EUR 309.e

EUROPEAN ATOMIC ENERGY COMMUNITY - EURATOM

MONTE CARLO CALCULATION OF THE NUCLEAR TEMPERATURE COEFFICIENT IN FAST REACTORS

by

W. MATTHES

1963

Joint Nuclear Research Center
Ispra Establishment - Italy
Applied Mathematical Physics Service

Paper presented at the third Symposium "Reactor Theory"
organized by the Deutsches Atomforum e.V., Bad Nauheim (Germany)
2. - 4. April 1963

LEGAL NOTICE

This document was prepared under the sponsorship of the Commission of the European Atomic Energy Community (EURATOM).

Neither the EURATOM Commission, its contractors nor any person acting on their behalf :

1° — Make any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this document, or that the use of any information, apparatus, method, or process disclosed in this document may not infringe privately owned rights ; or

2° — Assume any liability with respect to the use of, or for damages resulting from the use of any information, apparatus, method or process disclosed in this document.

This report can be obtained, at the price of Belgian Francs 50,—, from : PRESSES ACADEMIQUES EUROPEENNES — 98, Chaussée de Charleroi, Brussels 6.

Please remit payments :

— to BANQUE DE LA SOCIETE GENERALE (Agence Ma Campagne) — Brussels — account No 964.558,

— to BELGIAN AMERICAN BANK AND TRUST COMPANY — New York — account No 121.86,

— to LLOYDS BANK (Foreign) Ltd. — 10 Moorgate, London E.C.2,

giving the reference : « EUR 309 . e — Monte Carlo calculation of the nuclear temperature coefficient in fast reactors ».

Printed by L. VANMELLE S.A., Ghent
Brussels, May 1963

E U R 3 0 9 . e

MONTE CARLO CALCULATION OF THE NUCLEAR TEMPERATURE COEFFICIENT IN FAST REACTORS
by W. MATTHES

European Atomic Energy Community — EURATOM
Joint Nuclear Research Center — Ispra Establishment (Italy)
Applied Mathematical Physics Service
Paper presented at the third Symposium « Reactor Theory »
organized by the Deutsches Atomforum e.V.,
Bad Nauheim (Germany) 2. - 4. April 1963
Brussels, May 1963 — pages 28

In this report we describe a Monte Carlo program for the calculation of the nuclear temperature coefficient for fast reactors. The special difficulties for this problem are the energy and space dependence of the cross sections and the calculation of differential effects. These difficulties are discussed in detail and the way for their solution chosen in this program is described.

A second report will contain the results of the numerical calculations and their interpretation.

E U R 3 0 9 . e

MONTE CARLO CALCULATION OF THE NUCLEAR TEMPERATURE COEFFICIENT IN FAST REACTORS
by W. MATTHES

European Atomic Energy Community — EURATOM
Joint Nuclear Research Center — Ispra Establishment (Italy)
Applied Mathematical Physics Service
Paper presented at the third Symposium « Reactor Theory »
organized by the Deutsches Atomforum e.V.,
Bad Nauheim (Germany) 2. - 4. April 1963
Brussels, May 1963 — pages 28

In this report we describe a Monte Carlo program for the calculation of the nuclear temperature coefficient for fast reactors. The special difficulties for this problem are the energy and space dependence of the cross sections and the calculation of differential effects. These difficulties are discussed in detail and the way for their solution chosen in this program is described.

A second report will contain the results of the numerical calculations and their interpretation.

EUR 309.e

EUROPEAN ATOMIC ENERGY COMMUNITY - EURATOM

MONTE CARLO CALCULATION OF THE NUCLEAR TEMPERATURE COEFFICIENT IN FAST REACTORS

by

W. MATTHES

1963

Joint Nuclear Research Center
Ispra Establishment - Italy
Applied Mathematical Physics Service

Paper presented at the third Symposium "Reactor Theory"
organized by the Deutsches Atomforum e.V., Bad Nauheim (Germany)
2. - 4. April 1963

C O N T E N T S

MONTE CARLO CALCULATION OF THE NUCLEAR TEMPERATURE COEFFICIENT IN FAST REACTORS

SUMMARY

In this report we describe a Monte Carlo program for the calculation of the nuclear temperature coefficient for fast reactors. The special difficulties for this problem are the energy and space dependence of the cross sections and the calculation of differential effects. These difficulties are discussed in detail and the way for their solution chosen in this program is described.

A second report will contain the results of the numerical calculations and their interpretation.

A. Statement of the problem

We want to calculate the nuclear temperature coefficient of a fast reactor with the Monte Carlo method. The reactor considered consists of thin fuel needles (about 3 mm diameter) arranged in a square lattice (lattice pitch about 4 mm) cooled with sodium. The temperature distribution in a fuel element has approximately a parabolic shape (e.g. 500°C at the surface, 1000°C in the center of the fuel element). A small variation of this temperature distribution gives rise to a change in the multiplication factor of the reactor. We try to find some information about the relation connecting a change in the temperature distribution with the corresponding change in the multiplication factor.

