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EVALUATION OF THE ACCURACY OF GROUP CALCULATIONS

FOR REACTOR CRITICALITY PERTURBATIONS

V.A. Dulin

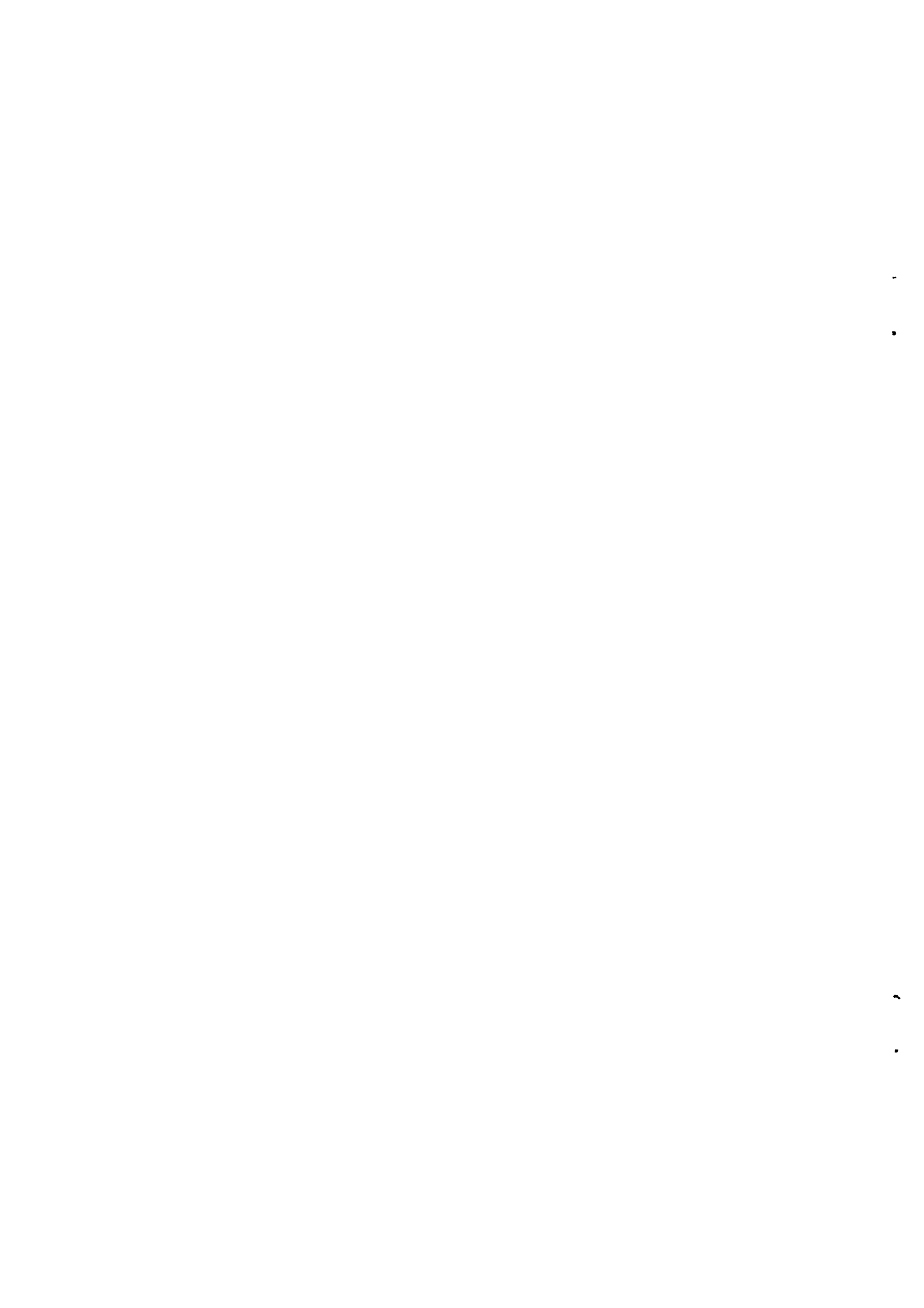Translated by the IAEA

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ABSTRACT

For calculations of criticality perturbations it is necessary to
use group constants which take into account not only the
peculiarities of the intra-group flux but also those of the behaviour
of the adjoint flux. A new method is proposed for obtaining
bilinear-averaged constants of this type on the basis of the
resonance characteristics of the importance function and the
difference between the value of neutron importance at the group
boundary and the group-averaged value (the b^{+j} factor). A number
of calculations are made for the ratios of reactivity coefficients in
the BFS assemblies. Values have been obtained for the difference
between the results of calculation with bilinear-averaged constants
and those averaged conventionally (over flux). In many cases, this
difference exceeds the experimental error.

At the present time the Bondarenko-Nikolaev-Abagyan-Bazazyants (BNAB)
26-group system of constants is used extensively for fast reactor
calculations [1, 2]. The method of preparation of the macroconstants
envisages the maximum possible accuracy in describing K_{eff} and the
functionals of the neutron flux. The resonance self-shielding of the
group cross-section is calculated here by means of the asymptotic spectrum

$$\varphi_a(u) = 1/\Sigma_t(u),$$
(1)

while the elastic slowing-down cross-section from one group to the next is obtained by calculating the difference between the flux at the group boundary and the group-averaged flux [3, 4]. Repeated verifications of the accuracy of the method of preparation of the BNAB constants by means of calculations with a substantially larger number of groups have shown that in its current version the methodological error in the group calculation of reactor characteristics (K_{eff}, the ratios of the average cross-sections of the main absorbing and fissile materials and the neutron group spectra) is lower by several factors than the error in the corresponding macroexperiments [4, 5].

The flux-averaged group constants thus obtained are also used for calculations by the perturbation theory. The problem of the error in these calculations of criticality perturbations was studied in Refs [6-15]. This is still of interest since exepriments on reactor (assembly) criticality perturbations caused by samples of elements introduced into the reactor continue to be in effect the main source of data on the capture cross-sections of non-activated elements (the higher isotopes of plutonium, most of the fission products and structural materials). The problem of the adequate calcuation of them in the group approximation has in principle been solved [6, 7]. Small-group constants are obtained here from the multigroup (10^4-10^5 groups) constants by bilinear averaging. However, such calculations have not yet been performed.

