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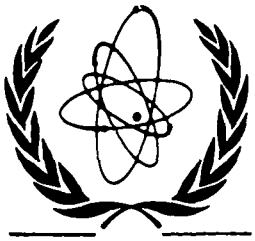

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CALCULATION OF SELF-SHIELDING FACTORS FOR CROSS-SECTIONS IN THE UNRESOLVED RESONANCE REGION USING THE GRUCON APPLIED PROGRAM PACKAGE

Translated from Nuclear Constants 5(54) 3 (1983)
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CALCULATION OF SELF-SHIELDING FACTORS FOR CROSS-SECTIONS IN THE UNRESOLVED RESONANCE REGION USING THE GRUCON APPLIED PROGRAM PACKAGE

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ABSTRACT

The author gives a scheme for the calculation of the self-shielding factors in the unresolved resonance region using the GRUCON applied program package. Some typical examples of calculation are considered and the results are compared with those of other authors. The calculation accuracy is better than 2%.

Computerization of the process of conversion of evaluated neutron cross-section data into multigroup microscopic constants is an important component in developing a system of providing constants for reactor neutron-physics and radiation safety calculations [1]. Since the end of the seventies the Institute of Power Physics (Obninsk) has been working on GRUCON, an applied program package designed for the solution of this problem. The first operative version of the package [2-4] made is possible to perform computerized calculations of the microscopic unshielded group cross-sections on the basis of computerized evaluated data libraries in the ENDF/B format [5]. It was used in late 1982 to carry out a preliminary conversion of the foreign libraries available to the author (the US libraries ENDL-78 [6] and ENDF/B [7], certain files of the ENDF/B library [8] and the Japanese JENDL-1 library [9]) into 28-group unshielded cross-sections averaged with the weight of the standard spectrum in the Bondarenko-Nikolaev-Abagyan-Bazazyants grouping [10].

The purpose of the second stage of the work on the GRUCON package was to be able, on the basis of the evaluated data libraries in the ENDF/B format, to obtain the values of multigroup shielded cross-sections and also other functionals of cross-sections of practical interest, for example the experimentally measured transmission and self-indication functions. When calculating these values it is necessary to take into account their dependence on the composition and temperature of the material. A slight complication in the form of the functionals leads to very large calculation difficulties - the volume of calculations is hundreds of times bigger and much more complex procedures and calculation schemes are required. This comment refers mostly to the unresolved resonance region considered in this paper.

For a solution of the problem of computerized calculation of group constants on the basis of evaluated data libraries, the algorithms and calculation schemes should satisfy the following requirements:

- The calculation model used should be consistent with the physical concepts on which the initial evaluated data library is based;
- The data processing scheme should be sufficiently universal to make it possible to obtain any functionals for micro-cross-sections of practical interest;
- The calculation accuracy should be higher than the accuracy of the data in order to preclude substantial distortions of the data during conversion (the actual calculation accuracy is about 1%);
- The time of conversion of the library unit of information - material - should be acceptable from the standpoint of the existing practice in preparing the group constants, for example, it should not exceed 1 h on the BEhSM-6 computer.

Very careful consideration of procedures recommended for the processing of unresolved resonance parameters from the ENDF/B library [11-13] revealed that they only had a narrow sphere of application [11], or that they did not ensure the requisite calculation accuracy for the functionals of interest to us [12], or else that they were not sufficiently fast (the computer time spent was more than 10 h for the BEhSM-6 when ten-point quadrupole formulae were used [13]). The present study proposes a set of algorithms and calculation schemes satisfying all the above requirements. It is used in the second version of the GRUCON package [14], which has been operating in the BEhSM-6 computer since the beginning of 1983, in the *U/D-F, *F/G-E and *F/C-F modules.

1. FORMULATION OF THE PROBLEM

In the region of unresolved resonances the ENDF/B library format provides for the storage of the following characteristics of target nuclei and parameters of their interactions with neutrons: atomic weight A; target nucleus spin I; effective scattering radius R_{ef} used for calculation of the scattering phase ϕ_ℓ (see also the note at the end of section 2), and orbital moment ℓ. For a given state of the compound nucleus and its decay probability along the different channels for each level system determined by the values of moment J and parity π, we give the average resonance parameters as a function of incident neutron energy: the average distance D between neighbouring resonances; reduced neutron width Γ_n^o; radiative capture width Γ_γ; fission width Γ_f; and width Γ_{com} of all processes competing with those mentioned earlier (usually inelastic scattering). The energy dependence of these parameters is given in tabular form.

In addition to the average values of the resonance parameters, the laws governing their probabilistic distributions are also given: the Porter-Thomas distribution with the parameter - number of degrees of freedom ν for resonance widths, and the Wigner distribution for distances between neighbouring resonances. The Breit-Wigner formula is recommended for calculation of the energy dependence of cross-sections (see section 2).

The purpose of the calculation is to find the values of functionals of the shielded cross-section type and transmission functions as a function of parameters of the material: temperature T; dilution cross-section σ_o; and target thickness t. For calculation of the shielded cross-sections they take the form:

$$\overline{\langle 1/[\sigma(E,T)+\sigma_0]^n\rangle_g}\,, \qquad \overline{\langle \sigma_r(E,T)/[\sigma(E,T)+\sigma_0]^n\rangle_g}\,, \tag{1}$$

while for the transmission and self-indication functions

$$T^g(t,T)=\overline{\langle \exp[-\sigma(E,T)t]\rangle_g}, \quad T_r^g(t,T)=\overline{\langle \sigma_r(E,T)\exp[-\sigma(E,T)t]\rangle_g}\,, \tag{2}$$

where $\sigma(E,T)$ is the total cross-section and $\sigma_r(E,T)$ the cross-section for a reaction of type r; the line denotes averaging over the distribution of resonance parameters; $\langle \ldots \rangle_g$ is averaging over energy with the weight of the standard spectrum in the group interval ΔE_g. Most of the quantities encountered

in practice are associated with these functionals by simple relationships. For example, the resonance self-shielding factors for the total cross-section and for the r-type reaction cross-section are expressed in terms of functionals as follows:

$$f^g(\sigma_0,T)=\frac{\langle\sigma(E,T)/[\sigma(E,T)+\sigma_0]^2\rangle_g}{\langle\sigma(E,T)\rangle_g\langle 1/[\sigma(E,T)+\sigma_0]^2\rangle_g},\qquad f_r^g(\sigma_0 T)=\frac{\langle\sigma_r(E,T)/[\sigma(E,T)+\sigma_0]\rangle_g}{\langle\sigma_r(E,T)\rangle_g\langle 1/[\sigma(E,T)+\sigma_0]\rangle_g}. \quad (2A)$$

2. CALCULATION MODEL

The calculations of the functionals of cross-sections (1) and (2) are based on the assumption that there is no correlation in the energy dependence of cross-sections of structures due to the different systems of levels. On this assumption we can calculate the functionals independently for each cross-section component determined by a particular system of levels, and obtain the integral quantities sought by means of convolution procedures (see section 6). Confining ourselves to one system of levels, we shall assume that the values of cross-sections $\sigma(E)$ and $\sigma_r(E)$ at a given energy point E are determined by the following factors:

- The distance from point E to the two nearest resonances situated below (L) and above (H) energy E: $E-E_L$ and E_H-E (hereafter we shall also use an equivalent set of variables: $S = E-E_L$ the position of the L-resonance and $D = E_H-E_L$ the distance between neighbouring resonances);
- The value of the resonance widths of the two nearest resonances: neutron Γ_{nL} and Γ_{nH}, radiative $\Gamma_{\gamma L}$ and $\Gamma_{\gamma H}$ and so on; the total sets of these widths for each resonance will be denoted in the form of vectors $\vec{\Gamma}_L$, $\vec{\Gamma}_H$.

The contributions of all other resonances over the energy range limited by these two resonances will be regarded as small. We write the Breit-Wigner formula for the J-system of resonances at T = 0 with allowance for the above limitations and the data of Ref. [15] in the form:

$$\sigma^J(E)=\sigma_p^J+4\pi\lambda^2 g_J\sum_\lambda\frac{\Gamma_{n\lambda}}{\Gamma_\lambda}\frac{G_\lambda^J+x_\lambda H_\lambda^J}{1+x_\lambda^2}+\delta\sigma^J;$$

$$\sigma_r^J(E)=4\pi\lambda^2 g_J\sum_\lambda\frac{\Gamma_{n\lambda}\Gamma_{r\lambda}}{\Gamma_\lambda^2}\frac{1}{1+x_\lambda^2}+\delta\sigma_r^J,\quad r\neq\ell; \quad (3)$$

$$\sigma_\ell^J(E)=\sigma^J-\sum_{r\neq\ell}\sigma_r^J(E),$$

where $x_\lambda = (E-E_\lambda)/\Gamma_\lambda$; $\sigma^J(E)$, $\sigma_r^J(E)$, $\sigma_\ell^J(E)$ are the total-interaction, r-type reaction and elastic-scattering cross-sections, respectively; $\sigma_p^J = 4\pi\lambda\!\!\!^{-2} g_J \sin^2\phi_J$ is the potential-scattering cross-section; $\delta\sigma^J$, $\delta\sigma_r^J$ are the contributions of distant resonances to the total cross-section and the r-type reaction cross-section; $\lambda\!\!\!^-$ is the incident-neutron wavelength; $g_J = (2J+1)/[2(2I+1)]$ is a statistical factor; G_λ^J, H_λ^J are terms for the interference of the two resonances:

$$G_\lambda^J = \sum_{\lambda' \neq \lambda} \frac{\Gamma_{n\lambda'}(\Gamma_\lambda + \Gamma_{\lambda'})/2}{(E_\lambda - E_{\lambda'})^2 + (\Gamma_\lambda + \Gamma_{\lambda'})^2/4} + \cos 2\phi_J ,$$

$$H_\lambda^J = \sum_{\lambda' \neq \lambda} \frac{\Gamma_{n\lambda'}(E_\lambda - E_{\lambda'})}{(E_\lambda - E_{\lambda'})^2 + (\Gamma_\lambda + \Gamma_{\lambda'})^2/4} + \sin 2\phi_J ; \qquad (3A)$$

subscript λ has the values of L and H.

