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ON CORRECTNESS OF SOME PROCESSING OPERATIONS FOR TWO-STEP CASCADE INTENSITIES DATA FROM THE (n_{th}, 2γ) REACTION

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О корректности некоторых операций обработки данных
по интенсивностям двухквантовых каскадов из реакции (n_{th}, 2γ)

Рассматривается влияние некоторых некорректностей анализа экспериментальных гамма-спектров на извлекаемые плотности уровней и радиационные силовые функции. Показано, что для получения достоверных данных об этих параметрах из реакции (n, 2γ) требуется выделять из экспериментальных распределений интенсивностей двухквантовых каскадов их зависимость от энергии первичного гамма-перехода. Оценено влияние некоторых условий анализа экспериментальных гамма-спектров реакции (^{3}He, α) на ожидаемые значения этих параметров. Предложены пути уменьшения соответствующих погрешностей.

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On Correctness of Some Processing Operations
for Two-Step Cascade Intensities Data from the (n_{th}, 2γ) Reaction

An influence of some incorrectness of analysis on the level densities and radiative strength functions derived from the experimental γ spectra is considered. It was shown that the obtaining of reliable data from the reaction (n, 2γ) requires one to derive dependence of the two-step cascade intensities on their primary transition energy. The influence of some conditions of an analysis of the experimental γ-spectra from reaction (^{3}He, α) on the expected value of both level density and radiative strength functions was estimated. The ways to decrease these uncertainties are suggested.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

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INTRODUCTION

The form of γ spectra measured in different experiments is ambiguously determined by the level density $\rho = D^{-1}$ and radiative strength functions $k = \langle\Gamma_{\lambda i}\rangle/(E_\gamma^3 \cdot A^{2/3} \cdot D_\lambda)$ (or in equivalent form $f = k \cdot A^{2/3}$) for the γ transitions between the levels $\lambda \to i$ in a nucleus with the mass A. The intensity of any such spectrum for a given γ-transition energy E_γ is determined by folding of these two parameters of the γ decay of a nucleus under study. Therefore, these parameters can be determined for any nucleus only jointly from the solution of reversed mathematical problem. In that case, the correspondence of the shape of functional relation between the measured intensity of spectrum and required mean values of ρ and k to the experiment is postulated.

In all known cases this relation includes the product ρ and k. That is why, any errors of, for example, ρ are completely or partially compensated in measured spectrum by corresponding errors of k. As a consequence, any method used for simultaneous determination of these parameters of the γ decay by the solution of reverses problem cannot give unique functional dependence between ρ and k for given excitation and γ-transition energies. Moreover, all existing methods of the analysis allow one to determine with acceptable precision only the sum of level densities of both parities in some spin window and sum of radiative strength functions for dipole electric and magnetic γ transitions. The uncertainty in level density partially decreases if one uses additional experimental data on the ρ below the excitation energy 1–2 MeV and spacing D_λ between neutron resonances. The use of the experimental ratio $k(E1)/k(M1)$ in vicinity of the neutron binding energy B_n leads to decrease in error of strength functions.

Principle impossibility to determine unique quantities of ρ and k was directly fixed in method [1] used to extract these parameters from the dependence of the two-step cascade intensities

$$I_{\gamma\gamma}(E_1) = F(E_1) = \sum_{\lambda,f}\sum_i \frac{\Gamma_{\lambda i}}{\Gamma_\lambda}\frac{\Gamma_{if}}{\Gamma_i} = \sum_{\lambda,f}\frac{\Gamma_{\lambda i}}{\langle\Gamma_{\lambda i}\rangle m_{\lambda i}} n_{\lambda i}\frac{\Gamma_{if}}{\langle\Gamma_{if}\rangle m_{if}}, \quad (1)$$

following thermal neutron capture on the energy E_1 of their primary transitions. This should be taken into account also in the analysis [2] of the primary γ-transition spectra of nuclear reactions. This conclusion follows from from testing [3]

of possible use of the conventional multidimensional fitting of parameters of the Gauss method instead of the so-called «Oslo method» [2].

Multidimensional distribution of probabilities of random ρ and k values for the case of ensembles [2] of the primary γ-transition spectra, depopulating arbitrary excited level $E_{\rm ex}$, is degenerate even for surplus number of experimental points. As a result, equal value of χ^2 is observed [3] for different ρ and k even in the case when ensemble of data [2] includes experimental total radiative widths, densities of low-lying levels and density [4] of neutron resonances extrapolated into some spin interval.

