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Neutron cross sections and related topics.

Part 1

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# Part I: Neutron cross sections and related topics

#### **Exercise I.1**

The velocity  $v_n$  of a neutron can be determined from the time-of-flight  $t_n$  over a given flight distance L by:

$$v_n = \frac{L}{t_n}$$

The relativistic relation between the kinetic energy  $E_n$  and the velocity  $v_n$  of the neutron is:

$$E_n = m_n c^2 \left( \frac{1}{\sqrt{1 - (v_n / c)^2}} - 1 \right) = m_n c^2 (\gamma - 1)$$
 with  $\gamma = \frac{1}{\sqrt{1 - (v_n / c)^2}}$ 

where  $m_n$  is the rest mass of the neutron and c is the velocity of light. The first term of a series expansion gives the classical expression :

$$E_{n} = \frac{1}{2}m_{n}v_{n}^{2} = \alpha^{2}\frac{L^{2}}{t_{n}^{2}}$$

- (a) Calculate the value of the constant  $\alpha$  when the energy  $E_n$  is given in eV, the distance L in m and the time  $t_n$  in  $\mu s$
- (b) Calculate the kinetic energy exactly and in the classical approximation for neutrons with a time of flight of  $2\mu s$  and  $2000\mu s$  for a flight path length of 30 m and 200m.

t <sub>n</sub> /μs	L/m	E <sub>n,das</sub> / eV	E <sub>n,rel</sub> / eV	$E_{n,rel}/E_{n,clas}$
2 2000	30 30			
2	200			
2000	200			

At a measurement station with a nominal flight path length of 30m the following observations were made: the signal from the gamma-flash was observed at a time-of-flight  $t_{\gamma,exp}$  = 298.4 ns and the time-of-flight of the 20.864 eV resonance of  $^{238}$ U at a time-of-flight  $t_{n,exp}$ = 467129.2 ns. The observed time-of-flight  $t_{exp}$  is related to the real time-of-flight t by the relation :  $t_{exp}$  =  $t_0$  + t

- (a) Determine the to value
- (b) Determine a more precise value of the flight path length.

Parameter
Flight path length, L
Time offset, t <sub>o</sub>

The vertical displacement  $\Delta s$  of a body subject to the gravitational force is given by:

$$\Delta s = \frac{1}{2}g_n t_n^2$$

with  $g_n$  the standard acceleration of free fall and  $t_n$  the time.

Calculate the vertical displacement of a 25 meV and 1 eV and 100 eV neutron for flight path lengths L = 30 m and 200 m.

(Assume that the start velocity has only a horizontal component and only the gravitational force has on impact on the kinematics)

Neutron energy /eV	L = 30 m		L = 200 m	
	t <sub>n</sub> / μs	Δs / mm	t <sub>n</sub> /μs	Δs/mm
0.025				
1				
100				

The Maxwell-Boltzmann distribution of the velocity v of a particle with mass m in equilibrium at a temperature T is:

$$P(v)dv = C v^2 exp(-\frac{mv^2}{2kT})dv$$

where k is the Boltzmann constant and C is a normalization constant of the distribution :

$$C=\sqrt{\frac{2}{\pi}}(\frac{m}{kT})^{3/2}$$

- (a) Show that the maximum of the distribution P(v)dv occurs at a velocity  $v_{max}$  corresponding to a kinetic energy  $E_{max} = kT$
- (b) What is the energy  $E_{\text{max}}$  if the temperature is 300 K?
- (c) Thermal cross sections  $\sigma_{th}$  are often given at a standard energy, e.g. corresponding to a neutron velocity v = 2200 m/s. What is the corresponding neutron energy and temperature.

The Maxwell-Boltzmann distribution can be used to describe the neutron flux in a thermal reactor:

$$\varphi(v)dv = C'vP(v)dv$$

where C' is a normalization constant.

In the thermal energy region most of the absorption cross sections are directly proportional to 1/v. For 1/v cross sections, the cross section  $\sigma(E)$  at an energy E relates to a reference cross section  $\sigma_R$  at an energy E<sub>R</sub> as:

$$\sigma(E) = \sigma_R \sqrt{\frac{E_R}{E}}$$

(a) Show that the energy distribution of the neutron flux becomes:

$$\phi(E)dE = C'' E exp(-\frac{E}{kT})dE$$

where k is the Boltzman constant and C" is a normalization constant.

