

An Analysis of U-233 Resonance Absorption

Kun Joong Yoo and Mann Cho

Reactor Physics Laboratory, Korea Atomic Energy Research Institute

Chang H. Kim

Dept. of Nuclear Engineering, Seoul National University

Chang Yul Chi

Dept. of Physics, Seoul National University

Abstract

The low-lying resolved resonance structure of U-233 is investigated in terms of the Adler-Adler multilevel formalism. The resonance capture and fission cross sections of U-233 below 60 eV are calculated using Adlers' effective resonance parameters. The infinite dilution resonance integrals of U-233 are computed with the use of the Alders' parameters adjusted to fit the cross section data. It is found that the agreement of calculations with experiments is generally good over most of the energy region covered.

A transformation of the Adlers' multilevel parameters into an equivalent set of the single level pseudoparameters is made for the use of the existing computer codes which are useful in the reactor calculations but do not have capability to use the multilevel parameters. The results of this transformation are presented in the form of a table.

요 약

U-233에 관한 저에너지에 있어서의 분리가 가능한 공명구조를 다 준위 이론을 고려한 아들라-아들라 이론에 의하여 조사하였다. 아들라-아들라의 유효 공명 매개변수를 이용하여 60 eV 이하의 에너지 영역에 있어서의 U-233의 공명 흡수 및 핵분열 단면적을 계산하였다. 또한 상기 단면적을 잘 표시하여 줄 수 있도록 정하여진 아들라-아들라 매개변수를 이용하여 U-233에 관한 무한 희석 공명적분을 구하였으며, 이는 여기서 고려한 대부분의 공명 에너지 영역에서 실험과 잘 일치하였다. 또한 원자코 계산에는 유용하나 다 준위 이론을 적용할 수는 없는 현존의 전자계산 코드들을 활용하기 위하여 아들라-아들라의 다 준위 이론에 따른 매개변수를 단일 준위 이론에 의한 가매개변수로 변환하여 이 결과를 표로 표시하였다.

1. Introduction

The low-lying resolved resonance cross sections of the heavy nuclides are generally described by the Breit-Wigner single level

formula¹. This description is very satisfactory when resonances are well separated from one another. However, when resonances are not too well separated, as encountered in the fissile isotopes even at low energies, the

adjacent resonances do not contribute independently but interfere with one another. In these circumstances the simple Breit-Wigner formula becomes inadequate for describing the interference effects on resonances². Instead, the multilevel formalism of the Wigner-Eisenbud type³ must be used for representing better the resonance structure of the experimental cross sections.

There are several multilevel formalisms suitable for this purpose⁴⁻⁷. Among those, the Adler-Adler⁷ formalism is known to be the simplest and is widely used both for analyzing the cross section data and for performing the reactor physics calculations. For example, Saussure and his coworkers⁸⁻¹⁰ analyzed the cross section data of U-233 and U-235, using this formalism. Frogner and Børresen¹¹ used this formalism to study the Doppler effects of U-235.

In this note we are presenting an analysis for the integral resonance absorption data of U-233, using the Adler-Adler formalism. In fact, Reich and Moore⁵ have applied the Wigner-Eisenbud formalism to analyzing the resonance structure of U-233. Also, Saussure and Perez¹⁰ analyzed the cross section data of U-233 in terms of the Adler-Adler formalism⁷. But they did not extend their study to the analysis of the integral resonance absorption data.

Therefore we consider it interesting to extend the Adler-Adler formalism to computing the integral resonance absorption data of U-233. In particular, we have computed the infinite dilution resonance integral of U-233 and compared the results with the available data.

We also converted the Adler-Adler multilevel parameters into an equivalent set of single level parameters, using a method

developed by Saussure and Perez¹². As discussed in ref. 12, this has a sole purpose of making useful many existing computer codes which are operative only for the single level parameters but do not have the capability to use the multilevel parameters in reactor physics calculations¹³.

