REICH-MOORE AND ADLER-ADLER REPRESENTATIONS OF THE ^{235}U CROSS SECTIONS IN THE RESOLVED RESONANCE REGION

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ABSTRACT

In the first part of this paper, a reevaluation of the low-energy neutron cross sections of ^{235}U is described. This reevaluation was motivated by the discrepancy between the measured and computed temperature coefficients of reactivity and is based on recent measurements of the fission cross section and of η in the thermal and subthermal neutron energy regions. In the second part of the paper, we discuss the conversion of the Reich-Moore resonance parameters, describing the neutron cross sections of ^{235}U in the resolved resonance region, into equivalent Adler-Adler resonance parameters and into equivalent momentum space multipole resonance parameters.

INTRODUCTION

A new evaluation of the ^{235}U resolved resonance range for the neutron cross sections of ^{235}U was recently completed and submitted for ENDF/B-VI. This evaluation was described in detail elsewhere.[1] Since completion of the evaluation, new very low energy measurements of the fission and total cross sections[2,3] and of η[4,5] have become available and have led to a reevaluation of the low-energy region. The first part of this paper concerns this reevaluation. In the second part of the paper, alternative representations of the evaluation of the ^{235}U neutron cross sections in the resolved resonance range are discussed.

THE LOW-ENERGY CROSS SECTIONS OF ^{235}U

Reactor physicists have pointed out for some time that a significant discrepancy existed between the computed and measured values of the temperature coefficient of reactivity in thermal reactors.[6] A careful examination of the sensitivities of this reactor parameter to differential neutron cross sections has led several authors to suggest that the discrepancy was due, at least in part, to an erroneous shape of the evaluated uranium cross sections and of η for ^{235}U in the thermal region.[7,8,9] Such considerations led to a program of careful measurements of the uranium cross sections and of η in the thermal and subthermal neutron energy ranges.[2,4,5] At the time of this writing the corrections on one of the new η measurements[5] are not yet finalized, and there is a new measurement of η in progress;[4] yet there is already some evidence[5] that η increases by 1 or 2% with energy in the range 1 to 100 meV. This is just the behavior suggested by the reactor physicists to improve the calculation of the moderator coefficient of reactivity.

Gwin et al.[10] have measured the variation of $\bar{\nu}$ for ^{235}U from a few meV up and found this parameter constant to a fraction of 1% below 1 eV; therefore the variation of η must be due to a variation of the ratio of the capture to the fission cross sections. Since the contribution of the distant levels to the fission or capture cross sections in the meV energy range is proportional to $1/v$, the variation of the ratio of the capture to the fission cross sections in that region implies the existence of a small resonance in the vicinity of the binding energy.

In order to represent the measured variation of η at low energy, a small level was introduced near the binding energy, and the parameters of that level and of the nearby resonances were searched using the resonance analysis code SAMMY[11] to fit the low energy fission cross section measurement of Wagemans et al.,[2] the transmission measurement of Spencer et al.[12] and a derived capture cross section obtained from the η measurement of Weigmann[5] and the fission cross section of Wagemans et al., assuming a constant value of 2.432 for $\bar{\nu}$.[13]

The resonance parameters given in Table I describe the new evaluated data up to 4.0 eV. Note that the parameters of the levels above 4.0 eV, like those of the bound levels, have been adjusted to compensate for the truncated levels so that the parameters of Table I are not intended to represent the cross sections outside the range 0 to 4.0 eV. To represent the cross sections above 4.0 eV, the previous evaluation should be used unchanged, with the previously defined resonance parameters for the levels below 4.0 eV.

A comparison of η computed from the resonance parameters of Table I with the measurements of Weigmann is shown in Fig. 1. The error bars are the sum of the statistical and systematic errors, added linearly as suggested by Weigmann.[5] The data were obtained in two measurements: one measurement, done at the Central Bureau for Nuclear Measurements Electron Linear Accelerator of Geel (Belgium), covers the energy range 1.8 to 465 meV; the other measurement, done at the Institut Laue-Langevin reactor at Grenoble, covers the range 1.5 to 150 meV. A comparison of the fission cross section computed from the same resonance parameters, with the recent measurement of Wagemans et al.,[2] is shown in Fig. 2. As seen in Figs 1 and 2, the evaluation is consistent with the fission measurement in the subthermal energy range and with the new η measurements.

The values of the fission and capture widths of the level nearest the binding energy are very small. These widths are somewhat constrained by the requirements of reproducing the cross-section values at 0.0253 eV and the Westcott g-factors recommended by the ENDF/B-VI standards committee,[13] as well as the measured shape of η in the subthermal region. The values obtained for the thermal parameters with the resonance parameters of Table I are compared to the values recommended by the ENDF/B-VI standards committee in Table II.

