22.211 Lecture 1

Nuclear Data

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Outline

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Outline

1. Objectives
2. Fission
3. Nuclear data evaluations
4. Resolved resonance range
5. Unresolved resonance range
6. Doppler Broadening

Objectives

- Understand nuclear data evaluation process
- Identify key elements of nuclear cross sections
- Differentiate physical phenomena in different energy ranges

Goals of Reactor Physics

Reactor Physics is the discipline devoted to the study of interactions between neutrons and matter in a nuclear reactor.

- Determine power distribution in the entire reactor
- Determine reactivity coefficients
- Determine power profile behavior during transients
- Calculate optimal loading patterns and cycle lengths
- Determine fuel composition prior to disposal
- Provide source of heat for multi-physics simulations

Pre-Requisites

Ideally, you should have taken 22.11 and something equivalent to 22.05

- It is expected that students will take necessary step to catch up and fill knowledge gaps. A good starting point is the DOE fundamentals handbook:
  - Volume 1: `https://www.standards.doe.gov/standards-documents/1000/1019-bhdbk-1993-v1`
  - Volume 2: `https://www.standards.doe.gov/standards-documents/1000/1019-bhdbk-1993-v2`
- In 22.211, we will not cover these topics in great detail:
  - Basic nuclear physics
  - Definition of micro, macro cross-sections
  - One group diffusion theory and 4 factor definitions
  - One group diffusion theory
  - Decay rate, activity, half-life

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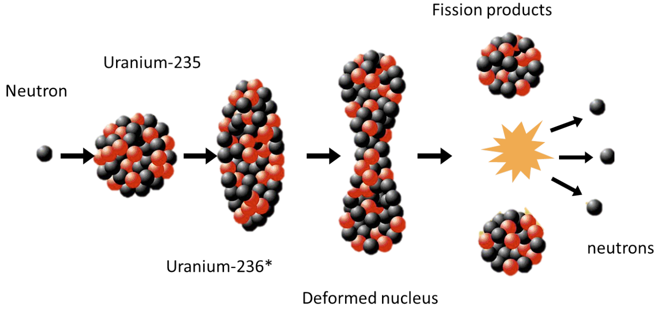
Most important reaction

$$ {}_0^1n + {}_Z^A X \rightarrow {}_{Z_1}^{A_1} Y_1 + {}_{Z_2}^{A_2} Y_2 + 200 MeV + neutrons $$



Activation Energy

Target Nucleus	Critical Energy E_{crit}	Binding Energy of Last Neutron BE_n	BE_n - E_{crit}
$^{232}_{90}Th$	7.5 MeV	5.4 MeV	-2.1 MeV
$^{238}_{92}U$	7.0 MeV	5.5 MeV	-1.5 MeV
$^{235}_{92}U$	6.5 MeV	6.8 MeV	+0.3 MeV
$^{233}_{92}U$	6.0 MeV	7.0 MeV	+1.0 MeV
$^{239}_{94}Pu$	5.0 MeV	6.6 MeV	+1.6 MeV

U-233, U-235 and Pu-239 are fissile since a neutron of any energy will exceed the activation energy of the formed compound nucleus. Th-232 and U-238 will exhibit thresholds to fission at around 1-2 MeV.

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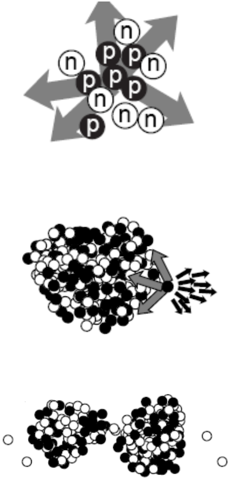
Nuclear forces

- Electromagnetic repulsion of protons
- Strong nuclear forces between nucleons
- If the particle gets too large and excited, the repulsive forces can cause the nucleus to split.



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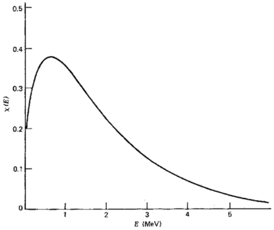
Prompt neutron spectrum

Watt spectrum

$$p(E')dE' = ce^{\frac{E'}{a(E)}} sinh(\sqrt{b(E)E'})dE'$$



More recent model: Madland-Nix model

	Incident Neutron Energy (MeV)	a(MeV)	b(MeV^{-1})
n + ^{232}Th	Thermal	1.0888	1.6871
	1	1.1096	1.6316
	14	1.1700	1.4610
n + ^{233}U	Thermal	0.977	2.546
	1	0.977	2.546
	14	1.0036	2.6377
n + ^{235}U	Thermal	0.988	2.249
	1	0.988	2.249
	14	1.028	2.084
n + ^{238}U	Thermal	0.88111	3.4005
	1	0.89506	3.2953
	14	0.96534	2.8330
n + ^{239}Pu	Thermal	0.966	2.842
	1	0.966	2.842
	14	1.055	2.383

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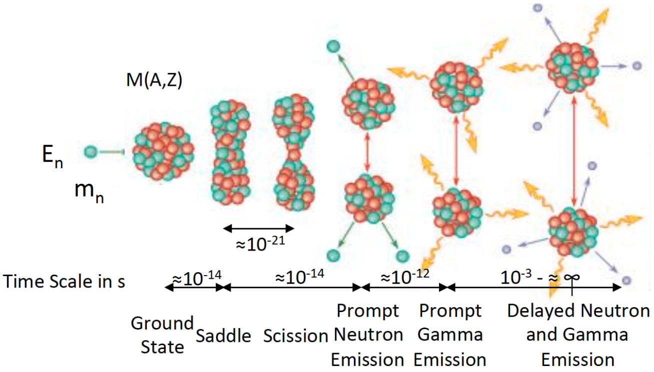
Delayed neutrons

Numbers to remember

- U235: 0.65%
- U238: 1.57%
- Pu239: 0.21%
- U233: 0.26%

Spectrum are stored as PDFs in 6 or 8 groups with different yields for each fissile species. Average energy is around 0.1 MeV.



