Fundamental aspects of the thermal neutron scattering

Florencia Cantargi
cantargi@cab.cnea.gov.ar

Departamento de Física de Neutrones
Gerencia de Ingeniería Nuclear
Instituto Balseiro (UNCuyo)

Centro Atómico Bariloche
Comisión Nacional de Energía Atómica

ARGENTINA

Joint ICTP-IAEA School on Nuclear Data Measurements for Science and Applications
October 27th, 2015


ARCTIC OCEAN
Greenland (DEN.)
U.S.
CANADA
UNITED STATES
MEXICO
ICELAND
NORWAY
SWEDEN
FINLAND
RUSSIA
UNITED KINGDOM
IRELAND
FRANCE
PORTUGAL
SPAIN
GER.
POL.
BELARUS
UKRAINE
ROM.
ITALY
GREECE
TURKEY
KAZAKHSTAN
MONGOLIA
CHINA
N. KOREA
S. KOREA
JAPAN
UZB.
TURKM.
KYRGYZSTAN
TAJIKISTAN
AFG.
IRAN
IRAQ
SYRIA
JOR.
PAKISTAN
NEPAL
INDIA
BURMA
LAOS
THAILAND
VIETNAM
CAMBODIA
PHILIPPINES
Taiwan
MALAYSIA
INDONESIA
PAPUA NEW GUINEA
SOLOMON ISLANDS
AUSTRALIA
NEW ZEALAND
NORTH PACIFIC OCEAN
NORTH ATLANTIC OCEAN
SOUTH PACIFIC OCEAN
SOUTH ATLANTIC OCEAN
INDIAN OCEAN
Equator
THE BAHAMAS
CUBA
DOMINICAN REPUBLIC
HAITI
JAM.
Puerto Rico (U.S.)
BELIZE
HONDURAS
GUATEMALA
EL SALVADOR
NICARAGUA
COSTA RICA
PANAMA
TRINIDAD AND TOBAGO
VENEZUELA
GUYANA
SURINAME
French Guiana (FRANCE)
COLOMBIA
ECUADOR
PERU
BRAZIL
BOLIVIA
PARAGUAY
CHILE
URUGUAY
ARGENTINA
MOROCCO
Western Sahara
ALGERIA
TUNISIA
LIBYA
EGYPT
MAURITANIA
MALI
NIGER
CHAD
SUDAN
SENEGAL
THE GAMBIA
GUINEA-BISSAU
GUINEA
SIERRA LEONE
LIBERIA
CÔTE D'IVOIRE
BURKINA FASO
GHANA
TOGO
BENIN
NIGERIA
CAMEROON
C.A.R.
EQ. GUINEA
GABON
REP. OF THE CONGO
DEM. REP. OF THE CONGO
UGANDA
KENYA
RWANDA
BURUNDI
TANZANIA
ETHIOPIA
ERITREA
DJIBOUTI
SOMALIA
YEMEN
OMAN
SAUDI ARABIA
QATAR
U.A.E.
KUWAIT
ANGOLA
ZAMBIA
MALAWI
MOZAMBIQUE
ZIMBABWE
NAMIBIA
BOTSWANA
SOUTH AFRICA
LESOTHO
SWAZILAND
MADAGASCAR
COMOROS
SEYCHELLES
MALDIVES
SRI LANKA
Antarctica
Scale 1:134,000,000
Robinson Projection
standard parallels 38°N and 38°S
Boundary representation is not necessarily authoritative.

Research Reactors in Argentina

RA-0

Cordoba National University
Academic use

RA-1

First RR in Latin America (1958)
Training professionals for NPPs

RA-3

10 MW
4% of world's Mo-99 production

RA-4

1 MW - Rosario National University
Training, research, services for industry

RA-6

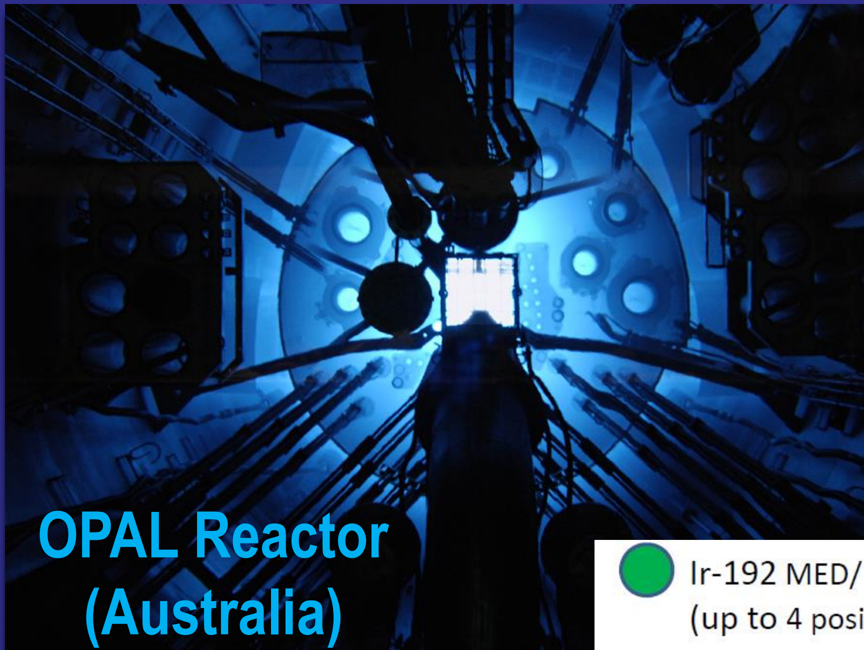
1 MW - Bariloche Atomic Center & Instituto Balseiro
Training of Nuclear Engineers
Experimental facilities: PGAA, BNCT, difractometer, neutrography

RA-8

Critical facility.
Test of CAREM reactor fuel design

RA-10

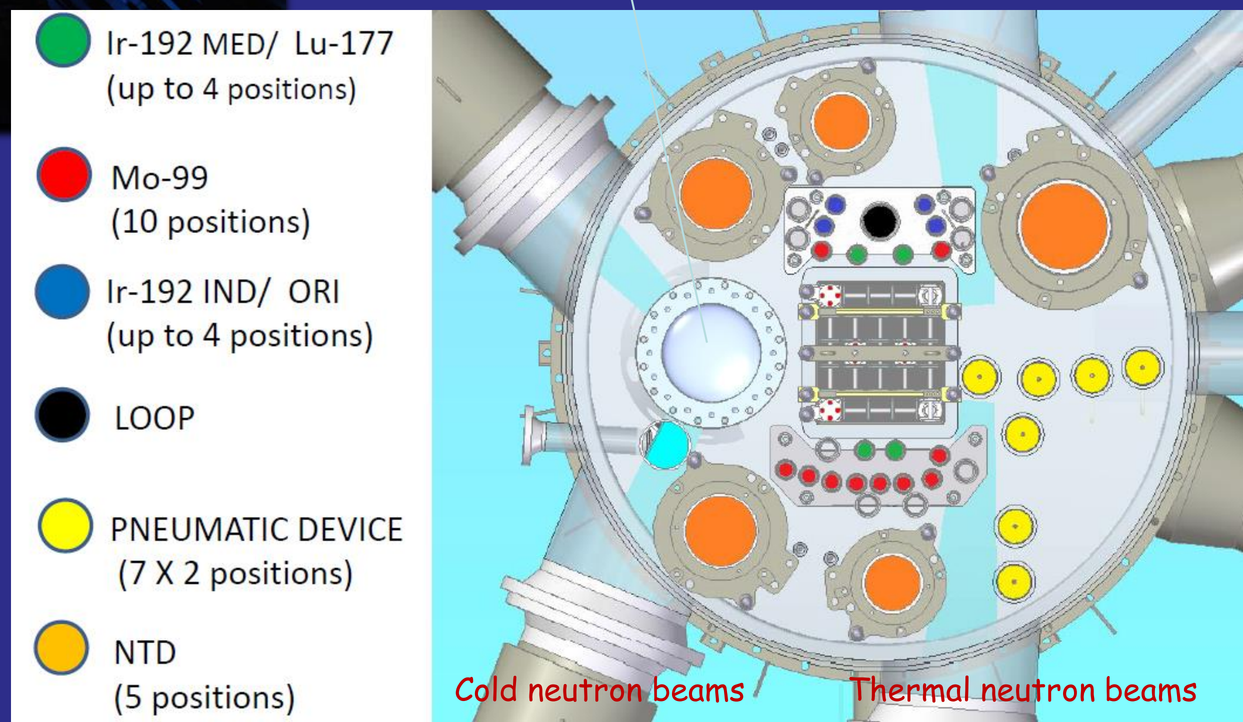
30 MW Multipurpose RR
Under construction in Ezeiza. ARG