The elastic scattering phase ϕ_ℓ can be calculated by the equation $\phi_o = \hat{\rho}$; $\phi_1 = \hat{\rho} - \text{arctg}\,\hat{\rho}$; $\phi_2 = \hat{\rho} - \text{arctg}[\hat{\rho}/(3-\hat{\rho}^2)]$, where $\hat{\rho} = kR_{ef}$; R_{ef} is the effective scattering radius given in the data library and k the wave number. Neutron widths Γ_n^ℓ are associated with the reduced neutron widths Γ_n^o by the relation $\Gamma_n^\ell = \Gamma_n^o \sqrt{E} v_\ell \nu$, where E is incident-neutron energy, eV, ν the number of elastic-scattering channels, v_ℓ the penetrability factor for a neutron with orbital moment ℓ. To calculate v_ℓ we can use the approximation of an even spherical nucleus: $v_o = 1$, $v_1 = \rho^2/(1+\rho^2)$, $v_2 = \rho^4/(9+3\rho^2+\rho^4)$. Here $\rho = kR$, R being the radius of interaction calculated by the formula $R = (1.23\,A^{1/3} + 0.8)10^{-13}$ cm, where A is ratio of nuclear mass to neutron mass.

Hereafter we shall consider only one system of levels and subscript J will be dropped.

In the unresolved resonance region there is no information about the exact position and width of resonances and therefore parameters E_L, E_H, $\vec{\Gamma}_L$, $\vec{\Gamma}_H$ are regarded as random quantities governed by the well-known theoretical probabilistic distributions [16]. For resonance widths Γ_r (components of vector $\vec{\Gamma}$) it is the Porter-Thomas distribution (Fig. 1a):

$$P_{\Pi T}(x) = \frac{\nu}{2\Gamma(\nu/2)} \left(\frac{x\nu}{2}\right)^{\nu/2-1} \exp\left(-\frac{x\nu}{2}\right), \quad x = \Gamma_z/\bar{\Gamma}_z , \quad x \in [0, \infty) ; \qquad (4)$$

For distances D between neighbouring resonances we have the Wigner distribution (Fig. 1b); $P_B(y) = (\pi/2)y \exp(-\pi y^2/4)$; $y = D/\bar{D}$, $y\in[0,\infty)$; for resonance shift S we shall assume an equiprobable distribution over the whole range of variation from 0 to D: $\phi_s(z) = 1$; $z = S/D$, $z\in[0,1]$. We write the expected value of the functional of cross-section in the form of a multiple integral

$$\overline{F(E,\vec{P})} = \int \ldots \int \langle F(E,\vec{P},S,\vec{R})\rangle P(\vec{R})d\vec{R}\,, \tag{5}$$

where the form of function F is determined by relationships (1) and (2); $\vec{P}$ is the set of parameters of the functional, $\vec{R}$ the set of resonance parameters and $\langle\ldots\rangle$ averaging over resonance shift S.

The group average values of the functionals can be obtained by averaging with the weight of the standard spectrum $\phi(E)$ over the group interval ΔE_g

$$\overline{\langle F(E,\vec{P})\rangle_g} = \int_{\Delta E_g} \overline{F(E,\vec{P})}\varphi(E)dE \Big/ \int_{\Delta E_g} \varphi(E)dE\,. \tag{5A}$$

3. FLUCTUATIONS IN RESONANCE PARAMETERS

The multiplicity of the integral in expression (5) is determined by the number of fluctuating resonance widths N and equals 2N + 1. The ENDF/B library format allows N = 4. Calculation of the integrand is a laborious operation, which includes computing the complex functions for Doppler broadening and integration over the resonance parameters. Under these conditions it is natural that the nine-fold integral can only be calculated by taking careful account of the behaviour of the integrand. So far in the calculation programs for constants only the form of the weighting function has governed the selection of the system mesh points for integration, the number of those mesh points being generally ten [17, 18]. An attempt was made in Ref. [19] to take into account the special form of the integrable function for the given problem in constructing the quadrature formulae. It was shown that to attain an accuracy of about 1% in evaluating the average values of cross-sections one could use two to six mesh points, instead of ten, depending on the value of parameter ν for any ratios of the average resonance parameters. When determining the parameters of the quadrature formulae the new version of the GRUCON package takes into account not only the shape of the dependence of the integrand on the integration parameters, but also the ratios between the average resonance parameters. For example, let us consider the dependence of the expected value

of the radiative-capture cross-section on the parameter $\alpha = \overline{\Gamma}_\gamma / \overline{\Gamma}_n$, which characterizes the ratios between the average resonance parameters for elastic scattering and radiative capture. We will assume that Γ_γ does not fluctuate ($\Gamma_\gamma = \overline{\Gamma}_\gamma$). The expected value of the radiative capture cross-section can then be represented in the form

$$\langle \overline{\sigma_\gamma} \rangle_s = \sigma_{\gamma 0} \int_0^\infty \frac{x}{x+\alpha} P_{n\tau}(x) dx , \tag{6}$$

where $x = \Gamma_n / \overline{\Gamma}_n$, $\sigma_{\gamma 0}$ is a constant. Figure 2 shows the dependence of the cross-section $\overline{\langle \sigma_\gamma \rangle_s}$ on parameter α for $\nu = 1$ degrees of freedom. As will be seen from the figure, the fluctuation effect can be as much as 30% approximately.

The integration on the right-hand side of Eq. (6) can be performed with the help of the quadrature formula

$$\int_0^\infty \frac{x}{x+\alpha} P_{n\tau}(x) dx \approx \sum_i a_i \frac{x_i}{x_i+\alpha} , \tag{7}$$

where a_i, x_i are the weights and mesh points of quadrature formula (7), which we shall determine by the Gauss scheme [20]. Considering the form of the integrable function in formula (6), we redefine the weighting function as:

$$P(x) = C_0 P_{n\tau}(x) / (x+\alpha_0)^L , \tag{7A}$$

where α_0, L are the optimization parameters (the choice of their values is discussed below);

$$C_0^{-1} = \int_0^\infty \frac{P_{n\tau}(x)}{(x+\alpha_0)} dx \quad \text{normalization constant.} \tag{7B}$$

The moments obtained for the weighting function are expressed in terms of the degenerate hypergeometric functions [21] and can be calculated by the formula (see section 9)

$$M_n = \int_0^\infty x^n P(x) dx . \tag{7C}$$

The parameters sought a_i, x_i are determined from the system of non-linear equations:

$$M_n = \sum_{i=1}^{N} a_i x_i^n , \quad n = 0, 1, \ldots, 2N-1 ; \tag{8}$$

where N is the number of mesh points. The values of the optimization parameters can of course be made equal to: $\alpha_o = \bar{\Gamma}_\gamma/\bar{\Gamma}_n$, $L = -1$ since in this case the cross-section can be expressed in terms of moment M_1 ($\langle \bar{\sigma}_\gamma \rangle = \sigma_{\gamma o} C_o^{-1} M_1$) and calculated accurately by formula (7) for $N = 1$.

If there are several fluctuating widths, the expected value of the cross-section can be represented in the form of a multiple integral over each of the variables $x_r = \Gamma_r/\bar{\Gamma}_r$. Let $x_{r'}$ be one of the variables x_r. When considering the dependence of the cross-section on resonance parameters (see Eq. (3)) we can see that the integrand in formula (6) retains its form if we take parameter α to mean not simply the ratio of average widths but the linear combination of all integration variables except the one selected

$$\alpha = \sum_{z \neq z'} \alpha_z x_z , \qquad \alpha_z = \bar{\Gamma}_z / \bar{\Gamma}_{z'} . \tag{9}$$

Thus, in the presence of several fluctuating widths, parameter α in the integrand will no longer be a constant but a variable lying in the interval $[0, \infty)$, and the calculation accuracy of the expected cross-section value will be goverened by the accuracy of the quadrature approximation of dependence (7) on parameter α in some range of its variation. This range is determined by the distribution width of random parameters x_r entering into α and by the ratio of the average resonance parameters α_r (see formula (9)). From the form of the distributions (see Figs 1a, 1b) it follows that the distribution of the random quantity α has a clearly expressed maximum, the position of which we shall denote by x_{ro} (x_{ro} is the most probable value of x_r). For the Porter-Thomas distributions from Eq. (4) we obtain $x_{ro} = 1-2/\nu_r$ for $\nu_r > 2$, $x_{ro} = 0$ for $\nu_r < 2$ and $\alpha_o = \sum_{r \neq r'} \alpha_r x_{ro}$ for the most probable value of α. It is this value which we shall use to determine the moments and parameters of the quadrature formulae for the selected variable $x_{r'}$.

