NEWGTOL

Introduction

The work has been done by the Data Center group (Petersburg Nuclear Physics Institute of the Russian Academy of Sciences). The group is involved into the activity of the International Network of Nuclear Structure and Decay Data Evaluators. The network includes 18 centers and groups which are working with the latest published nuclear data and producing the evaluation of properties of nuclear levels for all isotopes.

The data include the bibliography information (Nuclear Science References, NSR) and the evaluated nuclear data (Evaluated Nuclear Structure Data File, ENSDF). These data have a computer-oriented form. The newest version may be obtained via Internet from the site of Brookhaven National Laboratory, http:/www.nndc.bnl.gov. The printed version of the evaluated data is presented in the journal Nuclear Data Sheets.

Algorithm of the *GTOL* program

One of the basic tools for the nuclear data evaluators is the *GTOL* program [1] which is used for calculation of energies of levels and their uncertainties from the measured values of the energies of transition and corresponding experimental uncertainties.

Mathematically the problem may be reduced to the solution of system of linear equations

$$\boldsymbol{AX} = \boldsymbol{B}, \qquad (1)$$

where $\boldsymbol{X}$ is a vector of N_L numbers of level energies, $\boldsymbol{B}$ is a vector of N_G numbers of measured values of transition energies, $\boldsymbol{A}$ is a matrix with dimension ($N_G \times N_L$). Elements of the matrix $\boldsymbol{A}$ are:

$$a_{ij} = \begin{cases} 0, & \text{if the transition } i \text{ is not connected with the level } j; \\ 1, & \text{if the transition } i \text{ depopulates the level } j; \\ -1, & \text{if the transition } i \text{ populates the level } j. \end{cases} \qquad (2)$$

The necessary condition of resolvability of the system (1) is

$$N_G \geq N_L. \qquad (3)$$

The system is overdetermined and the least squares method was used for resolving the system (1). Solution may be found as

$$\boldsymbol{X} = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{B} \qquad (4)$$

where $\boldsymbol{W}$ is a matrix of weights of the equations. It is defined by the experimental uncertainties of the transition energies. It should be marked, that the independence of experimental values of the energies of the transitions is supposed in the *GTOL* program. That means that $\boldsymbol{W} = \mathrm{diag}(1/dE_G^2)_1^N$ is a diagonal matrix with elements equal to $1/dE_G^2$, where dE_G are the experimental uncertainties of the transition energies. The solution defined by the expression (4) corresponds to the minimum of the functional

$$Q = \sum_{i=1}^{N} \delta_i^2 \quad \text{or, which is the same, } Q_{norm} = Q/N_{st} \qquad (5)$$

where

$$\delta = \Delta/dE_G, \quad \Delta = E_G + E_{rec} - (E_{L,top} - E_{L,bot}), \qquad (6)$$

and

E_G is γ-ray energy,
E_{rec} is recoil energy,
$E_{L,top}$ is the energy of the initial level,
$E_{L,bot}$ is the energy of the final level,
N_{st} is the number of degrees of freedom. It is defined as

$$N_{st} = \begin{cases} N_G - (N_L - N_{L_0} - N_{K_F}), & N_G > N_{L_0} - N_L - N_{L_F} \\ 1, & N_G \le N_L - N_{L_0} - N_{L_F} \end{cases} \qquad (7)$$

where N_G and N_L are stated above, N_{L_0} is the number of levels which are not connected with any level in the scheme, N_{L_F} is the number of levels with the energy fixed a priori, from any considerations.

The level scheme may be found as ideal, if the discrepancies Δ are in agreement with experimental uncertainties of the transition energies, i.e. for the given scheme the quantity δ is distributed under the normal law with the average is equal to zero and the dispersion is equal to 1. In this case, the value Q is distributed under the χ^2-law with the average equal to N_{st} and the dispersion equal to $2N_{st}$. Here the expected value of Q_{norm} is equal to 1.

The problem of solvability of the system (1) concerns to the class of the incorrect mathematical problems. It makes the use of various regularizing algorithms necessary. For example, in the *GTOL* program, some of the energies of

levels may be fixed equal to the *a priori* defined value. It may be determined by the attribute (flag) in the input data. The energy of the ground state always obviously equals to zero; energies of levels which are not connected by any transitions with the level scheme are fixed automatically. Here is the necessary condition of solvability of the system (1):

$$N_L \leq N_G + F, \qquad (8)$$

where the numbers N_L and N_G (except for doubtful transitions) are stated above; F is the number of levels with the fixed values of the energy.

