Dynamics of a scattering reaction

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Content (week 3)

- Basic approximations of neutron transport
- Common approximations of neutron transport
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- Collision of a neutron on a nucleus initially at rest
- The collision law of the scattering reaction

Basic approximations

1. Relativistic effect can be neglected. The kinetic energy of a neutron is generally smaller than 10 MeV in a nuclear reactor. This value is $<< E_0 = mc^2 = 939.55$ MeV).
2. The neutron-neutron interactions can be neglected. This approximation is justified by the small number density of neutrons, compared to the number density of nuclei.
3. The neutron trajectories between collision are straight lines.
4. The materials are isotropic in space. Consequently, the effects of a neutron-nucleus collision are not function of the initial direction of the neutron.
5. The lifetime of a neutron in a nuclear reactor is smaller than the radioactive half-life of the neutron ($\simeq$10.25 m) by many orders of magnitude. Radioactive decay of neutrons is therefore neglected.
6. The nuclei are always in thermal equilibrium with the material and their velocity distribution is given by the Maxwell-Boltzmann law at absolute temperature T.

Maxwell-Boltzmann law

The Maxwell-Boltzmann law is a probability density written as

$$p(\boldsymbol{V}_\mathrm{A}) = \left(\frac{mA}{2\pi kT}\right)^{\frac{3}{2}} \exp\left(-\frac{mAV_\mathrm{A}^2}{2kT}\right)$$

where

$V_\mathrm{A} =$ module of $\boldsymbol{V}_\mathrm{A}$, the velocity of the nucleus in the LAB

$k =$ Boltzmann constant ($= 8.617065 \times 10^{-5}$ eV/$^\circ$ K $= 1.38054 \times 10^{-23}$J/K)

$T =$ absolute temperature of the mixture (K)

$m =$ neutron mass ($= 1.6749544 \times 10^{-27}$kg)

$A =$ atomic mass ratio (nucleus mass in units of the neutron mass)

$p(\boldsymbol{V}_\mathrm{A})\, d^3V_\mathrm{A} =$ probability for a nucleus to have a velocity $\boldsymbol{V}_\mathrm{A}$ (within a d^3V_A interval) in the LAB.

This probability density is normalized as

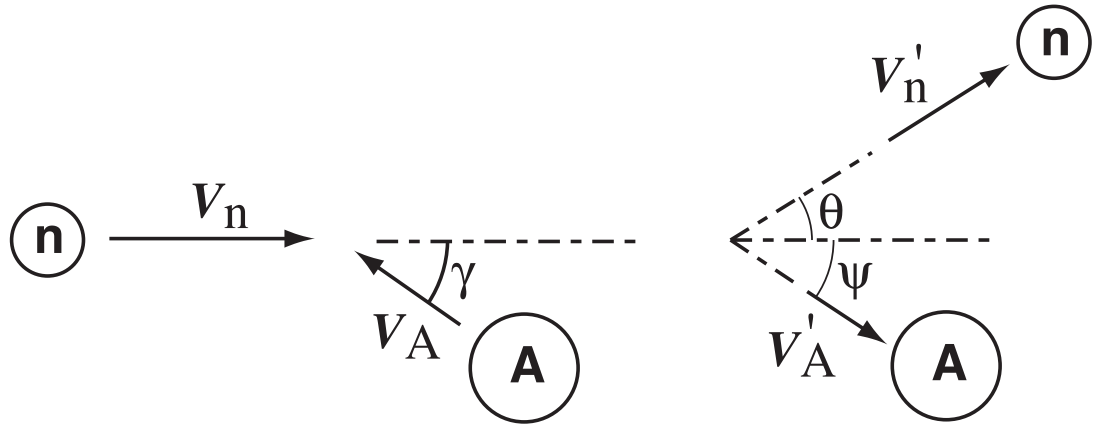
$$\int_\infty d^3V_\mathrm{A}\; p(\boldsymbol{V}_\mathrm{A}) = 1 \;\; .$$

Common approximations 1

These new approximations are less fundamental than the preceding ones and may be defeated in some practical cases.