The present paper deals with a method of obtaining the macroconstants for calculations of criticality perturbations that is based on the use of the asymptotic spectrum (1) and the asymptotic neutron importance

$$\varphi_a^+(u) = \frac{\beta \nu \Sigma_f(u) + \Sigma_s(u)}{\Sigma_t(u)} \tag{2}$$

to take into account the resonance effects and on redetermination of the elastic slowing-down cross-section with allowance for the importance function. The group equations for flux and neutron importance here

remain adjoint, and the calculations give the same values of K_{eff} and group fluxes as calculations with flux-averaged constants and other, more correct group importance and criticality perturbation values.

BILINEAR-AVERAGED GROUP CONSTANTS

The rules for averaging group constants preserving K_{eff}, group fluxes, neutron importance and criticality perturbations in the diffusion approximation were obtained in Ref. [6] (see also Ref. [7]):

$$\widetilde{\widetilde{\Sigma}}_t^j = \frac{1}{\varphi^j \varphi^{+j}} \int_{u_{j-1}}^{u_j} \varphi^+(u) \Sigma_t(u) \varphi(u) du; \quad \widetilde{\widetilde{D}}^j = \frac{1}{\varphi^j \varphi^{+j}} \int_{u_{j-1}}^{u_j} \varphi^+ D(u) \varphi du;$$

$$\nu \widetilde{\widetilde{\Sigma}}_f^j = \frac{1}{\varphi^j} \int_{u_{j-1}}^{u_j} \nu \Sigma_f(u) \varphi(u) du; \quad \widetilde{\chi}^j = \frac{1}{\varphi^{+j}} \int_{u_{j-1}}^{u_j} \chi(u) \varphi^+(u) du; \tag{3}$$

$$\widetilde{\Sigma}^{i \to j} = \frac{1}{\varphi^i \varphi^{+j}} \int_{u_{j-1}}^{u_j} \varphi^+(u) du \int_{u_{i-1}}^{u_i} \Sigma_s(u' \to u) \varphi(u') du',$$

where

$$\varphi^j = \int_{u_{j-1}}^{u_j} \varphi(u) du; \quad \varphi^{+j} = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \varphi^+(u) du. \tag{4}$$

Clearly, the law of preservation is satisfied only if $\varphi(u)$ and $\varphi^+(u)$ are exact solutions. We shall confine ourselves hereafter to the slowing-down equation in the B^2 approximation and to its adjoint equation, and for simplicity we shall consider only elastic slowing-down:

$$\left[D(u)B^2 + \Sigma_t(u)\right] \varphi(u) = \int_{u-\varepsilon}^u \Sigma_s(u') f(u-u') \varphi(u') du' + \frac{\chi(u)}{R} \int_0^\infty \nu \Sigma_f(u') \varphi(u') du'; \tag{5}$$

$$\left[D(u)B^2 + \Sigma_t(u)\right] \varphi^+(u) = \int_u^{u+\varepsilon} \Sigma_s(u) f(u'-u) \varphi^+(u') du' + \frac{\nu \Sigma_f(u)}{R} \int_0^\infty \chi(u') \varphi^+(u') du'. \tag{6}$$

Multiplying Eq. (5) by $\varphi^+(u)$, integrating over group j and using Eq. (3), we can write down the equation for the group flux φ^j:

$$\widetilde{\widetilde{\Sigma}}_t^j \varphi^j \varphi^{+j} = \widetilde{\widetilde{\Sigma}}^{j \to j} \varphi^j \varphi^{+j} + \widetilde{\widetilde{\Sigma}}^{j-1 \to j} \varphi^{j-1} \varphi^{+j} + \frac{\widetilde{\chi}^j \varphi^{+j}}{R} Q \ . \qquad (7)$$

Here

$$\widetilde{\widetilde{\Sigma}}^{j \to j} \varphi^j \varphi^{+j} + \widetilde{\widetilde{\Sigma}}^{j-1 \to j} \varphi^{j-1} \varphi^{+j} =$$

$$= \int_{u_{j-1}}^{u_j} \varphi^+(u) du \int_{u-\tau}^{u} \Sigma_s(u') f(u-u') \varphi(u') du' ; \quad Q = \sum_{i=1}^{G} \nu \Sigma_f^i \varphi^i \ . \qquad (7A)$$

This form of notation is not convenient unless the exact solutions $\varphi(u)$ and $\varphi^+(u)$ are known, and we have only $\varphi_a(u)$ and $\varphi_a^+(u)$.
Changing the order of integration in the double integral, we obtain:

$$\int_{u_{j-1}}^{u_j} \varphi^+(u) du \int_{u-\tau}^{u} \Sigma_s(u') f(u-u') \varphi(u') du' = \int_{u_{j-1}}^{u_j} \Sigma_s(u') \varphi(u') du' \int_{u'}^{u'+\tau} \varphi^+(u) f(u-u') du -$$

$$- \int_{u_j-\tau}^{u_j} \Sigma_s(u') \varphi(u') du' \int_{u_j}^{u'+\tau} \varphi^+(u) f(u-u') du + \int_{u_{j-1}-\tau}^{u_{j-1}} \Sigma_s(u') \varphi(u') du' \int_{u_{j-1}}^{u'+\tau} \varphi^+(u) f(u-u') du \ . \qquad (8)$$

By definition the difference between the first and the second integral on the right-hand side of relationship (8) is $\widetilde{\widetilde{\Sigma}}^{j \to j} \varphi^j \varphi^{+j}$ and the last integral is $\widetilde{\widetilde{\Sigma}}^{j-1 \to} \varphi^{j-1} \varphi^{+j}$ (see Eq. (3)). Transferring these terms to the left-hand side of Eq. (7) and using the definitions $\Sigma_t(u) = \Sigma_a(u) + \Sigma_s(u)$ and the normalization of the distribution function $f(u-u')$: $\int_{u'}^{u'+\tau} f(u-u') du = 1$, instead of Eq. (7) we obtain:

$$\widetilde{\widetilde{\Sigma}}_a^j \varphi^j \varphi^{+j} + \int_{u_{j-1}}^{u_j} \Sigma_s(u') \varphi(u') du' \int_{u'}^{u'+\tau} \left[\varphi^+(u') - \varphi^+(u) \right] f(u-u') du +$$

$$+ \widetilde{\widetilde{\Sigma}}^{j \to j+1} \varphi^j \varphi^{+j+1} = \widetilde{\widetilde{\Sigma}}^{j-1 \to j} \varphi^{j-1} \varphi^{+j} + \frac{\widetilde{\chi}^j \varphi^{+j}}{k} Q \ . \qquad (9)$$

