A GENERALIZATION OF THE LIVOLANT-JEANPIERRE THEORY FOR RESONANCE ABSORPTION CALCULATION

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A GENERALIZATION OF THE LIVOLANT-JEANPIERRE
THEORY FOR RESONANCE ABSORPTION CALCULATION

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ABSTRACT

Because of the large number of heavy nuclide resonances a detailed neutron flux calculation in the epithermal range cannot be made by standard nuclear reactor codes : it would need several tens of thousand of energy points. However, by using pre-calculated effective reaction rates only a few tens of groups are sufficient for accurate spectrum and reaction rate calculations, if a consistent formalism is used. Such a formalism was elaborated in the 1970s by M. Livolant and F. Jeanpierre (L.-J.)[1] for the "one resonant nuclide - one resonant zone" problem, and was implemented in the APOLLO code.[2]

In practical cases there are several resonant nuclides and often resonant zones of different characteristics, e.g. a lattice constituted with different kinds of pins, a lattice with irregular "water-holes", a fuel element with temperature (therefore Doppler effect) gradients,...

Since these problems cannot be correctly treated by APOLLO, a generalization of the formalism was derived. The basic principles were retained, and our aim was to construct an algorithm which would not require too expensive calculations.

After a brief recall of the L.-J. theory, equations for the most general case are presented, somme approximations for practical calculations proposed, and numerical tests on significant examples commented.

L.J. FORMALISM[1,3]

HOMOGENEOUS CASE

Let 0 be the resonant nuclide and 1 the non-resonant nuclide(s). The flux is given by :

$$R_0 \, \phi + R_1 \, \phi = (\Sigma_0 + \Sigma_1) \, \phi \qquad (1)$$

where R is the slowing-down operator, the other notations being as usual. Let

us write :

$$\dot{\phi} = \varphi \, \psi \tag{2}$$

where φ is the fine-structure and ψ the macroscopic (regular) flux. An adequate choice is :

$$\psi = R_1 \, \phi / \Sigma_1 \tag{3}$$

for Σ_1 is pratically constant and R_1 (a long range integral operator) smoothes ϕ. Since 0 has a short range slowing-down the approximation

$$R_0 \, \phi \simeq \psi \, R_0 \, \varphi \tag{4}$$

can be made. Using (2), (3) and (4) in (1) yields the fine structure equation :

$$\frac{1}{N_0} R_0 \, \varphi + \sigma_e = (\sigma_0 + \sigma_e) \, \varphi \tag{5}$$

which depends only on $\sigma_e = \Sigma_1 / N_0$, the constant equivalent cross-section.

It is possible (first step of the calculations) to solve (5) for a few values of σ_e and store the results (effective reaction rates). It is expensive but made only once.

For a new value of σ_e (second step) an interpolation allows to get the effective reaction rates. Re-writing (5) in a (large) multigroup form one can derive the effective cross-sections for the resonant nuclide in such a way that the exact effective reaction rates are obtained in the multigroup form : it is continuous-multigroup equivalence. Finally using these effective cross-sections in (1) re-written in a multigroup form allows to get a very accurate multigroup solution because the equivalence was performed on a fondamental problem (5) very close to the actual problem (1).

HETEROGENEOUS CASE

Let us now suppose that 0 is in the zone 0 and 1 in the zone 1. Using first-collision probabilities the flux is now given by :

$$\left. \begin{array}{l} V_0 \, P_{0C} \, R_0 \, \phi_0 + V_1 \, P_{10} \, R_1 \, \phi_1 = V_0 \, \Sigma_0 \, \phi_0 \\[2mm] V_0 \, P_{01} \, R_0 \, \phi_0 + V_1 \, P_{11} \, R_1 \, \phi_1 = V_1 \, \Sigma_1 \, \phi_1 \end{array} \right\} \, . \tag{6}$$

If we write $\phi_0 = \varphi \, \psi$ and use (3), (4) and take the medium to be perfectly reflected we get again (5) but with :

$$\sigma_e = \frac{1}{N_0} \cdot \frac{\Sigma_0 (1 - P_{00})}{P_{00}} \tag{7}$$

which now depends on Σ_0 and therefore on energy. However σ_e varies only a few percent while Σ_0 varies on several decades (figure) and therefore one can replace σ_e by a constant $\overline{\sigma}_e$, and the preceeding procedure can be applied : interpolation in the stored effective reaction rates, then continuous-multigroup equivalence.

