687 INDC (RUM)-51/L



NR-48-1973

TWO-CHANNEL-MULTILEVEL CALCULATION OF THE 235U NEUTRON FISSION CROSS-SECTION

I.M.MIHĂILESCU, M.PETRAȘCU



Bucharest - ROMANIA

The ²³⁵U fission cross-section is calculated for low energy neutrons, using the Reich-Moore formalism. A single neutron channel, two fission channels and many capture channels were taken into account. The fission cross-section values, computed with a FORTRAN IV PROGRAM, were represented in a figure. We have considered the contribution of two bound levels, using a Breit-Wigner formula, and of nine resonance levels, at positive energy, of the same spin and parity, which interfer. In the same figure, the fission cross-section curve, assuming a single fission channel, wes drawn.

TWO-CHANNEL-MULTILEVEL CALCULATION OF THE 235U NEUTRON FISSION CROSS-SECTION

I.M.Mihăilescu, M.Petrașcu

Institute for Atomic Physics

The shape of the neutron cross-sections for fissile elements impose to take into account the interference between the resonance levels. Reich and Moore /l/ obtained the multilevel formalee of the total and fission cross-sections for low energy neutrons, admitting the existence of a single neutron channel, a single fission channel and many capture channels. In this case, the collision matrix U can be written /2/:

$$U = \Omega \frac{1 + i P^{1/2} R P^{1/2}}{1 - i P^{1/2} R P^{1/2}} \Omega$$
(1)

where the R-matrix is given by the relation:

$$R = \sum_{\lambda} \frac{f_{\lambda} \times f_{\lambda}}{B - B - \frac{1}{2} f_{\lambda f}}$$
(2)

and the diagonal matrices P and Ω are defined by the components: P_c, the penetration factor and Ω_c , the phase factor, respectively.

The approximation of a single fission channel is justified by the theory of Bohr /3/, according to which the fission proceeds through a limited number of channels. The same conclusion was drawn by Porter and Thomas /4/, which have shown that the size distribution of the partial widths is related to the number of channels for the given process. They found that the size distribution of the fission widths can be fitted by a chi-squared distribution of

y = 2.3 degrees of freedom, thus indicating that fission is a process defined by two or three reaction channels.

This paper presents the calculation of the ²³⁵U neutron fission cross-section, supposing a single neutron channel, two fission channels and many capture channels.

In the R-matrix theory, the reaction cross-section from an incident channel c to an outgoing channel c', is given by the general expression:

$$\sigma_{cc} = \frac{\pi}{k_c^2} \sum_{J} \varepsilon_J / \frac{J}{Ucc}$$
(3)

so that in the case of two fission channels, the neutron fission cross-section formula has the form:

$$\mathcal{G}_{nf} = \frac{\pi}{k_n^2} \sum_{J} g_{J} \left\{ / U_{12}^{J} / ^2 + / U_{13}^{J} / ^2 \right\}$$
(4)

where the channels 1,2 and 3 represent the neutron channel and two fission channels, respectively, the rest being capture channels.

The resonance levels can not be devided into two spin groups, as sufficient information is not available. We can use a statistical spin factor, $\bar{g} = 1/2$, averaged on the two values corresponding to the two possible values of $J = I \pm 1/2$, where the spin of the ²³⁵U nucleus is I = 7/2. Replacing c/E for π/k_n^2 , where $c = 6.52 \times 10^5$, when the cross-section and the neutron energy are given in barns and electron-volts, respectively, the formula (4) becomes:

$$\sigma_{nf} \sqrt{E} = \frac{c}{\sqrt{E}} \quad \bar{g} \left\{ / v_{12} / ^2 + / v_{13} / ^2 \right\}$$
(5)

To find the collision matrix U, we introduce a matrix C:

$$C = P^{1/2} R P^{1/2}$$
 (6)

defined by the elements:

$$C_{ij} = \sum_{\lambda} \frac{\beta_{\lambda i}}{B_{\lambda} - E - \frac{i}{2} f_{\lambda f}} \equiv e_{ij} + ib_{ij}$$
(7)

where the indices i, j = 1 represent the neutron channel and i, j=2,3 the fission channels.