Dividing by φ^{+j} term by term, we can write down the equation for determination of group flux φ^j and flux φ^{j+1}:

$$\left\{ \widetilde{\widetilde{\Sigma}}_a^j + \frac{1}{\varphi^j \varphi^{+j}} \int_{u_{j-1}}^{u_j} \Sigma_s(u')\varphi(u')du' \int_{u'}^{u'+\tau} \left[\varphi^+(u')-\varphi^+(u)\right] f(u-u')du + \right.$$

$$\left. + \widetilde{\Sigma}^{j \rightarrow j+1} \varphi^{+j+1} \Big/ \varphi^{+j} \right\} \varphi^j = \widetilde{\Sigma}^{j-1 \rightarrow j} \varphi^{j-1} + \frac{\widetilde{\chi}^j}{k} Q \; ; \qquad (10)$$

$$\left\{ \widetilde{\widetilde{\Sigma}}_a^{j+1} + \frac{1}{\varphi^{j+1} \varphi^{+j+2}} \int_{u_j}^{u_{j+1}} \Sigma_s(u')\varphi(u')du' \int_{u'}^{u'+\tau} \left[\varphi^+(u')-\varphi^+(u)\right] f(u-u')du + \right.$$

$$\left. + \widetilde{\Sigma}^{j+1 \rightarrow j+2} \varphi^{+j+2} \Big/ \varphi^{+j+1} \right\} \varphi^{j+1} = \widetilde{\Sigma}^{j \rightarrow j+1} \varphi^j + \frac{\widetilde{\chi}^{j+1}}{k} Q \; . \qquad (11)$$

After addition and subtraction of $\widetilde{\Sigma}^{j \rightarrow j+1} \varphi^j$ on the left-hand side of (10) and of $\widetilde{\Sigma}^{j+1 \rightarrow j+2} \varphi^{j+1}$ in (11) we get the ordinary form of the group equations:

$$\left(\widetilde{\widetilde{\Sigma}}_a^j + \delta\Sigma_a^j + \widetilde{\Sigma}^{j \rightarrow j+1} \right) \varphi^j = \widetilde{\Sigma}^{j-1 \rightarrow j} \varphi^{j-1} + \frac{\widetilde{\chi}^j}{k} Q \; ; \qquad (12)$$

$$\left(\widetilde{\widetilde{\Sigma}}_a^{j+1} + \delta\Sigma^{j+1} + \widetilde{\Sigma}^{j+1 \rightarrow j+2} \right) \varphi^{j+1} = \widetilde{\Sigma}^{j \rightarrow j+1} \varphi^j + \frac{\widetilde{\chi}^{j+1}}{k} Q \; . \qquad (13)$$

Here $\widetilde{\widetilde{\Sigma}}_a^j$ and $\widetilde{\Sigma}^{j \rightarrow j+1}$ are bilinear-averaged absorption and elastic slowing-down cross-sections. The cross-section $\widetilde{\widetilde{\Sigma}}_a^j$ is averaged as $\widetilde{\widetilde{\Sigma}}_t^j$, while $\delta\Sigma_a^j$ denotes a fictitious addition to the absorption cross-section:

$$\delta\Sigma_a^j = - \frac{1}{\varphi^j \varphi^{+j}} \int_{u_{j-1}}^{u_j} \Sigma_s(u')\varphi(u')du' \int_{u'}^{u'+\tau} \left[\varphi^+(u)-\varphi^+(u')\right] f(u-u')du +$$

$$+ \widetilde{\Sigma}^{j \rightarrow j+1} \left(\varphi^{+j+1} - \varphi^{+j} \right) \Big/ \varphi^{+j} \; ; \qquad (14)$$

$$\widetilde{\widetilde{\Sigma}}_a = \frac{1}{\varphi^j \varphi^{+j}} \int_{u_{j-1}}^{u_j} \varphi^+(u)\Sigma_a(u)\varphi(u)du \; ; \qquad (15)$$

$$\widetilde{\Sigma}^{j \to j+1} = \frac{1}{\varphi^j \varphi^{+j+1}} \int_{u_j - \tau}^{u_j} \Sigma_s(u') \varphi(u') du' \int_{u_j}^{u'+\tau} \varphi^+(u) f(u-u') du \,. \qquad (16)$$

For the energy-independent importance function $\varphi^+(u) = $ const we obtain the normal rules for averaging cross-sections over flux [1, 3]:

$$\bar{\Sigma}_a^j = \frac{1}{\varphi^j} \int_{u_{j-1}}^{u} \Sigma_a(u) \varphi(u) du \,; \qquad (17)$$

$$\bar{\Sigma}^{j \to j+1} = \frac{1}{\varphi^j} \int_{u_j - \tau}^{u_j} \Sigma_s(u') \varphi(u') du' \int_{u_j}^{u'+\tau} f(u-u') du = \frac{\xi \bar{\Sigma}_s^j}{\Delta u_j} \beta^j \,, \qquad (18)$$

and the addition $\delta \Sigma_a^j$ to the absorption cross-section (see Eq. (14)) becomes zero.

EVALUATION OF THE DIFFERENCE BETWEEN GROUP MACROCONSTANTS OBTAINED BY BILINEAR AVERAGING AND BY AVERAGING OVER FLUX

Let us evaluate the difference between the bilinear-averaged absorption and elastic slowing-down cross-sections (15) and (16), and the flux-averaged cross-sections (17) and (18).

Let us assume that for strong resonance absorbers the main effect of using bilinear constants will be associated with the variation in Σ_a^j when averaging with weight $\varphi^+(u)$, in accordance with Eq. (15), and that to evaluate this effect we have to know the behaviour of the flux and neutron importance in intervals of the order of the resonance width Γ. The fictitious addition $\delta \Sigma_a^j$ will, on the other hand, be substantial chiefly for scattering elements, and for its calculation one needs to know the intra-group behaviour of the flux and neutron importance over an interval of the order of the variation in lethargy during scattering τ. For narrow intervals $\Gamma \ll \tau$, and these two effects will be almost independent. Let us tentatively call them the resonance and non-resonance bilinear additions to the absorption cross-section.

