Fundamental aspects of the thermal neutron scattering

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Comisión Nacional de Energía Atómica

ARGENTINA

Joint ICTP-IAEA School on Nuclear Data Measurements for Science and Applications
October 27th, 2015
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
OPAL Reactor (Australia)

RA-10 Reactor

Cold Neutron Source
(See poster by A. Marquez)

- Ir-192 MED/ Lu-177 (up to 4 positions)
- Mo-99 (10 positions)
- Ir-192 IND/ ORI (up to 4 positions)
- LOOP
- PNEUMATIC DEVICE (7 X 2 positions)
- NTD (5 positions)

Cold neutron beams

Thermal neutron beams
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

Florence 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

<table>
<thead>
<tr>
<th>Particle</th>
<th>Wave</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge</td>
<td>0</td>
</tr>
<tr>
<td>Mass</td>
<td>$m_n = 1.675 \times 10^{-27}$ kg</td>
</tr>
<tr>
<td>&quot;Radius&quot;</td>
<td>$r_0 = 6 \cdot 10^{-16}$ m</td>
</tr>
<tr>
<td>Spin</td>
<td>1/2</td>
</tr>
<tr>
<td>Magn. Moment</td>
<td>$\mu = -1.9 \mu_N$</td>
</tr>
</tbody>
</table>

**Momentum**

$\vec{p} = m \cdot \vec{v}$

**Energy**

$E = \frac{1}{2} m_n v^2$

$E = \frac{p^2}{2m_n} = kT = \frac{h^2}{2m_n \lambda^2}$

Mean life as a free particle: $T = (888 \pm 3)$ 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 self-sustaining.
<table>
<thead>
<tr>
<th></th>
<th>Ultracold</th>
<th>Cold</th>
<th>Thermal</th>
<th>Epithermal</th>
<th>Fast</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Energy</strong></td>
<td>0.25 μeV</td>
<td>1 meV</td>
<td>25 meV</td>
<td>1 eV</td>
<td>2 MeV</td>
</tr>
<tr>
<td><strong>Temperatura</strong></td>
<td>3 mK</td>
<td>12 K</td>
<td>290 K</td>
<td>12000 K</td>
<td>2.32 $10^{10}$ K</td>
</tr>
<tr>
<td><strong>Longitud de onda</strong></td>
<td>570 Å</td>
<td>9 Å</td>
<td>1.8 Å</td>
<td>0.29 Å</td>
<td>2.03 $10^{-4}$ Å</td>
</tr>
<tr>
<td><strong>Velocidad</strong></td>
<td>6.9 m/seg</td>
<td>440 m/seg</td>
<td>2200 m/seg</td>
<td>14000 m/seg</td>
<td>10$^7$ m/seg</td>
</tr>
</tbody>
</table>
Neutron spectra in a nuclear reactor
Neutron spectra in a nuclear reactor
Neutron Scattering Theory

**Incident flux** ($\Phi$): neutrons crossing per unit area and per unit time

*Double differential cross section*

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

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

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.

\[
\sigma_{\text{tot scatt}} = \int \frac{d\sigma}{d\Omega} d\Omega = \int \frac{d\sigma}{dE'} dE''
\]

The effective area presented by a nucleus to an incident neutron is the total cross section.
Scattering by a Single (fixed) Nucleus

Range of nuclear force (~1 fm) \ll \text{thermal neutron wavelength (~2 } 10^{-10} \text{ 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 \rightarrow \text{scattering is elastic}

\text{Incident wave function} \\
\psi_{inc} = e^{ikr}

\text{Scattered wave function} \\
\psi_{inc} = -\frac{b}{r} e^{ikr}

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 $\theta$ or $\phi$

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 $Z$. **BIG advantage over X-rays**

$b$ is the analog of the “form factor” in X-rays which is not isotropic.

