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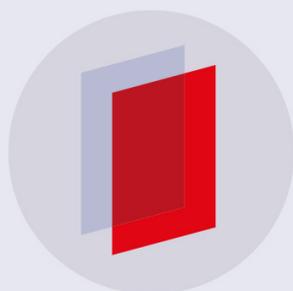
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# Diffusion of neutrons by a slab of moderating material: an application of the Monte Carlo method

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## Abstract

An application of the Monte Carlo method to the diffusion of neutrons passing through a slab of a moderating material is presented. This method can be used as a tool to improve the student's comprehension of the statistical properties of many particle systems, showing the necessity of simulation procedures to obtain information on the expected results of real experiments. We have chosen a very simple example to illustrate it: the evaluation of the transmission, reflection and absorption probabilities of a monochromatic beam of neutrons diffusing through a slab of a moderator material. After a collision with a nucleus of the moderator the neutron may be either elastically scattered or captured. The transmission, reflection and absorption properties of the neutrons diffused by different moderating materials are visualized with the help of an appropriate animation program.

## 1. Introduction

In these last years, much effort has been made by physics teachers in engineering and other scientific faculties to improve methods and tools for teaching physics by using simulation methods and interactive computer-based virtual labs. Active learning techniques have been shown to develop students' meaningful understanding and problem-solving skills [1]. Most of the innovative educational materials have been addressed to standard topics of introductory physics courses; however, some good examples have also been developed in the field of statistical physics [2, 3], structure of matter [4, 5], deterministic chaos [6–9] and quantum physics [8, 9]. In this paper we present the first step of our educational research project involving the application of the Monte Carlo method to problems of nuclear physics.

The random-sampling technique, generally known as the Monte Carlo method, has found widespread application in many fields of science, complementing both analytical theories and experiments. Nowadays, it is used routinely in different fields of applied research as, for instance, the design of nuclear reactors, radiation cancer therapy and financial risk management. The foundation of the method relies on the fact that behaviours of arbitrary complexity may often be ultimately traceable to very simple rules. This is mainly the case of many body systems, where the elementary physical events are well defined and can be easily understood by students at undergraduate level. Mathematical problems emerge when the synthesis of these elementary events is attempted. In a computer simulation, synthesis is realized implicitly in the logical design of the fundamental computational flow sequence used to define the conceptual model being studied. Physical values are obtained by averaging the set of values occurring in each of a very large number of particular computational sequences. The Monte Carlo method allows us to perform experiments with models and, in many cases, allows us to deal with very complicated physical phenomena resulting from the interplay of a large number of elementary processes. Moreover, the use of the Monte Carlo method is mandatory in problems where the quantities of interest depend on the microscopic properties and on the geometry of the moderating material, as will be shown in the following for the simple problem of neutron beams crossing a moderating slab.

Recently, Peralta [10] has proposed an educational Monte Carlo simulation of neutron thermalization in matter through elastic collisions. In this paper, we provide a Monte Carlo method application to the simulation of the diffusion process of a neutron beam through an infinite plate. The result is the beam slowing down due to the interactions with the moderator material of the plate.

We implemented a simplified non-commercial Monte Carlo code and present our results using an appropriate animation interface in JAVA code (<http://griaf/dft.unipa.it>). The simulation is devoted to undergraduate students: its main goal is to show that it is possible to describe the collective behaviour of a neutron beam passing through a slab of a moderating material, starting from a microscopic description of the interaction of a single neutron with a nucleus. Section 2 reports a simple description of the neutron–nucleus collision process and of the characteristic physical quantities, as mean free path and collision time. Section 3 outlines the main features of the Monte Carlo method and how it is applied to our problem. Section 4 describes the results of our simulation and analyses them in terms of the microscopic properties of the moderating materials.