To express this problem suitable for Monte Carlo calculation we proceed as follows : let N fission neutrons start in the reactor. During moderation some of these N fission neutrons get absorbed and others generate new fission neutrons. Divide the energy axis in small energy intervals ΔE_i and denote by N_i the number of fission neutrons produced in the energy interval ΔE_i. The sum $\sum_i N_i$ gives us the total number of fission neutrons produced, where the summation has to be extended over all energy intervals. The multiplication factor is then defined by :

$$K = \frac{1}{N} \sum_i N_i$$

If we change the temperature distribution and we let again start N fission neutrons we shall get another value for the multiplication factor : $K' = \left\{1/N\right\} \sum_i N_i'$. The change in K is then given by :

$$\Delta K = K' - K = \left\{1/N\right\} \sum_i (N_i' - N_i) = \left\{1/N\right\} \sum_i \Delta N_i$$

It turns out (1) that we have an appreciable change ΔN_i only in an energy range below some value E_o. So the summation in ΔK needs only to be extended over the energy intervals below E_o. Thus we can write :

$$\Delta K = \frac{1}{N} \sum_{E_i \leq E_o} \Delta N_i = \left(\frac{N_o}{N}\right) \frac{1}{N_o} \sum_{E_i \leq E_o} \Delta N_i$$

where we introduced the number of neutrons N_o slowing down below E_o. This expression tells us how to proceed for the calculation of ΔK :

S1) Let N fission neutrons start and calculate the number N_o of these neutrons which slow down below E_o (this gives us the factor N_o/N).

S2) Let N_o neutrons start with an energy within a collision interval around E_o and follow these neutrons through moderation counting hereby the produced fission neutrons.

S3) Change temperature distribution and

S4) Do the same as in S2) for the changed temperature distribution.

The calculation of the quantity (N_o/N) of S1) is straightforward adn a description of the program for doing this will not be given here. So we take the necessary probability for a fission neutron to slow below E_o ($S = N_o/N$) as given and turn to the study of how to performp the remaining statements S2, S3 and S4.

B. Specific difficulties of the program

We consider first the specific difficulties of our program which are common to the three subprograms S2, S3 and S4.

α) Energy dependence of the cross sections

Fundamental for all Monte Carlo applications in neutron physics is the knowledge of the cross sections. In our case (energy range below E_o, about 50 Kev) we are in the unluchy situation that we have only a statistical description of the behaviour of the cross section. This means that all the resonance parameters, necessary to calculate the (Breit-Wigner) shape of the cross-section curves are distributed according to distribution functions. We have to choose from these distribution functions for a special resonance :

1) the position E_r
2) the spin of the compound nucleus J
3) the width Γ_x for the reaction (n,x) (γ-absorption, fission, inelastic scattering, resonance scattering).

β) Space dependence of the cross sections

Let us decide for a set of values for the quantities E_r, J, Γ_x. Then we can calculate the cross section near the resonance out of the Breit-Wigner formulas if we know the temperature T of the material. Provided with this information we can calculate the probabilities for the different kinds of reactions at a collision point. But as stated in section A we have a spatial temperature distribution in the fuel element and this results in a spatial dependence of the cross sections.

γ) Differential effects

If we take for the moment the problems mentioned under α) and β) to be solved, we are still confronted with another difficulty inherent to our program :

The calculation of the multiplication factor K can now be done. The value of K is provided with a statistical error. We only can say that the real value of the multiplication factor lies in a small interval δK around K : $K \pm \delta K$.

If we make next the calculation of the multiplication factor for the changed temperature distribution we shall find another value K'. This value K' will usually lie in the range $K \pm \delta K$ so that we may not simply perform the difference K' - K to find the real value of K. These unavoidable statistical fluctuations of results in Monte Carlo calculations force us therefore to invent a special method for the calculation of differential effects.

C. Energy dependence of the cross sections

We take the cross section in the neighbourhood of the resonance energy E_r of a compound nucleus of total spin J to be described by the doppler-broadened Breit-Wigner formula. The cross section for the reaction (n,x) is then given by :

$$\sigma(n,x) = \sigma_{0c} \frac{\Gamma_x}{\Gamma} \phi$$

and for the different parts of the scattering cross section

$$\sigma(n,n) = \sigma_{Reo} + \sigma_{Int} + \sigma_{Pot}$$

we have

$$\sigma_{Reo} = \sigma_{0c} \frac{A}{\Gamma \Gamma_n} \phi$$

(we include only neutrons with orbital angular momenta $\ell = 0, 1$)

$$\sigma_{Int} = \sigma_{oe} \frac{2}{\Gamma_n} \{ B\psi - C\phi \}$$

$$\sigma_{Pol} = \sum_{\ell=0}^{\infty} 4\pi\lambda^2 (2\ell+1) \sin^2\delta_\ell = \frac{2601.5507}{E[Kev]} \{ \sin^2\delta_0 + 3\sin^2\delta_1 \}$$