The possibility of a local approximation in the neighbourhood of α_o is illustrated in Fig. 2, from where it will be seen that the number of mesh points $N = 3$ enables us to describe the exact curve with an error of up to 1% for a variation of parameter α by a factor of about 10 for any values of α_o. To compensate for the integration error we have made the approximation for α sign-variable by choosing the right value of parameter $L = -3$ (in the general case $L = -N$).

We have so far been looking at calculation of the expected values of the linear functionals of cross-sections. It is natural to ask how far the integration schemes given above are applicable to the evaluation of functions of a more complex form, which determine the values of the self-shielding factors (for example, functional (1)). It was shown in Ref. [19] that the n-th moment of cross-sections of form (1) for a selected integration variable x could be represented in the form of a linear combination of integrals

$$C_{k,m}(\alpha,\beta)=\int_0^\infty \frac{x^k P_{n\tau}(x)dx}{[(x+\alpha)(x+\beta)]^{m/2}},\quad m=2t+1,\quad i=0,1,\ldots,n;\quad k=1,2,\ldots,2n+1, \qquad (10)$$

where α, β are the linear combinations of integration variables which do not coincide with the selected variable.

The form of the integrand in Eq. (10) shows that the systems of mesh points found for the linear functionals will be sufficiently effective here also. The verification was performed in the most critical case (for zero temperature and undiluted material) for the resonance width ratio and the form of distribution corresponding to the maximum fluctuation effect. The moments of $\langle 1/\sigma\rangle$ and $\langle \sigma_\gamma/\sigma\rangle$ were calculated for different numbers of mesh points: N = 2, 3, ..., 10. The results are shown in Fig. 3a. In the critical case considered an accuracy of about 1% is attained for N = 5.

Distributions with higher values of ν and the Wigner distribution require a smaller number of mesh points. In particular, N = 2 is always sufficient for averaging over the Porter- Thomas distribution with $\nu > 5$ and over the Wigner distribution (Fig. 3b). For calculation of moments up to and including the second order at approximately 1% required accuracy the GRUCON package uses the following dependence of the number of mesh points on the form of distribution:

$$N = \begin{cases} 5 - E(\nu/2) & \text{for } \nu < 5 \\ 2 & \text{for } \nu \geqslant 5 \\ 2 & \text{for the Wigner distribution} \end{cases}$$

4. THE DOPPLER EFFECT

In order to allow for the dependence of the cross-section on the temperature of the material, we need to integrate its energy dependence over the energy distributions of the target nuclei $\sigma(E,T) = \int \sigma(E')F(E-E',T)dE'$. In the ideal-gas model this distribution takes the form

$$F(E-E',T)=\frac{1}{\sqrt{\pi}\Delta}\exp\left[-\left(\frac{E-E'}{\Delta}\right)^2\right], \qquad (11)$$

where $\Delta = 2\sqrt{K_B TE/A}$; $K_B = 8.61735 \times 10^{-5}$ eV is the Boltzmann constant; T the target temperature, K; E the incident neutron energy, eV; and A the ratio of the target nucleus mass to the neutron mass.

For the Breit-Wigner formula (3) consideration of the target temperature amounts to replacement of functions $1/(1 + x_\lambda^2)$ and $x_\lambda/(1 + x_\lambda^2)$ determining the resonance shape by the functions

$$\psi(x,\xi) = \frac{\sqrt{\pi}\xi}{2} u\left(\frac{x\xi}{2} + i\frac{\xi}{2}\right),$$
$$\chi(x,\xi) = \frac{\sqrt{\pi}\xi}{2} v\left(\frac{x\xi}{2} + i\frac{\xi}{2}\right), \qquad (12)$$

where $\xi = \Gamma/\Delta$; u(z) and v(z) are the real and imaginary parts of the complex probability integral:

$$w(z) = u(z) + iv(z) = e^{-z^2}\left[1 + (2i/\sqrt{\pi})\int_0^z e^{t^2} dt\right]. \qquad (12A)$$

The method proposed in Ref. [22] is used to calculate functions $\Psi(x,\xi)$ and $\chi(x,\xi)$.

When the temperature dependence is taken into account, the calculation volume increases because of the multiple calculations of functions $\Psi(x,\xi)$ and $\chi(x,\xi)$ and also because of going over from the explicit expression of the integral to the numerical integration scheme in the calculation of functionals of form $\langle \sigma_r/(\sigma + \sigma_o)^n \rangle$ (only the numerical scheme is applicable in any case to functionals of form $\langle \sigma_r \exp(-\sigma t) \rangle$). Changing to the numerical integration scheme involves an increase in the amount of calculation by several factors of 10, thereby making it necessary to optimize the computational scheme even at this stage of calculation. In the GRUCON package the optimization problem is solved by selecting a more or less rigorous approximation for the cross-section calculations, depending on the calculation accuracy for a particular cross-section component. Since the sensitivity of the resulting functional to the different corss-section components varies by several orders, the possible approximations may have a very wide spectrum. Below we give only those which have at present been used in the program.

Approximation by the Lorentz function

Kolesov and Luk'yanov [23] suggested an approximate method for consideration of the Doppler effect, which enables us in some cases to avoid the laborious

calculations of functions $\Psi(x,\xi)$ and $\chi(x,\xi)$. Essentially, it consists of the following. In integral (12) we replace distribution (11) by the Lorentz function: $\tilde{F}(E-E') = \tilde{\Delta}/2\pi\{1/[(E-E')^2 + \tilde{\Delta}^2/4]\}$. The resonance shape functions will then take the form: $\tilde{\Psi}(x,\xi) = (1 + \tilde{\xi}^{-1})/[x^2 + (1 + \tilde{\xi}^{-1})^2]$, $\chi(x,\xi) = x/[x^2 + (1 + \tilde{\xi}^{-1})^2]$, $\tilde{\xi} = \Gamma/\tilde{\Delta}$, and this is equivalent to the replacement in Eq. (3) of the total resonance widths: $\Gamma \to \tilde{\Gamma} = \Gamma + \tilde{\Delta}$. The question is only how to determine the effective Doppler width $\tilde{\Delta}$. The authors of the method suggested the determination of $\tilde{\xi}$ from the equality

$$\int \Psi^2(x,\xi)dx = \int \tilde{\Psi}^2(x,\bar{\xi})dx, \qquad (12B)$$

which gives us the dependence $\bar{\xi}^{-1}(\xi) = \Psi^{-1}(0,\xi/2)-1$. This method of determining $\bar{\xi}$ was verified by comparison with the results of exact calculations of the temperature dependence of the moments of cross-sections, i.e. using functions $\Psi(x,\xi)$ and $\chi(x,\xi)$ (Fig. 4a, 4b).

The nature of the deviations of the quantity being approximated from the exact curve indicates that it is possible to obtain a better approximation by introducing an adjusting parameter γ: $\tilde{\xi}^{-1}(\xi) = \Psi^{-1}(0,\gamma\xi) - 1$. For $\gamma = 2.0$ the deviation of the quantity being approximated from the exact curve decreased by several factors and did not exceed 5%.

Approximation of equidistant identical resonances

Consideration of the Doppler effect through redetermination of resonance widths does not change the shape of the dependence of the cross-section on energy for T = 0 so that the explicit expressions for the integrals over energy can be used to calculate the functionals $\langle 1/(\sigma + \sigma_0)^n \rangle$ and $\langle \sigma_r/(\sigma + \sigma_0)^n \rangle$. It is most convenient to obtain these expressions in the approximation of equidistant identical resonances proposed in Refs [16, 24]. Assuming $\Gamma_\lambda = \tilde{\Gamma}$, $\Gamma_{r\lambda} = \Gamma_r$, $x_\lambda = 2(S - \lambda D)/\Gamma$, $\delta\sigma = \delta\sigma_r = 0$ in Eq. (3), we sum over all the resonances. The resonance shape functions with allowance for the Doppler effect take the form

$$\tilde{\psi}^\infty = \sum_{\lambda=-\infty}^{\infty} \frac{1}{1+x_\lambda^2} = \frac{\pi\tilde{\Gamma}}{2D} \frac{\mathrm{sh}(\pi\tilde{\Gamma}/D)}{\mathrm{ch}(\pi\tilde{\Gamma}/D) - \cos(2\pi S/D)},$$

$$\tilde{\chi}^\infty = \sum_{\lambda=-\infty}^{\infty} \frac{x_\lambda}{1+x_\lambda^2} = \frac{\pi\tilde{\Gamma}}{2D} \frac{\sin(2\pi S/D)}{\mathrm{ch}(\pi\tilde{\Gamma}/D) - \cos(2\pi S/D)}. \qquad (13)$$

The interference terms

$$G^{\infty}=\frac{\Gamma_n}{\Gamma}\left[\frac{\pi\Gamma}{D}\operatorname{cth}\left(\frac{\pi\Gamma}{D}\right)-1\right]+\cos 2\phi;\qquad H^{\infty}=\sin 2\phi \tag{14}$$

after substitution into Eqs (3) enable them to be written in the form:

$$\sigma=\sigma_p+\sigma_m(G^{\infty}\tilde{\psi}^{\infty}+H^{\infty}\tilde{\chi}^{\infty});\qquad \sigma_z=\sigma_m(\Gamma_z/\Gamma)\tilde{\psi}^{\infty},\quad z\neq\ell;$$
$$\sigma_\ell=\sigma-\sum_{z\neq\ell}\sigma_z,\quad \text{где}\qquad \sigma_m=4\pi\lambda^2 g(\Gamma_n/\tilde{\Gamma}). \tag{14A}$$