7. In a neutron-nucleus collision, both momentum and kinetic energy of the system are conserved. Such a reaction is said to be elastic. Note that this approximation may be defeated in some nuclear reactions, such as inelastic scattering, where gamma energy is produced.
8. The neutron-nucleus collision is isotropic in the center of mass frame of reference (CM) of the colliding pair. This approximation means that all the emission angles of the secondary particles are equiprobable in the CM frame of reference. This approximation is known to be defeated for energies of the incident neutron greater than 1 MeV.
9. The nuclei are free between impacts. This approximation consists to assume that the nuclides are free from any atomic or molecular binding forces. However, for energies of the incident neutron smaller than 4 eV, molecular or metallic binding forces do have an effect if the nuclide is used as a moderator (e.g., H_2O, D_2O, Graphite, etc.).

Neutron-nucleus collision in the LAB



The collision law will be obtained in term of the following quantities:

$\boldsymbol{V}_\mathrm{n}, \boldsymbol{V}_\mathrm{n}{}' =$ initial and final velocity of the neutron in the LAB. We will also define the modulus of these vectors as $V_\mathrm{n} = |\boldsymbol{V}_\mathrm{n}|$ and $V'_\mathrm{n} = |\boldsymbol{V}_\mathrm{n}{}'|$.

$E, E' =$ initial and final kinetic energy of the neutron in the LAB. They are computed as $E = \frac{1}{2}mV_n^2$ and $E' = \frac{1}{2}mV_n'^2$.

$\boldsymbol{V}_\mathrm{A}, \boldsymbol{V}_\mathrm{A}{}' =$ initial and final velocity of the nucleus in the LAB.

$\psi, \theta =$ deviation angles in the LAB for the nucleus and the neutron, as shown in figure.

The collision law

- The collision law is a probability density written $P_{\rm e}(E' \leftarrow E, \mu)$ where $\mu = \cos\theta$.
- The quantity $P_{\rm e}(E' \leftarrow E, \mu)\, dE'\, d\mu$ is the probability for a neutron of initial energy E and undergoing an isotropic collision in the CM to have a final energy equal to E' (within a dE' interval) and a deviation cosine equal to μ (within a $d\mu$ interval) in the LAB.
- This collision law is a distribution with respect of variables E' and μ but a function with respect to E.
- It may also be a function of other quantities such as the absolute temperature on the underlying material.
- Its support is $0 \leq E' \leq \infty$ and $-1 \leq \mu \leq 1$.

Neutron-nucleus collision in the CM 1

It is easier to obtain the collision law by studying the same collision in the CM. The position $\boldsymbol{r}_{\rm CM}$ of the center of mass in the LAB is defined by

$$(A+1)\,\boldsymbol{r}_{\rm CM} = \boldsymbol{r}_{\rm n} + A\,\boldsymbol{r}_{\rm A}$$

where $\boldsymbol{r}_{\rm n}$ and $\boldsymbol{r}_{\rm A}$ are the position of the neutron and of the nucleus, respectively. The velocity of the center of mass in the LAB is

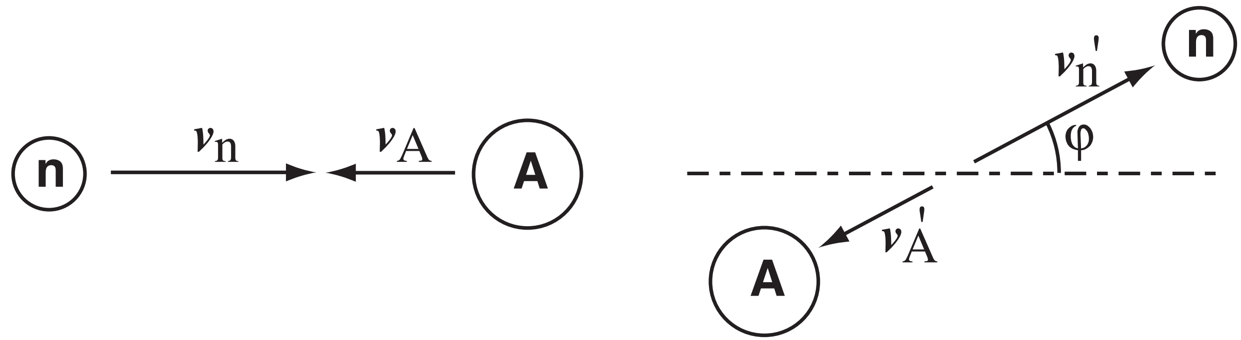
$$(A+1)\,\boldsymbol{V}_{\rm CM} = \boldsymbol{V}_{\rm n} + A\,\boldsymbol{V}_{\rm A} = \boldsymbol{V}_{\rm n}{}' + A\,\boldsymbol{V}_{\rm A}{}'$$