TABLE I

Evaluated Reich-Moore Resonance Parameters for the Energy Region 0 to 4.0 eV in ENDF/B Format

E (eV)	Γ_γ (meV)	Γ_n (meV)	Γ_{f1} (meV)	Γ_{f2} (meV)	J
−100.00	38.92	11.458	0.123	72.264	3
−90.00	37.00	2.422−3	56.114	−216.68	4
−4.2976	35.00	7.1641	318.98	−115.23	4
−3.4934	38.00	8.472−5	−6.753	12.973	3
−1.5043	37.87	8.520−5	−7.004	12.309	3
−0.41161	30.00	0.14875	−1.026	−155.26	3
−0.19428	35.22	5.045−4	198.76	−1.692	4
3.657−5[a]	30.00	6.505−8	−0.526	0.964	4
0.28190	38.57	0.00444	106.43	−4.845	3
1.1389	38.69	0.01381	−0.005	112.6	4
2.0361	37.76	8.950−3	−8.046	−1.637	3
2.7767	37.00	1.274−3	62.366	−43.82	4
3.1566	38.00	0.02422	−82.492	17.706	3
3.6208	36.00	0.04129	−27.76	29.516	4
4.8508	35.97	0.07169	0.048	−3.828	4
5.4497	37.00	0.03840	−80.508	−369.36	4
6.2094	38.00	0.16621	−110.94	75.912	3
6.3913	36.71	0.25177	10.327	0.163	4
7.0860	38.54	0.14362	0.226	29.959	4
7.6394	38.00	4.768−3	104.92	155.15	3
8.7726	32.77	1.5832	27.581	−70.354	4
12.400	39.02	3.4064	−2.701	26.655	3
19.293	37.00	12.113	−5.849	57.741	4

[a] Read 3.657−5 as 3.657*10.**−5.

Table II

Comparison of 2200 m/s cross sections and Westcott g-factors

Cross Section	Standards* (b)	This Evaluation (b)
Total	698.67 ± 1.71	697.48
Scattering	15.46 ± 1.06	14.32
Absorption	683.22 ± 1.34	683.16
Fission	584.25 ± 1.11	584.35
Capture	98.96 ± 0.74	98.81
Westcott g_f	.9771 ± .0008	.9777
Westcott g_a	.9790 ± .0008	.9793

*ENDF/B-VI Standards Committee (ref. 13).

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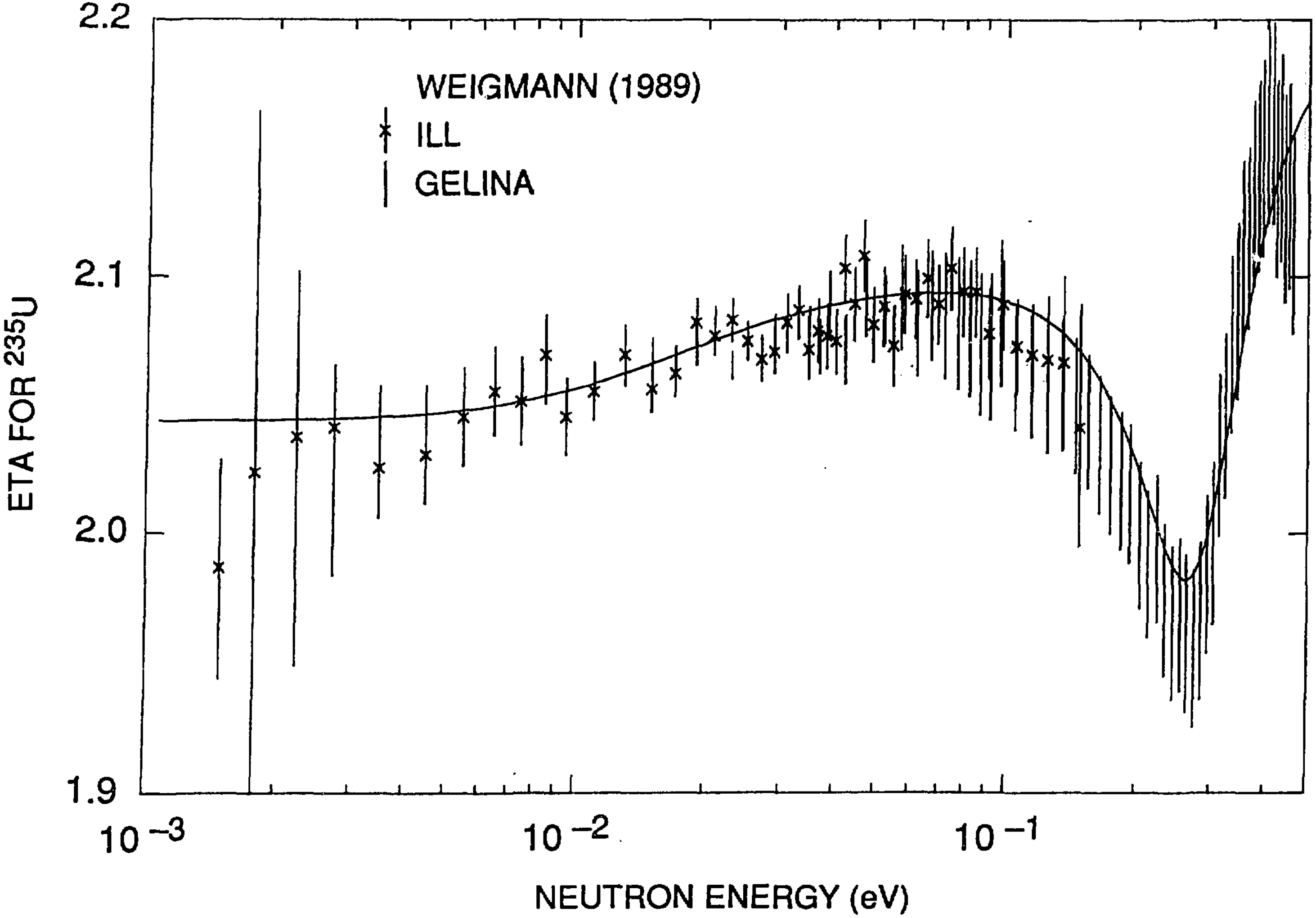