2. Method of Analysis

When the level spacing between the adjacent resonances is comparable to or less than the level width, the resonances do not contribute independently but interfere with one another^{2, 14}. Such interference effects are important for the reaction cross sections of some of heavy nuclides, and particularly for the fission cross sections of the fissile nuclides. In these circumstances, the Breit-Wigner single level formula becomes inadequate for describing the resonance structure of the experimental cross sections.

As a means of getting around this difficulty, D.B. Adler and F.T. Adler⁷ proposed that, for the low-lying resolved resonances, it is possible to fit the cross section data by a sum of the shifted quasi-resonances with asymmetrical shape factors. In other words, the reaction cross section of x -type for nuclei at rest and at neutron energy E is given by⁹

$$\sigma_x(E) = \frac{1}{\sqrt{E}} \sum_i \frac{1}{\nu_i} \cdot \frac{G_i^x \nu_i + H_i^x (E_i - E)}{(E_i - E)^2 + \nu_i^2} \quad (1)$$

E_i is the energy of i th quasi-resonance. ν_i , G_i^x , and H_i^x are Adlers' effective resonance parameters. The numerical values of the parameters are determined by a least-square fitting analysis of the cross section data⁸.

Eq. (1) is called the Adler-Adler multilevel formula. The advantage of this formula becomes clear when the Doppler effect due

Table 1. Adler-Adler Parameters

μ (eV)	ν (eV)	G_c (b·eV ^{3/2})	H_c (b·eV ^{3/2})	G_f (b·eV ^{3/2})	H_f (b·eV ^{3/2})	μ (eV)	ν (eV)	G_c (b·eV ^{3/2})	H_c (b·eV ^{3/2})	G_f (b·eV ^{3/2})	H_f (b·eV ^{3/2})
-2.79	0.37	120.75	-3.51	-1511.99	-513.24	30.76	0.15	11.69	0.88	52.79	51.39
0.18	0.07	0.27	-0.04	-0.19	-0.83	31.20	0.47	12.41	-4.82	149.57	-72.18
1.43	0.35	2.70	-7.24	65.91	-31.81	31.97	0.15	23.63	-8.15	113.99	6.79
1.78	0.12	26.06	5.47	111.08	-1.78	32.74	0.43	-1.78	-10.47	42.61	-96.58
2.29	0.05	37.05	1.89	42.47	17.64	34.03	0.66	-22.26	-21.40	112.79	26.70
3.29	0.51	1.26	1.12	36.93	-42.08	34.53	0.42	6.33	13.71	168.73	21.71
