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TRANSLATION OF SELECTED PAPERS

PRESENTED AT THE FOURTH ALL-UNION CONFERENCE ON NEUTRON PHYSICS

Kiev, 18-22 April 1977

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FOURTH ALL-UNION CONFERENCE ON NEUTRON PHYSICS

CALCULATION OF CROSS-SECTIONS FOR THE REACTIONS (n,n'), (n,2n), (n,3n), (n,n'f), (n,2nf), (n,3nf) ON THE BASIS OF THE EXCITON MODEL OF PRE-EQUILIBRIUM NUCLEAR DECAY

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ABSTRACT

The exciton model of pre-equilibrium decay is generalized for fissionable nuclei. The probability of transition of a non-equilibrium excited nuclear system into the equilibrium and then into the ground state is calculated by the Monte Carlo method. The inelastic interaction with ^{238}U of neutrons with energies of 6-30 MeV is analysed on the basis of the proposed model.

The model of pre-equilibrium decay developed in recent years [1-2] can successfully be used for predicting the cross-sections and spectra of emitted particles formed in inelastic reactions in the medium energy range. So far, however, only nuclear reactions in mass number ranges where the fission process could be ignored have been studied. This paper presents a generalization of the exciton model of pre-equilibrium decay to fissionable nuclei. The most successful model for this purpose is that proposed in Ref. [3], in which a link is established between stochastic Markov processes and the process of transition of a non-equilibrium nuclear system to the equilibrium state. Thus the Monte Carlo method could be used for a detailed description of the evolution of an excited system in time, including the successive emission of particles at the stage of steady statistical equilibrium. Further advantages of the exciton model of Ref. [3] are that, unlike other approaches, it makes it possible to take into account the deficit of the state due to the emission of particles in the pre-equilibrium stage, and that it allows for the possibility of a transition of the system both to a higher and to a lower number of excitons. Since fission is, by its very nature, a collective process it will clearly occur most often after the system has reached the equilibrium state.

Usually the transition of highly excited nuclei to the ground state is well described on the basis of Weisskopf's statistical theory. The Monte Carlo method yields a more detailed description of the successive emission of particles, of the concurrent changes in the properties of the excited nucleus, and also of the competition between the processes of evaporation and fission. The partial fission widths Γ_f were calculated using the Bohr-Wheeler formula [4]:

$$\Gamma_f = \frac{1}{2\pi\rho(E)} \int_0^{E-B_f} \rho_s(E - B_f - x)\, dx$$

where $\varrho(E)$ is the level density of the compound nucleus for an excitation energy E, B_f is the fission barrier, and ϱ_s is the level density in the saddle point. The probability of neutron emission is given by the expression:

$$\Gamma_n = \frac{1}{h} \int_0^{E-B_n} W_n(\varepsilon)\, d\varepsilon,$$

$$W_n(\varepsilon) = \sigma(E,\varepsilon)\, g m \varepsilon \left(\frac{1}{\pi^2\hbar^3}\right) \left[\rho(E - B_n - \varepsilon)/\rho(E)\right];$$

where E is the excitation energy of the initial compound nucleus, B_n is the neutron binding energy within it, $\sigma(E,\varepsilon)$ is the inverse reaction cross-section, g the statistical weight of the spin states, m the neutron mass and $\varrho(E-B_n-\varepsilon)$ the level density of the nucleus remaining after neutron emission. The inverse reaction cross-section $\sigma(E,\varepsilon)$ was taken in the form proposed by Dostrovskij [5].

For the level density of the evaporating and the fissioning nucleus an expression from the Fermi-gas model was used:

$$\rho_i(E) = \text{Const} \exp\left\{2\sqrt{a\varepsilon}\right\},$$

where a is the level density parameter. It should be noted that when the level density is calculated it is necessary to make a distinction between the parameter a in the fission point: a_f, and

the parameter for the nucleus remaining after neutron emission: a_n. The values of a obtained by analysing the experimental data on the basis of the equilibrium model lie in the range $\frac{A}{7} - \frac{A}{20}$ MeV^{-1}, where A is the mass number [6].

The neutron binding energy was calculated with Cameron's formula, taking into account shell corrections [7]. The fission barrier values obtained from analysing the experimental data on actinide fission were taken from Ref. [8].

The cross-sections of the reactions (n,n'), (n,n'f), (n,2n), (n,2nf), (n,3n), (n,3nf) were calculated in terms of the developed model for various assumptions about the parameters of level density, a_n and a_f, and of initial exciton number, $n_o (n_o = P + h)$. The influence of pairing effects on the reaction characteristics was also evaluated.

Taking as an example the ^{238}U nucleus, let us look at the cross-sections that are of greatest importance in considering non-equilibrium processes, namely the cross-sections for the reactions (n,n'), (n,2n) and (n,3n), on which there is the greatest body of experimental data. Figure 1 gives the theoretical results on the inelastic scattering cross-section for ^{238}U obtained for $a = \frac{A}{7}$, $a = \frac{A}{10}$, $n_o = 3$, for $a = \frac{A}{10}$, $n_o = 2$ and for $a_f = 0.11$ A, $a_n = 0.1$ A, $n_o = 3$.

The figure shows that calculation with $a = \frac{A}{7}$, $n_o = 3$ gives a sharply reduced value in comparison with the experimental data for 14 MeV. The results for $a_n = \frac{A}{10}$ and $a_f = 0.11A$, $a_f = a_n = \frac{A}{10}$ agree with the experimental data at 7 and 14 MeV. Figure 1 also gives the cross-sections for the (n,n') reaction calculated without taking account of pre-equilibrium processes (dotted curve). It can be seen that when the excitation energy rises the contribution of pre-equilibrium processes increases sharply. The dependence of the calculation results on n_o (number of excitons in initial state) is striking. For $n_o = 2$ the results of calculating σ nn' are higher than the experimental values and higher than the calculation results for $n_o = 3$. This is because the average energy of the emitted neutrons is greater at the stage of reaching equilibrium with $n_o = 2$ than when $n_o = 3$ (the excitation energy is redistributed over a smaller number of excitons in the initial state) (see Fig. 2).

It should be noted that the probability of emission of pre-equilibrium particles in the 14-MeV range is close to the values determined from experimental data on neutron spectra from inelastic interaction (~20% for ^{238}U) for $n_o = 2$, and somewhat lower for $n_o = 3$.

Figure 3 gives calculated and experimental data on the cross-sections of the reactions (n,2n) for $a_n = a_f = \frac{A}{10}$, $n_o = 3$ and $a = \frac{A}{7}$, $n_o = 3$.

Calculation for $a = \frac{A}{7}$ and $n_o = 3$ gives an absolute value of the cross-section lower by a factor of about 2. The closest agreement on the (n,2n) reaction cross-section is obtained for $a = \frac{A}{10}$, $n_o = 3$ and for $a_n = a_f = \frac{A}{10}$, $n_o = 2$.

Figure 3 also gives values of σ_{n2n} calculated for the equilibrium model of nuclear reactions (dotted curve). It is seen that as the initial energy increases the importance of pre-equilibrium processes grows, and that on the whole the proposed model makes it possible to describe the behaviour of the cross-section $\sigma_{n,2n}$.

Figure 4 gives results of calculating $\sigma_{n,2n}$ taking into account pairing effects, i.e. when the excitation energy is replaced by the effective energy:

$$E^* = \begin{cases} E - 2\Delta & \text{for even-even nuclei} \\ E - \Delta & \text{for A-odd nuclei} \\ E & \text{for odd-odd nuclei} \end{cases}$$

where Δ is the odd-even mass parameter, the values of which were taken from Ref. [8].

The Figure shows that although the shape is the same as the experimental one, there is a shift of the calculated points towards higher energies. It must be emphasized that this conclusion also follows from the calculations of σ_{n3n}. That is why we ignored pairing effects in all the calculations, and the curve in Fig. 4 is given merely to illustrate the influence of even-even effects.

The dependence of the (n,2n) reaction cross-sections on the initial exciton number ($n_o = 2$ and $n_o = 3$) was also evaluated. It was found that up to 15 MeV the theoretical values agree more closely with the experimental data for $n_o = 2$, and the calculated values themselves are lower in absolute magnitude for $n_o = 2$ than for $n_o = 3$. At energies higher than 15 MeV, σ_{n2n} is higher for $n_o = 2$ than for $n_o = 3$, although the difference between them is small. This dependence on n_o is due to the fact that the spectrum of the emitted particles in the pre-equilibrium stage is harder up to 15 MeV for $n_o = 2$, and therefore some channels with a large number of particles are closed, whereas at higher energies the new channel (n,3n) is opened, which leads to a reduction of $\sigma_{n,2n}$ for $n_o = 3$.

Figure 5 shows the experimental and calculated values of σ_{n3n} for $a_n = a_f = \frac{A}{10}$ and $n_o = 3$.

As high values of a are approached near the reaction threshold the (n,3n) reaction cross-section exceeds the cross-section calculated for lower values of a owing to the softer spectrum of the emitted particles. On the whole the calculated values of σ_{n3n} are somewhat higher than the scanty experimental data available.

The cross-sections of the (n,n'f), (n,2nf) and (n,3nf) reactions were also calculated in terms of this model. They depend to a large extent on the form of the energy dependence Γ_n/Γ_f. Figure 6 shows the energy dependence Γ_n/Γ_f for ^{238}U, ^{239}U and ^{237}U used in our calculations; it was obtained, without taking pairing effects into account, from the experimental values of the fission barriers B_f and the binding energies calculated according to Cameron's formula.

Figure 7 gives the energy dependence of the cross-sections of the (n,n'f), (n,2nf) and (n,3nf) reactions.

Further development of the model will involve taking into account the dependence of the level density parameter on the excitation energy and the structure of the fission barrier.

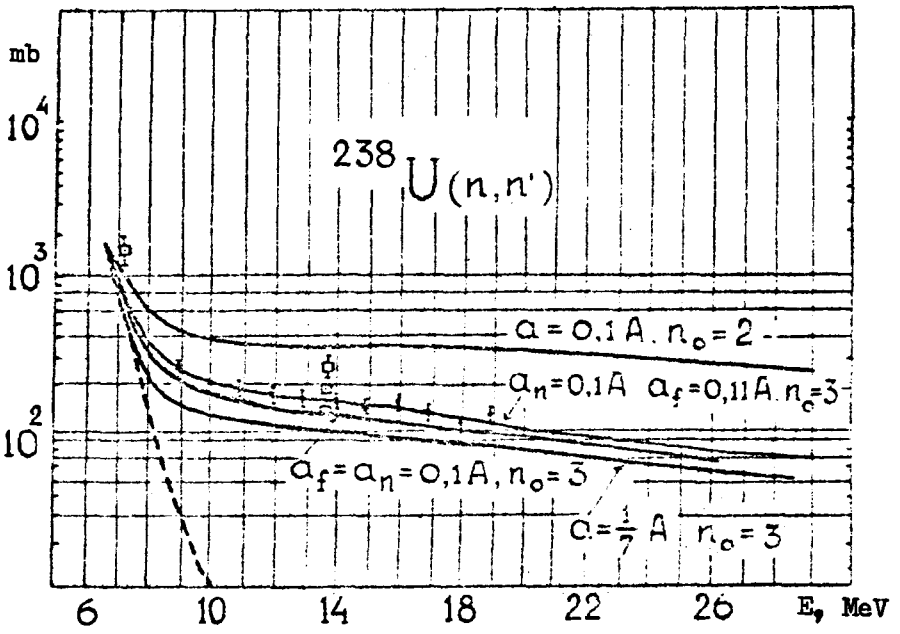

Fig. 1. Dependence of the inelastic scattering cross-section $\sigma_{nn'}$ on the initial neutron energy E_o. The values of the level density parameters a_n and a_f and also the initial exciton number n_o are shown. The experimental values symbolized by $\frac{J}{I}$ are taken from Refs [9-12].