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8 groups delayed neutrons yields

Modern trend is to use fixed decay constants (based on physical fission products) for all species with only yields that vary.

Group	Half-Life (s)	U-235 thermal $\beta_i = \nu_i / \nu_t$	U-238 thermal $\beta_i = \nu_i / \nu_t$	Pu-239 thermal $\beta_i = \nu_i / \nu_t$
1 (Br-87)	55.6	0.0218	0.0139	0.0072
2 (I-137)	24.5	0.1023	0.1716	0.0533
3 (Br-88)	16.3	0.0605	0.0619	0.01859
4 (Br-89)	5.21	0.1310	0.2260	0.0410
5 (Br-90)	2.37	0.2200	0.4850	0.0662
6 (Y-98)	1.04	0.0600	0.3270	0.01836
7 (Rb-95)	0.424	0.0540	0.2110	0.0162
8 (Rb-96)	0.195	0.0152	0.1536	0.00416
Total		**0.665**	**1.650**	**0.255**

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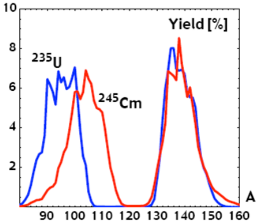
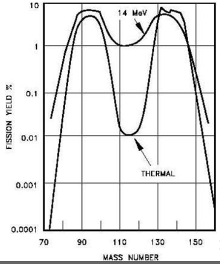
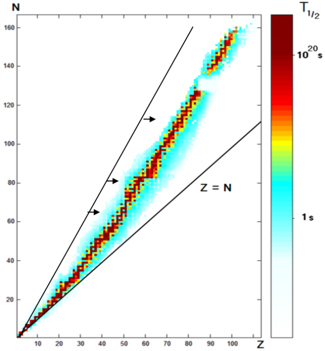
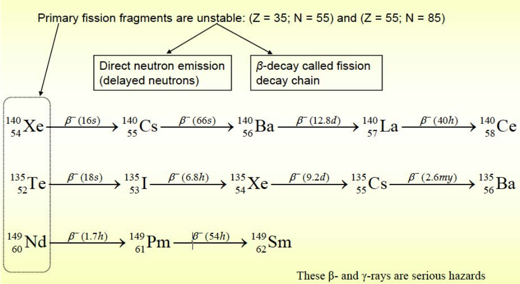
Fission product yields

- Fission yields depend on isotope and incoming neutron energy
- Stored in database as independent and cumulative yields
- Developed from a combination of experiment and models









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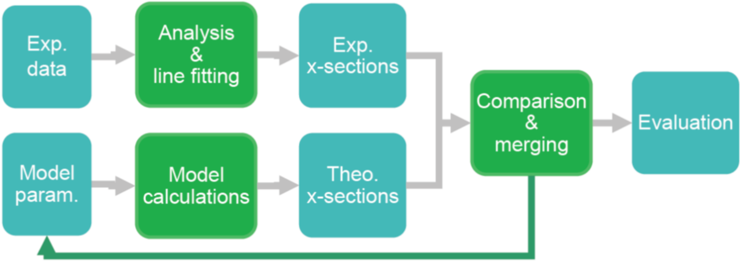
Spontaneous Fission

Element-A	Half-life years	Spontaneous fission	
		Fraction	Rate per kg per second
uranium-233	2×10^{5}	1.6×10^{-12}	0.5
uranium-235	7.0×10^{8}	7×10^{-11}	0.06
uranium-238	4.5×10^{9}	5.4×10^{-7}	6
plutonium-239	2.4×10^{4}	4.4×10^{-12}	10
plutonium-240	6.6×10^{3}	5.0×10^{-8}	4.1×10^{5}
californium-252	2.6	0.03	2.3×10^{15}

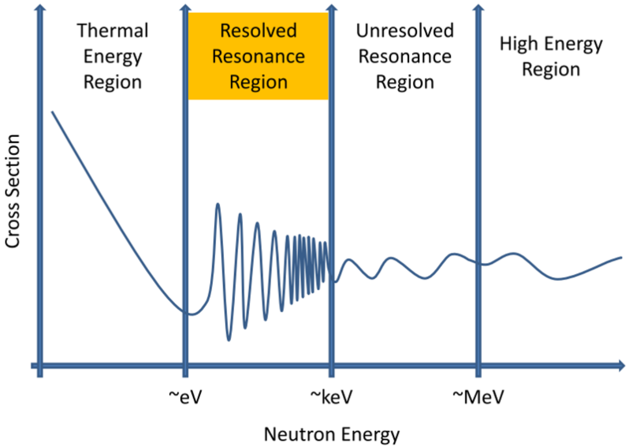
Outline

Evaluation Process



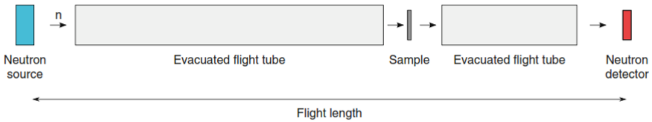
Cross sections are a combination of theory and experiments.

