22.05 P-SET 3

Jacob Miske

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1 3rd Largest Resonance

Using only the 36.68eV resonance and the energy range of [25.0eV to 50.0eV], compute by approximation and by integration the U-238 group capture cross section.

$$\sigma_{\gamma,g}^{-}(E) = \frac{\int_{E1}^{E2} \sigma_{\gamma}(E) \frac{1}{E} dE}{\int_{E1}^{E2} \frac{1}{E} dE}$$
(1)

1.1 Compute Analytically

Approximating both 1/E terms of the numerator as constants over the range of the integral, compute analytically the U-238 group capture gross section.

In U-238, the third resonance peak's energy is at $E_0 = 36.68eV$, $\Gamma_{\gamma} = 0.023$, $\Gamma_n = 0.03355$, $E_1 = 25.0eV$, and $E_2 = 50.0eV$. The microscopic cross section as defined by SLBW,

$$\sigma_{\gamma} = \sqrt{\frac{E_0}{E}} r_0 \frac{\Gamma_n * \Gamma_{\gamma}}{(\Gamma)^2} [\Psi(\chi)]$$

Where $\Psi = \frac{1}{1+\chi^2}$, $\Gamma_{\gamma} + \Gamma_n = \Gamma$, and $\chi = \frac{2(E-E_0)}{\Gamma}$.

$$\sigma_{\gamma,g}^{-} = \frac{\int_{E_1}^{E_2} \sigma_{\gamma}(E) \frac{1}{E} dE}{\ln \frac{E_2}{E_1}}$$
 (2)

$$\sigma_{\gamma,g}^{-} = \frac{1}{E_0} r_0 \frac{\Gamma_n * \Gamma_{\gamma}}{(\Gamma)^2} \frac{\int_{E_1}^{E_2} \frac{1}{1 + \chi^2} dE}{\ln \frac{E_2}{E_1}}$$
(3)

Substitute $u = \chi$ and $du = \frac{2dE}{\Gamma}$

$$\sigma_{\gamma,g}^{-} = \frac{1}{E_0} r_0 \frac{\Gamma_n * \Gamma_{\gamma}}{(\Gamma)^2} (\Gamma/2) \frac{\int_{u_1}^{u_2} \frac{1}{1 + u^2} du}{\ln \frac{E_2}{E_1}}$$
(4)

Use the identity $\int_{x_1}^{x_2} \frac{1}{1+x^2} dx = arctan(x_2) - arctan(x_1)$

$$\sigma_{\gamma,g}^{-} = \frac{1}{E_0} r_0 \frac{\Gamma_n * \Gamma_{\gamma}}{(\Gamma_n + \Gamma_{\gamma})^2} (\Gamma/2) \frac{\arctan(\frac{2(E_2 - E_0)}{\Gamma_n + \Gamma_{\gamma}}) - \arctan(\frac{2(E_1 - E_0)}{\Gamma_n + \Gamma_{\gamma}})}{\ln \frac{E_2}{E_1}}$$
(5)

Where
$$r_0 = \frac{2603911}{E_0} \frac{A+1}{A}^2$$
. A =238 for U-238.

When values are substituted into the equation and rounded accordingly $\sigma_{\gamma,g} = 60.263$ barns.

1.2 Compute Numerically

Approximating both 1/E terms in the numerator as constants over the range of the integral, compute the U-238 group capture cross section numerically.

Using the equation computed analytically above, an integration over the energy range can be solved in MatLab's native function library. The method implemented should underestimate the value of the group capture cross section as assuming the 1/E values in the numerator are constant

From MatLab,

```
%From analytical, constant 1/E assumption solution of the group capture
%cross section function
sigmaGammaA = (1/E_0)*r_0*((gammaN*gammaY)/(gammaTotal^2))*(gammaTotal/2)*((tan(Chi2)^-1) - (tan(Chi
sigmaGammaA =
60.2647 barns
```

1.3 Including 1/E Terms, compute numerically the U-238 group capture cross section

In order to efficiently incorporate the 1/E terms into the numerical calculation, I used the MatLab native function of 'integral'. Integral(fun,xmin,xmax) numerically integrates function fun from xmin to xmax using global adaptive quadrature and default error tolerances [MatLab Documentation].