It should be pointed out that in the *GTOL* program the dimension of the matrix $\boldsymbol{A^T WA}$ always equals to ($N_L \times N_L$). In complex schemes the number of levels N_L can reach some hundreds.

The analysis of calculations with the *GTOL* program

All data sets from ENSDF file (March, 2008) [2] have been calculated with the *GTOL*-7.2e program. The database *ANGTOL* and special subroutines for sorting out the information were used [3]. The total number of datasets which satisfy the inequality (8) is about 6 000, including 1 633 ADOPTED LEVELS datasets. It was found that the *GTOL*-7.2e program meets fatal problems in the solution of system (1) in 4.2 % of all cases. According to the *GTOL* diagnostics, four types of "problem" files have been detected.

In the Table 1 the number of datasets which are "problem" cases for *GTOL* is shown. It is marked that there is a significant number of ADOPTED LEVELS datasets which cause "problems" for calculations with *GTOL*.

Table 1.

GTOL-7,2e diagnostics		Number of datasets	Number of ADOPTED LEVELS datasets
I	"*Matrix is singular*"	238	45
II	"*Negative diagonal matrix elements*"	80	11
III	"*Unrealistic large diagonal matrix elements*"	77	13
IV	"*Negative Elevel after matrix mul.* "	25	4

The *GTOL* program does not calculate the level energies with the least squares method in these “problem” cases because of problems with the inversion of the matrix $\boldsymbol{A^T WA}$**.** For these datasets *GTOL* recommends: "*Fixing one or more*

of the preceding levels may solve matrix problem". The task appears to be non-trivial, if the level scheme consists of more than hundred of levels. Besides, it should be noted that the procedure of rigid fixation of value of energy of any level is the artificial reception for resolving a problem. The physical interpretation of this procedure is not so clear.

The solution of problems with the inversion of a matrix in the *NEWGTOL* program

Mathematical model of the level scheme is a graph which nodes are the levels, and edges are the transitions between the levels. In most number of cases for such a graph the subgraph may be determined. Such subgraph consists of group of nodes coupled with each other, but not coupled with all the rest.

Examples:

1. The isolated level which is not connected with other by any transitions;
2. The level which is introduced by the only transition to the ground state;
3. The isolated rotational band.

Except for these obvious cases, some level schemes consist of groups of levels connected among themselves only through the ground state.

Thus, the analysis of matrix $\boldsymbol{A}$ has shown that in many cases it has a block structure. Hence, the system (1) may be separated into a number of independent subsystems of essentially smaller dimension which may be solved independently. The algorithm of automatic splitting of the system (1) into a number of independent subsystems is realized in the *NEWGTOL* program.

Below the results of the analysis, arranged according to *GTOL* diagnostics (Table 1), are presented.

I. "*Matrix is singular*". For 45 ADOPTED LEVELS datasets the *GTOL*-7.2e program gives diagnostics "*Matrix is singular. Least-squares fit will not be done*". The *NEWGTOL* program, which takes into account the block structure of the matrix $\boldsymbol{A}$**,** solves the problem in the majority of cases. They are listed in the Table 2.

Notations in the Table 2:

N_{st} is the number of degrees of freedom for whole level scheme; eq. (7).

Q_{norm} was calculated for whole level scheme, eq. (5); energies of levels are from ENSDF.

R is the number of independent fragments in the level scheme.

$N_{L\,i}$ is the number of levels in the fragment of the level scheme; i is number of the fragment.

$N_{G\,i}$ is the number of the transitions which connect levels in the fragment *i*.
χ_i^2 is the normalized value of χ^2 for the fragment *i* calculated with the *NEWGTOL* program.

Table 2.

