Fusion-energy reaction $^3H(d,\alpha)n$ at low energies

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We have extended our past measurements of the $^2H(t,\alpha)n$ reaction near the low-energy $\frac{3}{2}^+$ resonance by measuring eight more data points over the lab deuteron energy range 80—116 keV. This was accomplished by bombarding a tritium gas target with deuterons, in contrast to the previous measurements in which a deuterium gas target was bombarded with tritons. The present data are accurate to 1.6%. The results of including the present data in a simple two-channel, two-level, R-matrix analysis and also in a large three-channel, multilevel, R-matrix analysis are presented. The resonance is characterized by giving the S-matrix poles from the R-matrix analyses. Of interest is the discovery that both analyses give two resonance poles on different (unphysical) Riemann sheets, one of them being a so-called "shadow pole." This is the first experimental observation of a shadow pole in nuclear and particle physics. Maxwellian reactivities up to a plasma temperature of 20 keV are presented.

I. INTRODUCTION

The $^3H(d,\alpha)n$ reaction, dominated at low energies by a $J^\pi=\frac{3}{2}^+$ resonance, will no doubt be the reaction used to fuel the first fusion reactors. In a previous publication[1] we presented an accurate, detailed study of the $^2H(t,\alpha)n$ reaction. Those data covered a range of triton bombarding energies from 12.5 to 117 keV, which corresponds to an equivalent deuteron bombarding energy range from 8.3 to 78.1 keV along the low-energy side of the $\frac{3}{2}^+$ resonance. The center-of-mass energy at the high end was limited by the facts that our low-energy accelerator has a maximum voltage of about 117 kV and that we bombarded the lighter target, deuterium, with the heavier projectile, the triton. Later, we began to study[2,3] the $^3H(t,\alpha)nn$ reaction, and for that purpose we developed a system to flow tritium gas through our windowless gas target.[1] We were then able to augment the $^2H(t,\alpha)n$ data at the high energy end by bombarding the tritium target with deuterons. The cross sections at eight deuteron bombarding energies from 80 to 116 keV were measured to an absolute accuracy of 1.6%. We present here the results of these new measurements and their influence on R-matrix analyses and reactivity calculations. We also use a recently developed code to study the analytic properties of the S matrix generated by three different R-matrix analyses. This allows one to study whether the "character" of different R-matrix results are similar or not.

II. EXPERIMENT

The experiment was performed using the Low-Energy Fusion Cross Section (LEFCS) system installed at the Los Alamos Ion Beam Facility. Details of the apparatus, data-taking procedure, and data reduction techniques are given in Ref. 1. In brief, the experiment is performed by accelerating negatively charged deuterium ions through a windowless, cryogenically pumped, flowing gas target of tritium and into a beam calorimeter. The reaction α particles are detected at six fixed angles with silicon surface-barrier detectors. The accelerating voltage is determined using a 10^5 to 1 resistive divider whose calibrated is traceable to the National Bureau of Standards. The beam calorimeter is used to determine the beam intensity and is calibrated to 0.1% using the heat generated by a precision resistor embedded in it.

The main difference between the procedure for the present experiment and that of Ref. 1 is the manner in which the gas target density was determined. Even though we operated the target at a tritium flow rate equal to the deuterium flow rate used in Ref. 1 (5 std cm^3/min as read by a thermal-gradient flowmeter), the tritium target density was not necessarily the same as the deuterium target density. This is because (a) it was necessary to operate the tritium target at a temperature about 1 K higher than that of the deuterium target because of the higher freezing point for tritum, (b) the flow characteristics of tritium are different from those of deuterium, and (c) the presence of contaminants of 0.5% deuterium and a few percent helium-3 also affects the relationship between the measured flow rate and the density. To determine the number of tritium atoms per cm^3 here, we simply measured the $^3H(d,\alpha)n$ reaction rate at four of the energies previously used in Ref. 1 and then used the Ref. 1 cross sections to determine the density. Over the time period during which we performed the present experiment, we found the tritium density to average only about 3% higher than that of the deuterium in Ref. 1.