Energy Ranges

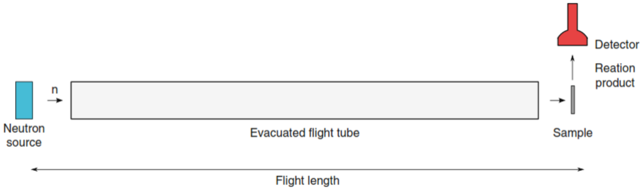


Time-of-flight (ch1, sect 5)

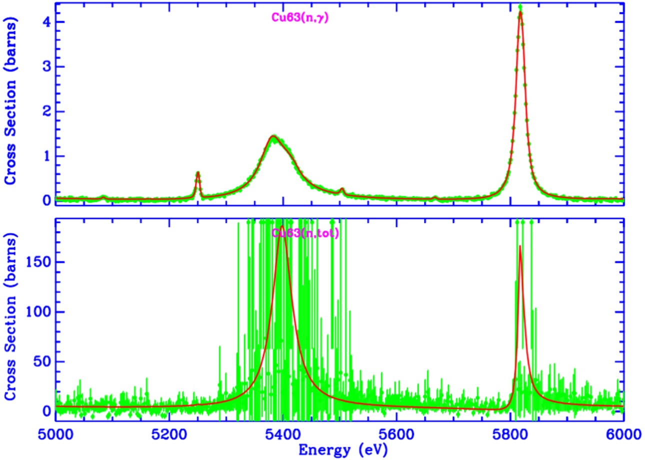
Transmission



Capture

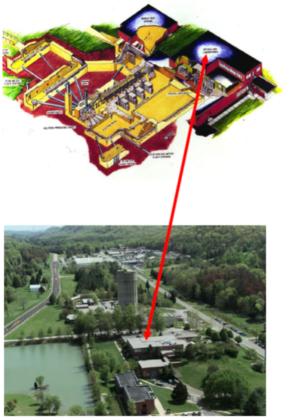


These experiments are referred to as differential experiments.

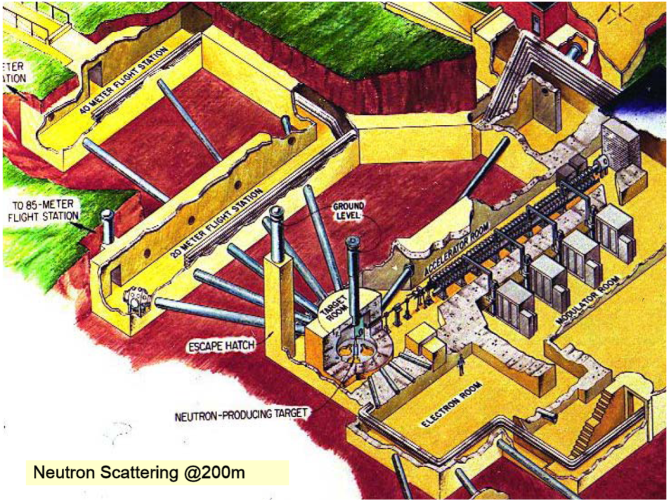

Cu63(n,γ)
Cross Section (barns)
0
1
2
3
4
Cu63(n,tot)
Cross Section (barns)
0
50
100
150
5000
5200
5400
5600
5800
6000
Energy (eV)

ORELA facility

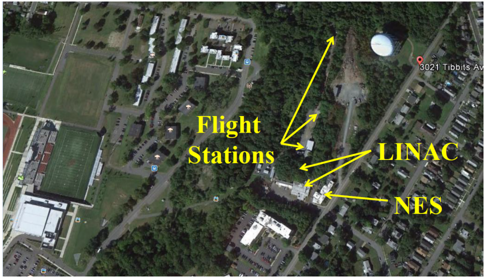
- High flux (10^{14} n/s)
- Spectrum from 0.01 eV to 80 MeV
- Good time resolution (2-30 ns)
- Well characterize background
- Simultaneous measurements in many beam lines
- Measurements performed on over 180 isotopes