3

The vectors β_{λ} are given by the expression:

$$\beta_{\lambda} = \mathbf{p}^{1/2} \ \mathbf{r}_{\lambda} \tag{8}$$

From the identity (7) we find:

$$\mathbf{s}_{1j} = \sum_{\lambda} \frac{\beta_{\lambda 1} \beta_{\lambda j} (\mathbf{B}_{\lambda} - \mathbf{B})}{(\mathbf{B}_{\lambda} - \mathbf{B})^{2} + \frac{1}{4} \Gamma_{\lambda T}^{2}}$$
(9)

$$\mathbf{b}_{ij} = \sum_{\lambda} \frac{\frac{1}{2} \beta_{\lambda i} \beta_{\lambda j} \Gamma_{\lambda r}}{(\mathbf{B} - \mathbf{E})^2 + \frac{3}{4} \Gamma_{\lambda r}^2}$$
(10)

The resonance paremeters $\beta_{\lambda i}$ are expressed in terms of neutron and fission widths:

$$\beta_{\lambda \mathbf{i}}^2 = \frac{1}{2} \int_{\lambda \mathbf{i}}$$
(11)

Defining a neutron reduced width:

$$\Gamma_{\lambda n}^{0} = 2 \bar{g} \Gamma_{\lambda n} B^{-1/2}$$
(12)

in case of 2350 we obtain:

$$\beta_{\lambda 1} \equiv \beta_{\lambda n} \equiv \sqrt{\frac{\Gamma_{\lambda n}}{2}} = \frac{1/2}{2}$$
(13)

The interference between the resonance levels is taken

$$\Gamma_{\lambda}^{(c)} = 2 \dot{P}_{c} \gamma_{\lambda}^{(c)2}$$
(11)

we obtain :

$$E P_{c} \Upsilon_{\lambda}^{(c)} \Upsilon_{\mu}^{(c)} = \frac{1}{2} E \Gamma_{\lambda}^{(c) 1/2} \Gamma_{\mu}^{(c) 1/2} = \Gamma_{\lambda}^{(\gamma)} \delta_{\lambda\mu}$$
(12)
c(\gamma) c(\gamma)

The assumption (11) is justified by the great numbers of capture channels. Thus we can introduce a diagonal matrix F:

$$\mathbf{F} = \frac{1}{2} \Gamma$$
(13)

so that the relation (8) becomes :

$$A^{-1} = e - E - F - \frac{1}{2} \sum_{c \neq c(\gamma)} u^{(c)} v^{(c)}$$
(14)

In a case of a single neutron channel and a single fission channel, the sum over c contains only two terms, resulting :

$$\mathbf{A^{-1}} = (\mathbf{e} - \mathbf{E} - \mathbf{F})^{-1} \left\{ \mathbf{I} - \frac{1}{2} (\mathbf{e} - \mathbf{E} - \mathbf{F})^{-1} (\mathbf{u}^{(n)} \cdot \mathbf{v}^{(n)} + \mathbf{u}^{(\mathbf{F})} \cdot \mathbf{v}^{(\mathbf{F})}) \right\}$$
(15)

where I represent the unit matrix.

Defining a diagonal matrix D, with the elements :

$$d_{\lambda} = (E_{\lambda} - E - \frac{1}{2} \Gamma_{\lambda}^{(\gamma)})^{-1} = \frac{E_{\lambda} - E + \frac{1}{2} \Gamma_{\lambda}^{(\gamma)}}{(E_{\lambda} - E)^{2} + \frac{1}{4} \Gamma_{\lambda}^{(\gamma)2}}$$
(16)

we obtain for the level matrix the expression :

$$A = \left[I -, \frac{1}{2} D(u^{(n)} \cdot v^{(n)} + u^{(F)} \cdot v^{(F)}\right]^{-1} \cdot D$$
 (17)

We introduce the vectors column and line, respectively :

4 –

$$\begin{cases} \alpha^{(i)} = \frac{i}{2} D u^{(i)} & \begin{pmatrix} \alpha^{(i)}_{1} \\ \alpha^{(i)}_{2} \\ \vdots \\ \alpha^{(i)}_{n} \end{pmatrix} & i = 1,2 \quad (18) \\ \beta^{(i)} = v^{(i)} & (v^{(i)}_{1}, v^{(i)}_{2} \dots v^{(i)}_{n}) \end{cases}$$

with the components :

$$\begin{cases} \alpha_{\lambda}^{(1)} = \frac{1}{2} d_{\lambda} I_{\lambda}^{(n) 1/2} \\ \beta_{\lambda}^{(1)} = \Gamma_{\lambda}^{(n) 1/2} \\ \alpha_{\lambda}^{(2)} = \frac{1}{2} d_{\lambda} \Gamma_{\lambda}^{(F) 1/2} s_{\lambda} \\ \beta_{\lambda}^{(2)} = \Gamma_{\lambda}^{(F) 1/2} s_{\lambda} \end{cases}$$
(19)

where s_{λ} are the interference resonance parameters, which represent the sign of the product $\Gamma_{\lambda}^{(n)1/2}$. $\Gamma_{\lambda}^{(F)1/2}$ relative to a reference resonance level.

We define a matrix C by the relation :

$$C = (I - \alpha^{(1)}, \beta^{(1)} - \alpha^{(2)}, \beta^{(2)})$$
(21)

. . .

• •

and we can obtain its components using the rank annihilation method.