RA-10 Reactor

Cold Neutron Source
(See poster by A. Marquez)

RA-10



NPPs in Argentina

Atucha - I

357 MWe PHWR
First NPP in Latin America (1974)

Embalse

648 MWe CANDU (1983)

Atucha - II

748 MWe PHWR (2014)

4th NPP

To be constructed
Agreements with Chinese National Nuclear Corporation (CNNC)

Argentinian RR’s in the world

OPAL (Australia)

20 MW
Multi-purpose

ETRR-2 (Egypt)

22 MW
Radioisotopes, BNCT, Fuel Testing.

NUR (Argelia)

1 MW
Training and research

RP-0 (Peru)

The Neutron Physics Department at Centro Atómico Bariloche was founded in 1969 by Hector Antunez , one of the alumni of the legendary neutron physics group at General Atomics in San Diego.

The group was created towards a small pulsed neutron source, a 25 MeV electron LINAC, similar to the accelerator at RPI.

Now we are 23 people (counting researchers, students and technical staff) working on neutron physics and applications to condensed matter research, materials science and nuclear engineering.

The main current group activity is the development of neutron scattering instruments for the forthcoming RA-10 reactor, which will be similar to the OPAL reactor that the Argentine company INVAP built in Australia.

Thermal scattering nuclear data group (cross section libraries generation)

Rolando Granada
Scattering theory and advanced neutron sources

Florencia Cantargi
Cold moderator materials and neutron filters

Ignacio Marquez
Nuclear reactor applications and benchmarking

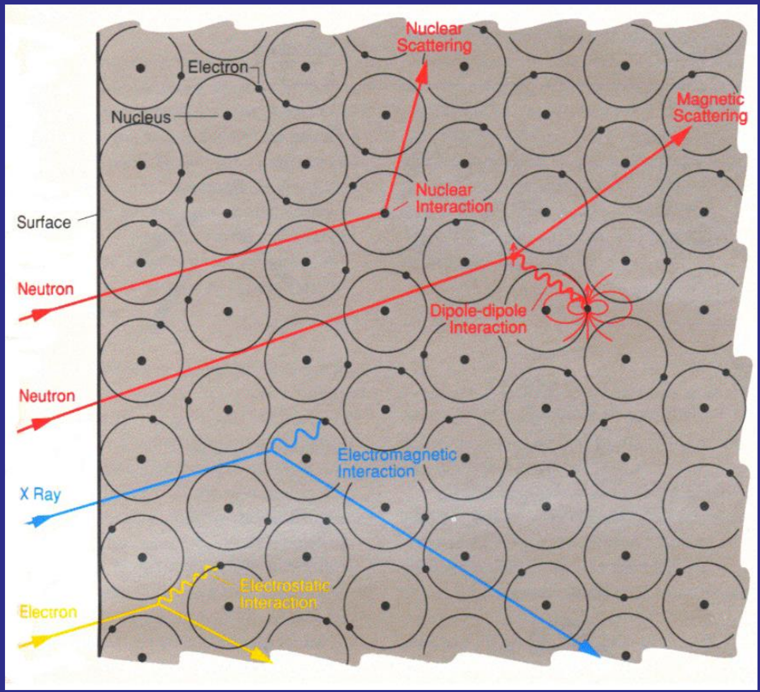
Past members:

- Monica Sbaffoni (currently at IAEA),
- Victor Gillette (currently at University of Sharjah, U.A.E).

Characteristics of neutrons

	Particle		Wave
Charge	0		
Mass	$m_n = 1.675 \times 10^{-27}$ kg		
"Radius"	$r_0 = 6 \cdot 10^{-16}$ m	Wave length	$\lambda = \frac{h}{m \cdot v}$
Spin	1/2	Wave number	$k = \frac{2\pi}{\lambda}$
Magn. Moment	$\mu = -1{,}9\,\mu_N$		
Momentum	$\vec{p} = m \cdot \vec{v}$	Momentum	$\vec{p} = \frac{h \cdot \vec{k}}{2\pi} = \hbar \cdot \vec{k}$
Energy	$E = \frac{m}{2} v^2$	Energy	$E = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 \cdot k^2}{2m}$

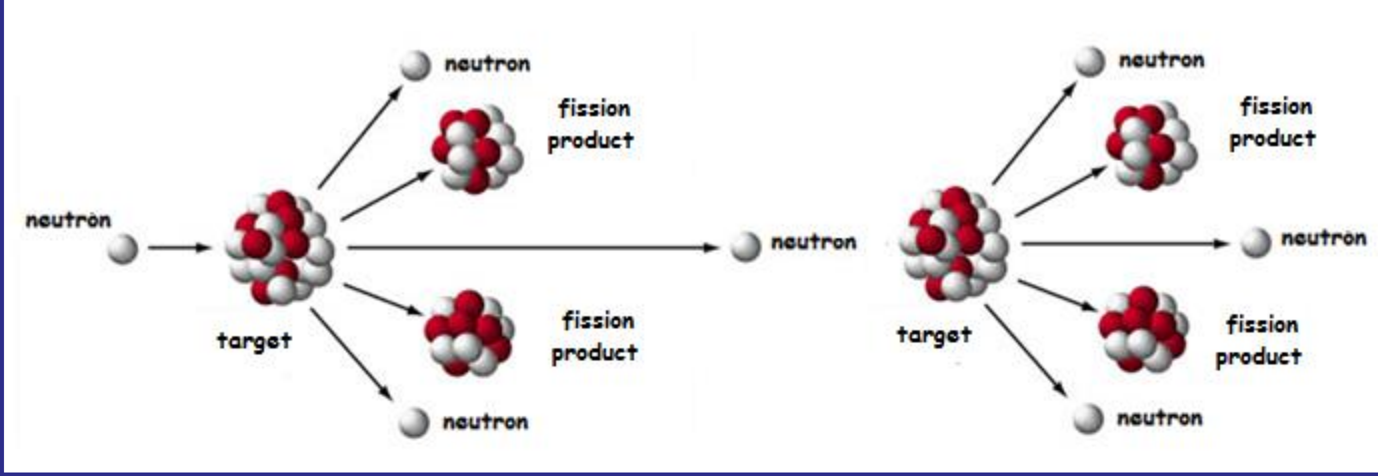
(v = velocity) (h = Plank´s constant)



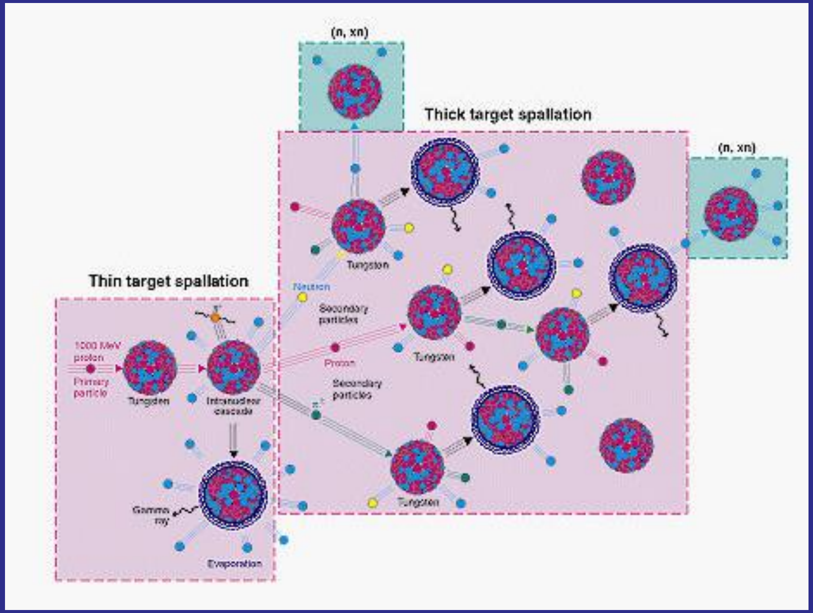
$$E = \frac{1}{2} m_n v^2 = \frac{p^2}{2m_n} = KT = \frac{h^2}{2 m_n \lambda^2}$$