Non-resonance effects

As will be seen from Eqs (14) and (16), $\delta\Sigma_a^j$ and $\widetilde{\Sigma}^{j\rightarrow j+1}$ are associated with the peculiarities of averaging the elastic scattering cross-sections. If we had the exact solutions $\varphi(u)$ and $\varphi^+(u)$, the calculations with bilinear-averaged constants would, as we know, give the same values of K_{eff} and group fluxes as the calculation with flux-averaged constants.

Let us define b^{+j} as the relationship

$$\delta^{+j} = \widetilde{\Sigma}^{j\rightarrow j+1} \Big/ \overline{\Sigma}^{j\rightarrow j+1} . \tag{19}$$

The values of b^{+j} and $\widetilde{\chi}^j$ can be found by applying the solution $\overline{\varphi}^{+j}$ obtained with flux-averaged constants. This procedure is similar to the one used for calculation of the factors b^j. Linearly integrating $\overline{\varphi}^{+j}$ and χ^j (here it is necessary for the intra-group values of χ^j to remain unchanged), we obtain:

$$\left.
\begin{array}{l}
\delta^{+j} = \left(\overline{\varphi}^{+j} + \overline{\varphi}^{+j+1}\right)\Big/ 2\overline{\varphi}^{+j+1} ; \\[2mm]
\delta\Sigma^{j\rightarrow j+1} = \widetilde{\Sigma}^{j\rightarrow j+1} - \overline{\Sigma}^{j\rightarrow j+1} = \overline{\Sigma}^{j\rightarrow j+1}(\delta^{+j}-1) ;
\end{array}
\right\} \tag{20}$$

$$\delta\chi^j = \widetilde{\chi}^j - \chi^j = (\chi^{j+1} - \chi^{j-1})(\overline{\varphi}^{+j+1} - \overline{\varphi}^{+j-1})\Big/ 48\,\overline{\varphi}^{+j} . \tag{21}$$

Let us determine $\delta\Sigma_a^j$ in Eq. (14) from the requirement of preservation of K_{eff} and φ^j with use of the bilinear-averaged elastic slowing-down cross-sections in calculations of φ^j and φ^{+j}. For this purpose, we will equate the expresssion for φ^j as calculated with flux-averaged constants (with allowance for inelastic scattering),

$$\varphi^j = \frac{\chi^j + \sum\limits_{i=1}^{j-1} \Sigma_{in}^{i\rightarrow j}\varphi^i + \overline{\Sigma}^{j-1\rightarrow j}\varphi^{j-1}}{\Sigma_a^j + \left(\overline{\Sigma}_{in}^j - \Sigma_{in}^{j\rightarrow j}\right) + \overline{\Sigma}^{j\rightarrow j+1} + D^j B^2} , \tag{22}$$

and as calculated with the bilinear-averaged constants

$$\varphi^j = \frac{\chi^j + \delta\chi^j + \sum\limits_{i=1}^{j-1}\bar{\Sigma}_{in}^{i \to j}\varphi^i + \left(\bar{\Sigma}^{j-1\to j} + \delta\Sigma^{j-1\to j}\right)\varphi^{j-1}}{\bar{\Sigma}_a^j + \delta\Sigma_a^j + \left(\bar{\Sigma}_{in}^j - \Sigma_{in}^{j\to j}\right) + \bar{\Sigma}^{j\to j+1} + \delta\Sigma^{j\to j+1} + D^j B^2} \quad , \tag{23}$$

where $\delta\Sigma^{j\to j+1}$ and $\delta\chi^j$ are given by relationships (20) and (21), and $\delta\Sigma_a^j$ must be determined. Equating the right-hand sides we obtain

$$\left(\chi^j + \sum\limits_{i=1}^{j-1}\bar{\Sigma}_{in}^{i\to j}\varphi^i + \bar{\Sigma}^{j-1\to j}\varphi^{j-1}\right)\left(\bar{\Sigma}_y^j + \delta\Sigma_a^j + \delta\Sigma^{j\to j+1}\right) =$$

$$= \bar{\Sigma}_y^j\left(\chi^j + \delta\chi^j + \sum\limits_{i=1}^{j-1}\bar{\Sigma}_{in}^{i\to j}\varphi^i + \bar{\Sigma}^{j-1\to j}\varphi^{j-1}\right) + \bar{\Sigma}_y^j\delta\Sigma^{j-1\to j}\varphi^{j-1}. \tag{23A}$$

Hence, with allowance for Eq. (22), we obtain

$$\left.\begin{array}{l} \delta\Sigma_a^1 = -\delta\Sigma^{1\to2} ; \\[6pt] \delta\Sigma_a^j = \left(\varphi^{j-1}\delta\Sigma^{j-1\to j}/\varphi^j\right) - \delta\Sigma^{j\to j+1} + \delta\chi^j Q/\varphi^j k_{\text{эф}} ; \\[6pt] \delta\Sigma_a^j = \varphi^{25}\delta\Sigma^{25\to26}/\varphi^{26} ; \qquad 1 < j < 26 . \end{array}\right\} \tag{24}$$

The value of K_{eff} determined in its case from relation (12) as

$$K_{eff} = Q = \sum\limits_{j=1}^{26}\nu\bar{\Sigma}_f^j\varphi^j = Q^+ = \sum\limits_{j=1}^{26}\chi^j\varphi^{+j} , \tag{25}$$

is also preserved since in bilinear averaging (3), the values of $\nu\bar{\Sigma}_f^j$ are taken as flux-averaged. Hence it follows that the difference between φ^{+j} as calculated with bilinear-averaged constants (21) and (23) and the earlier $\bar{\varphi}^{+j}$ $\delta\varphi^{+j} = \varphi^{+j} - \bar{\varphi}^{+j}$ should be sign-alternating in nature and satisfy the condition

$$\sum\limits_{j=1}^{26}\tilde{\chi}^j\delta\varphi^{+j} = 0 . \tag{26}$$

This is confirmed by the practice of numerical calculations.