For deformed nucleus, this extrapolation requires also the knowledge of dependence of coefficient of rotational enhancement of level density [4] on their spin. The lack of necessary experimental data on parameters of rotational bands even for the excitation energy 2–3 MeV and some higher results in unknown additional uncertainty in determination of ρ and k. Of course, this question is more serious for the region $E_{\rm ex} \simeq B_n$ [2].

Rather considerable nonlinearity of the task, solution of which is described in [2], limits the variation interval of ρ and k even at the correlation coefficient $|R_{\rm corr}| = 1$ (as compared with the degenerate system of linear equations). Because the relation between the ρ and k for the primary transition spectra [2] and intensities of the two-step cascades [1] are essentially different, then involving of these heterogeneous experimental data in the united likelihood function could increase reliability in determination of ρ and k. The type and magnitude of the most important statistics errors at both obtaining of experimental spectra in the frameworks of these methods and their further use for determination of ρ and k are partially separated. This also can provide increase in reliability of the results.

Very important problem for any method for simultaneous determination of ρ and k is the minimization of additional systematic errors caused by inaccuracy in data processing. This follows from incompatibility of conclusions made by investigation [1] and [5] of two-step γ cascades following thermal neutron capture and by the study of the primary γ-transition spectra of nuclear reactions [6]. This is reduced to the following: according to [1], cascade γ decay of, for example, deformed compound nucleus is characterized by clearly expressed step-like structure in level density (predicted [7] by A. V. Ignatyuk and Yu. V. Sokolov and related by them with breaking of the next Cooper pair of nucleons). But in accordance with [5, 6], the main peculiarity of γ decay is the presence of «pygmy» resonance in radiative strength function at «smooth» level density. As the authors of [1] and the authors of [5, 8] use the same type of experimental data then all observed discrepancies should be related with incorrectness of a method of their analysis. This incorrectness appears to a great extent due to ignoring [5, 8] of specific of the experiment on investigation of $I_{\gamma\gamma}$.

1. SPECIFIC OF THE EXPERIMENT ON INVESTIGATION OF THE TWO-STEP γ CASCADES

Main properties of this experiment are the following:

1. The impossibility to determine ordering of two successive quanta with sum energy of several MeV measured with HPG detectors directly in experiment.

2. The dependence of intensity of every cascade on the ρ and k values over all excitation region of a nucleus.

3. The connection of variation $\delta I_{\gamma\gamma}$ with variations $\delta\rho$ and δk through incoherent sum of derivatives of cascade intensities with respect to all possible values of ρ and k.

1. As a result, every experimental spectrum $I_{\gamma\gamma}(E_\gamma)$ of cascades (see Fig. 1) with the total cascade energy $E_c = E_1 + E_2 = B_n - E_f$ can be reproduce by a sum of 2^N different symmetrical distributions $F(E_1)$ and $S(E_2)$ corresponding to registration of one or other cascade quanta as primary or secondary transitions, respectively (here N are total number of cascades). Decomposition of the spectrum $I_{\gamma\gamma}(E_\gamma)$ into two parts corresponding to solely primary $F(E_1)$ and solely secondary $S(E_2) = F(E_c - E_1)$ transitions can be realized with some uncertainty. Practical determination of function $F(E_1)$ with small enough uncertainty is quite possible in modern experiment like [10] with the help of the nuclear spectroscopy methods using the numerical method [11] for improvement of energy resolution. Probable error of this procedure is determined by extrapolation [12] of cumulative sums of intensities of cascades (experimentally resolved in form of pair of peaks) for small energy intervals of their intermediate levels $E_i < 0.5B_n$ to the zero detection threshold of their intensity.

It should be noted that any from 2^N possible variants of functions $F(E_1)$ and $S(E_2)$ can be always reproduced by some set of functional dependencies $\rho(E_{\rm ex})$ and $k(E_1)$. Level density for any function $F(E_1)$ is defined as the number of cascade intermediate levels in a given interval of excitation energy independently on the truth in determination of their primary transition energy. Because the value of F is always determined for any variant of quanta ordering in cascades then in any case are also determined and radiative strength functions. This means that the experimental spectra of the two-step cascades can be reproduced, in principle, with its experimental precision by ρ and k from [6] independently on the magnitude of systematical errors of these parameters.