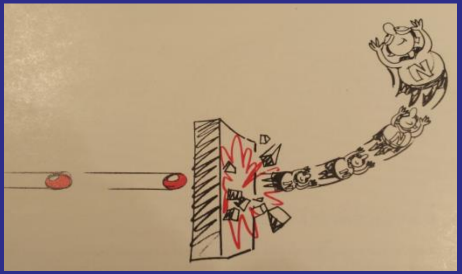
Mean life as a free particle: T=(888 ± 3) sec

Neutrons for scattering experiments can be produced either by nuclear fission in a nuclear reactor



or by spallation when high-energy protons strike a heavy metal target (W, Ta, or U).





About 1.5 useful neutrons are produced by each fission event in a nuclear reactor whereas about 25 neutrons are produced by spallation for each 1-GeV proton incident on a tungsten target

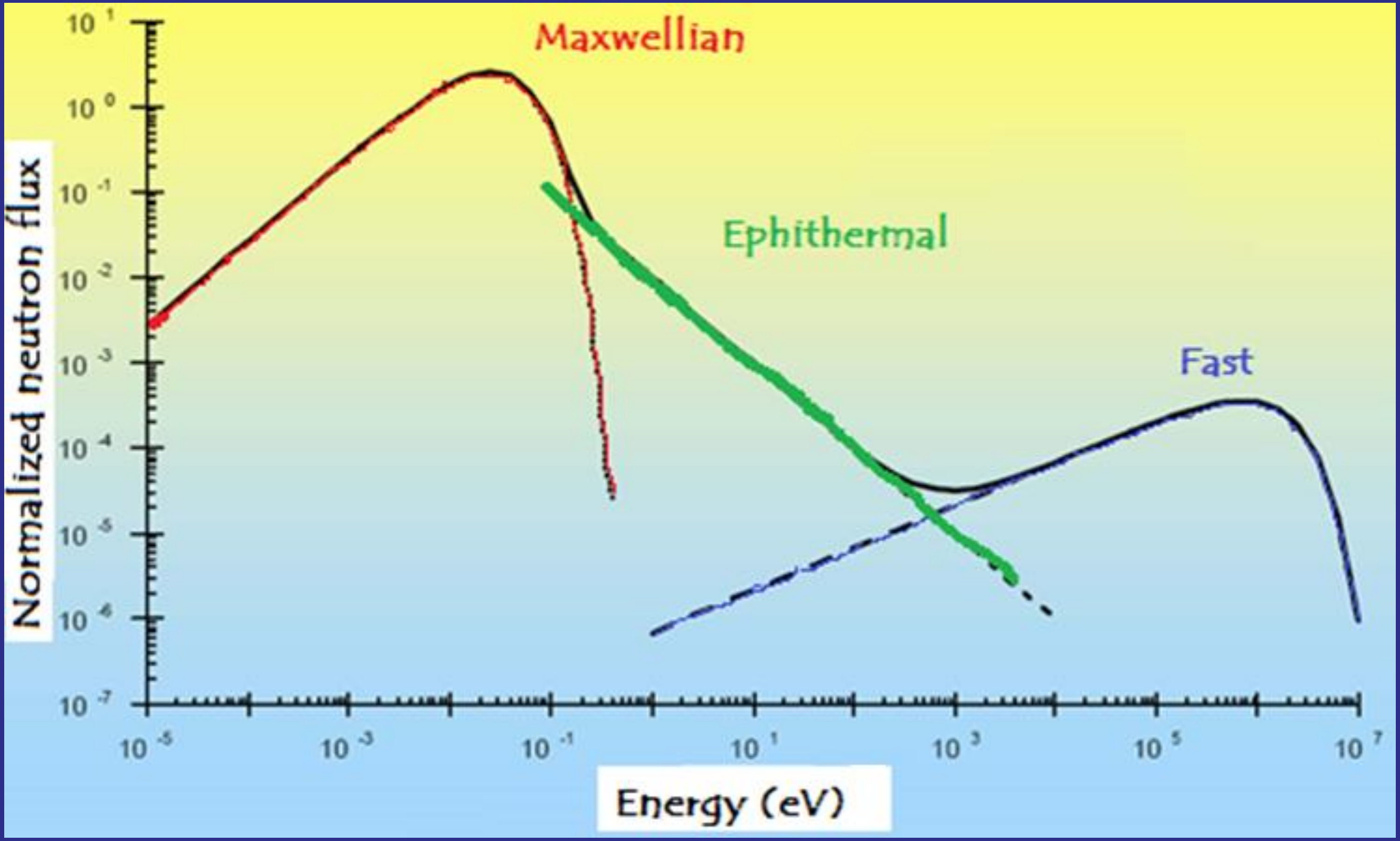
In general, reactors produce continuous neutron beams and spallation sources produce beams that are pulsed between 20 Hz and 60 Hz

Fission neutrons must be moderated to thermal energies to cause fission in other nuclei

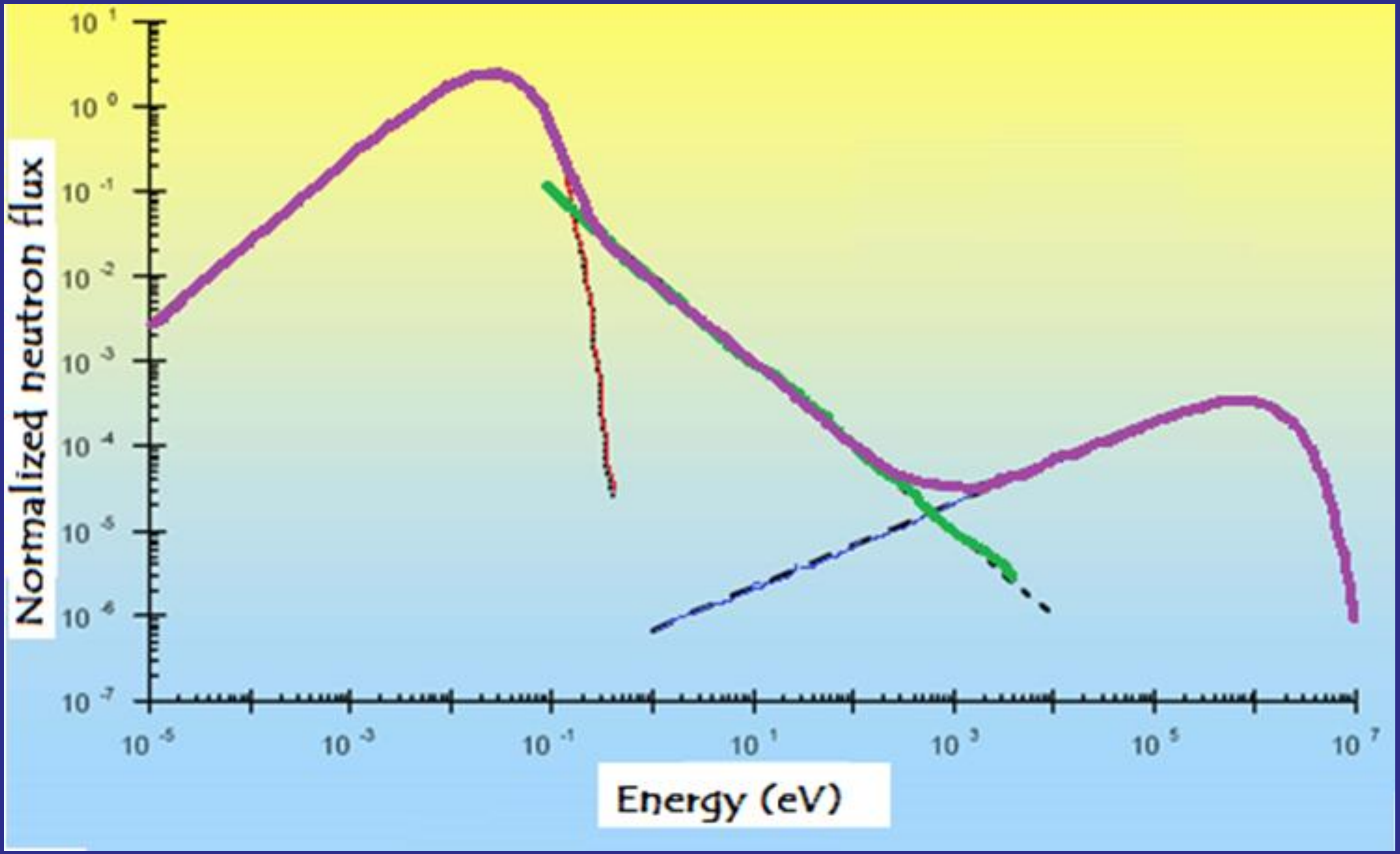
In contrast to fission, spallation cannot be selfsustaining