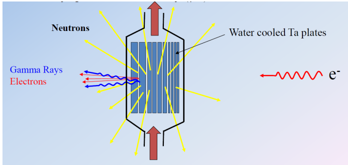


ORELA facility

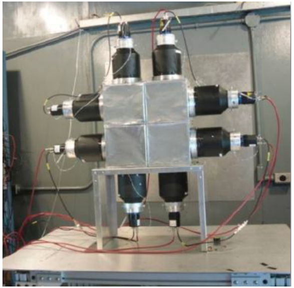


RPI LINAC

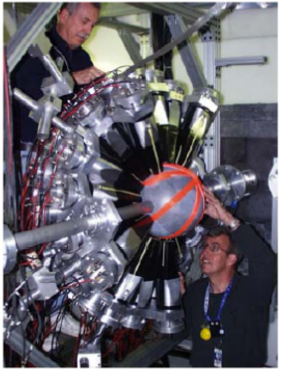

3021 Tibbits Av
Flight
Stations
LINAC
NES

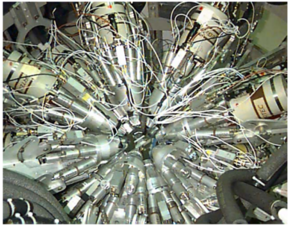

Neutrons
Water cooled Ta plates
Gamma Rays
Electrons
e-

Detectors

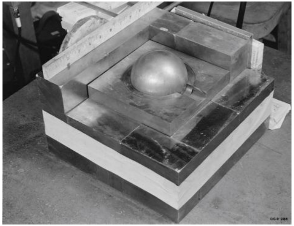


Detectors





Integral Validation



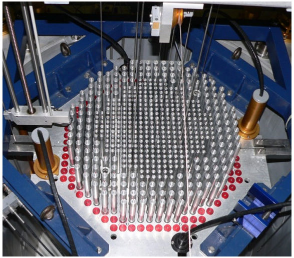


Figure 2. Manual Loading of the ZPPR Matrix.

Figure 3. Photograph of Typical Plate-Loaded ZPPR Drawer.

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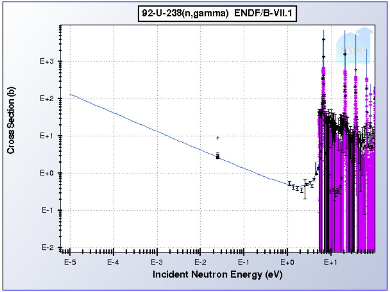
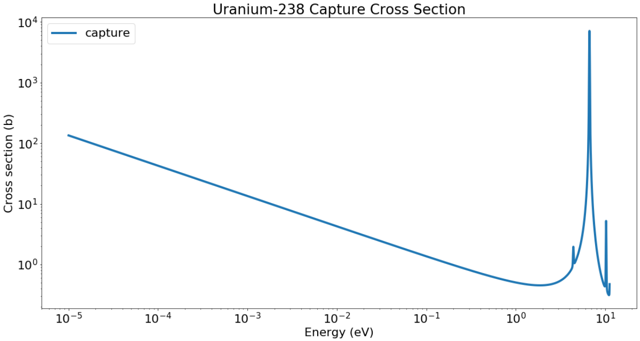
Thermal measurements are often done using a single point at 0.025eV

- Irradiate sample to saturation activity
- Pull sample and measure activity (and reaction rate)
- Assuming 1/v capture cross section and flux magnitude, we can calculate the cross section at a given energy point (0.025eV is the most probable energy of a Maxwellian distribution at 293K).

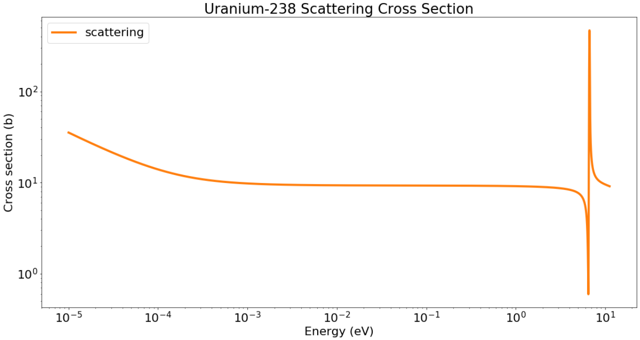


1/v cross sections

The "1/v" behavior is a first order approximation at low energy (see 1948 Wigner paper for details) commonly observed for neutron capture. It is valid for s-wave only and in the absence of thermal resonances. It shows up as the energy dependence of the neutron width ($\Gamma_n(E) \approx 1/\sqrt{E}$).



Potential scattering



Potential scattering is flat and corresponds approximately to the size of the nucleus ($4\pi R^2$), except for H-1. The radius can be approximated by

$$R = r_0 A^{1/3} \quad r_0 = 1.25x10^{-13} cm$$

SLBW at 0K

$$\sigma_\gamma(E) = \frac{\Gamma_n}{\Gamma}\frac{\Gamma_\gamma}{\Gamma}\sqrt{\frac{E_0}{E}}\left[r\psi(x)\right]$$

$$\sigma_n(E) = \frac{\Gamma_n}{\Gamma}\frac{\Gamma_n}{\Gamma}\left[r\psi(x) + \frac{\Gamma}{\Gamma_n}q\chi(x)\right] + \sigma_{pot}$$

where

$$\psi(x,\xi) = \frac{1}{1+x^2}$$

$$\chi(x,\xi) = \frac{x}{1+x^2}$$

$$r = \frac{h^2}{2\pi m E_0}\frac{A+1}{A} = \frac{2603911}{E_0}\frac{A+1}{A}$$

$$q = 2\sqrt{r\sigma_{pot}}$$

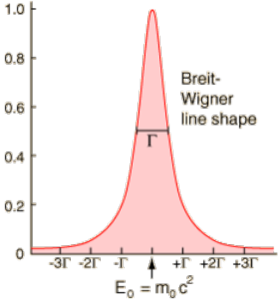
$$x = \frac{2(E-E_0)}{\Gamma}$$

$$\Gamma = \Gamma_n + \Gamma_\gamma \quad \sigma_{pot} = 4\pi a^2$$

Resonance Models

Resonance models are derived from Schrodinger equation. Experimental data fills the knowledge gap (i.e. nuclear potential) and the model allows extension beyond the measurement range (e.g. temperature effects).