with :

$$\Gamma_n = \sum_{\ell,j} \Gamma_{n\ell j}$$

$$\Gamma = \Gamma_{Rn} + \Gamma_\gamma + \Gamma_n$$

$$\sum_{\ell,j} = \sum_{\ell=|J-\frac{1}{2}|}^{J+\frac{1}{2}} \sum_{s=|J-I|}^{J+I}$$

$$A = \sum_{\ell,j} \Gamma_{n\ell j}^2$$

(I = spin of the target nucleus)

$$B = \sum_{\ell,j} \Gamma_{n\ell j} \sin\delta_\ell \cos\delta_\ell$$

$$C = \sum_{\ell,j} \Gamma_{n\ell j} \sin^2\delta_\ell$$

$$\sigma_{oe} = 4\pi\lambda^2 \frac{(2J+1)}{2(2I+1)} \frac{\Gamma_n}{\Gamma} = \frac{2601.5507}{E[Kev]} \cdot \frac{2J+1}{2(2I+1)} \cdot \frac{\Gamma_n}{\Gamma} \quad [6]$$

The functions ϕ and ψ are given by

$$\phi = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{+\infty} e^{-(q-x)^2/4t} \frac{1}{1+x^2} dx$$

$$\psi = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{+\infty} e^{-(q-x)^2/4t} \frac{x}{1+x^2} dx$$

$$q = \frac{E - E_R}{\Gamma/2}$$

$$t = \frac{4kT E_R}{A \Gamma^2}$$

$$= \frac{0.3446 \cdot T[^\circ K] E_R[KeV]}{A \Gamma^2[eV]}$$

and are transformed with x = tg z into :

$$\phi = \frac{1}{\sqrt{4\pi t}} \int_0^{\pi/2} \left\{ e^{-(y z - q)^2/4t} + e^{-(y z + q)^2/4t} \right\} dz$$

$$\psi = \frac{1}{\sqrt{4\pi t}} \int_0^{\pi/2} \left\{ e^{-(y z - q)^2/4t} - e^{-(y z + q)^2/4t} \right\} \lg z \, dz$$

for numerical integration with Simpson's Rule.

In appendix 1 we give a simple derivation for the Breit-Wigner formulas as used in our program.

The $\Gamma_{nej}(J, E_r)$ are calculated in the simplified theory of Blatt-Weisskopf. So we put :

$$\Gamma_{nej}(E_r, J) = \sqrt{E[eV]}\; v_l\; \Gamma_n^0(J, E_r)$$

and take the Γ_{nej} to be independent of j.

For v_l we need only the values for l = 0 and l = 1.

$$v_0 = 1$$

$$v_1 = \frac{k^2 R^2}{1 + k^2 R^2} \qquad k = \frac{1}{\lambda}, \; R = \text{nuclear radius}$$

The δ_l are given for l = 0, 1 by : $\delta_0 = kR$

$$\delta_1 = kR - \operatorname{arc\,tg} kR$$

So far we have only collected the necessary formulas used in the program. The next task is to fix the values for all the parameters. This is now the point where we have to enter statistics. Without going into the theory of the statistical distribution functions for the nuclear parameters (2), we show what calculations are done for the program.

The reduced neutron width Γ_n^0 is picked out of a chisquare distribution (see appendix 2) with one degree of freedom and the mean value :

$$\langle \Gamma_n^0(J, E_r) \rangle = 10^{-4} \langle S \rangle_{J, E_r}$$

with $\langle S \rangle$ as the mean level spacing for a compound nucleus of total spin J in the energy range of E_r. The energy and spin dependence of $\langle S \rangle$ is taken from (2).

The Γ_γ width's are assumed to be independent fo E_r and J and are taken to be 0.033 [ev] for U235 and 0.028 [ev] for U238.

The Γ_f width is assumed to be independent of J for U235 and zero in the energy range considered for U238. The energy dependence of Γ_f for U235 is taken from (2).

The position of the resonance energy E_r nearest to the neutron energy is found in the following way :

The distance S between two neighbouring resonances is distributed according to a chisquare distribution with a certain number ν of degree of freedom and certain mean value $\langle S \rangle$. (ν = 8 for U235, ν = 10 for U238, the energy dependence of $\langle S \rangle_E$ is taken from (2)). So we pick a value S out of the corresponding distribution function (for U235 resp. U238) and identify the point ξS on S with E, where ξ is a random number uniformly distributed between 0 and 1.

Then we make the assumption that only the resonance nearest to E is responsible for the cross sections for the energy E. So we neglect the overlapping of two or more resonances.

Once the position of the resonance is fixed, we have to determine the spin J of the compound nucleus.

This is done by the assumption that the total level structure is a random superposition of the levels due to the different J's. So the total level density w is given by :

$$w = \sum_J w_J$$

The additional assumption that w_J is proportional to $(2J + 1)$ gives us the distribution function for the values of J by : $1 = \sum p(J)$ with $p(J) = (2J + 1) / \sum_K (2K + 1)$.