III. RESULTS

The methods of data reduction and error determination are discussed in great detail in Ref. 1 and will not be mentioned here. The present cross sections have a relative error (standard deviation) of 0.8% and a scale error of 1.4%, resulting in an overall error of 1.6%. The deuteron bombarding energies are accurate to 15 eV, and the energy spread is about 40 eV [full width at half maximum

(FWHM)]. As discussed in Ref. 1, it is useful for comparison purposes to convert the cross sections to the so called astrophysical S function, which factors out from the cross section the energy dependences of the de Broglie wavelength and the Coulomb penetrability. For reactions having a d + t incident channel, S is given by

$$S = 0.599\,62 \sigma E_{\rm d} \exp(1.40411 E_{\rm d}^{-1/2}) , \quad (1)$$

where σ is the cross section in b (barns), $E_{\rm d}$ is the deuteron bombarding energy in MeV, and S is expressed in MeV b. The present measurements are listed in Table I, and the S function extracted from the present and previous[1] data is plotted in Fig. 1. These 25 data points will be referred to as the LEFCS data. We find that the cross section peaks near 107.5 keV with a value of about 4.9 b; the S function peaks at a lower energy, around 81 keV.

In Ref. 1 our data were compared in detail with those of others. Here we will not illustrate such comparisons, but will restrict ourselves to the following comments. The present data agree with those of Argo *et al.*,[4] Arnold *et al.*,[5] and Kobzev *et al.*,[6] but are systematically a few percent below those of Conner *et al.*[7] and of Katsaurov.[8] Taking into account both the present data and our earlier data of Ref. 1, which together cover the deuteron lab energy range of from 8 to 116 keV, we find the best overall agreement with the work of Arnold *et al.*[5]

IV. CALCULATIONS

A. Two-channel, two-level, R-matrix analysis

R-matrix theory[9] has been used extensively in describing reactions among light nuclei, and, in particular, has been used to increase our understanding of reactions important for fusion energy.[10] As in Ref. 1, we have assembled a data base for use in an R-matrix analysis with deuteron bombarding energies up to about 250 keV. Besides the present data, we include, as before,[1] the data from Refs. 1 and 5–8. To remain consistent with the method used in Ref. 1, total errors were used in the fitting procedure.

An attempt to perform a single-level fit to this database showed that with the present data in the base it was not possible to obtain a minimum in χ^2 space with reasonable values of the parameters, the indication being that a background level was needed at an energy some distance from the $\frac{3}{2}^+$ resonance. It is known from the multilevel approach to this problem[10] that a $\frac{3}{2}^+$ background is present with a level energy around 10 MeV. Thus we performed a two-level ($\lambda = 1$ and 2), two-channel (d + t, denoted by d, and α + n, denoted by α) fit to the database with the $\lambda = 2$ level energy E_2 fixed at 10 MeV. With the channel radii a_c and the boundary-condition parameters B_c chosen as in Ref. 1, there remain the following five fitting parameters: the level energy E_1 for $\lambda = 1$, and four reduced widths $\gamma_{\lambda c}$, with $\lambda = 1,2$ and $c = {\rm d},\alpha$. A fit to the database was achieved with a χ^2 per degree of freedom of 1.34 for 185 data points. The value of 1.34 represents two standard deviations in χ^2 space, which is a reasonably good fit considering the amount of disagreement among the data sets used (see Fig. 11 of Ref. 1 for an illustration of the database). This fit is shown as the dashed curve in Fig. 1, and the R-matrix parameters are listed in Table II. The solid curve in Fig. 1 is discussed in Sec. IV B. The two-level fit reproduces the low-energy (< 80 keV) data of Ref. 1 somewhat better than does the single-level fit of that reference. However, the fit is systematically one to two standard deviations above the present high-energy (> 80 keV) data. Varying the level energy E_2 of the background level by several MeV in either direction does not change this conclusion. It appears that the data at energies above our measurements (up to 250 keV) exert

TABLE I. Integrated cross section σ and astrophysical S function for the ^{3}H(d,α)n reaction. The relative error (standard deviation) is 0.8% and the scale error is 1.4%, giving a total error of 1.6%. The lab deuteron energy $E_{\rm d}$ is accurate to 15 eV.