The functionals of the cross-sections sought are calculated by the equations

$$\left\langle\frac{1}{(\sigma+\sigma_0)^n}\right\rangle=\frac{1}{\pi C^n}\sum_{k=0}^{n}\binom{k}{n}(1-B)^{n-k}(1+B)^k\int_{-\infty}^{\infty}\frac{x^{2k}dx}{R^n(1+x^2)},$$
$$\left\langle\frac{\sigma_z}{(\sigma+\sigma_0)^n}\right\rangle=\frac{C_z}{\pi C^n}\sum_{k=0}^{n}\binom{k}{n-1}(1-B)^{n-k-1}(1+B)^k\int_{-\infty}^{\infty}\frac{x^{2k}dx}{R^n},\quad z\neq\ell, \tag{15}$$
$$\left\langle\frac{\sigma_\ell}{(\sigma+\sigma_0)^n}\right\rangle=\left\langle\frac{1}{(\sigma+\sigma_0)^{n-1}}\right\rangle-\sigma_0\left\langle\frac{1}{(\sigma+\sigma_0)^n}\right\rangle-\sum_{z\neq\ell}\left\langle\frac{\sigma_z}{(\sigma+\sigma_0)^n}\right\rangle.$$

Here $C=\sigma_m(\pi\Gamma_n/2D)$; $C_z=C(\Gamma_z/\Gamma)\operatorname{th}(\pi\tilde{\Gamma}/D)$; $B=1/\operatorname{ch}(\pi\tilde{\Gamma}/D)$; $R=\alpha x^2+\beta x+\gamma$,

where $\alpha=A+(\sigma_p+\sigma_0)(1+B)/C$, $\beta=-2BH^{\infty}$, $\gamma=A+(\sigma_p+\sigma_0)(1-B)/C$, $A=G^{\infty}\operatorname{th}(\pi\tilde{\Gamma}/D)$.

(For calculation of the integrals on the right-hand side of equalities (15) see section 10).

Approximation of fluctuation factors

Let us consider as an example the functional $\langle 1/\sigma(E,T,S,\Gamma,D)\rangle$. We will write down for it the identity

$$\langle 1/\sigma(E,T,S,\Gamma,D)\rangle=\frac{\overline{\langle 1/\sigma(E,T,S,\Gamma,D)\rangle}}{\langle 1/\sigma(E,T,S,\bar{\Gamma},\bar{D})\rangle}\langle 1/\sigma(E,T,S,\bar{\Gamma},\bar{D})\rangle, \tag{15A}$$

where $\bar{\Gamma}$, $\bar{D}$ are the average values of resonance widths and distances between levels. The ratio of the functionals

$$R(E,T)=\frac{\overline{\langle 1/\sigma(E,T,S,\Gamma,D)\rangle}}{\langle 1/\sigma(E,T,S,\bar{\Gamma},\bar{D})\rangle} \tag{15B}$$

is the fluctuation factor for the moment of cross-section $\langle 1/\sigma(E,T,S,\bar{\Gamma},\bar{D})\rangle$. The fluctuation factors for any of the functionals of interest to us are

determined similarly. There are grounds to assume that the dependence of factor R(E,T) on temperature T of the material is weaker than the dependence of the functionals of cross-sections entering into the factor. This means that for evaluation of its value the accuracy of the approximate methods given earlier may be quite sufficient. The example in Fig. 5a and b confirms this assumption. The second multiplier $\langle 1/\sigma(E,T,S,\bar{\Gamma},\bar{D})\rangle$ can be calculated by any exact, though laborious, algorithm since it does not require multiple integration over the resonance parameter distributions.

5. CONTRIBUTION OF DISTANT RESONANCES

In order to calculate $\delta\sigma$ and $\delta\sigma_r$ in Eqs (3) we use the approximation of identical equidistant resonances. Excluding from sums (13) the two terms corresponding to the L-resonance ($\lambda = 0$) and H-resonance ($\lambda = 1$) for the line shape function due to the contribution of distant resonances in the interval $[E_L, E_H]$ we obtain

$$\delta\tilde{\psi}^{\infty} = \tilde{\psi}^{\infty} - 1\Big/\left[1+(2S/\tilde{\Gamma})^2\right] - 1\Big/\left\{1+\left[2(S-D)/\tilde{\Gamma}\right]^2\right\};$$

$$\delta\tilde{\chi}^{\infty} = \tilde{\chi}^{\infty} - (2S/\tilde{\Gamma})\Big/\left[1+(2S/\tilde{\Gamma})^2\right] - \left[2(S-D)/\tilde{\Gamma}\right]\Big/\left\{1+\left[2(S-D)/\tilde{\Gamma}\right]^2\right\}, \tag{15C}$$

and, respectively, for the contributions of distant resonances to cross-sections:

$$\delta\sigma \approx \delta\tilde{\sigma}^{\infty} = \sigma_m(\delta\tilde{\psi}^{\infty}\cos 2\phi + \delta\tilde{\chi}^{\infty}\sin 2\phi),$$
$$\delta\sigma_z \approx \delta\tilde{\sigma}_z^{\infty} = \sigma_m(\Gamma_z/\Gamma)\delta\tilde{\psi}^{\infty} \tag{15D}$$

When calculating $\delta\sigma$ and $\delta\sigma_r$ the effect of fluctuations in the resonance parameters is not taken into account. This is quite acceptable since the ratio of the contribution of distant resonances to that of the nearest two is about Γ/D and it is consequently small in the sphere of application of the Breit-Wigner equation.

6. CONVOLUTION OF FUNCTIONALS

The functionals of cross-sections obtained for some systems of equations $\nu = J^{\pi}$ are used for the calculation of the functionals sought by convolution procedures corresponding to their forms. This procedure appears

to be the simplest for the transmission and self-indication functions. On the assumption that the distributions of the energy structures of cross-sections due to independent systems of equations are independent we write:

$$T(t)=\overline{\left\langle \exp\left(-\sum_{\nu}\sigma^{\nu}t\right)\right\rangle}=\prod_{\nu}\left\langle \exp(-\sigma^{\nu}t)\right\rangle=\prod_{\nu}T^{\nu}(t);$$

$$T_{z}(t)=\overline{\left\langle \sum_{\nu}\sigma_{z}^{\nu}\exp\left(-\sum_{\mu}\sigma^{\mu}t\right)\right\rangle}=\sum_{\nu}\overline{\left\langle \sigma_{z}^{\nu}\exp(-\sigma^{\nu}t)\right\rangle}\prod_{\mu\neq\nu}\overline{\left\langle \exp(-\sigma^{\mu}t)\right\rangle}=T(t)\sum_{\nu}\frac{T_{z}^{\nu}(t)}{T^{\nu}(t)}. \qquad (16)$$

For functionals of form $\overline{\langle 1/(\sigma+\sigma_{o})^{n}\rangle}$ and $\overline{\langle \sigma_{r}/(\sigma+\sigma_{o})^{n}\rangle}$ the convolution procedure is based on the use of an intermediate representation of the cross-section structure in the form of sub-group parameters. To obtain sub-group components a_{i}^{ν} and cross-sections σ_{i}^{ν}, σ_{ri}^{ν} it is convenient to use the scheme proposed in Ref. [25] with modifications to suit the specific features of the problem in hand: here, in the convolution procedure the sub-group parameters can be determined independently for each reaction r, dilution cross-section σ_{o} and temperature T. Having set these values, we consider the following system of non-linear equations as the initial system

$$\overline{\left\langle \frac{\sigma_{z}^{\nu}}{(\sigma^{\nu}+\sigma_{0})^{n}}\right\rangle}=\sum_{i=1}^{N}\frac{C_{zi}}{x_{i}^{n}}, \quad n=N, N-1, \ldots, -N+1. \qquad (16A)$$

By simple transformations this system can be reduced to the form of (8) and solved with the help of the same algorithms. The set of values of x_{i} found is then substituted into the system of linear equations

$$\overline{\left\langle \frac{1}{(\sigma^{\nu}+\sigma_{0})^{n}}\right\rangle}=\sum_{i=1}^{N}\frac{C_{i}}{x_{i}^{n}}, \quad n=-1,0,\ldots,N-2, \qquad (17)$$

from where the values of c_{i} are determined. The sub-group parameters sought are found from the relationships $a_{i}^{\nu}=c_{i}$, $\sigma_{i}^{\nu}=x_{i}-\sigma_{o}$, $\sigma_{ri}^{\nu}=c_{ri}/c_{i}$.