- SLBW: Only accounts for channel interference at a given level
- MLBW: Accounts for channel interference at a given level and level-level interference within a channel
- Reich-Moore: Accounts for interference across channels and levels but neglects interference with gamma channels



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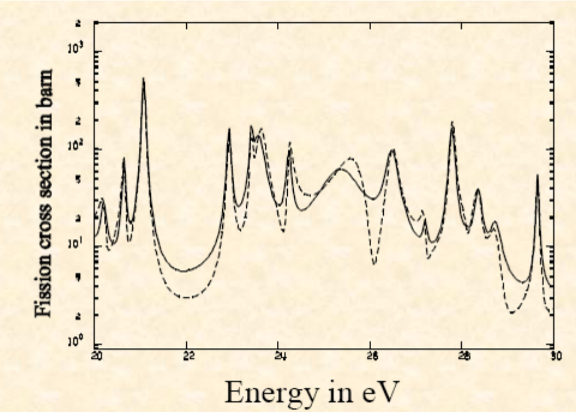
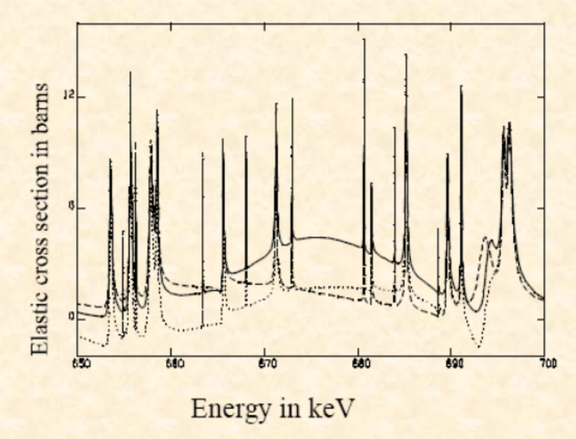
- Physical significance of resonances: `https://www.youtube.com/watch?v=XggxeuFDaDU`
- Geometrically, an eigenvector, corresponding to a real nonzero eigenvalue, points in a direction in which it is stretched by the transformation and the eigenvalue is the factor by which it is stretched.

Interference effects on U235



Solid line (RM), Dash line (SLBW)



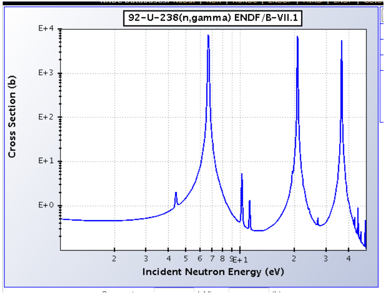
Solid line (RM), Dash line (MLBW), Dot line (SLBW)

Outline

1. Objectives
2. Fission
3. Nuclear data evaluations
4. Resolved resonance range
5. Unresolved resonance range
6. Doppler Broadening

U238 resonances

- Why are there negative values?
- Are these physical?



eV	J	GN	GG	GFA	GFB
-4.405250+3	5.000000-1	1.393500+2	2.300000-2	0.000000+0	0.000000+0
-4.133000+2	5.000000-1	5.215449-2	2.300000-2	0.000000+0	0.000000+0
-3.933000+2	5.000000-1	4.993892-2	2.300000-2	0.000000+0	0.000000+0
-3.733000+2	5.000000-1	4.764719-2	2.300000-2	0.000000+0	0.000000+0
-3.533000+2	5.000000-1	4.527354-2	2.300000-2	0.000000+0	0.000000+0
-3.333000+2	5.000000-1	4.281115-2	2.300000-2	0.000000+0	0.000000+0
-3.133000+2	5.000000-1	4.025348-2	2.300000-2	0.000000+0	0.000000+0
-2.933000+2	5.000000-1	3.759330-2	2.300000-2	0.000000+0	0.000000+0
-2.733000+2	5.000000-1	2.551450-2	2.300000-2	0.000000+0	0.000000+0
-2.533000+2	5.000000-1	2.397198-2	2.300000-2	0.000000+0	0.000000+0
-2.333000+2	5.000000-1	2.234626-2	2.300000-2	0.000000+0	0.000000+0
-2.133000+2	5.000000-1	2.062684-2	2.300000-2	0.000000+0	0.000000+0
-1.933000+2	5.000000-1	1.879962-2	2.300000-2	0.000000+0	0.000000+0
-1.733000+2	5.000000-1	1.685164-2	2.300000-2	0.000000+0	0.000000+0
-1.533000+2	5.000000-1	1.476751-2	2.300000-2	0.000000+0	0.000000+0
-1.333000+2	5.000000-1	1.253624-2	2.300000-2	0.000000+0	0.000000+0
-1.133000+2	5.000000-1	1.015824-2	2.300000-2	0.000000+0	0.000000+0
-9.330000+1	5.000000-1	7.658435-3	2.300000-2	0.000000+0	0.000000+0
-7.330000+1	5.000000-1	5.086118-3	2.300000-2	0.000000+0	0.000000+0
-5.330000+1	5.000000-1	2.932955-3	2.300000-2	0.000000+0	0.000000+0
-3.330000+1	5.000000-1	1.004548-2	2.300000-2	2.010000-6	0.000000+0
-7.000000+0	5.000000-1	1.685000-4	2.300000-2	0.000000+0	0.000000+0
6.673491+0	5.000000-1	1.475792-3	2.300000-2	0.000000+0	9.990000-9
2.087152+1	5.000000-1	1.009376-2	2.286379-2	5.420000-8	0.000000+0
3.668212+1	5.000000-1	3.354568-2	2.300225-2	0.000000+0	9.770000-9
6.603118+1	5.000000-1	2.417823-2	2.330763-2	5.265000-8	0.000000+0
8.074744+1	5.000000-1	1.873989-3	2.338714-2	0.000000+0	6.049000-8
1.025586+2	5.000000-1	7.077051-2	2.408178-2	0.000000+0	0.000000+0
1.168923+2	5.000000-1	2.535360-2	2.227601-2	0.000000+0	0.000000+0
1.456649+2	5.000000-1	8.857229-4	2.382470-2	0.000000+0	0.000000+0
1.653167+2	5.000000-1	3.190336-3	2.437384-2	0.000000+0	0.000000+0
1.896804+2	5.000000-1	1.701848-1	2.357967-2	0.000000+0	3.573000-8
2.085250+2	5.000000-1	4.988164-2	2.283536-2	8.347000-8	0.000000+0
2.373985+2	5.000000-1	2.644844-2	2.517753-2	0.000000+0	3.542000-8
2.736794+2	5.000000-1	2.486493-2	2.440783-2	0.000000+0	0.000000+0