	Ultracold	Cold	Thermal	Epithermal	Fast
Energy	0.25 μeV	1 meV	25 meV	1 eV	2 MeV
Temperatura	3 mK	12 K	290 K	12000 K	$2.32\ 10^{10}$ K
Longitud de onda	570 Å	9 Å	1.8 Å	0.29 Å	$2.03\ 10^{-4}$ Å
Velocidad	6.9 m/seg	440 m/seg	2200 m/seg	14000 m/seg	10^{7} m/seg

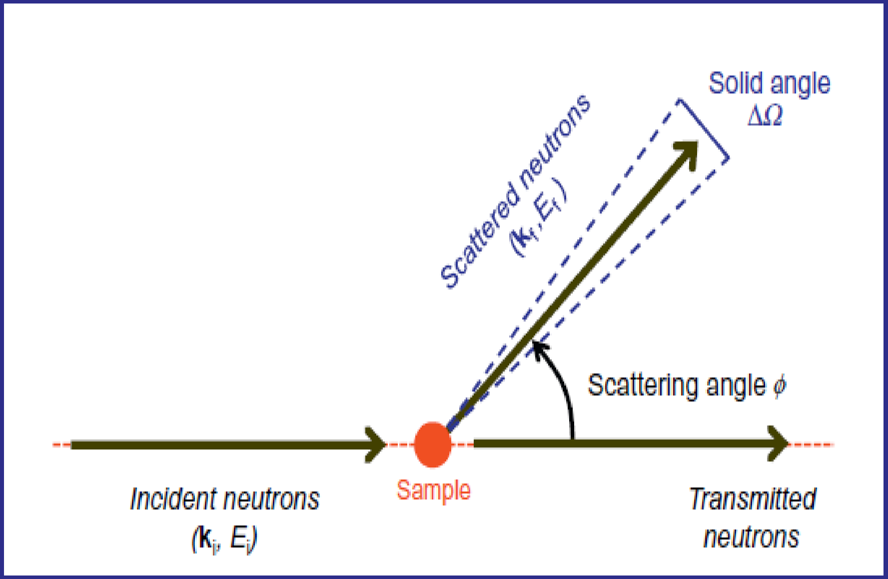
Neutron spectra in a nuclear reactor



Neutron spectra in a nuclear reactor



Neutron Scattering Theory



Incident flux (Φ) : neutrons crossing per unit area and per unit time

Double differential cross section

$$\frac{d^2\sigma}{dEd\Omega} = \frac{\text{number of neutrons scattered per second into the solid angle } d\Omega \text{ in the } (\theta, \varphi) \text{ direction and with final energies between } E' \text{ and } E'+dE'}{\Phi\, d\Omega\, dE}$$

$$\frac{d\sigma}{d\Omega} = \int \frac{d^2\sigma}{d\Omega dE'} dE'$$

Differential cross section ***is the number of scattered neutrons per second*** **into the solid angle dΩ in the (θ, φ) direction / ΦdE**

The energy kernel is the number of scattered neutrons per second and energy unit and with final energies between E' and E'+dE'

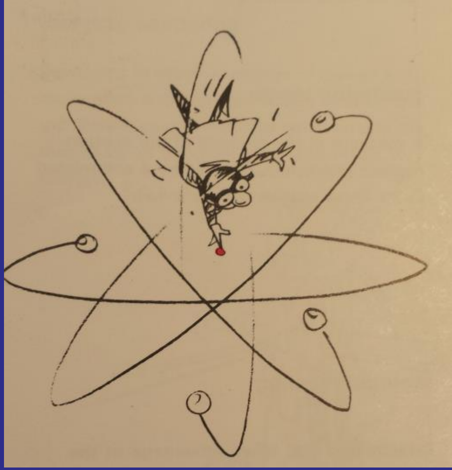
$$\frac{d\sigma}{dE'} = \int \frac{d^2\sigma}{d\Omega dE'} d\Omega$$

Total scattering cross section is the total number of scattered neutrons per second in any direction and with any energy .

$$\sigma_{\substack{tot \\ scatt}} = \int \frac{d\sigma}{d\Omega} d\Omega = \int \frac{d\sigma}{dE'} dE'$$

The effective area presented by a nucleus to an incident neutron is the ***total cross secction.***

Scattering by a Single (fixed) Nucleus



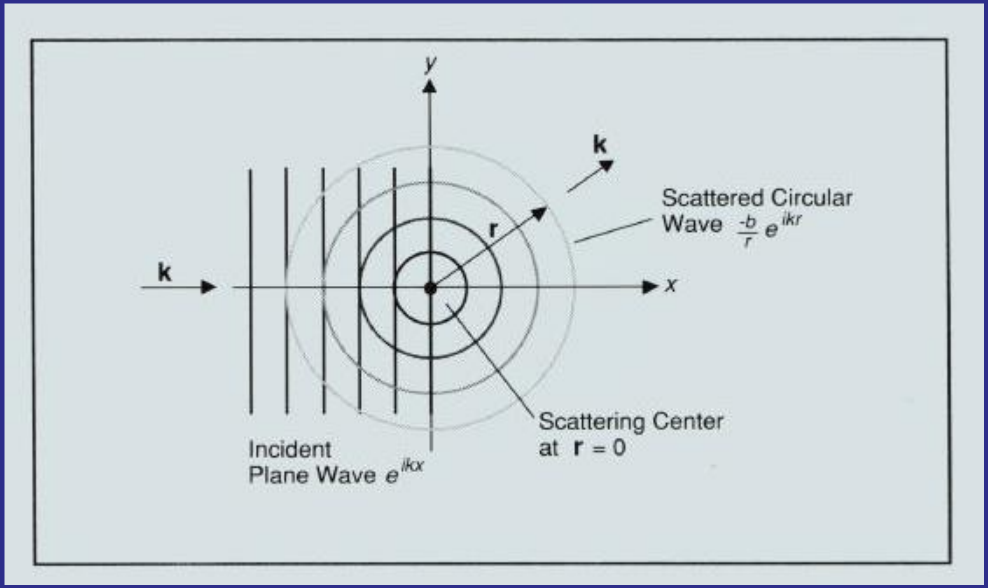
Range of nuclear force (~ 1fm) << thermal neutron wavelength (~2 10^{-10} m)

scattering is "point-like"

Energy of neutron is too small to change energy of nucleus & neutron cannot transfer kinetic energy to a fixed nucleus → scattering is elastic

Incident wave function

$\psi_{inc}=e^{ik \cdot r}$



Sacttered wave function

$\psi_{inc}=-b/r \,.e^{ik \cdot r}$

b : **scattering length of the scattering nucleus**

Scattering length characteristics

It is a constant that depends on the nucleid and on the spin of the neutron-nucleus system

It is a constant, it does not depend on θ or ϕ

It is a complex number. The imaginary part is related to resonance phenomena between certain nuclei and the neutron (a few cases)

When b is positive the potential V(r) is repulsive

In some cases b is negative: this allows for contrast (e.g. Ti-Zr alloys)

There is not a theory of nuclear forces that allows predicting the value of b. It is taken as a phenomenological parameter and determined experimentally for each nucleus (tabulated).