For functionals dependent only on the total cross-section, parameters a_{i}^{ν}, σ_{i}^{ν} are determined from the system of equations of the form of (17) which is non-linear with respect to c_{i} and x_{i} but has variation limits n = N,N - 1, ..., -N + 1. The functionals of cross-sections are calculated from the sub-group components and cross-sections found in accordance with the values of their parameters (type of reaction, dilution cross-section and temperature) by the formulae

$$\langle 1/(\sigma+\sigma_{0})^{n}\rangle=\sum_{i}a_{i}/(\sigma_{i}+\sigma_{0})^{n}; \quad \overline{\langle \sigma_{z}/(\sigma+\sigma_{0})^{n}\rangle}=\sum_{i}a_{i}\sigma_{zi}/(\sigma_{i}+\sigma_{0})^{n}, \qquad (17A)$$

where $a_{\vec{i}} = \prod_{\nu} a^{\nu}_{i_\nu}$, $\sigma_{\vec{i}} = \sum_{\nu} \sigma^{\nu}_{i_\nu}$, $\sigma_{r\vec{i}} = \sum_{\nu} \sigma^{\nu}_{ri_\nu}$; the summation is performed over all possible positions of sub-group vector $\vec{i} = \{i, i_2, \ldots, i_M\}$ where i_ν is the number of the sub-group for the ν-th system of levels and M the number of systems of levels. The convolution procedure using the sub-group representation of the cross-section structure does not presuppose any definite form for the resulting functional and is in this sense more universal than the preceding one. In particular, for the transmission and self-indication functions the following relationships are valid

$$T(t) \approx \sum_{\vec{i}} a_{\vec{i}} \exp(-\sigma_{\vec{i}} t);$$
$$T_\gamma(t) \approx \sum_{\vec{i}} a_{\vec{i}} \sigma_{\gamma\vec{i}} \exp(-\sigma_{\vec{i}} t) \qquad (18)$$

$\vec{i}$

The dependences of these functions on target thickness t, as calculated by expressions (18), can be regarded as sub-group approximations of exact curves (16). In order to see how well the sub-group approximation describes the exact functions, we obtained for the same set of resonance parameters the values of the transmission functions T(t) and the self-indication function for capture $T_\gamma(t)$ from exact Eqs (16) and approximate formulae (18) with a number of sub-groups N = 2 and N = 3. The calculation results are shown in Fig. 6a, 6b. Thus, the sub-group approximation satisfactorily describes the exact dependences for a small target width and is sign-variable (since it retains the exact values of the integrals of these functions) but yields exceedingly large relative errors for high values of t. This is understandable if we take into account the fact that the asymptotic behaviour of the transmission function cannot be represented by a finite number of sub-groups since it takes the form

$$T(t) \xrightarrow[t\sigma_{max} \gg 1]{} \frac{C}{\sqrt{\sigma_{max} t}} \exp(-\sigma_{min} t), \qquad (18A)$$

where σ_{min}, σ_{max} are the minimum and maximum values of the cross-sections over the averaging interval and C is a constant with respect to t [24].

7. PROGRAMMING

The calculation of the group functionals of cross-sections on the basis of the unresolved resonance parameters in the GRUCON applied program package is made with the help of three modules performing the following operations: calculation of detailed behaviour of the functionals of cross-sections from the unresolved resonance parameters for some systems of levels (module *U/D-F);

calculation of group average values of the functionals of cross-sections on the basis of the detailed dependences for a given group structure and shape of the standard spectrum (module *F/G-F); convolution of the functionals of cross-sections obtained for some systems of levels into functionals of total cross-sections (module *F/C-F). When the sub-group convolution scheme is used, it is possible to transform the functional.

The basic part of the calculation work is performed with the *U/D-F module; it is therefore quite sufficient to consider this module in order to have an idea of the way in which the approximations and calculation schemes described in the preceding sections are used and the interrelationships between them. Figure 7 shows a schematic of the functional module *U/D-F. The individual program modules have the following functions:

UXDXF - general command of the calculation; organization of loops for systems of levels and energy points;

LOADU - retrieval of average resonance parameters from the GRUCON data library;

LOADF - recording of calculation results in the GRUCON data library;

FMOM - calculation of moments at a given energy point by one of the possible schemes (for selection logic see end of section 7);

OPTIM - calculation of parameters of quadrature formulae for integration over distributions of resonance widths and distances between levels;

SUM - calculation of sums of arbitrary multiplicity with given boundaries of variation of summation indices;

UBRWI - calculation of functionals of cross-sections of form $\langle 1/(\sigma + \sigma_0)^n \rangle$ and $\langle \sigma_r/(\sigma + \sigma_0)^n \rangle$ by analytical formulae in the approximation of identical equidistant resonances for given resonance parameter values;

DELTA - calculation of effective values of total widths for a given temperature T of the material;

UFORM - calculation of functionals of cross-sections having any of forms $\langle F \rangle$ given in the task, with the use of the numerical scheme of integration over energy;

FBF - selection of energy points over the integration interval in accordance with the given calculation accuracy;

UFUN - calculation of functions of cross-sections at some energy point indicated by the FBF program for a given set of parameters of the material (the form of the dependence F on cross-sections and parameters of the material is determined by the type of functional being calculated);

BRWI - calculation of cross-section values by the Breit-Wigner equation for a given energy point and a given set of temperatures;

PSICHI - calculation of resonance shape functions $\Psi(x,\xi)$ and $\chi(x,\xi)$;

REMO - calculation of cross-section values by the Reich-Moore formula for non-fissioning nuclei.

Within the framework of this structure we executed several calculation schemes which can be used to compute functionals with different degrees of accuracy for different times (varying from 0.1 to 1 min for one system of levels, one energy point and the standard set of parameters of the material containing 30 values). The scheme can be given as an instruction in the task set, indicating one of the three possible calculation variants considered in section 4, namely:

Variant 1. The functionals are calculated by a numerical scheme for integration over energy; the Doppler effect is taken into account with the help of functions $\Psi(x,\xi)$ and $\chi(x,\xi)$ (the most exact, although the most laborious, variant).

Variant 2. The functionals are calculated by analytical formulae in the approximation of identical equidistant resonances with allowance for the Doppler effect through effective resonance widths. Although it is faster than variant 1 by several factors of ten, it can be used only for calculation of functionals of the shielded cross-section type. The Doppler effect is taken into account with an error of about 10%.

Variant 3. The functionals are obtained by multiplying the fluctuation factors obtained in the approximation of variant 2 by the values calculated (disregarding fluctuations in the resonance parameters) by the scheme of variant 1. This variant is a few times slower than variant 2 and can be used only for functionals of the shielded cross-section type. The Doppler effect is taken into account with an accuracy of about 5%.

If the calculation scheme is not specified, a particular variant is selected by the FMOM program, depending on the contribution of the system of levels to the resulting functional. This contribution is evaluated approximately from the ratio of the penetrability coefficient v_ℓ of the system under consideration to that of the s-wave $v_o = kR$: if $r = v_\ell/kR > 0.05$, variant 1 is taken; if $r < 0.05$, variant 2 is adopted. Moreover, for $r < 0.1$ the single-resonance cross-section model is used and the number of mesh points for calculation of integrals over systematic distributions is taken to be the minimum: $N = 2$ for resonance widths and $N = 1$ for distances between levels.

By virtue of this approach, the time requirements for the conversion of evaluated data into group constants are satisfied.

8. THE MODEL'S POTENTIAL AND CALCULATION ERRORS

The model adopted for the calculation of the functionals of cross-sections in the unresolved resonance region enables us to take into account: the statistical fluctuations of resonance widths in one- and two-level approximations using the Porter-Thomas distributions; the dependence of the functionals on the temperature of the material by the methods of ψ- and χ-functions and redetermination of the total resonance width; the statistical fluctuations in distances between the neighbouring levels using the Wigner distribution; the effect of inter-level interference in the two-level approximation of the Breit-Wigner formula; the contribution of distant resonances in the multilevel approximation of identical equidistant resonances. The main sources of calculation errors within the framework of this model are: integration over resonance parameter distributions; consideration of the temperature dependence of cross-sections; integration over resonance shift; convolution of functionals using the sub-group representation of the cross-section structure; integration over the group interval. We use the model problem proposed by Muñoz et al. [26] in order to make a quantitative evaluation of the physical effects and calculation errors. After obtaining the resonance sequences by the Monte Carlo method, and on the basis of the average resonance parameters for ^{238}U from the ENDF/B-V library (Table 1), they used a different method to obtain the values of the resonance self-shielding factors for the total and radiative-capture cross-sections as a function of temperature of the material (Table 2). This method reduces the problem to calculation of the functionals of cross-sections in the resolved resonance region; therefore it has almost no need for special calculation schemes and highly accurate models can be used. Thus,

the main source of error in its case is that of integration over resonance parameter distributions; for the Porter-Thomas distribution this error depends on the number of resonances involved N. The form of this dependence is $\sqrt{N/2}$. Here, for the necessary accuracy to be attained a much larger number of resonances are required than in the proposed method, and the time spent clearly exceeds the permissible limits for large-scale computations. Nevertheless, the approach can be used with success for adjusting the approximate methods.

Table 2 gives the self-shielding factors for ^{238}U obtained by our method. The maximum disagreement (about 3%) is attained in the extreme case of the even-even ^{238}U nucleus, the low-energy boundary of the unresolved resonance region (4 keV) as well as the minimum values of the dilution cross-section (σ_o = 1 b) and of the temperature of the material (T = 300 K). This agrees with the stated 2% accuracy of de Saussure's results [26] and with the specified accuracy of calculations by our method, which is approximately 1% for the cross-section moments entering into the self-shielding factors (here the error in the factors themselves is also about 2%).

In Table 3 we give the relative deviations of the self-shielding factors obtained by the "standard" and "non-standard" calculation schemes for ^{238}U. By standard we mean the scheme which is selected by the program on the basis of resonance parameter values and calculation conditions. The latter conditions were taken to be: temperature T = 300 K, dilution cross-section σ_o = 1 b and calculation accuracy ε = 1%. The following calculation schemes were chosen with allowance for the values of the average resonance parameters.

For calculation of the s-wave we use the Breit-Wigner formula with allowance for inter-level interference, making a correction for the contribution of distant resonances. The resonance widths of the neighbouring resonances fluctuate independently of each other, and the fluctuation of the distance between resonances is taken into account; allowance is made for the Doppler effect by means of the ψ- and χ-functions; the numerical scheme of integration over resonance shift is used; the number of mesh points for integration over neutron width distribution N_Γ = 5 and over the distribution of distances between levels N_D = 2; the number of sub-groups for representation of the cross-section structure N = 2.