Now we are provided with all the details to calculate the cross section. Actually we proceed as follows:

1) choose the position of the nearest resonance for the different isotopes present (U235 and U238 in this case)
2) choose the spin J of the compound nucleus
3) choose $\Gamma_n^0(J, E_r)$
4) calculate the parameters for the cross sections and the cross sections themselves.

D. Space dependence of the cross sections

The Breit-Wigner formula tells us that we have with increasing temperature a decrease of the cross section in the center of the resonance and an increase of the cross section in the wings of the resonance shape. Now remember that we have a parabolic shape of the temperature distribution inside a fuel rod. So if we move from the surface towards the center of the rod we have an increase of temperature and therefore an increase (or decrease) of the cross section. This leads

us to the assumption that we could approximate the real spatial dependence of the cross section also by a parabolic shape. This assumption opens the possibility to treat the travelling of neutrons inside a rod to a good deal by analytical methods. We put :

$$\Sigma(\rho) = a\rho^2 + b$$

where ρ is the distance of the point in question from the axis of the rod. The constants a and b are found by putting $\rho = 0$ (center of the rod) resp. $\rho = R$ (surface of the rod) to be :

$$b = \Sigma(0) \; ; \quad a = [\Sigma(R) - \Sigma(0)] / R^2$$

Now consider a neutron flying in the rod. Let the neutron start from the point κ_0 (in the rod) in the direction ν. The number M(S) of mean free path's necessary for the neutron to pass the geometrical distance s is defined by :

$$M(s) = \int_0^s \Sigma(\kappa_0 + \nu t)\, dt$$

We denote the projection of the point $(\kappa_0 + \nu t)$ in the X-Y plane by $(\kappa_0' + \nu' t')$ and write the integral :

$$M(s) = \int_0^s \Sigma(\kappa_0' + \nu' t')\, dt = \int_0^s [a(\kappa_0' + \nu' t')^2 + b]\, dt$$

If we normalize ν' to unity : $\nu'^2 = 1$, we can use the relations

$$(\nu\nu') = \sin T \; ; \quad s \sin T = s' \; ; \quad t \sin T = t'$$

and transform the integral once more to :

$$M(s) = \int_0^{s'} [a(\kappa_0' + \nu' t')^2 + b]\, dt' / \sin T$$

Evaluation of the integral gives :

$$M(s) = \alpha s^3 + \beta s^2 + \gamma s$$

with :

$$\alpha = a \sin^2 \tau / 3$$
$$\beta = a \sin \tau \, (r_0' w)$$
$$\gamma = a r_0'^2 + b$$

The application of this result in the Monte Carlo program goes as follows (see fig. 1 for geometrical visualization) :

A neutron starts from the point r_0 (inside the rod) in the direction w. We give the neutron a number of mean free path, let us say λ, and we look where the neutron makes its next collision. To find this next collision-point we first calculate the distance D from the starting point up to the crossing point of the flying line (in the direction w) with the surface of the rod. To travel this distance the neutron would need M(D) mean free paths. If this number of mean free path M(D) necessary to leave the rod is smaller than the number of mean free path λ given, the neutron leaves the rod and continues its flight outside the rod and has yet still λ - M(D) mean free paths available.

But if $M(D) > \lambda$, then the neutron makes its next collision inside the fuel rod and we have to find the geometrical distance s from the starting point to the collision point (in the direction w) out of the equation :

$$M(s) = \lambda$$

This equation is solved upon s within the program by an iteration method. If s is found out of this equation then the collision point is determined by :

$$\vec{r} = \vec{r}_0 + \vec{m} s$$

E. Differential effects

The fundamental ideas leading to a solution of this problem are well described in the article about Monte Carlo methods by H. Kalos and Goertzl (3). But for convenience we would like to explain the situation for our special case. We remember that we have to follow N_o fission neutrons through their life and to compute the multiplication factor K. Then we have to change the temperature distribution somewhat and to calculate K again to find another value, for instance K', which can lie within the range of the statistical error of K. How does this statistical error arise and what can we do about it when concentrating on differential effects ?

Let us picture the life of one fission neutron in phase space. We obtain a certain path L in this space. Under all possible pathes this one selected path L appears with a probability P(L). If we denote by K(L) the value for the multiplication factor found in the Monte Carlo calculation for this path, then the mean value for K can be expressed by :

$$\bar{K} = \sum_i P(L_i)\, K(L_i)$$

where we have to sum over all possible pathes consistent with the physical situation.

In the actual calculation we sum only over N_o pathes picked out of the distribution P(L). This finite sampling procedure is the reason for the fluctuations of the calculated quantity K.