## 2. Properties of the neutron–nucleus elementary collision process

The slowing down process of neutrons is a consequence of inelastic and elastic collisions. Since inelastic collisions are very difficult to handle, our simple model considers only elastic collisions and absorption of neutrons. In the kinematics of the elastic scattering, we assume the nucleus at rest in the laboratory frame. After the scattering event a neutron, with initial energy  $E_0$ , will possess an energy  $E$  and will be deflected by an angle  $\vartheta$ , in the centre-of-mass system. Velocity and direction of the neutron after the collision can be calculated using a simple geometrical method, called the momentum diagram [11], based upon energy and momentum conservations. The ratio between the neutron energy after and before the collision is

$$\frac{E}{E_0} = \frac{1}{(A+1)^2} (A^2 + 1 + 2A \cos \vartheta) \quad (1)$$

where  $A$  is the nucleus mass number. All the kinematic properties of the neutrons after the collision are determined by equation (1) together with the relationship existing between the

scattering angle in the laboratory system  $\vartheta_L$ , assumed isotropic, and the scattering angle in the centre-of-mass system  $\vartheta$

$$\cos \vartheta_L = \frac{A \cos \vartheta + 1}{(A^2 + 1 + 2A \cos \vartheta)^{1/2}}. \quad (2)$$

The other variables needed to perform Monte Carlo simulation are the average time  $\tau$  between two collisions and the mean free path  $\lambda$ . The average time  $\tau$  between two collisions is given by

$$\tau = \frac{T}{N} \quad (3)$$

with  $N$  the number of neutron–nuclei collisions in a given time interval  $T$ . For neutrons with a velocity  $v$  the mean free path  $\lambda$  is  $\lambda = v\tau$ . The probability that a neutron will undergo another collision in a time interval  $dt$ , after the previous collision, will then be  $dt/\tau$ , and the collision probability per unit time  $w = 1/\tau$ .

The average time  $\tau$  between two next collisions and the mean free path  $\lambda$  depends both on the details of the neutron–nucleus interaction and on the nuclei density in the material. The interaction of neutrons with matter is characterized by the effective cross section  $\sigma_T$ , representing the total collision area, that is related to the microscopic properties of the interacting particles. Since the neutron–nucleus interaction is short range, we can roughly approximate neutrons and nuclei as hard spheres. In this approximation the collision area can be taken as the largest area including the centre of the two colliding particles

$$\sigma_T = \pi(r_A + r_n)^2 \quad (4)$$

with  $r_A$  and  $r_n$  the nucleus and the neutron classic radii, respectively. A neutron moving across a material with  $n$  atoms per unit volume will encounter a number  $nv dt$  of target nuclei per unit area perpendicular to the direction of the incident neutron: consequently, the total cross section per unit area will be  $nv\sigma_T dt$ . Then, the probability  $dt/\tau$  that the neutron undergoes a collision in the time interval  $dt$  and the probability per unit time  $w$  will be, respectively,

$$\frac{dt}{\tau} = nv\sigma_T dt. \quad (5)$$

$$w = \frac{1}{\tau} = nv\sigma_T. \quad (6)$$

In a more realistic model the colliding particles cannot be considered as hard spheres. In fact several scattering processes such as inelastic, elastic, resonant, absorption, etc, should be taken into consideration. To keep our model simple we include only two independent processes, elastic collision and absorption of neutrons; the total cross section is just the sum  $\sigma_T = \sigma_c + \sigma_a$ , the total collision probability per unit time is  $w = w_c + w_a$  and the total mean free path will be

$$\frac{1}{\Lambda} = \frac{1}{\lambda_c} + \frac{1}{\lambda_a}. \quad (7)$$

### 3. The Monte Carlo simulation

Let us consider a flux of neutrons with energy  $E_0$  incident perpendicularly onto a homogeneous infinite plate of width  $d$ . After several scattering events the neutron either may cross the plate or may be reflected or captured inside the plate. The transmission, reflection and absorption probabilities,  $P_T$ ,  $P_R$ ,  $P_A$ , are defined respectively as

$$P_T = \frac{N_T}{N}, \quad P_R = \frac{N_R}{N}, \quad P_A = \frac{N_A}{N} \quad (8)$$

where  $N_T$  is the number of neutrons crossing the plate,  $N_R$  and  $N_A$  are the numbers of reflected and absorbed neutrons, while  $N$  is the total number of neutrons. Our simulation calculates  $N_T$ ,  $N_R$  and  $N_A$  using the Monte Carlo method.