For calculation of the p-wave we use the Breit-Wigner formula in the approximation of identical equidistant resonances. The temperature dependence is taken into account by the method of redetermination of the total width; the integrals are calculated by a shift method with the help of analytical formulae; $N_\Gamma = 3$, $N_D = 2$, $N = 2$.

For calculation of the d-wave we use the Breit-Wigner formula, as in the case of the p-wave, with $N_\Gamma = 2$, $N_D = 1$, $N = 1$. From the data given in Table 3 for ^{238}U we can draw the following conclusions:

- The Doppler effect and neutron width fluctuations have the strongest influence on the values of the self-shielding factors;
- The values of the resonance self-shielding factors for the total cross-section are affected by the correlations of the widths of the neighbouring resonances and by fluctuations in distances between resonances; for this reason, the approximation of identical equidistant resonances cannot be used for calculating the s-wave component;
- The values of the functionals are not affected substantially by the use of more accurate calculation schemes (increasing the number of integration mesh points and the number of sub-groups) and of numerical integration for calculation of the p- and d-waves, and this confirms that the calculation scheme is chosen correctly;
- The calculation time can be roughly halved by optimizing the calculation scheme.

9. CALCULATION OF MOMENTS FOR RESONANCE PARAMETER DISTRIBUTIONS

The general expression for moments takes the form

$$N_n = \int_0^\infty (x + x_0)^n P(x)dx, \quad n = 0, \pm 1 \ldots \tag{18B}$$

If $P(x)$ is the Porter-Thomas distribution, the moments are represented in terms of the degenerate hypergeometric function $M_n = x_o^n (x_o \nu/2)^{\nu/2} U(\nu/2, \nu/2 + n + 1; x_o \nu/2)$. To calculate $U(a,b,z)$ we use the recurrence formula $(b-a-1)U(a,b-1;z)+(1-b-z)U(a,b;z)+zU(a,b+1;z) = 0$ with the initial values: $U(a,a+1;z) = z^{-a}$, $U(a,a;z) = e^z \Gamma(1-a,z)$ where $\Gamma(a,z)$ is an incomplete gamma function. Parameter $a = \nu/2$ can take only integer and semi-integer values. Function $\Gamma(a,x)$ is calculated by the recurrence formula $\Gamma(a+1;x) = \Gamma(a,x) + x^a e^{-x}$ with the initial values:

$\Gamma(0.5,x) = \sqrt{\pi}\,\mathrm{erfc}(\sqrt{x})$; $\Gamma(0,x) = E_1(x)$. To calculate erfc(x) for $x \leq 2$ we use the rational approximation: $e^{x^2}\,\mathrm{erfc}(x) = a_1 t + a_2 t^2 + a_3 t^3 + a_4 t^4 + a_5 t^5$, where $t = 1/(1 + px)$, $a_1 = 0.254829592$, $a_2 = -0.284496736$, $a_3 = 1.42141374$, $a_4 = -1.45315203$, $a_5 = 1.06140543$, $p = 0.3275911$. For $x > 2$ we use an expansion into a continued fraction

$$e^{x^2}\mathrm{erfc}(x) = \frac{1}{\sqrt{\pi}}\,\frac{1/2}{x+}\,\frac{1/2}{x+}\,\frac{1}{x+}\,\frac{3/2}{x+}\,\cdots \tag{18C}$$

In order to calculate function $E_1(x)$ we use the rational approximations:

$$x \leq 1, \qquad E_1(x) + \ln(x) \approx a_1 + a_2 x + a_3 x^2 + a_4 x^3 + a_5 x^4 + a_6 x^5,$$

$a_1 = -0,57721566$; $a_2 = 0,99999193$; $a_3 = -0,24991055$; $a_4 = 0,05519968$; $a_5 = -0,00976004$; $a_6 = 0,00107857$;

$$1 < x \leq 10, \qquad x e^x E_1(x) \approx \frac{x^2 + b_1 x + b_2}{x^3 + b_3 x^2 + b_4 x},$$

$b_1 = 2,334733$; $b_2 = 0,25062$; $b_3 = 3,330657$; $b_4 = 1,68154$; (18D)

$$10 < x, \qquad x e^x E_1(x) \approx \frac{x^2 + b_1 x + b_2}{x^3 + b_3 x^2 + b_4 x}$$

$b_1 = 4,03640$; $b_2 = 1,15198$; $b_3 = 5,03637$; $b_4 = 4,19160$.

To calculate the moments of the Wigner distribution we use the recurrence relationships $M_n = (2r/\pi)\,M_{n-2}$, $n = 1,2, \ldots$ with the initial values $M_{-1} = \pi/2$, $M_0 = 1$.

10. CALCULATION OF INTEGRALS

We consider the calculation of integrals of form

$$\int_{-\infty}^{\infty} \frac{x^{2m}\,dx}{R^n(1+x^2)} \quad (R = ax^2 + bx + c, \ \Delta = 4ac - b^2 > 0).$$

With the help of the recurrence formula

$$\int \frac{x^{2m}\,dx}{R^n(1+x^2)} = \int \frac{x^{2m-2}\,dx}{R^n} - \int \frac{x^{2m-2}\,dx}{R^n(1+x^2)} \tag{18E}$$

the problem can be reduced to calculation of the integrals

$$\int \frac{dx}{R^n(1+x^2)} \quad \text{and} \quad \int \frac{x^m\,dx}{R^n}. \tag{18F}$$

To calculate the integral $\int \frac{dx}{R^n(1+x^2)}$ we use the recurrence formulae

$$\int \frac{dx}{(1+x^2)R^n} = \frac{1}{(c-a)^2+b^2}\left[\frac{b^2-2a(c-a)}{2}\int \frac{dx}{R^n} + (c-a)\int \frac{dx}{(1+x^2)R^{n-1}} - b\int \frac{dx}{(1+x^2)R^{n-1}}\right] \tag{18G}$$

$$\int \frac{x\,dx}{(1+x^2)R^n} = \frac{1}{(c-a)^2+b^2}\left[-\frac{b(c-a)+2ab}{2}\int \frac{dx}{R^n} + b\int \frac{dx}{(1+x^2)R^{n-1}} + (c-a)\int \frac{x\,dx}{(1+x^2)R^{n-1}}\right]$$

For these the initial integrals are $\int \frac{dx}{R(1+x^2)}$ and $\int \frac{xdx}{R(1+x^2)}$, which are calculated by the formulae

$$\int \frac{dx}{R(1+x^2)} = \frac{1}{(c-a)^2+b^2}\left[\frac{b^2-2a(c-a)}{2}\int \frac{dx}{2} + x(c-a)\right];$$

$$\int \frac{xdx}{R(1+x^2)} = \frac{1}{(c-a)^2+b^2}\left[-\frac{b(c-a)+2ab}{2}\int \frac{dx}{R} + xb\right]. \qquad (18H)$$

The following recurrence formula is used to calculate the integrals $\int \frac{x^m dx}{R^n}$

$$\int \frac{x^m dx}{R^n} = \frac{(m-1)c}{(2n-m-1)a}\int \frac{x^{m-2}}{R^n} dn - \frac{(n-m)b}{(2n-m-1)a}\int \frac{x^{m-1}}{R^n} dx \qquad (18I)$$

With the initial integrals $\int \frac{dx}{R^n}$ and $\int \frac{xdx}{R^n}$ calculated by the formulae

$$\int \frac{dx}{R^n} = 2\left(2-\frac{1}{n-1}\right)\frac{a}{\Delta}\int \frac{dx}{R^{n-1}}, \quad \int \frac{xdx}{R^n} = -\left(2-\frac{1}{n-1}\right)\frac{b}{\Delta}\int \frac{dx}{R^{n-1}}. \qquad (18J)$$

For n = 1 we obtain: $\int \frac{dx}{R} = \frac{2\pi}{\sqrt{\Delta}}$; $\int \frac{xdx}{R} = -\frac{2\pi b}{2a\sqrt{\Delta}}$, where $\Delta = 4ac - b^2 > 0$.

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Table 1. Values of average resonance parameters

Orbital moment ℓ	Total moment J	Average distance between levels D	Reduced neutron width $\overline{\Gamma}_n^o$	Radiative width $\overline{\Gamma}_\gamma$
0	1/2	20.0	$0.0^2 21$	0.0235
1	1/2	20.0	$0.0^2 1549$	0.0235
	3/2	10.0	$0.0^3 7745$	0.0235
2	3/2	10.0	$0.0^2 25$	0.0235
	5/2	6.67	$0.0^2 167$	0.0235

N.B. Ratio of nuclear mass to neutron mass A = 236.006; effective scattering radius $R_{ef} = 8.9 \times 10^{-13}$ cm; value of the cross-section of the background for elastic scattering $\Delta\sigma_{e\ell} = 1.444$ b.

Table 2. Resonance self-shielding factors for total cross-section f_t and radiative-capture cross-section f_γ

Dilution cross-section b	Temperature of surrounding material, K					
	300		1000		2000	
	f_t	f_γ	f_t	f_γ	f_t	f_γ
1	55±01	52±01	62±01	62±01	67±01	69±01
	57±01	51±01	63±01	61±01	67±01	68±01
10	64±01	60±001	69±01	70±01	72±01	76±01
	65±01	60±01	70±01	70±01	72±01	75±01
100	79±01	83±02	84±01	89±01	87±01	92±01
	79±01	83±01	84±01	89±01	87±01	92±01

N.B. Figures after the decimal point are given; the first value is data from Ref. [26] and the second is results of calculation by the proposed method.

