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THE LIBRARY OF EVALUATED AND EXPERIMENTAL DATA ON CHARGED PARTICLES FOR FUSION APPLICATION (SaBa)

by

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Abstract: An electronic version of the evaluated and experimental data on charged particles for thermonuclear applications (SaBa) was prepared on the base of handbook "Nuclear Physics Constants for Thermonuclear Fusion", INDC(CCP)-326/L+F, VIENNA, 1991.

Data on 100 channels for 52 reactions are presented in the Library. Program code was performed using the object-oriented programming environment Borland C^{++} Builder for Microsoft Windows 95 and Windows NT operating systems.

Optimal set of data processing procedures and friendly interface provide remarkable possibilities for the active use of this program for various applications in the field of thermonuclear fusion. It is available online (http:/www-nds.iaea.or.at/reports/data/saba/disk1.zip, ../disk2.zip, ../disk3.zip, on CD-ROM or on a set of PC diskettes from the IAEA Nuclear Data Section, costfree, upon request.

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Data References

Most of the data included in this system is based on the International Databases EXFOR (version of January, 1999), ENDF/B-VI, Rel.5, 1998).

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The library of evaluated and experimental data on charged particles for fusion application (SaBa)

Version 1 of 1999

by
A.G. Zvenigorodskij, V.A. Zherebtsov, L.M. Lazarev, S.A. Dunaeva,
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Introduction

An electron version of the evaluated and experimental data on charged particles for thermonuclear applications (SaBa) was prepared on the base of handbook "Nuclear Physics Constants for Thermonuclear Fusion" //INDC(CCP)-326/L+F, VIENNA, 1991, with taking into account new experimental data, revealed errors and misprints.

An electron version was convenient for making figures to scientific reports (articles), obtaining express-information about the current status of evaluated and experimental data on cross-sections of charged particles for light nuclei. Available analytical presentation of the evaluated curve makes convenient adaptation of the data incorporated in this handbook for the using in the other software products. For this a polynomial presentation (cubic spline) was chosen for approximation of excitation functions of evaluated integral cross-sections. It allows evaluated curves to be combined with other descriptions presented as analytical ones.

Theoretical models were used in cases when the experimental data did not allow to define univocally a shape of the excitation function for cross-sections of some reactions. The spline was built according to the theoretical curve normalized by weight-average experimental values.

For a qualified user of the library we can propose a capability to obtain his "own" evaluated curve. It could be achieved by using a graphic interface enclosed in this library. It allows to obtain your "own" evaluated curve in a dialogue mode. For this purpose the library is supplied with programs allowing to input new experimental data, and modify the existing ones.

The available “help” allows to master this library.

The authors will be grateful for any remarks related with both factographic materials of the handbook, and technique for the work with it.

1. SaBa OBJECTS

Experimental and adopted data are considered in SaBa. Any value of user's interest could be calculated in any desired point. Usually the approximation error is evaluated along with data evaluation.

1.1 Experimental data

In the new version of SaBa experimental data are presented in the form of tables of total cross-sections depending on the energy, or coefficients of Legendre polynomials depending on the energy for expansion of angular distributions in these polynomials. The

energy is considered in the laboratory coordinate system in **MeV**, cross-sections are measured in **mb** (millibarn). If the original authors' data are preset in another coordinate system they are transformed to the desired presentation before input to SaBa.

Errors of function measurement (experimental errors) are also stored with the experimental data, while errors of argument measurement are not written in SaBa even if they are given by the authors. Evaluator's errors are also stored with the data, but are used only for evaluation, as well as the systematic errors.

Each **set of data** contains a list of author's names participated in the experiment and a reference. This list is used for the experiment identification, for example, on the plot. Moreover, only the first name from the list is written, and if there are some others, they are replaced by symbol **'+'**. Most of the SaBa data are input from EXFOR files /2/, text of record AUTHOR in this file corresponds to the list of SaBa authors. A reference corresponds to record REFERENCE of EXFOR file. The reference text is enclosed in brackets. Appropriated EXFOR Subent number follows after the closed bracket.

It is assumed that each **j** set of data could contain a systematic error. It is random value, which normally distributed with zero mathematical expectation. Square mean deviation of this random value is a systematic error designated as δ_j.

Evaluator's errors are also stored with the data, but are used only for evaluation, as well as the systematic errors. Evaluator's errors may differ from those experimental, since they are nominated basing on the relation between a specific set of data and the totality of data.

In most cases systematic errors are not mentioned by authors of experiment, they are additional fitting parameters for an evaluator for evaluation performance. Varying their values the evaluator may build a curve differently with regard to the set of data: from set with a considerable systematic error the evaluation curve will go further, that from set with the less error. In this case however the curve shape will also take into account the data with a considerable systematic error.