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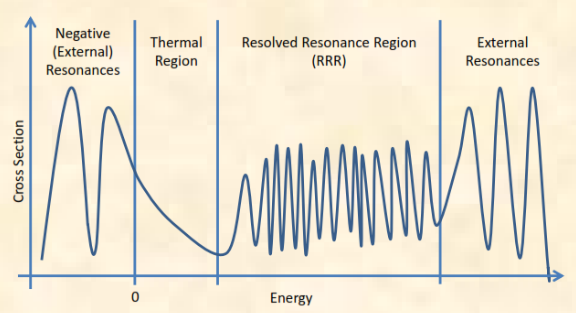
External resonances

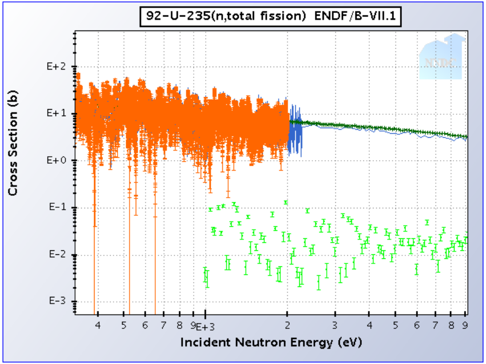


External resonances are added to provide additional degrees of freedom in the fitting process.

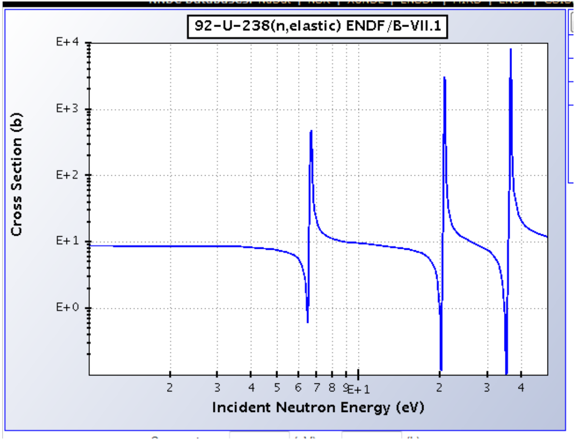
Nuclear data evaluation

- Evaluations in the resolved resonance range are a giant data fit
- Experiments are used to find position of resonances and shape of the resonances (width, spin, angular momentum ...)
- Theoretical models are used to compress data, to provide accurate fitting functions, to supplement data gaps (interpolation and extrapolation), ...
- Data is provided at 0K or in the form of resonance parameters

Not all experimental data is of equal value

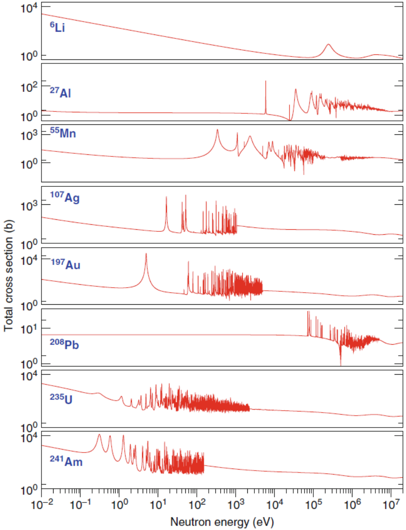


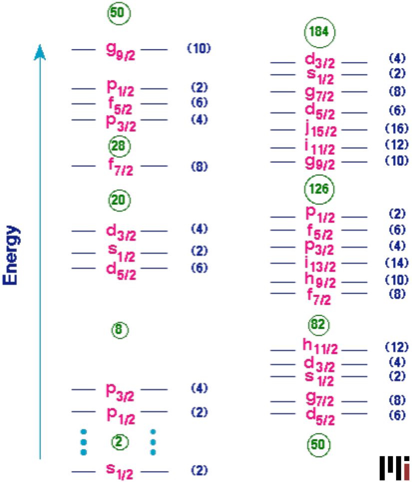
Data fitting is very complicated and is considered an "art". Bayesian statistics and expert judgment comes in to play in obtaining an evaluation.