(b) Show that for a 1/v cross section the average cross section  $<\sigma(T)>$  in a flux with a Maxwellian distribution, which is characterized by a temperature T, can be expressed as a function of the cross section  $\sigma_R$  at a given temperature  $T_R$  by:

$$<\sigma(T)> = \frac{\int \sigma(E)\phi(E)dE}{\int \phi(E)dE} = \frac{\sqrt{\pi}}{2}\sigma_R\sqrt{\frac{T_R}{T}}$$

Note that :  $\int x^{\alpha-1}e^{-x}dx = \Gamma(\alpha)$  with  $\Gamma(2) = 1$  and  $\Gamma(3/2) = \sqrt{\pi}/2$ 

(c) How much does the average cross section  $<\sigma(T)>$  deviates from the cross section  $\sigma(kT)$  at temperature kT.

A disc-shaped sample of natural gold has a diameter of (40.00  $\pm$  0.10) mm and a mass of (5.0000  $\pm$  0.0002)g. The atomic mass of  $^{197}\text{Au}$  is (m\_{Au}=196.966543  $\pm$  0.000004) u.

- (a) Calculate the mass per unit area or the thickness of the sample in g/cm<sup>2</sup>
- (b) Calculate the number of atoms per unit area in atoms per barn (at/b)

Isotope	m <sub>X</sub> /u	isotopic abundance, a <sub>i</sub>	thickness / (g/cm <sup>2</sup> )	thickness / (at/b)	m / g
<sup>197</sup> Au	196.966543	1			

A sample is made out of a pure element  $_ZX$  containing the isotopes  $_Z^{A_i}X$  i = 1,...,n. The isotopic abundance  $_X$  of the isotope  $_Z^{A_i}X$  in the element  $_ZX$  is defined as the fraction of the number of nuclei  $_Z^{A_i}X$  in element  $_ZX$ . The mass fraction  $_X$  corresponds to the ratio of the mass  $_X$  (m( $_X$ )) of isotope  $_Z^{A_i}X$  to the total mass m( $_X$ ) of element  $_X$ .

- (a) Determine the atomic mass  $(m_X)$  of element  $_ZX$  in case the isotopic abundance  $x_i$  and atomic mass  $m_{Xi}$  of the isotopes are given
- (b) Determine the relation between the isotopic abundance  $x_i$  and the weight fraction  $w_i$  of the isotopes  ${}^{A_i}_Z X$  of element  ${}_Z X$ .

A disc-shaped sample of natural silver ( $^{nat}Ag$ ) has a diameter of 80 mm and a mass of 50g. Natural silver consists of  $^{107}Ag$  and  $^{109}Ag$ . The natural isotopic abundance and atomic mass of  $^{107}Ag$  and  $^{109}Ag$  are given in the

Isotope	atomic mass / u	isotopic abundance	thickness / (at/b)	weight fraction	mass /g
<sup>107</sup> Ag	106.905093	0.51839			
<sup>109</sup> Ag	108.904756	0.48161			
Ag	107.868151	1		1	50

- (a) Calculate the atomic mass of <sup>nat</sup>Ag
   (b) Calculate the number of <sup>nat</sup>Ag atoms per unit area (in at/b)
   (c) Calculate the number of atoms for each isotope per unit area (in at/b)
- (d) Calculate the mass fraction and mass of each isotope

**Exercise I.9** A disc-shaped sample of  $ZrO_2$  has a diameter of 2.54 cm and a mass of 6.595 g. The isotopic abundance of Zr and O are given in the table together with the atomic mass of the Zr- and O-isotopes present in the sample..