Fig. 1. Comparison of η for ^{235}U obtained from the resonance parameters of Table I, with the results of the two measurements of Weigmann.[5] The error bars represent the sum of the statistical and systematic uncertainties.

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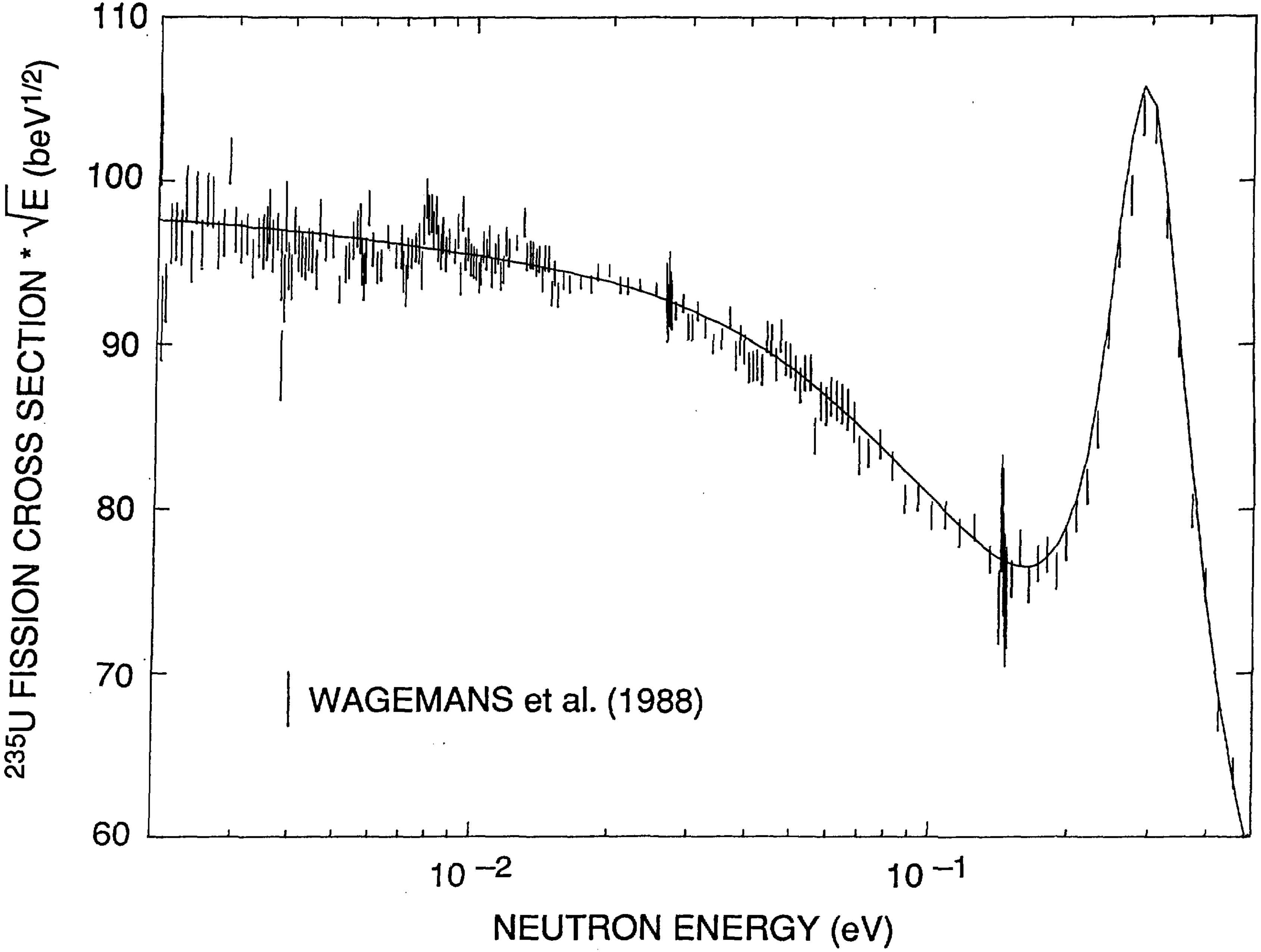