For each incident neutron the free path  $l$  is stochastically determined as well as the interaction process. If the interaction process is an elastic collision, we determine stochastically the diffusion angle and the next free path and so on iteratively.

In the Monte Carlo method, the crucial point is the choice of the different variables characterizing the process: in our case the quantities of interest are the neutron free path and the scattering angles. For each of these variables it is necessary to know the probability density function. These functions can be determined from experimental data or from the theoretical model describing the physics of the process. In the appendix we give the derivation of the probability density functions for the variables of interest. The probability density function related to the free path  $l$  between two collisions results (see (A.12)) in

$$\rho(l) = n\sigma \exp(-n\sigma l). \quad (9)$$

To select the direction of the neutron trajectory after the collision it is necessary to know the probability density functions related to the scattering angles  $\vartheta$  and  $\varphi$ . The density probabilities are given respectively as (see (A.15) and (A.16))

$$\rho(\vartheta) = \frac{\sin \vartheta}{2} \quad (10)$$

and

$$\rho(\varphi) = \frac{1}{2\pi}. \quad (11)$$

The angle  $\varphi$  is then uniformly distributed in the interval  $(0, 2\pi)$  and, due to the infinite extension of the slab, is inessential to the simulation.

In order to calculate for each neutron a value of the free path  $l$  and of the scattering angles  $\theta$  and  $\varphi$  after the collision, we map the relative probability densities (equations (9)–(11)) to the standard one, using the uniform distribution of a random variable  $\gamma$  between 0 and 1, as

$$\int_0^\xi \rho(x) dx = \int_0^\gamma 1 dx = \gamma \quad (12)$$

where  $\xi$  assumes the values  $l$ ,  $\theta$  and  $\varphi$  for the three different variables.

The relation between the random variable  $\gamma$  and the free path variable  $l$  is

$$l = -\Lambda \ln \gamma \quad (13)$$

where  $\Lambda(\lambda_a, \lambda_c)$  is given by equation (7).

The relation between the random variable  $\gamma$  and the angle  $\varphi$  is

$$\varphi = 2\pi \gamma \quad (14)$$

and the relation between the random variable  $\gamma$  and the angle  $\theta$  is

$$\cos \vartheta = 2\gamma - 1. \quad (15)$$

Figure 1 shows the block diagram of the program used to simulate the neutron motion. The index  $j$  indicates the trajectory number, i.e. identifies the neutron undergoing a scattering process, while  $k$  indicates its collision number. For each neutron the initial coordinate  $x_0$  and scattering angle  $\vartheta_L = 0$ , in the laboratory frame, are assigned; then its free path length  $l_k$  between two collisions and the scattering angle  $\vartheta_k$  are stochastically chosen according to the probability densities given by equations (13) and (14); finally the scattering angle  $\vartheta_k$  is expressed in terms of the laboratory system one  $\vartheta_L$  using equation (2), (see [11]), and the

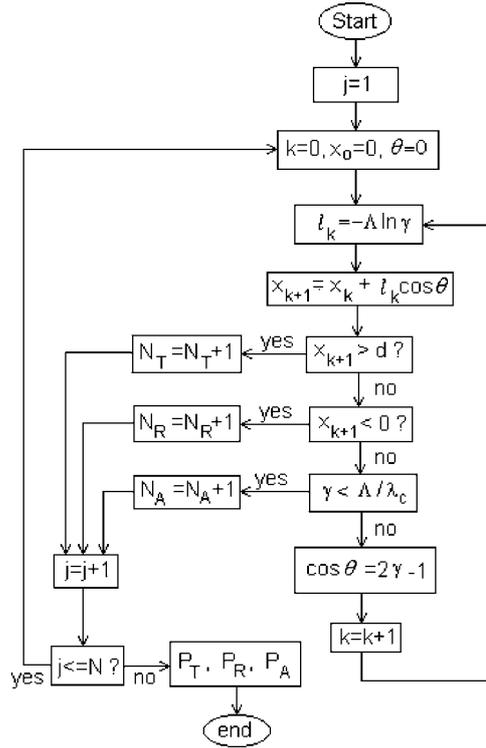


Figure 1. Flow chart of the simulation.

