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SOME PROBLEMS OF EXTRACTING LEVEL DENSITY AND RADIATIVE STRENGTH FUNCTIONS FROM THE γ SPECTRA IN NUCLEAR REACTIONS

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Хитров В. А. и др. Некоторые проблемы извлечения плотности уровней и радиационных силовых функций из гамма-спектров ядерных реакций

Установлены наиболее важные систематические ошибки определения плотности уровней и радиационных силовых функций из гамма-спектров ядерных реакций типа срыва и подхвата.

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Khitrov V. A. et al. Some Problems of Extracting Level Density and Radiative Strength Functions from the γ Spectra in Nuclear Reactions

The most important systematical errors in determination of level density and radiative strength functions for deformed nuclei have been estimated from the gamma-ray spectra in nuclear reactions like the stripping or pickup reactions.

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

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INTRODUCTION

At the excitations below the neutron binding energy $E_{\rm ex} \leq B_n$ the radical complication of the structure of the nuclear excited states occurs. Simple, practically one-component low-lying levels transform into the extremely complicated Bohr's high-lying compound states. For understanding of the main properties of this transition, it is necessary to determine density ρ of levels for a given interval of their quantum numbers and the mean widths of populating and depopulating them γ transitions, at least, with systematical error provided by the modern experimental technique. Only on the basis of such reliable and precise information one can develop adequate theoretical model of the process under consideration. Unfortunately, more or less systematical errors are inherency of any method for data treatment.

The reliable and precise data on level density ρ and probability of emission of any reaction products are important not only for verification and development of theoretical notions but also to the practical point of view. In particular, reliable and precise enough evaluation of interaction cross-section of neutrons with fissile nuclei will permit one to raise the efficiency of exploitation of nuclear reactors. Modern analysis [1] of a bulk of the experimental data shows, however, that the quality of the evaluation of the required parameters depends on the degree of correspondence of the used model notions to the experiment.

The analysis [2] of these cross-sections with a great probability points out at rather considerable underestimate of the pairing interaction effect by existing models and, as a consequence, at visible discrepancy of conventional notions of the energy dependence of level density of, at least, fissile nuclei with the experiment.

The problem of reliable experimental determination of the level density excited in some nuclear reaction below the energy $E_{ex} \simeq 6-8$ MeV has not been solved yet. The analysis of evaporation spectra in reactions like (n, n'), (p, n)and so on used for this purpose contains unknown systematical errors caused by impossibility of correct accounting for the reaction mechanism and precise calculation of the penetration coefficients of nuclear surface for reaction products below B_n . As a result, corresponding experimental data can contain strongly underestimated inherent uncertainty. This problem is, probably, of special impor-

tance [3] for low (3–4 MeV) excitation energy of a nucleus-reaction product. This quite unambiguously follows from the fact that the areas of spectra in method [3] are (in the first approach) inversely proportional to the level density, but just in this excitation region of deformed nuclei, this method has maximal sensitivity, and the maximal discrepancy between the obtained ρ is observed.

The systematical errors manifest themselves in any other experiments, for example, in investigations of intensity $I_{\gamma\gamma}$ of two-step cascades [3], and in analysis of spectra S of γ transitions depopulating levels with energies E_i excited in the (d, p) [4] or (³He, α) reactions [5,6].

The last method must give also considerable systematical errors in determination of the absolute width of γ transitions with the energy $E_{\gamma} \leq E_i$, owing to their strong correlations with errors of level density (and vice versa).

1. ON SOME SYSTEMATICAL ERRORS IN DETERMINATION OF ρ AND k IN MODERN EXPERIMENT

It is obvious that the correspondence between ρ and the radiative strength function $k = f/A^{2/3} = \Gamma_{\lambda}/(D_{\lambda}E_{\gamma}^3A^{2/3})$ obtained within different methods in the limits of corresponding uncertainties is one of criterions of their confidence. Unfortunately, the ρ and k values determined according to Ref. [3] and to Refs. [5, 6] do not obey this condition. So, the $I_{\gamma\gamma}$ values cannot be reproduced within experimental accuracy using level density from [5, 6] due to the strong difference with ρ from [3]. For example, the main peculiarity of the data [2, 3] — clearly expressed the «step-like» structure in ρ — practically is absent in the data [5, 6]. Comprehensive enough analysis of systematical errors of ρ and k determined with the use of the two-step cascade intensities was performed in [3]. But it cannot explain the source of this discrepancy of the observed results.