The first step is to calculate the matrix :

$$C_1 = (I - \alpha^{(1)}, \beta^{(1)})^{-1}$$
 (22)

s magnese a

. .

and applying the formula (7) we obtain :

a series de la companya de la compan

$$C_1 = I + \frac{\alpha^{(1)} \cdot \beta^{(1)}}{1 - \beta^{(1)} \cdot \alpha^{(1)}}$$
 (23)

The matrix C is found by writting the definition (21) in the form :

$$C = (C_1^{-1} - \alpha^{(2)}, \beta^{(2)})^{-1}$$
(24)

- 5 -

With a subroutine using the Gauss-Jordan method, we can find the inverse matrix:

$$B' = G'^{-1} = \begin{pmatrix} b_1 & b_2 \\ \hline b_3 & b_4 \end{pmatrix}$$
(29)

By an analogous procedure, the inverse matrix in the complex form:

$$B = G^{-1} = \alpha + i\beta$$
 (30)

is defined by the relations:

$$\begin{cases} c = b_1 = b_4 \\ \beta = b_2 = b_3 \end{cases}$$
(31)

The correctness of the inversion procedure can be checked imposing the condition that the found submatries have to satisfy the above equalities.

The last step is to obtain the collision matrix elements using the relation (21):

$$W_{ij} = \sum_{k} F_{ik} (G^{-1})_{kj}$$
(32)

so that the formula (5) becomes:

.

$$\tilde{v}_{nf} \sqrt{B} = \frac{\sigma}{\sqrt{E}} \sum_{kk'} F_{1k} (G^{-1})_{1k'}^{\#} \left[(G^{-1})_{k2} F_{k'2}^{\#} + (G^{-1})_{k3} F_{k'3}^{\#} \right]$$
(32)

In the low energy region the fit of the calculated fission cross-section to the experimental points, need to take into account some bound levels. Their contribution to the fission crosssection is given by the Breit-Wigner formula:

$$\mathcal{O}_{nf}^{\prime} \sqrt{\mathbf{B}} = c \sum_{\lambda} \frac{\int_{\lambda n}^{o} \int_{\lambda f}}{(E_{\lambda} - E)^{2} + \frac{f_{\lambda}^{2}}{4}}$$
(34)

where the fission width $\Gamma_{\lambda f}$ is the sum of $\Gamma_{\lambda f_1} + \Gamma_{\lambda f_2}$ and Γ_{λ} represents the total width:

 $\Gamma_{\lambda} = \Gamma_{\lambda n} + \Gamma_{2f_1} \mathbf{s}_1 + \Gamma_{\lambda f_2} \mathbf{s}_2 + f_{\lambda f_3}$

Finally, we obtain the neutron fission cross-section formula as the sum of two terms:

$$\mathcal{O}_{nF} \quad \sqrt{\mathbf{B}} = c \left\{ \sum \frac{\int_{\lambda \mathbf{B}} \left(\int_{\lambda f_1} + \int_{\lambda f_2} \right)}{\left(\mathbf{B}_{\lambda} - \mathbf{B} \right)^2 + \frac{\int_{\lambda}^2}{4}} + (35) \right\}$$

+
$$\frac{1}{\sqrt{B}} = \sum_{kk'} \mathbf{P}_{1k} (\mathbf{G}^{-1})_{1k'}^{\underline{m}} [(\mathbf{G}^{-1})_{k2} \mathbf{P}_{k'2}^{\underline{m}} + (\mathbf{G}^{-1})_{k3} \mathbf{P}_{k'3}^{\underline{m}}]$$

The appendix of this paper presents a code for calculating the 235 U neutron fission cross-section using the formula (35) and the resonance parameters listed in the paper of de Saussure /5/.

We have cosidered two bound levels and nine resonance levels at positive energy, of the same spin and parity, which interfere according to the relation (35). The fission cross-section values computed for neutron energy less than 2 eV, are shown in the figure (1). In table (1) the resonance parameters used in computation are given. In the same figure, the fission cross-section calculated in the case of a single fission channel /6/ is drawn, too.

Comparing the two curves with the experimental data, we can conclude that the essumption of two fission channels diminishes the assimetry of the resonances of the 2350 fission cross-section, so that the resonances are better fitted supposing a single fission channel. A better information on the spin of resonances could improve the result.

The advantage of the present calculation consists in using the inversion of a complex matrix of order 3x3, whichever the number of resonances would be and this lead to the pessibility of



This successful result of applying the rank annihilation method in the above calculation has determined us to generalize it to other cases.

8

9	.