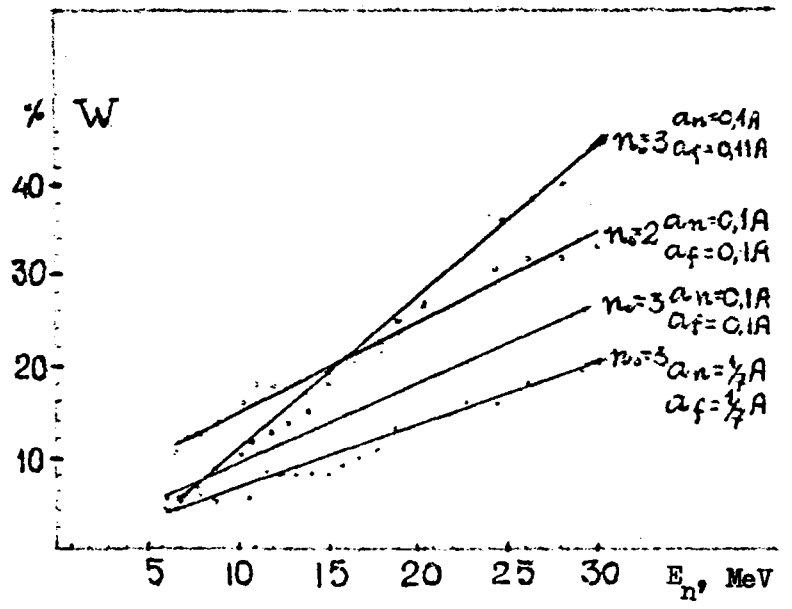

Fig. 2. Dependence of the contribution of pre-equilibrium processes on the initial neutron energy.

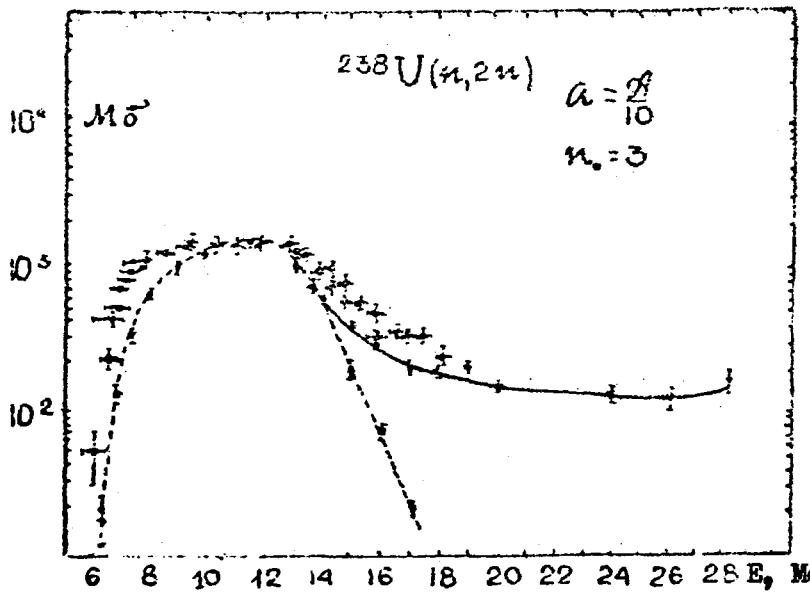

Fig. 3. Dependence of σ_{n2n} on E_o (dotted curve = calculation based on equilibrium model).

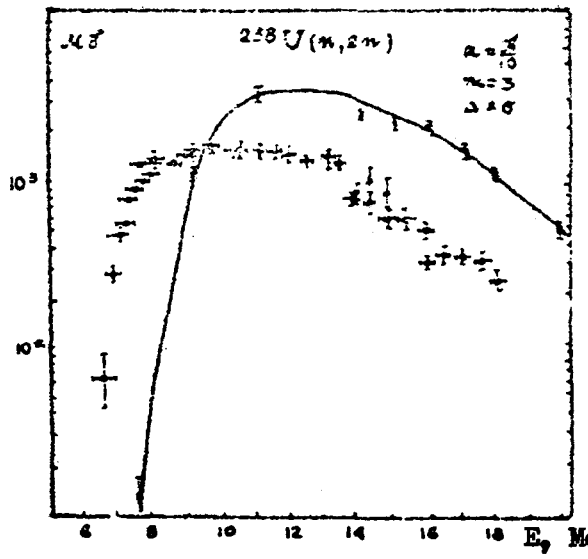

Fig. 4. Dependence of σ_{n2n} on E_o (■ = calculation based on statistics, taking pairing into account, o = experimental points from Refs [13, 18-21]).

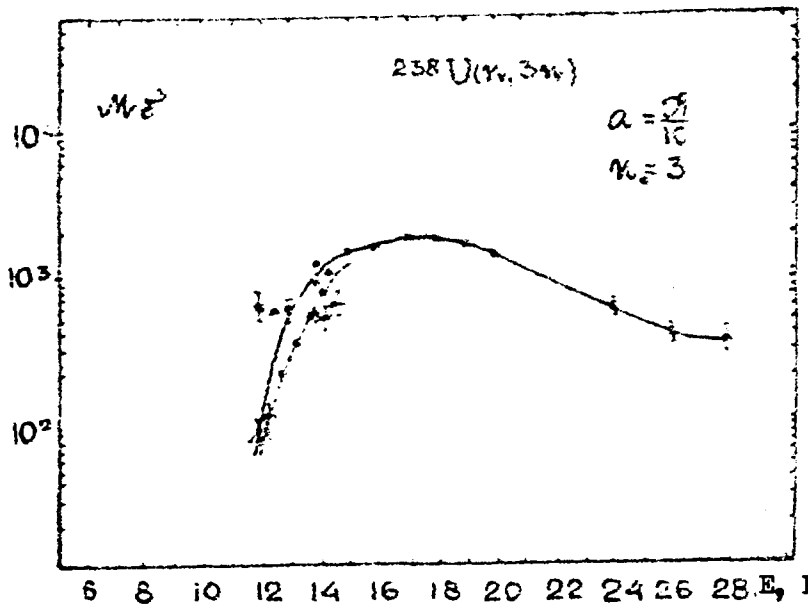

Fig. 5. Dependence of σ_{n3n} on E_o (■ = calculation based on pre-equilibrium model; experimental points taken from Refs [13-17]).

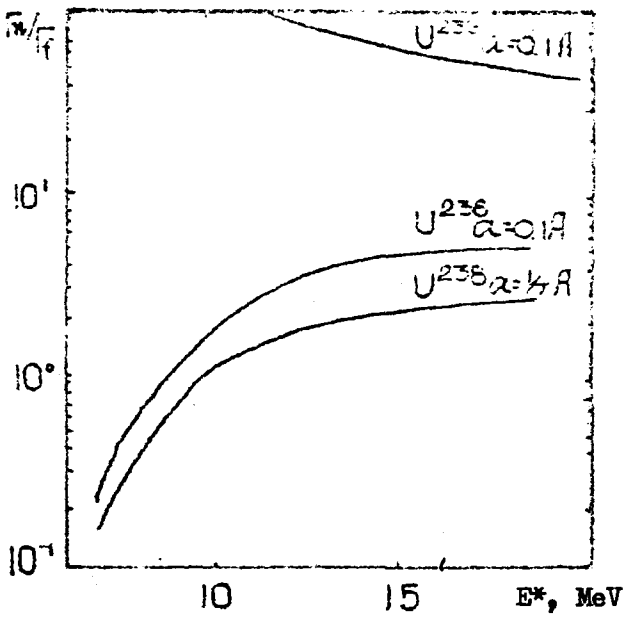

Fig. 6. Functions for Γ_n / Γ_f used in these calculations.

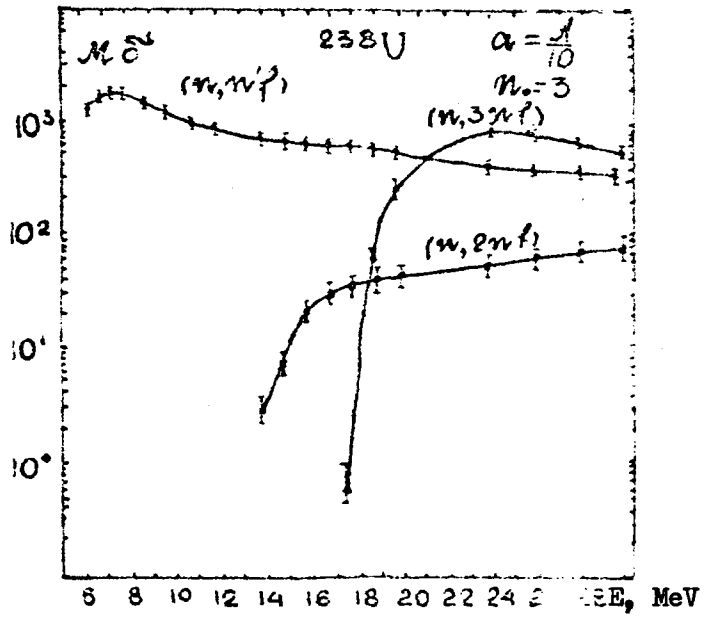

Fig. 7. Energy dependence of the cross sections of the reactions (n,n'f), (n,2nf) and (n,3nf).

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GROUP CONSTANTS FOR ^{235}U, ^{239}Pu, ^{240}Pu AND ^{241}Pu; COMPARISON WITH DATA FROM OTHER LIBRARIES

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ABSTRACT

The results of calculation of the 26-group cross-sections for ^{235}U, ^{239}Pu, ^{240}Pu and ^{241}Pu are given. Detailed information for the calculations was taken from the evaluated neutron data files completed in the INPE of the Byelorussian Academy of Sciences.

As complete files of evaluated nuclear data are accumulated, work is proceeding on translating them into group constants. For this purpose we have set up the GREKO system of computer programs by which constants can be obtained for any group subdivision and any shape of the spectrum. The algorithm for obtaining group constants which was taken as a basis for the present calculations is explained in detail in Refs [1, 2]. For this reason the main differences between the group constants obtained and the available data are attributable to the initial data on cross-sections, energy and angular distributions of secondary neutrons, and on mean resonance parameters. In the derivation of inelastic transition matrices account was taken of the possible pre-equilibrium emission of neutrons leading to a hardening of the spectrum and consequently to an increase in the value of the matrix elements for transition into the adjacent group.

Numerical integration in the region of the resolved resonances was performed by the Gauss method, in terms of intervals whose boundaries consisted of the energy values of the resonances. In this way the calculation time could be shortened.

A set of weighting functions of the type E^n (where n = -1, 0, 1) and the fission neutron spectrum were used in averaging the evaluated data. It would appear that these can be used to break down the real spectrum with sufficient accuracy for the calculations. The coefficients of the breakdown of the real spectrum can be made more precise by means of an iteration method.

In the derivation of the group cross-sections the integration was performed with an accuracy of 10^{-3}; and with an accuracy of 10^{-2} in deriving the resonance self-shielding factors. A higher degree of accuracy demands an unjustifiably large amount of computer time, since the factors of resonance self-shielding cannot be obtained with high precision from the available resonance parameters.

The table gives the group constants for the nuclei indicated above, obtained by averaging in terms of the 1/E spectrum (for E<2.5 MeV) and the fission spectrum (E>2.5 MeV). Only group cross-sections and values of $\bar{\nu}_t$ in the range of energies characteristic of fast reactors are shown here. The group constants for other weight spectra throughout the energy range, the matrices for inelastic transitions, and the coefficients for resonance self-shielding have been transmitted to the Nuclear Data Centre.

