PARAMETERS OF THE BEST APPROXIMATION FOR DISTRIBUTION OF THE REDUCED NEUTRON WIDTHS. SPECIFICITY OF FULL-SCALE METHOD OF ANALYSIS

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Abstract

The method is described and tested for analysis of statistical parameters of reduced neutron widths distributions accounting for possibility of coexistence of superposition of some functions with non-zero mean values of neutron amplitude and its arbitrary dispersion. The possibility to obtain reliable values of distribution parameters at variation of number of resonances involved in analysis and change of registration threshold of resonances with the lowest widths is studied.

1 Introduction

Experimentally measured reduced widths $\Gamma_0^n$ ($\Gamma_1^n$) of neutron resonances – strongly fluctuating values. This circumstance very much complicates determination of their mean values (the averaged spacing $D$ and strength function $S_0 = \langle \Gamma_0^n \rangle / D_0$) from real experimental data distorted by different systematical uncertainties. The generally accepted notion of shape of their distribution was suggested in 1956 [1] and was not up to now tested in full scale.

This test is non-trivial procedure because only the part of the measured distribution is observed in experiment but its independent parameter $X$ can be determined only for the total spectrum of possible values of widths. Id est, approximation of experimental data is performed at presence of unknown error parameter $X = \Gamma_0^n / \langle \Gamma_0^n \rangle$. Real value and error $\langle \Gamma_0^n \rangle$, of cause, cannot be determined experimentally. And value of the $\delta X$ depends on accepted model notions.

The ordinary test of distribution $\Gamma_0^n$ consists in determination of effective value of number of degrees of freedom $\nu$ of $\chi^2$-distribution for given set of widths (with fixed orbital momentum $l$) and rather subjective choice of neutron energy interval where distortions of $D$ and $S$ are minimal. The deeper test must answer the questions, in what degree are realized the conditions of applicability of $\chi^2$-distribution to real data. Id est:

(a) whether mathematical expectation of amplitude $A = \sqrt{\Gamma_0^n}$ is equal to zero,

(b) its dispersion – to mean value $\langle \Gamma_0^n \rangle$ and

(c) whether the function providing description of experimental data with maximum possible precision is the unique?
It should be also taken into account that practical investigation of nucleus properties includes obligatory stage – creation of mathematical model of process under study. By this, any model is created on limited basis of data having non-estimated systematical errors which are inevitably projected on the following investigation of nucleus properties.

Therefore, predictive ability of a model and its quality are strongly correlated values. It follows from this the necessity to test hypothesis \[1\] whether real distribution \(A\) can be composition of several Gauss distributions with different mean values and dispersions.

2 Choice of experimental data presentation form

Analysis of status of the problem from the point of view of both theoretical ideas and totality of experimental data allows one to expect for maximal discrepancy between experimental data and hypothesis \[1\] in region of maximal widths. In practice, it can be caused by influence \[2\] of large components of wave functions of nuclear states with maximal number of quasi-particles and phonons owing to their weak fragmentation \[3\] in the excitation energy region \(E_{ex} \approx B_n\).

Distribution \(\Gamma_0^n\) can be approximated in both its “differential” and “integral” forms in function of width or square root from this resonance parameter. Experimental data contain fixed quantity of information. Therefore, the volume of available information does not depend on form of data presentation and its choice is determined only by mathematical problems of obtaining of the sought values and visualization of results. In principle, it is possible to analyse both distribution itself or large enough set of its momentums.

Specific problem of distribution analysis of changeable values at presence of threshold of their registration - the lack of information on portion of distribution of neutron width is really observed in experiment. As a consequence, there appears the problem of unit of measurement for random value it does not depend on form of distribution presentation. The most suitable form for presentation of the data for the problem under solution is cumulative sum of experimental values of \(X = \Gamma_0^n / \langle \Gamma_0^n \rangle\), increasing when increases \(X\). This sum includes all the observed experimentally and included in the used compilation (for example, in \[4\] or library ENDF/B-VII \[5\]) values of widths.