$E_{\rm d}$ (keV)	σ (mb)	S (MeV b)
79.913	3849	26.48
84.912	4259	26.84
89.904	4444	25.89
94.903	4698	25.50
99.902	4779	24.33
104.901	4882	23.44
109.901	4836	22.02
115.901	4734	20.34

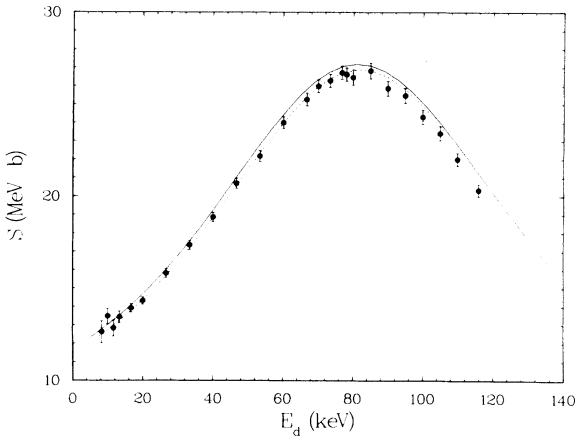

FIG. 1. S function [Eq. (1)] vs deuteron lab energy $E_{\rm d}$ for the ^{3}H(d,α)n reaction. The eight highest-energy points show the present data, and the remaining points are those of Ref. 1, having been measured with essentially the same apparatus as used in the present experiment. Total errors are shown. The dashed curve is from a two-level, two-channel, R-matrix fit to a database including the data shown and other data selected from the literature (see Ref. 1) up to a deuteron energy of 250 keV. The solid curve is from a three-channel, multilevel, R-matrix fit using a much larger database extending up to a deuteron lab energy of 8 MeV. The single-level fit of Ref. 1 (not shown) falls between the two curves at the lowest energies, drops to 0.7% below the dashed curve as the energy is raised to 30 keV, rises to 0.3% above the solid curve as the energy is further raised to 90 keV, and then drops again to about 0.4% below the dashed curve at 140 keV.

TABLE II. Parameters for the two-level fit discussed in Sec. IV A. The level energies E_λ are channel independent. E_2 was held fixed in the fit.

Channel	a_c (fm)	B_c	L	γ_{1c} (MeV$^{1/2}$)	E_1 (MeV)	γ_{2c} (MeV$^{1/2}$)	E_2 (MeV)
d + t	5.00	−0.278 64	0	0.958 38	0.021 626	0.483 04	10.0000
α + n	3.00	−0.557 00	2	0.277 81	0.021 626	1.517 53	10.0000

enough influence on the fit to widen slightly the resonance structure over that indicated by the present data alone. This happens even though the LEFCS data have errors significantly smaller than those of the other data.

The covariance matrix,[11] or error matrix,[12] for the two-level fit is listed in Table III. This matrix is defined as being twice the inverse of the matrix of second derivatives of χ^2 with respect to the fitting parameters, the derivates being evaluated at the χ^2 minimum. Often the square root of the diagonal elements of the error matrix are quoted as the errors in the fitting parameters; however, that procedure does not take the correlations among the parameters into account. We use the full covariance matrix to compute the error in the fitted curve, and to account for "poorness of fit" we increase that result by multiplying by 1.157, the square root of χ^2 per degree of freedom. The result is as follows: The absolute standard deviation in the S function or in σ is about 0.8% near the highest energy (E_d=250 keV) of the database, drops gradually to about 0.4% as E_d drops to 100 keV, and then rises to about 0.7% as E_d decreases to 8 keV. For S_0, the S function extrapolated to zero energy, we find 11.45±0.08 MeV b, which is 1.75 standard deviations below the value obtained from the single-level fit of Ref. 1.