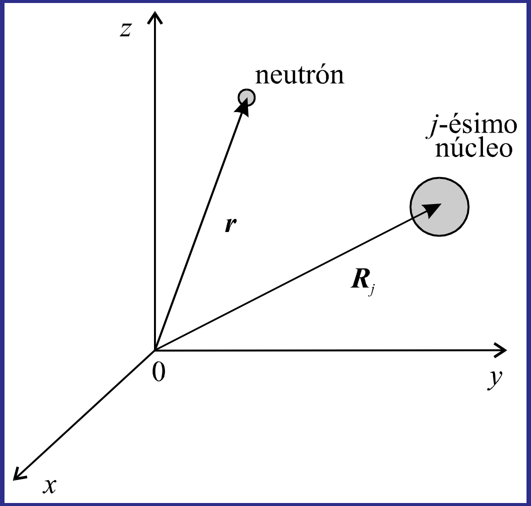
b varies erratically as a function of Z. <u>BIG advantage over X-rays</u>

b is the analog of the "form factor" in X-rays which is not isotropic.

$$\sigma_{\substack{scatt \\ tot}} = 4\pi b^2$$

NUCLEAR SCATTERING

	Initial state		Final State	
Neutron:	$\mathbf{k}$	ψ_k	$\mathbf{k}'$	$\psi_{k'}$
Scattering system	λ	χ_λ	λ'	$\chi_{\lambda'}$



The diferential cross section represents the sum of all processes in which the state of the scattering system changes from λ to λ', and the state of the neutron changes from $\mathbf{k}$ to $\mathbf{k}'$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\rightarrow\lambda'} = \frac{1}{\Phi}\frac{1}{d\Omega}\sum_{\substack{\mathbf{k}' \\ \text{en } d\Omega}} W_{\mathbf{k},\lambda\rightarrow\mathbf{k}',\lambda'}$$

where $W_{\mathbf{k},\lambda\rightarrow\mathbf{k}',\lambda'}$ is the number of transitions per second from the state $\{\mathbf{k},\lambda\}$ to the state $\{\mathbf{k}',\lambda\}$, and Φ is the incident neutron flux.

By means of **Fermi Golden Rule**:

$$\sum_{\substack{\mathbf{k}' \\ \text{en } d\Omega}} W_{\mathbf{k},\lambda\to\mathbf{k}',\lambda'} = \frac{2\pi}{\hbar}\rho_{\mathbf{k}'}\left|\langle\mathbf{k}'\lambda'|V|\mathbf{k}\lambda\rangle\right|^2$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2\left|\langle\mathbf{k}'\lambda'|V|\mathbf{k}\lambda\rangle\right|^2$$

$$E_\lambda + E = E_{\lambda'} + E'$$

$$\left(\frac{\mathbf{d}^2\sigma}{\mathbf{d}\Omega\mathbf{d}E'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar}\right)^2\left|\rangle\mathbf{k}'\lambda'|V|\mathbf{k}\lambda\langle\right|^2\delta\left(E_\lambda - E_{\lambda'} + \hbar\omega\right)$$

$$\text{where } \hbar\omega = E - E'$$

The interaction potential between the neutron and the j-th nucleus is proportional to $V_j(\boldsymbol{r}-\boldsymbol{R}_j)$, in such a way that for the whole system

$$V(\boldsymbol{r}) = \sum_j V_j(\boldsymbol{r}-\boldsymbol{R}_j)$$

j-th nucleus position

Fermi Pseudopotencial

$$V_j(\mathbf{r}-\mathbf{R}_j) = \frac{2\pi\hbar^2}{m} b_j \delta(\mathbf{r}-\mathbf{R}_j)$$

Neutron position

Scattering length of the j-th nucleus

Fourier Transform

$$V(Q) = \frac{2\pi\hbar^2}{m} \sum_j b_j$$

$$\text{where } \hbar Q = \hbar(k - k')$$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\sum_{j,j'} b_{j'}^{*}\, b_j \langle\lambda'|\exp(-i\boldsymbol{Q}\cdot R_{j'})|\lambda\rangle\langle\lambda'|\exp(i\boldsymbol{Q}\cdot R_j)|\lambda\rangle$$

$$\times\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\exp\left(i\frac{E_{\lambda'}-E_{\lambda}}{\hbar}t\right)\exp(-i\omega t)\,\mathrm{d}t$$

In a real case, we have to sum all the final states keeping the initial state fixed and then average over all initial states of the target.

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_{j'}\, b_j \int_{-\infty}^{\infty}\left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j'}(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)\right)\right\rangle \exp(-i\omega t)\,\mathrm{d}t$$

This is the **master formula** and it is the basis for the interpretation of all neutron-scattering experiments.

Each scatterer has it own b which varies between one nucleus to another (different isotopes, nuclear spin, different species)

$$\frac{d^2\sigma}{d\Omega\, dE'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}\overline{b_{j'}\, b_j}\int_{-\infty}^{\infty}\exp(-i\omega t)\;\chi_{jj'}(t)\, dt$$

$$\chi_{jj'}(t) = \left\langle \exp\left(-i\mathbf{Q}\cdot\mathbf{R}_{j'}(0)\right)\exp\left(i\mathbf{Q}\cdot\mathbf{R}_j(t)\right)\right\rangle$$

The system will have an average $\overline{b}$ and averaged $\overline{b^2}$

The measured cross-section will be an average. Taking that there is NO correlation among the b of different nuclei then

$$\overline{b_j b_{j'}} = \overline{b}^2 \qquad j' \neq j$$

$$\overline{b_j b_{j'}} = \overline{b^2} \qquad j' = j$$

Coherent scattering: depends of Q direction

$$\left(\frac{d^2\sigma}{d\Omega\, dE'}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}\int_{-\infty}^{\infty}\exp(-i\omega t)\,\chi_{jj'}(t)\,dt$$

$$\sigma_{coh} = 4\pi\bar{b}^2$$

Interference effects

Incoherent scattering: independent of Q

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{inc} = \frac{\sigma_{inc}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j}\int_{-\infty}^{\infty}\exp(-i\omega t)\chi_{jj}(t)dt$$

$$\sigma_{inc} = 4\pi\left\{\overline{b^2} - \bar{b}^2\right\}$$

No interference effects

We can also write

$$\frac{d^2\sigma}{d\Omega\, dE'} = \frac{1}{4\pi}\frac{k'}{k} N \left(\sigma_{coh}\, S_{coh}(\boldsymbol{Q},\omega) + \sigma_{inc}\, S_{inc}(\boldsymbol{Q},\omega)\right)$$

where $S_{coh}(Q\omega)$ and $S_{inc}(Q\omega)$ are the coherent and incoherent scattering laws

$$S_{inc}(\boldsymbol{Q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp(-i\omega t)\, \chi_{inc}(\boldsymbol{Q},t)\, dt \qquad S_{coh}(\boldsymbol{Q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp(-i\omega t)\, \chi_{coh}(\boldsymbol{Q},t)\, dt$$

The Fourier transform are called *Intermediate Scattering Functions*

$$\chi_{coh}(\boldsymbol{Q},t) = \frac{1}{N}\sum_{j,j'} \left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j'}(0)\right) \exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)\right) \right\rangle \qquad \chi_{inc}(\boldsymbol{Q},t) = \frac{1}{N}\sum_{j} \left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j}(0)\right) \exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)\right) \right\rangle$$

These correlation functions, scattering laws and intermediate scattering functions contain all the information on the structure and dynamics of the scattering system. This information is obtained in a direct way in the measurement of the double differential scattering cross section.