The selective average \(\langle \Gamma_0^n \rangle\) for experimental cumulative sum was determined from this set without accounting for missed resonances and their unresolved multiplets. Its inevitable displacement with respect to unknown value is compensated at approximation by deflection of approximated \(\sigma\) value from the most probable value (in particularly, from \(\sigma = 1\)). This uncertainty does not influence \(\chi^2\) - the shape of relative difference between experimental and approximated distributions does not depend on units determining the width \(\Gamma_0^n\).

Approximation region in all calculations was limited by the interval from zero to twice maximal experimental values \(X_{max}\). Cumulative sum was normalized in point \(X_{max}\) to number of experimentally determined widths. The region \((0 - 2X_{max})\) included in all cases not less than 1000 points, in which was minimized the difference of experimental
cumulative sum and its approximating function. Dispersion of cumulative sum at this normalization changes from zero in extreme points to maximal value in region $X \sim 2 - 10$ (see Fig. 1). In given variant of analysis this change was ignored, and $\chi^2$ was calculated as a sum of squares of difference of experimental and approximated values of cumulative sums. Naturally, all statistical errors in region of the lowest widths in this case exert the lowest influence on determined parameters of distributions. For convenience of comparison of different data the value $\chi^2$ was divided by number of freedom degrees of approximation.

All the obtained experimentally values of widths were included in practical analysis except obvious errors of experiment (misprints in compilation, strong discrepancy in different data sets). Practically, the latter can be revealed only in region of maximal values of $\Gamma^0_n$, therefore corresponding correction decreases degree of discrepancy between experiment and [1].

This form of presentation of experimental data permits one to involve simply enough in approximation, in principle, any factor distorting width distributions. Besides, this allows determination of probable resonance parameters for any nucleus at presence of systematical errors of $\Gamma^0_n$, if only influence of such systematical error can be take into account in any (numerical or analytical) form of functional dependence with free parameters.

3 Model and method of suggested analysis

Experimental level density in region of neutron resonances of nuclei from mass region $40 \leq A \leq 200$ obtained in Dubna (within the model-free method for analysis of the two-step cascade intensities) is described [6, 7, 8] by sum of three (or more) partial level densities with different number of quasi-particles and phonons. Practically, it was accepted on calculation problems that in limit case the experimentally observed resonances can belong (as a maximum) to four different distributions of $\Gamma^0_n$ for even-even target-nuclei. This is true and for $A$ odd nuclei at equality of $< 2g \Gamma^0_n >$ for resonances with different spins $J$. In the other case the results of approximation contain and information on spin dependence of neutron strength functions.

Physically, according to the parameters of different approximation variants of the total set of level density obtained for $\approx 40$ nuclei in Dubna, it is also worth while to limit maximal value of $K$ by $K = 4$. In this case, the system of corresponding nonlinear equations will be most probably always degenerated. Therefore, instead of determination of the unique value of any parameter, it is necessary and possibly to determine the width of limited interval of their values corresponding to $\chi^2$ minimum.

A smallness of set of experimental values of the widths and exponential functional dependence of probability for their observation at different $\Gamma^0_n$ very strongly complicate process of determination of the parameters for approximating function. Therefore, it is worth while to perform this operation so that the algorithm of search for minimum of $\chi^2$ would permit stable approximation of the experimental data at presence of two and more distributions with practically coinciding parameters. Comparison of the data obtained for $K > 1$ with the results of their approximation by the only distribution can give new
information on nuclear structure in region $B_n$. First of all – information on possible existence of neutron resonances with different structures of their wave functions (as it was suggested in [9]).

Practical degeneration of the realized process together with exponential change of the analyzed dependencies complicate (but do not exclude) the use of the Gauss method for solution of systems of nonlinear equations in form of existing library programs. The problem of the use of this method is very complicated by events of appearance (as the most probable value) of near to zero values $\sigma$ and corresponding to them steps in cumulative sums. Id est – to some sets of non-random width values. There is easier realized the Monte-Carlo method for solution of systems of degenerated nonlinear equations. Namely – random set of elements correction vector of parameters of fitted function with arbitrary variation of their initial values.