where the RHS part of this equation is an application of the conservation of linear momentum. The velocity $\boldsymbol{V}_{\rm CM}$ of the center of mass is constant in the LAB, before and after the collision.

If the nucleus is initially at rest, $\boldsymbol{V}_{\rm A} = \boldsymbol{0}$ and

$$\boldsymbol{V}_{\rm CM} = \frac{1}{A+1}\boldsymbol{V}_{\rm n}$$

Neutron-nucleus collision in the CM



The new dynamics relations will be obtained in term of the following quantities:

$\boldsymbol{v}_{\rm n}, \boldsymbol{v}_{\rm n}{}' =$ initial and final velocity of the neutron in the CM. We will also define the modulus of these vectors as $v_{\rm n} = |\boldsymbol{v}_{\rm n}|$ and $v'_{\rm n} = |\boldsymbol{v}_{\rm n}{}'|$.

$e_{\rm n}, e_{\rm n}{}' =$ initial and final kinetic energy of the neutron in the CM. They are computed as $e_{\rm n} = \frac{1}{2} m v_n^2$ and $e_{\rm n}{}' = \frac{1}{2} m v_n'^2$.

$\boldsymbol{v}_{\rm A}, \boldsymbol{v}_{\rm A}{}' =$ initial and final velocity of the nucleus in the CM.

$e_{\rm A}, e_{\rm A}{}' =$ initial and final kinetic energy of the nucleus in the CM. They are computed as $e_{\rm A} = \frac{1}{2} m A v_A^2$ and $e_{\rm A}{}' = \frac{1}{2} m A v_A'^2$.

Neutron-nucleus collision in the CM

The velocities in the CM are

$$\boldsymbol{v}_{\rm n} = \boldsymbol{V}_{\rm n} - \boldsymbol{V}_{\rm CM} \; , \quad \boldsymbol{v}_{\rm A} = \boldsymbol{V}_{\rm A} - \boldsymbol{V}_{\rm CM}$$

$$\boldsymbol{v}_{\rm n}{}' = \boldsymbol{V}_{\rm n}{}' - \boldsymbol{V}_{\rm CM} \quad \text{and} \quad \boldsymbol{v}_{\rm A}{}' = \boldsymbol{V}_{\rm A}{}' - \boldsymbol{V}_{\rm CM} \quad .$$

Combining these Eqs., we can show that

$$\boldsymbol{v}_{\rm n} = \boldsymbol{V}_{\rm n} - \frac{\boldsymbol{V}_{\rm n} + A\,\boldsymbol{V}_{\rm A}}{A+1} = \frac{A}{A+1}\,\boldsymbol{V}_{\rm R} \quad \text{and} \quad \boldsymbol{v}_{\rm A} = \frac{-1}{A+1}\,\boldsymbol{V}_{\rm R}$$

where $\boldsymbol{V}_{\rm R}$ is the initial relative velocity between the neutron and the nucleus. It is defined as

$$\boldsymbol{V}_{\rm R} = \boldsymbol{V}_{\rm n} - \boldsymbol{V}_{\rm A} \quad .$$

We observe that $\boldsymbol{v}_{\rm n}$ and $\boldsymbol{v}_{\rm A}$ are colinear vectors of opposite direction in the CM.