The criticality perturbation due to the slight variation in the concentration of element α Δn_α (reactivity coefficient for element α) calculated with flux-averaged constants $\bar{\rho}_\alpha$, as we know, is given by the expression:

$$\bar{\rho}_\alpha \sim \frac{1}{k_{_{3\phi}}}\left(\sum_{j=1}^{26}\chi^j\bar{\varphi}^{+j}\right)\left(\sum_{i=1}^{26}\Delta n_\alpha\,\nu\bar{\sigma}_{f\alpha}^i\,\varphi^i\right) -$$

$$-\sum_{j=1}^{26}\bar{\varphi}^{+j}\Delta n_\alpha\,\bar{\sigma}_{a\alpha}^j\,\varphi^j + \sum_{j=1}^{26}\Delta n_\alpha\left(\bar{\sigma}_\alpha^{j-1\rightarrow j}\,\varphi^{j-1}-\sigma_\alpha^{j\rightarrow j+1}\,\varphi^j\right)\bar{\varphi}^{+j}. \qquad (27)$$

It can be shown that $\tilde{\rho}_\alpha$ calculated with bilinear-averaged constants and using φ^{+j} obtained by the above method is also described by an expresssion coinciding with (27) and differing from it only in that $\bar{\varphi}^{+j}$ is replaced by $\tilde{\varphi}^{+j}$. The difference

$$\delta\rho_\alpha = \tilde{\rho}_\alpha - \bar{\rho}_\alpha \qquad (28)$$

is the addition to the reactivity coefficient due to the use of the bilinear-averaged constants.

In this manner, the old flux-averaged perturbations of the absorption and elastic slowing-down cross-sections and new modified group neutron importance φ^{+j} are used in the calculation of criticality perturbations. The reactivity components for neutron generation and inelastic slowing-down are also calculated with the old group cross-sections and new group importance. This means that the whole effect of using bilinear-averaged constants in this approach is purely "spectral", i.e. when calculating the criticality perturbation only the group importance changes.

Equations (20), (21) and (23) and the above conclusions based on them are valid for any type of interpolation used to obtain b^{+j}, for example quadratic interpolation. Moreover, the use of different reasonable types of interpolation gives a natural evaluation of the methodological error in obtaining $\delta\Sigma^{j\rightarrow j+1}$ and $\delta\Sigma_a^j$ and in the bilinear functionals calculated thereby.

We will show that the fictitious addition $\delta\Sigma_a^j$ can be calculated directly from Eq. (14), and that for a linear interpolation it coincides with result (23). In fact, if the linear representation for the dependence

$$\varphi^+(u) = \varphi^+(u') + (u - u')\frac{d\varphi^+(u')}{du'}du' \tag{29}$$

is substituted into Eq. (14), then with allowance for Eqs (18) and (20) we obtain:

$$\delta\Sigma_a^j = -\frac{\xi}{\varphi^j\varphi^{+j}}\int_{u_{j-1}}^{u_j}\Sigma_s(u')\varphi(u')\frac{d\varphi^+(u')}{du'}du' + \frac{\xi\Sigma_s^j b^j b^{+j}}{\Delta u_j}\left(\frac{\varphi^{+j+1}}{\varphi^{+j}} - 1\right). \tag{30}$$

If for the determination of b^j we also use a linear approximation and determine b^j as the ratio of collision density x^j (see (18))

$$b^j = \frac{\bar\Sigma_s^{j+1}\varphi^{j+1} + \bar\Sigma_s^j\varphi^j}{2\bar\Sigma_s^j\varphi^j} = \frac{1}{2}\left(\frac{x^{j+1}}{x^j} + 1\right), \tag{31}$$

and represent the behaviour of collision density and neutron importance within the group j in the form of linear functions of u

$$\left.\begin{aligned}\Sigma_s(u')\varphi(u') &= \frac{\varphi^j}{\Delta u} + \frac{\bar\Sigma_s^{j+1}\varphi^{j+1} - \bar\Sigma_s^j\varphi^j}{\Delta u^2}u' ; \\[2mm]\varphi^+(u') &= \bar\varphi^{+j} + \frac{\bar\varphi^{+j+1} - \bar\varphi^{+j}}{\Delta u}u' ;\end{aligned}\right\}\ 0 < u' < \frac{\Delta u}{2} \tag{32}$$

$$\left.\begin{aligned}\Sigma_s(u')\varphi(u') &= \frac{\bar\Sigma_s^j\varphi^j}{\Delta u} + \frac{\bar\Sigma_s^j\varphi^j - \Sigma_s^{j-1}\varphi^{j-1}}{\Delta u^2}u' ; \\[2mm]\varphi^+(u') &= \bar\varphi^{+j} + \frac{\bar\varphi^{+j} - \bar\varphi^{+j-1}}{\Delta u}u' ,\end{aligned}\right\}\ -\frac{\Delta u_j}{2} < u' < 0$$

then substituting (32) into (30), integrating and making simplifications, with allowance for (20) and (31), we obtain

$$\delta\Sigma_a^j = \frac{\xi\bar{\Sigma}_s^j}{4\Delta u}\left[\left(\frac{x^{j+1}}{x^j}+1\right)\left(1-\frac{\bar{\varphi}^{+j}}{\bar{\varphi}^{+j+1}}\right)+\left(\frac{x^{j-1}}{x^j}+1\right)\left(\frac{\bar{\varphi}^{+j-1}}{\bar{\varphi}^{+j}}-1\right)\right].$$

(33)

For b^j and b^{+j} determined in accordance with Eqs (20) and (31) we can write down

$$\delta\Sigma^{j-1\to j} = \frac{\xi\bar{\Sigma}_s^{j-1}}{4\Delta u}\left(\frac{x^j}{x^{j-1}}+1\right)\left(\frac{\bar{\varphi}^{+j-1}}{\bar{\varphi}^{+j}}-1\right);$$

$$\delta\Sigma^{j\to j+1} = \frac{\xi\bar{\Sigma}_s^j}{4\Delta u}\left(\frac{x^{j+1}}{x^j}+1\right)\left(\frac{\bar{\varphi}^{+j}}{\bar{\varphi}^{+j+1}}-1\right).$$

(33A)

The first term in (33) is then simply $-\delta\Sigma^{j\to j+1}$ and, using Eq. (31), we obtain:

$$\delta\Sigma_a^j = -\delta\Sigma^{j\to j+1} + \frac{\xi\bar{\Sigma}_s^j}{4\Delta u}\left(\frac{x^{j-1}}{x^j}+1\right)\left(\frac{\bar{\varphi}^{+j-1}}{\bar{\varphi}^{+j}}-1\right) =$$

(33B)

$$= -\delta\Sigma^{j\to j+1} + \frac{\xi\bar{\Sigma}_s^j x^{j-1}}{4\Delta u\, x^j}\left(1+\frac{x^j}{x^{j-1}}\right)\left(\frac{\bar{\varphi}^{+j-1}}{\bar{\varphi}^{+j}}-1\right) = \varphi^{j-1}\delta\Sigma^{j-1\to j}/\varphi^j = \delta\Sigma^{j\to j+1}.$$

Hence the proposed method of obtaining the macroconstants is essentially one of using age approximation to solve the equation for the flux and its adjoint equation.