One of possible explanations for discrepancy between the results [5, 6] and [3] can be obtained from analysis of the suggested in Oslo method of extraction of the desired parameters which provide minimum value for χ^2 :

$$\frac{\chi^2}{N} = \frac{1}{N} \sum_{E_i} \sum_{E_\gamma} \left(\frac{S_{\rm th}(E_i, E_\gamma) - S_{\rm exp}(E_i, E_\gamma)}{\Delta S(E_i, E_\gamma)} \right)^2,\tag{1}$$

for the system of equations connecting experimental γ spectra S with the desired parameters ρ and k marked below as X:

$$S(X) = S_{\rm th}(E_i, E_\gamma) = \Gamma_i \times \rho_i / \sum (\Gamma_i \times \rho_i).$$
(2)

As was pointed out in [4], this system can be complemented by the expression for the experimental value of the total radiative width of neutron resonance. It should be noted that the system of some nonlinear equations (including system (1)) is solved in the framework of matrix algebra [7] using the Gauss-modified (regularized) methods and does not require any additional algorithms for fitting (like that suggested in [5]).

The value of vector-column X consisting of n parameters is determined in the vicinity of their actual values [7] for k + 1 iteration by the matrix equation

$$X_{k+1} = X_k - (J^T G J)^{-1} J^T G S(X_k),$$
(3)

where G is the matrix of weights; the Jacobi matrix J and corresponding transposed matrix J^T are the matrixes of derivatives from function (2) with respect to the desired radiative strength function k of transition and number ρ of levels in a given energy interval of corresponding spectrum. S is the vector-row of m experimental points in all spectra used for fitting of parameters. It is obvious [7] that Eq. (1) has a solution (unique) only upon condition of existence of covariant matrix $C = (J^T G J)^{-1}$.

The derivatives, with respect to *n* desired parameters in $m \ (m \ge n)$ points, are determined analytically from Eq. (2). Products of χ^2/N on diagonal elements of matrix *C* in point of minimum of (1) equal [7] variances of desired parameters, on nondiagonal elements equal covariants of these parameters. It is well known in mathematical statistics [8] that the shape of the multi-dimensional Gauss distribution used in the general case as a likelihood function depends also on nondiagonal elements of covariant matrix. In particular, Eq. (1) has maximum only if covariant matrix slightly differs from diagonal one. This is clearly seen from Eq. (4) for the Gauss distribution of two variables *u* and *v*, which equal random deviations of random values *X* from the mathematical expectation $\langle X \rangle$:

$$F(u,v) = \exp\left(-0.5((u^2/\sigma_u^2 - 2ruv/(\sigma_v\sigma_v) + y^2/\sigma_v^2))/(1-r^2))/(2\pi\sigma_v\sigma_v(1-r^2)).$$
 (4)

If correlation coefficient equals unity $r = \pm 1$, then covariant matrix becomes singular, and maximum of function F(u, v) can be obtained for any values of uand v which obey equation $u/\sigma_u \pm v/\sigma_v = 0$. At r = 0 it exists, of course, only for u = 0 and v = 0.

Correspondingly, at r = 1 the same maximum of the function is observed for a multitude values of variables. This situation, of course, is taken into account in any modern program of multi-parameter fitting. It should be noted that inversion of large matrix at $|r| \approx 1$ also brings a considerable loss in accuracy.

The conditions for invertibility of matrix (J^TGJ) for ¹⁷²Yb considered in [5] were studied by us for the model calculated spectra (2) with variations of possible accuracy in determination of the *S* values. It was established that even at 0.01% relative uncertainty of each point in the spectrum, the matrix (J^TGJ) is singular in the limits of precision of modern computers.

The corresponding covariant matrix includes a large enough number of correlation coefficients which are near or equal to unity (in limits of calculation precision) and, therefore, it is singular. According to definition [8] of covariant matrix, there is a multitude of ensembles of different values of parameters ρ and k which lead to the same magnitude of χ^2 in (1).

The complete compensation of random deviation of one parameter from its experimental value by corresponding deviation of other parameter is possible in the only case when |r| = 1. However, change in the desired parameters leads to the change in the correlation coefficients, due to nonlinear connection between level density and radiative strength functions. As a consequence, the region of possible change in level density completely compensated by change in strength functions is limited by some intervals of values of ρ and k for a given excitation energy of a nucleus. But the correlation coefficients approach on absolute value to unity at other values of desired parameters from Eq. (2), and covariant matrix stays singular.