B. Three-channel, multilevel R-matrix analysis

A three-channel, multilevel R-matrix analysis[10] of reactions in the ^{5}He system has been in progress for the past several years, with the experimental database being continually updated as new measurements became available. For example, the stage of the analysis as it existed at the time of publication of Ref. 1 was such that the fit was about 7% below the data of Ref. 1. Recently, the database has stabilized, and the analysis has converged to a relative minimum in the χ^2 surface, having a χ^2 value of 1.55 per degree of freedom. Details of the analysis will be reported elsewhere, but we can summarize some of the features as follows.

The multilevel analysis employs three arrangement channels and contains data for the reactions ^{3}H(d,d)^{3}H, ^{3}H(d,n)^{4}He, and ^{3}H(d,n)^{4}He*(0$^+$, 20.1 MeV) at deuteron lab energies up to about 8 MeV, and contains data for ^{4}He(n,n)^{4}He scattering and the n + ^{4}He total cross section up to a lab neutron energy of 28 MeV. Although the database, comprising 2520 points, is not exhaustive, it contains many polarization measurements as well as the most recent n + ^{4}He total cross-section measurements,[13] and the ^{3}H(d,n)^{4}He integrated cross sections reported here and in Ref. 1. These data are fitted simultaneously by 97 free R-matrix parameters, which are required to describe numerous states of the compound system found in this energy range and to describe the contributions of distant-level background poles. Most of the levels above the d + t threshold have positive parity, like the low-energy $\frac{3}{2}^+$ resonance of interest here.

Because the present data and those of Ref. 1 represent the most accurate ^{3}H(d,n)^{4}He reaction cross sections yet measured, it was decided to treat those data in the most consistent way possible in the multilevel fit. Therefore, those 25 points, along with the four overlap points taken to determine the normalization of the present data (see Sec. III), were entered into the database with their relative errors only. Two variable normalizations that multiply the data were then treated as follows. The 17 lowest energy data points[1] were tied to one normalization N_1 with their scale error of 1.26%. The eight present data points plus the four overlap points were tied to a second normalization N_2. Although this second normalization was unrestricted in the sense that no scale error was specified, it is, in fact, restricted through the presence of the four overlap

TABLE III. Elements of the symmetric covariance matrix for the two-level fit discussed in Sec. IV A. The elements have units of MeV$^{1/2}$ and are indexed as follows: 1=$\sqrt{E_1}$, 2=γ_{1d}, 3=γ_{2d}, 4=$\gamma_{1\alpha}$, and 5=$\gamma_{2\alpha}$. The level energy E_2 was held fixed in the fit. The numbers in square brackets give the power of 10 by which the preceding number is to be multiplied.

	1	2	3	4	5
1	0.217 78[−5]				
2	−0.351 13[−5]	0.400 25[−3]			
3	0.631 10[−4]	0.241 11[−2]	0.281 02[−1]		
4	0.280 73[−6]	0.800 92[−4]	0.580 10[−3]	0.170 80[−4]	
5	0.114 52[−4]	0.557 31[−3]	0.686 96[−2]	0.132 42[−3]	0.174 71[−2]

points that occur in an energy region of restricted normalization. This procedure most closely represents the way the data were actually obtained. The resulting normalizations are

$$N_1 = 1.01781 \ , \quad N_2 = 1.02495 \ . \tag{2}$$

Thus this procedure gives a scale renormalization of the 17 low-energy points upward by 1.41 standard deviations and of the eight high-energy points upward by 1.78 standard deviations.[14]

The relative deviations of the 29 measured points from the fit are illustrated in Fig. 2. All the measured cross sections and errors are scaled by the appropriate normalization factor (N_1 or N_2) and divided by the calculated cross section. All but eight of the values lie within one standard deviation of unity, and they appear to be randomly distributed, except possibly for the upper-energy points. Thus, the multilevel analysis gives a very good fit to the energy dependence of the LEFCS data.