Resonance effects

Let us evaluate the bilinear-averaged absorption cross-section of resonance absorbers, using Eqs (1) and (2). The quantity β^j is the ratio of the average neutron importance $\bar{\varphi}_x^+$ weighted over the fission spectrum, to the neutron importance in the given group $\bar{\varphi}^{+j}$ [9, 10]:

$$\beta^j = \left(\sum_{i=1}^{26}\chi^i\bar{\varphi}^{+i}\right)\Bigg/\left[\bar{\varphi}^{+j}+\frac{\bar{\Sigma}^{j\to j+1}}{\bar{\Sigma}_s^j}(\bar{\varphi}^{+j+1}-\bar{\varphi}^{+j})\right].$$

(33C)

In a sub-group representation [2] we can easily calculate the difference between the bilinear-averaged resonance absorption cross-section and the flux-averaged cross-section (and the difference in the diffusion coefficients):

$$\delta\sigma^j_{a\tau\alpha} = \tilde{\tilde{\sigma}}^j_{a\tau\alpha} - \bar{\sigma}^j_{a\tau\alpha} =$$

$$= \left[\sum_{k\in j}\frac{a^j_{\alpha k}\sigma^j_{a\alpha k}A^j_{\alpha k}}{n_\alpha(B^j_{\alpha k})^2}\right]\Bigg/\left[\sum_{k\in j}\frac{a^j_{\alpha k}}{n_\alpha B^j_{\alpha k}}\right]\left[\sum_{k\in j}\frac{a^j_{\alpha k}A^j_{\alpha k}}{B^j_{\alpha k}}\right] -$$

$$- \left[\sum_{k\in j}\frac{a^j_{\alpha k}\sigma^j_{a\alpha k}}{n_\alpha B^j_{\alpha k}}\right]\Bigg/\left[\sum_{k\in j}\frac{a^j_{\alpha k}}{n_\alpha B^j_{\alpha k}}\right] , \tag{34}$$

where $A^j_{\alpha k} = \beta\nu\sigma^j_{f\alpha k} + \sigma^j_{s\alpha k} + \sigma^j_{1\alpha}$; $B^j_{\alpha k} = \sigma^j_{t\alpha k} + \sigma^j_{0\alpha}$;

$$\sigma^j_{0\alpha} = \sum_{\gamma\neq\alpha}\frac{n_\gamma}{n_\alpha}\sigma^j_{t\gamma}; \quad \sigma^j_{1\alpha} = \sum_{\gamma\neq\alpha}\frac{n_\gamma}{n_\alpha}(\beta\nu\sigma^j_{f\gamma} + \sigma^j_{s\gamma}). \tag{35}$$

The notations are as in Ref. [2]: $\sigma^j_{x\alpha k}$ is a cross-section of type x of element α in group j, sub-group k, $a^j_{\alpha k}$ the width of the sub-group and n_α the concentration of element α in the medium. Then

$$\delta\Sigma^j_{a\tau} = \sum_\alpha n_\alpha\delta\sigma^j_{a\tau\alpha}; \tag{36}$$

$$\delta D^j = \tilde{\tilde{D}}^j - \bar{D}^j = \sum_\alpha\left(\sum_{k\in j}\frac{a^j_{\alpha k}}{n_\alpha B^j_{\alpha k}}\right)\left\{\left[\sum_{k\in j}\frac{a^j_{\alpha k}A^j_{\alpha k}}{B^j_{\alpha k}}\right]\Bigg/\left[\sum_{k\in j}\frac{a^j_{\alpha k}A^j_{\alpha k}}{n^2_\alpha(B^j_{\alpha k})^3}\right] -$$

$$- 1\Bigg/\sum_{k\in j}\frac{a^j_{\alpha k}}{n^2_\alpha(B^j_{\alpha k})^2}\right\}. \tag{37}$$

The addition $\delta\sigma_{a\tau}$ can be expressed in terms of the resonance parameters:

$$\delta\sigma_{az} = \bar{\sigma}_{az} \left\{ \frac{\beta\nu\Gamma_f - \Gamma_a}{2\Gamma k} \left(h - \frac{1}{n}\right)\left[1 - \frac{\pi\Gamma h}{2DC} + \right. \right.$$

$$\left. \left. + \frac{2DCh}{\pi\Gamma(h^2 + c^2 D^2/\Gamma^2)} \right] \right\} \approx \frac{\bar{\sigma}_{az}(\beta\nu\Gamma_f - \Gamma_a)(1 - f_a^2)}{2\Gamma} ;$$

$$\bar{\sigma}_{az} = \pi\Gamma_a \sigma_0' / 2Dh \left[1 - \frac{\pi\Gamma}{2DC}\left(h - \frac{1}{n}\right)\right] = \frac{\pi\Gamma_a \sigma_0}{2D} f_a . \tag{38}$$

Here D is the average distance between resonances, $h^2 = 1 + (\sigma_0' C)/(\sigma_p + \sigma_0)$, σ_0' is the value of the cross-section at resonance energy and f_a the coefficient of resonance self-shielding [1, 2].

For capture resonance $\Gamma_f = 0$ and $\delta\sigma_{az} < 0$, and for fission resonance $\delta\sigma_{az} > 0$ if $\beta\nu\Gamma_f > \Gamma_a$.

For scattering resonances $(\Gamma_f = 0, \Gamma_a << \Gamma)$ the bilinear correction is small. For capture resonances $(\Gamma_a \simeq \Gamma)$ the bilinear-averaged cross-section can be appreciably smaller than the flux-averaged cross-section (approximately by a factor of two).

When there is no resonance structure (for example, when the cross-sections in the sub-groups of the given group j are constant), it follows from Eq. (34) that the value of $\delta\sigma_{az\alpha}^j$ becomes zero.