3.63	0.08	9.29	0.93	20.91	7.23	35.19	0.12	-2.92	1.08	27.07	-8.85
4.53	0.39	3.89	-2.24	44.29	-51.91	35.49	0.16	0.98	5.12	10.72	-24.48
5.74	0.18	3.41	-1.79	11.04	-24.25	36.52	0.09	20.52	4.03	59.13	11.50
6.80	0.09	57.38	3.05	168.68	35.89	37.46	0.19	4.64	1.81	64.70	14.44
7.50	0.11	1.97	1.33	5.93	2.23	39.48	0.22	1.39	-2.51	67.55	76.24
8.67	0.26	2.50	-0.76	15.01	4.05	39.71	0.11	-2.94	0.50	34.07	-27.73
9.15	0.15	3.77	-0.44	17.63	-15.41	40.15	0.45	4.87	7.67	97.39	-80.00
10.35	0.16	55.23	3.35	276.95	7.65	41.08	0.10	10.80	4.27	19.88	13.37
11.20	0.27	2.68	-3.19	41.21	-4.76	42.62	0.11	17.35	3.72	62.23	15.86
12.76	0.16	32.11	2.06	226.13	44.65	43.47	0.13	6.76	0.67	32.49	6.16
13.51	0.14	7.76	1.11	-12.21	4.42	44.70	0.56	7.79	12.83	93.00	36.62
13.63	0.24	5.49	-2.16	101.85	3.03	45.21	0.25	2.46	-3.23	1.91	-23.98
15.28	0.12	46.08	-2.03	118.40	-33.36	45.99	0.12	17.43	-6.39	33.33	-26.17
16.15	0.22	6.91	-1.14	105.78	7.14	47.17	0.23	3.55	-4.39	75.74	-9.08
16.51	0.13	20.72	2.55	97.21	17.74	48.64	0.13	80.38	2.44	167.38	-21.20
17.92	0.10	8.63	1.66	37.37	4.27	49.12	0.09	-2.74	-4.94	9.68	-6.64
18.46	0.25	10.00	2.14	78.36	20.69	50.21	0.45	-3.19	-4.48	55.75	-31.14
18.85	0.15	36.00	0.17	213.21	-61.33	50.99	0.38	-2.27	-6.83	16.84	-4.13
20.53	0.21	20.01	1.15	116.58	6.91	51.95	0.62	-17.85	3.73	12.00	-41.84
21.85	0.13	34.39	13.11	131.87	95.43	52.93	0.22	8.85	4.14	53.45	-62.43
22.23	0.24	66.98	-8.29	545.37	-90.62	53.97	0.11	11.77	2.99	61.95	-25.09
22.94	0.38	-6.43	-7.82	96.53	-6.68	54.77	0.09	20.52	3.05	61.08	6.13
23.54	0.33	5.05	1.07	61.03	-95.86	56.09	0.27	3.83	2.11	69.62	128.22
25.13	0.19	15.88	0.18	85.00	-44.81	56.35	0.30	25.61	6.04	211.98	-60.39
26.57	0.28	13.75	1.21	58.70	19.73	57.38	0.49	17.92	3.53	282.72	20.92
28.42	0.28	17.47	6.33	29.85	86.46	58.51	0.23	11.03	-2.43	91.51	26.41
28.91	0.31	13.81	-15.88	233.67	-62.48	61.30	0.40	8.35	-1.18	185.51	47.48
29.68	0.11	2.97	-0.04	-0.16	16.34	62.50	0.20	56.08	-2.62	107.86	-14.96
30.15	0.10	-0.96	-1.11	2.27	-0.71	64.30	0.40	35.51	-16.18	228.02	-22.05

