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MULTIGROUP CROSS SECTIONS FOR RESONANCE ABSORBERS

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Discussion

The nuclear cross sections used in multigroup calculations are customarily obtained by numerically averaging the lethargy dependent cross section over the proper lethargy interval. In the case of resonance absorbers such as hafnium, the numerical work is considerable and the results are probably somewhat inaccurate. The labor can be greatly reduced and accurate results obtained by using an analytical formula expressed in terms of the resonance parameters. The purpose of this work is to obtain this formula in a nearly exact form and then reduce it to a more simple form for practical usage. The Breit-Wigner one-level formula is assumed to apply.

The results have been applied to obtain multigroup cross sections for hafnium isotopes 177, 178, and 179. Experimental data taken at Argonne, Brookhaven, and Harwell on hafnium resonances in the 1-100 volt region was used. The data, as evaluated by Dr. John Harvey of Brookhaven, is given in Table 1. The calculated multigroup cross sections are given in Table 2.

II. Derivation of an Analytical Formula for Obtaining Multigroup Cross Sections in Terms of Resonance Parameters.

For a given isotope the contribution of the i^{th} resonance to the total average isotopic cross section of the j^{th} group is

$$\Delta\bar{\sigma}_{ij} = \frac{1}{u_{j+1} - u_j} \int_{u_j}^{u_{j+1}} \sigma_i \, du \qquad (1)$$

and the total average isotopic cross section is

$$\bar{\sigma}_j = \frac{1}{u_{j+1} - u_j} \sum_i \Delta \bar{\sigma}_{ij} \qquad (2)$$

where u_j and u_{j+1} are the lower and upper limits of the j^{th} lethargy interval.

We now turn our attention to the principal part of the problem which is is to find an expression for $\int_{u_j}^{u_{j+1}} \sigma_i \, du$. To avoid confusion with other subscripts which are to be introduced, the subscript i will now be dropped .

The Breit-Wigner one-level formula can be written in the following form:

$$\sigma_i = \pi \lambda^2 g \frac{\Gamma_n \Gamma_i}{(E-E_0)^2 + (\frac{\Gamma}{2})^2} \qquad (3)$$

where σ_i is the cross section for the decay of the compound nucleus by process i.

λ is related to the neutron wave length at energy E by

$\lambda = \hbar / \sqrt{2mE}$ (m is the mass of the neutron)

Γ_n is neutron width at energy E.

Γ_i is the partial width for process i.

Γ is the total level width.

g is a statistical weight factor depending on the spins involved.

E_0 is the resonance energy.

The neutron width at energy E is assumed to be related to the neutron width at resonance by $\Gamma_n(E) = \Gamma_n^0 \sqrt{\frac{E}{E_0}}$

Since we are interested in resonance absorbers, Γ_i is replacedby the radiation width Γ_γ which is assumed to be constant with energy.

A subscript or superscript o indicates that the value of the quantity at resonance applies.

It is convenient to write the cross section for absorption in the following form:

$$\sigma_a = \sigma_0 \beta_0^2 \left(\frac{\Gamma_\gamma^0}{\Gamma^0}\right) \frac{1}{\sqrt{\frac{E}{E_0}}\left[\left(\frac{E}{E_0}-1\right)^2 + \beta^2\right]} \qquad (4)$$

where

σ_0 is the peak total cross section.

$\beta = \Gamma/2E_0$

Substituting expression 4 for σ_a and changing variables to $x = \sqrt{\frac{E}{E_0}}$ gives

$$\int_{u_1}^{u_2} \sigma_a \, du = 2\sigma_0 \beta_0^2 \frac{\Gamma_\gamma^0}{\Gamma^0} \int_{x_1}^{x_2} \frac{dx}{x^2\left[(x^2-1)^2 + \beta_0^2\right]} \qquad (5)$$

The integral in (5) can be put into standard form by forming partial fraction from the quantity $\frac{1}{(x^2-1)^2 + \beta_0^2}$

let

$$\frac{1}{(x^2-1)^2+\gamma_0^2} = \frac{1}{2ab}\left[\frac{b+x}{x^2+bx+a} + \frac{b-x}{x^2-bx+a}\right] \quad (6)$$

where $a = \sqrt{1+\gamma_0^2}$

$b = \sqrt{2(1+\sqrt{1+\gamma_0^2})}$

Note that in the integral in equation 5, γ has been approximated by the constant value γ_0. The quantity γ is usually not significant except at, or very close to, resonance where it is well approximated by the constant value γ_0.