K_{eff} and φ^j can be preserved in this case, too, by redetermining the elastic slowing-down cross-section and the bilinear-averaged fission spectrum $\tilde{\chi}^j$, as is shown in Ref. [15]. For values of $\delta\Sigma_{az}^j$ and δD^j specified in the limited interval of groups $n \leqslant j \leqslant m$, if we stipulate that the group flux φ^j calculated with constants modified in this manner

$$\varphi^j = \frac{\chi^j + \delta\chi^j + \sum_{i=1}^{j-1}\Sigma_{in}^{i \to j}\varphi^i + (\bar{\Sigma}^{j-1 \to j} + \delta\Sigma^{j-1 \to j})\varphi^{j-1}}{\bar{\Sigma}_a^j + \delta\Sigma_{az}^j + \Sigma_{in}^j + \bar{\Sigma}^{j \to j+1} + \delta\Sigma^{j \to j+1} + (D^j + \delta D^j)B^2} , \tag{39}$$

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should coincide with the result of calculation with the flux-averaged constants (22), we then get [15]

$$
\left.
\begin{aligned}
\delta\Sigma^{m-1\to m} &= \varphi^m(\delta\Sigma_a^m + \delta D^m)/\varphi^{m-1}; \\
\delta\Sigma^{i-1\to i} &= \varphi^i(\delta\Sigma_a^i + \delta D^i + \delta\Sigma^{i\to i+1})/\varphi^{i-1}; \\
\delta\chi^n &= \varphi^n(\delta\Sigma_a^n + \delta D^n + \delta\Sigma^{n\to n+1}). \quad (n \leqslant i < m)
\end{aligned}
\right\}
\quad (40)
$$

The minimum number of groups n up to which the slowing-down cross-section has to be redetermined is, in this case, undetermined. The redetermination can be made, for example, up to the fourth group, starting from which the calculation of factor b^j takes place in the BNAB 26-group method. It is physically justified rather to redetermine the slowing-down cross-sections (40) up to an energy of about 100 keV, i.e. up to the eighth group, when the resonance structure of the fertile and fissile materials virtually vanishes. The uncertainty in the importance function and in the value of the bilinear functionals (let us recall that the values of K_{eff} and group fluxes remain unchanged) obtained during change in group number n may describe the accuracy of corrections of this type.

RESULTS OF CACLULATIONS WITH BILINEAR-AVERAGED CONSTANTS AND DISCUSSION

Figure 1 shows the group fluxes φ^j and neutron importance $\bar{\varphi}^{+j}$ for the critical assembly BFS-44, which is similar in structure to the model for the fast power reactor ZPR-VI-7 [16], calculated with the BNAB-78 system of constants in the sub-group representation, as well as for the critical assembly BFS-33-2 [17, 18] consisting mainly of uranium dioxide with about 8% enrichment giving $K_\infty \approx I$.

For the same assemblies Fig. 2 gives the $\varphi^{+j}/\bar{\varphi}^{+j}$ ratios obtained with allowance for non-resonance bilinear effects (calculation with modified cross-sections (20), (21) and (24) for linear and parabolic interpolation when calculating b^{+j}) as well as the consequences of making allowance for resonance effects (Eqs (34)-(37)), with

redetermination of the slowing-down cross-section up to the fourth and the seventh BNAB group. The resonance structure was calculated from the eighth to the twenty-second group.

The second column in Table 1 presents the evaluated experimental values of the ratios (in relation to ^{235}U) of the central reactivity coefficients for a number of elements corresponding to the conditions for homogeneous calculations by the first-order perturbation theory [17, 19, 20]. The evaluation was performed by the methods described in Refs [14, 21].

The results of calculations by the perturbation theory with flux-averaged constants are given in the third column. The fourth and fifth columns contain the additions to the calculation needed when allowing for resonance (fourth column) and non-resonance bilinear (fifth column) effects.

In all the cases given, the uncertainty in the corrections due to selection of the model for obtaining b^{+j} or group number n does not exceed 20% of the experimental error.

The agreement between the value of the resonance bilinear effects and the results of "exact" (228-group [12] and 300-group [14]) calculations lies within 20 and 30%.

It would seem sufficient to increase the number of the BNAB groups by a factor of 10-20 in order to dispense with the concept of b^j (and, of course, b^{+j}), and there will be no need to take into account the non-resonance bilinear effects. It will still be necessary, for some time to come, to take account of the resonance bilinear effects, especially when interpreting experimental data for assemblies with "soft" neutron spectra.

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Table 1

Comparison of experiment and calculations with
flux-averaged and bilinear-averaged constants for the ratios of
reactivity coefficients in critical assemblies

Ratio ρ_i/ρ_{235_U}	Experiment	BNAB-78 calculation	Bilinear addition	
			Resonance	Non-resonance
BFS—26				
^{239}Pu	1,376±0,040	1,363	0,012	0,019
^{238}U	-	-0,331	0,0080	-0,0150
^{10}B	-3,43±0,13	-3,181	-0,069	-0,208
^{12}C	0,0239±0,0010	0,0217	0,0005	0,0022
BFS—33—2				
^{239}Pu	0,248±0,012	1,268	0,005	0,006
^{10}B	-0,87±0,03	-0,831	-0,007	-0,015
^{12}C	-0,0045±0,0004	-0,0059	0,0004	0,0010
^{6}Li	-0,352±0,003	-0,340	-0,006	-0,003
BFS—35				
^{239}Pu	1,460±0,015	1,463	0,000	-0,003
^{10}B	-0,51±0,02	-0,452	0,000	+0,004
^{12}C	-0,0224±0,0011	-0,0230	0,0001	-0,0006
BFS—38				
^{239}Pu	1,44±0,01	1,441	0,000	-0,005
^{10}B	-0,404±0,015	-0,397	0,000	0,011
^{12}C	-0,0300±0,0011	-0,0321	0,0001	-0,0015
^{240}Pu	0,218±0,005	0,241	0,000	-0,0002
^{241}Pu	1,54±0,03	1,81	0,000	-0,005
^{238}U	-0,0553±0,0015	-0,0580	-0,0001	0,0012
BFS—39				
^{239}Pu	1,350±0,015	1,348	0,009	0,005
^{238}U	-0,090±0,003	-0,0900	-0,0015	-0,0021
^{10}B	-1,260±0,035	-1,151	-0,034	-0,025
^{12}C	0,0033±0,0004	0,00226	0,00065	0,00090
^{6}Li	-0,466±0,007	-0,460	-0,012	-0,006
BFS—41				
^{239}Pu	1,207±0,012	1,199	-0,001	0,000
^{238}U	-0,058±0,002	-0,0613	-0,0002	0,0007
^{10}B	-0,70±0,03	-0,612	-0,007	0,000
^{12}C	-0,0104±0,0004	-0,0124	0,00027	0,0008
^{240}Pu	0,108±0,016	0,116	-0,0004	-0,0004
^{241}Pu	1,850±0,013	1,780	-0,002	0,001
BFS—44				
^{239}Pu	1,273±0,015	1,265	0,003	0,002
^{238}U	-0,067±0,003	-0,0670	-0,0009	-0,0002
^{10}B	-0,920±0,025	-0,816	-0,012	-0,010
^{12}C	-0,0063±0,0004	-0,0075	0,0002	0,0005
^{6}Li	-0,352±0,003	-0,347	-0,004	0,000
Ta	-0,0049±0,0004	-0,0061	0,0002	0,0003