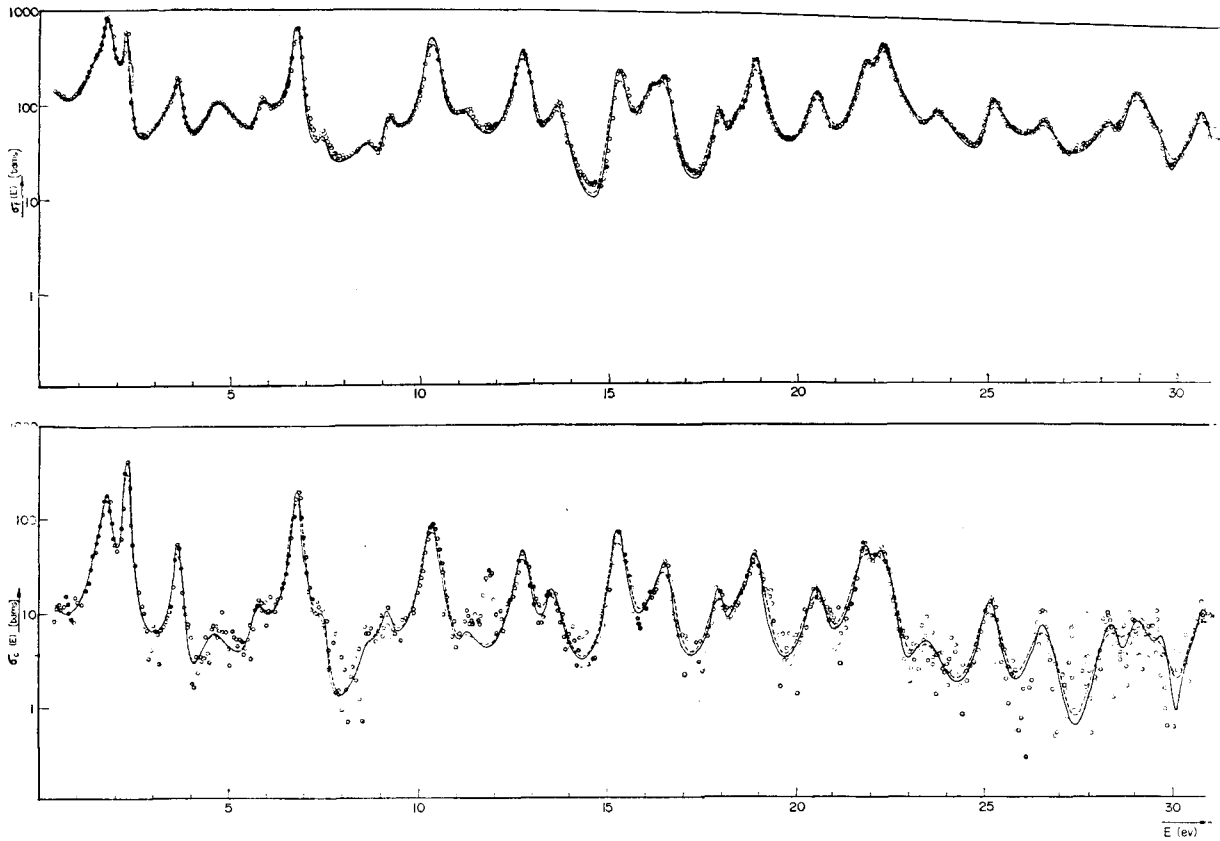


Fig. 1. Resonance Cross-sections

to the thermal motion of the nuclei, is taken into account. When the Maxwellian velocity distribution is assumed for the thermal motion of the nuclei, it can be shown⁹ that the Doppler broadened cross section $\sigma_x(E, T)$ becomes

$$\sigma_x(E, T) = \frac{1}{\sqrt{E}} \sum_i \frac{1}{\nu_i} \times [G_i^2 \Psi(T_i, X_i) - H_i^2 \phi(T_i, X_i)]. \quad (2)$$

$$T_i = \frac{kT}{A\nu_i^2}$$

$$X_i = \frac{E_i - E}{\nu_i}$$

k = Boltzmann constant

T = sample temperature

A = the atomic mass number

The shape function, Ψ and ϕ , are given by

$$\Psi(T_i, X_i) \equiv \frac{1}{\sqrt{4\pi T_i}} \int_{-\infty}^{\infty} \frac{e^{-(X_i - y)^2 / 4T_i}}{1 + y^2} dy,$$

