Neutron Thermalization: A Fractional Calculus

Theoretical Approach

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Abstract

One of the technologically most important interactions of neutrons with matter is their loss of energy ("slowing down") by a series of elastic collisions. These can be treated by the methods of classical mechanics, assuming the interacting particles as perfectly elastic spheres. The energy loss is an important subject, and is discussed in several books where numerical tables and graphs are presented. Formulas are found semiempirically with several correction coefficients. Despite all efforts, no direct, exact formula has so far been obtained analytically. The purpose of this paper is to introduce just such a direct formula of the energy loss analytically by using a recently introduced method of the quantization of nonconservative systems based on fractional calculus.
1. Introduction

The distance that a fast neutron will travel, between its introduction into the slowing-down medium (moderator) and thermalization, is dependent on the number of collisions and the distance between collisions. Though the actual path of the neutron slowing down is tortuous because of collisions, the average straight-line distance can be determined; this distance is called the fast diffusion length or slowing-down length. The distance traveled, once thermalized, until the neutron is absorbed, is called the thermal diffusion length.

Fast neutrons rapidly degrade in energy by elastic collisions when they interact with low atomic number materials. As neutrons reach thermal energy, or near thermal energies, the likelihood of capture increases. In present day reactor facilities the thermalized neutron continues to scatter elastically with the moderator until it is absorbed by fuel or non-fuel material, or until it leaks from the core.

Most of these interactions individually transfer only minute fractions of the neutron's kinetic energy, and it is convenient to think of the neutron as losing its kinetic energy gradually, often referred to as "continuous slowing-down approximation". Because of the multitude of interactions undergone by each neutron in slowing down, its path length tends to approach the expectation value that would be observed as a mean for a very large population of identical particles. That expectation value is called the range.

The purpose of this paper is to introduce a direct analytical formula related the energy loss with the range analytically by using Ajlouni's theory of quantization of nonconservative systems depending on fractional calculus (Ajlouni, 2004, Ajlouni, 2010, Ajlouni, 2011, Rabei et al., 2006).

2. Neutron Slowing Down and Thermalization

Fission neutrons are produced at an average energy level of 2 MeV and immediately begin to slow down as the result of numerous scattering reactions with a variety of target nuclei. After a number of collisions with nuclei, the speed of a neutron is reduced to such an extent that it has approximately the same average kinetic energy as the atoms (or molecules) of the medium in which the neutron is undergoing elastic scattering. This energy, which is only a small fraction of an electron volt at ordinary temperatures, 0.025 eV at 20°C, is frequently referred to as the thermal energy, since it depends upon the temperature. Neutrons whose energies have been reduced to values in this region (< 1 eV) are designated thermal neutrons. The process of reducing the energy of a neutron to the thermal region by elastic scattering is referred
Neutron thermalization to as thermalization, slowing down, or moderation. The material used for the purpose of thermalizing the neutrons is called a moderator. A good moderator reduces the speed of neutrons in a small number of collisions, but does not absorb them to any great extent. Slowing the neutrons in as few collisions as possible is desirable in order to reduce the amount of neutron leakage from the core and also to reduce the number of resonance absorptions in non-fuel materials.

The ideal moderating material (moderator) should have the following nuclear properties (DEO, 1993):

1. Large scattering cross section
2. Small absorption cross section
3. Large energy loss per collision

A convenient measure of energy loss per collision is the logarithmic energy decrement. The average logarithmic energy decrement is the average decrease per collision in the logarithm of the neutron energy, represented by the symbol $\xi$ (DEO, 1993):

$$\zeta = \ln E_i - \ln E_f = \ln \frac{E_i}{E_f}$$

where $E_i$ and $E_f$ are the average initial and final neutron energy, respectively.

Since the fraction of energy retained by a neutron in a single elastic collision is a constant for a given material, $\xi$ is also a constant. Because it is a constant for each type of material and does not depend upon the initial neutron energy, $\xi$ is a convenient quantity for assessing the moderating ability of a material.