We have a **Bravais lattice** with only one atom in the unit cell, where each position is determined by a vector l_j

Allowing the thermal moving of the j-th nucleus, its position will be $R_j = l_j + u_j$, where u_j is the displacement from the equilibrium position and l_j is a constant.

U and V are operators related to displacements of the nuclei from equilibrium at time 0 and t

Coherent scattering

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\exp\langle U^2\rangle \sum_{l} \exp(i\kappa\cdot\mathbf{l}) \int_{-\infty}^{\infty} \exp\langle UV\rangle \exp(-i\omega t)\,dt$$

Debye Waller Factor: related to the mean-square displacement of each atom around its equilibribum position → depends on the temperature

$$\exp\langle U^2\rangle = \exp(-2W) = \exp(-\langle (Q.u_0(0))^2\rangle)$$

Related to the creation of phonons

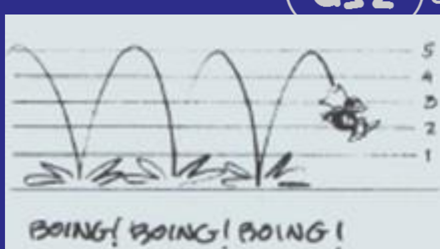
Coherent elastic scattering

No phonon creation → elastic scattering $|\mathbf{k}| = |\mathbf{k}'|$

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\substack{elas\\coh}} = \frac{\sigma_{coh}}{4\pi} N \exp\langle U^2\rangle \sum_j \exp\,(iQ.l_j)\ \delta(\hbar\omega)$$

$$\int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\substack{elas\\coh}} dE' = \left(\frac{d\sigma}{d\Omega}\right)_{\substack{elas\\coh}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\substack{elas\\coh}} = \frac{\sigma_{coh}}{4\pi} N \frac{(2\pi)^3}{V} \boxed{\exp\,(-2W)} \sum_\tau \delta(Q-\tau)$$



Unit cell volume

Debye Waller Factor

Reciprocal lattice vectors

Bragg Scattering

(for non- Bravais crystals a form factor appears in this expresion)

Mean-square displacements are associated to the oscillation modes. Since the number of degrees of freedom is close to 10^{23}, oscillation modes are expressed as an integral over all the frequencies by means of the density of states $Z(\omega)$ (or frequency spectra)

$Z(\omega)\, d\omega$ is the fraction of normal modes between w and $w+dw$

The Debye Waller factor is written as:

$$2W = \frac{\hbar Q}{2M}\int_0^\infty \langle 2\, n(\omega) + 1\rangle \frac{Z(\omega)}{\omega} d\omega$$

Bose occupation number

Incoherent inelastic scattering

Debye Waller Factor

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{inc} = \frac{\sigma_{inc}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\exp\langle U^2\rangle \int \exp\langle UV_0\rangle \exp(-i\omega t)dt$$

Phonons creation

Incoherent elastic scattering

No phonon creation → elastic scattering $|\mathbf{k}| = |\mathbf{k}'|$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\substack{elas\\incoh}} = \frac{\sigma_{incoh}}{4\pi} N \exp(-2W)$$

The only dependence in the scattering direction apears in the Debye Waller factor.

At low temperatures exp(-2W) is close to 1 → scattering es isotropic scattering

Phonons

Through a Taylor expansion of exp<UV> y exp<UVo> in the coherent and incoherent scattering expresions respectively

$$\exp\langle UV\rangle = 1 + \langle UV\rangle + \frac{1}{2}\langle UV\rangle^2 + \ldots\ldots + \frac{1}{p!}\langle UV\rangle^p$$

elastic

1 phonon

2 phonons

p phonons

Coherent elastic 1 phonon scattering

$$\left.\frac{d^2\sigma}{d\Omega dE'}\right|_{coh\pm1f} = \frac{\sigma_{coh}}{4\pi}\frac{k'}{k}\frac{(2\pi)^3}{v_o}\frac{\hbar}{2M}e^{-2W}\sum_s\sum_\tau \frac{(\mathbf{Q}\cdot\hat{\mathbf{e}}_s)^2}{\omega_s}\left\{\begin{array}{c}<n_s+1>\\ <n_s>\end{array}\right\}\delta(\hbar\omega\mp\hbar\omega_s)\delta(\mathbf{Q}\mp\mathbf{q}-\tau)$$

Incoherent inelastic 1 phonon scattering

$$\left.\frac{d^2\sigma}{d\Omega dE'}\right|_{inc\pm1f} = \frac{\sigma_{inc}}{4\pi}\frac{k'}{k}\frac{N}{4M}Q^2 e^{-2W}\frac{Z(\omega)}{\omega}\left[\coth\left(\frac{\beta\hbar\omega}{2}\right)\pm1\right]$$

Density of states →

Information of the dynamics of the scattering system

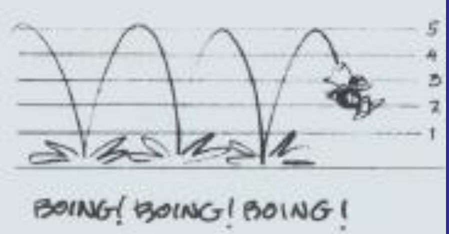
Summary

coherent scattering

Scattering in which an incident neutron wave interacts with all the nuclei in a sample in a coordinated fashion; that is, the scattered waves from all the nuclei have definite relative phases and can thus interfere with each other.

incoherent scattering

Scattering in which an incident neutron wave interacts independently with each nucleus in the sample; that is, the scattered waves from different nuclei have random, or indeterminate, relative phases and thus cannot interfere with each other.



elastic scattering

Scattering with no change in the energy of the incident neutron; or, in terms of the wave vector of the neutron, scattering in which the direction of the vector changes but not its magnitude.

inelastic scattering

Scattering in which exchange of energy and momentum between the incident neutron and the sample causes both the direction and the magnitude of the neutron's wave vector to change.

The NJOY Nuclear Data Processing System is a commercial code that generates scattering laws, kernels and cross sections for different materials at different temperatures

It is a modular computer code designed to read evaluated data in ENDF format, transform the data in various ways, and output the results as libraries designed to be used in various applications.

Each module performs a well defined processing task. The modules are essentially independent programs, and they communicate with each other using input and output files, plus a very few common variables.

$$\alpha = \frac{E' + E - 2\sqrt{E'E}\mu}{AK_B T} \qquad \beta = \frac{E' - E}{K_B T}$$

$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\beta t} e^{-\alpha\Gamma(t)} dt$$

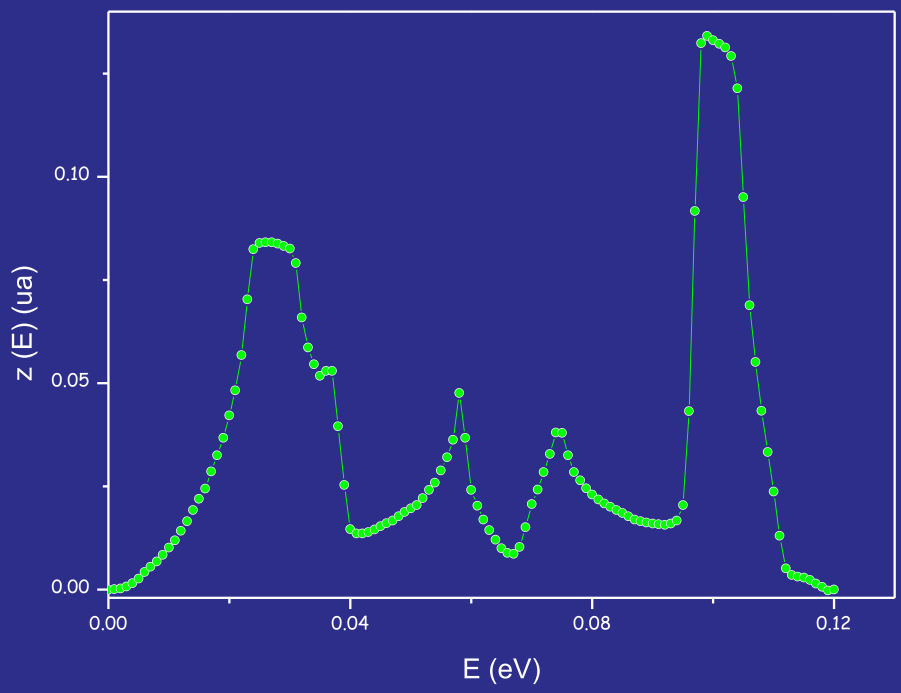
The dynamics of the scattering system is in the frequency spectra

$$Z(E) = \omega_{cont} Z_{cont}(E) + \sum_{vibr_i=1}^{N} \omega_{vibr_i} Z_{vibr_i}(E)$$