ADOPTED LEVELS	Data from ENSDF		Results of *NEWGTOL* optimization						
	N_{st}	Q_{norm}	R	Main fragment			"Problem" fragment		
				$N_{G\,i}$	$N_{L\,i}$	χ_i^2	$N_{G\,i}$	$N_{L\,i}$	Diagnostics
^{22}Na	237	1.47	2	323	85	0.31	1	2	$N_{G\,i} < N_{L\,i}$
^{40}Ar	143	1.8	41	212	79	0.56	1	2	$N_{G\,i} < N_{L\,i}$
^{48}Mn	3	0.003	2	10	7	0	6	7	$N_{G\,i} < N_{L\,i}$
^{51}Cr	108	4.4	8	181	78	1.5	–	–	
^{55}Fe	35	1.2	6	72	37	0.49	1	2	$N_{G\,i} < N_{L\,i}$
^{59}Ni	217	2.3	5	305	91	1.99	5	6	$N_{G\,i} < N_{L\,i}$
							6	7	$N_{G\,i} < N_{L\,i}$
^{65}Zn	77	0.66	6	90	40	0.42	2	3	$N_{G\,i} < N_{L\,i}$
							6	7	$N_{G\,i} < N_{L\,i}$
^{66}Ni	–	–	2	11	11	0	1	2	$N_{G\,i} < N_{L\,i}$
^{79}Se	40	3.6	2	92	55	1.7	1	2	$N_{G\,i} < N_{L\,i}$
^{86}Zr	60	1.7	5	131	65	1.0	5	6	$N_{G\,i} < N_{L\,i}$
^{103}Ru	120	1.6	4	193	73	0.83	6	7	$N_{G\,i} < N_{L\,i}$
							1	2	$N_{G\,i} < N_{L\,i}$
^{105}Ru	86	1.9	3	133	46	1.5	5	6	$N_{G\,i} < N_{L\,i}$
							1	2	$N_{G\,i} < N_{L\,i}$
^{110}Pd	104	1.4	2	116	38	0.7	2	3	$N_{G\,i} < N_{L\,i}$
^{110}Cd	190	12	5	357	177	4.6	2	3	$N_{G\,i} < N_{L\,i}$
^{114}Te	22	2.4	2	123	100	0.68	4	5	$N_{G\,i} < N_{L\,i}$
^{125}Pr	12	0.03	5	27	18	0	–	–	
^{135}Sm	18	3	4	32	23	3.5	5	6	$N_{G\,i} < N_{L\,i}$
				17	10	3			
				5	5	0			
^{136}Ce	59	2.4	4	88	55	0.98	5	6	$N_{G\,i} < N_{L\,i}$
^{139}Gd	24	0.3	3	61	42	0.33	7	6	The matrix is singular
							6	7	$N_{G\,i} < N_{L\,i}$
^{146}Nd	148	5.3	4	275	127	0.91	1	2	$N_{G\,i} < N_{L\,i}$
^{158}Er	100	4.3	4	193	107	1.8	10	11	$N_{G\,i} < N_{L\,i}$
^{158}Tm	26	0.22	3	48	28	0.23	11	7	The matrix is singular

^{159}Er	117	6.9	3	237	143	2.3	–	–	
				28	20	0.12			
				28	15	1.55			
^{161}Gd	–	–	8	3	2	0.1	1	2	$N_{G\,i} < N_{L\,i}$

Table 2 (continuation 1)

ADOPTED LEVELS	Data from ENSDF		Results of *NEWGTOL* optimization						
	N_{st}	Q_{norm}	R	Main fragment			"Problem" fragment		
				$N_{G\,i}$	$N_{L\,i}$	χ_i^2	$N_{G\,i}$	$N_{L\,i}$	Diagnostics
^{161}Er	88	0.84	4	144	62	0.69	14	15	$N_{G\,i} < N_{L\,i}$
							15	16	$N_{G\,i} < N_{L\,i}$
^{162}Er	162	1.4	5	232	77	1.3	11	12	$N_{G\,i} < N_{L\,i}$
							16	17	$N_{G\,i} < N_{L\,i}$
							2	3	$N_{G\,i} < N_{L\,i}$
							1	2	$N_{G\,i} < N_{L\,i}$
^{165}Lu	151	5.4	7	417	272	1.63	10	11	$N_{G\,i} < N_{L\,i}$
							4	5	$N_{G\,i} < N_{L\,i}$
^{166}Er	244	2.4	2	343	102	1.24	1	2	$N_{G\,i} < N_{L\,i}$
^{171}Yb	133	2.3	3	245	119	1.99	1	2	$N_{G\,i} < N_{L\,i}$
^{174}Hf	240	1.1	10	383	142	0.46	2	3	$N_{G\,i} < N_{L\,i}$
							12	13	$N_{G\,i} < N_{L\,i}$
^{175}Hf	147	0.74	4	344	164	0.56	1	2	$N_{G\,i} < N_{L\,i}$
^{177}Yb	46	0.64	2	127	98	0.39	1	2	$N_{G\,i} < N_{L\,i}$
^{177}Hf	102	0.48	4	185	93	0.3	5	6	$N_{G\,i} < N_{L\,i}$
							6	7	$N_{G\,i} < N_{L\,i}$
^{186}Os	138	0.6	2	260	135	0.46	1	2	$N_{G\,i} < N_{L\,i}$
^{190}Ir	30	16.8	5	82	56	14.2	1	2	$N_{G\,i} < N_{L\,i}$
				9	8	0.04			
				9	8	3.5			
				10	8	2.5			
^{190}Tl	7	2.3	8	14	9	2.8	4	5	$N_{G\,i} < N_{L\,i}$
^{191}Bi	5	0.05	4	11	7	0.04	4	5	$N_{G\,i} < N_{L\,i}$
^{196}Pb	165	0.37	4	425	268	0.27	13	14	$N_{G\,i} < N_{L\,i}$
^{202}Bi	3	3.3	3				44	38	The matrix is singular
^{208}Rn	13	0.94	2	51	38	0.09	2	3	$N_{G\,i} < N_{L\,i}$
^{239}Pu	28	3.7	4	58	33	0.27	4	5	$N_{G\,i} < N_{L\,i}$
							4	5	$N_{G\,i} < N_{L\,i}$
							5	4	The matrix is singular
^{240}Pu	135	10.5	5	145	64	0.48	1	2	$N_{G\,i} < N_{L\,i}$
				55	32	2.1			
^{248}Bk	2	186	5	4	3	0.11	2	3	$N_{G\,i} < N_{L\,i}$
^{253}No	2	0	2	6	6	0	5	6	$N_{G\,i} < N_{L\,i}$