The spectra for the studied even-odd and even-even nuclei demostrate [10] relatively small density of peaks for the cascades with $E_i \leqslant 0.5B_n$. This allows one to expect that the asymptotic value of error of function $I_{\gamma\gamma}(E_1)$ will aspire to zero as the detection threshold of individual cascade also aspires to zero. The portion of unobserved cascade intensity is determined by the detection threshold and form of distribution of deviations of the random γ-quanta intensities from the average for any decaying level $E_{\rm ex}$. If this distribution depends on the structure

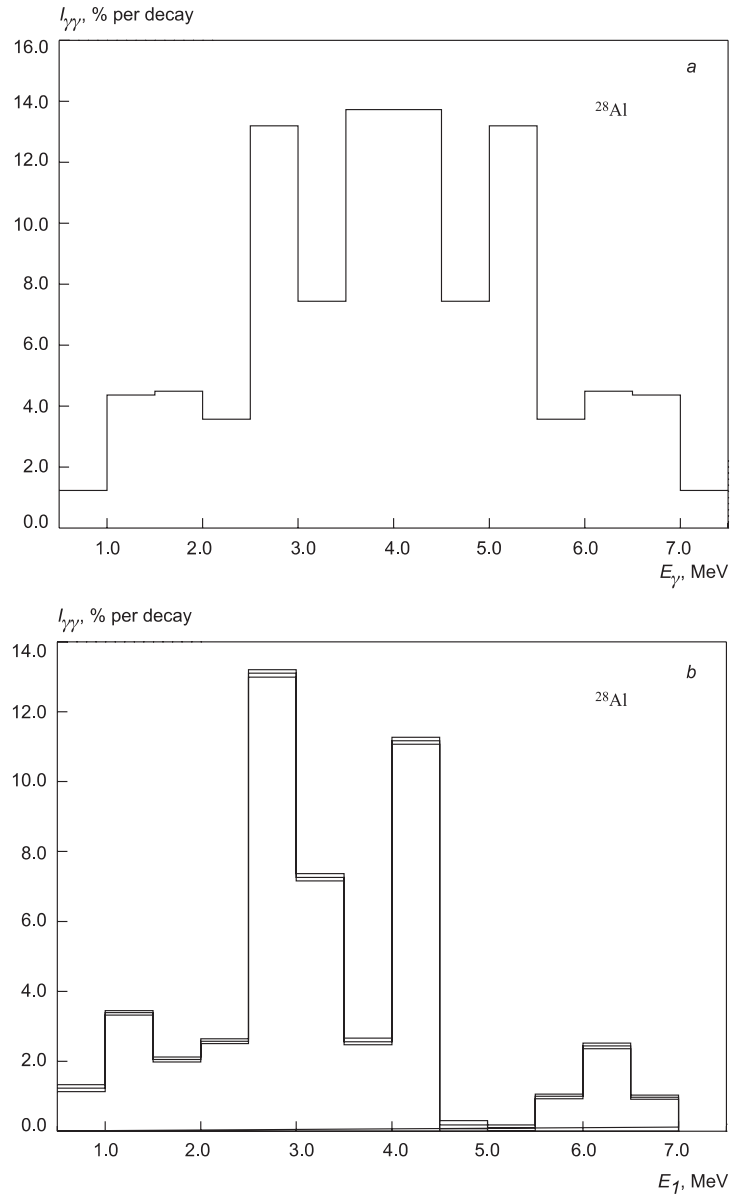

Fig. 1. a — the experimental spectrum of the two-step γ cascades terminating at the first and ground states of ^{28}Al. b — distribution [9] of the same intensity in function of the primary transition energy only