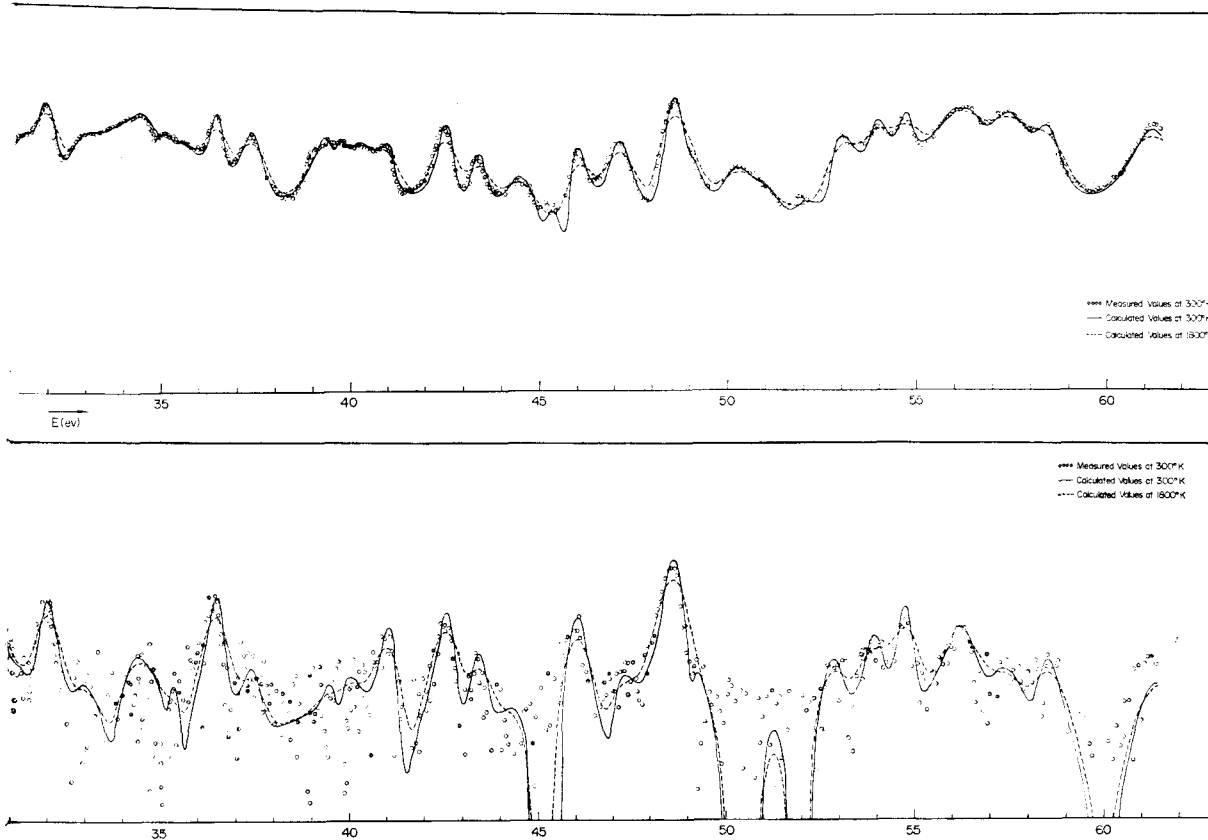
and

$$\phi(T_i, X_i) \equiv \frac{1}{\sqrt{4\pi T_i}} \int_{-\infty}^{\infty} \frac{ye^{-(X_i - y)^2 / 4T_i}}{1 + y^2} dy.$$

The numerical values of these functions are available in the form of table⁵. Efficient numerical methods of computing them are also available^{16, 17}. In this note we evaluated these functions, adopting the complex probability technique of O'Shea and Thacher¹⁶.

3. Results and Discussions

So far experimental informations on Adlers' effective resonance parameters are available only for a few heavy nuclei⁸⁻¹⁰.



of U-233 vs Energy E

Therefore, there have been very limited applications of the Adler-Adler multilevel formalism^{8,9} to studying the integral resonance absorptions, the Doppler coefficients, etc.

Recently de Saussure⁸ measured the fission and the capture cross sections of U-233 covering the resolved resonance energy region below 60 eV. He analyzed the cross section data in terms of the Adler-Adler formalism, and determined the effective resonance parameters by a least square fitting process. The parameters he obtained are listed in Table 1. We made use of this table to calculate the integral resonance absorption by U-233 nuclei.

First of all, a serious test of the Adler-Adler formalism is to show how well the

formalism can represent the experimental resonance structure of U-233. Therefore, we computed the capture and the fission cross sections of U-233, using the numerical values listed in Table 1. The results are compared with the cross section data in Fig. 1. The circles in Fig. 1 are room temperature data and the solid curves the present calculations at 300°K. It is clearly shown that the agreements of calculations (solid curves) with experiments are very excellent. As a consequence, it can be said that the least squares fitting analysis for the resonance structure in combination with the Adler-Adler formalism of U-233 is quite satisfactory. We have also computed the cross sections at 1800°K, as denoted by the dotted curves in