Calculations for these 45 ADOPTED LEVELS datasets were made using the *NEWGTOL* program. *NEWGTOL* did not found any problems in ADOPTED LEVELS datasets for ^{51}Cr, ^{125}Pr, ^{159}Er. In other cases the necessary condition of solvability (8) appears broken for a fragment of the level scheme (51 cases). In most number of cases the level scheme has a "floating" fragment consisting of 2–3 levels connected by 1–2 transitions and not connected with other part of the scheme. The second typical case is a rotational band with unknown energy of band head. The fixing of energy of one level in the "floating" fragment may help to solve the problem in both cases.

There are 4 fragments for which the *NEWGTOL* program has given the diagnostics "*Matrix is singular*". In three cases the dimension of a "problem" fragment essentially lower than a dimension of the whole matrix. In ^{139}Gd there are 6 levels and 7 transitions, in ^{158}Tm there are 6 levels and 11 transitions, in ^{239}Pa there are 4 levels and 5 transitions. All these fragments are "floating" and are not connected in any way with other levels. The unique ^{202}Bi scheme has a "problem" fragment having 38 levels and 44 transitions. It has three low excited states which are not connected by transitions. These states are introduced to the scheme from α-decay data. There are rotational bands built on these states. The level scheme of ^{202}Bi needs additional investigations.

II. "*Negative matrix element*" diagnostics have 11 ADOPTED LEVELSdatasets.

Negative values of the diagonal elements of the matrix $\boldsymbol{(A^{T}WA)^{-1}}$ have no physical sense. These values appear as a result of *GTOL* program using the algorithm of Gauss–Jordan for the inversion of a symmetric matrix. However, the method of rotation for the inversion of a symmetric matrix seems to be more suitable for computer calculations. The *NEWGTOL* program uses standard subroutine of the symmetric matrix inversion *SMXIN*V.

The datasets with diagnostics "*Negative matrix element*" and results of calculations with the *NEWGTOL* program are presented in the Table 3.

It was found that the level scheme of ^{164}Tm consists of 5 independent fragments, and each of them may be processed with good χ^2. Five of level schemes have fragments with the number of levels exceeding the number of transitions; five other schemes have "problem" fragments for which the *NEWGTOL* gives the message "*Matrix is singular*". In these cases the dimension of the "problem" fragment is significantly less than the dimension of the full matrix.

Example: ^{64}Zn scheme has 103 levels and 210 transitions in the main fragment and 12 levels connected by 17 transitions in the "problem" fragment. The problem of analysis of these schemes appears significantly simplified.

Table 3.