Fig. 2. Comparison of the ^{235}U fission cross section computed with the resonance parameters of Table I with the results of the measurement of Wagemans et al.[2]

ALTERNATE REPRESENTATIONS OF THE ^{235}U RESOLVED RESONANCE REGION

Several multilevel formalisms are available to describe the neutron cross sections of the fissile nuclides. The most frequently used are the Reich-Moore and Adler-Adler formalisms which are specializations of the general dispersion theory of Wigner and Eisenbud.[14]

The resonance analysis of the cross sections was done with the code SAMMY,[11] using the Reich-Moore formalism,[15] because this formalism is unitary and yields R-matrix resonance parameters which are easier to interpret than the parameters of the Adler-Adler formulation.[16] Indeed, up to 500 eV the statistical distributions of the partial widths and level spacings were found consistent with the distributions expected from R-matrix theory,[17] increasing the confidence in the results of the analysis. Furthermore, much use was made of the Dyson-Metha Δ_3 statistics[18] to assign the spin of resonances where the spin separated fission data were ambiguous and to determine where small resonances should be added to improve the fit to the data. As was observed by several authors, the Δ_3 statistics is very sensitive to missing levels.[19,20]

For describing the cross sections for practical applications such as reactor calculations, the Adler-Adler representation might be more convenient because it is particularly well suited for the calculation of Doppler-broadened and self-shielded cross sections, using Voigt profiles and the generalized J-function. Fröhner[21] has demonstrated a technique for the direct calculation of Doppler-broadened Reich-Moore cross sections which is as fast as the Adler-Adler calculation with Voigt profiles. Fröehner's method is most efficient when the cross sections are broadened on a specific predetermined energy mesh. For reactor calculations, the Adler-Adler formulation or the multipole expansion recently proposed by Hwang[22] may be more suitable.

The Adler-Adler representation of the cross sections is not rigorously equivalent to the Reich-Moore representation since it neglects the momentum dependance of the neutron width contribution to the total width. Adler and Adler[23] have investigated the effect of this approximation and found that the effect on the cross sections was small as long as the reduced neutron width was smaller than the other partial widths. This condition is generally fulfilled for ^{235}U and for the other fissile nuclei.

Hwang[22] has described a rigorous formalism based on a rational expansion of the Reich-Moore cross-section formula in momentum space. The problems with this approach are that it is not an accepted formalism of ENDF/B[23] and that it requires twice as many resonance parameters as does the Adler-Adler formulation. However, the formalism represents rigorously the cross sections and can use the Voigt profiles for Doppler broadening. Hwang[22] has shown how the formalism can be made very similar in form to the Adler-Adler formulation, by taking advantage of the general characteristics of the resonance poles.

We have used the POLLA option of the code WHOPPER of Hwang[22] to transform the Reich-Moore resonance parameters describing the ^{235}U cross sections into equivalent Adler-Adler parameters. We have then compared the cross sections computed with the Adler-Adler parameters to those computed with the Reich-Moore parameters. The largest absolute differences between the two sets of cross sections are below 0.2 eV, where it may not be advisable to use the Adler-Adler parameters anyway since at these low energies the Doppler broadening is not represented correctly by the Voigt profiles. The largest relative differences in the unbroadened total absorption and fission cross sections, below and above 4.0 eV, are listed in Table III. The unbroadened fission cross sections below 4.0 eV and between 30 and 50 eV are shown on Figs. 3 and 4. The figures also show the absolute differences between the fission cross sections computed with the Reich-Moore formalism and the fission cross sections computed with the Adler-Adler formalism.