If for all sets $\delta_j = 0$, then the applied statistic model will coincide with the common method of least squares.

A full description of a statistical model is done in Appendix A.

Angular distributions are presented as Legendre polynomial expansion:

$$\sigma(\mu,E) = \sum_{i=0}^{n} a_i(E) P_i(\mu),$$

where $\mu = \cos\theta$,

P_i - Legendre polynomial of *i-th* degree.

From this expansion normalized presentations can be derived:

RS - normalization on a_0:

$$\sigma(\mu,E) = a_0(E)\left(1 + \sum_{i=1}^{n} a_{RS,i}(E) P_i(\mu)\right),$$

where $a_{RS,i}(E) = a_i(E) / a_0(E)$

RS0 - normalization on the cross-section under 0°:

$$\sigma(\mu,E) = \sigma(\mu = 1,E) \sum_{i=0}^{n} a_{RS0,i}(E) P_i(\mu),$$

where $a_{RS0,i}(E) = a_i(E) / \sigma(\mu = 1, E)$.

RSD - normalization on the cross-section under the angle of 90°:

$$\sigma(\mu, E) = \sigma(\mu = 0, E) \sum_{i=0}^{n} a_{RSD,i}(E) P_i(\mu),$$

where $a_{RSD,i}(E) = a_i(E) / \sigma(\mu = 0, E)$.

All types of presentation can be used in SaBa. Values of coefficients are input into the data base with mentioned normalization method. Only even or odd polynomial expansion coefficients for symmetrical distributions are written and it is indicated that a step of polynomial numeration is 2. For a general case the step is 1.

1.2 Adopted data

By adopted data are meant those obtained with the method of least squares over a collection of experimental data stored in the database in terms of systematic and statistic errors. As an approximation curve describing adopted data spline function is used.

Cross-section σ is expressed through an astrophysics factor *S* according to the formula:

$$\sigma(E_{cm}) = \frac{S(E_{cm})}{E_{cm}} exp\left(- \sqrt{\frac{E_g}{E_{cm}}} \right),$$

$$E_g = m \cdot (0.98948\ Z_1 Z_2)^2,$$

$$m = \frac{m_1 m_2}{m_1 + m_2},$$

$$E_{cm} = \frac{m_2}{m_1 + m_2} E_{lab}.$$

There are used the following designations:

m_1, Z_1 - mass and charge of the incident nucleus,

m_2, Z_2 - mass and charge of the target nucleus.

Mass is given in atomic mass units and charge is given in proton charge units.

Energies are measured in MeV.

The approximation of function *S(E)* is built as two functions:

for $E \geq E_{min}$ - spline;

for $0 \leq E < E_{min}$ - as usual, extrapolation in this case is carried out according to theoretical model, described in the corresponding reference for the reaction given.

E_{min} is usually equal to the minimal energy for which the experimental data are measured. If the extrapolation to *0* is not built for some reasons, the spline value in its left limit is taken as value *S* at $E < E_{min}$.

For evaluation of Legendre polynomial coefficients only splines are used.

1.3 Spline definitions

Spline is piecewise smooth functions with continuous derivatives of up to some order. Points, in which derivatives of highest orders breaks are called knots of the spline. Between knots the spline is presented by polynomials (each interval has its own polynomial) of the same degree. For building the approximate spline a statistical model is used according to which the data are split in set (usually these are the results of one experiment), each of which contains its own systematic error. Usually, this error is not given by authors of the experiment, but even if it is given, it requires a critical approach. Most frequently systematic errors serve as evaluation parameters, with which the evaluator can obtain the agreed (from the viewpoint of physics) result.

Knot of spline is a point, in which the spline derivative continuity is violated. To the left of the knot the spline-function is presented by one polynomial, to the right - by another. These two polynomials are related with each other by the expression providing the continuity of the function and some of its derivatives. A number of continuous derivatives in the knot depends on the spline order and the defect of the spline in the knot. Configuration of knots effects spline possibilities in presenting dependencies: the more nonuniformity and inflection points the function has, the greater amount of knots should be located in this interval to achieve the desired precision of the function presentation. On the other hand, the excess (as compared to the number of experimental points) amount of knots can lead to degeneration of the task related with the search of approximating spline and obtaining unjustified oscillations of the spline.

Spline order is a order of polynomials involved in the spline in the intervals between knots. Most frequently cubic splines are used, i.e. splines of the third order. However the use of other orders is also acceptable. In particular, spline of order *1* - it is a piecewise smooth function convenient for use in some calculation algorithms.