This mean value is generally characterized by the Bell factor $b = \sigma_e / \sigma_{e\infty}$ where $\sigma_{e\infty}$ is the limit value of (7) for large Σ_0. The $\overline{\sigma}_e$ is defined such that

(5) written with the true σ_e and with $\bar{\sigma}_e$ give the same absorption rates : it is the heterogeneous-homogeneous equivalence. Usual approximations such as the narrow resonance assumption, are used to implement this equivalence.

It is easy to show that a more complicated heterogeneous case can be treated similarly as far as there are only one resonant nuclide and one resonant zone.
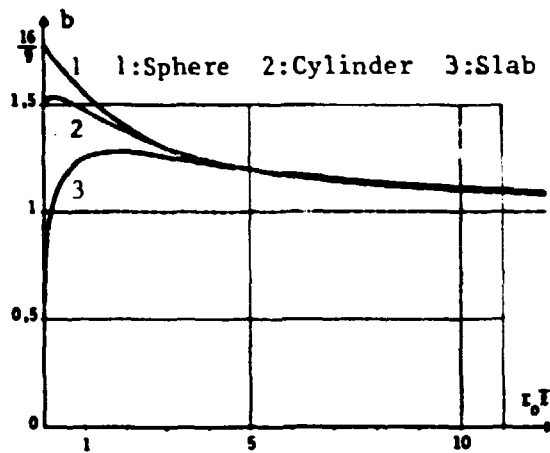
Bell factor as a function of opacity for usual shapes

GENERAL FORMALISM

We now consider a general case with any number of resonant nuclides, non-resonant nuclides and zones (zone : volume small enough for a flat-flux assumption). The subscripts x,y,... stand for the resonant nuclides ; i,j,... for the non-resonant nuclides ; ℓ,m,... for nuclides of any kind. In order to simplify the formalism we put a nuclide subscript for the fluxes, but it is clear that the fluxes are the same for nuclides mixed together in a same zone, and this fact is taken into account in the practical calculations.

MACROSCOPIC FLUXES AND FINE STRUCTURES

The equations to be solved are :

$$\sum_m V_m P_{m\ell} R_m \phi_m = V_\ell \Sigma_\ell \phi_\ell. \tag{8}$$

Here V_ℓ is the volume of the zone containing nuclides ℓ and $P_{m\ell}$ is the first-flight collision probability for neutrons born isotropically and uniformly in volume m to undergo a collision with nuclides ℓ. After use of the reciprocity relation for the $P_{m\ell}$, this equation reads :

$$\sum_m P_{\ell m} \frac{R_m \phi_m}{\Sigma_m} = \phi_\ell. \tag{8a}$$

For the non-resonant nuclides we define the macroscopic fluxes :

$$\psi_i = R_i \phi_i / \Sigma_i \tag{9}$$

Alike the ψ defined by (3) the ψ_i have no fine structure.

To get $\varphi = 1$ between resonances one must define the resonant nuclide macroscopic fluxes by :

$$\sum_y P_{xy} \psi_y + \sum_j P_{xj} \psi_j = \psi_x. \tag{10}$$

We will see later that the ψ_x, also, have no significant fine structure.

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Putting $\phi_x = \varphi_x \psi_x$ and assuming $R_x \phi_x \simeq \psi_x R_x \varphi_x$ we get :

$$\sum_y P_{xy} \psi_y \left(1 - \frac{R_y \varphi_y}{\Sigma_y}\right) = \psi_x (1 - \varphi_x) \qquad (11)$$

Since the slowing-down uniformizes the neutron distributions, the ψ_i and therefore the ψ_x are very close to each other for a given lethargy. Assuming $\psi_x = \psi$ ($\forall x$) we get the fundamental situation :

$$\sum_y P_{xy} \left(1 - \frac{R_y \varphi_y}{\Sigma_y}\right) = 1 - \varphi_x \qquad (12)$$

GENERALIZATION OF THE BELL FACTOR

As in the simple case it is useful to introduce quantities varying slowly with Σ_y. This goal is reached if we define :

$$A_{xy} = \overset{::}{P}_{xy}/\Sigma_y \qquad (13)$$

with

$$\overset{::}{P}_{\ell m} = P_{\ell m} + \sum_y P_{\ell y} \overset{::}{P}_{ym} \qquad (14)$$

$\overset{::}{P}_{\ell m}$ can be interpreted as the collision rate on m for one neutron born in ℓ when absorption by the resonant nuclides is replaced by scattering. $A_{\ell m}$ is the corresponding flux in m : its fine structure is not significant because resonant absorption has been eliminated (a mathematical justification is proposed in the third part).