We have also used the POLLY option of the code WHOPPER to obtain the expansion in momentum space of the cross-section representations and verified that the cross sections computed with the multipole parameters were numerically equal to the cross sections computed with the Reich-Moore parameters. The Adler-Adler resonance parameters describing the cross sections below 4.0 eV and corresponding to the Reich-Moore parameters of Table I are given in Table IV. The corresponding momentum space multipole parameters are listed in Table V. The evaluated Reich-Moore resonance parameters and the equivalent Adler-Adler and multipole parameter sets describing the cross sections above 4.0 eV are available from the authors.

We believe that the accurate representation of the ^{235}U evaluations with Adler-Adler parameters and the exact representation with multipole parameters in momentum space should provide useful alternatives to the Reich-Moore formalism for reactor codes, like MC^2,[23] which use the Voigt profiles and J-functions.

Table III

Comparison of cross sections computed with Reich-Moore resonance parameters and equivalent Adler-Adler parameters

For each energy range the maximum relative differences are listed:

$$\delta = \frac{|\sigma_{AA} - \sigma_{RM}|}{\sigma_{RM}}.$$

(The energy of that maximum difference is given in parentheses.)

Cross section	0–4 eV	4–110 eV	110–300 eV	300–500 eV
Total	0.00013 (10^{-5} eV)*	0.0067 (81 eV)	0.0022 (209 eV)	0.0029 (425 eV)
Absorption	0.0023 (10^{-5} eV)*	0.018 (110 eV)	0.034 (283 eV)	0.0091 (321 eV)
Fission	0.00009 (10^{-5} eV)*	0.00004 (19.4 eV)	0.00002 (262 eV)	0.00002 (627 eV)

*Minimum value at which the cross sections were computed.

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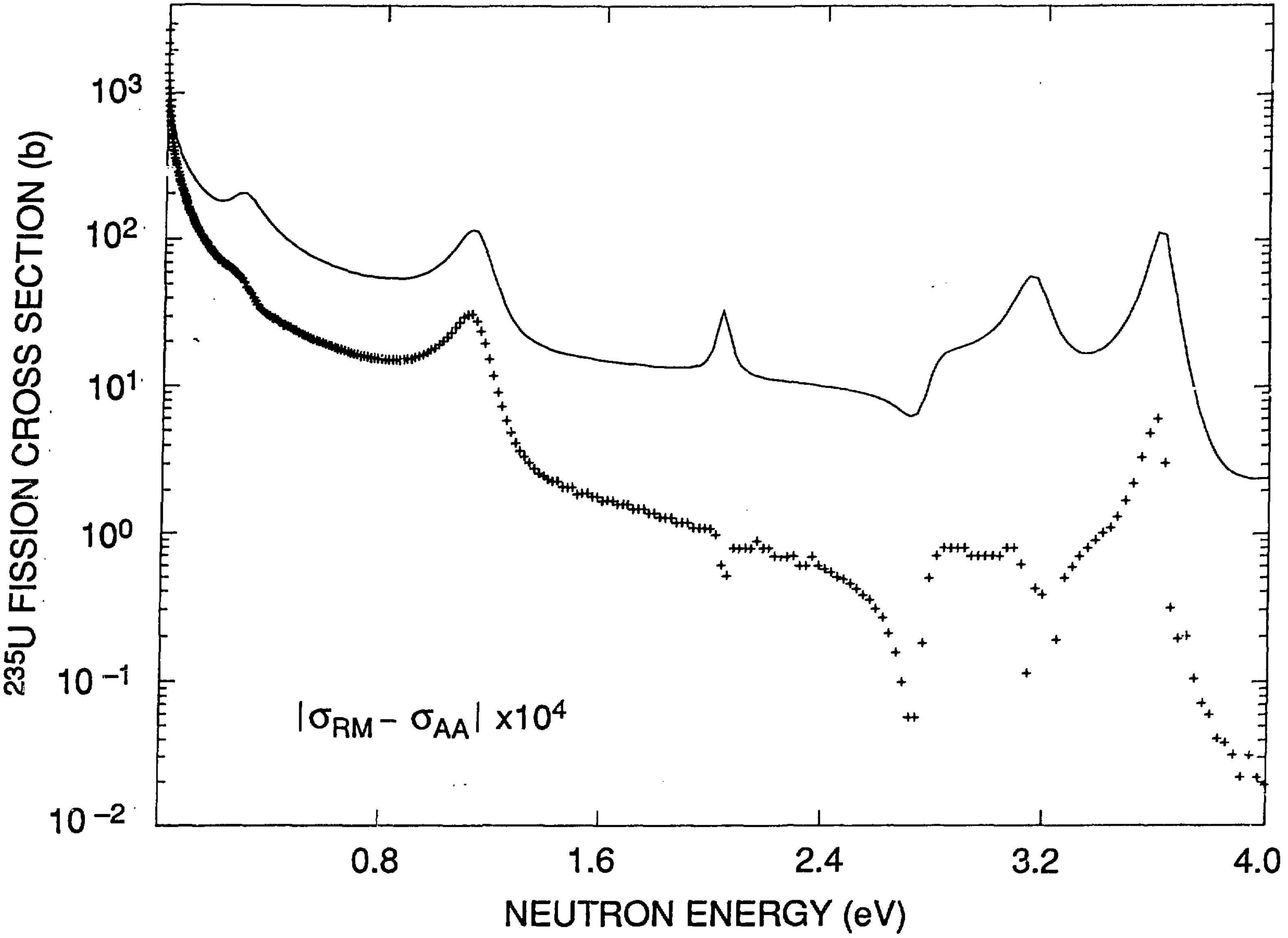