new  $x$  coordinate is determined as

$$x_{k+1} = x_k + l_k \cos \vartheta_L. \quad (16)$$

After each collision the neutron position is checked. Three different conditions are possible:

$$x_{k+1} > d, \quad x_{k+1} < 0, \quad \text{and} \quad 0 \leq x_{k+1} \leq d. \quad (17)$$

If the first condition is satisfied, the computation of the trajectory for the neutron is terminated and a unit is added to the counter of the transmitted particles  $N_T$ . If the second condition is satisfied, the computation of the trajectory for the neutron is terminated and a unit is added to the counter of the reflected particles  $N_R$ . In the third case it is necessary to establish if the neutron will be absorbed, or if it will undergo one more elastic scattering event. Another random number  $\gamma$  is then sorted out and the condition

$$\gamma < \frac{\Lambda}{\lambda_a} \quad (18)$$

is checked.

If the above inequality is satisfied, the neutron is absorbed, the trajectory is terminated and a unit is added to the counter of the absorbed particles  $N_A$ . Otherwise, the neutron has been scattered and equation (15) is used to calculate another scattering angle in the centre-of-mass system. Equation (2) transforms this angle into the laboratory frame system and determines the new direction of the neutron velocity. Since the target nuclei are considered at rest, each elastic collision results in a transfer of kinetic energy to the target and a consequent slowing down of the incident neutrons takes place. For each neutron the slowing down process

continues until it is absorbed or its energy reaches a value comparable with the thermal energy of the moderator (0.025 eV). The simulation continues until a statistically significant number of absorbed, transmitted and reflected neutrons is reached.

#### 4. Simulation results

The simulation has been performed for three different materials: water (H<sub>2</sub>O), heavy water (D<sub>2</sub>O) and graphite. In order to determine the mean free path values equations (7) and (4) can be used. However, the cross section values obtained using the geometric cross-sectional area of the involved atomic nuclei are generally small, of the order of 5 to 10 barns. These values are in agreement with those obtained experimentally or using a more accurate model (within the framework of the nuclear quantum theory), only at high energies or for massive nuclei (see any textbook of nuclear physics [11, 12]). Moreover, neutron elastic, inelastic and absorption cross sections exhibit resonance peaks for particular values of the energy; besides the values of the cross sections are inversely proportional to the velocity.

Since we want just to give a hint of the educational usefulness of this method we assume that the cross sections of interest are constant and we use the averaged values of the elastic scattering and absorption free paths taken from [11]. They are  $\lambda_c = 1.1$  cm for water,  $\lambda_c = 2.6$  cm for heavy water and  $\lambda_c = 2.6$  cm for graphite. For the absorption free paths we have used  $\lambda_a = 170$  cm for water,  $\lambda_a = 34977$  cm for heavy water and  $\lambda_a = 3854$  cm for graphite. All values are assumed to be independent of the neutron energy. In the simulation we follow the history of  $10^4$  neutrons and assume an initial neutron energy of 1 MeV.

Figure 2 reports the transmission, reflection and absorption probabilities as a function of the slab's thickness  $d$  for the three materials considered. For all the materials, the reflection and the absorption probabilities increase with the increase of the slab's thickness, while the transmission probabilities decrease. For large values of  $d$  the reflection and absorption probabilities saturate while the transmission probability goes to zero.

For graphite the absorption probability goes to zero and the transmission and reflection probabilities become equal to 0.5 for  $d \simeq 4$  cm. This indicates that graphite may be used as a good moderator because the neutrons can easily thermalize without being absorbed.

A different behaviour is obtained for water: the absorption probability for  $d > 2$  cm becomes much larger than the transmission and the reflection probabilities and, for large values of  $d$ , the neutrons are either reflected or absorbed.