If we now change the physical situation somewhat (by changing for instance the temperature distribution) we find a changed probability distribution for the pathes L. The expression for the multiplication factor K (mean value) reads now :

$$\overline{K'} = \sum_i P'(L_i)\, K'(L_i)$$

We have for the difference :

$$\Delta\overline{K} = \sum_i P'(L_i) K'(L_i) - \sum_\ell P(L_\ell) K(L_\ell) \qquad (A)$$

which can be written :

$$\Delta\overline{K} = \sum_i P(L_i) \left\{ \frac{P'(L_i)}{P(L_i)} K'(L_i) - K(L_i) \right\}$$

As we can only average over a finite set of neutron pathes, we have two possibilities to calculate ΔK, according to formula A or B.

Formula A means : α) pick N pathes out of $P'(L)$ and form $\overline{K'}$

β) pick N pathes out of P(L) and form $\overline{K}$

γ) subtract $\overline{K'} - \overline{K}$ to obtain $\Delta\overline{K}$

Formula B means : pick N pathes out of P(L) and form

$$\overline{\frac{P'}{P} K' - K}$$

For an infinite set of pathes (A) and (B) would naturally give the same result. This is no more valid for a finite N but in this case we get a smaller variance for $\Delta\overline{K}$ if we sample due to the scheme of formula B.

So we follow formula (B) and play the game dictated by P(L) for the unchanged situation. This means in our case that we have to take the same set of neutron pathes in geometrical space for the unchanged and changed reactor. If we do so, we sample with a wrong distribution function for the collision points in the changed case. To correct for this we must modify the weight of the neutron between two collisions in the changed reactor. This modification of the weight is expressed by the factor P'/P in formula (B). The correction factor can easily be determined.

Consider N neutrons starting at r_0 in the direction ω. In the unchanged case (index zero)

$$N_0 = N\, e^{-\tau_0(r_0,s)}\, \Sigma_0(r_0+\omega s)\, ds$$

neutrons would make the first collision in ds, where

$$\tau(r_0,s) = \int_0^s \Sigma(r_0+\omega t)\, dt =$$

number of mean free paths necessary to reach the point $r = r_0 + \omega s$. In the changed case (index one) we would have

$$N_1 = N\, e^{-\tau_1(r_0,s)}\, \Sigma_1(r_0,s)\, ds$$

collisions in ds.

If we sample in the changed case with the distribution function for the unchanged case we would have N_o collisions instead of N_1. So we provide each incoming neutron with a weight g in such a way that : $N_o \cdot g = N_1$ which gives us :

$$g = e^{-[\tau_1(x_0,s) - \tau_0(x_0,s)]} \frac{I_1}{I_0} = e^{-\Delta\tau} \left(\frac{I_1}{I_0}\right)_{\text{at the collision point.}}$$

As we have no change of the number of mean free path in the moderator, we have

$$\Delta\tau = \sum_i \left[M_1(s_i) - M_0(s_i) \right]$$

where we have to sum over all those pieces s_i of the way between two collisions which lie in fuel rods.

The program makes the necessary calculations as follows :

1) two neutrons are started from the same point in the same direction with the same energy and the same weight
2) the next collision is found by picking from the transport kernel for the unchanged case
3) the difference in the number of mean free path for the two cases is calculated
4) the neutron n_0 running for the unchanged case enters the next collision point with the weight as it left the last collision point
5) the neutron n_1 running for the changed case enters the next collision point with the weight as it left the last collision point multiplied with the factor:

$$g = \exp(-\Delta\tau) \cdot (I_1/I_0)_{\text{at the collision point.}}$$

The change of the weight's at the collision point itself is treated according to :

6) the neutron n_0 (entering with W_0) leaves the collision with $w_0 (\Sigma_s/\Sigma_t)_0$ and leaves back the portion $w_0(\Sigma_a/\Sigma_t)_0$ as absorbed weight. The neutron n_1 (entering with W_1) leaves the collision point with $w_1(\Sigma_s/\Sigma_t)_1$ and leaves back the portion $w_1(\Sigma_a/\Sigma_t)_1$ as absorbed weight.

Analogue correction factors, as for the geometrical distribution function, have to be applied as soon as one samples after a wrong distribution function. In our program we made use of this fact when choosing the isotope that scatters the neutron and when terminating the histories by Russian Roulette. In both cases we sample with distribution functions for the unchanged case and correct by weight factors for the changed case.

Appendix 1

Derivation of the Breit-Wigner formulas as used in this report (we neglect parity factors)

Consider a neutron of orbital angular momentum l and spin s (= 1/2) moving towards a target nucleus with spin I. s and I combine to the channel spin S. The energy E of the neutron may lie near an energy value E_r which would lead to a resonance level of the compound nucleus, where this level may belong to a spin J of the compound nucleus. If the two angular momenta l and S add up to J, then the neutron feels the resonance and if they do not add up to J then the neutron does not feel the resonance and makes no resonance reaction. In this case it suffers only potential scattering. We denote the range of l, S values in which they can combine to J by A (see fig. 2). If l and S lie outside of this range, the neutron suffers only potential scattering. Let P(l,S/J) be the probability that the two angular momenta l and S add up to J :

$$P(l,s/J) = P(I,s/S)\,P(l,S/J)$$

$$= \frac{2S+1}{(2s+1)(2I+1)} \cdot \frac{2J+1}{(2l+1)(2S+1)} = \frac{2J+1}{(2l+1)(2s+1)(2I+1)}$$