Fig. 3. Unbroadened fission cross section of ^{235}U up to 4.0 eV. The upper curve is the unbroadened fission cross section computed with the evaluated Reich-Moore resonance parameters of Table I. The lower curve is the difference between the cross section computed by the Reich-Moore formalism and the cross section computed by the Adler-Adler formalism with the parameters of Table IV. The absolute value of the difference was multiplied by 10000 so as to be on the scale of the figure.

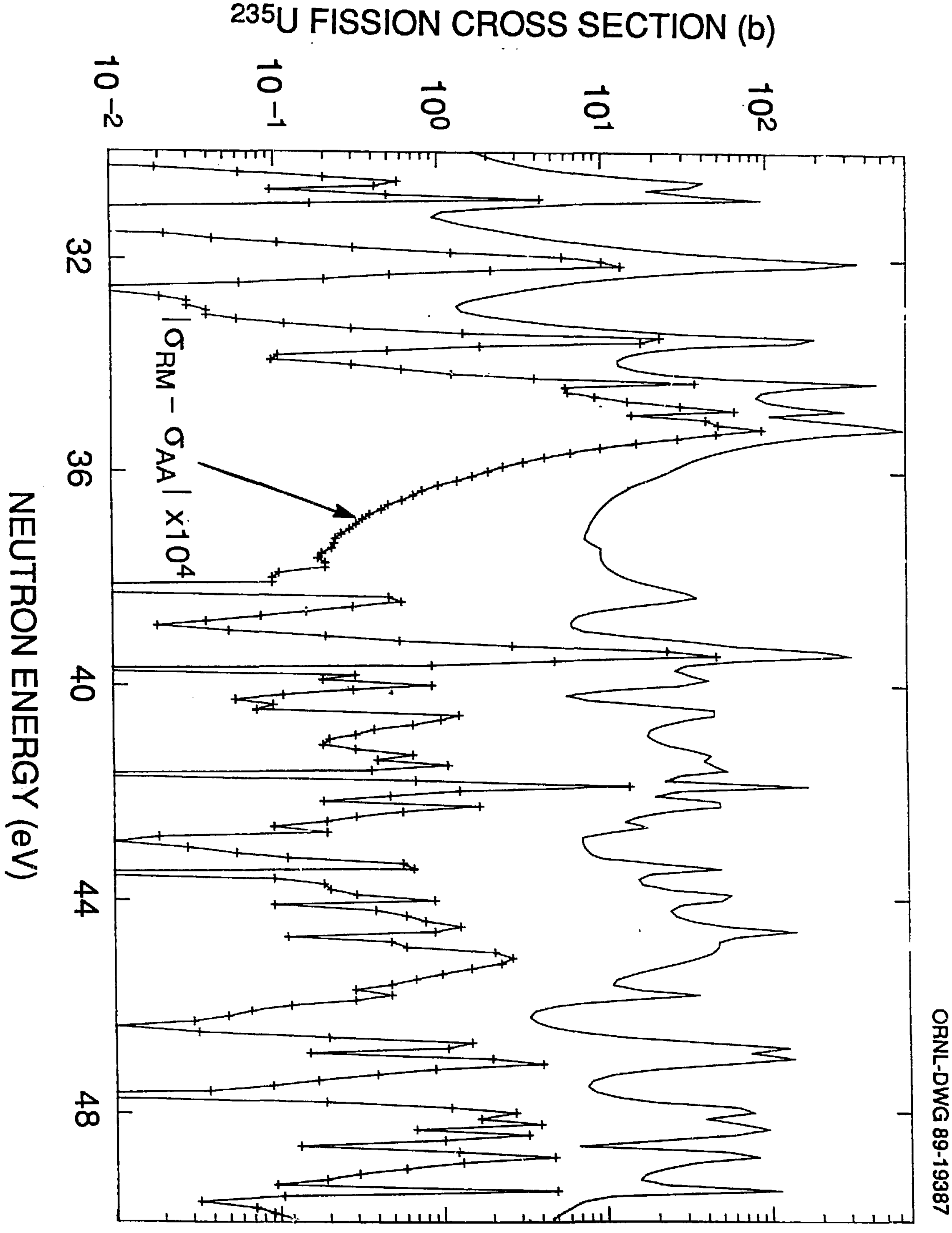
^{235}U FISSION CROSS SECTION (b)
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
32
36
40
44
48
NEUTRON ENERGY (eV)
$|\sigma_{RM} - \sigma_{AA}| \times 10^4$
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Fig. 4. Unbroadened fission cross section of ^{235}U between 30 and 50 eV. The upper curve is the unbroadened fission cross section computed with evaluated Reich-Moore resonance parameters. The lower curve is the difference between the cross section computed by the Reich-Moore formalism and the cross section computed by the Adler-Adler formalism. The absolute value of the difference was multiplied by 10000 so as to be on the scale of the figure.