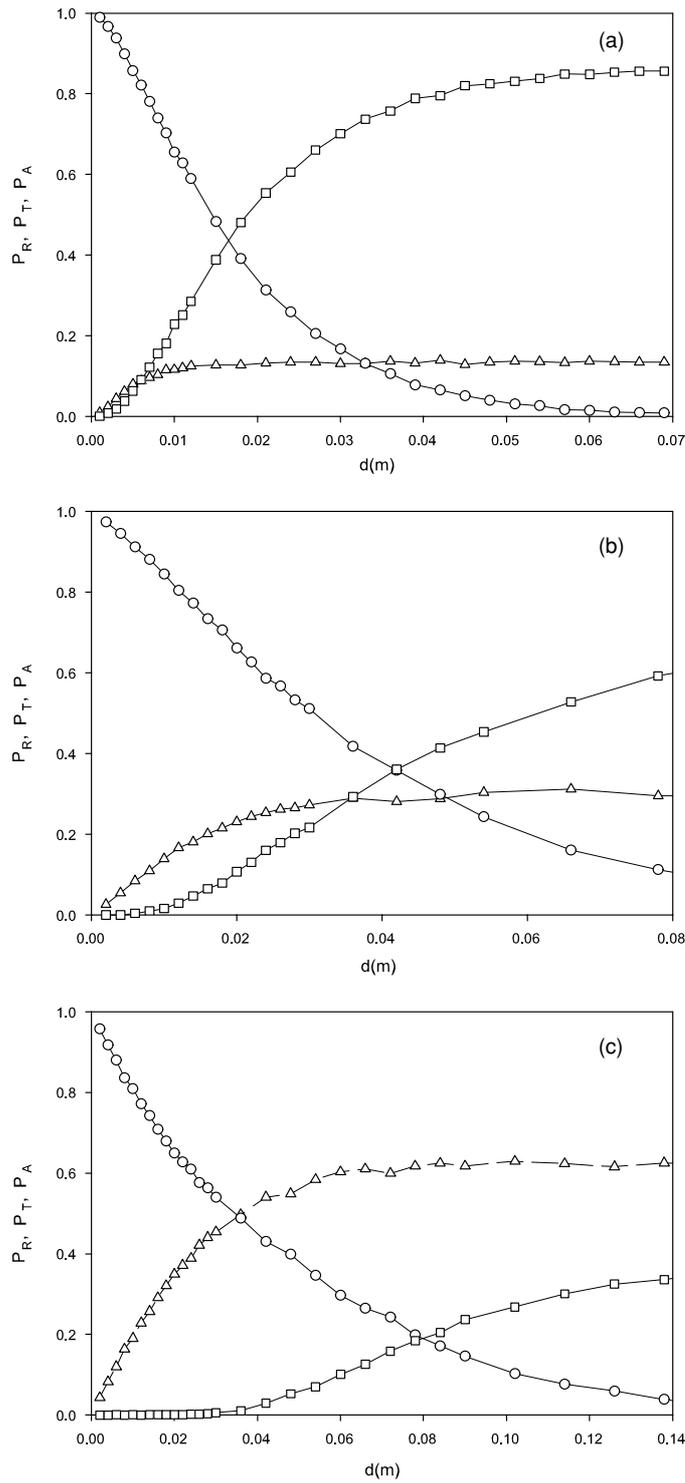
For heavy water the absorption probability is not as low as for graphite, but due to the smaller mass of the deuterium nucleus (see equation (1)), the collisions are more efficient and fewer collisions are necessary to thermalize the neutrons; consequently, heavy water can also be used as a moderator.

The transmission, reflection and absorption probabilities, as said before, depend both on the microscopic properties and on the geometry of the moderating material. In order to obtain an analytical expression for the transmission probability as a function of the slab thickness an easy procedure could be the following: given the flux density  $N_0$  of neutrons impinging on the target and the layer thickness  $d$ , at a depth  $x$  from the surface, the variation of the flux can be represented as