Table 2. Comparison of the Infinite Dilution Resonance Integrals for U-233

Energy Interval (eV)	$\int_{E_1}^{E_2} \frac{dE}{E} = \sum_i \frac{\sigma_{fi}}{E_i} \cdot \frac{(E_{i+1} - E_i)}{2}$ (b)					$\int_{E_1}^{E_2} \frac{dE}{E} \sigma_c$ (b)				
	ORNL- RPI ¹⁸	Nifene- cker ¹⁹	Moore ²⁰	Brooks ²¹	Calculated Values		ORNL- RPI ¹⁸	Brooks ²¹	Calculated Values	
					300° K	1800° K			300° K	1800° K
0.414-0.532	33.34	—	34.20	35.14	33.64	33.65	3.08	3.64	2.91	2.92
0.532-0.683	30.50	—	31.47	32.29	30.37	30.40	2.77	2.84	2.60	2.60
0.683-0.876	28.84	—	29.53	30.84	29.32	29.37	2.80	2.12	2.53	2.54
0.876-1.125	34.76	—	35.54	37.17	34.15	34.30	3.19	3.11	3.14	3.16
1.125-1.455	56.61	—	54.63	53.87	59.65	59.85	6.15	6.38	7.26	7.35
1.455-1.855	138.23	—	140.54	139.95	136.49	134.50	27.48	25.41	27.90	27.38
1.855-2.382	97.56	97.63	92.02	95.05	96.40	96.60	34.93	30.40	36.09	35.14
2.382-3.059	14.55	13.18	17.19	15.22	13.80	15.22	5.39	6.04	4.92	6.10
3.059-3.927	26.14	23.11	25.82	25.54	26.04	25.95	4.33	5.45	4.53	4.52
3.927-5.043	20.41	17.92	19.86	20.07	20.11	20.10	1.15	1.84	1.17	1.18
5.043-6.475	22.10	19.92	20.83	22.07	22.24	22.56	2.91	2.02	2.34	2.42
6.475-8.313	35.09	33.44	31.55	30.98	34.58	34.33	9.40	10.73	9.54	9.46
8.313-10.675	30.48	28.43	25.85	28.59	30.84	30.51	5.04	6.36	5.22	5.16
10.675-13.706	27.61	26.98	23.17	—	27.11	27.37	4.20	—	3.45	3.49
13.706-17.599	18.99	19.30	16.36	—	18.64	18.75	4.11	—	4.15	4.18
17.599-22.597	32.47	30.87	23.21	—	32.55	32.19	5.03	—	4.98	4.92
22.597-29.014	16.76	17.53	15.12	—	16.03	16.31	1.26	—	1.25	1.29
29.014-37.254	15.18	15.54	11.77	—	14.88	14.94	1.23	—	1.45	1.45
37.254-47.834	6.78	7.27	5.90	—	6.71	6.67	0.71	—	0.79	0.79
47.834-61.419	11.29	10.91	8.23	—	10.75	10.73	1.25	—	1.29	1.29
61.419-78.862	9.77	—	7.14	—	—	—	1.38	—	—	—
78.862-101.258	8.74	—	6.51	—	—	—	2.03	—	—	—
101.258-130.016	—	—	8.09	—	—	—	—	—	—	—
130.016-166.940	—	—	4.70	—	—	—	—	—	—	—
166.940-214.351	5.82	—	4.07	—	—	—	0.75	—	—	—
214.351-275.227	5.51	—	4.59	—	—	—	1.15	—	—	—
275.227-353.391	5.42	—	4.51	—	—	—	0.87	—	—	—
353.391-453.755	3.65	—	3.77	—	—	—	0.83	—	—	—
453.755-582.621	3.54	—	2.80	—	—	—	1.34	—	—	—
582.621-748.085	3.84	—	3.17	—	—	—	1.16	—	—	—
748.085-960.541	3.26	—	—	—	—	—	0.92	—	—	—
960.541-1225.335	2.44	—	—	—	—	—	0.89	—	—	—

Fig. 1. We have done this in order to see the effects of thermal motions on the individual resonances of U-233 nuclei. It is noted that the resonances of U-233 are broadened as temperature increases from 300°K to 1800°K.