Table IV

Adler-Adler Resonance Parameters corresponding to the Reich-Moore Parameters of Table I

μ (eV)	ν (eV)	GT (b*eV3/2)	HT (b*eV3/2)	GF (b*eV3/2)	HF (b*eV3/2)	GC (b*eV3/2)	HC (b*eV3/2)
−99.9999	0.0614	658.2420	0.1097	388.1400	0.0596	208.6640	0.0279
−89.9993	0.1549	0.1827	0.0649	0.1596	0.0648	0.0231	0.
−4.2896	0.2382	2556.6499	2.4581	2329.7900	1.1530	188.3700	−0.4589
−3.4930	0.0288	0.0244	−0.0153	0.0052	−0.0152	0.0193	0.
−1.5036	0.0285	0.0111	−0.0795	−0.0448	−0.0767	0.0559	−0.0029
−0.4106	0.0933	133.3380	−1.7793	111.7600	−1.8025	21.4699	−0.0025
−0.1961	0.1180	−1.8762	−3.0185	−2.3741	−3.0592	0.5008	0.0395
−6.88−5[a]	0.0157	−0.0041	0.0398	−0.0408	0.0382	0.0367	0.0016
0.2835	0.0749	4.7196	−1.2730	3.4821	−1.2670	1.2370	−0.0059
1.1422	0.0755	9.2286	3.0268	6.7055	3.0193	2.5204	0.0102
2.0362	0.0237	3.5922	0.0255	0.7362	0.0244	2.8553	0.0003
2.7757	0.0717	−0.0723	−1.1185	−0.3650	−1.1093	0.2925	−0.0092
3.1569	0.0692	7.7725	1.4761	5.6005	1.4741	2.1708	−0.0001
3.6183	0.0464	16.2850	2.8601	9.7871	2.8423	6.4907	0.0114
4.8512	0.0198	23.7335	0.5463	2.1320	0.5200	21.5586	0.0095
5.4488	0.2442	12.0009	−2.3868	11.0516	−2.3555	0.9438	−0.0407
6.2068	0.1125	38.3881	1.9092	31.8716	1.8957	6.4883	−0.0023
6.3908	0.0236	73.8810	0.1598	16.0678	0.0901	57.4141	−0.0071
7.0842	0.0342	39.8103	0.1244	17.1529	0.1042	22.5710	−0.0144
7.6382	0.1491	0.9453	0.4602	0.8122	0.4599	0.1333	−0.0001
8.7696	0.0660	393.7580	−19.7083	290.9340	−19.7250	98.0757	−0.1292
12.3996	0.0359	555.7460	−0.8336	227.1290	−0.7522	302.2380	−0.0006
19.2922	0.0563	2037.4600	16.9521	1148.9900	18.4169	669.3000	−0.4539

[a] Read -6.88-5 as -6.88*10**-5.

The G's and H's in Tables IV and V include the constant $c = 652000$ b*eV and should be divided by that number to conform to ENDF/B-Format.