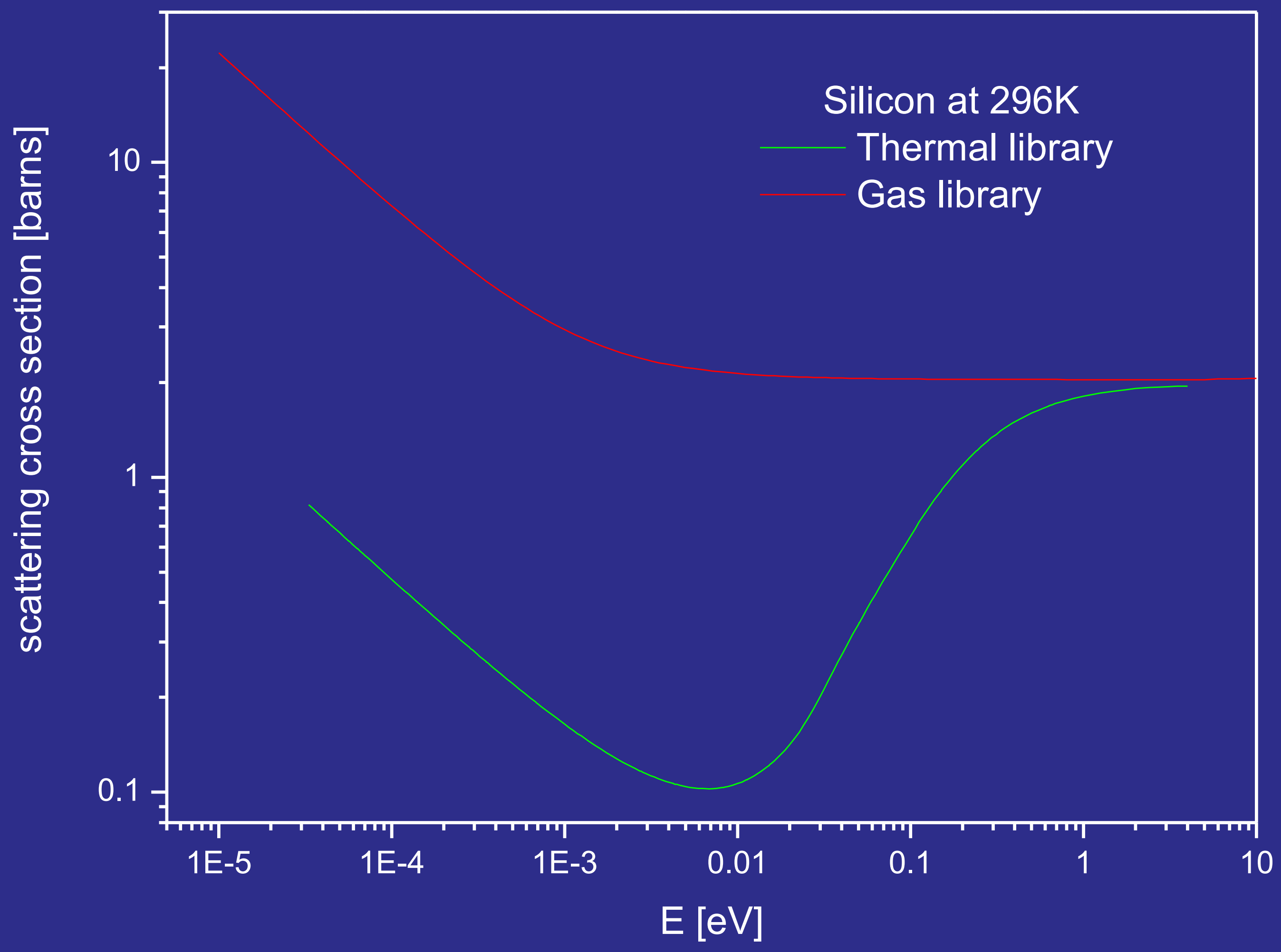
Each spectrum is composed of a continuous part, associated to translational and rotational motions of the molecular system

and a set of discrete oscillators related to the molecule's internal degrees of freedom