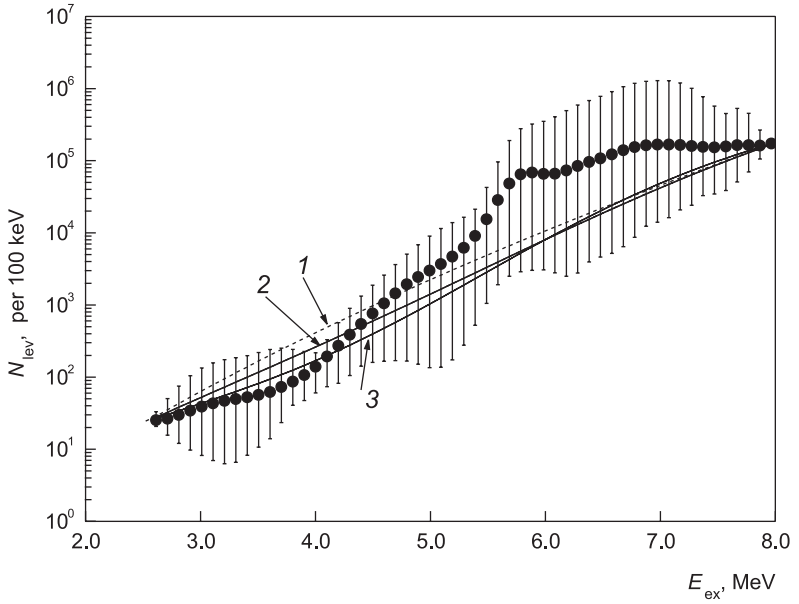

Fig. 2. The interval of variations of the level density providing reproduction of the experimental intensities [8] of the two-step cascades to the ground and first excited state of ^{172}Yb (points with bars). Line *1* represents predictions according model [14], lines *2* and *3* show the data used in calculations for Figs. 4 and 5, respectively

of the level $E_{\rm ex}$ then the model notions of the γ decay must be corrected both in [1] and [6].

It is very important that the specific form of dependence of $I_{\gamma\gamma}(E_1)$ on its parameters allows one precisely ($\chi^2/f \ll 1$) reproduce this function with the help of ρ and k varying in narrow enough intervals of magnitudes. (Up to now, intensities of cascades $F(E_1)$ were calculated [1] for several millions of pairs of different functional dependencies of ρ and k.)

Quite different situation is observed at direct in analysis of the experimental spectra of the two-step γ cascades $I_{\gamma\gamma}(E_\gamma) = F(E_1) + S(E_2)$ whose amplitudes in any interval of γ-transition energy depend on both E_1 and E_2. Any algorithm for search of random functions (like that used in [1]) allows one to be convinced that the precise reproduction of the sum of all possible values of functions F and S is possible only when the maximum values of the obtained ρ and k exceed the minimum values by a factor of several tens (Figs. 2, 3). It is not difficult to check that at the fixation of ρ on the ground of any additional information, the

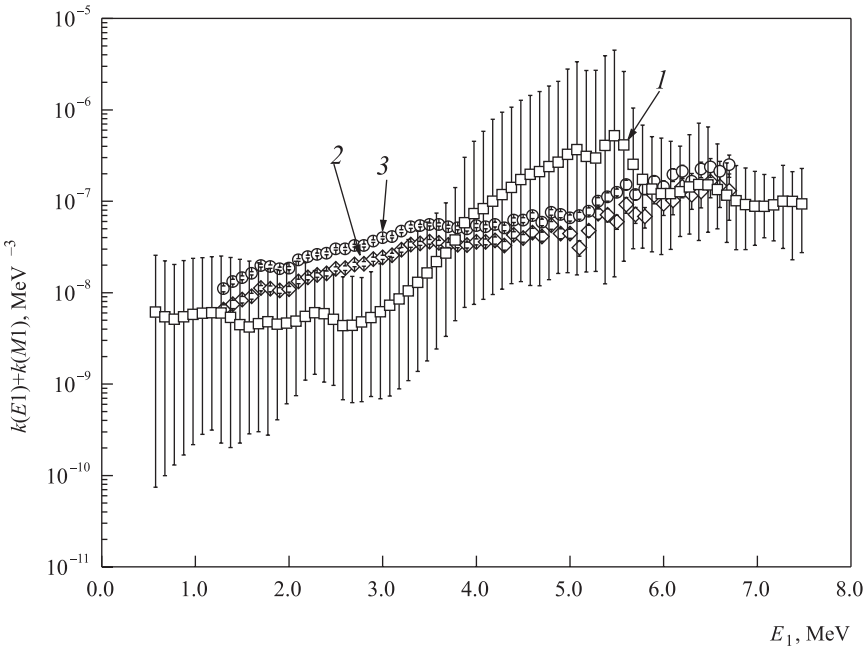

Fig. 3. Interval of variations of the strength functions (points *1* with bars). Points *2* and *3* represent strength functions from [6] and [8], respectively

spectra of cascade intensities also can be exactly reproduced for all E_γ by wide ensemble of k. Maximum value of these k is (Fig. 4, 5) 2–10 times higher than minimum values (any systematic errors of ρ shift location and distort the shape of the region of possible k values).