Spline defect in the knot is a number of discontinuous derivatives in the preset knot of a spline beginning from derivative of the maximum order. The minimal defect value is *1*, since if there are no discontinuous derivatives in the knot, then there is no the knot itself, and polynomials to the left and to the right of the knot are one polynomial. In the knot of defect *1* derivative *p-1* is breakable, where *p* - is the spline order. The maximal defect is *p+1*, in this case the function itself is also breakable, and the spline splits in two unrelated polinomials. Thus, a number of continuous derivatives in the knot of defect *d* is *p-d+1*, assuming that the function is *0* derivative.

It is recommended to preset initially defects of all knots be equal to *1* before building the spline. While fitting the nearby knots may merge. In this case these knots could be replaced by one knot with defect equal to the sum of merged ones. Thus, during fitting optimal defects are preset automatically.

A full description of a spline presentation of a fitting curve is done in Appendix B.

Polynomial presentation of the spline

The spline is presented as a set of polynomials. If $x = \{x_0 < x_1 < \ldots < x_n\}$ is the spline grid, then the spline-function of p order $S(x), x \in [x_0, x_n]$ is defined as

$$S(x) = P_i(x), \;\; x_{i-1} \le x < x_i, i = 1,\ldots n,$$

where $P_i(x) = a_{i0} + a_{i1}(x - x_{i-1}) + \ldots a_{ip}(x - x_{i-1})^p$.

Polynomial coefficients are related by dependencies providing continuity of required derivatives in the knots. This presentation is most convenient for calculations with the existing spline, but it is inconvenient for spline defining since it demands to solve sets of equations for observing continuity conditions.

Basic presentation of the spline

Spline function of *p* order is written as a linear combination of basic splines. Let's designate: $(a-x)_+^p = \begin{cases} (a-x)^p, & x \le a \\ 0, & x > a \end{cases}$, then the basic spline will present the function:

$$B_k(x) = \sum_{j=1}^{p+1-k} \frac{(x_j - x)_+^p}{(x_j - x_0)^k \prod_{l=0, l\neq j}^{p+1-k} (x_j - x_l)} .$$

$B_k(x)$ equals to *0* outside the interval $\lfloor x_0, x_{p+1-k} \rfloor$, in knot x_0 it has defect $k+1$, in knots $x_i, i = 1, p+1-k$ the defect is *1*. To preset a spline on the selected spline's grid with a set of defects a relevant set of basic splines should be chosen, so all the required conditions will be fulfilled automatically. Therefore, the basic presentation is convenient when defining the spline. However for calculation of the function value in the indicated point with the existing splines the expressions for basic splines are complicated. Therefore, after the spline is defined the basic presentation is transformed to the polynomial one.

2. MAIN FUNCTIONS OF SaBa

Working with the SaBa program is a process of data manipulation through a set of embedded windows standard for Windows environment. Each window includes a set of commands, control buttons, graphic or text fields. Any window except the performance of specific functions provides for the execution of the following commands:

- **Help** - obtaining specific information on the program.
- **Exit** - completion of operation with the current window and return to the previous one.

The last command could be executed by the standard close button - .

The main window of the program titled **" Thermonuclear Reaction"** consists of three parts: at the top there is a menu bar; at the left there is given a list of all available reactions in the form of a tree; at the right there is a set of buttons with which all manipulations with data are made.

2.1 Commands of the Main Menu

Main menu includes the following menu names:

- **Language** - change of the language for communication with the program. While addressing to this command a list of available languages is displayed, where the desired one should be noted. The changing of the language will not effect some subscriptions on

standard Windows dialogue panels, for example, panels for choosing the file name, the language of which is defined by the applied version of the operating system.

- **Help** - obtaining specific information on the program.
- **Exit** - completion of operation with the program.

Two last commands from the menu are common for the most of programs operating in Windows.

2.2 Data selection by reaction name

The list of data is arranged like a tree (see Fig. 1). The tree contains nodes. The node is displayed on the screen as a small picture followed with a subscription - a name of the preset node. The node may involve other nodes, then before designating this node there will be a little square, enclosing sign **'+'** or **'-'**. One can control the displayed nodes. Click (with the mouse) the square, and you will be able to control the demonstration of nodes belonging to the given one: if '+' is displayed the nodes of the next level are invisible, clicking the mouse will activate their display. Clicking the sign '-' will cause the opposite action: the displayed subnodes of the preset node will be hidden. To indicate the node click the left button of the mouse on the nodes name, or the picture presenting it. Colors of the indicated node change in accordance with preset colors in Windows. One can manipulate the node by pressing the required big button to the right of the window.