Element	Isotope	atomic mass / u	isotopic abundance	fraction	thickness / (at/b)	weight fraction	mass (g)
Zr	<sup>90</sup> Zr	89.90470	0.0229				
	<sup>91</sup> Zr	90.90564	0.1861				
	<sup>92</sup> Zr	91.90504	0.1895				
	<sup>93</sup> Zr	92.9	0.1998				
	<sup>94</sup> Zr	93.90632	0.2050				
	<sup>96</sup> Zr	95.90828	0.1967				
0	<sup>16</sup> O	15.99491463	0.99762				
	<sup>17</sup> O	16.9991312	0.00038				
	<sup>18</sup> O	17.9991603	0.00200				
$ZrO_2$				1		1	6.595

- (a) Calculate the atomic mass of Zr and O for the isotopic abundance given in the table.
- (b) Calculate the molar mass of ZrO<sub>2</sub>
- (c) Calculate the number of ZrO<sub>2</sub> molecules in the target
- (d) Calculate the number of Zr- and O-isotopes per unit area (in at/b)
- (e) Calculate the weight fractions and mass of the Zr- and O-isotopes

For a neutron induced reaction on a target nucleus with spin I and parity  $\pi_0$ , the angular momentum J of a resonance is given by the vector sum of the angular momenta:

$$\vec{J} = \vec{I} + \vec{i} + \vec{\ell}$$

with i the spin of the neutron and  $\ell$  the angular momentum of the incident neutron. A neutron with angular momentum quantum number  $\ell = 0$ , 1 and 2 is denoted as a s-, p-and d-wave neutron, respectively.

Defining with s the channel spin, the momenta satisfy the relations:

Since the neutron has a positive parity, the resonance parity  $\pi$  is defined by:

$$\pi = \pi_{o} (-1)^{\ell}$$

- (a) Calculate the possible spin and parity combinations  $J^{\pi}$  of resonances induced by a s-, p-and d-wave neutron on a target nucleus with spin and parity  $I^{\pi o} = 0^+$ ,  $1/2^+$  and  $1^+$
- (b) Determine also the spin factor g<sub>J</sub>, which is defined by:

$$g_J = \frac{2J+1}{2(2I+1)}$$

Target nucleus	Incide neutro		Channel spin	Resonance		
$I^{\pi}$	i	$\ell$	S	$J^{\pi}$	<b>g</b> J	$\Sigma \ g_J$
0*	1/2	0 1 2				
1/2+	1/2	0				
		2				
1+	1/2	0				
		2				

Neutron induced cross sections in the resonance region are determined by resonance parameters corresponding to the properties of excited nuclear levels. The cross section for a reaction (n,r) of an isolated resonance with spin J for a non-fissile nucleus can in first approximation be described by the Single Level Breit-Wigner (SLBW) form:

$$\sigma_r(E_n) = \frac{\pi}{k^2} g_J \frac{\Gamma_n \Gamma_r}{(E_n - E_R)^2 + \frac{(\Gamma_n + \Gamma_r)^2}{4}}$$

where  $E_R$  is the resonance energy,  $\Gamma_n$  is the neutron width,  $\Gamma_r$  is the reaction width,  $g_J$  is the statistical factor and k is the angular wave number of the neutron.

The reaction cross section at thermal ( $E_n = E_{th} = 0.025 \text{ eV}$ ) is composed out of a contribution from unbound and bound ("negative resonances") states. Based on the SLBW expression (assuming  $|E_R| > E_n$  and  $\Gamma_n + \Gamma_r << E_R$ ) the cross section (in units of a barn) at thermal is a sum over all contributions:

$$\sigma_r(E_{th}) \approx 4.099 \text{x} 10^6 \left(\frac{A+1}{A}\right)^2 \sum_{i=1}^{N} \frac{g_{J,i} \; \Gamma_{n,i} \; \Gamma_{r,i}}{\left|E_{R,i}\right|^{5/2}}$$

with A nucleus-neutron mass ratio In this expression the resonance energy, reduced neutron and radiation width are expressed in eV.