The quadrature approach continues to increase dE size until error is reduced into the fourth decimal place. This is because the values used in Γ values have up to four significant digits past the zero.

```
% Problem 1, Part 3
funcsigmaGamma1overE = @(E) sqrt(E_0./E).*(1./E).*r_0.*(gammaN./gammaTotal).*(gammaY./gammaTotal).*
func1overE = @(E) 1./E;
sigma_groupCapture = integral(funcsigmaGamma1overE, 25.0, 50.0)./integral(func1overE, 25.0, 50.0);
sigma_groupCapture =
60.2811 barns
```

2 Include All Three Major Resonances to Cross Sections at All Energies

2.1 Plot 0K U-238 Capture Cross Section

From 0.1eV to 50.0eV, what are the peak capture cross sections for each resonance?

I started by running a loop that would calculate the cross section from each resonance at intervals of dE = 0.05eV. This loop populated a list for each resonance. The combination of these lists is an overall U-238 group capture cross section that can be used to determine facets of what the cross sections are between resonances. Figure two shows the impact of each resonance and figure three shows the total cross section.

Looking through the lists that hold each resonances cross section values over the energy range, the MatLab 'max' function can be used to spot the highest cross section value calculated.

```
maxRes1 = 6.1025e + 03 barns; maxRes2 = 1.0811e + 04 barns; maxRes3 = 1.1510e + 04 barns;
%RI_inf^(E1,E2) = int from E1 to E2 of { sigma_gamma(E) 1/E dE
E_1res1 = 1.0; E_2res1 = 6.0; E_1res2 = 6.0; E_2res2 = 10.0; %eV
E_1res3 = 10.0; E_2res3 = 25.0; E_1res4 = 25.0; E_2res4 = 50.0; %eV
%Run step wise integration
dE = 0.05; numOfESplits = (0.1:dE: 50.0); %eV
XSplaceholder = [];
resInt1numerator = (sqrt(E_0res1./E).*(1./E).*r_0res1.*(gammaNres1./gammaTotalres1).*(gammaYres1./gamma
resInt2numerator = (sqrt(E_0res2./E).*(1./E).*r_0res2.*(gammaNres2./gammaTotalres2).*(gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gammaYres2./gamm
resInt3numerator = (sqrt(E_0res3./E).*(1./E).*r_0res3.*(gammaNres3./gammaTotalres3).*(gammaYres3./gamma
%for Resonance Int 1
res1numOfESplits = numOfESplits(1:119)
for i = 1:size(res1numOfESplits,2)
         E = res1numOfESplits(i);
         XSplaceholder(i) =(1/dE)*(resInt1numerator + resInt2numerator + resInt3numerator);
end
XSresInt1 = XSplaceholder;
XSresInt1sum = sum(XSplaceholder)
%for Resonance Int 2
XSplaceholder = [];
res2numOfESplits = numOfESplits(119:199)
for i = 1:size(res2numOfESplits,2)
         E = res2numOfESplits(i);
         XSplaceholder(i) = (1/dE)*(resInt1numerator + resInt2numerator + resInt3numerator);
end
XSresInt2 = XSplaceholder;
XSresInt2sum = sum(XSplaceholder)
%for Resonance Int 3
XSplaceholder = [];
res3numOfESplits = numOfESplits(199:499)
for i = 1:size(res3numOfESplits,2)
```

```
E = res3numOfESplits(i);
   XSplaceholder(i) = (1/dE)*(resInt1numerator + resInt2numerator + resInt3numerator);
end

XSresInt3 = XSplaceholder;
XSresInt3sum = sum(XSplaceholder)

%for Resonance Int 4

XSplaceholder = [];
res4numOfESplits = numOfESplits(499:999)
for i = 1:size(res4numOfESplits,2)
   E = res4numOfESplits(i);
   XSplaceholder(i) = (resInt1numerator + resInt2numerator + resInt3numerator);
end

XSresInt4 = XSplaceholder;
XSresInt4sum = sum(XSplaceholder)
```

Taking the sum of the integral equation points across each energy range gives RSI_{calc} .

2.2 Compute Numerically, the Resonance Integrals for Energy Groups

Consider the ranges, [1-6], [6-10], [10-25], and [25-50]eV. This should match closely with the published ENDF-B/VII Resonance Integrals.

$$RI_{\infty}^{E1,E2} = \int_{E1}^{E2} \sigma_{\gamma}(E) \frac{1}{E} dE \tag{6}$$

In evaluating the equation 6 numerically, we can use the numerator evaluation from earlier in problem 1 to map out how these integrals sum up over the different energy groups.