TABLE V

Multipole Momentum Space Resonance Parameters Corresponding to the Reich-Moore Resonance Parameters of Table I (see Table IV for definitions of G's and H's)

μ (eV1/2)	ν (eV1/2)	GT (b*eV3/2)	HT (b*eV3/2)	GF (b*eV3/2)	HF (b*eV3/2)	GC (b*eV3/2)	HC (b*eV3/2)
−4.3923	−0.0050	1018.7400	10.3319	732.0140	9.2093	426.3620	0.0011
−3.5213	−0.0046	277.8730	−0.3156	125.4760	−0.3761	166.9700	0.
−2.9614	−0.0109	196.8870	−9.7987	149.0650	−9.8635	50.2484	0.
−2.7639	−0.0270	0.4728	0.2298	0.4061	0.2299	0.0666	0.
−2.6616	−0.0064	19.9048	0.0488	8.6136	0.0521	11.3346	0.
−2.5280	−0.0046	36.9420	0.0407	8.1232	0.0451	29.0206	0.0088
−2.4915	−0.0225	19.1944	0.9433	15.9597	0.9478	3.2490	0.
−2.3349	−0.0523	5.9977	−1.1971	5.5270	−1.1778	0.4726	−0.0185
−2.2025	−0.0045	11.8673	0.2673	1.0704	0.2600	10.8187	0.0084
−1.9022	−0.0122	8.1427	1.4303	4.8988	1.4213	3.2482	0.0079
−1.7769	−0.0195	3.8865	0.7371	2.8014	0.7371	1.0857	0.
−1.6662	−0.0215	-0.0360	−0.5593	−0.1825	−0.5547	0.1464	−0.0046
−1.4270	−0.0083	1.7962	0.0125	0.3683	0.0122	1.4282	0.0004
−1.0693	−0.0353	4.6134	1.5169	3.3540	1.5099	1.2606	0.0053
−0.5370	−0.0697	2.3600	−0.6360	1.7414	−0.6335	0.6187	−0.0028
−0.1280	−0.4609	-0.9374	−1.5103	−1.1873	−1.5298	0.2499	0.0199
−0.0883	−0.0887	-0.0020	0.0199	−0.0204	0.0191	0.0184	0.0008
−0.0723	−0.6448	66.6587	−0.8975	55.9248	−0.9455	10.7438	−0.0053
−0.0566	−2.0710	1277.3000	0.5567	1182.4100	−17.4759	95.6056	−1.4892
−0.0116	−1.2263	0.0056	−0.0398	−0.0224	−0.0383	0.0280	−0.0014
−0.0082	−9.4868	0.0913	0.0324	0.0798	0.0324	0.0116	0.
−0.0077	−1.8690	0.0122	−0.0077	0.0026	−0.0076	0.0096	0.
−0.0028	−9.9997	329.0730	0.0298	211.8040	−21.7745	113.8660	−11.7220
0.0028	10.0003	329.1700	0.0298	211.8040	21.8341	113.8660	11.7220
0.0077	1.8690	0.0122	−0.0077	0.0026	−0.0076	0.0096	0.
0.0082	9.4868	0.0914	0.0324	0.0798	0.0324	0.0116	0.
0.0116	1.2263	0.0056	−0.0398	−0.0224	−0.0383	0.0280	−0.0014
0.0566	2.9728	1279.3300	0.5388	1182.4100	18.6291	95.6056	1.4315
0.0723	0.6449	66.6785	−0.8986	55.9247	−0.8571	10.7438	0.0117
0.0883	0.0887	−0.0020	0.0199	−0.0204	0.0191	0.0184	0.0008
0.1280	0.4609	−0.9371	−1.5093	−1.1871	−1.5298	0.2499	0.0200
0.5370	0.0698	2.3597	−0.6366	1.7411	−0.6335	0.6186	−0.0028
1.0693	0.0353	4.6143	1.5132	3.3528	1.5097	1.2603	0.0053
1.4270	0.0083	1.7961	0.0126	0.3681	0.0122	1.4276	0.0004
1.6662	0.0215	−0.0363	−0.5593	−0.1825	−0.5546	0.1464	−0.0046
1.7769	0.0195	3.8863	0.7377	2.8003	0.7371	1.0854	0.0003
1.9022	0.0122	8.1429	1.4279	4.8936	1.4212	3.2450	0.0078
2.2025	0.0045	11.8669	0.2694	1.0660	0.2600	10.7792	0.0084
2.3349	0.0523	6.0000	−1.1954	5.5258	−1.1777	0.4723	−0.0184
2.4915	0.0226	19.1942	0.9530	15.9358	0.9478	3.2441	0.0003
2.5280	0.0047	36.9405	0.0671	8.0339	0.0451	28.7070	0.0089
2.6616	0.0064	19.9051	0.0551	8.5764	0.0521	11.2855	−0.0002
2.7639	0.0270	0.4727	0.2301	0.4061	0.2299	0.0666	0.
2.9614	0.0111	196.8750	−9.9275	145.4660	−9.8624	49.0410	−0.0001
3.5213	0.0051	277.8730	−0.4363	113.5640	−0.3761	151.1190	0.0001
4.3923	0.0064	1018.7300	8.0880	574.4950	9.2084	334.6420	0.0010

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