The total number of collisions necessary for a neutron to lose a given amount of energy may be determined by dividing $\xi$ into the difference of the natural logarithms of the energy range in question. The number of collisions ($N$) to travel from any energy, $E_{\text{high}}$, to any lower energy, $E_{\text{low}}$, can be calculated as (DEO, 1993):

$$N = \frac{\ln E_{\text{high}} - \ln E_{\text{low}}}{\xi} = \frac{\ln \left(\frac{E_{\text{high}}}{E_{\text{low}}}\right)}{\xi}$$

Sometimes it is convenient, based upon information known, to work with an average fractional energy loss per collision as opposed to an average logarithmic fraction. If the initial neutron energy is $E_0$, and the average fractional energy loss per collision is
known, $X$, the final energy for a given number of collisions, $E_N$, may be computed using the following formula (DEO, 1993):

$$E_N = E_0 (1 - X)^N$$

<table>
<thead>
<tr>
<th>Material</th>
<th>$\xi$</th>
<th>Number of Collisions to Thermalize</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$O</td>
<td>0.927</td>
<td>19</td>
</tr>
<tr>
<td>D$_2$O</td>
<td>0.510</td>
<td>35</td>
</tr>
<tr>
<td>Helium</td>
<td>0.427</td>
<td>42</td>
</tr>
<tr>
<td>Beryllium</td>
<td>0.207</td>
<td>86</td>
</tr>
<tr>
<td>Boron</td>
<td>0.171</td>
<td>105</td>
</tr>
<tr>
<td>Carbon</td>
<td>0.158</td>
<td>114</td>
</tr>
</tbody>
</table>

3. Quantization of Nonconservative Systems: Free Particle in a Dissipative Medium

According to Ajlouni’s theory of the quantization of nonconservative systems, the Hamiltonian can be written as follows (Ajlouni, 2004, Ajlouni, 2010, Ajlouni, 2011, Rabei et al., 2006):

$$H = \sum_{i=0}^{N-1} \frac{d}{dt} \delta^{(i+1) - (i)} q_{r, a(i)} P_{r, a(i)} - L, \quad 0 \leq i \leq N-1$$

$$= \sum_{i=0}^{N-1} q_{r, a(i + 1)} P_{r, a(i)} - L, \quad (4)$$

and the Schrödinger equation reads [6]

$$i\hbar \frac{\partial}{\partial t} \Psi = H \Psi. \quad (5)$$

Consider a free particle moving in a dissipative medium where dissipation is proportional to velocity (Ajlouni, 2004, Ajlouni, 2010, Ajlouni, 2011, Rabei et al., 2006), i.e.,

$$F = -\gamma q_1, \quad (6)$$
\( \gamma \) being a positive constant. The potential related to this dissipation is (Ajlouni, 2004, Ajlouni, 2010, Ajlouni, 2011, Rabei et al., 2006)

\[
U = \frac{i\gamma}{2} q_{1/2}^2,
\]


\[
L = \frac{1}{2} m q_i^2 - \frac{i\gamma}{2} q_{1/2}^2,
\]

where

\[
q_0 = x, \quad q_i = \frac{dx}{dt}, \quad q_{1/2} = \frac{d^{1/2}x}{d(t-b)^{1/2}};
\]


\[
p_0 = \frac{\partial L}{\partial q_{1/2}} + i \frac{d^{1/2}}{d(t-a)^{1/2}} \frac{\partial L}{\partial q_0} = i\gamma q_{1/2} + imq_{1/2};
\]

and

\[
p_{1/2} = \frac{\partial L}{\partial q_1} = mq_1.
\]


\[
H = \frac{(p_{1/2})^2}{2m} + q_{1/2} p_0 + \frac{\gamma}{2i} q_{1/2}^2.
\]

Here \( p_0 \) and \( p_{1/2} \) are the canonical conjugate momenta to \( q_0 \) and \( q_{1/2} \), respectively.