Neutron-nucleus collision in the CM

During the collision, the two particles will stay at rest in the CM. If a compound nucleus is formed, it will stay at rest in the CM, so that all the kinetic energy of the particles will be available as excitation energy. This quantity is the available kinetic energy for excitation $e_{\rm exc}$ defined as

$$e_{\rm exc} = e_{\rm n} + e_{\rm A} = \frac{1}{2}\frac{mA}{A+1}V_{\rm R}^2 \quad .$$

We will see later that $e_{\rm exc}$ is only one component of the excitation energy for the compound nucleus. Morever, $e_{\rm exc}$ is not the sum of $E_{\rm n}$ and $E_{\rm A}$, as the compound nucleus is moving in the LAB. The kinetic energy of the compound nucleus in the LAB is not available as excitation energy.

Assuming conservation of linear momentum in the CM, we write

$$\boldsymbol{v}_{\rm n} + A\,\boldsymbol{v}_{\rm A} = \boldsymbol{v}_{\rm n}{}' + A\,\boldsymbol{v}_{\rm A}{}' = \frac{A}{A+1}\boldsymbol{V}_{\rm R} - A\,\frac{1}{A+1}\boldsymbol{V}_{\rm R} = \boldsymbol{0}$$

so that

$$\boldsymbol{v}_{\rm n} = -A\,\boldsymbol{v}_{\rm A} \quad \text{and} \quad \boldsymbol{v}_{\rm n}{}' = -A\,\boldsymbol{v}_{\rm A}{}' \quad .$$

Neutron-nucleus collision in the CM 5

Assuming conservation of energy in the CM, we write

$$e_{\mathrm{n}} + e_{\mathrm{A}} = e'_{\mathrm{n}} + e'_{\mathrm{A}} = e_{\mathrm{exc}}$$

so that

$$\frac{1}{2} m {v'_{\mathrm{n}}}^2 + \frac{1}{2} m A {v'_{\mathrm{A}}}^2 = \frac{1}{2} \frac{mA}{A+1} V_{\mathrm{R}}^2 \quad .$$

We finally find

$$v'_{\mathrm{n}} = v_{\mathrm{n}} = \frac{A}{A+1} V_{\mathrm{R}} \quad \text{and} \quad v'_{\mathrm{A}} = v_{\mathrm{A}} = \frac{1}{A+1} V_{\mathrm{R}} \quad .$$

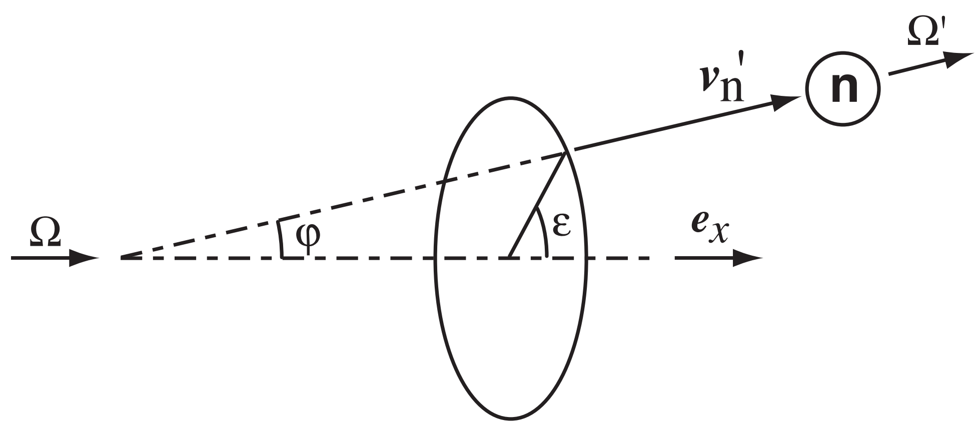
The last two Eqs. are scalar relations demonstrating the conservation of the CM velocity modules for each particle during the collision.