- (a) Calculate the contribution of the positive s-wave resonances for  $^{197}$ Au(n, $\gamma$ ) with  $I^{\pi} = 3/2^{+}$ , which are given in the table.
- (b) Adjust the neutron width of a negative resonance (or bound state) to match the capture cross section at thermal ( $E_{th} = 0.025 \text{ eV}$ ), which is  $\sigma(E_{th}, \gamma) = 98.66 \text{ b}$ . (Assume that the direct capture component can be neglected)
  - for a negative resonance at -60 eV with spin J= 2 and radiation width  $\Gamma_v$  = 0.125 eV
  - for a negative resonance at -120 eV with spin J=2 and radiation width  $\Gamma_{\gamma}$  = 0.125 eV

E <sub>R</sub> / eV	J	$\Gamma_{n}$ / eV	$\Gamma_{\gamma}$ / eV	Contribution to the thermal cross section	
			•	$\sigma_{\gamma}$ (E <sub>th</sub> ) / b	Relative
4.890	2	0.01520	0.124		
57.921	1	0.00435	0.112		
60.099	2	0.06640	0.110		
78.271	1	0.01667	0.120		
107.000	2	0.00760	0.110		

The total cross section for an s-wave in the SLBW-formalism is given by:

$$\sigma_{tot}\!\left(E_{n}\right) = g_{J} \frac{\pi}{k_{n}^{2}} \frac{\Gamma_{n}\Gamma}{\left(E_{n} - E_{R}\right)^{2} + \left(\Gamma/2\right)^{2}} + g_{J} \frac{4\pi}{k_{n}} \frac{\Gamma_{n}(E_{n} - E_{R})R}{\left(E_{n} - E_{R}\right)^{2} + \left(\Gamma/2\right)^{2}} + g_{J} 4\pi R^{2}$$

The last term in this equation is the contribution due to the potential scattering ( $\sigma_{pot}$ ).

In the SLBW-formalism the peak cross section  $\sigma_0$ , which reflects the maximum of the resonance part of the total cross section, is:

$$\sigma_{o} = \frac{4\pi}{k_{n}^{2}} \frac{g_{J}\Gamma_{n}}{\Gamma} \approx \frac{2.608x10^{6}}{E_{R}} \left(\frac{A+1}{A}\right)^{2} \frac{g_{J}\Gamma_{n}}{\Gamma}$$

where in the last expression the peak cross section is given in barn and the resonance energy in eV. This peak cross section can be used to estimate the maximum total  $(\sigma_{max,tot})$ , capture  $(\sigma_{max,\gamma})$  and elastic  $(\sigma_{max,n})$  cross section becomes:

$$\begin{split} &\sigma_{\text{max,tot}} = \sigma_{\text{o}} + \sigma_{\text{pot}} \\ &\sigma_{\text{max},\gamma} = \sigma_{\text{o}} \, \frac{\Gamma_{\gamma}}{\Gamma} \\ &\sigma_{\text{max,n}} = \sigma_{\text{o}} \, \frac{\Gamma_{\text{n}}}{\Gamma} \end{split}$$

- (a) Calculate the peak cross sections  $\sigma_o$ ,  $\sigma_{o\gamma}$  and  $\sigma_{on}$  for the resonances of  $^{238}U$  given in the table.
- (b) Compare the peak cross section  $\sigma_0$  with the maximum of the cross sections given in the figure.
- (c) Can the parity of the resonances at 66.02 eV and 80.73 eV be determined from the shape of the total cross sections?
- (d) What about the resonances at 83.68 eV and 89.24 eV?
- (e) How much does the potential scattering contribute to the total cross section for the resonance at 66.02 eV ? (the effective scattering radius for <sup>238</sup>U: R= 9.6 fm).

	$^{238}$ U: $I^{\pi} = 0^{+}$	R = 9.6  fm					
E <sub>R</sub>	J	gл	$\Gamma_{n}$	Γγ	$\sigma_{o}$	$\sigma_{max,\gamma}$	$\sigma_{max,n}$
(eV)			meV	meV	barn	barn	barn
66.02	1/2	1	24.6	24.0			
80.73	1/2	1	1.8	25.0			
83.68	1/2	1	0.01	25.0			
89.24	1/2	1	0.09	25.0			

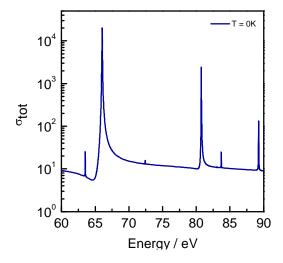


Figure: The neutron induced total cross section for 238U in the energy region between 60 eV and 90 eV.