Let us make a brief comparison between the group constants derived and data obtained from the English library [3] (experimental data up to 1970), the German library [4] (1968) and the BNAB-70 system.

^{239}Pu - the fission corss-section σ_f agrees with BNAB-70 and with the data in Ref. [3] for the first 12 groups, on average, to within 3%; in lower energy groups the agreement is less satisfactory and the discrepancy reaches ~7%; the degree of agreement with the German library [4] is considerably lower (up to 10%). The capture cross-section $\sigma_\gamma(^{239}\text{Pu})$ in the energy range below 1 MeV agrees on average to within 10% with BNAB-70 and within 15% with the data in Ref. [3]; the agreement with the data in Ref. [4] is considerably less satisfactory.

^{235}U - the fission cross-section σ_f agrees with BNAB-70 and with the data in Ref. [3] to within 2-3% (except for groups 10-11); the data in Ref. [4] are consistently higher. The capture cross-section σ_γ (^{235}U) in the energy range below 1 MeV is, on average, consistently 7% smaller than the BNAB data; agreement with the data in Ref. [3] is to within 10%, except for groups 14-15, for which the data in [3] are ~25% lower. The data in Ref. [4] for the range above 5 keV agree with our data on average to within 5%.

^{240}Pu - the fission cross-section σ_f agrees with BNAB-70 data to within 2% for the first 6 groups; below the fission threshold the discrepancy reaches 80-100%. In the BNAB-70 data the capture cross-section σ_γ (^{240}Pu) is consistently larger by ~50%; the data in Ref. [3] agree with our data to within ~5% for the range above 100 keV; in the lower energy range the data in [3] are approximately twice as high.

^{241}Pu - in the BNAB data the fission cross-section σ_f is consistently ~13% smaller for the energy range above 0.2 MeV but considerably larger (by ~40%) for energy values below 0.2 MeV. The values in Ref. [3] are consistently 5-10% higher for the entire energy range. The discrepancy for σ_γ (^{241}Pu) is as much as 40% for the BNAB-70 data and for the data in Ref. [3].

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Table

Group constants for ^{235}U, ^{239}Pu, ^{240}Pu and ^{241}Pu

i	ΔE	U-235					Pu-239				
		$\bar{\sigma}_{f,\delta}$	$\bar{\sigma}_{\gamma,\delta}$	$\bar{\sigma}_{el,\delta}$	$\bar{\sigma}_{in,\delta}$	$\bar{\nu}_t$	$\bar{\sigma}_{f,\delta}$	$\bar{\sigma}_{\gamma,\delta}$	$\bar{\sigma}_{el,\delta}$	$\bar{\sigma}_{in,\delta}$	$\bar{\nu}_t$
I	6,5-I0,5 MeV	I,680	0,009	3,335	I,429	3,525	2.I74	0,00I	3,455	I,0I9	4,045
2	4,0-6,5	I,II8	0,0I8	4,28I	2,2I6	3,069	I,772	0,002	4,52I	I,624	3,645
3	2,5-4,0	I,202	0,030	4,52I	2,094	2,800	I,828	0,003	4,506	I,682	3,360
4	I,4-2,5	I,266	0,053	4,059	I,754	2,626	I,928	0,0I3	3,8I4	I,586	3,I07
5	0,8-I,4	I,2I8	0,I03	3,950	I,66I	2,535	I,784	0,048	4,004	I,4I2	3,02I
6	0,4-0,8	I,I64	0,I60	4,955	I,569	2,470	I,609	0,097	5,672	I,I03	2,947
7	0,2-0,4	I,279	0,253	6,826	I,238	2,455	I,504	0,I55	7,679	0,8I8	2,907
8	0,I-0,2	I,474	0,388	8,9I5	0,624	2,436	I,496	0,2I0	9,530	0,642	2,886
9	46,5-I00 keV	I,75I	0,539	I0,360	0,I66	2,423	I,569	0,296	I0,32I	0,448	2,875
I0	2I,5-46,5	2,074	0,754	II,3I9	0,009	2,4I8	I,596	0,492	II,I70	0,376	2,868
II	I0,0-2I,5	2,549	I,00I	I2,I2I	0,0	2,4I6	I,68I	0,685	I2,I03	0,349	2,864
I2	4,65-I0,0	3,472	I,305	I2,228	0,0	2,4I6	2,I54	I,623	I2,235	0,054	2,862
I3	2,I5-4,65	5,029	I,729	I2,384	0,0	2,4I6	3,040	2,76I	I2,633	0,0	2,862
I4	I,0-2,I5	7,042	3,403	I2,620	0,0	2,4I6	3,982	3,793	I3,225	0,0	2,862
I5	0,465-I,0	II,523	4,550	II,654	0,0	2,4I6	8,3I2	6,563	I4,829	0,0	2,862
I6	0,2I5-0,465	I6,488	7,435	I2,605	0,0	2,4I6	I3,056	II,3I9	I4,2I3	0,0	2,862
I7	0,I-0,2I5	22,034	II,I76	I4,208	0,0	2,4I6	I9,393	I4,999	I4,747	0,0	2,862

(Continuation of table)

i	ΔE	Pu-240					Pu-241				
		$\bar{\sigma}_{f,\delta}$	$\bar{\sigma}_{\gamma,\delta}$	$\bar{\sigma}_{el,\delta}$	$\bar{\sigma}_{in,\delta}$	$\bar{\nu}_t$	$\bar{\sigma}_{f,\delta}$	$\bar{\sigma}_{\gamma,\delta}$	$\bar{\sigma}_{el,\delta}$	$\bar{\sigma}_{in,\delta}$	$\bar{\nu}_t$
I	6,5-I0,5 MeV	I,980	0,007	3,365	I,I2I	3,956	I,844	0,006	3,45I	I,337	4,0I5
2	4,0-6,5	I,532	0,0I4	4,5I8	I,466	3,562	I,394	0,007	4,676	I,899	3,606
3	2,5-4,0	I,579	0,030	4,464	I,587	3,304	I,493	0,0II	4,525	I,954	3,358
4	I,4-2,5	I,58I	0,078	3,742	I,739	3,I24	I,679	0,058	3,8II	I,853	3,I84
5	0,8-I,4	I,454	0,I73	3,753	I,68I	3,I88	I,608	0,098	3,995	I,525	3,070
6	0,4-0,8	0,569	0,I66	5,762	I,545	3,I36	I,5I6	0,096	5,69I	I,I56	3,002
7	0,2-0,4	0,I35	0,I87	8,I69	I,I86	2,889	I,737	0,II6	7,859	0,63I	2,963
8	0,I-0,2	0,076	0,254	I0,086	0,843	2,868	2,0I5	0,224	9,748	0,277	2,944
9	46,5-I00 keV	0,08I	0,425	II,I46	0,324	2,857	2,293	0,359	I0,944	0,I35	2,934
I0	2I,5-46,5	0,II7	0,750	I2,2I5	0,002	2,852	2,70I	0,5I0	II,704	0,0I2	2,929
II	I0,0-2I,5	0,II7	I,085	I2,888	0,0	2,850	3,238	0,703	I2,292	0,0	2,926
I2	4,65-I0,0	0,097	I,374	I3,945	0,0	2,848	4,3I9	I,063	I2,750	0,0	2,924
I3	2,I5-4,65	0,I53	I,882	I5,674	0,0	2,847	6,I49	I,636	I3,I02	0,0	2,924
I4	I,0-2,I5	0,287	3,273	I8,242	0,0	2,847	8,4I6	I,947	I3,3I6	0,0	2,924
I5	0,465-I,0	0,269	4,8I4	I8,528	0,0	2,847	I2,046	3,904	I3,703	0,0	2,924
I6	0,2I5-0,465	0,059	7,852	22,048	0,0	2,847	22,624	6,0I8	I4,299	0,0	2,924
I7	0,I-0,2I5	0,I30	24,044	29,I89	0,0	2,847	26,5I5	9,2I3	I3,954	0,0	2,924

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EVALUATION OF NUCLEAR DATA ON ^{241}Pu FOR THE COMPILATION OF A COMPLETE FILE OF CONSTANTS

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ABSTRACT

On the basis of the available experimental data and of theoretical models the neutron cross-sections of ^{241}Pu in the energy range 10^{-4} eV-15 MeV were evaluated. The evaluated data are presented in the SOKRATOR format and transmitted to the Obninsk Nuclear Data Centre.

This paper is a further step in the work on evaluating nuclear data for heavy nuclei which is being performed at the Institute of Nuclear Power Engineering (IAEh) of the Byelorussian SSR Academy of Sciences [1-3]. Here the evaluation results are only briefly summarized, with indications of the methods used. The full text of the paper in the traditional form of a detailed report has been sent to the Nuclear Data Centre together with a machinable information carrier containing the evaluated data in the SOKRATOR format.

In the thermal neutron energy range 10^{-4}-1 eV the cross-sections σ_t, σ_f, σ_a and σ_γ and the derived quantities α and η were evaluated on the basis of the available experimental data on σ_t and σ_f. The results were normalized to the thermal (E = 0.0253 eV) cross-section values recommended by Lemmel [4].

In the range of allowed resonances of ^{241}Pu the cross-sections were self-consistently parametrized using a modified Adler-Adler-type formalism. The resonance parameters were obtained from previously selected experimental data. These self-consistent parameters make it possible to establish the cross-sections σ_t, σ_f, σ_γ and σ_n for any temperature in the energy range up to 150 eV.

In the forbidden resonance range (0.1-100 keV) the average resonance parameters were obtained with which all types of average cross-sections can be calculated and the presence of a forbidden resonance structure in this range taken into account. The average resonance parameters were evaluated on the basis of experimental data on $<\sigma_f>$ using the average resonance parameters obtained in the allowed resonance range ($<D>_{obs}$ = 1.34 ± 0.10 eV, $<\Gamma_\gamma>$ = 0.043 ± 0.005 eV, $S_o = (1.16 \pm 0.19) \times 10^{-4}$, $S_1 = (2.0 \pm 0.5) \times 10^{-4}$. The average widths $<\Gamma_f>_{J\pi}$ were calculated in accordance with channel theory). The criterion for the quality of the evaluated average parameters is comparison of the calculated value of α with the experimental value of Ref. [5] (see Fig. 1).

For the fission cross-section σ_f there are only two absolute measurements [6, 7]. All other references discuss measurements of the ratio $\sigma_f(^{241}Pu)/\sigma_f(^{235}U)$. The best description of this ratio was therefore obtained initially. From this $\sigma_f(^{241}Pu)$ was then obtained using our evaluation of $\sigma_f(^{235}U)$ [2]. The data obtained in this way, together with the data from the absolute measurements, were then used to obtain the final evaluated curve for $\sigma_f(^{241}Pu)$.

The evaluated energy dependence of the average number of neutrons on fission, $\nu_t(E)$, is based on experimental data and approximated by the expression:

$$\nu_t(E) = 2.9243 + 0.13471\ E + 0.001125\ E^2 (E \text{ in MeV}).$$

The cross-sections of radiative capture σ_γ, and of inelastic scattering, $\sigma_{n'}$, were calculated using the statistical model of nuclear reactions in the region of both discrete and continuous level spectra of the target nucleus (up to 5 MeV). In the calculation of σ_γ the competition of the $(n,\gamma f)$ and $(n,\gamma n')$ reactions needed to be taken into account in order to achieve a more accurate calculation of the cross-sections σ_γ and σ_f and of the quantity α for fissionable nuclei. Thus taking account of the $(n,\gamma f)$ process at an energy of 1 MeV reduces σ_γ by a factor of 1.6, and taking account of the $(n,\gamma f)$ and $(n,\gamma n')$ processes at 3 MeV leads to a reduction by a factor of 6 (see Fig. 2).