Azimuthal reduction

We have now reached the point where the collision law can be obtained. Assuming the isotropic emission of the secondary neutron in the CM, a first probability density can be written as

$$\mathcal{P}_{\rm e}(\boldsymbol{\Omega}' \leftarrow \boldsymbol{\Omega}) = \frac{1}{4\pi} \tag{1}$$

where the solid angles are defined in term of the deviation angle φ and on the azimuth ϵ in the CM. The two angles are defined in the figure



Assuming that $\boldsymbol{\Omega} = \boldsymbol{i}$, we see that $\boldsymbol{\Omega}' = \cos\varphi\, \boldsymbol{i} + \sin\varphi\, \cos\epsilon\, \boldsymbol{j} + \sin\varphi\, \sin\epsilon\, \boldsymbol{k}$. The support of $\mathcal{P}_{\rm e}$ is $0 \le \varphi \le \pi$ and $0 \le \epsilon \le 2\pi$. $\mathcal{P}_{\rm e}(\boldsymbol{\Omega}' \leftarrow \boldsymbol{\Omega})d^2\Omega'$ is the probability for a neutron of initial direction $\boldsymbol{\Omega}$ and undergoing an isotropic collision in the CM to have a final direction equal to $\boldsymbol{\Omega}'$ (within a $d^2\Omega'$ interval) in the CM.

Azimuthal reduction

A distribution reduction is performed to get the probability density in term of the deviation cosine $\cos\varphi = \mathbf{\Omega}\cdot\mathbf{\Omega}'$ in the CM. We obtain

$$\mathcal{P}_{\rm e}(\cos\varphi) = \int_0^{2\pi} d\epsilon\, \mathcal{P}_{\rm e}(\mathbf{\Omega}' \leftarrow \mathbf{\Omega}) = \frac{1}{2} \tag{2}$$

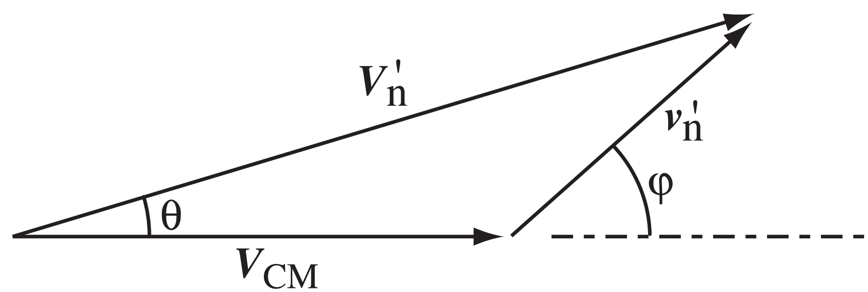
over the support $-1 \le \cos\varphi \le 1$. $\mathcal{P}_{\rm e}(\cos\varphi)\, d(\cos\varphi)$ is the probability for a neutron undergoing an isotropic collision in the CM to have a deviation cosine equal to $\cos\varphi$ (within a $d(\cos\varphi)$ interval) in the CM. As expected, this probability density is normatized to one:

$$\int_{-1}^{1} d(\cos\varphi)\, \mathcal{P}_{\rm e}(\cos\varphi) = 1 \quad .$$

Nucleus initially at rest

We first study the collision of a neutron on a nucleus initially at rest. In this case, the preceding equations still applied, with $\boldsymbol{V}_{\rm A} = \boldsymbol{0}$ in the LAB. Expressions of $V_{\rm CM}$ and $v'_{\rm n}$ are now written

(3) $$V_{\rm CM} = \frac{1}{A+1} V_{\rm n} \quad \text{and} \quad v'_{\rm n} = v_{\rm n} = \frac{A}{A+1} V_{\rm n} \quad .$$



We can also apply the cosines law. We obtain

(4) $$V_{\rm n}'^{2} = V_{\rm CM}^2 + v_{\rm n}'^{\,2} + 2V_{\rm CM}\, v'_{\rm n} \cos\varphi$$

where $V_{\rm CM}$ and $v'_{\rm n}$ are independent of φ. Taking the derivative of Eq. (4) and substituting Eqs. (3) leads to