The fitted function is sum $K$ of the distributions $P(X)$ of normally distributed random values with independent variables $X_k$ each. The required parameters in compared variants are the most probable value $b_k$ of the amplitude $A = \sqrt{\Gamma_0^N/ <\Gamma_0^N>}$, its dispersion $\sigma_k$ and total contribution $C_k$ of function number $k$ for variable

$$X_k = ((A_k - b_k)^2)/\sigma_k^2$$

in the total experimental cumulative sum of widths.

The number of distribution and sign of amplitude $A_k$ for given resonance are unknown. Further was used its positive value because (1) is invariant with respect to simultaneous change of signs of $A_k$ and $b_k$. But, it was everywhere supposed that in the considered distribution number $K$ can exist the only value of $b_k$. I.e., any distribution of widths $K$ has only one maximally possible value of amplitude. There is the main (and absolutely necessary) hypothesis of the performed by us analysis of distributions of the resonance reduced widths. Concrete value of function $P(X)$ for variable (1) in the described analysis was obtained by compression and shifting of the generally known Euler gamma-function. The obtained in this way value corresponds to the magnitude of this mention function for the variable $X = (A \times \sigma + b)^2$. At present the basis for this algorithm for setting of parameters of approximating function is excellent degree of description of all known experimental distributions of the widths. In addition it should be noted that the modules of the $b_k$ and $\sigma_k$ values are strongly correlated variables, at least, for large enough $b_k$ values.

4 Results of test of analysis method

The test of analysis method was performed by approximation of different sets of random $X$ values. By this, the mean values of normally distributed random values, their dispersion, number of variables in sets and distortions of different types appearing in the experiment are easily varied.

The random value $X = \xi^2$, corresponding to the $\chi^2$-distribution with one degree of freedom and unit dispersion and corresponding average was generated from the normally
distributed random values $\xi$. The later were set using Neumann algorithm as a product of two random numbers: $\delta_1 = \sin(2\pi\gamma)$ and $\delta_2 = -2\ln(\gamma)$, where $\gamma$ – the uniformly distributed in interval $[0,1]$ random value. Modeling of experimental distortions of widths in the case under consideration reduces to corresponding arithmetic operations with $\xi$ and approximation of cumulative sums of the distorted values $X_d$ with necessary repetition number of this process. For example, below modeling of influence of the observation threshold of resonance was done using linear function of number $X$ with the parameters providing in sum exclusion from the tested set $L = 30\%$ of the lowest random $X$ values. The spectrum of possible values of cumulative sums for any practically achievable values of number of observed resonances can be obtained by interpolation of the data presented in Fig. 1.

Fig. 1. Thin lines – the example of cumulative sums for some tens of sets from 150, 500 and 2000 random $X$ values (upper row) Thick lines – the minimal and maximal values with corresponding parameters $\sigma$. Cumulative sums for the same sets after exclusion of 30\% of the lowest $X$ values (lower row).

Large dispersion of random values $X$ brings to large fluctuations of cumulative sums of both experimental data and model distributions. And, respectively, to essential variations of the best values of the parameters (1). Therefore, the conclusion about possible deviations of the parameters $b$ and $\sigma$ from the expected values 0 and 1, respectively, can have only probabilistic character.

Frequency distributions of these parameters were obtained from modeling sets for the $N=150$, 500 and 2000 random values $X$. Modeling was performed for variant of the non-distorted values $X$ and omission which corresponds to exclusion of $L = 30\%$ of their lowest values (linearly changing with number of random value). The results of approximation of these distributions (corresponding to practical maximum of $\chi^2$) are given in Fig. 2.
Fig. 2. The examples of approximation of cumulative sums from the sets presented in Fig.1 curves for case of maximal $\chi^2$ values. The upper row – for zero threshold, the lower row – with exclusion of 30% of the least random $X$ values. Dotted curves – partial distributions for $K = 4$, points – their sum, solid curves – approximation for $K = 1$.