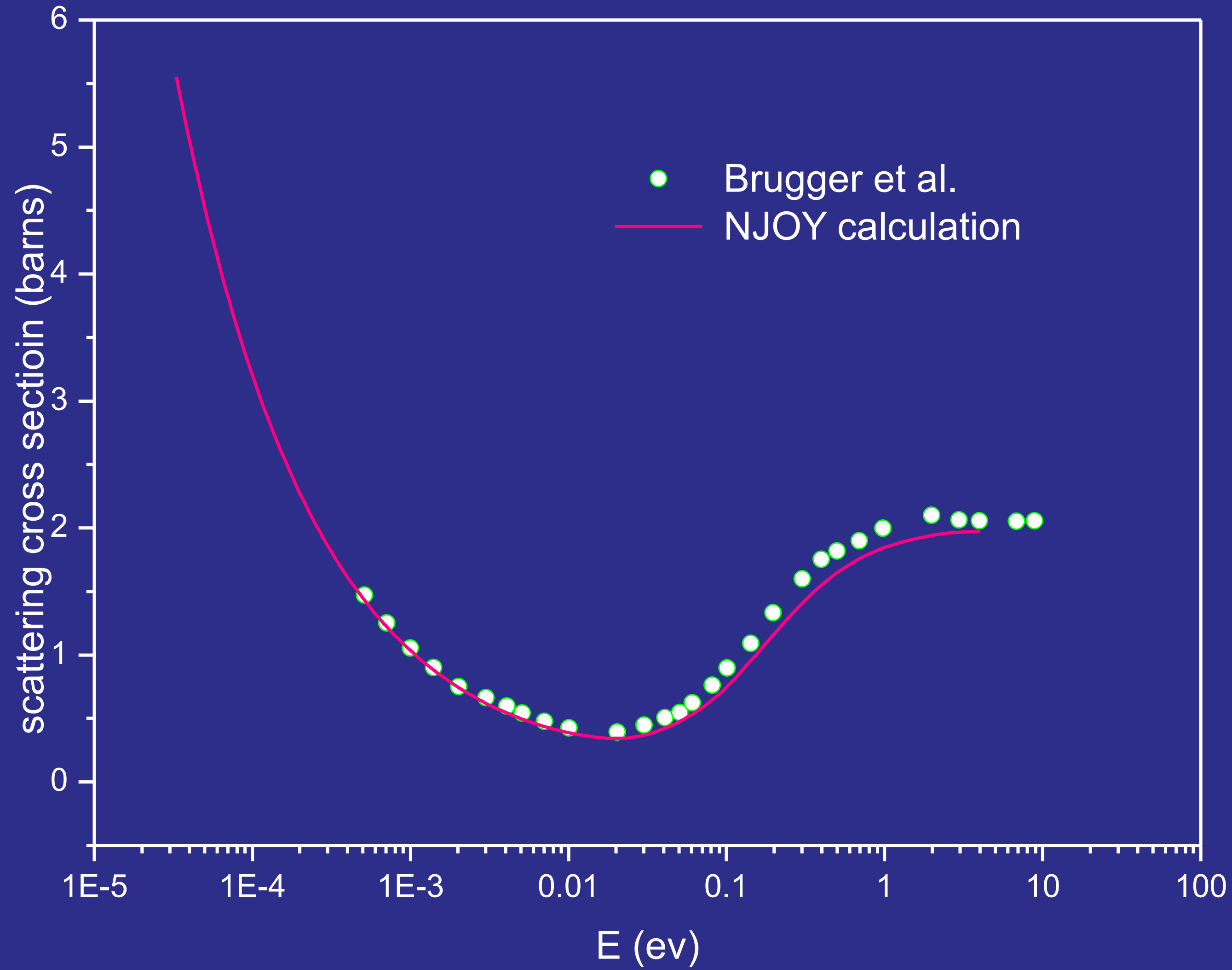
Silicon single-crystal



R. Meyer y D. Comtesse, Phys. Rev. B **83** (2011) 014301

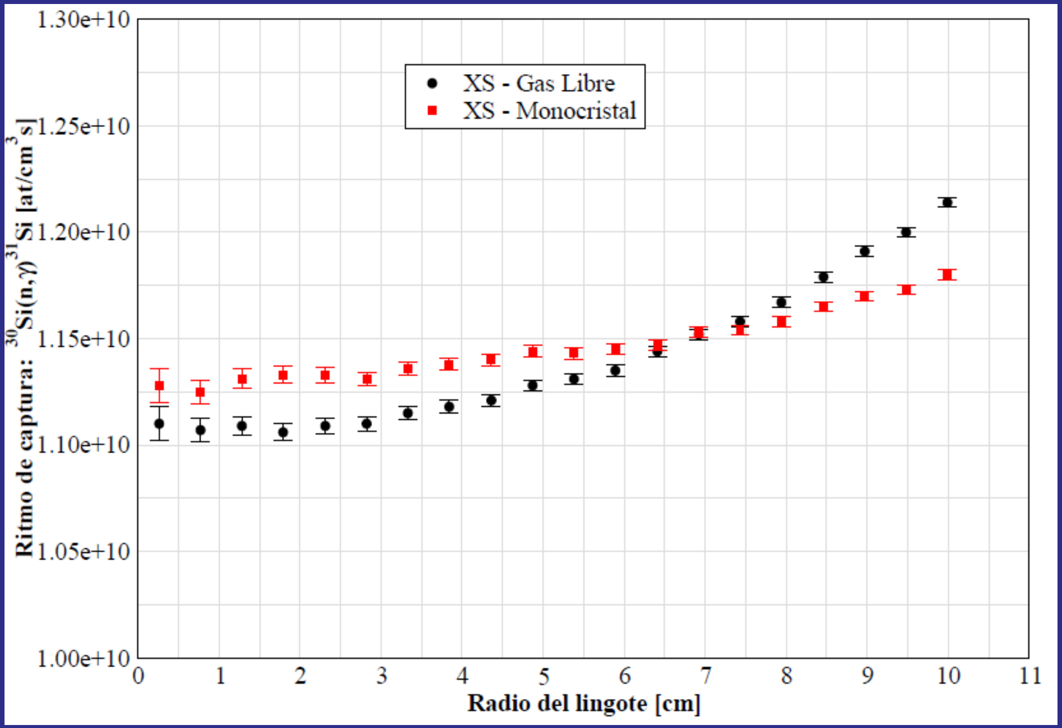


Silicon at 296K
Thermal library
Gas library
scattering cross section [barns]
10
1
0.1
1E-5
1E-4
1E-3
0.01
0.1
1
10
E [eV]


Brugger et al.
NJOY calculation
scattering cross sectioin (barns)
E (ev)
0
1
2
3
4
5
6
1E-5
1E-4
1E-3
0.01
0.1
1
10
100

Capture reaction rate for $^{30}Si\ (n,\gamma)\ ^{31}Si$ with both libraries in the RA10 MCNP model

The reaction rate indicates the amount of ^{31}P generated in the silicon lingote.



Los Alamos NATIONAL LABORATORY EST. 1943

T-2 Nuclear Information Service

T-2 Home

NIS Home

RESOURCES

Tour area

Data area

Codes area

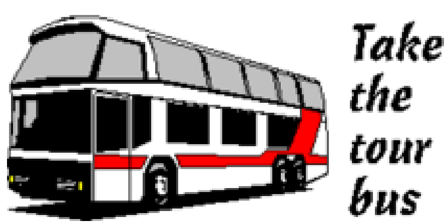
Publications area

Training area

T-2 Home » T-2 Nuclear Information Service

The Tour Area

The School Bus takes you on an educational tour of the subject of nuclear data. What are nuclear data? Where are nuclear data used? Who does nuclear data? Most of the content is aimed toward scientists who are not familiar with the nuclear data field, the general public, and secondary school students, but some more specialized review articles are also available here.

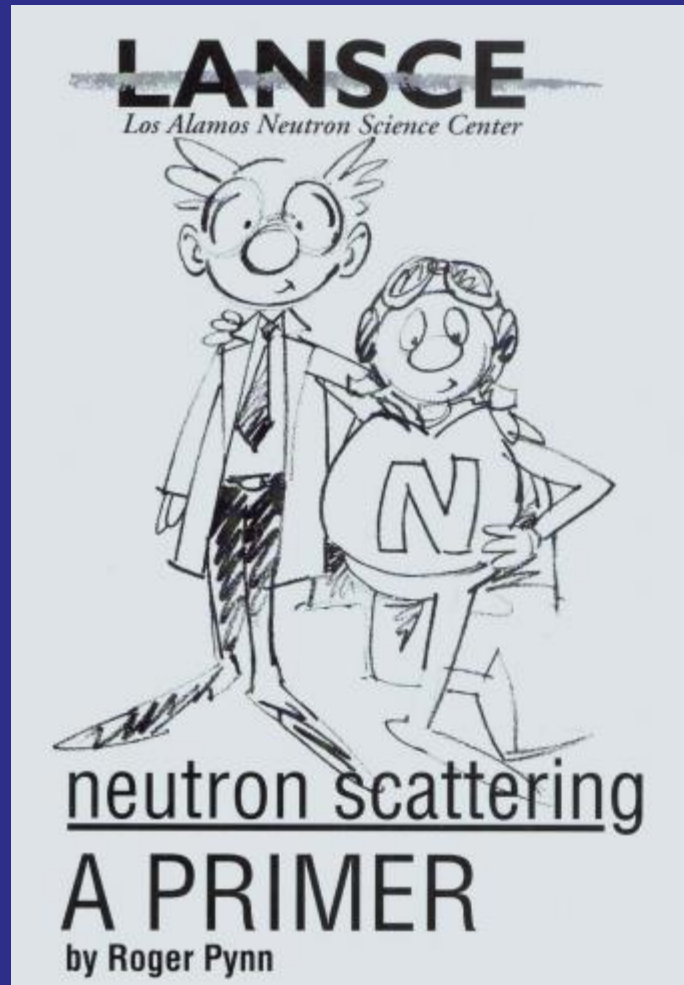


The Tour Bus is for people with some understanding of nuclear physics, nuclear data, or nuclear engineering who want to learn how to find their way around in the T-2 Nuclear Information Service. How do you obtain or prepare plots of cross sections? Where are the evaluated data files? What about radioactivity information? How do you find nuclear masses?

Featured Articles

See the article *Interactions Between Nuclear Radiation and Matter* from the School Bus for an introduction to particles, isotopes, cross sections, angle and energy distributions, and the other creatures that inhabit our world of nuclear data.

See the article *Graphing Nuclear Data* from the Tour Bus to find out how to use the convenient, online, interactive Nuclear Data Viewer to make a wide variety of plots from evaluations and experimental data.


LANSCE
Los Alamos Neutron Science Center
neutron scattering
A PRIMER
by Roger Pynn