Presentation of data in a form of a "tree"

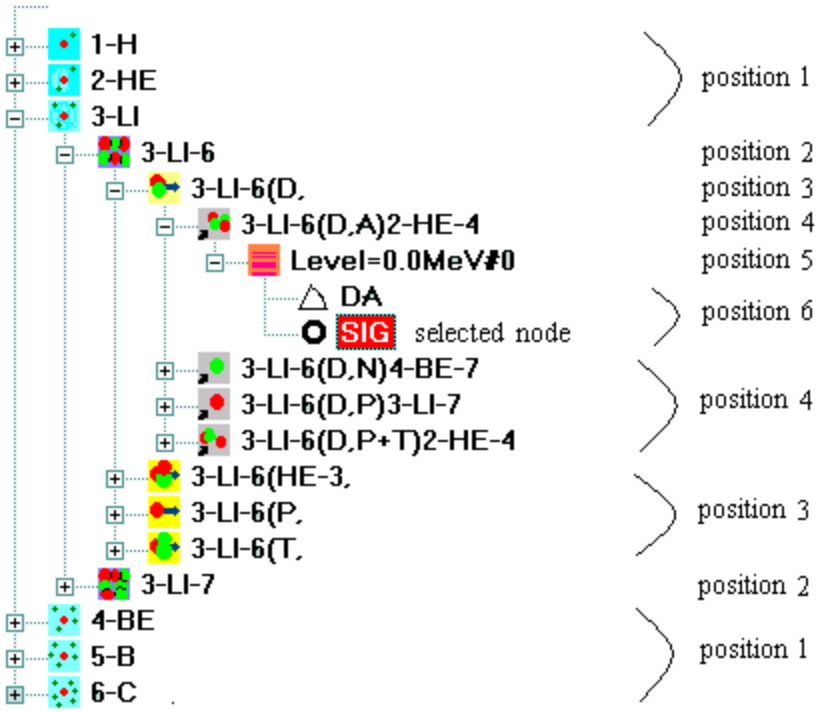

Fig. 1

Let us introduce a term called the node position. In this case all the nodes involved in some node (called parents') have the same position, it is one unit more than the parent's node

position (Fig.1). On the tree the nodes of high positions are shifted to the right as compared to those from lower positions. In SaBa positions from 1 to 6 are used (see Fig. 1).

Node position

Position 1 - target element. The node name consists of the nucleus atomic number, followed via **'-'** by the element symbol, for example **1-H** (Fig.1, position 1).

Position 2 - target isotope. The node name is created according to the common scheme of isotope designation: atomic number- symbol- mass number, for example, **3-LI-6** (Fig.1, position 2).

Position 3 - incident particle, for example, **3-LI-6 (D,** - (Fig.1, position 3).

Such designation is a beginning of the common designation of nuclear reactions. Symbols of incident particles used in database are given in Table 1.

Table 1 - Designation of the incident particles

Designation	Incident particle
P	Nucleus H-1 (proton)
D	Nucleus H-2 (deuteron)
T	Nucleus H-3 (triton)
HE-3	Nucleus He-3
A	Nucleus He-4 (alpha-particle)
G	Gamma-quantum
N	Neutron

Two last particles are not used in the Library of charged particle reactions. They are given for completeness of data presentation. SaBa software may be used for further library development.

Position 4 - outgoing particle (particles), or a process. For a particle full designation of the nuclear reaction is written in the name node according to EXFOR /2/, for example, 3-LI-6(D,N)4-BE-7. List of outgoing particles for reactions presented in SaBa is given in Table 2. At a later time there may appear other combination of particles produced from the basic ones by the sign **'+'** and coefficient, for example, **P+2N**. If the reaction product is neutron, it is designated as **0-NN-1**. In the case of gamma-quantum the designation is the following: **0-G-0**, according to EXFOR rules.

Table 2 - Designation of the outgoing particles

Designation	Outgoing particle
G	Gamma-radiation
N	Neutron
P	Proton
D	Nucleus H-2
T	Nucleus H-3
HE-3	Nucleus He-3
A	Nucleus He-4
N+N	Two neutrons
N+P	Neutron and proton
P+T	Proton and triton
G+2N	Gamma and 2 neutrons

List of available processes is given in Table 3.

Table 3 - Designation of processes

Designation	Process
ABS	Absorption
EL	Elastic scattering
F	Fission
INL	Inelastic scattering
NON	Nonelastic
PAI	Pair production
SCT	Total scattering
THS	Thermal neutron scattering
TOT	Total reaction cross-section
X	This symbol is used for designation of total cross-section measurement for reaction of product formation
XN	Variable number of emitted neutrons
YP	Variable number of emitted protons

Position 5 - an excitation level. Node name "undef level" designates indefinite level, i.e. a mixture of all levels. The level name begins with "Level=" for the data of the definite excitation level, and the level value in MeV will follow, afterwards - symbol **'#'** and a number of the excitation level. The number of the ground state level is *0*. (For example, Fig.1, position 5).