It should be especially noted that at reproducing of intensities of two-step cascades in ^{172}Yb listed in [8], «pygmy» resonance does not appear. Irremovable ambiguity of the experiment causes a necessity of transition from the analysis of the spectra $I_{\gamma\gamma}(E_\gamma)$ to analysis of spectra in function of the primary transitions energy $I_{\gamma\gamma}(E_1)$ only. This circumstance is ignored by the authors of both [5] and [8]. The authors of [8] make conclusion about correspondence of the functions $\rho^r = f(E_{\rm ex})$ and $k^r = \phi(E_\gamma)$ obtained by them from γ-ray spectra of reaction $(^3{\rm He}, \alpha)$ to the experimental values only on the grounds that they provide reproduction of the untransformed experimental distributions of two-step cascade intensities in limited [5, 8] interval of energies of their intermediate levels. The statement about correspondence between the experimental and tested values of ρ and k made on the ground of equality $I^{\rm exp} = I^{\rm cal}$ than it is equivalent to

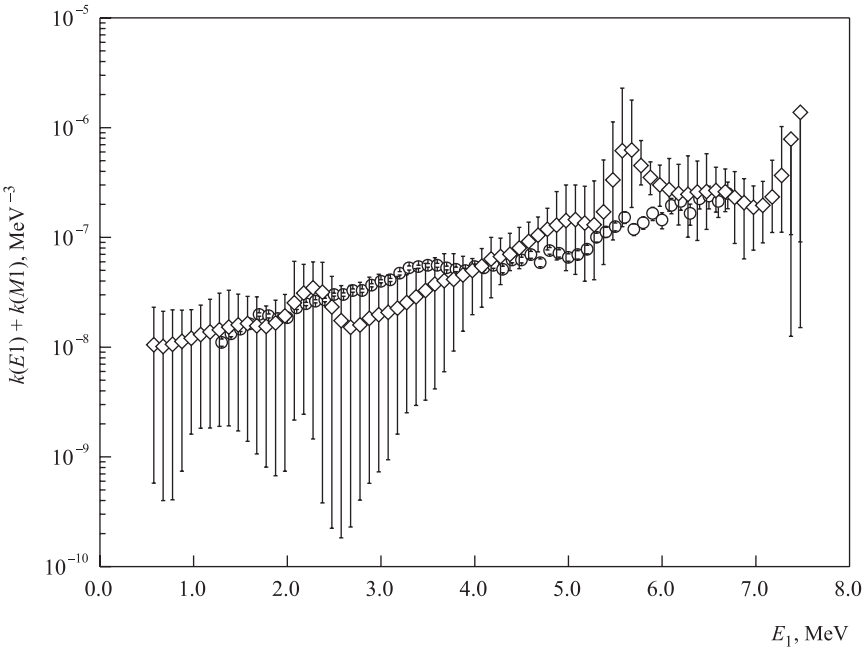

Fig. 4. The same as in Fig. 3. Calculation with level density shown in Fig. 2 by line *2*

execution of conditions $F^{\rm exp} = F^{\rm cal}$ and $S^{\rm exp} = S^{\rm cal}$ for any energies of the cascade γ transitions, i. e., from the multitude of possible solutions of Eq. (2) with two unknown values of functions F and S, the authors of [5, 8] choose the unique solution. It is wrong mathematical operation. Inequality of the experimental and calculated values of F and S always will mean that the ρ and k parameters used for calculation of cascade intensities do not correspond to their unknown experimental values. Therefore, such reproduction ($\chi^2/f \ll 1$) of the experimental intensities $I_{\gamma\gamma} = F(E_1) + S(E_2)$ for any energies of cascade transitions is necessary but not enough criterion of correspondence between the desired and unknown experimental values of ρ and k. Only analysis of the experimental distribution $I_{\gamma\gamma}(E_1)$ with accounting for its total error allows determination of ρ and k with minimum possible systematic error.

2. The total width of the decaying initial (or intermediate) cascade level can be presented as $\Gamma = \Gamma_{\rm in} + \Gamma_{\rm out}$ where two items represent sum of partial widths of cascade transitions in limits of energy interval chosen in [5] or [8] and out of it, respectively. These sums are the items of functional relation (1) of $I_{\gamma\gamma}$ with ρ and k. If experimental distribution $I_{\gamma\gamma}$ is reproduced with the use of some ρ and