Number of level	E _λ (eV)	$\Gamma^0_{\lambda n}$ (10 ⁻⁶ eV)	$\Gamma_{\lambda f}$ (10 ⁻³ eV)	^Γ λΥ (10 ⁻³ eV)	$(10^{-3} eV)$	relative sign of the pro- $\Gamma_{\lambda}^{\text{duct}} 1/2 \Gamma_{\lambda}^{(F)} 1/2$
1	-1.45	2770	223	33	256	
2	-0.02	0.72	63	34	97	
3	+0.282	4.49	71.8	27.9	.99.7	+ 1
4	1.138	12.9	92.1	41.9	134	- 1
5	2.036	5.3	6.8	34.6	41.4	- 1
6 👘	3.599	23.4	45	37	· 8 1.4	- 1
7	4.847	25	2.3	25.5	27.8	- 1
8	6.4	100	\$	33	4	- 1
9	8.795	257	бо	33	93	- 1

REFERENCES

- /1/ E.P.Wigner, L.Eisenbud, Phys.Rev. 72, 29 (1947)
- /2/ C.W.Reich, M.S.Moore, Phys.Rev. 104, 483 (1956)
- /3/ A.Bohr, Proc.Geneva, vol.2, p.151 (1953)
- /4/ C.Porter, R.G.Thomas, Phys.Rev. 111, 929 (1958)
- /5/ I.M.Mihailescu, Stud.Cerc.Fizica, vol.23, p.1075 (1971)
- /6/ H.S.Wilf, J.Soc.Indust.Appl.Math. 7, p.149-151 (1959)
- /7/ J.Bela, Rezolvarea Numerica a Ecuatiilor Liniare, E.A.Bucuresti
- /8/ T.Watanabe, IN-1098 (1967)
- /9/ F.J.Shore, V.L.Sailor, Phys. Rev. 112, 191 (1958)
- /lo/ I.M.Mihailescu, M.Petrașcu, "Multilevel Calculation of ²³⁵U Neutron Fission Cross Section", to be published.

```
DIMENSION G (6, 6), A(3, 3), B(3, 3), G(3, 3), Y(3, 3), G(3, 3), Y(3, 3), G(3, 3), G
31
32
21
  51
    52
    16
      11
    12
    13
    14
    20
  48
    46
      49
    45
    44
    42
```

IF [AES (GR1 [I, J] - GR2 [I, J]) - 0.0001] 41,40,40
41 1F [AES [GT1 [I, J] - GI2 [I, J]] - 0.0001] 39,40,40
40 WRITE [J, 60]
60 FORMAT[', 'MATBICE INVERSA GFESITA']
9 D0 57 J=1,3
D0 57 J=1,3
D0 57 J=1,3
C0 NJG (F1[J]) (I, J) (I, J))
61 [I, J] = CHELX (S [I, J], V (I, J))
62 [I, J] = CONJG (G1[I, J])
63 J=1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 JJ = 1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 JJ = 1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 JJ = 1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 JJ = 1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 AJ = 1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 AJ = 1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 AJ = 1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 AJ = 1,3
3 SUH1= SUH1+ F1(1,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 AJ = 1,3
3 SUH1= SUH1+ F1(I,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 AJ = 1,3
3 SUH1= SUH1+ F1(I,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
D0 AJ = 1,3
3 SUH1= SUH1+ F1(I,I) *G2(1,J) *(G1(I,2)*F2(J,2)+G1(I,3)*F2(J,3))
S0 FORMAT(I') * G2(F1(I)*GHAF1(I)*IS(I,1)+GANAF2(I)*IS(I,2))/((E(I)
1 = F1(J,2))/((E(I))*IS(I,1)+GANAF2(I)*IS(I,2))/((E(I))*IS(I,2))/((E(I))*IS(I,2))/((E(I))*IS(I,1)+GANAF2(I)*IS(I,2))/((E(I))*I

11

_

-

٠.

.

•• •

•



Table 1. 235U resonance parameters used in computing the multilevel neutron fission cross-section for two fission channels.

Number of	E ₁	Γ ⁰ 2π	1-28	r _{kft}		r _{afz} '	
level	(ev)	(20 ⁻⁶ eV)	(eV)	sign	(eV)	вign	(eV)
1	-1.947	5036	0.021		0.179		0.024
2	-0.020	0	0.034	ł	0.003		0.576
3	0.282	5.16	0.032	+	0.022	+	0.060
4	1.140	13	0.034	-	0.042	-	0.063
5	2.028	5	0.042	-	0.002	-	0.010
6	2.736	Q	0.004	• •	0.010	-	0.063
7	3-135	14	0.033	-	0.007	+	0.112
8	3.605	27	0.039	-	0.043		0.023
9	4-840	29	0.094	+	0	+	0.005
10	5.351	18	0.025	-	0.230	+	0.682
n ·	. 6.222	ü	0-038	+	0.150	-	0.015
12	6.373	<u>]]</u> 4	0.045	•	0 002	-	0.014