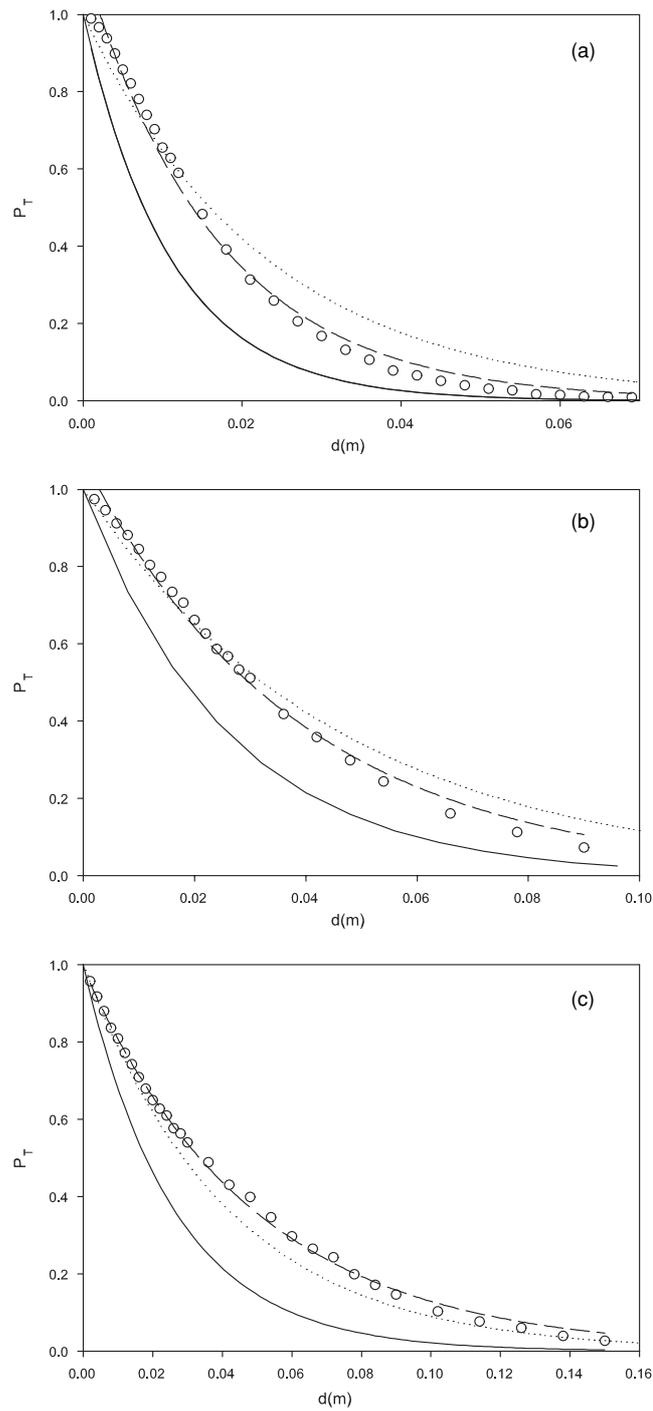
$$dN = -N(x)n\sigma_T dx \quad (19)$$

where  $n$  is the material density and  $\sigma_T$  is the total cross section. By integrating the above equation, the number of neutrons reaching the target layer at the depth  $x$  results in

$$N(x) = N_0 \exp(-\Lambda x) \quad (20)$$



**Figure 2.** Transmission ( $\circ$ ), reflection ( $\Delta$ ) and absorption ( $\square$ ) probabilities as a function of the slab's thickness  $d$  for three different materials: water (a), heavy water (b) and graphite (c).



**Figure 3.** Transmission probability obtained from the numerical Monte Carlo simulation ( $\odot$ ) as a function of the slab's thickness  $d$  where (---) is the best exponential fitting. The full curve (—) is obtained using equation (21) with the 'exact' total mean free path  $\Lambda$ . The dotted curve ( $\cdots$ ) is obtained using equation (21) with the 'empirical' value  $\Lambda_M$  (equation (22)). The plots are for the three different materials: water (a), heavy water (b) and graphite (c).