These quantities allow us to write the solution of (10) as

$$\psi_x = \sum_j \overset{::}{P}_{xj} \psi_j \qquad (15)$$

which shows that indeed the ψ_x have practically no fine structure.

This leads to a new form of the fondamental equations :

$$\sum_y A_{xy} (\Sigma_y \varphi_y - R_y \varphi_y) = 1 - \varphi_x \qquad (16)$$

The A matrix generalizes the equivalent cross-section $\overline{\sigma}_e$: since it varies very little (see numerical examples below), it can be replaced by a constant matrix $\overline{A}$ obtained by a generalized heterogeneous-homogeneous equivalence. We propose in the third part a simple procedure to perform this equivalence easily.

TABULATIONS

The reactions rates for the fondamental problem can be obtained by interpolation in tables. Of course these tables depend on a greater number of parameters than in the L.-J. case, but simplifications can be suggested.

RESOLUTION OF THE ACTUAL PROBLEM

At the present stage we know the reaction rates for the fundamental situation. Thanks to a continuous-multigroup equivalence they can be used as precee-

dingly to get the set of effective cross-sections which will be used to solve the actual problem (8).

An alternative way which allows to avoid this second equivalence consists of calculating directly the macroscopic fluxes. We derived the equations for these functions. They contain only the $P_{ij}^{::}$ and the effective reaction rates :

$$\alpha_x = \Sigma_x \, \varphi_x - R_x \, \varphi_x \tag{17}$$

which are very close to the absorption rates and that can be tabulated :

$$\sum_j \frac{P_{ij}^{::}}{\Sigma_j} \, R_j \left[U_j - \sum_x \frac{P_{jx}^{::}}{\Sigma_x} \, U_x \, \alpha_x \right] = U_i \tag{18}$$

where $U_\ell = \sum_j P_{\ell j}^{::} \, \psi_j$.

These equations are similar to the initial ones (8a). But the absorptions do not appear in the same way (left instead of right hand side).

Note that $U_x \equiv \psi_x$, therefore an actual reaction rate is obtained by multiplying U_x by the effective reaction rate.

SIMPLIFIED PROCEDURES AND NUMERICAL TESTS

EXAMPLES OF A MATRICES

We calculated the elements of A for three typical PWR situations.

i. Cylindrical Cells of Various Sizes

Four examples were chosen with the following characteristics, the radius of the pin being the unit of length :

Case	a	b	c	d
Cell radius	1.4	1.7	2	2
Moderator macroscopic cross-section	0.3	0.3	0.3	5

"c" is a standard PWR cell. For "d" the Dancoff effect is suppressed. "a" and "b" are representative of a very and a slightly undermoderated PWRs. The unique element of A is given in table 1 as a function of the macroscopic cross-section Σ in the pin. In column "d" we find $\sigma_{e\infty}/\sigma_e = 2/b$, where b is the usual Bell factor. It can be noticed in the other columns that the Dancoff effect only shifts of an approximatively constant amount the "d" values. As a similar remark can be made for the following tests we will only report the results for "a" where this effect is maximum.

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ii. Chessboard Pattern of Two Types of Pins

The calculation was made with the usual Roth approximation which is sufficient to appreciate the variations. Table 2 presents the results as functions of Σ_1 and Σ_2, the macroscopic cross-sections in these two types of pins (note that $A_{21} = A_{12}$ and $A_{22}(\Sigma_1, \Sigma_2) = A_{11}(\Sigma_2, \Sigma_1)$).

A_{11} practically depends only on Σ_1 and behaves similarly to A in table 1. A_{12} is almost constant.

iii. Cell with Two Zones in the Pin

This case is the same as the first one but two zones of equal volumes are distinguished in the pin. Table 3 shows that A_{12} and A_{22} depend only on Σ_2, the macroscopic cross-section in the peripheral zones, but A_{11} depends on both cross-sections. All the variations are always similar to the preceeding ones.

This fact can be easily understood if we assume isotropic currents at the interfaces : then one can indeed establish that

$$A = A^+ + (1 - C^+)^{-1} C^+ \overline{\ell} \tag{19}$$

where A^+ is the value without Dancoff effect, C^+ the Dancoff matrix (independant of the resonant cross-sections) and $\overline{\ell}$ the mean chords (diagonal matric).

We conclude that the present and well tested procedure for the "one resonant zone" problem, i.e. replacing A by a constant $\overline{A}$, remains valid for the general problem where A behaves very similarly.