\[
\sigma_{\text{scatt}} = 4\pi b^2
\]
NUCLEAR SCATTERING

<table>
<thead>
<tr>
<th>Initial state</th>
<th>Final State</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutron:</td>
<td></td>
</tr>
<tr>
<td>( k )</td>
<td>( k' )</td>
</tr>
<tr>
<td>( \psi_k )</td>
<td>( \psi_{k'} )</td>
</tr>
<tr>
<td>Scattering system</td>
<td></td>
</tr>
<tr>
<td>( \lambda )</td>
<td>( \lambda' )</td>
</tr>
<tr>
<td>( \chi_\lambda )</td>
<td>( \chi_{\lambda'} )</td>
</tr>
</tbody>
</table>

The differential cross section represents the sum of all processes in which the state of the scattering system changes from \( \lambda \) to \( \lambda' \), and the state of the neutron changes from \( k \) to \( k' \)

\[
\left( \frac{d\sigma}{d\Omega} \right)_{\lambda \rightarrow \lambda'} = \frac{1}{\Phi} \frac{1}{d\Omega} \sum_{k'} W_{k, \lambda \rightarrow k', \lambda'}
\]

where \( W_{k, \lambda \rightarrow k', \lambda'} \) is the number of transitions per second from the state \( \{ k, \lambda \} \) to the state \( \{ k', \lambda' \} \), and \( \Phi \) is the incident neutron flux.
By means of Fermi Golden Rule:

\[ \sum_{k'} W_{k,\lambda \rightarrow k',\lambda'} = \frac{2\pi}{\hbar} \rho_{k'} \left| \langle k' \lambda' | V | k \lambda \rangle \right|^2 \]

\[ \text{en } d\Omega \]

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

\[ E_{\lambda} + E = E_{\lambda'} + E' \]

\[ \left( \frac{d^2\sigma}{d\Omega dE'} \right)_{\lambda \rightarrow \lambda'} = \frac{k'}{k} \left( \frac{m}{2\pi\hbar} \right)^2 \left| \langle k' \lambda' | V | k \lambda \rangle \right|^2 \delta(E_{\lambda} - E_{\lambda'} + \hbar\omega) \]

where \( \hbar\omega = E - E' \)
The interaction potential between the neutron and the \( j \)-th nucleus is proportional to \( V_j(r-R_j) \), in such a way that for the whole system

\[
V(r) = \sum_j V_j(r-R_j)
\]

\[
V_j(r-R_j) = \frac{2\pi \hbar^2}{m} b_j \delta(r-R_j)
\]

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

where \( \hbar Q = \hbar (k - k') \)
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.

\[
\frac{d^2\sigma}{d\Omega \, dE'} = \frac{k'}{k} \, \frac{1}{2\pi \, \hbar} \sum_{j,j'} b_j^* \, b_j \langle \lambda' | \exp(-iQ \cdot R_j) | \lambda \rangle \langle \lambda' | \exp(iQ \cdot R_j) | \lambda \rangle \times \frac{1}{\hbar} \int_{-\infty}^{\infty} \exp\left(\frac{E_{\lambda'} - E_{\lambda}}{\hbar} t\right) \exp(-i\omega t) \, dt
\]

This is the master formula and it is the basis for the interpretation of all neutron-scattering experiments.
Each scatterer has its own \( b \) which varies between one nucleus to another (different isotopes, nuclear spin, different species)

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

\[\chi_{jj'}(t) = \langle \exp(-iQ \cdot R_j(0)) \exp(iQ \cdot R_{j'}(t)) \rangle\]

The system will have an average \( \bar{b} \) and averaged \( \bar{b}^2 \)

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

\[
\begin{align*}
\bar{b}_j \bar{b}_{j'} &= \bar{b}^2 \\
\bar{b}_j \bar{b}_{j'} &= \bar{b}^2 \\
\end{align*}
\]

\( j' \neq j \)

\( j' = j \)
**Coherent scattering:** depends of Q direction

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

\[
\sigma_{\text{coh}} = 4\pi b^2
\]

**Interference effects**

**Incoherent scattering:** independent of Q

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

\[
\sigma_{\text{inc}} = 4\pi \left\{ b^2 - \bar{b}^2 \right\}
\]