where  $\Lambda$  is the total mean free path for absorption and for elastic scattering given by equation (7). The transmission probability as a function of  $d$  will result in

$$P_T(d) = \frac{N(d)}{N} = \exp(-\Lambda d). \quad (21)$$

In figure 3 we compare the transmission probability obtained from the numerical Monte Carlo simulation with the expression given in equation (21) for the three different materials (solid curve). It is clear that the agreement is very poor. Then, the simulation data have been fitted with an exponential function  $P_T = a \exp(-bx)$  where the parameter  $b$  is related to an effective mean free path  $\Lambda_e = 1/b$  (dashed curve). The best fitting gives the following values for  $\Lambda_e = 1/b$ : for water  $\Lambda_e = 1.7$  cm, for heavy water  $\Lambda_e = 3.9$  cm and for graphite  $\Lambda_e = 4.9$  cm. These values are larger than those used in the simulation. The reason is that in deriving equation (21) we have assumed that the neutron disappears from the incident beam after the first collision while the simulation shows that, on average, the neutrons undergo several collisions before they are transmitted, reflected or absorbed.

A better agreement (dotted curve) with the simulation results is obtained if, in equation (21), we replace the total mean free path  $\Lambda$  with a different value  $\Lambda_M$  that takes into account the fact that the neutrons are removed from the incident beam only after several collisions. An empirical value of  $\Lambda_M$  is obtained by averaging, over a large number of neutrons, the sum of the different forward free paths covered by each neutron before undergoing the first backward scattering or absorption.

$$\Lambda_M = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^{N_i} \Lambda_{i,j} \quad (22)$$

where  $N_i$  is the number of collisions that the  $i$ th neutron undergoes before the first backward or absorption collision and  $\Lambda_{i,j}$  is the  $j$ th free path of the  $i$ th neutron. The different values of  $\Lambda_M$  are found following the evolution of  $10^4$  neutrons in a slab of infinite thickness. We have found  $\Lambda_M = 2.3$  cm for water,  $\Lambda_M = 4.6$  cm for heavy water and  $\Lambda_M = 4.1$  cm for graphite.

For water and heavy water the agreement is good only for small values of  $d$ . A better agreement is obtained for heavy water ( $d < 3$  cm) than for water ( $d < 1.5$  cm), while for graphite the agreement is quite good for small and also for large values of  $d$  ( $d < 2$  cm,  $d > 12$  cm).

The agreement for low values of  $d$  may be easily understood as due to the fact that, once a backward collision occurs, the chance that the neutron is reflected is very high. The agreement at high values of  $d$  for graphite is mainly due to the fact that the collisions at large angles are more likely with the increase of the target mass. Moreover, once a backward scattering has occurred, the probability that the neutrons, after several scattering events, will be again aligned in a given forward direction (allowing the transmission or the reflection) becomes very low: then the neutrons become trapped and will sooner or later be absorbed.

## 5. Conclusions

We have presented a simple application of the Monte Carlo method to the computation of the transmission, reflection and absorption probabilities of a monoenergetic beam of neutrons incident on a slab of moderating materials. The transmission, reflection and absorption properties of the neutrons interacting with slabs of different moderating materials have been obtained. The results show that for each material, the transmission, reflection and absorption probabilities change with the increase of slab width and the changes depend upon the microscopic properties. We have shown the necessity of using a Monte Carlo method to get

information on the behaviour of the quantities of interest as a function of the slab thickness  $d$ . In fact, due to the inclusion of two different scattering processes such as the elastic and absorption ones, the neutrons will undergo a random number of elastic collisions before being absorbed. Then, in principle, it is possible to find, for the transmission probability, an analytical solution of the rate equation (19) as that given in equation (21) that fits well the simulation results. Analytical solutions, showing the expected decrease in the transmission probability as function of  $d$ , are instead easily obtained in the cases when, at each scattering event, a particle is removed from the incident beam. This happens, for example, in the absorption of a radiation beam from a material slab or in our problem if we consider, in the simulation, only the absorption process. We have shown that we can keep using the solution (21) of the rate equation only if we adopt an empirical value of the mean free path that takes into account the possibility for the neutron to undergo several elastic scatterings before being absorbed.

This is the first step of our research project aimed at the application of the Monte Carlo method to problems of nuclear physics suitable for students of master courses as well as at undergraduate level. Moreover, this method has revealed a particular efficacy in improving understanding of the statistical properties of many particle systems by students of our physics courses.