Making the subsitution indicated by equation (6) gives

$$\int_{u_1}^{u_2} \sigma_a \, du = \frac{\sigma_0 \gamma_0^2}{ab} \frac{\pi^2}{\Gamma^2}\left[b\int_{v_1}^{v_2}\frac{dv}{v^2 X^+} + b\int_{v_1}^{v_2}\frac{dv}{v^2 X^-} + \int_{v_1}^{v_2}\frac{dv}{v X^+} - \int_{v_1}^{v_2}\frac{dv}{v X^-}\right] \quad (7)$$

where $X^+ = x^2+bx+a$

$X^- = x^2-bx+a$

The integrals are now expressed in standard form. Performing the integration over the indicated range and collecting terms gives

$$\int_{u_1}^{u_2} \sigma_a \, du = \frac{\sigma_0 \gamma_0^2}{1+\gamma_0^2} \frac{\sqrt{\gamma}}{\Gamma^0} \left\{ \frac{(2+\sqrt{1+\gamma_0^2})\sqrt{2(\sqrt{1+\gamma_0^2}-1)}}{2\sqrt{1+\gamma_0^2}\,\gamma_0} \log \sqrt{\frac{X^+(\chi_2)\,X^-(\chi_1)}{X^-(\chi_2)\,X^+(\chi_1)}} + \right.$$

$$2\left(\frac{1}{\chi_1} - \frac{1}{\chi_2}\right) + \frac{(2-\sqrt{1+\gamma_0^2})\sqrt{2(\sqrt{1+\gamma_0^2}+1)}}{2\sqrt{1+\gamma_0^2}\,\gamma_0} \times$$

$$\left[\tan^{-1}\left(\frac{\chi_2\sqrt{2(\sqrt{1+\gamma_0^2}+1)} + (\sqrt{1+\gamma_0^2}+1)}{\gamma_0} \right) + \tan^{-1}\left(\frac{\chi_2\sqrt{2\sqrt{1+\gamma_0^2}+1} - (\sqrt{1+\gamma_0^2}+1)}{\gamma_0} \right) \right.$$

$$\left. \left. - \tan^{-1}\left(\frac{\chi_1\sqrt{2(\sqrt{1+\gamma_0^2}+1)} + (\sqrt{1+\gamma_0^2}+1)}{\gamma_0} \right) - \tan^{-1}\left(\frac{\chi_1\sqrt{2(\sqrt{1+\gamma_0^2}+1)} - (\sqrt{1+\gamma_0^2}+1)}{\gamma_0} \right) \right] \right\}$$

(8)

The only approximation involved in obtaining equation (8) other than basic assumptions, is that of neglecting the energy dependence of γ . There is little error introduced by this approximation for resonances which are primarily absorbing rather than scattering. In such cases the total level width is mainly the radiation width which is fairly constant with energy.

The integral in equation (5) has been evaluated by Dr. John Sampson by a different method than that used here. The limits of integration, however, were such as to give an expression for the total resonance integral. An equivalent expression is obtained from equation (8) by substituting the proper values of χ_1 and χ_2 . For this case the two results were found to be the same.

For numerical work equation (8) is rather complicated. Simple forms valid for specified situations will now be obtained.

The quantity γ_0 is usually quite small. For hafnium, γ_0 is less than a tenth. When γ_0 is of this order or smaller, then equation (8) reduces to

$$\int_{u_1}^{u_2} \sigma_a \, du = \sigma_0 \gamma_0^2 \frac{\Gamma^0}{\Gamma_0} \left\{ \frac{3}{4} \log \left[\frac{(x_2+1)(x_1-1)}{(x_2-1)(x_1+1)} \right] + 2\left(\frac{1}{x_1} - \frac{1}{x_2} \right) + \right.$$
$$\left. \frac{1}{\gamma_0} \left[\tan^{-1} \frac{2}{\gamma_0}(x_2-1) - \tan^{-1} \frac{2}{\gamma_0}(x_1-1) \right] \right\} \qquad (9)$$

The first two arc tangent terms have been dropped because they will essentially cancel each other for small values of γ_0. The quantity $\sqrt{1+\gamma_0^2}$ has been approximated by either 1 or $1+\frac{\gamma_0^2}{2}$, whichever was appropriate in taking the limiting form. Further simplification is possible. Away from the $1/v$ region the term $\left(\frac{1}{x_1} - \frac{1}{x_2}\right)$ is negligible. Also when the contribution of a resonance to the total cross section of the group in which it lies is wanted, and the resonance lies well within the group, the following form is quite accurate;

$$\int_{u_1}^{u_2} \sigma_a \, du = \pi \sigma_0 \gamma_0 \frac{\Gamma^0}{\Gamma_0} = \frac{\pi}{2} \left(\frac{\sigma_0 \Gamma^0}{\Gamma^0 E_0} \right) \frac{\Gamma^0}{\Gamma_0} \qquad (10)$$

The log term is negligible and the two arc tangent terms are approximately equal to π.