SIMPLIFIED HETEROGENEOUS-HOMOGENEOUS EQUIVALENCE

The goal of this equivalence is to obtain the mean value $\overline{A}$ of A. For the case of a single resonant nuclide this value is given in the L.-J. theory by the equation "effective absorption rate with A function of Σ_x" = "effective absorption rate with $\overline{A}$ constant". This equation is simple when the narrow-resonance (NR) approximation is used to express both terms. This approximation appears to be sufficient to get a correct value of $\overline{A}$ (if necessary, a better intermediate-resonance approximation could be used).

For the general case the equivalence equation is more complicated, even in the NR approximation, because of the greater number of unknowns. This is the reason why an approximate "one-by-one" procedure has been considered : supposing that only one nuclide x is resonant, we carry out the present procedure which gives one $\overline{A}$ value. From $\overline{A}$ we get $\overline{\Sigma}_x$ by (14) and (13) written with x only. Similarly we get $\overline{\Sigma}_y$, $\overline{\Sigma}_z$,... Then we can get the $\overline{A}_{xy}$ by (14) and (13) used with the $\overline{\Sigma}$.

We have tested this approximation for a mixture of two resonant nuclides in a pin (we have seen that the A functions are similar whatever the geometry is ; also, if the procedure is correct for 2, it is - recurrently - correct for N resonant nuclides). For the sake of simple numerical calculations we represented both resonant cross-sections by sets of three values of equal probabilities (see table) and used the NR approximation. In column α we give the errors on the total effective reaction rate with this procedure (first of all $\overline{\Sigma}_1$ is calculated with $\Sigma_2 = 0$; then $\overline{\Sigma}_2$ is calculated with $\Sigma_1 = \overline{\Sigma}_1$: it is the reason why the cases 2a

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and 2b, for example, have to be distinguished). These errors are smaller than 1%
but for two cases where the effective reaction rate is small. The results are gene-
rally better when the more absorbing nuclide is treated first (for instance, 2a is
better than 2b), but not very significantly. In columns β and γ we give the errors
when the procedure is iterated ($\overline{\Sigma}_1$ is recalculated with $\Sigma_2 = \overline{\Sigma}_2$; etc...). No si-
gnificant improvement appears (the iteration converges but not towards the exact
result).

SIMPLIFICATION OF THE EFFECTIVE REACTION RATE TABULATIONS

Equations (16) relative to the fundamental situation contain a great number
of parameters if several resonant nuclides are taken into account. The effective
reaction rate tables should be built with all these parameters and therefore they
would be very large and expensive to create and to interpolate from. It is the
reason why we suggested a factorization approximation in order to have only binary
(two resonant nuclides) factors to calculate and store ; that is to say : we
assume that interference effects between resonances are practically uncorrelated.

Let $\tau_x^{y+z+t+\cdots}$ be the effective reaction rate for x in presence of y,z,t,...
and $f_x^{y+z+t+\cdots} = \tau_x^{y+z+t+\cdots}/\tau_x^0$ be the interference factor (τ_x^0 is relative to x
alone). Our hypothesis is

$$f_x^{y+z+t+\cdots} \simeq f_x^y \, f_x^z \, f_x^t \, \cdots$$

It is clear that heterogeneity effects are independant of these interference
effects. Consequently numerical tests were performed with a homogeneous mixture.
We chose the following one with a 20b non-resonant cross-section (which gives
a great self-shielding and therefore one of
the most severe cases that can be encoun-
tered). The calculations where performed by
J. Mondot and R. Sanchez[4] with a very fine
mesh slowing-down code.

Nuclide at %	
^{235}U	0.98
^{236}U	0.54
^{238}U	90.63
^{237}Np	0.35
^{239}Pu	4.36
^{240}Pu	1.70
^{241}Pu	0.92
^{242}Pu	0.52

From the numerous results we present
(in Table 5) the binary factors and the
comparison of their product with the exact
global factor for ^{238}U and ^{239}Pu on the
whole resonant range (1.5 keV - 2.8 eV). It
can be seen that the errors of the factori-
zation approximation are small. A group by
group analysis shows a slight dispersion of

the errors around these mean values.

Remark. R. Sanchez and J. Mondot[5] proposed another method : calculate the inter-
ference $f_x^{y+z+t+\cdots}$ factors with the wide resonance approximation. The precision
is similar (differences for the same examples : - 0.1 ; - 0.2 ; 2.3 ; 1.2%) ;
the amount of data to be stored is also similar.