The cross-sections for the reactions (n,n'), (n,2n'), (n,3n'), (n,n'f) and (n,2n'f) and the spectra of the corresponding neutrons in the energy range above 5 MeV were calculated in accordance with the statistical theory of compound nucleus decay generalized for the case of multiparticle decay. The calculations took into account the possibility of pre-equilibrium emission of neutrons from the nucleus and used experimental information on the nuclei produced in the successive stages of decay.

The spectra of gamma rays accompanying the reactions (n,γ), (n,f), (n,n'), (n,2n') and (n,3n') were also calculated in accordance with the statistical model.

The results of this evaluation of the cross-sections σ_{γ}, $\sigma_{n'}$ and $\sigma_{n,2n'}$ differ substantially from other available evaluations. A comparison is made to illustrate this in Figs 3-5.

FIGURE CAPTIONS

Fig. 1. Comparison of calculated and experimental data [5] on α for ^{241}Pu in the range 0.1-100 keV.

Fig. 2. Radiative capture cross-section for ^{241}Pu, calculated with (1) and without (2) account of the $(n,\gamma f)$ process.

Fig. 3. Comparison of various evaluations of σ_γ for ^{241}Pu.
1 - this paper, 2 - Prince [8], 3 - Kaner and Yiftah [9].

Fig. 4. Comparison of various evaluations of $\sigma_{n'}$ for ^{241}Pu. (Curves identified as in Fig. 3.)

Fig. 5. Comparison of various evaluations of $\sigma_{n,2n}$ for ^{241}Pu. (Curves identified as in Fig. 3.)

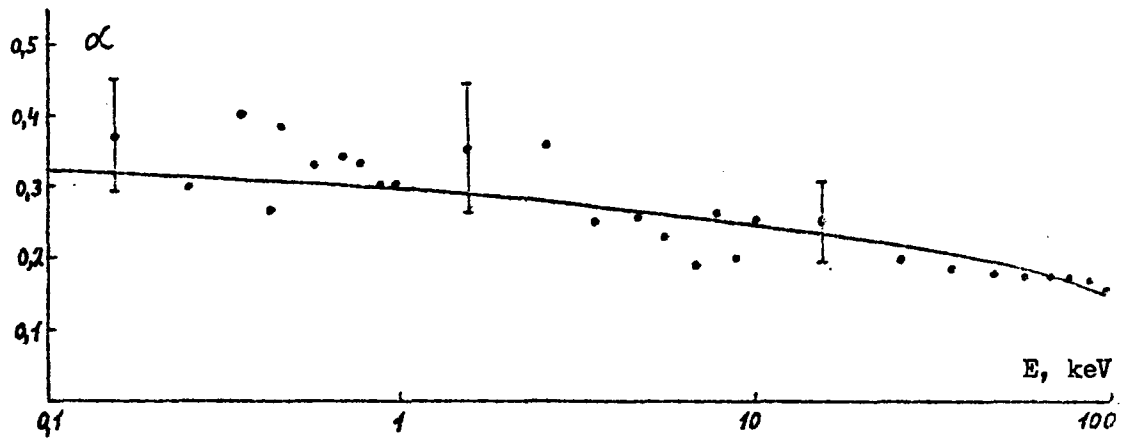

Рис.I. Сравнение расчетных и экспериментальных / 5 / данных по величине α ^{241}Pu в области 0,I-I00 кэВ.

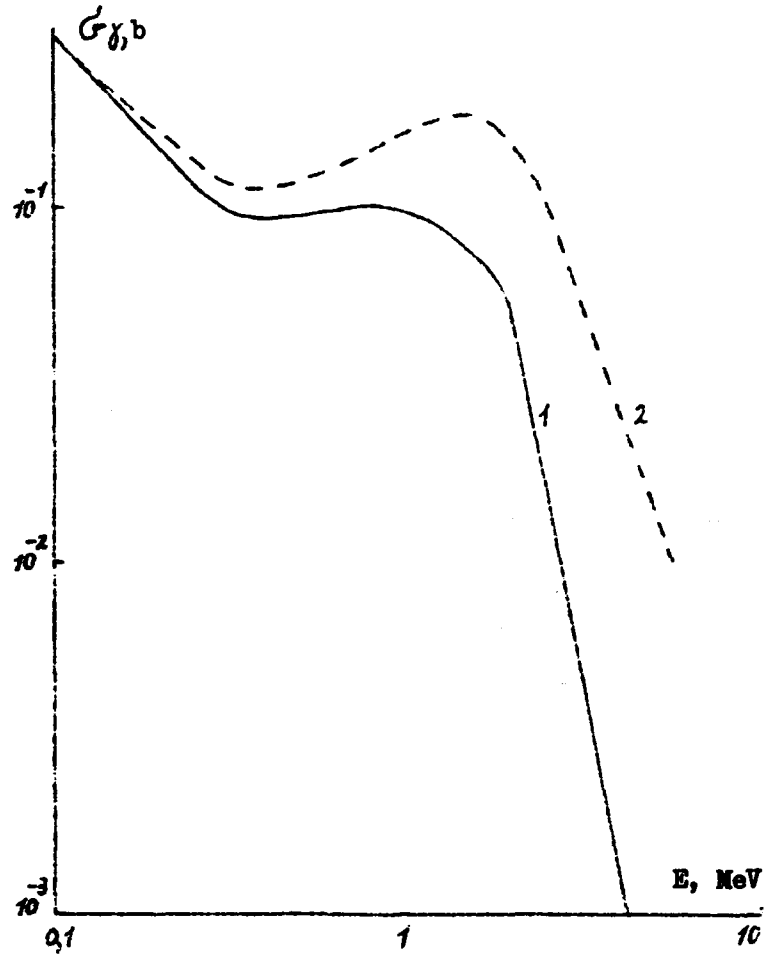

Рис.2. Сечение радиационного захвата ^{241}Pu, рассчитанное с учетом процесса (n,γf) - I и без учета - 2.

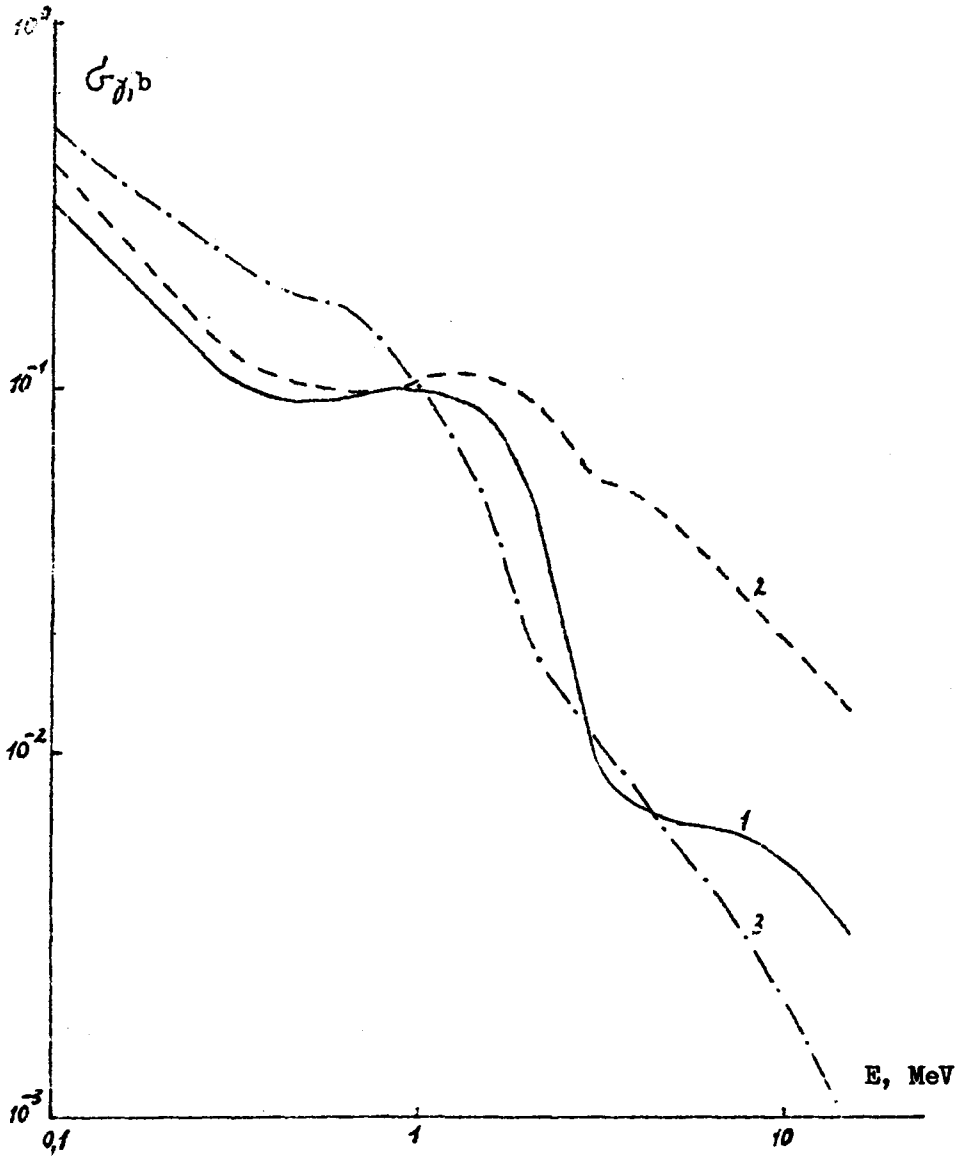

Рис.3. Сравнение различных оценок сечения σ_{γ} ^{241}Pu.
1 - настоящая работа, 2 - Принс / 8 /,
3 - Канер и Ифта / 9 /.

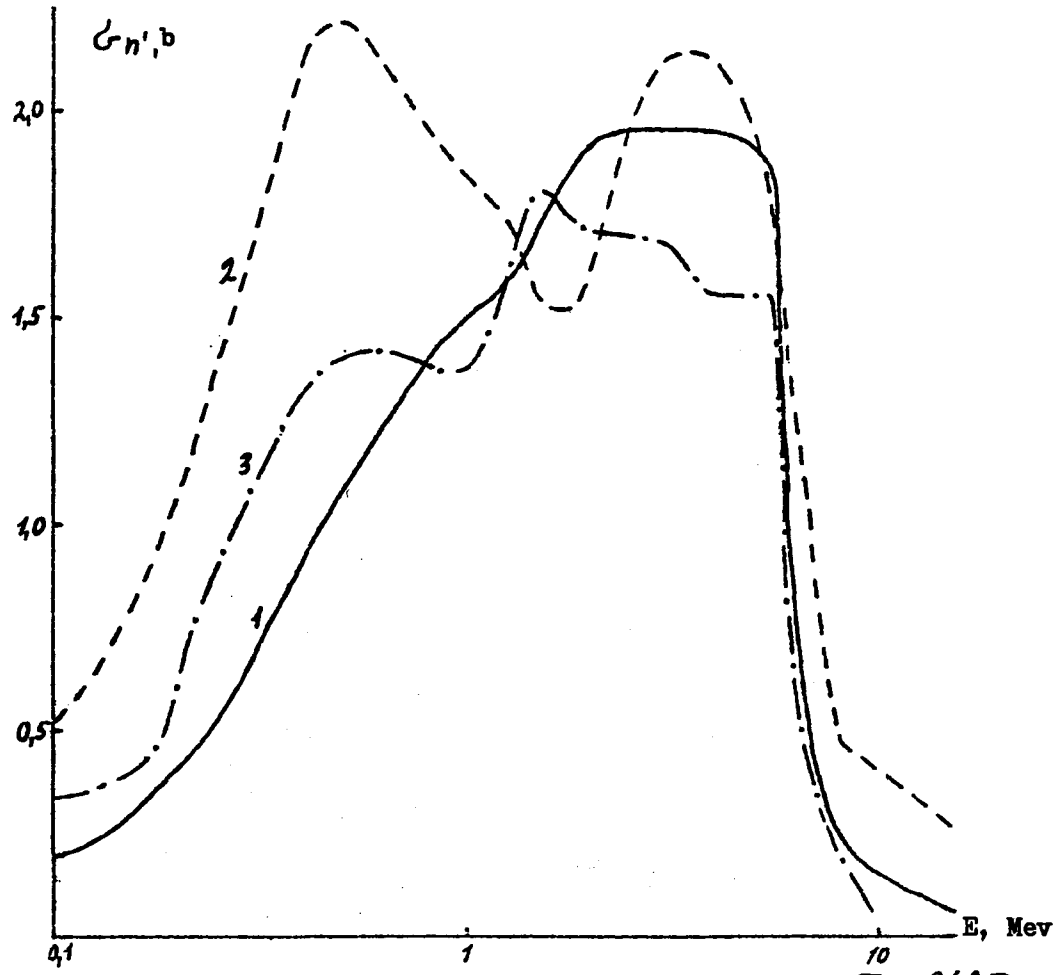

Рис.4. Сравнение различных оценок сечения $\sigma_{n'}$ ^{241}Pu. Обозначения кривых аналогично рис.3.