**No interference effects**
We can also write

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

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

\[
S_{\text{inc}} (Q, \omega) = \frac{1}{2\pi \hbar} \int_{-\infty}^{\infty} \exp(-i\omega t) \chi_{\text{inc}} (Q, t) \, dt \quad \quad S_{\text{coh}} (Q, \omega) = \frac{1}{2\pi \hbar} \int_{-\infty}^{\infty} \exp(-i\omega t) \chi_{\text{coh}} (Q, t) \, dt
\]

The Fourier transform are called \textit{Intermediate Scattering Functions}

\[
\chi_{\text{coh}} (Q, t) = \frac{1}{N} \sum_{j,j'} \left\langle \exp(-iQ \cdot R_j (0)) \exp(iQ \cdot R_j (t)) \right\rangle \quad \quad \chi_{\text{inc}} (Q, t) = \frac{1}{N} \sum_{j} \left\langle \exp(-iQ \cdot R_j (0)) \exp(iQ \cdot R_j (t)) \right\rangle
\]

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.

**Coherent scattering**

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

**Debye Waller Factor:** related to the mean-square displacement of each atom around its equilibrium position \( \rightarrow \) depends on the temperature

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

**Related to the creation of phonons**

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

$Q$ represents the momentum transfer and $u_0(0)$ is the displacement at time 0.
Coherent elastic scattering

No phonon creation $\rightarrow$ elastic scattering $|k| = |k'|$

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

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

$$\frac{d\sigma}{d\Omega}_{\text{elas coh}} = \frac{\sigma_{\text{coh}}}{4\pi} N \frac{(2\pi)^3}{V} \exp(-2W) \sum \delta(Q - \mathbf{Q})$$

Debye Waller Factor

Bragg Scattering

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

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

The Debye Waller factor is written as:

$$2W = \frac{\hbar Q}{2M_0} \int_0^\infty \left\{ 2n(\omega) + 1 \right\} \frac{Z(\omega)}{\omega} \, d\omega$$

Bose occupation number
Incoherent inelastic scattering

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

Debye Waller Factor

Phonons creation

Incoherent elastic scattering

No phonon creation \(\rightarrow\) elastic scattering \(|k| = |k'|\)

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

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

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

Through a Taylor expansion of $\exp<UV> \cdot y \cdot \exp<UVo>$ in the coherent and incoherent scattering expressions respectively,

\[
\exp<UV> = 1 + \langle UV \rangle + \frac{1}{2} \langle UV \rangle^2 + \ldots + \frac{1}{p!} \langle UV \rangle^p
\]

elastic 1 phonon 2 phonons $p$ phonons
Coherent elastic 1 phonon scattering

\[
\frac{d^2\sigma}{d\Omega dE'}|_{coh \pm 1f} = \frac{\sigma_{coh} k'}{4\pi} \frac{(2\pi)^3}{k} \frac{\hbar}{2M} e^{-2W} \sum_s \sum_r \frac{(Q \cdot \hat{s})^2}{\omega_s} \left\{ \begin{array}{l} \langle n_s + 1 \rangle \\ \langle n_s \rangle \end{array} \right\} \delta(\hbar\omega \mp \hbar\omega_s) \delta(Q \mp q - \tau)
\]

Incoherent inelastic 1 phonon scattering

\[
\frac{d^2\sigma}{d\Omega dE'}|_{inc \pm 1f} = \frac{\sigma_{inc} k'}{4\pi} \frac{N}{k} Q^2 e^{-2W} \frac{Z(\omega)}{\omega} \left[ \coth \left( \frac{\beta \hbar \omega}{2} \right) \right] \pm 1
\]

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.

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.

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.

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.

\[ \alpha = \frac{E' + E - 2\sqrt{E'E}\mu}{AK_BT} \]
\[ \beta = \frac{E' - E}{K_BT} \]

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

Silicon at 296K

- Thermal library
- Gas library

Scattering cross section [barns] vs. Energy [eV]
scattering cross section (barns) vs. E (ev)

Brugger et al.
NJOY calculation
Capture reaction rate for $^{30}\text{Si} (n,\gamma) ^{31}\text{Si}$ with both libraries in the RA10 MCNP model.

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

**Take the school bus**

**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?
neutron scattering
A PRIMER
by Roger Pynn