Table 3. Analysis of deviations in the self-shielding factors for the total cross-section and the radiative-capture cross-section

Calculation conditions	Deviations, %		Calculation time, relative units*/
	$\Delta f_t/f_{tCT}$	$\Delta f_\gamma/f_{\gamma CT}$	
Neutron widths do not fluctuate	11.5	-9.8	0.1
Distance between resonances does not fluctuate	-2.3	0.5	0.6
Doppler effect absent (T = 0)	-23.4	-46.3	1.3
Neutron widths of neighbouring resonances are correlated	9.1	-1.8	0.2
Resonances do not interfere	1.1	-0.8	0.6
Contribution of distant resonances absent	0.1	0.0	0.9
Contribution of p- and d-waves absent	-6.8	-18.6	0.9
s-wave is calculated by the scheme for p- and d-waves: $N_\Gamma = 5$, $N_D = 2$, $N = 2$ (see section 8)	12.2	1.1	0.03
Number of mesh points $N_\Gamma = 6$	-0.3	0.2	2.0
Number of mesh points $N_D = 3$	-0.7	-0.6	1.4
Accuracy of integration over energy increased by a factor of 10	0.0**/	0.0	2.8
p- and d-waves are calculated by the scheme for s-wave (see section 8)	0.0	0.8	2.0

*/ Relative to calculation time by the standard scheme.

**/ Deviations not exceeding 0.1% are taken as zero.

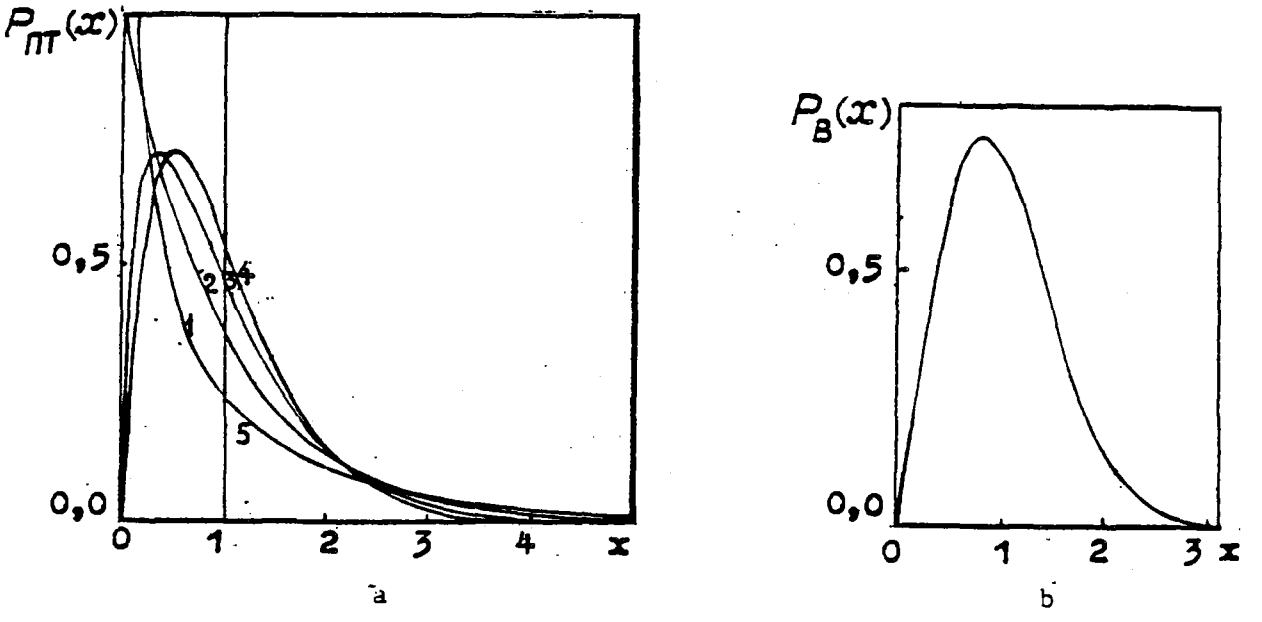

Fig. 1. Shapes of distributions: (a) Porter-Thomas distribution as a function of the number of degrees of freedom ν, (1) $\nu = 1$; (2) $\nu = 2$; (3) $\nu = 3$; (4) $\nu = 4$; (5) $\nu = \infty$; (b) Wigner distribution.

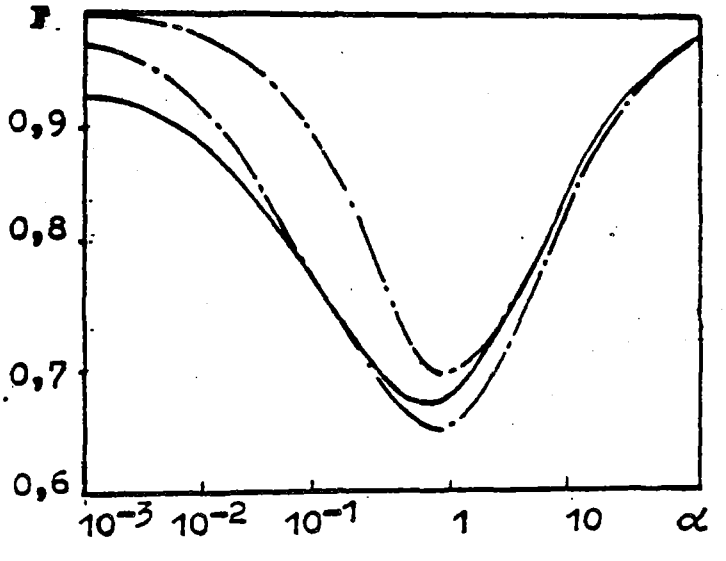

Fig. 2. Dependence of fluctuation factor $F = (1 + \alpha)\frac{x}{x+\alpha}$ for the radiative capture cross-section on the ratio of the average resonance widths $\alpha = \overline{\Gamma}_\gamma / \overline{\Gamma}_n$.

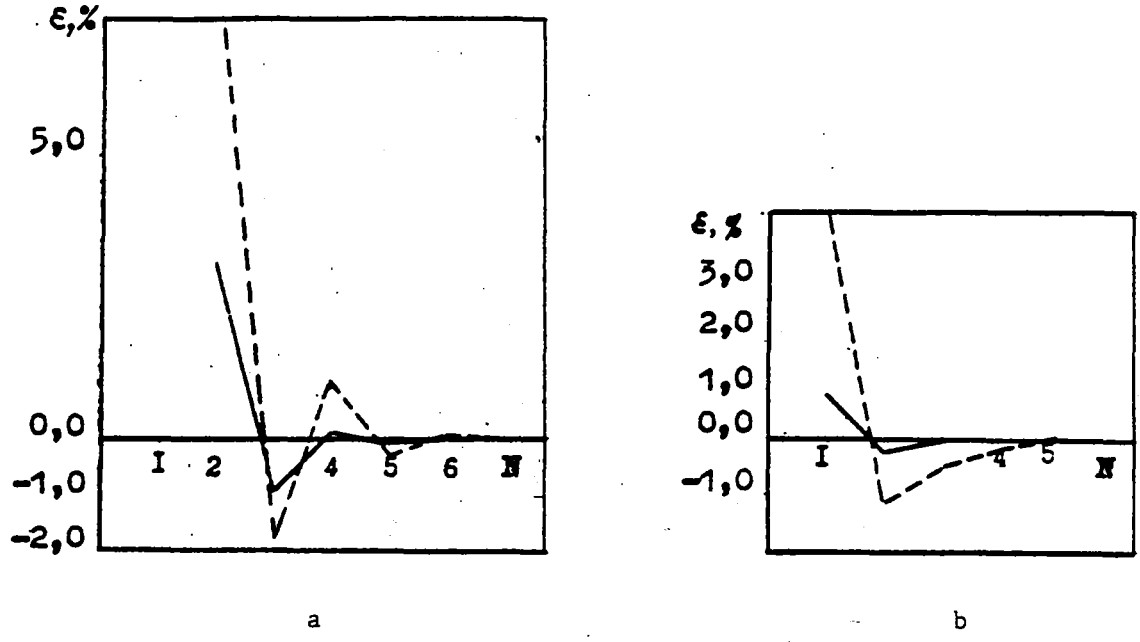

Fig. 3. Dependence of the accuracy of integration over the distributions of resonance widths (a) and distances between levels (b) on the number of mesh points N; ———— moments of cross-sections $\langle 1/(\sigma+\sigma_0)\rangle$; --- moments of cross-sections $\langle \sigma_\gamma/(\sigma+\sigma_0)\rangle$.