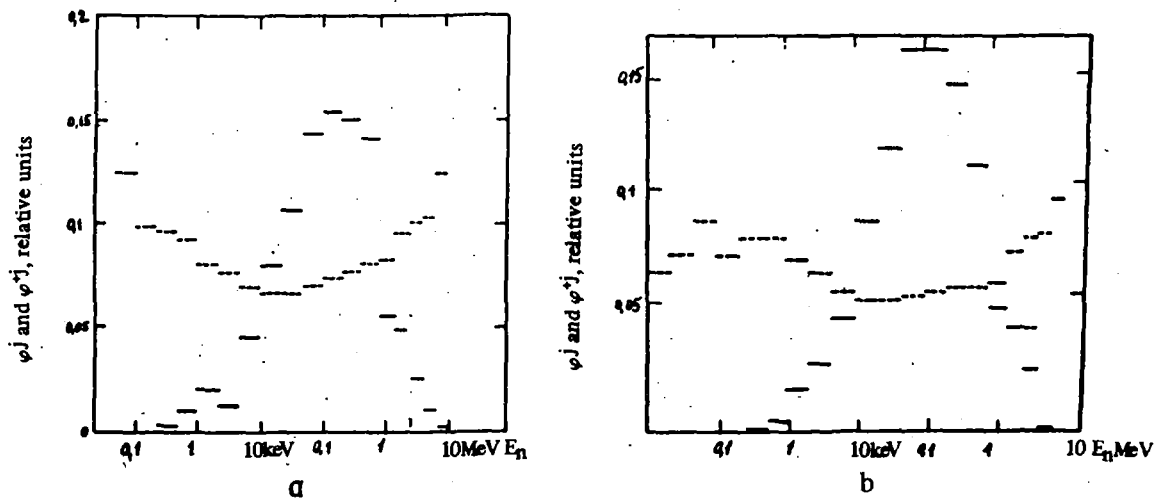| Ratio ρ_i/ρ_{235_U}	Experiment	BNAB-78 calculation	Bilinear addition	
			Resonance	Non-resonance
^{240}Pu	0,137	0,14I	0,000I	-0,00I0
^{241}Pu	I,860±0,040	I,860	0,003	0,002
KBR—3—3				
^{10}B	-I,73±0,06	-I,786	-0,066	-0,005
^{12}C	-0,0025±0,0003	-0,00I9I	0,000I2	0,00000
Fe	-0,00365±0,000I2	-0,00329	+0,000II	0,0000I
Ni	-0,00790±0,00020	-0,00936	-0,00045	-0,00004
Cr	-0,00580±0,00030	-0,00566	0,00007	-0,0000I

Fig. 1. Group fluxes φ^j (————) and neutron importance $\bar{\varphi}^{+j}$ (- - -) in the BFS-44 (a) and BFS-33 (b) critical assemblies.
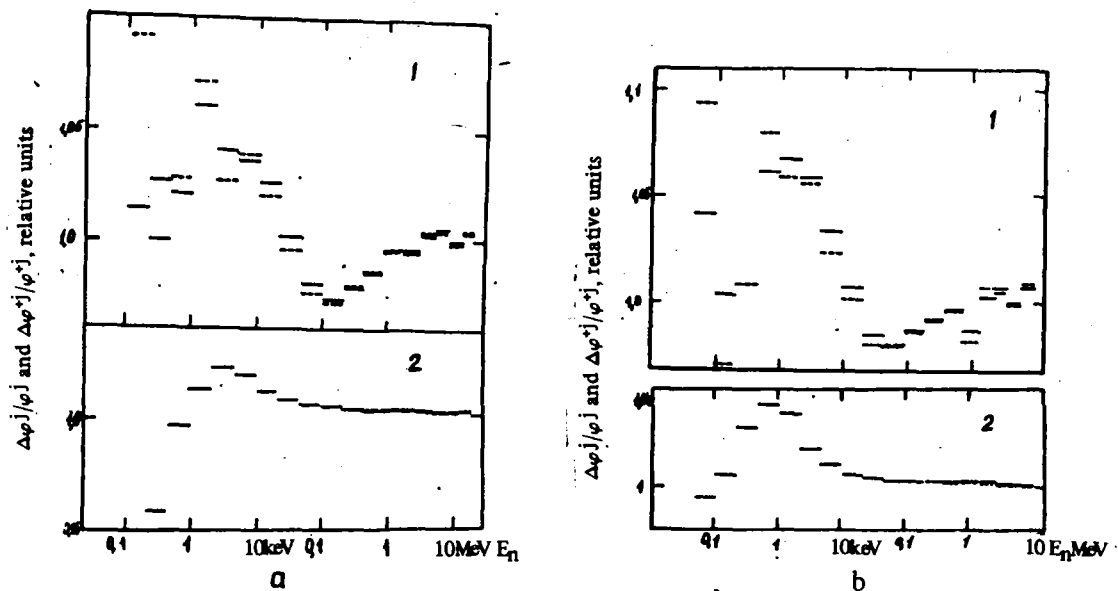
Fig. 2. Variation in neutron imporance $\varphi^{+j}/\overline{\varphi}^{+j}$ with allowance for: (1) Non-resonance bilinear effects (- - - linear and _____ parabolic interpolation); (2) resonance effects (_____ redetermination of the slowing-down cross-section up to the 4th and - - - up to the 7th group) in the BFS-44 (a) and BFS-33-2 (b) critical assemblies.