Notice the interference effect that exists between potential scattering and compound nucleus resonant scattering.

Resonance location and spacing





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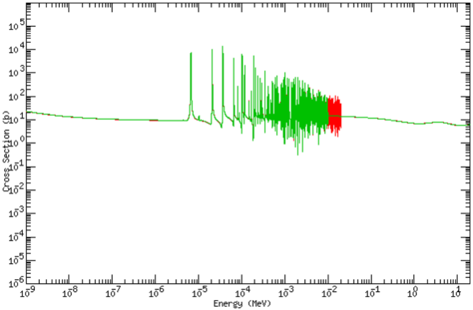
Outline

U238 ENDF6 vs ENDF7

- Why does the resolved resonance range end?
- How do we determine the end point?
- Why does it vary from library to library?



URR distributions

- Wigner distribution on level spacing
- χ^2 distribution of partial widths
- Parameters are determined from an extension of the resolved resonance range and statistical models

Unresolved Parameters
all parameters are energy dependent

Spin: 0.000000+0
Scattering length AP: 9.433790-1
Potential scattering 4*pi*AP**2: 1118.36072
LSSF: 1
Number of l states: 3

L = 0 (1 J states)

J = 5
Interpolation law: log-log

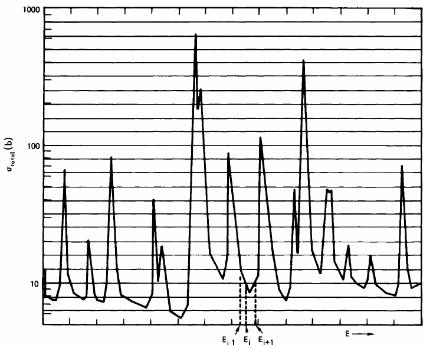
Degrees of freedom

zero	zero	AMUX	AMUN	AMUG	AMUF
0.000000+0	0.000000+0	2.000000+0	1.000000+0	0.000000+0	0.000000+0

S	D	GX	GN0	GG	GF
2.000000+4	2.199760+1	0.000000+0	2.063460-3	2.281190-2	0.000000+0
2.300000+4	2.185120+1	0.000000+0	2.043260-3	2.284390-2	0.000000+0
2.600000+4	2.170590+1	0.000000+0	2.023690-3	2.287600-2	0.000000+0
3.000000+4	2.151390+1	0.000000+0	1.998440-3	2.291910-2	0.000000+0
3.500000+4	2.127610+1	0.000000+0	1.967970-3	2.297280-2	0.000000+0
4.000000+4	2.104110+1	0.000000+0	1.938570-3	2.302660-2	0.000000+0
4.500000+4	2.080860+1	0.000000+0	1.910100-3	2.308050-2	0.000000+0
4.509020+4	2.080440+1	0.000000+0	1.909600-3	2.308140-2	0.000000+0
5.000000+4	2.057890+1	1.097450-5	1.882470-3	2.313450-2	0.000000+0
5.500000+4	2.035200+1	6.242520-5	1.855610-3	2.318890-2	0.000000+0

Probability tables

- Generate a fake cross section set using SLBW model
- Compute probability of cross section being in each band
- Repeat the process multiple times and take average probability table



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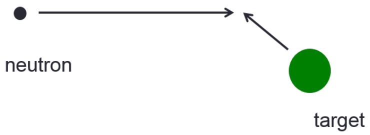
Outline

Cross sections depend on target motion



Assumptions

- Medium is in thermal equilibrium
- Medium can be characterized by a Maxwellian distribution
- Medium is isotropic (no preferential direction)
- Target atoms are not part of a lattice or molecule (free gas)
- Neutron is not at relativistic velocities

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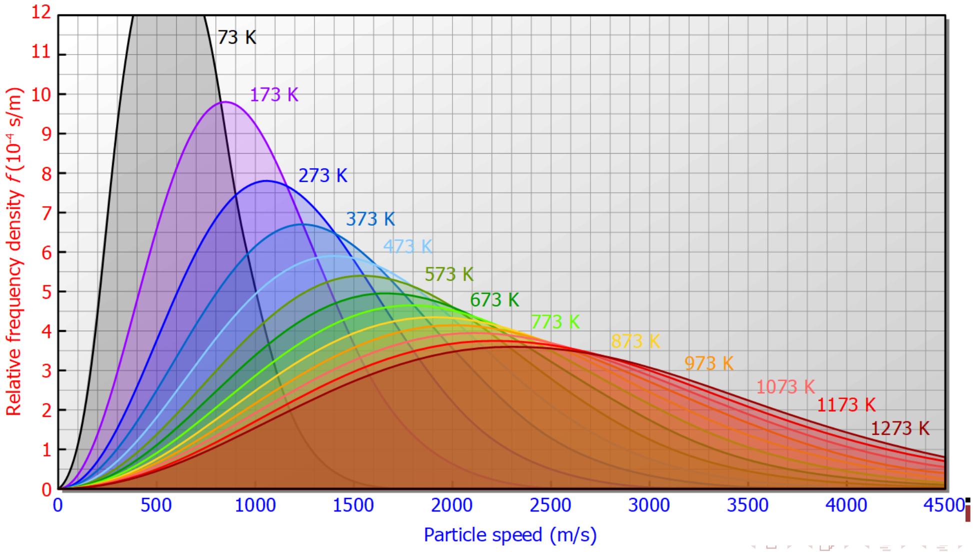
Convolution integral