ADOPTED LEVELS	Data from ENSDF		Results of NEWGTOL optimization						
	N_{st}	Q_{norm}	R	Main fragment			"Problem" fragment		
				$N_{G\,i}$	$N_{L\,i}$	χ_i^2	$N_{G\,i}$	$N_{L\,i}$	Diagnostics
^{64}Zn	131	2.63	6	210	103	1.1	16	12	The matrix is singular
^{145}Gd	64	0.14	3	169	105	0.07	15	16	$N_{G\,i} < N_{L\,i}$
^{153}Ho	27	0.42	7	65	41	0.07	13	14	$N_{G\,i} < N_{L\,i}$
							14	15	
^{161}Yb	13	1.24	2	41	34	0.47	42	37	The matrix is singular
^{164}Tm	118	1.18	5	28	14	0.82	–	–	
				96	58	0.8			
				114	70	0.8			
				48	29	0.83			
				5	3	1.4			
^{176}Ir	61	68.3	5	39	26	59	10	11	$N_{G\,i} < N_{L\,i}$
				38	29	52			
				90	53	38			
^{181}Re	140	5	3	271	137	4.9	25	23	The matrix is singular
^{186}Au	44	0.25	5	17	13	0.7	19	14	The matrix is singular
				31	22	0.7			
				52	28	0.03			
^{189}Tl	32	1.8	3	75	50	0.32	8	9	$N_{G\,i} < N_{L\,i}$
							8	9	$N_{G\,i} < N_{L\,i}$
^{193}Pb	69	0.6	2	176	125	0.18	12	13	$N_{G\,i} < N_{L\,i}$
				35	26	0.16			
^{197}Pb	106	2	6	246	147	0.92	51	45	The matrix is singular

III. The *GTOL* program gives the diagnostics "*Unrealistic large diagonal matrix elements*" for 13 ADOPTED LEVELS datasets which are listed in the Table 4.

Table 4.

ADOPTED LEVELS	Data from ENSDF		Results of NEWGTOL optimization						
	N_{st}	Q_{norm}	R	Main fragment			"Problem" fragment		
				$N_{G\,i}$	$N_{L\,i}$	χ_i^2	$N_{G\,i}$	$N_{L\,i}$	Diagnostics
^{40}Ca	592	0.93	8	582	140	0.21	4	5	$N_{G\,i} < N_{L\,i}$
^{49}Cr	48	157	2	61	31	5.9	2	3	$N_{G\,i} < N_{L\,i}$
^{140}Nd	69	3.67	7	226	163	0.67	17	18	$N_{G\,i} < N_{L\,i}$
^{144}Ho	3	1.2	2	4	3	0.9	5	6	$N < M$
^{149}Tb	123	0.56	6	217	99	0.52	12	13	$N < M$
^{149}Dy	43	0.4	8	80	46	0.44	23	17	The matrix is singular
^{151}Dy	22	1.4	6	60	41	0.52	20	21	$N_{G\,i} < N_{L\,i}$
^{158}Ho	95	777	4	148	82	0.36	27	13	Q_{norm}=3681 level 438
				20	11	0.01	15	10	The matrix is singular
^{176}Re	78	0.24	3	39	24	0.4	–	–	
				122	66	0.05			
				27	20	0.03			
^{177}Ta	190	0.46	2	321	152	0.4	29	19	The matrix is singular
^{183}Tl	–	–	1	–	–		9	9	The matrix is singular
^{195}Hg	238	1.8	6	345	136	1.8	15	16	$N_{G\,i} < N_{L\,i}$
							17	18	$N_{G\,i} < N_{L\,i}$
^{212}At	28	0.04	5	8	7	0.05	72	49	The matrix is singular
				12	11	0.03			

Results of calculations with the *NEWGTOL* are:

The level scheme of ^{176}Re consists of 3 independent fragments and does not cause any problems; "problem" fragments are found and localized for other cases.

IV. The *GTOL* program gives the diagnostics "*Negative Elevel after matrix mul.*" For four ADOPTED LEVELS datasets *NEWGTOL* did not found problem

for ^{90}Tc; for the level schemes of ^{60}Co and ^{183}Hg "problem" fragments are localized. The diagnostics "*Elevel = -0.00053*" is given for the famous ^{229}Th.

Discussion and conclusions

During the *NEWGTOL* program testing it was found that taking into account the block structure of the matrix (or, which is the same, of the level scheme) and using the method of rotation for matrix inversion instead of the Gauss–Jordan method completely excludes appearance of negative or abnormal great values of diagonal elements in the inverted matrix. Main part of "problem" datasets for the *GTOL* program was completely clarified with the *NEWGTOL*. In other cases, the "problem" fragments are localized which simplifies work for evaluators in the analysis of the level schemes.

Fragments of schemes, which the *NEWGTOL* program determines as "problem", may be divided into two types:

1. Fragments, in which the number of levels is more than the number of transitions connecting these levels; here the condition of solvability (8) is broken. The scheme should be analyzed for the correspondence of numbers of transitions and levels.
2. The condition of the solvability (8) is formally satisfied, but matrix is singular. Here methods for regularization (see [4, 5]) should be used; for these calculations the fixation of one or more values of energies of levels may be useful.

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