Therefore, at the analysis of the S_{exp} values, one should take into account the possibility of existence of the region of possible values ρ and k, where a complete mutual compensation of their random deviations from true value is observed.

A simple possibility to test this statement is provided by the Monte Carlo method. Some variant of this method was used by authors [3], namely, for determination of region of possible ρ and k values which allow reproduction of the same value of $I_{\gamma\gamma}$. Fig. 1 shows several pairs of random functional dependencies of ρ and k obtained in accordance with the iterative procedure [3] for different input values of these parameters. The spectra S_{if} (2) is calculated using these parameters represented in Fig. 2. It is natural that all pairs of ρ and k values allow reproduction of the total radiative width of ¹⁷²Yb chosen for modelling. As is seen from Fig. 2, uncertainty of reproduction of the spectra S_{if} , using the data given in Fig. 1, is at least 5-10 times less than the error of the experimental data [5] in spite of rather significant deviation of ρ and k from the input values, (as compared with estimations of errors in [6]). Therefore, one can assume that the set of the ρ and k values, allowing reproduction of the experimental spectra $S_{\rm if}$, is considerably wider than that given by authors [6]. It should be noted that the fluctuations of the S values in Fig. 2 partially result from the random fluctuations of the data in Fig. 1, owing to the use of the Monte Carlo method for their calculation.

The authors [5,6] point out that without the use of the experimental level densities at two excitation energies, their experimental spectra can be reproduced with infinite number of ρ and $k = f A^{2/3}$ even if the number of points in experimental spectra is ten times higher then the number of desired parameters. Hence, reliability of the physical conclusions in [6] directly depends on systematical uncertainty of two experimental values of ρ used in [5,6]. It should be noted that level density for the considered 172Yb in vicinity of B_n was deter-



Fig. 1. Some random functional dependencies of level density in ¹⁷²Yb with $J = 2 \div 6$ (a) and radiative strength functions (b), which allow reproduction of the spectra of primary transitions in Fig. 2. Curve *I* represents the desired values of ρ and *k*

mined experimentally only for neutron resonances with $J^{\pi} = 0^{-}$ and 1^{-} . The reaction (³He, α) used in [5, 6] excites (as it is pointed out by authors) mainly levels with spin 2 to 6. All conclusions of authors, however, directly depend on the accuracy in determination of level density in vicinity of B_n just for the spin interval and parity of levels excited in the reaction. But now it is impossible to evaluate the well-known effect of rotational enhancement of level density in deformed nuclei on the results [6]. According to Ref. [9], its value amounts to 10 for the complete level density. Assuming that the parameters of rotational bands built on the excited states J < 6 of this nucleus insufficiently differ from that of rotational bands of known low-lying states, and they do not depend on the parity of head level one can estimate that rotation of the nucleus increases density of levels J = 2-6 by a factor of at least 2.5, as compared with the known model spin dependencies.

An additional uncertainty can be also introduced in the results of this analysis and if level density of even-even deformed nuclei at $E_{\rm ex} \approx 3-4$ MeV is less than that predicted by the simplest extrapolations of ρ . This possibility follows from the results [10] of extrapolation of the number of their cascade intermediate levels to the zero detection threshold of the experiment.



Fig. 2. The calculated spectra of the primary transitions for the energy E_i , corresponding to that given in [5]. Points with the error bars represent calculation for curves l in Fig. 1 with the 10% interval of their deviations. All spectra are shifted right to value $B_n - E_i$

Hence, in spite of this uncertainty in level density at $E_{\rm ex} \approx 8$ MeV, all the data in Fig.1 is mathematically equivalent (including level density in the vicinity of B_n). And rejection from «superfluous» solutions is possible only at the presence of the complementary physics information. Therefore, the question arises about the obtaining more reliable information on the desired parameters of the cascade γ decay process.

CONCLUSION

Correct estimation of systematical errors of the data like those given in Refs. [5, 6], first of all, requires taking into account both sharp increase of interval of values for ρ and k, which allow reproduction of the experimental spectra with the same precision, due to their strong correlation, and possible change in the extrapolated level density in given spin and parity intervals, due to known rotational (and, probably, vibrational) effect.

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