As an application of the Adlers' formalism we have computed the integral resonance absorption of U-233, e.g., the infinite dilution

resonance integral,

$$I_{\infty}(T) = \int \sigma_r(E, T) \frac{dE}{E}$$

In Table 2 we have shown both calculational and experimental results¹⁸⁻²¹ on this quantity. The experimental values for the infinite dilution resonance integral show some fluctuations from one experiment from the

Table 3.1. Infinite Dilution Resonance Integrals for Capture

E(eV)	$I_{c, \infty}(300^\circ\text{K})$	$I_{c, \infty}(1800^\circ\text{K})$	$\Delta I_{c, \infty}$	$\Delta I_{c, \infty}/I_{c, \infty}(300^\circ\text{K})$
0.414—61.419	127.509	127.419	0.090	0.0007

Table 3.2. Infinite Dilution Resonance Integrals for Fission

E(eV)	$I_{f, \infty}(300^\circ\text{K})$	$I_{f, \infty}(1800^\circ\text{K})$	$\Delta I_{f, \infty}$	$\Delta I_{f, \infty}/I_{f, \infty}(300^\circ\text{K})$
0.414—61.419	694.301	694.266	0.035	0.00005

other. However, the agreement of calculation with experiment is generally good over most of the energy range covered. It is noted that the agreement is better in the fission resonance integral than in the capture one. In Table 3 the infinite dilution resonance integrals at 300°K and 1800°K are compared. The resonance energy region covered in this calculation ranges from 0.4 eV to 61.5 eV. It is shown that $I_{c, \infty}(300^\circ\text{K})$ and $I_{c, \infty}(1800^\circ\text{K})$ are nearly the same. Considering that for the well-separated isolated resonances the infinite dilution resonance integral should be temperature-independent, the resonances of U-233 are nearly resolved over the energy region under consideration.

The above calculations are based on the multilevel representation of the resonance cross section of U-233 nuclei. However, many computer codes for the reactor physics calculations do not presently have the capability to use the multilevel parameters¹³ like the Adlers' effective resonance parameters. In order to make them useful in the reactor calculations, one needs to find the equivalent set of single level parameters from the multilevel parameters. We have done this for the U-233 nuclei, using a method recently developed by Saussure and Perez¹². The results are shown in Table 4.

The notations are the same as those defined in the ref. 12. The first five columns of this table contains the single level pseudoparameters. In the sixth column of the table, the value $\Gamma^* = \Gamma^0 \sqrt{E} + \Gamma_f + \Gamma_\gamma$ is given. As pointed out in the ref. 12, there is an ambiguity in choosing the total width as either Γ or Γ^* . But the difference between the values of Γ and Γ^* is only a few percents. Therefore, either values can be used in the reactor calculations. The negative values of the partial widths are fortuitous. Note that the total or the reaction cross section is the sum of the single level cross section and a smooth background.

4. Conclusions

We have evaluated a resonance integrals of U-233 at 300°K and 1800°K. As expected for the case of resolved resonances of U-233, the infinite dilution resonance integrals are nearly temperature-independent. So far as the numerical calculations are concerned, we found that an efficient computing procedure for the Doppler shape functions is highly desirable for a satisfactory application of the Adler-Adler formalism. Otherwise one can not avoid a long computing time in the applications of this formulation. It is found