To calculate reaction probabilities the thermal motion of the target nucleus has to be taken into account. Therefore, for practical applications resonance cross sections are mostly needed in Doppler broadened form. In the most simple approximation, the classical ideal gas model, it is assumed that the target nuclei have the same velocity distribution as an ideal gas at an effective temperature  $T_{\text{eff}}$ . The thermal motion of the target nuclei gives rise to a broadening  $\Delta_D$ :

$$\Delta_D = \sqrt{\frac{4kT_{eff}E_R}{A}}$$

with A the nucleus-neutron mass ratio en k the Boltzman constant.

- (a) Calculate the Doppler broadening for the resonances in the table
- (b) Compare the Doppler broadening with the total natural line width of the resonance

238 <b>U</b> : Ι <sup>π</sup>	$= 0^+ R =$	9.6 fm				
E <sub>R</sub>	J	gл	$\Gamma_{n}$	$\Gamma_{\gamma}$	$\Gamma_{\gamma}$ + $\Gamma_{n}$	$\Delta_{D}$
(eV)			meV	meV	meV	meV
66.02	1/2	1	24.6	24.0		
80.73	1/2	1	1.8	25.0		
83.68	1/2	1	0.01	25.0		
89.24	1/2	1	0.09	25.0		

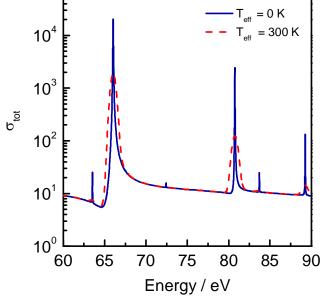
The self-shielding factor for a parallel neutron beam on a target with target thickness n (in at/b) is defined by:

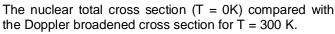
$$f = (1 - e^{-n\sigma_{tot}})$$

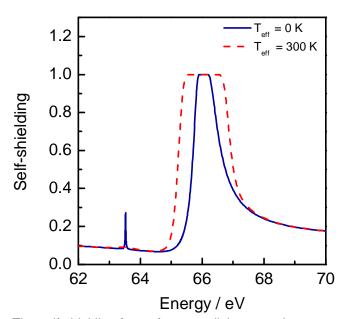
For practical application the calculation of the self-shielding factor requires the Doppler broadened cross sections. In figure 14.1 the total nuclear cross for <sup>238</sup>U+n is compared with the Doppler broadened cross section. In the figure the peak cross sections are indicated.

- (a) Calculate the self-shielding factor for a parallel neutron beam on a 0.5 cm thick UO<sub>2</sub> sample for the resonances at 66.02, 80.73 and 89.24 eV in <sup>238</sup>U. Perform the calculations for the nuclear and Doppler broadened total cross sections. The sample is made of natural uranium and has a density of 10 g/cm<sup>3</sup>.
- (b) Discuss the impact of an increase in temperature on the self-shielding factor around the resonance at 66 eV (see figure)

E <sub>R</sub> (eV)	J	σ <sub>ο</sub> (0 K) barn	σ <sub>o</sub> (300 K) barn	f (0 K)	f (300 K)
66.02	1/2	20245	1900		
80.73	1/2	2420	125		
89 24	1/2	135	14		



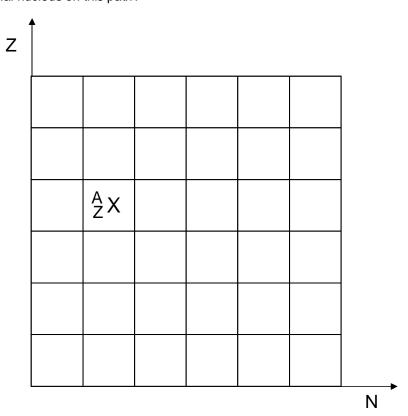




The self-shielding factor for a parallel neutron beam on a 0.5 cm thick  $UO_2$  sample around the 66.02 eV resonance for T=0 and 300 K.