The widths of corresponding distributions decrease as $N$ increases and at small $X$ depend on value $L$. One can conclude from the data presented in figures 1 and 2 that a deviation of the experimental distribution of widths from the Porter-Thomas distribution appears itself mainly at $X = (\Gamma_n^0 / < \Gamma_n^0 >)^2 - 5$.

Discrepancy between the experimental data and hypothesis at smaller $X$ values can be related, first of all, with omission of weak resonances or other systematical errors of the experiment. But, it is not excluded and possibility of real deviation of parameters $b$ and $\sigma$ from values corresponding to hypothesis [1].

Probabilistic conclusions on this account can be made only from comparison between frequency distribution of the parameters (1) for different model distributions and experimental data. For the case $b = 0$ and $\sigma = 1$ they are shown in figures 3 and 4.

5 Test of method for determination of number of unobserved resonances

Any errors of experimental values of the tested set inevitably increase dispersion of the obtained best values of $b$ and $\sigma$. But, in principle they can be taken into account by determination of the most probable parameters even for distorted distribution $\Gamma_n^0$. 
Fig. 3. Comparison of frequency distributions of given values of $b$ (upper) and $\sigma$ (lower) rows, respectively for $K = 1$. Left column – all possible random values are included in modeling, right column – $L = 30\%$ of the lowest random values are excluded from each tested set.

Fig. 4. The same, as in Fig. 3, for $K = 4$. 
For example, the problem of resonance omission can be solved easily enough at presence of reliably established dependence of threshold of its registration on neutron energy. A possibility to realize of this computational process follows from the data presented in Fig. 5. As it is seen from comparison of mean values of cumulative sums, their form for the same number of resonances (in given case $N_{exp} = 350$) depends on presence/lack of omitted resonances.

Direct estimation of the most probable number of omitted resonances in any experiment does not call troubles and can be simple if only functional dependence of their portion $\delta \psi_{th}$ from the total number $S$ is set on the ground of some data or hypotheses for concrete intervals of resonance energies. Then

$$\chi^2 = (S - \psi(A, b, \sigma) - \delta \psi_{th})^2$$

(2)

Here $\psi(A, b, \sigma) = \int X \cdot P(X) dX$ for any fitted distribution $P$ in function of ratio $X$. The value $\delta \psi_{th}$ depends only on difference of $N_t - N_{exp}$ for varied from variant to variant expected number of resonances $N_t$ in interval $\delta E$ and determined in the experiment $N_{exp}$. A number of these intervals was varied in interval 5-20 in dependence on bulk of the experimental width values. Moreover, negative values $N_t - N_{exp}$ in any intervals were changed by zero. The desired value $D = \sum \delta E / \sum N_t$ corresponds to minimum of $\chi^2$.

Naturally, function $\delta \psi$ can take into account and other factors distorting experimental width distribution. This accounting can be performed in frameworks of both some model approaches and concrete experimental data.

Modeling of the process of determination of the most probable $D$ value was performed by approximation of cumulative sums of sets of the random $X$ values for $\chi^2$ distributions with some different $N_t$ values. Approximately 30% of their lowest values were excluded from every set (the threshold – linearly increasing with number of random value).

Direct use of equation (2) for determination of the most probable $N_t$ with high reliabil-
ity, most probably, is not worth-while without solution of, as a minimum, two problems:

(a) The set of the precise enough (relative or absolute) dispersion of cumulative sum for every value of $X$ and

(b) The guarantied determination of location of absolute minimum of $\chi^2$ corresponding to the desired $N_t$ value.

Although these problems are not irresistible of principle but their solution is not found up to now.

6 Conclusion

The described and tested method of the reduced neutron widths distributions analysis allows one to get new of principle information on properties of neutron resonances. In particular to suppose that the values of the distribution parameters of their neutron amplitudes can correspond to the set of several distributions with their different mean values and dispersions.

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