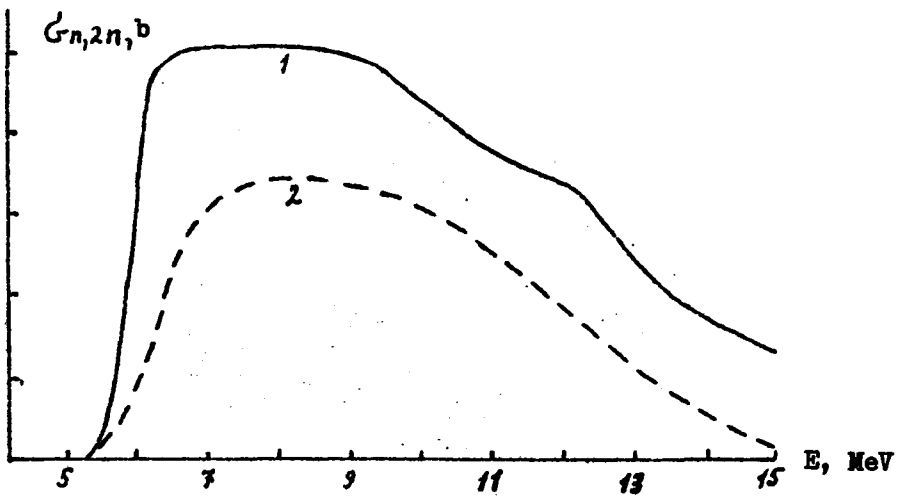

Рис.5. Сравнение различных оценок сечения $\sigma_{n,2n}$ ^{241}Pu. Обозначения кривых аналогично рис.3.

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ALLOWANCE FOR CORRELATIONS IN THE DETERMINATION OF THE ERRORS IN EVALUATED DATA

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ABSTRACT

A method is proposed for evaluating quantities and their associated errors on the basis of information on the correlations between the partial errors in the experimental data; the method also enables the correlation coefficients between the errors at different points on the evaluated curve to be calculated. An example is given of the evaluation of the quantity $\alpha(^{259}Pu)$ and its associated error.

One of the problems in the evaluation of nuclear constants which has received the least attention is that of determining the errors in the evaluated results and of finding the proper "weights" for the experimental data used in the evaluation.

The use of "weights" which are inversely proportional to the squares of the errors in the experimental data is a procedure which is only correct if the errors are uncorrelated. In fact, however, the errors in the experimental data are often strongly correlated because identical measuring techniques are used.

The method proposed in Ref. [1], which makes use of the detailed information on the correlations between the errors in the experimental data, is employed in this paper to evaluate the quantities $\sigma_f(^{235}U)$, $\sigma_f(^{239}Pu)$, $\alpha(^{235}U)$ and $\alpha(^{239}Pu)$ and their associated errors. In addition, correlation coefficients between the errors at different points of the evaluated curves are also obtained. We give below a short account of the method used in the evaluation.

Suppose that there are N measurements of a quantity σ_o (the unknown, true value of the measured quantity), equal to σ_i(i=1, ..., N). The result of each particular measurement, σ_i, is a functional of some set of the actually measured quantities f_{ik}(k=1, ..., M) with error Δf_{ik}, where M is the total number of parameters required to obtain the values σ_i. Then, restricting ourselves to a linear approximation, we have

$$\sigma_i = \sigma_o + \sum_{k=1}^{M} \frac{\partial \sigma_i}{\partial f_{ik}} \Delta f_{ik} \tag{1}$$

The quantity $\frac{\partial \sigma_i}{\partial f_{ik}} \Delta f_{ik}$ is the part of the error of the i-th experiment caused by the uncertainty in our knowledge of the k-th measured parameter (denoted below by $\Delta \sigma_{ik}$).

Suppose now that the evaluated result is obtained by averaging the experimental values with "weights" a_i^2, such that $\sum_{i=1}^{N} a_i^2 = 1$. Then

$$\sigma_{o4} = \sum_{i=1}^{N} \sigma_i a_i^2 \tag{2}$$

Summing Eq. (1) over i, we obtain:

$$\sum_{i=1}^{N} \sigma_i a_i^2 = \sum_{i=1}^{N} \sigma_o a_i^2 + \sum_{i=1}^{N} \sum_{k=1}^{M} \Delta \sigma_{ik} a_i^2 \tag{3}$$

Then,

$$\overline{|\sigma_{o4} - \sigma_o|^2} = \overline{\left|\sum_{i=1}^{N} \sum_{k=1}^{M} \Delta \sigma_{ik} a_i^2\right|^2} = \sum_{i=1}^{N} \sum_{k=1}^{M} \sum_{j=1}^{N} \sum_{m=1}^{M} a_i^2 a_j^2 \overline{\Delta \sigma_{ik} \Delta \sigma_{jm}}$$

$$= \sum \sum \sum \sum a_i^2 a_j^2 K_{ikjm} \sqrt{\overline{|\Delta \sigma_{ik}|^2}} \sqrt{\overline{|\Delta \sigma_{jm}|^2}} \tag{4}$$

where K_{ikjm} is a correlation coefficient, defined by the relationship

$$K_{ikjm} = \frac{\overline{\Delta\sigma_{ik}\,\Delta\sigma_{jm}}}{\sqrt{\overline{|\Delta\sigma_{ik}|^2}}\,\sqrt{\overline{|\Delta\sigma_{jm}|^2}}} \qquad (5)$$

Equation (4) gives the error in the evaluated quantity in terms of the standard deviation of the partial measurement errors $\overline{|\Delta\sigma_{ik}|^2}$, the correlation coefficient between these partial errors K_{ikjm} and the weights a_i^2 used in the evaluation.

It is natural to use for the experimental data the "weights" which minimize the error in the evaluated quantity (see Eq. (4)). These "weights" of course depend on the partial errors of the experiments and on the correlations between them, i.e. they reflect the actual experimental situation and indicate the value of a particular experiment.

In the case where there is no correlation, $K_{ikjm} = 0$, for $k \neq m$ and $i \neq j$, and $K_{ikjm} = 1$ for $k = m$ and $i = j$, this method gives "weights" which are inversely proportional to the squares of the errors in the experimental data, i.e. it is equivalent to the least-squares method.

We assume that it is possible to divide the total error into partial errors in such a detailed way that $K_{ikjm} = 0$ for $k \neq m$. This assumption implies that the errors in any two different parameters which are needed for calculating the cross-section are mutually uncorrelated. Using the notation $K_{kij} = K_{ikjk}$, we can re-write Eq. (4) as:

$$\overline{|\sigma_{ay} - \sigma_0|^2} = \sum_{k=1}^{M} \sum_{i=1}^{N} \sum_{j=1}^{N} a_i^2 a_j^2 K_{kij} \sqrt{\overline{|\Delta\sigma_{jk}|^2}} \cdot \sqrt{\overline{|\Delta\sigma_{jk}|^2}} \qquad (6)$$

Equation (6) gives the error in the evaluated quantity for an individual point on the curve. We define the correlation coefficient between the errors at any two evaluated points, B_{nm}, as

$$B_{n,m} = \frac{\overline{\Delta\sigma_n\,\Delta\sigma_m}}{\sqrt{\overline{|\Delta\sigma_n|^2}} \cdot \sqrt{\overline{|\Delta\sigma_m|^2}}} \qquad (7),$$

where the subscripts n and m denote the serial numbers of the points for which the correlation coefficient is being calculated, and $\Delta\sigma_n$ and $\Delta\sigma_m$ are the errors in the evaluated quantities at these points. Using expression (3) for the evaluated errors, we obtain:

$$\mathcal{B}_{n\,m} = \frac{\sum_{j=1}^{N}\sum_{l=1}^{M}\sum_{i=1}^{N}\sum_{k=1}^{M} a_{jn}^2\, a_{im}^2\, \overline{\Delta\sigma_{jlm}\,\Delta\sigma_{ikm}}}{\sqrt{|\Delta\sigma_n|^2}\;\sqrt{|\Delta\sigma_m|^2}} \qquad (8),$$

where $\Delta\sigma_{jln}$ is the l-th partial error of the j-th experiment at point n and a_{jn}^2 is the "weight" of the j-th experiment when used in the evaluation at point n.

If we use the definition,

$$K_{jlnikm} = \frac{\overline{\Delta\sigma_{jln}\cdot\Delta\sigma_{ikm}}}{\sqrt{|\Delta\sigma_{jln}|^2}\;\sqrt{|\Delta\sigma_{ikm}|^2}} \;,$$

and assume as before that errors of a particular type are correlated, i.e. $K_{jlnikm} = 0$ for $l \neq k$, then with $K_{kjimn} = K_{jlnikm}$, we get the following expression for the correlation coefficient between the errors of the two evaluated points:

$$\mathcal{B}_{n,m} = \frac{\sum_{k=1}^{M}\sum_{j=1}^{N}\sum_{i=1}^{N} a_{jn}^2\, a_{im}^2\, K_{kjinm}\sqrt{|\Delta\sigma_{jkn}|^2}\;\sqrt{|\Delta\sigma_{ikm}|^2}}{\sqrt{|\Delta\sigma_n|^2}\;\sqrt{|\Delta\sigma_m|^2}} \qquad (9)$$

Thus the correlation coefficient between the errors of two evaluated points can be expressed in terms of the values of the partial errors of the experiments used in the evaluation, the "weights" with which these experiments are used in the evaluation, and the correlation coefficients between the partial errors at these points.