Position 6 - in this position the data are split in angular, with the node name "DA", and total cross-sections with the node name "SIG". The node for manipulations with data should be selected just in this position. (For example, Fig.1, position 6).

2.3 Function keys of the Main Menu

Not all the buttons for manipulations with the data are activated. The button availability depends on the mode of data processing. There are the following buttons:

- **Information on isotopes and reactions [Ctrl-H]** - is active for each position. The reference is given by WinHelp Windows system and, therefore its working order is the same as for the standard Windows-based application.
- **Output of a reaction list [Ctrl-L]** -is active for positions from 1 to 4.
- **Review and output of tables and plots [Ctrl-O]** - is active for position 6. A window is displayed where one can select the mode of data processing: data selecting from the database, data analysis, executing tables and graphs for reports.
- **Creation of the ENDF file [Ctrl-E]** - is active for positions from1 to 6. If in SaBa there is no evaluation for any reaction referring to the indicated node, then this button will be passive.
- **Editing and evaluating of data [Ctrl-P]** - is active for position 6. This mode provides for editing data, input data from file, deleting the whole sets of data, building a new spline.

  Any button involves designation of a Hot key, which you may use instead of pressing the mouse button. For example, instead of clicking the mouse on **"View and output of tables and plots"**, you may simultaneously press **Ctrl** and **O.**

3. INFORMATION ABOUT ISOTOPS AND REACTIONS

Depending on the current position in reaction (see data tree) one or another information about the reactions and experimental data sources stored in the database is presented. For example, clicking on the button **"Information about isotopes and reactions"** from position 1 of the tree node causes displaying of data for corresponding isotope, and from position 6 causes displaying of information about the specific reaction, reference list of experimental data and etc.

Output of these information is supported by WinHelp Windows system, therefore the working order in this case is the same as for a standard Windows-based application.

4. OUTPUT OF THE REACTION LIST

A list involving all the reactions referring to the selected node is output. Output is going to a separate window supplied with control buttons:

All - output the list with overall SaBa reactions;

Print - print out of list;

Write - output to the file;

Font - change the font with which the list will be printed (this setting doesn't effect the list image on the screen);

Help - help for the commands of current menu;

Close - come back to the main menu.

The following information is given in the table: data type, value of reaction energy and excitation energy.

The energy of reaction Q is calculated by the formula:

$$Q = 931.5016(m_t + m_i - m_e - m_r),$$

where m_t - mass of the target nucleus;

m_i - mass of the incident particle;

m_e - mass of the emitted particle (particles);

m_r - mass of the residual nucleus.

Mass is measured in atomic mass units, energy - in MeV. Mass values are taken from the Wapstra tables /3/.

5. REVIEW AND OUTPUT OF TABLES AND PLOTS

The output window is divided in two parts. In the left one there is a **"Menu for data selection"**, the right is intended for the data editing and named the **"Working field"**. From the **"Menu for data selection"** one can select the objects, which will be displayed in the **"Working field"**, and, possibly, output as a report. Placing the cursor on the line separating the titles of these parts and shifting to the left or to the right, parts' widths could be changed.

The main activities can be performed using buttons in these fields.

5.1 Commands of the Menu

Menu offers additional capabilities involving the following commands:

- **ViewData**- for the output differing from that offered at the moment of the window initiation: for total cross-sections - tables with cross-sections, for angular distributions - tables with coefficients of Legendre polynomials.
- **AdditionalTables** - output of tables with the spline coefficients.
- **Report** - transfer report to WinWord for printing and writing to a file. Transferring some tables to Excel or writing them into a text file. This command is not active while there is nothing in the working field.
- **Comparison** - comparison of data from SaBa with those from other libraries.
- **Help** - obtaining specific information on the program.
- **Exit** - come back to the previous window.

5.1.1 Selection of the data presentation (Command "ViewData")

Commands of this menu involves descriptions of various options for data presentation, which are incompatible with each other for displaying on the same graphic. Therefore, with the displaying at least one of the curves on the graphic in the working field this command becomes unable and is activated only after the mentioned graphic is clean.

For operations with total cross-sections (SIG, Fig.1) two options of function presentation are possible:

Cross-section

S-factor

And two systems for energy defining:

ENERG-LAB

ENERG-SCM

The initial combination preset automatically when opening the window:

Cross-section and **ENERG-LAB**.

As S-factor in SaBa is given in the center of mass system, then while selecting **"S-factor"** going over to energy measurement units in **"ENERG_SCM"** occurs automatically.