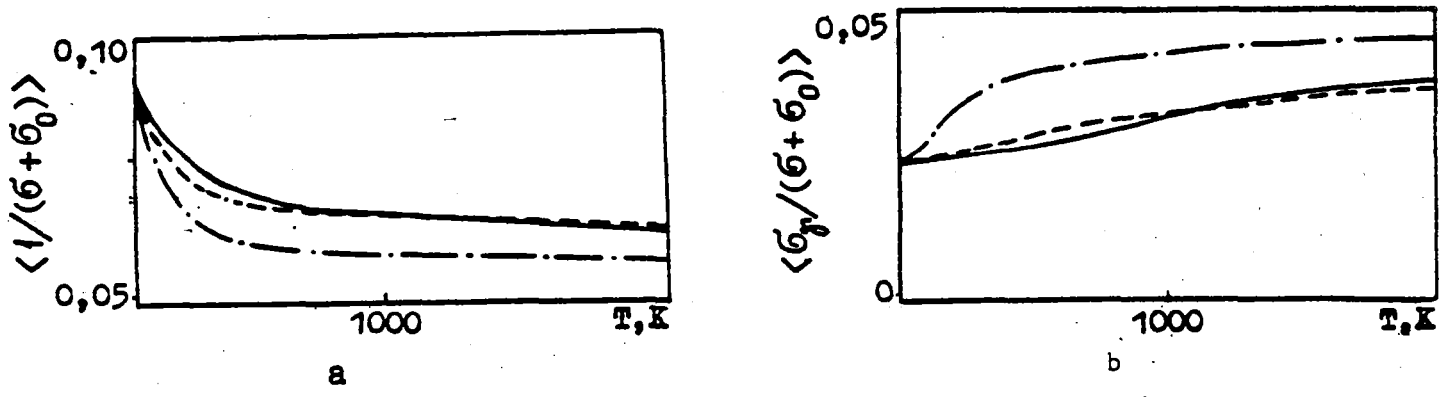

Fig. 4. Dependence of the values of functionals $\langle 1/(\sigma+\sigma_0)\rangle$ (a), $\langle \sigma_\gamma/(\sigma+\sigma_0)\rangle$ (b) on temperature T of the material: ———— calculation using functions Ψ and χ; -.- calculation by the method of redetermination of the total width; --- calculation by the method of redetermination of the total width with adjusted parameter γ.

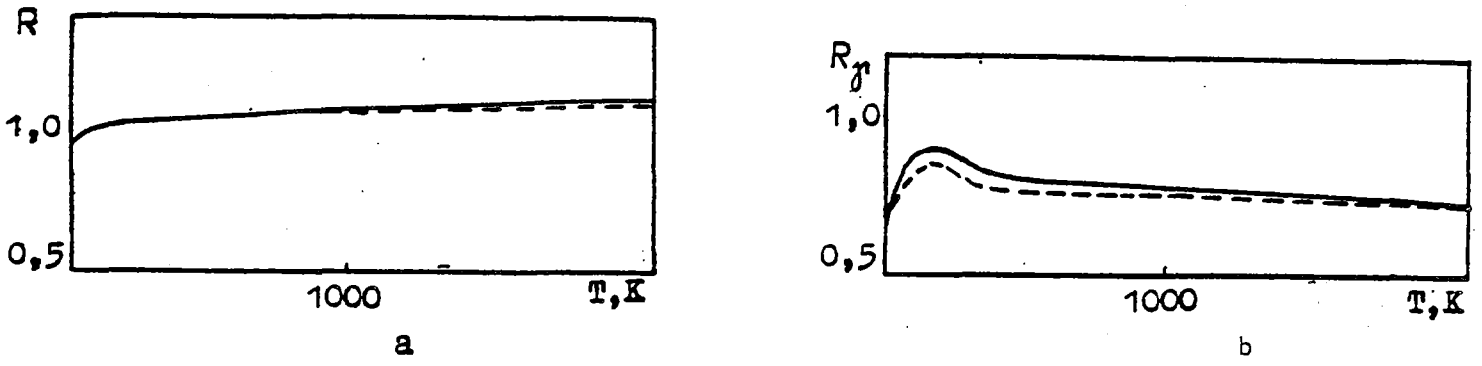

Fig. 5. The dependence of fluctuation factors R for functionals $\langle 1/(\sigma+\sigma_o)\rangle$ (a) and functionals $\langle \sigma_\gamma/(\sigma+\sigma_o)\rangle$ (b) on temperature T of the material: ———— calculation using functions Ψ and χ; --- calculation by the method of redetermination of the resonance width.

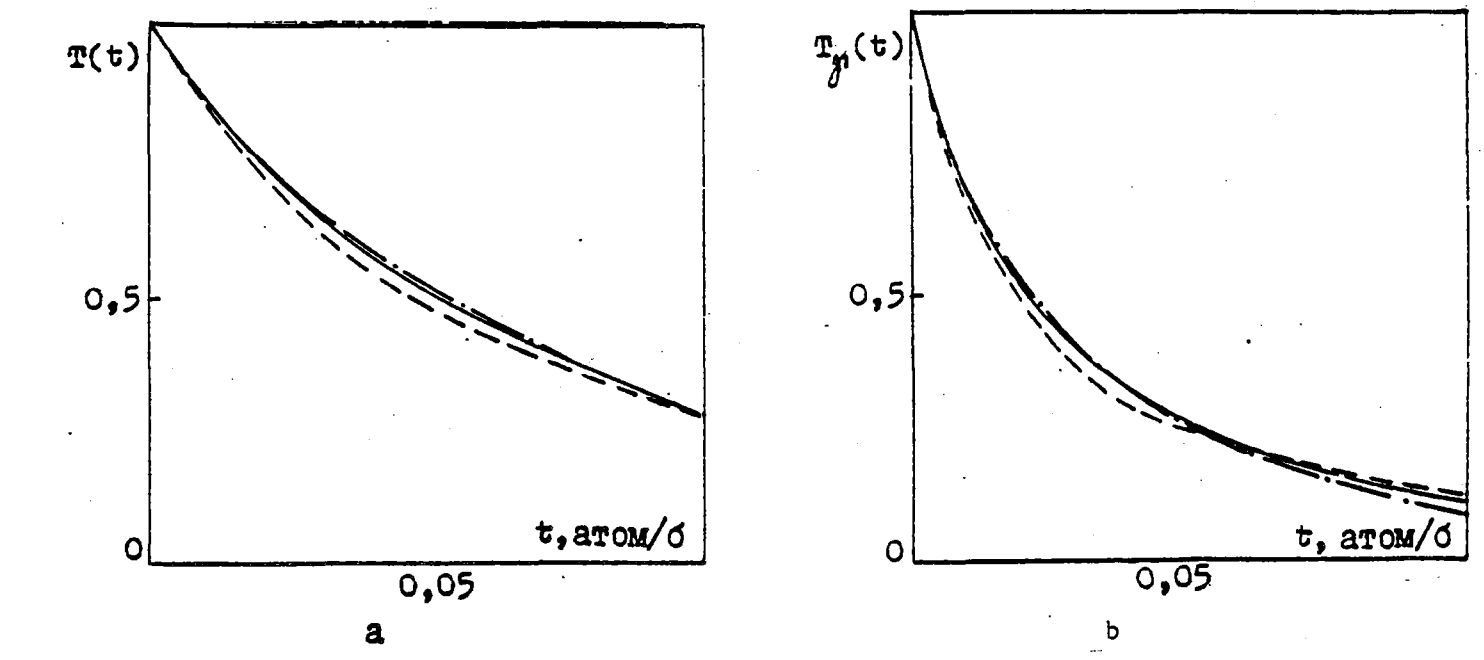

Fig. 6. Sub-group approximation of the dependence of transmission function T(t) (a) and self-indication function for capture $T_\gamma(t)$ (b) on target width t; ———— exact curve; --- sub-group approximation N = 2; -.- sub-group approximation N = 3.

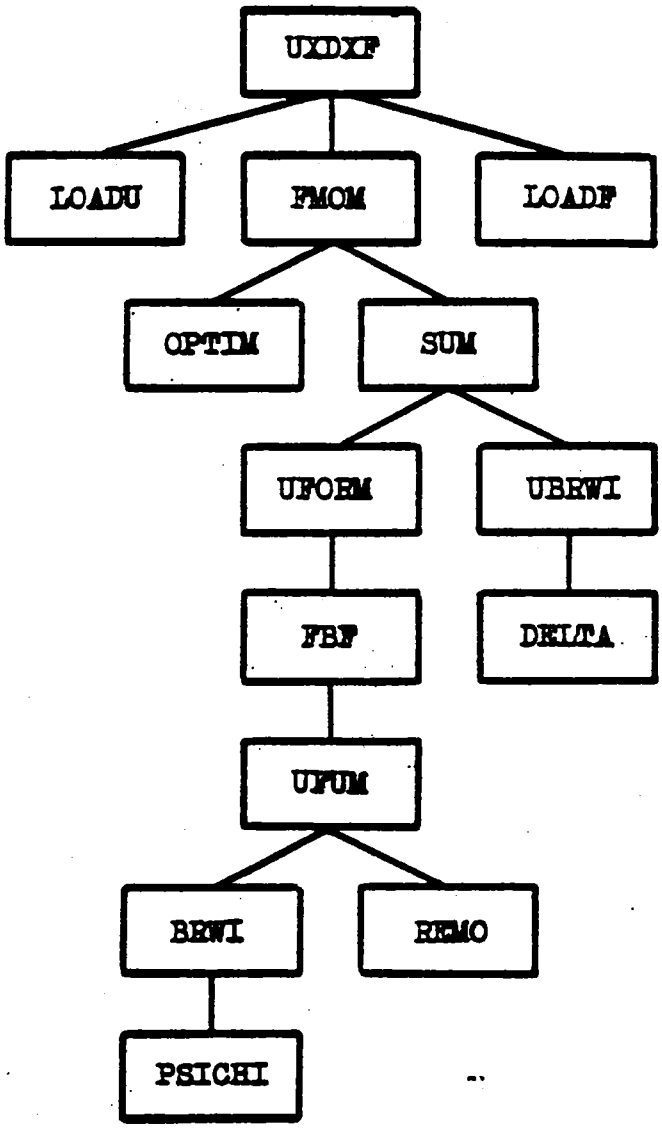

Fig. 7. Structure of the functional module *U/D-F.