(5) $$2V'_{\rm n}\, dV'_{\rm n} = 2V_{\rm CM}\, v'_{\rm n}\, d(\cos\varphi) = \frac{2A}{(A+1)^2} V_{\rm n}^2\, d(\cos\varphi) \quad .$$

Nucleus initially at rest

The last equation can be written in term of initial and final energies of the neutron in the LAB. We obtain

$$2dE' = \frac{4A}{(A+1)^2} E\, d(\cos\varphi) = (1-\alpha)\, E\, d(\cos\varphi) \tag{6}$$

where

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 \quad . \tag{7}$$

We perform a change of variable toward $E' = f(\cos\varphi)$, so that

$$\frac{d}{dE'}(\cos\varphi) = \frac{2}{(1-\alpha)\, E} > 0\ ; \quad \text{with} \quad -1 \le \cos\varphi \le 1 \tag{8}$$

and Eq. (2) becomes

$$P_{\rm e}(E' \leftarrow E) = [\mathcal{P}_{\rm e}(\cos\varphi)] \left[\frac{d}{dE'}(\cos\varphi)\right] = \frac{1}{(1-\alpha)\, E} \tag{9}$$

with $E'_{\rm min} \le E' \le E'_{\rm max}$.

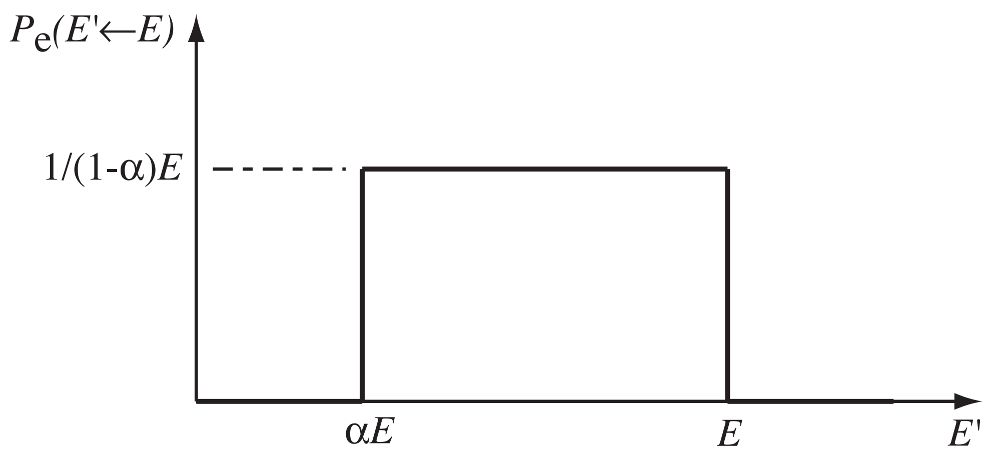
Nucleus initially at rest

The support of E' can also be found using the vector diagram. If $\cos\varphi = -1$, then

$$V'_{\rm n} = v'_{\rm n} - V_{\rm CM} = \frac{A-1}{A+1} V_n \quad \text{so that} \quad E'_{\rm min} = \alpha\, E \quad .$$

At the other limit, $\cos\varphi = 1$, and

$$V'_{\rm n} = v'_{\rm n} + V_{\rm CM} = V_n \quad \text{so that} \quad E'_{\rm max} = E \quad .$$



The probability density is uniform in the support $\alpha\, E \le E' \le E$. The collision of a neutron on a nucleus initially at rest has the effect to slow down this neutron. The slowing-down effect is more important for light nuclides, as they are characterized by small values of α.