CONCLUSION

The generalized formalism herein proposed will allow to treat with the same proved precision than the L.-J. theory any complicated situation. It will be introduced in the entirely new version of our code, APOLLO 2, presently in progress. Then we will at least be able to correctly calculate the well known difficult problems drastically imposed to the physicists by the designers of nuclear reactors !

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Σ	Case a	Case b	Case c	Case d
0.1	4.30	2.63	2.03	1.30
0.2	4.33	2.65	2.05	1.30
0.5	4.41	2.73	2.11	1.36
1	4.52	2.84	2.22	1.46
2	4.68	3.00	2.39	1.62
5	4.87	3.20	2.59	1.82
10	4.95	3.28	2.67	1.90
20	5.00	3.33	2.72	1.95
50	5.02	3.35	2.74	1.98

Table 1 : A for Cells

A_{11}

Σ_1 \ Σ_2	0.1	0.5	2	10	50
0.1	2.51	2.50	2.50	2.50	2.50
0.5	2.59	2.59	2.58	2.58	2.58
2	2.86	2.86	2.85	2.85	2.85
10	3.14	3.13	3.13	3.13	3.13
50	3.22	3.21	3.21	3.21	3.21

$A_{12} = A_{21}$

	0.1	0.5	2	10	50
0.1	1.79	1.80	1.81	1.81	1.81
0.5	1.81	1.82	1.83	1.82	1.82
2	1.81	1.83	1.83	1.83	1.83
10	1.81	1.82	1.83	1.82	1.82
50	1.81	1.82	1.83	1.82	1.82

Table 2 : A for a Chessboard Pattern

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Σ_2 / Σ_1	0.1	0.5	2	10	50
0.1	2.49	2.58	2.88	3.40	3.44
0.5	2.53	2.61	2.89	3.42	3.46
2	2.69	2.76	3.03	3.57	3.61
10	2.93	3.01	3.28	3.81	3.84
50	3.00	3.08	3.35	3.88	3.92

A_{11}

	0.1	0.5	2	10	50
0.1	2.12	2.14	2.23	2.43	2.50
0.5	2.11	2.14	2.23	2.43	2.50
2	2.11	2.13	2.23	2.43	2.51
10	2.10	2.13	2.23	2.43	2.50
50	2.10	2.13	2.23	2.43	2.51

A_{22}

	0.1	0.5	2	10	50
0.1	2.01	2.07	2.24	2.50	2.52
0.5	1.99	2.06	2.23	2.50	2.52
2	1.99	2.05	2.22	2.51	2.53
10	1.99	2.06	2.23	2.51	2.52
.50	1.99	2.06	2.23	2.51	2.53

$A_{12} = A_{21}$

Table 3 : A for a Cell with Two Zones in the Pin

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Case	Σ_1 set			Σ_2 set			Errors (%) (See text)		
							α	β	γ
1	0.1	0.5	2	0.1	0.5	2	− 1.6	2.1	1.3
2a	0.5	2	10	0.1	0.5	2	− 0.8	0.8	0.8
2b	0.1	0.5	2	0.5	2	10	− 1.2	0.9	0.8
3	0.5	2	10	0.5	2	10	− 0.6	0.1	0.2
4a	2	10	50	0.1	0.5	2	0.3	− 0.0	− 0.0
4b	0.1	0.5	2	2	10	50	− 0.8	− 0.3	− 0.0
5a	2	10	50	0.5	2	10	0.5	− 0.2	− 0.3
5b	0.5	2	10	2	10	50	− 0.2	− 0.3	− 0.3
6	2	10	50	2	10	50	0.4	− 0.2	− 0.3

Table 4 : Errors from an "One-by-One" Procedure

238	Absorption	Scattering
I_{eff} ::	12.4	53.8
239	.958	.935
241	.977	.979
240	.985	.986
235	.988	.988
236	.993	.995
237	.994	.994
242	.997	.996
Product	.897	.878
Exact	.895	.881
Difference	0.2%	-0.3%

239::::	Absorption	Scattering
I_{eff} ::	179.9	50.9
238	.855	.887
241	.976	.982
235	.989	.990
240	.993	.991
236	.997	.995
242	.999	.998
Product	.816	.848
Exact	.797	.835
Difference	2.5%	1.6%

:: Effective Resonance Integral in the Mixture (barns).

:::: Without ^{237}Np in the Mixture.

Table 5 : Errors from a Factorization of the Interference Factors

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