic forms. This calulation cannot be done in a model-independent fashion, but even a simple model of the internal behavior of the bound-state wavefunctions gives qualitatively different effects.

We have assumed S-wave, square-well eigenfunctions (sine functions) for the internal bound-state wavefunctions. The depths (V^0) and ranges (c) of the square wells were determined by matching the binding energies and asymptotic normalization constants ($\tilde{C}^2$) for d-α binding in ^{6}Li and for n-d binding in ^{3}H. These values are given in Table III.

TABLE III

SQUARE-WELL POTENTIAL PARAMETERS FOR ^{6}Li AND ^{3}H BOUND STATES

	V_i^0 (MeV)	c_i (fm)	B_i (MeV)	$\tilde{C}_i^2$	Recommended $\tilde{C}_i^{2(a)}$
^{6}Li(d-α)	5.08	4.45	1.474	4.62	4.60
^{3}H(n-d)	38.51	1.95	6.258	2.57	2.59

(a) Taken from M. P. Locher and T. Mizutani, Phys. Rep. 46, 43 (1978).

The Born-approximate T matrix in this model is given by

$$T_{31}^{BA}(\theta) = \frac{1}{4\pi^2} V_1^0 V_3^0 (1-\alpha)^3 \frac{\hbar^4}{\mu_1\mu_3}(\beta_1\beta_3)^{\frac{1}{2}} \frac{K_1 K_3}{D(\varepsilon,\theta)[D(\varepsilon,\theta)-(1-\alpha)V_1^0][D(\varepsilon,\theta)-(1-\alpha)V_3^0]} \qquad (1)$$

in which the label 1 refers to n-^{6}Li, 3 refers to α-t, μ_1 is the d-α reduced mass, μ_3 is the n-d reduced mass, B_1 is the binding energy of α and d in ^{6}Li, B_3 is the binding energy of n and d in ^{3}H, and $\beta_i^2 = \frac{2\mu_i}{\hbar^2} B_i$. The energy denominator is

$$D(\varepsilon,\theta) = B_1 + B_3 + (1+\alpha)\varepsilon - 2\sqrt{\alpha(\varepsilon+B_1)(\varepsilon+B_3)}\cos\theta \quad , \tag{2}$$

in terms of the total center-of-mass energy ε (relative to the n+d+α mass), and scattering angle θ between the incident neutron and outgoing triton. We also have the residue factors

$$K_i = \tilde{C}_i \left(\cos q_i c_i + \frac{\beta_i}{q_i}\sin q_i c_i\right)e^{-\beta_i c_i} \quad , \tag{3}$$

which are functions of momentum transfer

$$q_i = \left[\frac{2\mu_i}{(1-\alpha)\hbar^2} D(\varepsilon,\theta) - \beta_i^2\right]^{1/2} \quad , \tag{4}$$

and the mass factor $\alpha = \frac{m_n m_\alpha}{m_t m_{^6Li}} = \frac{2}{9}$.

Using the identity

$$\frac{(1-\alpha)^2 V_1^0 V_3^0}{D[D-(1-\alpha)V_1^0][D-(1-\alpha)V_3^0]} = \frac{1}{D} - \frac{V_3^0}{V_3^0-V_1^0}\frac{1}{D-(1-\alpha)V_1^0} + \frac{V_1^0}{V_3^0-V_1^0}\frac{1}{D-(1-\alpha)V_3^0} \quad , \tag{5}$$

Eq. (1) can be reduced to a sum of pole terms, in which D gives the negative -energy pole in the squared momentum transfer ($q_i^2 = -\beta_i^2$), and the other terms give positive-energy poles, the lowest of which has a residue with opposite sign from that of the D^{-1} term since $V_3^0 > V_1^0$. This is qualitatively the same as the pole structure seen in our R-matrix analysis for the spin-½ transitions although the comparison is quite approximate. The point is, however, that including the internal behavior of the bound-state wavefunctions appears to broaden the energy range over which particle exchange contributes to a reaction, so that its effects need not be concentrated just at low energies in negative-energy poles, but may be manifest in positive-energy poles as well.

V. CONSISTENT R-MATRIX APPROACH

The similarities between our R-matrix amplitudes for the spin-½ transi-ions and a PWBA calulation including internal behavior of the bound-state avefunctions lead one to seek a more definitive correspondence within the nitary framework of R-matrix theory. The deuteron exchange mechanism in the Li(n,t) reaction belongs to a larger class of effects that come from non-rthogonal channels that are neglected in conventional R-matrix theory. This s because the equations used to relate the R matrix to the T (or S) matrix ome from matching to an asymptotic scattering solution that is valid only at nfinity, where the channel overlap effects vanish.

When a consistent R-matrix formulation of the scattering equations in the cternal (asymptotic) region is matched to the R-matrix solutions in the inter-il region, additional terms due to channel overlap appear in the relation etween the T matrix and R matrix, which can be considered as off-diagonal con-ributions to the "hard-sphere" amplitude. These terms are mathematically imilar to the PWBA T-matrix contributions from particle exchange, except that ey are properly unitary. We are presently reducing the integrals for the rtial-wave amplitudes of these terms to computational form so that they can included in our R-matrix calculations. The expectation is that these terms ll account for most of the spin-½ transition strength presently coming from les in our conventional R-matrix analysis.

SUMMARY AND CONCLUSIONS

A comprehensive, conventional R-matrix fit to reactions in the ^{7}Li system ves a good representation of almost all the data included. In this analysis, e 1/v cross section for the ^{6}Li(n,t) reaction at low energies comes primarily om the constructive interference of J = ½ S-wave levels below the t-α thresh-d and above the n-^{6}Li threshold. Similar levels for the J = ½ P-wave transi-ons provide the forward-peaked background underlying the behavior of the i(n,t) angular distributions, although this contribution appears to be some-at too small in the region $0.4 \lesssim E_n \lesssim 1$ MeV.

A PWBA calculation of the deuteron exchange contribution to the reaction at takes into account the behavior of the internal bound-state wavefunctions gives, in addition to the pole normally encountered at negative squared momentum-transfer ($q^2 = -\beta^2$), poles at positive q^2 that interfere constructively (residues with opposite sign) with it. This is qualitatively the pole structure we see for the $s = \frac{1}{2}$ transitions in the R-matrix analysis, and suggests, along with the similarity of the shapes of the angular distributions calculated for those transitions with the PWBA results, that the dominant mechanism for the $s = \frac{1}{2}$ transitions in the Li(n,t) reaction is deuteron exchange.

Channel overlap terms that correspond to deuteron exchange in a simple model of the bound states for this reaction arise naturally in R-matrix theory with a properly consistent treatment of the scattering equations in both the internal and external regions. These terms, which are similar to the PWBA results except that they are unitary, may account for most of the $s = \frac{1}{2}$ transition strength observed in the ^{6}Li(n,t) reaction. The final results of the Los Alamos ^{7}Li R-matrix analysis, including these channel overlap effects, will be used in the combined ENDF/B-VI standards evaluation and in the Version VI general-purpose cross-section evaluation for ^{6}Li.

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