For operations with angular distributions (DA, Fig.1) the energy is always set in the laboratory coordinate system and for differential cross-sections the energy is given in the center of mass system. For data presentation there are 4 options:

- **Legendre coefficients** - accepted default.
- **Angular (many energies, few angles)** and
- **Angular (many angles, few energies)** - The first option differs from the second one by the fact that angles will be located in columns of the table and energy in lines. Of course, understanding "many" and "few" is relative and depends on how many points have been preset for one or another variable. The goal is that a number of columns will be less, otherwise the page of the report couldn't enclose the table.
- **Comparison with ECPL** - comparison with the data from ECPL library entered according to the following format.

Format description for input of data obtained from the ECPL library

Two directories are provided for placing the files with data obtained from the ECPL library. First directory is for the files containing total cross section data and second is for those including angular distribution ones. Such separation is due to the particularities of SaBa working.

File containing total cross-section data should include:

- title, where the reaction name is given, for example, H-3(D,N);
- numeric data written as a pair "energy-cross-section", for example,

1.10000+ 0 2.00000- 1 1.30000+ 0 2.00000- 1 1.40000+ 0 2.30000- 1

Energy is given in MeV, cross-section value is in barn. No more than 6 columns may be in a line. E12.5 format is used for data representation.

File containing total cross-section data should include:

- title, (see above);
- numeric data written in the following order:
  - in the 1-st line there are given the value of incident particle energy and a number of pairs "angle-function value";
  - in subsequent lines there are presented the value of angle cosine and the value of $F(E,\mu)$,

$$F(E,\mu) = 2\pi\delta(E,\mu) / \delta_{tot},$$

where $\delta(E,\mu)$ - value of angular distribution;

δ_{tot} - value of total cross-section.

No more than 6 columns may be in a line. E12.5 format is used for data representation. Example of a table is presented below:

```
3.00000-1      6.00000+0
-1.00000+ 0  6.10367- 1   -9.11940- 1   5.80745- 1   -7.22930- 1   5.29779- 1
-5.94850- 1  5.02404- 1   -4.48720- 1   4.77425- 1   -2.04600- 1   4.50050- 1
```

5.1.2 Output of spline coefficients(Command "AdditionalTables")

Now while using the command **AdditionalTables** there is possible to obtain the spline coefficients only.

Spline coefficients are presented as polynomials. For Legendre polynomial expansion there are created as many tables as there polynomials in expansion are.

A request is output **"Write coefficients to a file?"**. The text file structure is as follows:

- 1-st line - integer number indicating how many lines follow the heading. This heading is a text description of the reaction, excitation level etc. Presence of this number makes possible to pass the heading for computer processing of the file.
- The spline coefficients follow the heading. All splines for coefficients of Legendre polynomials are written into one file, but prior to the writing of each spline the additional line is inserted. It contains an integer to denote a polynomial degree.

The spline coefficients themselves are written as follows:

- First a line with 4 integers delimited with commas. The meanings of these integers are: a number of lines in the following table, a number of columns in it, an indicator of scale along X, an indicator of scale along *Y*. Indexes may have two meaning: 1- logarithmic, 0 - linear.
- The first column of the table with spline coefficients involves an integer to denote a defect in the knot.
- The second column involves knot X_i. If the logarithmic scale is along *X*, then there is written not the knot itself but its natural logarithm.
- Then coefficients of polynomial in $X - X_i$ degree follow, beginning with zero degree.

5.1.3 Input of the new data (Command "Comparison")

This menu name involves the following commands:

- **Text file** - table input from file for comparison with tables obtained in SaBa (see below).
- **Choice of directory** - for files involving data from ECPL library. It involves two commands allowing to set separately directories for angular distributions and total cross-sections. A system dialogue is output for selecting the file name with which one can go over to the desired directory, and indicated there any file, since file selection is needed only to obtain the directory name from it.
- **ECPL** - comparison with the data from the ECPL (see above).

Input table from the file

The file should be in the text format. It is assumed that it involves the information from which the table title can be taken, and a numerical part in the form of columns, which

could be assigned as an argument, function or the function error. The table from this file is transferred to the table field in two phases.

For opening the file a system dialogue will be output.

Phase 1 for obtaining the table from the text file

The main goal of this phase is to select the information part from the file for making the table heading, and a numerical one for the table itself.

The window **"Creation tables for comparison"** is an edit field with the control buttons:

- **Write -** output data to the file, if changes in the data have been made.
- **Next>>** - Button **Next>>** will be active if the **data** are selected (presence of heading lines is not obligatory). Pressing the button will begin fulfillment of Phase 2 in obtaining the table from the text file.
- **Help -** obtaining specific information on the program.
- **Exit -** come back to the previous window without transferring entered data to the table field of the program.