An interesting feature of both the two-level and multilevel fits is the fact that the unitary limit is nearly attained by the reaction S matrix near 135 keV deuteron bombarding energy (i.e., $|S_{d,\alpha}^{3/2+}|$ is close to unity). In fact, for the multilevel fit this approach is so close that the error corridor narrows significantly at the energy. Both fits give a maximum cross section very close to 5.0 b at 107.5 keV. The multilevel fit gives a value for S_0, the S function extrapolated to zero energy, of 11.71 ± 0.08 MeV b, which is 2.3% higher than the S_0 from the two-level fit (Sec. IV A).

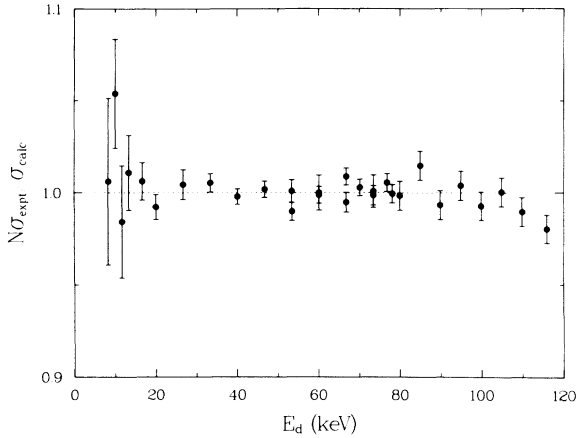

FIG. 2. Ratio of the normalized experimental cross section to the cross section calculated from the three-channel, multilevel, R-matrix fit for the LEFCS data plus the four overlap points. E_d is the lab deuteron energy, and the bars indicate relative errors.

C. Poles of the S matrix

It has been pointed out[1,15] that it is not always easy to interpret the parameters of the R matrix, especially for a complicated multilevel analysis, and that it would be better to extract resonance parameters from an asymptotic quantity such as the S matrix. One of us (G.M.H.) has used the elegant complex Coulomb function routine of Thompson and Barnett[16] to develop a computer code that finds the poles and residues of the S matrix given a set of R-matrix parameters as input. The definitions of Humblet and Rosenfeld[17] are used to relate the poles and residues to resonance energies and widths. We have applied this code to the single-level fit reported in Ref. 1 and to both the two-level and multilevel analyses described here. The results are listed in Table IV.

In each case, a single R-matrix level contributes more than 99% of the pole structure associated with the $\frac{3}{2}^+$ resonance. Two poles are found on different (unphysical) Riemann sheets in complex energy space for the many-channel S matrix. The pole designated "M" in Table IV, with a width of about 74 keV, is clearly the main pole associated with the structure observed in the low-energy ^{3}H(d,n)^{4}He cross section and in the n + ^{4}He total cross section at neutron energies near 22.13 MeV. The other pole, designated "S" for "shadow" pole in the terminology introduced by Eden and Taylor,[18] lies close to the real energy axis of a different unphysical sheet at a c.m. energy of about 80 keV, and is indirectly responsible for driving the reaction S-matrix element close to its unitary limit near $E_d = 135$ keV. This is the first experimental evidence for the existence of shadow poles in nuclear and particle physics. A more complete discussion of the properties of these poles and their interpretation is given elsewhere.[19]

TABLE IV. S-matrix resonance parameters. The resonance energy E_r, the partial widths Γ_d and Γ_α, and the total width Γ are given in keV in the center-of-mass system.

Fit	Pole	E_r	Γ_d	Γ_α	Γ
Ref. 1	M	48.24	33.07	38.83	71.90
	S[a]	78.05	10.01	8.14	18.15
Two-level	M	48.10	25.77	48.39	74.16
	S	78.94	16.10	0.42	16.52
Multilevel	M	46.97	27.69	46.51	74.20
	S	81.57	7.11	0.17	7.28

[a]This shadow pole appears on a different Riemann sheet from the one on which the shadow pole lies in the two-level and multilevel analyses.