III. Calculation of Multigroup Cross Sections for Hafnium

Experimental data taken at Argonne, Brookhaven and Harwell has been considered by D. John Harvey of Brookhaven. From the various data he has selected "best values" for the resonance parameters in the 1-100 volt region. These values are summarized in Table 1. These values were used in equations 9 and 10 above, to calculate multigroup absorption cross sections for hafnium isotopes 177, 178, and 179 in the 1-100 volt region. Cross sections for groups lying outside this region were calculated by methods described below.

A. Low energy region - the measured thermal cross section was used and a $1/v$ variation with energy assumed.

B. Energies greater than 100 volts - average values of resonance parameters were calculated from the data taken in the 1-100 volt region. An effective cross section vs. the region of a resonance (expressed in terms of the average values of the resonance parameters) was obtained as a continuous function of energy. This effective cross section was then averaged over the desired lethargy interval.

This method was used only for the 177 isotope for which data on several resonances as available. The cross sections obtained are given in Table 2.

The author wishes to acknowledge the assistance of Miss Irene Rouillard in performing the numerical calculations, and the beneficial discussions with Drs. H. Hurwitz, T. Snyder, J. Stehn, and H. L. Storm.

Table I

Resonance Parameters of Hafnium Isotopes*

Isotope	E_o (ev)	$g\Gamma_n^o$ (b-ev)	Γ^o (ev)	Γ_n^o (mv)
177	1.08 ± .02	110 ± 30	.05 ± .01	1.8
	2.36 ± .02	240 ± 30	.083 ± .01	5
	5.8 ± .1	70 ± 15	[Γ_γ = .07]	4.2
	6.5 ± .1	120 ± 20	.057 ± .013	11
	8.9 ± 1	45 ± 10	[Γ_γ = .07]	4.2
	13.9 ± .1	40 ± 5	.11 ± .03	3.9
	22.5 ± .2	17 ± 4	[Γ_γ = .07]	4.0
	23.6 ± .2	4 ± 2	"	1.0
	27.3 ± .3	9 ± 3	"	2.6
	33.2 ± .4	5 ± 2	"	1.8
	37.0 ± .5	46 ± 10	"	15
	46.8 ± .6	60 ± 20	"	23
	49.1 ± .7	210 ± 50	"	60
	56.0 ± .8	60 ± 20	"	27
	57.2 ± .9	20 ± 7	"	11
	64.6 ± 1.0	140 ± 30	"	55
	68.4 ± 1.1	90 ± 20	"	42
	71.3 ± 1.2	14 ± 4	"	10
	75.0 ± 1.3	38 ± 10	"	23

*Values given are "best values" as selected by Dr. John Harvey of Brookhaven from experimental data taken at Argonne, Harwell, and Brookhaven.

Table I

(contd.)

Isotope	E_0(ev)	$g \cdot \Gamma^{0 2}$(b-ev^2)	Γ^0(ev)	Γ_n^0(mv)
177	85.8 ± 1.6	12 ± 4	[Γ_γ = .07]	10
	87.4 ± 1.6	15 ± 5	"	12
	94 ± 2	12 ± 4	"	11
	100 ± 2	32 ± 10	"	26
178	7.8	1500	.082	55
179	5.7 ± .1	50 ± 20	[Γ_γ = .07]	3.0
"	17.7 ± .2	11 ± 3	"	2.1
	23.9 ± .2	29 ± 8	[Γ_γ = .07]	7
	26.5 ± .3	6 ± 2	"	1.7
	31.5 ± .4	18 ± 4	"	6
	36.9 ± .5	75 ± 15	"	23
	40.5 ± .5	80 ± 15	"	26
	42.6 ± .6	26 ± 8	"	11

Table 2

Hafnium Isotopic Absorption Cross Sections (barns)

Group	Lethargy Range	Isotope 177	178	179
1	0-.5	--	--	--
2	.5-1	--	--	--
3	1-2	--	--	--
4	2-3	--	--	--
5	3-4	--	--	--
6	4-8	2	--	--
7	8-11	26	--	--
8	11-12.5	109	--	23
9	12.5-13.75	69	--	62
10	13.75-15	611	963	146
11	15-16	2158	9	7
12	16-17	2604	15	12
13	17-17.75	119	26	19
14	17.75-18.7	163	35	26
15	18.7	213	46	35