In the current window there are also the lists with the following titles:

- **Delimiters -** involving a list of delimiters between numbers in columns. A standard set of delimiters: space, comma and semicolon. This window is an editing window, so additions may be inserted in it if other delimiters are used in the file. As additional delimiters first symbols of newly inserted line will be used. A group of symbols in the file consisting of delimiters will be taken as one delimiter. All other symbols will be interpreted as those involved in record of numbers, and these numbers will be translated to the computer presentation. If failed, a message will be output with the text, that could not be translated to a number. In this case the necessary changes should be made.
- **Limiting right position -** entering a position number in a file string, that will be a limit for data input in line. For example, let us suppose that the file consists of two data columns that take up positions from 1 to 19 and the comment that begins from the 20 position of each line. Setting the value of 20 in the field **"Limiting right position"** defines the data range, that will be transferred to the table at the second stage of data input from file.
- **Heading** - selecting the mode of table heading creation;
- **Data -** selecting the mode of forming the numeric data for a table.

  Two last fields allow to select the mode of data input:

  - Start - means that the selected information will be placed at the beginning of the appropriate section;

  - Add - the selected information should be added to those marked earlier;

  - Cancel - deletes the appropriate section.

While opening the window a file is read to the edit field. Any changes can be made in this field, as in any editor. Input sequence of tables is the following:

a) check the existence of corresponding delimiters in file in the field **"Delimiters"**;
b) check the necessity of input of position number in the field **"Limiting right position"** ;
c) headings or data from the table are selected. The selection is made as in any editor by pressing the left button of the mouse or by moving the cursor of the keyboard with the

button **Shift** pushed. Then select the corresponding mode from one of the fields: **"Title"** or **"Data"**.

If the changes are made, they may be written to the file using the menu command **Write**.

Phase 2 for obtaining the table from the text file

The edit field **"Creation tables for comparison"** is split into 2 parts: in the upper one the heading is placed, in the lower there is the main part: numerical data, separated in columns. A window is an edit field with the control buttons:

- <<**Finish -** finish data collecting. When the data have been entered to columns **X** and **Y**, button <<**Finish** activates, and the table may be sent to the table field. Thus, the available column of errors **DY** is not obligatory. If errors are set by a common percentage for all points, this percentage should be noted in the text format in the table title.
- **Back>>** - at any moment it is possible to be back to the previous window of pressing **Back>>.**
- **Help -** obtaining specific information on the program.
- **Exit -** come back to the previous window without transferring entered data to the program.

There are also the lists in this window with the following titles:

- **Cx** - Being transferred the data are multiplied by coefficients: **X** by **Cx**, the magnitude of which is assigned to 1 before the window is opened.
- **Cy -** Being transferred the data are multiplied by coefficients: **Y** and **DY** by **Cy**, the magnitude of which is assigned to 1 before the window is opened.
- **Step** - Created tables are arranged in increasing order for X. If there are too many points in the file they can be sent to the table with a step, the value of which could be entered in the editing field with subscription **"step"**. The first and last points are always sent to the table, even if the difference of their numbers is not a multiple to a step.
- **column X -** select **column X.**
- **column Y -** select **column Y.**
- **column DY -** select **column DY.**

  The last three fields allow to select the input mode for the table columns:

  - Start - start the definition of a column;

  - Add - add to the columns entered before;

  - Cancel - cancel input of columns made before.

  Working sequence is the following.

  a) Indicate the **column X, column Y**, and, possibly, **column DY**. It is reached by selecting line to **"start"** or **"add"** in the appropriate selection window. The cursor will change its shape, and it should be clicked on the desired column. Afterwards the column will be colored with the same color, as the title of the applied selection window, and the column will be titled: **X, Y** or **DY**.

  b) Enter needed coefficients for X and Y. Being transferred the data are multiplied into the following coefficients: X by Cx, Y and DY by Cy. Coefficient meanings are assigned a value of 1 before window opening. These coefficients could be replaced by the required ones for which purpose the edit fields titled correspondingly serve.

  c) Data are written according to the step chosen (see **step**).

d) Transfer created table to the table field or come back to the first stage. One should remember, that actions relating to the multiplying by coefficients are executed only at the moment of table's transferring to the table field of the program.

At the second stage any data editing (except multiplying by coefficients) is illegal. One should come back to the first stage for data editing.

5.1.4 Output of the selected data (Command "Report")

This command of menu remains inactive if **"Working field"** does not contain any information.

The first group of commands is intended for making the report as a WinWord file: (Warning: this version of Saba can work only with MSOffice95). There are three items:

- **WinWord** - create a WinWord file;
- **Plot Size** - set plot sizes;
- **Table Format** - choose a table format.