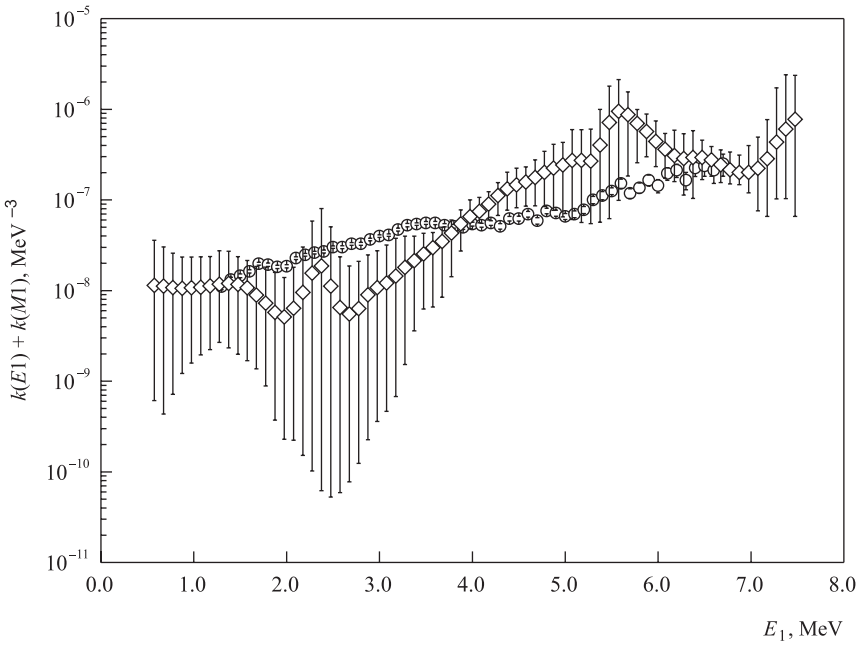

Fig. 5. The same as in Fig. 3. Calculation with level density shown in Fig. 2 by line *3*

k only for the part of energies of intermediate levels and is not reproduced over the whole energy interval then, most probably, this partial correspondence should be considered as the result of mutual compensation of errors. Porter–Thomas fluctuations of the primary transition widths have zero mean value and cannot lead to systematic discrepancy between the experimental and calculated cascade intensities.

So, discrepancy between experimental and calculated cascade intensities observed [8] at low and high energies of cascade transitions are caused by the error in determination of the sum $\Gamma_{\rm out}$ of partial widths of primary and/or secondary cascade transitions. In turn, this can manifest itself only at discrepancy between the experimental and used for calculation values of ρ and k.

3. As is known from mathematical statistics, error of function can be presented in the first approach as the product of its derivative by the argument of function. For Eq. (1), relative errors of ρ and k at any energy of excitation or transition lead through incoherent sum of derivatives to the different relative change in $I_{\gamma\gamma}$ simultaneously over all energy region of cascade transitions. If this sum is close to zero then small relative deviation of function $I_{\gamma\gamma}$, for example,

can be obtained only due to very wide variations of parameters or due to even small change in function S and necessary for this small variation of parameters of the calculation. In practice, in some cases [13] fixation of ρ makes impossible selection of k which provide reproduction of $I_{\gamma\gamma}(E_1)$ (especially at low energies of the primary transitions of cascades and large values of ρ). But there is no problem to achieve practically absolute agreement of the experimental and calculated sums $F + S$ for ρ and k with any systematic errors.

2. MAIN SOURCES OF SYSTEMATIC ERRORS IN DIFFERENT EXPERIMENTS

Discrepancy between the main properties of the ρ and k values obtained in [1] and [5, 6] means the presence of systematic error in corresponding experiments. The values of $\delta\rho$ and δk in method [1] are determined, first of all, by the following errors of the values of the used function $F(E_1)$ as:

a) the error in determination of absolute value (normalization of area);

b) distortion of the form of functional dependence $I_{\gamma\gamma}(E_1)$ on the energy of the cascade primary transition.

Both errors are limited only by the experimental conditions. At the absence of these errors, asymptotic values of δ_ρ and δ_k for method [1] equals about 20%.

Influence of the error in determination of the absolute value of $I_{\gamma\gamma}(E_1)$ on $\delta\rho$ and δk was studied in [13]. Most considerable result of this modeling is that the sign and magnitude of errors of desired parameters depend on the energy of excitation and cascade γ transition. Besides, they do not depend on the error in determination of absolute values of $I_{\gamma\gamma}(E1)$ at some these energies. This result confirms conclusion [1] that level density, for instance, cannot correspond to predictions of both model of noninteracting Fermi gas [14] and model of constant temperature.