## Appendix

The probability density function  $\rho(x)$  of a given random variable  $x$ , defined in the interval  $(a, b)$ , is obtained from the definition of the probability  $P$  that the value of  $x$  falls inside the interval  $(a', b')$  as

$$P(a' < x < b') = \int_{a'}^{b'} \rho(x) dx. \quad (\text{A.1})$$

The probability density function  $\rho(x)$  must satisfy the normalization condition

$$\int_a^b \rho(x) dx = 1. \quad (\text{A.2})$$

The expected value (mean value) of the random variable  $x$  is then obtained as

$$\bar{x} = \int_a^b x\rho(x) dx. \quad (\text{A.3})$$

First we derive the probability density function related to the time of flight  $t$ , i.e. the time interval between two next collisions. The time  $t$  can be divided into  $n$  small intervals. Using equation (4) we obtain the average time interval between two next collisions in terms of the total cross section and the nuclei density as

$$\delta t_1, \delta t_2, \delta t_3, \dots, \delta t_n. \quad (\text{A.4})$$

If  $w\delta t_i$  is the probability that the neutron undergoes a collision in the time interval  $\delta t_i$  the probability that it will not undergo a collision in the time interval  $\delta t_i$  will be

$$1 - w\delta t_i. \quad (\text{A.5})$$

The probability that the neutron will not collide during the total time of flight will be

$$S(t) = \prod_{i=1}^n (1 - w\delta t_i). \quad (\text{A.6})$$

Taking the logarithm of the above expression

$$\ln\{S(t)\} = \sum_{i=1}^n \ln(1 - w\delta t_i) \quad (\text{A.7})$$

as  $w\delta t_i \ll 1$  we get, for  $n \rightarrow \infty$ ,

$$S(t) = \exp \left\{ - \int_0^t w \, dt' \right\}. \quad (\text{A.8})$$

Since we have assumed that the total probability per unit time  $w$  is constant

$$S(t) = \exp(-wt) \quad (\text{A.9})$$

comparing this expression with (A.1)

$$S(t) = S(0 < t' < t) = \int_0^t \rho(t) \, dt, \quad (\text{A.10})$$

the probability density function related to the time of flight  $t$  will be

$$\rho(t) = w \exp(-wt). \quad (\text{A.11})$$

Consequently, using the relation between the average free path and the average collisions time, the probability density function related to free path  $l$  is

$$\rho(l) = n\sigma \exp(-n\sigma l). \quad (\text{A.12})$$

In order to choose the neutron direction after a collision event it is necessary to know the probability density functions related to the scattering angles  $\theta$  and  $\varphi$ . In the centre-of-mass frame the scattering can be assumed isotropic. This means that the unit vector  $P(\vartheta, \varphi)$ , indicating the scattering direction, will point uniformly over the surface of a sphere of unit radius. Denoting by  $\rho(\vartheta, \varphi)$  the density of the random point  $P(\vartheta, \varphi)$ , the probability of finding  $P$  in any element of surface  $dS = \sin \vartheta \, d\vartheta \, d\varphi$  will be

$$\rho(\vartheta, \varphi) \, d\vartheta \, d\varphi = \frac{dS}{4\pi} \quad (\text{A.13})$$

and

$$\rho(\vartheta, \varphi) = \frac{\sin \vartheta}{4\pi}. \quad (\text{A.14})$$

$\rho(\vartheta)$  and  $\rho(\varphi)$  are obtained integrating the total density probability  $\rho(\vartheta, \varphi)$  over  $\varphi$  and  $\theta$  respectively

$$\rho(\vartheta) = \int_0^{2\pi} \rho(\vartheta, \varphi) \, d\varphi = \frac{\sin \vartheta}{2} \quad (\text{A.15})$$

and

$$\rho(\varphi) = \int_0^\pi \rho(\vartheta, \varphi) \, d\vartheta = \frac{1}{2\pi}. \quad (\text{A.16})$$

The angle  $\varphi$  is then uniformly distributed in the interval  $(0, 2\pi)$ . Moreover, since  $\rho(\vartheta, \varphi) = \rho(\vartheta)\rho(\varphi)$ , the choice of the variables  $\theta$  and  $\varphi$  will be independent.

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