E_{range}	RI_{exp}	RI_{calc}
1.0 - 6.0	1.74	1.734
6.0 - 10.0	127.56	127.45
10.0 - 25.0	66.35	66.30
25.0 - 50.0	41.84	41.80

The integration of these ranges is done with a bin width of 0.05eV. As a result, around the peak of the resonance there may be a bin that is potentially underestimating the total value of the cross section around the area. This can be noted in the undershoot by all the numerically calculated values I provide in the table above.

```
%RI_inf^(E1,E2) = int from E1 to E2 of { sigma_gamma(E)    1/E dE

E_1res1 = 1.0; E_2res1 = 6.0; E_1res2 = 6.0; E_2res2 = 10.0; %eV

E_1res3 = 10.0; E_2res3 = 25.0; E_1res4 = 25.0; E_2res4 = 50.0; %eV

%Run step wise integration
dE = 0.05; numOfESplits = (0.1:dE: 50.0); %eV

XSplaceholder = [];
resInt1numerator = (sqrt(E_0res1./E).*(1./E).*r_0res1.*(gammaNres1./gammaTotalres1).*(gammaYres1./gammaresInt2numerator = (sqrt(E_0res2./E).*(1./E).*r_0res2.*(gammaNres2./gammaTotalres2).*(gammaYres2./gammaresInt3numerator = (sqrt(E_0res3./E).*(1./E).*r_0res3.*(gammaNres3./gammaTotalres3).*(gammaYres3./gammaYres3./gammaTotalres3).*(gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYres3./gammaYr
```

```
%for Resonance Int 1
res1numOfESplits = numOfESplits(1:119)
for i = 1:size(res1numOfESplits,2)
   E = res1numOfESplits(i);
   XSplaceholder(i) = resInt1numerator + resInt2numerator + resInt3numerator;
end
XSresInt1 = XSplaceholder;
XSresInt1sum = sum(XSplaceholder)
%for Resonance Int 2
XSplaceholder = [];
res2numOfESplits = numOfESplits(119:199)
for i = 1:size(res2numOfESplits,2)
   E = res2numOfESplits(i);
   XSplaceholder(i) = resInt1numerator + resInt2numerator + resInt3numerator;
XSresInt2 = XSplaceholder;
XSresInt2sum = sum(XSplaceholder)
%for Resonance Int 3
XSplaceholder = [];
res3numOfESplits = numOfESplits(199:499)
for i = 1:size(res3numOfESplits,2)
   E = res3numOfESplits(i);
   XSplaceholder(i) = integral(@(E) resInt1numerator + resInt2numerator + resInt3numerator);
end
XSresInt3 = XSplaceholder;
XSresInt3sum = sum(XSplaceholder)
%for Resonance Int 4
XSplaceholder = [];
res4numOfESplits = numOfESplits(499:999)
for i = 1:size(res4numOfESplits,2)
   E = res4numOfESplits(i);
   XSplaceholder(i) = resInt1numerator + resInt2numerator + resInt3numerator;
end
XSresInt4 = XSplaceholder;
XSresInt4sum = sum(XSplaceholder)
figure(4)
fplot(funcsigmaGammaCaptureXSRes1times1overE, 'r'); hold on
title('Resonance Integrals')
legend('Resonance Integral')
xlim([0 50]); ylim([0 10000]); grid on
xlabel('E (eV)'); ylabel('XS (barns)')
saveas(gcf,'Resonance Integrals Equation.pdf')
Bibliography
22.05 Lecture 4 and 5
Lamarsh chapter 6
```

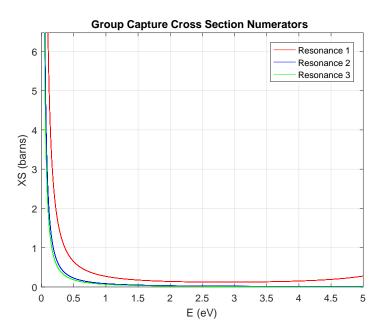


Figure 1: XS Numerator

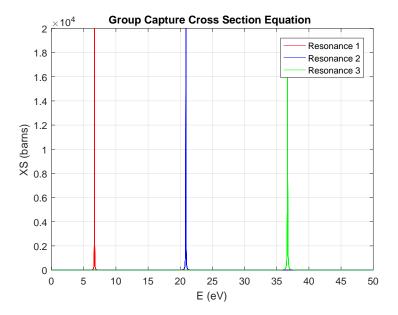


Figure 2: XS Equation

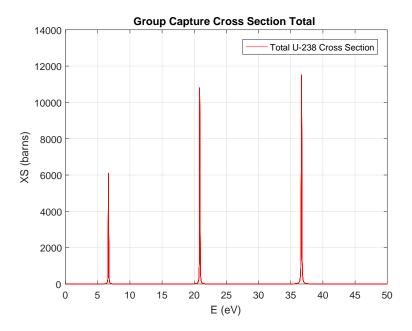


Figure 3: Total XS