Table 4. Single Level Pseudoparameters

E_0 (eV)	$2g\Gamma_n^0$ (mV)	Γ_r (mV)	Γ_f (mV)	Γ (mV)	Γ^* (mV)	E_0 (eV)	$2g\Gamma_n^0$ (mV)	Γ_r (mV)	Γ_f (mV)	Γ (mV)	Γ^* (mV)
0.18	0.0001	472.5	-332.5	140.0	140.0	30.76	0.0989	54.4	245.6	300.0	300.5
1.43	0.1052	27.5	672.5	700.0	700.1	31.20	0.2484	72.0	868.0	940.0	941.4
1.78	0.2103	45.6	194.4	240.0	240.3	31.97	0.2111	51.5	248.5	300.0	301.2
2.29	0.1220	46.6	53.4	100.0	100.2	32.74	0.0626	-37.5	897.5	860.0	860.4
3.29	0.0586	33.7	986.3	1020.0	1020.0	34.03	0.1388	-324.6	1645.0	1320.0	1321.0
3.63	0.0163	49.2	110.8	160.0	160.1	34.53	0.2685	30.4	809.6	840.0	841.6
4.53	0.0739	63.0	717.0	78.0	780.2	35.19	0.0370	-29.0	269.0	240.0	240.2
5.74	0.0222	85.0	275.0	360.0	360.1	35.49	0.0179	26.8	293.2	320.0	320.1
6.80	0.3467	45.7	134.3	180.0	180.9	36.52	0.1222	46.4	133.6	180.0	180.7
7.50	0.0121	54.9	165.1	220.0	220.0	37.46	0.1063	25.4	354.6	380.0	380.7
8.67	0.0269	74.2	445.8	520.0	520.1	39.48	0.1057	8.9	431.1	440.0	440.7
9.15	0.0328	52.9	247.1	300.0	300.1	39.71	0.0478	-20.8	240.8	220.0	220.3
10.35	0.5095	53.2	266.8	320.0	321.6	40.15	0.1568	42.9	857.1	900.0	901.0
11.20	0.0673	33.0	507.0	540.0	540.2	41.08	0.0471	70.4	129.6	200.0	200.3
12.76	0.3961	39.8	280.2	320.0	321.4	42.62	0.1221	48.0	172.0	220.0	220.8
13.51	-0.0068	-488.3	768.3	280.0	280.0	43.47	0.0602	44.8	215.2	260.0	260.4
13.63	0.1646	24.6	455.4	480.0	480.6	44.70	0.1546	86.6	1033.0	1120.0	1121.0
15.28	0.2523	67.2	172.8	240.0	241.0	45.21	0.0067	281.5	218.5	500.0	500.0
16.15	0.1744	26.7	413.3	440.0	440.7	45.99	0.7785	82.4	157.6	240.0	240.5
16.51	0.1809	45.7	214.3	260.0	260.7	47.17	0.1216	20.6	439.4	460.0	460.8
17.92	0.0706	37.5	162.5	200.0	200.3	48.64	0.3800	84.4	175.6	260.0	262.7
18.46	0.1355	56.6	443.4	500.0	500.6	49.12	0.0106	-71.1	251.1	180.0	180.1
18.86	0.3822	43.3	256.7	300.0	301.7	50.21	0.0806	-54.6	954.6	900.0	900.6
20.53	0.2095	61.5	358.5	420.0	420.9	50.99	0.0224	-118.4	878.4	760.0	760.2
21.85	0.2550	53.8	206.2	260.0	261.2	51.95	-0.0090	3784.0	-2544.0	1240.0	1240.0
22.23	0.9392	52.5	427.5	480.0	484.4	52.93	0.0956	62.5	377.5	440.0	440.7
22.94	0.1382	-54.2	814.2	760.0	760.7	53.97	0.1131	44.7	235.3	280.0	280.8
23.51	0.1013	50.4	609.6	660.0	660.5	54.77	0.1252	45.3	134.7	180.0	180.9
25.43	0.1547	59.8	320.2	380.0	380.8	56.09	0.1127	28.2	511.8	540.0	540.8
26.57	0.1111	106.3	453.7	560.0	560.6	56.35	0.3644	64.7	535.3	600.0	602.7
28.42	0.0726	206.7	353.3	560.0	560.4	57.48	0.4611	58.4	921.6	980.0	983.5
28.91	0.3796	34.6	585.4	620.0	622.0	58.51	0.1573	49.5	410.5	460.0	461.2
29.68	0.0043	232.5	-12.5	220.0	220.0	61.30	0.2973	34.5	765.5	800.0	802.3
30.15	0.0020	-146.6	346.6	200.0	200.0	62.50	0.2541	136.8	263.2	400.0	402.0
						64.30	0.4042	107.8	692.2	800.0	803.2

that the ordinary integral technique¹⁵ such as the Simpson's rule is not economic for this particular application of the Adlers' formalism. In this note we adopted the complex probability integral scheme of O'Shea and Thacher¹⁶.

We have also presented the single level pseudoparameters of U-233 resonance capture and fission cross sections. These parameters will be very useful for those reactor codes which do not presently have the capability to use the multilevel parameters in computing the resonance absorptions.

5. Acknowledgements

This work was supported by the Ministry of Science of Technology, Government of Republic of Korea under the contract number of R-73-70.

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