Let Q(l,S/J) be the probability that the two angular momenta do not add up to J. If $l < \alpha$ (see fig. 2) then

$$Q(l,S/J) = 1 - \sum_S P(l,S/J)$$

If $l \notin \alpha$ then : $Q(\ell, s/J) = 1$

We can now write for the cross sections :

$$\sigma_x(E/J,E_r) = \sum_{\ell,s} P(\ell,s/J)\,\sigma_{Res,x}(E/\ell,s,J,E_r)$$

where $\sigma_{Res,x}$ means resonance cross section for the reaction (n,x)

and for the scattering cross section :

$$\sigma_s(E/J,E_r) = \sum_{\substack{\ell,s\\ \ell',s'}} P(\ell,s/J)\,\sigma_{res,s}(E/\ell,s,J,E_r,\ell',s') + \sum_{\ell,s\subset A} Q(\ell,s/J)\,\sigma_{pot}(E,\ell) + \sum_{\ell\notin A}\sigma_{pot}(\ell)$$

where l' and S' denote the angular momenta of the outgoing channel.

We separate from the scattering cross section the term with l = l' and S = S' because this gives rise to interference scattering and we write :

$$\sigma_s(E/J,E_r) = \sum_{\ell,s} P(\ell,s/J)\,\sigma_{res}(E/\ell,s,J,E_r) + \sum_{(\ell,s)\neq(\ell's')} P(\ell,s/J)\,\sigma_{res}(E/\ell,s,J,E_r,\ell's')$$

$$+ \sum_{\ell,s} Q(\ell,s/J)\,\sigma_{pot}(\ell) + \sum_{\ell\notin A}\sigma_{pot}(\ell)$$

The Breit Wigner formula for the different partial cross sections reads :

$$\sigma_{res,x}(E/\ell,s,J,E_r) = \pi\lambda^2(2\ell+1)\,\frac{\Gamma_n(J,E_r)\,\Gamma_x(\ell,s,J,E_r)}{(E-E_r)^2 + (\frac{1}{2}\Gamma)^2}$$

this holds also for the resonance scattering for the case $(l,S) \neq (l',S')$

$$\sigma_{res,s}(E/\ell,s,J,E_r) = \pi\lambda^2(2\ell+1)\left|\frac{i\,\Gamma_n(\ell,s,J,E_r)}{(E-E_r)+i\,\Gamma/2} + e^{2i\delta_\ell} - 1\right|^2$$

This last term can be evaluated to lead to an additional resonance scattering :

$$\sigma_{res} = \pi \lambda^2 (2l+1) \frac{\Gamma_n^2(l,S,J,E_\nu)}{(E-E_\nu)^2 + (\frac{1}{2}\Gamma)^2}$$

the interference cross section :

$$\sigma_{int} = \pi \lambda^2 (2l+1) 2 \Gamma_n(l,S,J,E_\nu) \left[\frac{2(E-E_\nu)}{(E-E_\nu)^2 + (\Gamma/2)^2} \sin\delta_l \cos\delta_l - \frac{2 \cdot \Gamma/2}{(E-E_\nu)^2 + (\Gamma/2)^2} \sin^2\delta_l \right]$$

and a part of the potential cross section :

$$\sigma_{pot} = 4\pi \lambda^2 (2l+1) \sin^2\delta_l$$

We insert these expressions in our general formula for the scattering cross section and obtain for the first term :

$$\sigma_s = \sum_{l,S} p(l,S/J) \sigma_{res} + \sum_{l,S} p(l,S/J) \sigma_{int} + \sum_{l,S} p(l,S/J) \sigma_{pot} + \cdots$$

Now we remember that :

$$\sum_{l,S} g(l,S/J) \sigma_{pot}(l) = \sum_{l} \left[1 - \sum_{S} p(l,S/J) \right] \sigma_{pot}(l)$$

Inserting this and the explicite expression for P(1,S/J) gives us the following results for the different cross sections :

Resonance reaction cross section :

$$\sigma_x(E/J,E_\nu) = \sum_{l,S} 4\pi \lambda^2 \frac{2J+1}{2(2I+1)} \frac{\Gamma_n(lS/J)}{\Gamma} \frac{\Gamma_x}{\Gamma} \frac{1}{1+x^2}$$

Resonance scattering cross section :

$$\sigma_{scatt} = \sum_{\substack{l,s \\ l',s' \}<A}} 4\pi\lambda^2 \frac{2J+1}{2(2I+1)} \frac{\Gamma_n(l,s,J)}{\Gamma} \frac{\Gamma_n(l',s',J)}{\Gamma} \frac{1}{1+x^2}$$

Interference scattering cross section :

$$\sigma_{int} = \sum_{l,s} 4\pi\lambda^2 \frac{2J+1}{2(2I+1)} \frac{\Gamma_n(l,s,J)}{\Gamma} \left[\frac{2x}{1+x^2} \sin\delta_l \cos\delta_l - \frac{2}{1+x^2} \sin^2\delta_l \right]$$

Potential scattering cross section :

$$\sigma_{pot} = \sum_{l} 4\pi\lambda^2 (2l+1) \sin^2\delta_l \qquad x = \frac{E-E_r}{\Gamma/2}$$

As we restrict ourselves only to values of l = 0,1 we have no transitions of the kind $(l,S) \longrightarrow (l',S')$ with $(l,S \neq l' S')$ because of parity conservation. In this case we need only consider the $(l,S) = (l',S')$ terms in the summation of the resonance scattering cross section.