In practice, the minimum possible systematic errors of ρ and k in any experiment and with the use of the processing data [1] are to be expected under conditions that:

a) the γ-ray spectrum of the thermal neutron capture was measured within the method [15] (or within method with equivalent precision) and capture cross section was determined with minimal uncertainty;

b) statistics of useful events is so high that experimentally resolved peaks concentrate main portion of intensity of cascades with energy of intermediate levels $E_i \leqslant 0.5B_n$;

c) all other errors characterizing experiments on measurements of $\gamma - \gamma$ coincidences were minimized.

Because realization of both two last conditions in real experiment on measurement of $\gamma - \gamma$ coincidences is impossible then minimization of $\delta\rho$ and δk can be achieved at careful optimization of its geometry.

Quantitative estimation of all sources of systematic errors for the data [6] was not performed.

Systematic uncertainties of determination of ρ and k from the spectra h of the primary γ transitions from the $(^3\mathrm{He}, \alpha)$ reaction are mainly determined by the following:

a) distortion of form of the dependence of spectrum h on the primary transition energy at its extraction from the total experimental γ spectra f;

b) degeneracy of multidimensional distribution of random deviations of desired parameters from the expected value;

c) necessity of model extrapolation [2] of density of neutron resonances into the spin region where there are no experimental data.

These uncertainties can significantly change the conclusions on the cascade γ-decay process. So, Fig. 5 demonstrates estimation of interval of possible values of $k(E1) + k(M1)$ for level density used for calculation shown in Fig. 3 (this density is less than that given in [6, 8]). Its maximum deviation from the previous variant is observed at $E_{\mathrm{ex}} = 4$ MeV and is equal to about $2/3$ of the level density [6, 8]. But even so small change in the calculated level density brings noticeable change in mean values of radiative strength functions which are necessary for reproduction of the two-step cascade intensities listed in [8]. For example, it changes the derivative of the strength function with respect to the energy. This occurs due to two factors: a necessity simultaneously to reproduce in calculation for increased level density of both cascade intensity and total radiative width $\langle \Gamma_\lambda \rangle$. The data shown in Figs. 4 and 5 point to necessity of maximum possible minimization of errors of the experiments under consideration.

The authors of [2, 6] do not make doubts about necessity of transition from the experimental total γ spectra to spectra h of only primary transitions although this operation cannot be carried out [15] without bringing in of additional uncertainties in ρ and k even in principle. Besides, in some situations the nonlinearity of the error transfer (for instance, of the error in determination of reaction cross-section on the error of intensity of total γ spectra f) can lead even to increase in relative uncertainty of spectra $h(E_1)$ of primary γ transitions as compared with analogous value for the total spectra f_i of γ-rays depopulating levels E_{ex}. This conclusion follows from consideration of given in [16] and slightly modified equation

$$h_1 = f_1 - \sum_i (h_i f_i). \tag{2}$$

Here, i is the number of energy interval. The left and right parts of this equation must have the same dimension (events per one decay or per given number of decay in general case). Therefore, all spectra f_i must be normalized to the same value as spectrum F_1. If it was done with some error, for example, $f_i = \kappa_i \phi_i$, then it will be simply convinced that the renormalization of the determined from (3)

spectrum h to 100% will not have error in only case when $\kappa_i = \mathrm{const}$. Hence, the total spectra f_i must be normalized to one decay with maximum possible accuracy before calculation of the primary transition spectra h_i from Eq. (3). This operation must be carried out with a precision considerably exceeding the accuracy in determination of the γ-ray intensities of the thermal neutron radiative capture in modern [15] experiment.

Estimation of permitted δh for the distorted spectra of any kind can be easily obtained in the following way: the total γ-ray spectrum f for any energy interval is recurrently calculated for the arbitrary ρ and k without statistic errors beginning from the known γ-transitions depopulating decay of low-lying discrete levels according to the relation

$$f_1 = h_1 + \sum_i (h_i f_i). \tag{3}$$

Then, the spectra of primary transitions are restored from the spectra distorted by random error like $f_i = (1 + e_i) f_i$ according to Eq. (3). The worst variant is the case when the error e_i is proportional to the number of spectrum and increases its intensity as increasing i (for numeration used in [16]).

Using this technique one can obtain that maximum relative error of normalization of spectra to one decay must be considerably less than 1%. This follows from the fact that at increasing of E_{ex} small value of h for low energy E_γ is determined from difference of two much larger intensities of the total γ spectra with very intence low-energy secondary transitions. Moreover, the same energy of γ quantum in spectrum f can be related with the sum of intensities of the first, second, third and so on cascade quanta at increasing of their intensities when excitation energy decreases.