D. Reactivity calculations

As discussed in Ref. 1, the reactivity $\langle \sigma v \rangle$ of a d + t plasma in thermal equilibrium at temperature T can be written in a form in which its main temperature dependence, which arises from the energy dependences in the cross section produced by the de Broglie wavelength and the Coulomb penetrability, is factored out, leaving a Maxwell-Boltzmann averaged S function $\langle S \rangle$. For convenience we repeat here Eqs. (13) and (14) of Ref. 1,

$$\langle \sigma v \rangle = 5.967 \times 10^{-16} \langle S \rangle \tau^2 e^{-\tau} [1 + 5/(12\tau)] , \quad (3)$$

with

$$\tau = 19.983/(kT)^{1/3} , \quad (4)$$

where k is Boltzmann's constant, kT is in keV, $\langle \sigma v \rangle$ is in cm^3/s, and $\langle S \rangle$, which is a function of kT, is in MeV b.

In Ref. 1 the function $\langle S \rangle$ calculated from a single-level fit was compared with several other reactivity calculations from the literature over the plasma temperature range $kT = 0$–20 keV. Here in Fig. 3 we compare $\langle S \rangle$ from our two-level fit with $\langle S \rangle$ from the multilevel analysis. In those calculations, cross sections up to $E_d = 500$ keV were used, although the bulk of the contributions to the reactivity integral comes from data below a few hundred keV. As would be indicated from Fig. 1 or from the normalizations of Eq. (2), the multilevel fit gives reactivities a percent or two higher than those from the two-level fit. The reactivities from the single-level fit of Ref. 1 are close to those of the present two-level analysis.

E. Polynomial fits

In Ref. 1 (Tables IX and X; however, see the erratum for Table X) to make calculations easier for those who don't have access to an R-matrix code, polynomial expressions were given for the low-energy portion of the S function and for the reactivity function $\langle S \rangle$. In Tables V and VI we give the results of such fits for both the two-level and multilevel analyses. The cross section σ and reactivity $\langle \sigma v \rangle$ can then be calculated by applying Eqs. (1), (3), and (4). We should stress that Table V represents only the low-energy tail of the S function ($E_d < 78$ keV) and is *not* valid across the peak of the S function and down the high-energy side.

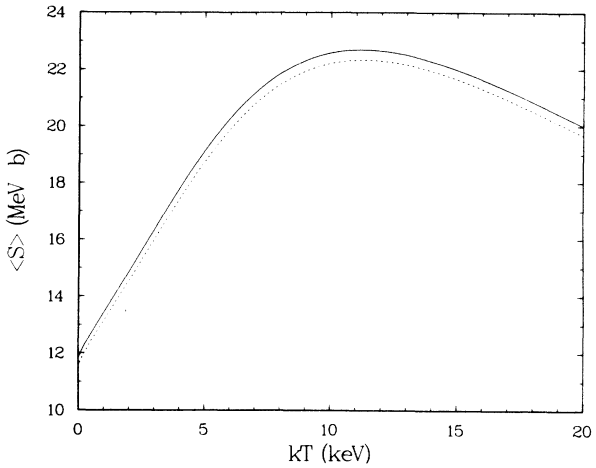

FIG. 3. Maxwell-Boltzmann averaged S function $\langle S \rangle$ vs plasma temperature from which the ^{3}H(d,α)n reactivity $\langle \sigma v \rangle$ can be calculated using Eqs. (3) and (4). The solid curve represents the calculation using the multilevel fit, and the dashed curve represents the calculation using the two-level fit. The result of the single-level fit of Ref. 1 (not shown) is closer to the dashed curve than to the solid curve, generally falling within 0.5% of the dashed curve. The single-level fit is below the dashed curve in the kT range of about 2–7 keV and is above the dashed curve over the rest of the range.