Consider a neutron beam with a neutron flux  $10^{14}$  cm<sup>-2</sup> s<sup>-1</sup> which hits a target consisting of nuclei  $^{A}_{Z}X$ . The nucleus  $^{A}_{Z}X$  undergoes a  $(n,\gamma)$  reaction; the nucleus formed in this way immediately decays via  $\beta$  decay. The nucleus obtained after this decay undergoes a  $(n,\gamma)$  reaction, leading to an unstable nucleus. This nucleus in turn decays via electron capture (EC) with  $T_{1/2}=8$  year but it also undergoes a  $(n,\gamma)$  reaction with an averaged cross section  $\langle \sigma(n,\gamma) \rangle = 10$  mb. Follow here the most probable path. The next nucleus again undergoes a  $(n,\gamma)$  reaction, leading to a short-living nucleus immediately decaying via  $\alpha$ -emission. The daughter nucleus undergoes a  $(n,\gamma)$  reaction. On the nucleus formed in this way two neutron induced reactions are possible: a  $(n,\gamma)$  reaction with an average cross section  $\langle \sigma(n,\gamma) \rangle = 1.8$  mb. Follow the most dominant process.

- (a) Draw the most probable path followed in the (N,Z)-diagram
- (b) What is the final nucleus on this path?



$$(n,\gamma) \qquad {}^{A}_{Z}X + n \,\rightarrow\, {}^{A+1}_{Z}X + \gamma$$

$$(n,p) \qquad {\overset{A}{Z}} X + n \, \rightarrow \, {\overset{A}{Z-1}} X + p$$

$$\beta^{-}$$
  $\overset{A}{Z}X \rightarrow \overset{A}{Z+1}X + e^{-}$ 

$$\beta^+$$
  ${}^A_Z X \rightarrow {}_{Z-1}^A X + e^+$ 

EC 
$${}^{A}_{Z}X + e^{-} \rightarrow {}_{Z-1}^{A}X$$

$$\alpha \qquad \quad {^{A}_{Z}X} \rightarrow \ {^{A-4}_{Z-2}X} + \alpha$$

Reaction rate (N = number of nuclei per volume) :  $N\phi\sigma$ Decay probability (decay constant  $\lambda = \ln 2 / T_{1/2}$ ) :  $\lambda N$ 

# Mills et al., "Quantities, Units and Symbols in Physical Chemistry" Useful constants (SI Units)

Quantity	Symbol	Value
Speed of light in vacuum	Co	299 792 458 m s <sup>-1</sup> (defined)
Planck constant	h	6.626 075 5 (40) x 10 <sup>-34</sup> Js
Elementary charge	е	1.602 177 33 (45 ) x 10 <sup>-19</sup> C
Electron rest mass	m <sub>e</sub>	9.109 389 7 (54) x 10 <sup>-31</sup> kg
Proton rest mass	$m_p$	1.672 623 1 (10) x 10 <sup>-27</sup> kg
Neutron rest mass	$m_n$	1.674 928 6 (10) x 10 <sup>-27</sup> kg
Atomic mass constant	$m_u = 1u$	1.660 540 2 (10) x 10 <sup>-27</sup> kg
(unified atomic mass unit)		
Avogadro constant	$N_A$	6.022 136 7 (36) x 10 <sup>23</sup> mol <sup>-1</sup>
Boltzmann constant	k	1.380 658 (12) x 10 <sup>-23</sup> J K <sup>-1</sup>
Standard acceleration of free fall	g <sub>n</sub>	9.806 65 m s <sup>-2</sup> (defined)

## **SI Prefixes**

Submultiple	Prefix	Symbol	Multiple	Prefix	Symbol
10 <sup>-2</sup>	centi	С			
10 <sup>-3</sup>	milli	m	10 <sup>3</sup>	kilo	k
10 <sup>-6</sup>	micro	μ	10 <sup>6</sup>	mega	М
10 <sup>-9</sup>	nano	n	10 <sup>9</sup>	giga	G
10 <sup>-15</sup>	femto	f			

## **Conversion tables for units**

Name	Symbol	Relation to SI
ångström	Å	= 10 <sup>-10</sup> m
barn	b	$= 10^{-28} \text{ m}^2$
gram	g	$= 10^{-3} \text{ kg}$
year	а	≈ 31 556 952 s
electronvolt	eV	$= e \times V \approx 1.602 \ 18 \times 10^{-19} \ J$
watt	W	= kg m2 s-1