One can try to achieve appropriate accuracy using normalization of total γ-ray spectrum to one decay with the help of condition $\sum(E_\gamma \times I_\gamma) = E_{\mathrm{ex}}$. Such normalization excludes the problems [16] of different multiplicity of quanta in total γ-ray spectra for different excitation energy of decaying levels and for precise determination of reaction cross-section. But this can be done, probably, only partially. Detailed investigation of influence of energy resolution of detectors and functions of their response on systematic error can be required in this case as well. The open question is systematic error connected with widening of spin window of levels excited by cascade transitions.

Statistic error of the h data given in [2] is larger than 1%. Therefore, it is worth while to make extraction of the primary γ-transition spectrum for minimization of systematic errors by means of minimization of sums $\chi^2 = \sum(f_1^{\mathrm{exp}} - (h_1 + \sum_i (h_i f_i^{\mathrm{exp}}))^2$ instead of mathematical method used in procedure [16].

3. SYSTEMATIC ERRORS OF JOINT ANALYSIS OF DIFFERENT EXPERIMENTS AND POSSIBILITIES OF THEIR DECREASING

Level densities and radiative strength functions presented in [6], in opinion of the authors of this work, correspond to their most probable values because uncertainties of method [2] were completely eliminated due to fixation of level density at two excitation energies and the use of the experimental total radiative width of neutron s resonances. Correctness of this statement depends only on the form of multidimensional distribution of probability of random values of desired parameters.

As was obtained in [3], deviation distribution of the ρ and k values from their averages for the experimental data [6] is generated owing to correlation of these parameters (even at the use in [6] of complementary with respect to [2] information). One can try to decrease this degeneracy or even eliminate it only by involving complementary information in the maximum likelihood function.

Effective search for its maximum and identification of false solutions is realized now by means of the Gaussian method for solving systems of nonlinear equations. At any their degeneracy, the region of possible solutions is found within the programs of multiparameter fitting with the use of the procedure of regularization of covariant singular matrix with obligatory variation of input values of desired parameters. The presence of exponentially changing parameters leads to appearance [3] of nonprinciple problems for the use of modern programs which realized the Gaussian method for determination of the most probable ρ and k values for the set of the data [6]. As the experience [3] shown, there is no grounds to wait principle obstacles for involving of derivatives of function $I_{\gamma\gamma}$ from Eq. (1) with respect to its parameters in the Jacoby matrix.

Unfortunately, there is no any grounds to hope for complete exclusion of systematic errors of ρ and k even in this variant of analysis. Any hypotheses about the cascade γ-decay process of an excited nucleus (directly or indirectly used in [1, 6, 8]) also lead to appearance of additional systematic errors of the desired parameters of the cascade γ-decay process. But the use of them is absolutely necessary, for instance, above the excitation energy 1–3 MeV of deformed nucleus due to the lack of any required experimental information in this region.

First of all this concerns the problem of the shape of the energy dependence of the radiative strength functions of equal multipolarity and γ-quantum energy for different energies of decaying levels. Available data (theoretical calculation of matrix elements, experimental data [4] and intensities of the cascade population of levels up to the excitation energy $\leqslant 1$ MeV [17] and higher [18]) show that influence of this factor on systematic error cannot be neglected.

This problem common for both methods [1] and [2]. But there is considerable difference: in the case of the data [6], resulting value of k is a superposition of

strength functions for γ transitions of equal energy but depopulating levels with sufficiently different energy and structure of wave functions. In the case [1], difference between the energy dependences of strength functions of the secondary transitions and analogous dependence of the primary transitions affects the desired parameters ρ and k only indirectly — through distortion of the Γ_{if} value. At low energy of the secondary transitions this distortion decreases due to both factor E_γ^3 and possible [17] different in sign change in the shape of dependence $k = \phi(E_\gamma)$ for different energy of γ transitions (for equal energy of decaying level).

CONCLUSION

Insufficient degree of correctness of using mathematics and mathematical statistics for extraction of the level density and radiative strength functions from the primary γ-transition spectra of nuclear reactions and spectra of the two-step γ cascades leads to mistaken conclusions about the process under study. Therefore, the use of the analysis procedure suggested in [19] cannot provide obtaining of the reliable data on the radiative strength functions.

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