By introducing

$$\sigma_{oc} = 4\pi\lambda^2 \frac{2J+1}{2(2I+1)} \cdot \frac{\Gamma_n}{\Gamma}$$

with $\Gamma_n = \sum_{l,s} \Gamma_n(l,s)$ we decide for the final formulation :

$$\sigma_x = \sigma_{oc} \frac{\Gamma_x}{\Gamma} \frac{1}{1+x^2}$$

now specializing for the l,S = l',S' term

$$\sigma_{res\,scatt} = \sigma_{oc} \frac{A}{\Gamma\Gamma_n} \frac{1}{1+x^2}$$

$$\sigma_{int} = \sigma_{oc} \frac{2}{\Gamma_n} \left[\frac{x}{1+x^2} B - \frac{1}{1+x^2} C \right]$$

where we have introduced :
(we turn from the summation over l and S to the summation over l and j

$$\sum_{l,S} = \sum_{l=|J-S|}^{J+S} \sum_{S=|I-\frac{1}{2}|}^{I+\frac{1}{2}} \longrightarrow \sum_{l,j} = \sum_{l=|j-\frac{1}{2}|}^{j+\frac{1}{2}} \sum_{j=|J-I|}^{J+I}$$

$$A = \sum_{l,j} T_{lj}^2$$

$$B = \sum_{l,j} T_{lj} \sin\delta_l \cos\delta_l$$

$$C = \sum_{l,j} T_{lj} \sin^2\delta_l$$

As T_{nlj} is independent of j, we have :

$$\sum_{l,j} T_{nlj}^2 = \sum_{l=|j-\frac{1}{2}|}^{j+\frac{1}{2}} T_{nl}^2 \sum_{j=|J-I|}^{J+I}$$

If the summation is extended only up to l = 1, we write :

$$T_n = \alpha T_{n0} + \beta T_{n1}$$

$$A = \alpha T_{n0}^2 + \beta T_{n1}^2$$

$$B = \alpha T_{n0} \sin\delta_0 \cos\delta_0 + \beta T_{n1} \sin\delta_1 \cos\delta_1$$

$$C = \alpha T_{n0} \sin^2\delta_l + \beta T_{n1} \sin^2\delta_1$$

These formulas applied to U235 (I = 7/2) and U238 (I = 0) lead explicitely to the following set of values for the parameters α and β :

U235

J	2	3	4	5
α	0	1	1	0
β	1	2	2	1

U238

J	1/2	3/2
α	1	0
β	1	1

Appendix 2

Chisquare distribution

The chisquare distribution of n degree of freedom and mean value $\langle s \rangle$ is defined by :

$$P_n(s)\,ds = \frac{n}{2^n \langle s \rangle\ \Gamma(\frac{n}{2})} \cdot \left(\frac{n.s}{2.\langle s \rangle} \right)^{\frac{n}{2} - 1} \cdot e^{-\frac{n.s}{2\langle s \rangle}} \cdot ds$$

$P_n(s)\,ds$ is the probability that the random variable s lies in the interval ds around s.

The transformation

$$X = \frac{n.s}{\langle s \rangle}$$

leads to the distribution function for the random variable x :

$$P_n(x)\,dx = \frac{1}{2^{n/2}\ \Gamma(\frac{n}{2})}\ x^{\frac{n}{2} - 1} \cdot e^{-\frac{x\pounds}{2}} \cdot dx$$

We pick a value for the random variable x out of this distribution with the routine described in (2) and find the value for the random variable s through :