Nucleus initially at rest

We will now compute the complete collision law $P_{\rm e}(E' \leftarrow E, \mu)$. In the case where the nucleus is initially at rest, the variables E' and μ are dependent one of the other and are related by a function of type $\mu = f(E')$. All the neutrons with a given final energy E' have the same deviation angle φ in the CM and the same deviation cosine μ in the LAB, for any given value of E. The probability density describing a known event is the Dirac delta density $\delta(x)$, so that

(10) $$P_{\rm e}(E' \leftarrow E, \mu) = P_{\rm e}(E' \leftarrow E)\, \delta\left[\mu - f(E')\right] \ .$$

The vector diagram and the cosines law will be used again as the starting point to compute $f(E')$. We write

(11) $${v'_{\rm n}}^2 = {V'_{\rm n}}^2 + {V_{\rm CM}}^2 - 2V'_{\rm n}\, V_{\rm CM}\, \mu \ .$$

which becomes

(12) $$\left(\frac{A}{A+1}\right)^2 {V_{\rm n}}^2 = {V'_{\rm n}}^2 + \left(\frac{1}{A+1}\right)^2 {V_{\rm n}}^2 - \frac{2}{A+1}\, V'_{\rm n}\, V_{\rm n}\, \mu$$

and which can be written in term of initial and final energy of the neutron in the LAB as

(13) $$-(A-1)\, E + (A+1)\, E' = 2\sqrt{E\, E'}\, \mu \ .$$

Nucleus initially at rest

The deviation cosine of the neutron in the LAB is obtained as a function of E'. We write

$$\mu = f(E') = \frac{1}{2}(A+1)\sqrt{\frac{E'}{E}} - \frac{1}{2}(A-1)\sqrt{\frac{E}{E'}} \quad . \tag{14}$$

Finally, we obtain the required collision law as

$$P_\mathrm{e}(E' \leftarrow E, \mu) = \begin{cases} \dfrac{1}{(1-\alpha)E}\,\delta\!\left[\mu - \frac{1}{2}(A+1)\sqrt{\frac{E'}{E}} + \frac{1}{2}(A-1)\sqrt{\frac{E}{E'}}\right] , & \text{if } \alpha E \le E' \le E; \\ 0\ , & \text{otherwise.} \end{cases} \tag{15}$$

This equation is often referred as the elastic slowing-down collision law. It can be used to study the slowing-down of neutrons in the energy range above 1 eV. At lower energies, the thermal agitation of nuclides can transmit kinetic energy to the neutrons, which can no longer be considered initially at rest. The support of this distribution is $0 \le E' \le \infty$ and $-1 \le \mu \le 1$ and its normalization condition is

$$\int_0^\infty dE' \int_{-1}^1 d\mu\, P_\mathrm{e}(E' \leftarrow E, \mu) = 1 \quad . \tag{16}$$

Change of variable 1

A neutron is loosing a fraction of its initial kinetic energy in each elastic scattering reaction. We define the lethargy of the neutron as

$$u = \ln \frac{E_0}{E}$$

where E_0 is a reference energy taken above the maximum energy of all neutrons in the reactor. The lethargy is generally defined in the LAB. A neutron emitted at energy E_0 has a zero lethargy. Its lethargy will increase as the neutron slow-down in the reactor.

The collision law can also be written in term of lethargy. $P_{\rm e}(u' \leftarrow u, \mu) du' \, d\mu$ is the probability for a neutron of initial lethargy u and undergoing an isotropic collision in the CM to have a final lethargy equal to u' (within a du' interval) and a deviation cosine equal to μ (within a $d\mu$ interval) in the LAB.

Change of variable

A change of variable on Eq. (15) leads to.

$$P_{\mathrm{e}}(u' \leftarrow u, \mu) = \begin{cases} \dfrac{\mathrm{e}^{-U}}{1-\alpha}\,\delta\left[\mu - \frac{1}{2}(A+1)\,\mathrm{e}^{-U/2} + \frac{1}{2}(A-1)\,\mathrm{e}^{U/2}\right] \ , & \text{if } 0 \le U \le \epsilon; \\ 0 \ , & \text{otherwise,} \end{cases}$$

where $U = u' - u$ is the actual lethargy gain of the neutron and

$$\epsilon = \ln \frac{1}{\alpha}$$

is the maximum gain of lethargy.