In the calculations, the correlation coefficient K_{kjimn} has been taken to be independent of n and m, i.e. $K_{kjimn} = K_{kji}$, and therefore Eq. (5) can be used for K_{kji}. In fact, if the correlation coefficient for the partial

errors depends on the point concerned (for example, some parameter used to determine a cross-section may be measured in different ways at the various points), we can formally consider that we are dealing with different experiments and we can convert the correlation coefficient between points into a relationship between experiments, i.e.

$$\beta_{nm} = \frac{\sum_{k=1}^{M}\sum_{j=1}^{N}\sum_{i=1}^{N} a_{jn}^2\, a_{im}^2\, K_{kji}\sqrt{|\Delta\sigma_{jkn}|^2}\cdot\sqrt{|\Delta\sigma_{ikm}|^2}}{\sqrt{|\Delta\sigma_{n}|^2}\cdot\sqrt{|\Delta\sigma_{m}|^2}} \qquad (10)$$

This algorithm has been incorporated into a computer program which uses the partial errors and the correlations between them to determine the "weights" for the experimental data which will minimize the error in the evaluated quantity, the errors in the evaluated data at the various points, and the correlation coefficients between them.

Let us consider briefly the evaluation of the quantity $\alpha(^{239}\mathrm{Pu})$. The data from Refs [3-13] which were used in our earlier evaluation [2] have been supplemented by new data from Refs [14-20]. An analysis of the methods and errors of the various experiments has enabled us to break down the total error for each case into the following partial errors: the background which depends on E_n (k=1), statistical errors which depend on the energy (k=2), the error in the normalization (k=3), background from delayed fission gamma-rays (k=4), indeterminacy in the relative neutron flux (k=5), scattering of neutrons in the sample and the detector walls (k=6), indeterminacy in the detector efficiency due to a possible change in the gamma-ray spectrum (k=7), an error in $\bar{\nu}$ leading to indeterminacy in α (k=8), the determination of the efficiency of the detector system (k=9), changes in the detector-system efficiency with time (k=10), indeterminacies in the correction for impurities in the sample (k=11), the probability of fission events occurring without the fission neutrons being recorded (k=12), and the energy resolution (k=13). The following correlations between the partial errors were noted: for k=1, the experiments in Refs [14] and [15], which were carried out on the same linear accelerator, were taken to have a correlation coefficient of 0.5, as were Refs [6] and [16], and [10] and [8]; for k=3, Ref. [3] is correlated

with Refs [14, 15, 4, 5, 16, 8, 10, 19] and also partially with [6, 7]. The data in Refs [9, 11] are relative and they have been renormalized to the weighted-average value of α at 30 $\pm$ 10 keV obtained from Refs [18, 12, 13] and are therefore correlated with them; for k=4 and k=7, it was assumed that the relevant partial error was fully correlated in all the experiments; for k=5, there is correlation between Refs [3] and [14], [15], [16], [5] and [6], and between [4] and [7] and [9]; for k=6, Ref. [14] is correlated with [3], and [16] with [6]; for k=8, Ref. [15] is correlated with Refs [4, 5, 6, 16, 10, 19, 9, 11]; for k=9, Ref. [3] is correlated with [14], and Refs [12, 13, 18] are partially correlated; for k=10, Ref. [3] is correlated with [14].

The table shows the evaluated magnitudes of $\alpha(^{239}Pu)$ and their associated errors, obtained with and without allowance for the correlations between the partial measurement errors. The errors in the evaluated $\alpha(^{239}Pu)$ at the different energy points are strongly intercorrelated. For example, for energies of 0.1–0.2 keV and 1–2 keV, B = 0.922; for 0.1–0.2 keV and 20–30 keV, B = 0.706; for 0.1–0.2 keV and 100–200 keV, B = 0.588; for 0.1–0.2 keV and 0.5 MeV, B = 0.199; and for 0.1–0.2 keV and 1 MeV, B = 0.075.

Table

Evaluated data for $\alpha(^{239}Pu)$ and the associated errors with and without allowance for the correlations between the partial errors (optimized "weights")

E_n, keV	α	$\Delta\alpha$, %	$\Delta\alpha_{stat}$, %	E_n, keV	α	$\Delta\alpha$, %	$\Delta\alpha_{stat}$, %
0,I-0,2	0,86	5,5	3,I	I5-20	0,33	8,8	5,8
0,2-0,3	0,93	5,4	3,0	20-30	0,36	7,I	4,7
0,3-0,4	I,I5	5,7	3,2	30-40	0,28	8,I	5,I
0,4-0,5	0,45	5,7	3,8	40-50	0,25	8,2	5,6
0,5-0,6	0,72	5,7	3,4	50-60	0,23	8,6	5,9
0,6-0,7	I,50	5,7	3,2	60-70	0,20	8,9	7,5
0,7-0,8	0,92	5,5	3,2	70-80	0,I8	9,4	8,0
0,8-0,9	0,80	5,7	3,5	80-90	0,2I	I3,6	I2,0
0,9-I,0	0,69	5,7	3,6	90-I00	0,I5	I3,0	II,9
I - 2	0,89	5,9	3,5	I00-200	0,I4	9,8	6,9
2 - 3	I,0I	6,0	3,6	250	0,II	I6,7	I6,7
3 - 4	0,78	6,0	3,8	300	0,I2	I2,7	II,5
4 - 5	0,84	6,0	3,7	400	0,085	I0,6	9,5
5 - 6	0,84	6,2	3,9	500	0,078	I4,I	I3,0
6 - 7	0,80	6,I	3,9	600	0,056	I5,6	I5,0
7 - 8	0,63	6,2	3,9	750	0,067	I7.2	I6,6
8 - 9	0,56	6,0	3,9	900	0,038	25,4	25,0
9 -I0	0,6I	6,0	3,9	I000	0,027	26,0	26,0
I0-I5	0,54	8,3	5,I				

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SOME QUESTIONS CONCERNING THE PARAMETRIZATION OF THE CROSS-SECTIONS OF FISSIONABLE NUCLEI IN THE RESOLVED RESONANCE ENERGY REGION WITH ^{235}U, ^{239}Pu AND ^{241}Pu AS EXAMPLES

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ABSTRACT

Parametrization problems of neutron cross-sections in the resonance energy region are discussed; negative level parameters are given for ^{235}U, ^{239}Pu and ^{241}Pu.

Parametrization - the representation of a great deal of experimental data on cross-sections by a relatively small number of energy-independent parameters - is particularly important in the case of the heavy fissionable elements used in reactors. Cross-section parametrization is carried out on the basis of one of the formalisms for describing cross-sections in the resonance region, which were analysed in detail in Ref. [1].

The Breit-Wigner formalism proved to be suitable for parametrization of the ^{239}Pu nucleus, where the distance between levels is great and the interference between levels is negligible. For nuclei with appreciable interference between levels (^{235}U and ^{241}Pu) we have developed a formalism [1, 2] which, in our opinion, combines the advantages of the Breit-Wigner formalism and the Adler-Adler formalism and is free of the disadvantages of the latter. The essence of the proposed formalism is as follows: formally keeping the expression for $\sigma(E)$ in the Adlerian form we assume the parameter G_x to be a purely Breit-Wigner parameter - i.e.

$$\sigma_x(E) = \frac{A}{\sqrt{E}} \sum_{i=1}^{n} (G_{xi}\Psi_i + H_{xi}\chi_i),$$

where

$$G_{xi} = \frac{g_i \Gamma_{ni}^{\circ} \Gamma_{xi}}{\Gamma_i^2}.$$

An expression based on Breit-Wigner parameters has also been derived for H_x, but here one encounters the usual difficulty of determining the pair interference sign, so we shall not present this expression. The number of resonances taken into account, N, is defined as the minimum number necessary for the adequate regeneration of cross-sections from the parameters obtained; the region between the resonances is the most sensitive to the value of N.

The main question which arises in connection with parametrization is that of the experimental data used to obtain the parameters. From all the series of experiments for which results are available we chose those which give the fullest representation of the behaviour of cross-sections in the region under consideration and which complement one another, account being taken of sample temperature, energy resolution and cross-section normalization. The series of experimental data chosen in this way are the basis for parametrization.

To obtain a reliable system of parameters it is first necessary to solve the question of interfering and omitted levels in the experimental data. Generally, it is not difficult to get rid of the interfering resonances - it is sufficient to compare the available sets of experimental data on cross-sections among themselves and with the resonance parameter systems of the elements making up a sample. The number of omitted levels in a given energy range (i.e. resonances omitted in existing systems of parameters) is determined both by the method described in Ref. [1] and by the least squares method, on the basis of the energy dependence of the growing sum of levels. After this, the omitted resonances are arranged over an energy scale, mean parameter values are assigned to them and they are included in the parametrization procedure in the usual way.

Let us now consider the problem of negative levels. They have to be introduced because it is not possible, with any combination of positive resonance parameters, to get a good description of the energy region below 0.1 eV (especially the point E = 0.0253 eV) and above 0.5 eV, i.e. the trough between the first and second resonances; this is particularly characteristic of ^{239}Pu and ^{241}Pu, where the distances between the first and second resonances are of the order of 7 eV and 4 eV respectively. The number of negative resonances, their

position on the energy scale and their parameters were adjusted in such a way as to compensate for the difference between the experimental values of the cross-sections for the corresponding reaction and the cross-section values obtained from the parameters of the positive resonances making a contribution to the region under consideration. It was found that one negative level with E = -1.6 eV, Γ = 0.192 eV, Γ_n = 0.00246 eV, Γ_f = 0.17347 eV, Γ_γ = 0.01607 eV and J = 1 is enough for ^{239}Pu.

For ^{235}U and ^{241}Pu, it was necessary to introduce two negative levels each, with the parameters given in the table below.

Table

parameter \ nucleus	^{235}U	^{241}Pu
E_r , eV	- 0,5	- 0.25
	- 0.0I	- 0.0I
Γ , eV	0.25	0.30
	0.0I	0.0I
G_Γ , б.eV$^{1/2}$	$0.3603 \cdot I0^{-7}$	$0.69759 \cdot I0^{-4}$
	$0.464235 \cdot I0^{-4}$	$0.6650 2 \cdot I0^{-4}$
H_Γ , б.eV$^{1/2}$	$0.85I7 \cdot I0^{-4}$	$0.40549 \cdot I0^{-4}$
	0	0.0
G_f , б.eV$^{1/2}$	$-0.I022I2 \cdot I0^{-3}$	$0.0465062 \cdot I0^{-4}$
	$0.49692 \cdot I0^{-4}$	$-0.327508 \cdot I0^{-4}$
H_f , б.eV$^{1/2}$	$0.850I \cdot I0^{-4}$	$0.438284 \cdot I0^{-4}$
	0	0
G_γ , б.eV$^{1/2}$	$0.I00009 \cdot I0^{-4}$	
	$0.5 \cdot I0^{-6}$	
H_γ , б.eV$^{1/2}$	$0.I00II7 \cdot I0^{-4}$	
	0	

These parameters were not reduced to the Breit-Wigner form and not made self-consistent since the levels in question are adjustment levels and their parameters were determined at a great distance from the resonance peaks, where the main contribution is made by interference terms; one cannot therefore demand that the parameters obtained be physical parameters, and consequently it is impossible to make them self-consistent and to convert them to Breit-Wigner parameters as was done for ^{239}Pu, where we did not take interference into account. The above parameters, together with the data presented in Refs [1, 2], enable one to obtain a good description of the variations in the cross-sections in the 0.01 eV-1 eV region when the corresponding number of resonances is taken into account.