$$s = \frac{\langle s \rangle}{n} \cdot x$$

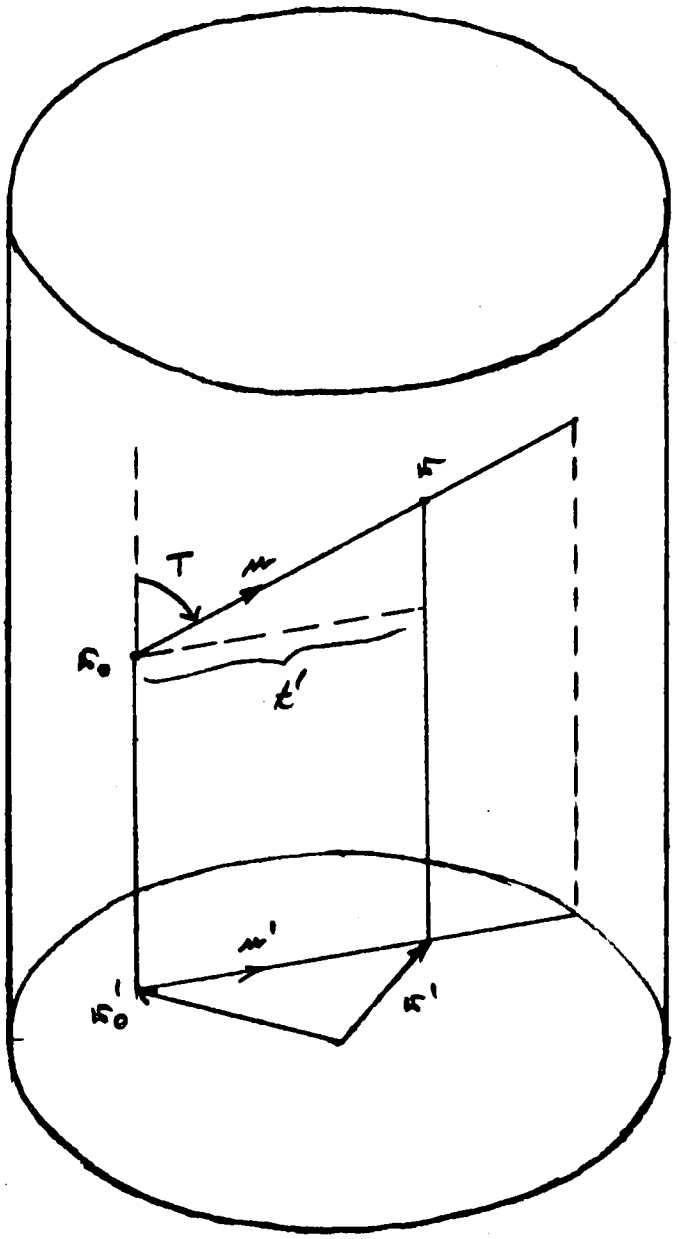
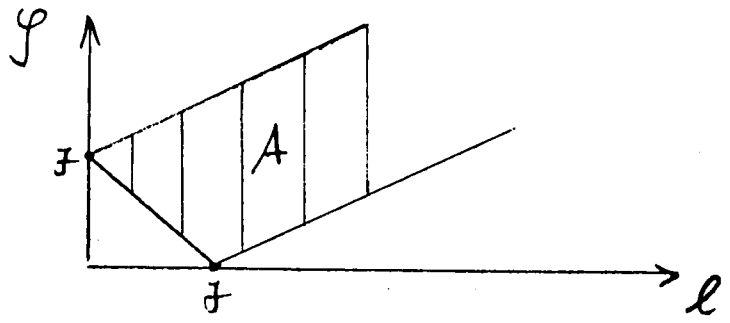


Fig. 1 : geometrical situation for a collision in a fuel rod

Let A be the range in the (l,S) plane, where (l,S) can add up to $\mathcal{J}$



In our case S is bounded between two extreme values $S_{min} = |I-S|$ and $S_{max} = |I+S|$ so that the region A looks like

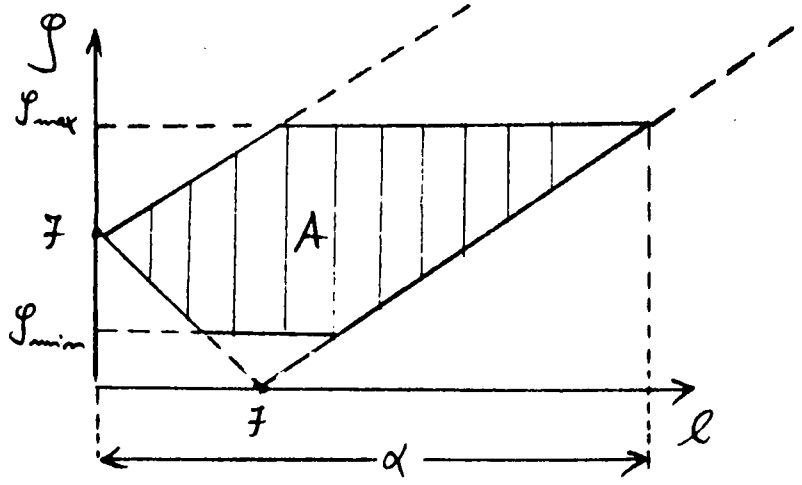


Fig. 2 : geometrical representation for the range A in which l and S can add up to $\mathcal{J}$

Literature

(1) R.B. Nicholson (1960) - The doppler effect in fast reactors, APDA 139

(2) L. Dresner - Resonance absorption of neutrons in nuclear reactors, ORNL-2659

(3) G. Goertzl and M.H. Kalos - Monte Carlo methods in transport problems, Progress in Nuclear Energy, Vol. 2 (1958).

CDNA00309ENC