V. CONCLUSION

The accurate measurements of Ref. 1 for the ^{3}H(d,α)n reaction near the low energy $\frac{3}{2}^+$ resonance have here been extended over the resonance peak. The same apparatus was used as in Ref. 1, with the windowless-target, gas-handling system having been modified to allow tritium to be used as a target in place of the deuterium of Ref. 1. The LEFCS data and data of others were formed into databases and were analyzed with R-matrix theory. A database of 185 points containing only ^{3}H(d,n)^{4}He reaction data up to a deuteron bombarding energy of 250 keV was used in a two-level, two-channel analysis. A broad-range, three-channel, multilevel analysis[10] was also carried out with a database of 2520 points containing data in addition to those for the ^{3}H(d,n)^{4}He reaction. The S-matrix poles

TABLE V. Coefficients e_n of a polynomial fit, $\sum e_n E^n$, in c.m. energy E to the low-energy portion of the S function for both the two-level and multilevel analyses. To convert to a series in deuteron bombarding energy E_d, multiply e_n by $(0.599\,62)^n$, or to convert to a series in triton bombarding energy E_t, multiply e_n by $(0.400\,38)^n$. The fit is valid for E, E_d, and E_t less than 46.8, 78.0, and 117.0 keV, respectively. The errors in reproducing S are less than 0.04% (two-level) and 0.06% (multilevel), except that right at the high end of the energy range those errors are twice as large. The units of e_n are such that S is in MeV b when the energies are in keV. The numbers in square brackets specify the power of 10 that multiplies the given coefficient.

Two-level	n:	0	1	2	3	4
	e_n:	11.4481	0.199 327	0.154 785[−2]	0.229 324[−3]	−0.435 653[−5]
Multilevel	n:	0	1	2	3	4
	e_n:	11.7055	0.200 546	1.83 398[−2]	0.229 448[−3]	−0.448 764[−5]

TABLE VI. Coefficients t_n of a fit in plasma temperature kT to the Maxwell-Boltzmann averaged S function $\langle S \rangle$ for both the two-level and multilevel analyses. The polynomial used is $\sum t_n z^n$ with $z=(kT)^{1/3}$. The series is valid for kT from 0 to 20 keV with a maximum error in reproducing $\langle S \rangle$ of 0.03%. The units of t_n are such that $\langle S \rangle$ is in MeV b when kT is in keV.

			Two-level			
n:	0	1	2	3	4	5
t_n:	11.460 964 04	1.379 083 402	−15.969 594 78	87.390 346 78	−240.913 021 7	406.473 976 1
n:	6	7	8	9	10	11
t_n:	−438.803 216 4	308.175 235 4	−139.195 696 4	38.789 040 70	−6.051 290 500	0.403 836 417
			Multilevel			
n:	0	1	2	3	4	5
t_n:	11.717 977 54	1.1477 016 57	−13.587 751 18	77.194 876 09	−216.758 259 9	371.800 188 4
n:	6	7	8	9	10	11
t_n:	−407.262 675 7	289.750 209 7	−132.349 737 5	37.233 710 70	−5.855 386 481	0.393 425 156

for these two fits were very similar and also very similar to the poles from the single-level fit of Ref. 1. Reactivities in a Maxwellian plasma for the ^{3}H(d,n)^{4}He reaction were computed for both fits. For convenience in applications of these results, polynomial expressions are given that reproduce the low energy portion of the S function and the calculated reactivities. Users of these cross sections and reactivities may choose the results of either fit depending on whether they prefer one that more closely represents the LEFCS data (two-level fit) or one that more closely represents a very broad range of data and requires a modest renormalization of the LEFCS data (multilevel fit). For applications at energies below the peak of the S function, we suggest using the results of the two-level fit.

We have completed data taking with the LEFCS apparatus for ^{2}H(d,t)^{1}H, ^{2}H(d,^{3}He)n, and ^{3}H(t,α)nn, and the data for these other fusion-energy reactions are in the process of being analyzed.

ACKNOWLEDGMENTS

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