Let us now turn to the question of identifying resonances by their spins, for without this procedure it is impossible to carry out the operation of making the parameters self-consistent correctly and to determine correctly the usual Breit-Wigner parameters from the G_x values obtained in parametrization. Data on level spins for heavy fissionable nuclei are not complete as a rule and are not always reliable; in some cases, however, the situation can be rectified. Let us take each of the above-mentioned nuclei separately:

1. In ^{239}Pu the spin of the ground state is $\frac{1}{2}$, so that two values are possible ($J = 0^+$ and $J = 1^+$) for the spins of the levels of the compound nucleus; at the same time there is a very distinct difference between the total widths of resonances with $J = 0^+$ (high values) and $J = 1^+$ (low values). Consequently, on the basis of the total widths it is possible to assign spins to resonances with a fairly high degree of confidence.
2. In ^{235}U the spin of the ground state is $7/2$ - i.e. resonances with $J = 3^-$ and $J = 4^-$ are formed. At the same time, judging by the avilable data on resonance spins, there is no clear separation of widths by spin state; this is due to the relative smallness of the total widths compared with the widths in ^{239}Pu. To determine the resonance spins we used the parameters $\{G_{Ti}\}$, $\{G_{fi}\}$ and $\{G_{\gamma i}\}$

obtained as a result of parametrization of the corresponding cross-section types with the help of our formalism. One can readily see that they are linked by the relation

$$G_{Ti} = G_{fi} + G_{\gamma i} + G_{Ti}^2 \sqrt{E_{ri}}/g_i ,$$

so that it is possible to determine g_i for each resonance at which this relation is satisfied best. Although we do not claim that they are absolutely reliable, the level spins obtained in this way offer the possibility of solving the problem of self-consistency and of obtaining Breit-Wigner parameters.

3. In ^{241}Pu the spin of the ground state is $5/2$ - i.e. we have resonances with $J = 2^+$ and $J = 3^+$. However, there are no experimental data on $\sigma_\gamma(E)$ and $\sigma_n(E)$, so that it is impossible to determine the level spins as was done for ^{235}U. In determining the resonance spins, the absolute majority of which is unknown, we started with the level density ratio as a function of J, assigning a spin of 2^+ to resonances with a larger total width. Here, as for ^{235}U, there is no clear separation of total widths by spin. We consider the assigned spin values to be tentative and in need of more precise determination.

Let us now consider the procedure for making parameters self-consistent, which is closely linked with the spin questions discussed above. In this case also we can obtain self-consistent sets of parameters only if there are three cross-section types. As in the preceding case, we use the relation

$$G_{Ti} = G_{fi} + G_{\gamma i} + G_{Ti}^2 \sqrt{E_{ri}}/g_i ;$$

then, on the basis of our knowledge of the accuracy of the experiments relating to each cross-section type, we specify the resolved interval of variation of the parameters, and the parameters themselves vary

within this interval in such a way that this relation is satisfied exactly. The resulting self-consistent values are used both for regenerating the cross-sections and, on the basis of the relation

$$G_{x,i} = \frac{g_i \Gamma_{n,i}^{\circ} \Gamma_{x,i}}{\Gamma_i^2} ,$$

for obtaining Breit-Wigner parameters which in turn are necessary both for verification of the quality of parametrization (together with the cross-section values regenerated from the parameters) and for obtaining the mean parameter values and the strength function S^{o} value used for calculations in the unresolved resonance region.

The agreement between the values of S^{o} calculated in two different ways - from the parameters in the resolved resonance region and from the experimental total cross-section values in the unresolved resonance region - is also a good criterion for the quality of parametrization. For example, for ^{235}U these values are $1.069 \cdot 10^{-4}$ and $1.08 \cdot 10^{-4}$ respectively.

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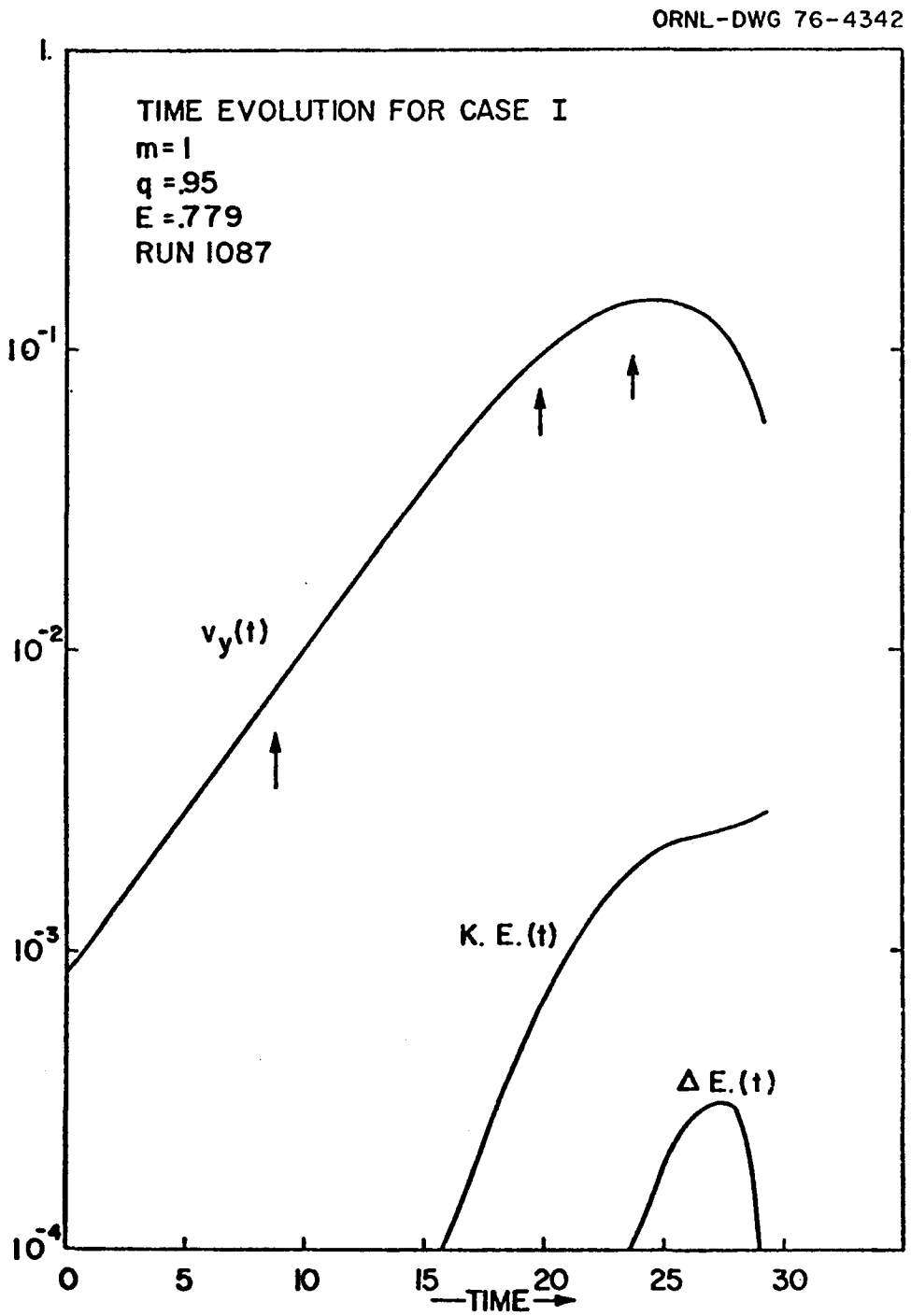
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RUN 1087
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10^{-2}
10^{-3}
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$v_y(t)$
K. E.(t)
Δ E.(t)
0
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10
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20
25
30
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CONSIDERATION OF THE (n,γf) PROCESS WHEN CALCULATING WIDTHS OF RADIATIVE CAPTURE AND MEAN CROSS-SECTIONS OF FISSIONABLE NUCLEI

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ABSTRACT

The widths and cross-sections of ^{239}Pu radiative capture and fission processes are calculated within the framework of a statistical model, with allowance for the (n,γf) process. The importance of taking this process into account for heavy nuclei with negative fission thresholds is shown.

The need for the (n,γn') process to be taken into consideration when calculating radiative widths for neutron energies higher than the mean energy of the gamma quanta emitted ($\bar{\varepsilon}\gamma \sim 1$ MeV) is well known. With fissionable nuclei the (n,γf) process must also be considered when, in terms of energy, fission of an excited compound nucleus is possible after primary gamma quantum emission. However, the theoretical estimates that have been made of widths for this process, where the excitation energy is equal to the binding energy, contradict each other [1,2,3].

The present paper contains an analysis of the influence of the (n,γf) process on calculations of the energy dependence of mean widths and cross-sections of radiative capture σ_γ, fission cross-sections σ_F, and the value of α.

It was assumed that the width of primary gamma quantum emission, with only EI transitions taken into account, can be represented as in Ref. [4]:

$$\Gamma_\gamma^{J\pi}(E)=\frac{1}{\rho(E+B_n,J,\pi)}\int_0^{E+B_n}\sum_{J_n=|J-1|}^{J+1} f(E,\varepsilon_\gamma)\rho(E+B_n-\varepsilon_\gamma,J_n,\pi)d\varepsilon_\gamma, \quad (I)$$

where $\rho(U,J,\pi)$ is the level density of a nucleus with excitation energy U, spin J and parity π. For the spectral factor $f(E,\varepsilon_\gamma)$, two concepts were

used: (a) that proposed by Weisskopf [5], where $f(E,\varepsilon_\gamma) \sim \varepsilon_\gamma^3$, and (b) the Lorentz dependence, which follows from the mode of the cross-section of an inverse (photonuclear) reaction generalized for the case of deformed nuclei [6]:

$$f(E,\varepsilon_\gamma) \sim \sum_{i=1}^{2} \frac{i}{3} \frac{\Gamma_{iG}\,\varepsilon_\gamma^4}{(\varepsilon_\gamma^2 - E_{iG}^2)^2 + (\Gamma_{iG}\,\varepsilon_\gamma)^2} \qquad (2)$$

The giant resonance parameters E_{iG} and Γ_{iG} were based on the mean for heavy nuclei [4]: E_{iG} = 11 MeV, Γ_{iG} = 2.9 MeV, E_{2G} = 14 MeV and Γ_{2G} = 4.5 MeV. The level density was chosen so as to accord with the model of non-interacting particles [7], for which it is assumed that there is no dependence on parity.

For the calculations of radiative widths it was assumed that, if after primary gamma quantum emission the residual excitation of a nucleus is greater than the neutron binding energy B_n, then only fission or the emission of a neutron will occur subsequently. For this reason the contribution of these gamma transitions to the radiative capture width is nil. For nuclei with a negative fission threshold, competition of the $(n,\gamma f)$ process in radiative capture is possible also when the residual excitation of a nucleus after primary gamma quantum emission is less than the neutron binding energy where $E-E_f > \varepsilon_\gamma$ (E_f = fission threshold energy).

In this case the probability of further gamma discharge is equal to $\Gamma_\gamma^{J\pi}(E-\varepsilon_\gamma)/\left(\Gamma_\gamma^{J\pi}(E-\varepsilon_\gamma) + \Gamma_f^{J\pi}(E-\varepsilon_\gamma)\right)$, and therefore the integrand in (1) can be multiplied by this value. Here $\Gamma_f^{J_K^\pi}(E-\varepsilon_\gamma)$ is the fission width of the channel $\{J_K,\pi\}$ at an excitation energy of $E+B_n-\varepsilon_\gamma$. The fission widths $\Gamma_f^{J_K^\pi}$ were calculated according to the Bohr-Hill-Wheeler channel theory [8], with the transitional state parameters taken from Ref. [9]. The width $\Gamma_\gamma^{J_K^\pi}$ was calculated from formula (1). Parity π in calculating the widths $\Gamma_f^{J_K^\pi}$ and $\Gamma_\gamma^{J_K^\pi}$ is the opposite of that of a compound nucleus, since an E1 gamma quantum is emitted in advance.