Schrödinger's equation reads [1, 5]

\[
i\hbar \frac{\partial}{\partial t} \Psi = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q_{1/2}^2} + \frac{\hbar}{i} q_{1/2} \frac{\partial}{\partial q_0} + \frac{1}{2i} \gamma q_{1/2} \right] \Psi.
\]

which is Schrödinger's equation for a dissipated free particle, has the following solution (Ajlouni, 2004, Ajlouni, 2010, Ajlouni, 2011, Rabei et al., 2006)
\[ \Psi_n = AH_n \left[ \frac{m\gamma}{i\hbar^2} \right]^{q/2} H_{\nu}^{2} \exp \left( -\frac{m\gamma}{i\hbar^2} \right) \exp \left( -\frac{i}{\hbar} E_s q_0 \right) \exp \left( -\frac{i}{\hbar} E_0 t \right). \] (14)

where \( H_n \) are Hermite polynomials.

5. Neutron thermalization

In this problem we assume that the free particle represents the neutron, the dissipative medium is the matter where the particle passes, and the dissipative effects result from a drag force influences the neutron motion inside the matter, similar to that take place, when an object moving through a fluid, and will generally experience a drag force proportional to its velocity. Despite the fact that, many processes may occur during particle passage, but, what we concern about, is the over all energy loss of the particle in matter.

The dissipation force and potential are found by velocity proportional law, i.e.,

\[ F = \gamma q_1 \] (15)

The potential corresponding to this dissipation is

\[ U = \frac{i\gamma}{2} q_{1/2}. \] (16)

which leads to Schrödinger's equation for a dissipated free particle, Eq. (13), has the solution, \( \Psi_n = AH_n \left[ \frac{m\gamma}{i\hbar^2} \right]^{q/2} H_{\nu}^{2} \exp \left( -\frac{m\gamma}{i\hbar^2} \right) \exp \left( -\frac{i}{\hbar} E_s q_0 \right) \exp \left( -\frac{i}{\hbar} E_0 t \right). \) (14)

Energy expectation value is:

\[ \langle E \rangle = \int \int \Psi^* H \Psi dx'dy'. \] (17)

Inserting Eq. (14) in Eq. (17), and using the relations (Dass, and Sharma, 1998, Arfken, 1985):

\[ H_n'(y) = 2nH_n(y), \] (18)
Neutron thermalization

\[ \int_{-\infty}^{\infty} e^{y^2} H_n(y) H_m(y) dy = \sqrt{\pi} n! 2^n \delta_{nm}, \quad (19) \]

and,

\[ \int_{-\infty}^{\infty} y^p e^{y^2} H_n(y) H_{n+p}(y) dy = \begin{cases} \sqrt{\pi} (n+r)! 2^n, & p = r \\ 0, & p > r \end{cases}, \quad (20) \]

that makes all the non-\( x \)-terms of Eq. (14), constants or zeros. The remainder part is the \( x \)-dependent terms, appears as:

\[ \langle E \rangle = \int_{x,x' \geq 0} H_n \exp \frac{\alpha^2 y^2}{2} \left( \exp \frac{i}{\hbar} E_x \frac{x'}{y} \right) \left[ \alpha^2 \frac{iE_x x'}{\hbar y} \left( \frac{E_x x'}{\hbar y^2} \right) + \frac{iE_x x'}{\hbar y^3} \right] \]

\[ H_n \exp \frac{\alpha^2 y^2}{2} \exp \frac{i}{\hbar} E_x \frac{x}{y} dy dx' \quad (21) \]


\[ \langle E \rangle = bx^3 - ax^2 - cx; \quad (22) \]

where \( a, b, \) and \( c \) are constants.

**Figure 1**: A schematic representation of average neutron energy loss as a function of distance through moderator.
6. Conclusion

Quantization of nonconservative free particle system, according to Ajlouni's recent theory is applied on neutron thermalization when passed through matter. The formula of energy loss versus distance traveled inside matter has been introduced and plotted. The figure agrees widely with the experimental results.

References


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