$$v_n \overline{\sigma_x(v_n)} = \int d^3 v_T P(v_T) |\vec{v_n} - \vec{v_T}| \sigma_x(|\vec{v_n} - \vec{v_T}|)$$

where $|\vec{v_n} - \vec{v_T}|$ is the relative velocity $\vec{v_R}$.

- Maxwellian distribution is commonly used for $P(v_T)$
- Integral can be performed analytically for the SLBW format
- MLBW and RM require conversion to multipole formalism or numerical integration (SIGMA1)

Maxwell Boltzmann Distribution



SLBW as a function of temperature

$$\sigma_\gamma(E,T) = \frac{\Gamma_n}{\Gamma}\frac{\Gamma_\gamma}{\Gamma}\sqrt{\frac{E_0}{E}}\left[r\psi(x,\xi)\right]$$

$$\sigma_n(E,T) = \frac{\Gamma_n}{\Gamma}\frac{\Gamma_n}{\Gamma}\left[r\psi(x,\xi) + \frac{\Gamma}{\Gamma_n}q\chi(x,\xi)\right] + \sigma_{pot}$$

where

$$\psi(x,\xi) = \sqrt{\pi}Re\left[\xi W\left((x+i)\xi\right)\right]$$

$$\chi(x,\xi) = \sqrt{\pi}Im\left[\xi W\left((x+i)\xi\right)\right]$$

$$r = \frac{h^2}{2\pi m E_0}\frac{A+1}{A} = \frac{2603911}{E_0}\frac{A+1}{A}$$

$$q = 2\sqrt{r\sigma_{pot}}$$

$$\xi = \frac{\Gamma}{4}\sqrt{\frac{A}{kTE_0}} \quad x = \frac{2(E-E_0)}{\Gamma}$$

$$\Gamma = \Gamma_n + \Gamma_\gamma \quad \sigma_{pot} = 4\pi a^2$$

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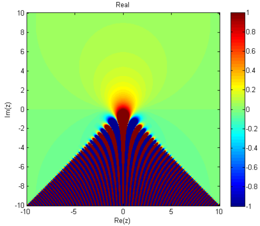
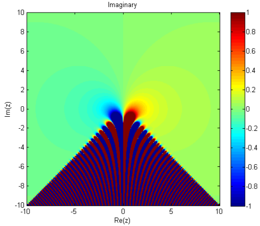
Faddeeva function

$$W(z) = e^{-z^2} erfc(-iz)$$

- You can use the following package

(http://ab-initio.mit.edu/wiki/index.php/Faddeeva_Package)





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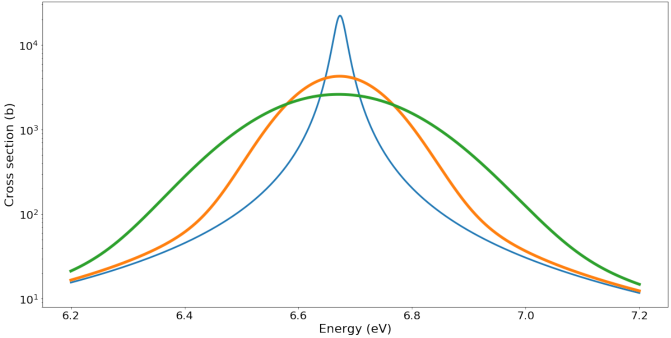
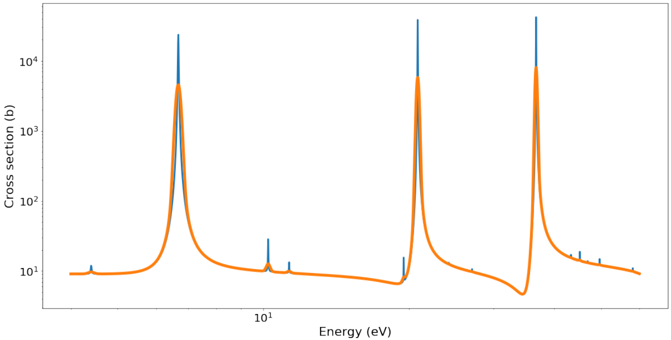
U238 Capture near 6.67eV resonance with Temperature



Blue (0K), Orange (1000K), Green (3000K)

U238 Capture near the three main s-wave resonances



Blue (0K), Orange (1000K)

HW1a - Using OpenMC on google colab

1. Email me with address you would like to use for shared data folder
2. Log in to colab.research.google.com
3. Upload OpenMC-install.ipynb notebook
4. Run notebook to verify install
5. Documentation can be found at (https://docs.openmc.org/en/latest/)

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