Let us now examine the influence of the $(n,\gamma n')$ and $(n,\gamma f)$ processes when calculating mean widths and cross-sections of the (n,γ) and (n,F) reactions for the ^{239}Pu nucleus. The calculations described below were

based on a statistical model with the following parameters: for a ^{239}Pu compound nucleus B_n = 5.655 MeV [10], the pairing energy Δ = 0.420 MeV [10,11], and the level density parameter a = 27.48 MeV^{-1}, which is found from the observed value $\langle D \rangle$ = 9.5 ± 0.7 eV [12]. For the ^{240}Pu compound nucleus B_n = 6.534 MeV [10], Δ = 0.919 MeV [10,11], a = 26.46 MeV^{-1} and the observed value for $\langle D \rangle$ = 2.38 ± 0.06 eV [13]. The optical potential parameters are taken from Ref. [14].

Since fission widths are a function of the spin and parity of a channel, it is seen that, when the competition of the (n,γf) process is considered, mean radiative widths are dependent on parity and that there is a greater spin dependence (see table).

The values given for widths are normalized to the experimental value of $\langle \Gamma_\gamma \rangle$ = 43.3 ± 3.0 MeV [12]. It will be seen that the figures for the two different concepts of the spectral factor $f(E,\varepsilon_\gamma)$ are very different. This follows from the difference in the mean energies of primary gamma quanta, which shows itself in the competition of the (n,γf) process in radiative capture. From this difference and from the experimental data available it is possible to draw certain conclusions about the type of spectral factor. In Ref. [15] measurements are quoted which show the difference in $\Gamma_{\gamma f}^{J\pi}$ widths for the 0^+ and 1^+ states, viz. $/\Gamma_{\gamma f}^{0+} - \Gamma_{\gamma f}^{1+}/ < 4$ MeV. Ref. [16] gives 4.1 ± 0.9 MeV as the value of $\Gamma_{\gamma f}^{1+}$. If the Weisskopf spectral factor is used for calculations, the values $\Gamma_{\gamma f}^{0+}$ = 20.3 MeV and $\Gamma_{\gamma f}^{1+}$ = 10.6 MeV are obtained. Use of equation (2) yields the values $\Gamma_{\gamma f}^{0+}$ = 10.2 MeV and $\Gamma_{\gamma f}^{1+}$ = 4.9 MeV, which are near the estimate of Lynn [1], who used Lorentz dependence for the spectral factor and obtained the values $\Gamma_{\gamma f}^{0+}$ = 8 MeV and $\Gamma_{\gamma f}^{1+}$ = 3 MeV. One can also compare calculations of $\Gamma_{\gamma f}^{J\pi}$ for ^{241}Pu with the experimental results in Ref. [17], viz. $\Gamma_{\gamma f}^{2+} \sim 7$ MeV and $\Gamma_{\gamma f}^{3+} \sim 2$ MeV. Calculations, with B_n = 6.301 MeV, Δ = 1.013 MeV, a = 26.90 MeV^{-1}, $\langle D \rangle_{obs.}$ = 1.34 ± 0.10 eV and $\langle \Gamma_\gamma \rangle_{exp.}$ = 43.0 ± 3.0 MeV, give $\Gamma_{\gamma f}^{2+}$ = 5.0 MeV and $\Gamma_{\gamma f}^{3+}$ = 2.9 MeV when the Lorentz dependence is used for the spectral factor and, when Weisskopf's concept is used, 10.4 MeV and 6.3 MeV respectively. Clearly the use of Weisskopf's concept of the spectral factor gives results which differ from experimental data, whereas good agreement with experimental data is found with the Lorentz dependence (2).

In Ref. [3] the opposite conclusion is drawn. The contradiction seems to be the result of the difference in the parameters employed. The parameters we used are optimized with reference to the latest experimental data and our conclusion has more justification.

When the $(n,\gamma f)$ and $(n,\gamma n')$ processes are taken into account the energy dependence of the mean radiative widths is seen to be different (Fig. 1) and, consequently, that of the cross-section σ_γ differs also (Fig. 2). It will be seen that calculations of σ_γ will differ by a factor of about two at an energy of 1 MeV, depending on whether the $(n,\gamma f)$ process is taken into account or not. With an energy of 3 MeV, where the $(n,\gamma n')$ process is significant, the results differ by a factor of approximately ten.

When low energies are involved, where the cross-section σ_γ constitutes an important part of the inelastic interaction cross-section, the $(n,\gamma f)$ process can make a significant contribution to the fission cross-section $\sigma_F = \sigma_f + \sigma_{\gamma f}$. Thus, calculations with mean resonance parameters for ^{239}Pu show that at an energy of 1 keV the contribution of the $(n,\gamma f)$ process cross-section to σ_F is about 10%. As the energy increases, the contribution of the $(n,\gamma f)$ process cross-section will of course diminish.

The difference in the cross-sections σ_γ and σ_F, depending on whether the $(n,\gamma f)$ process is taken into account or not, shows itself clearly in the calculated value $\alpha = \sigma_\gamma/\sigma_F$. Thus, calculations of α differ, depending on whether this process is taken into account or not, by 15% at 1 keV, by 10% at 40 keV, by 20% at 0.3 MeV and by 50% at 0.7 MeV. Below 100 keV the increase in the divergence in α with the decrease in energy is caused by the increase in the contribution of the cross-section $\sigma_{\gamma f}$ to σ_F. Above 100 keV, the increase in divergence as the energy increases is caused by the greater competition of the $(n,\gamma f)$ process in radiative capture.

Therefore, when calculating mean widths and cross-sections of radiative capture and fission for nuclei with negative fission thresholds, the $(n,\gamma f)$ process must be taken into account. Consideration of the $(n,\gamma f)$ process will show a clear dependence of radiative widths on channel characteristics. Calculations show that the concept of the spectral factor $f(E,\varepsilon_\gamma)$, which is based on the Lorentz dependence, is the preferable one.

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Table

Mean radiative widths for ^{239}Pu, calculated both with and without taking the (n,γf) process into account and with different concepts of the spectral factor for a neutron energy E = 0.1 keV

Channel	With allowance for (n,γf) process, MeV		Without allowance for (n,γf) process, MeV	
	Weisskopf concept	Lorentz dependence	Weisskopf concept	Lorentz dependence
0^+	36,58	39,73	43,47	43,53
0^-	56,I4	49.73	43,47	43,53
I^+	46,0I	44,65	43,24	43,22
I^-	35,I0	36,98	43,24	43,22
2^+	4I,22	4I,8I	42,8I	42,62
2^-	39,35	39,95	42,8I	42,62

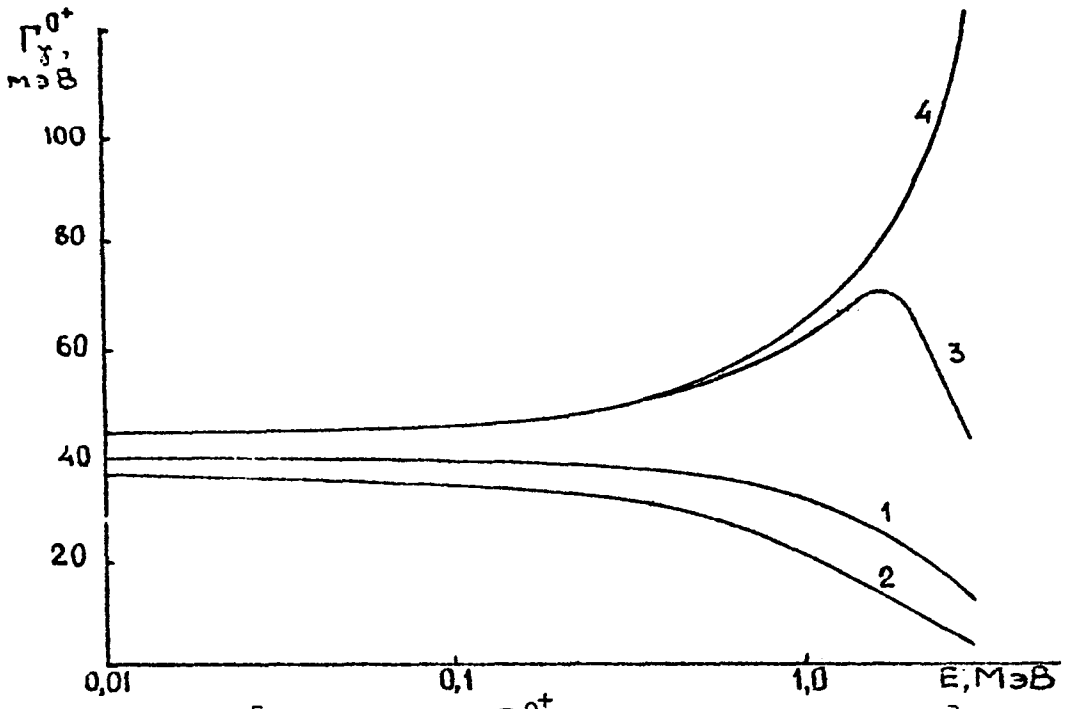

Fig. 1. [Vertical axis: $\Gamma_{\gamma}^{0^+}$, MeV; Horizontal axis: E,MeV]
The dependence of $\Gamma^{0^+}_{\gamma}$(E): 1. with consideration of (n,γf) and (n,γn'), $^{\gamma}$f(E,ε_{γ}) in mode (2); 2. with consideration of (n,γf) and $^{\gamma}$(n,γn'), f(E,ε_{γ}) in Weisskopf mode; 3. with consideration of (n,γn'), $^{\gamma}$f(E,ε_{γ}) in mode (2); 4. without consideration of (n,γf) and (n,γn'), f(E,ε_{γ}) in mode (2).

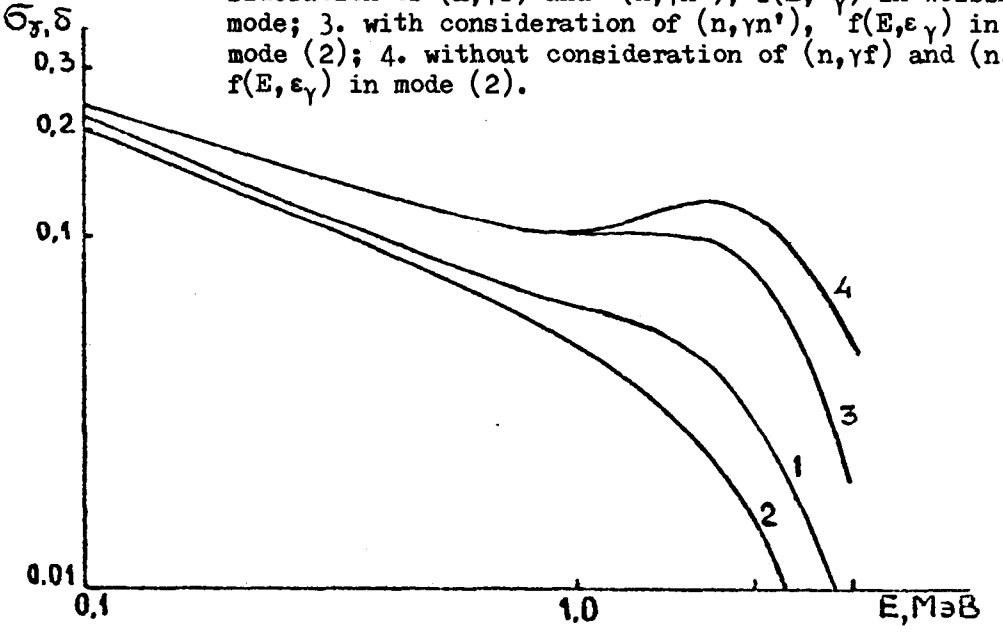

Fig. 2. [Vertical axis: σ_{γ},δ; Horizontal axis: E,MeV]
Radiative capture cross-section σ_{γ} for ^{239}Pu.
Designation of curves as in Fig. 1.