The rest commands are meant for a transfer of tables to other applications or files. They are enabled only when **Field of tables** is active.

- **What to transfer?** - setting rows or columns to transfer;
- **Transfer** - beginning to transfer data to the indicated text file;
- **Into a text file** - no action will be performed when this command is clicked. There will be changed only the command status: checked it or not. In addition to, when the command is checked a dialog window will be displayed, as described below. The transfer itself will be performed when one clicks the command **Transfer**. The window **"Format of table transfer"** contains a switch (radiogroup) to choose one from 4 delimiters between numbers in columns and headers of columns:

  comma
  space
  tab
  columns of equal widths.

  Selecting the forth item the editing field titled **"columns width"** will be displayed to enter a required number. Spaces will be added to a table content to achieve a required width of a column.

  Warning! Too long denotation of a number will be cut from right. No rounding will be made. If a number has an exponent part, a value of the number will be distorted. To avoid this one must agree a format of number representation in the table with the preset columns width.

  If the box titled **"save this setting as default"** will be checked, the format will be saved for all other tables.

  The button **Cancel** is designed to restore the format that was used before window displaying, not to cancel a table transfer.

WinWord

The following messages are displayed on the panel while transferring the report to ***WinWord***: **"Connecting with WinWord"**, **"Plot transferring"**, **"Output of tables"**. During the time of connection establishing and tables transferring any process in SaBa is

locked. Finally, a dialogue window for the choice of a file name is displayed. This file will be a ***WinWord*** document including the created report.

Transferred text is formatted using the specific SaBa styles stored in a template file **SabaTmpl.dot** from the SaBa working folder. This file may be edited with the help of ***WinWord*** to make the necessary modifications of styles for SaBa report.

Format of the tables is set using the menu command **Table Format**.

Changing plot sizes in SaBa with the help of command menu **Plot Size** is preferred over the same procedure in ***WinWord***, because of the appearance of the appreciable image distortions.

5.2 Functions of the data selection

The main part of the menu is occupied with a **plot** presenting all data available in SaBa for the reaction under consideration, and a **"list for selection"**, where authors of experimental data are listed. If there are processed coefficients of Legendre polynomial expansion, then the author's name is followed via a comma by a number of polynomial in the form "AN", where N is the polynomial number.

If in SaBa the evaluation for data exists, then in the list of selection it is designated as **Estimate** or **Spline**.

Delaying a cursor on the line in the selection list a window similar to the Window prompt appears for several seconds, which involves a reference to the appropriate data.

The desired lines in the selection list are selected by pressing the left button of the mouse (to select several lines the procedure should be performed with the **Ctrl** button pressed). The selected data are placed in the working field and then into a report.

For Legendre polynomials there are additional selection windows titled "**Authors:**" and "**Polynomials:**". Using them all polynomials of one author could be selected immediately, or polynomial of a specific degree for all authors. The line **"do not select"** means that selection is not performed.

Warning! While selecting one of the command **Angular…** only adopted data are displayed. Therefore there are no additional fields for selection in the window.

Processing of the data are performed with buttons listed below.

 - output of information on the reaction under consideration.

 - send the selected data to the **"Working field"**. If none of the lines is indicated in the selection list the button is not active.

 - send all the data displayed in the **"Menu of data selection"** to the **"Working field"**.

 - on the plot only the data indicated in the selection list will be shown. This button allows the user to orient in the huge amount of data with a large number of authors. It is possible to indicate one author by clicking twice the line in the selection list. To be back to the graphic menu one may press the same button for the second time, or select any information in the selection list.

 - remove from the working field data indicated in the selection list. Simultaneously the relevant table could be removed from the field of tables upon a request in the dialogue panel displayed for confirmation of the removal.

 - calculation of **adopted data table**. The table is placed in the **field of tables**, but it isn't output in the **"Working field"** automatically. It could be made from the table field.

 - going over to the table field. This field replaces **“Menu for data selection”**. The content of available tables can be reviewed in it. This button is invisible if there is no yet any table in the field of tables. When pressing this button an additional window appears. It will be described in section 5.2.1.

5.2.1 Functions of the "Adopted data tables"

It is necessary first to preset an output grid for the table creation. One grid (over energy) should be defined for total cross-sections. Two grids (over energy and the angle) should be defined for angular distributions and excitation functions of differential cross-sections. Each grid is preset in the window **“Set a grid for the table output”**.

The first line of this window is the following **“ Evaluation exists in…”** and involves information about the type of variable according to which the grid is built with its limiting values.

The grid can be preset by three ways, the option is chosen by activating switches titled **“Grid type”**. The following grid types are possible:

- **Linear**- arithmetic progression, difference between near-by points of the grid is **Step** (see below).
- **Logarithm** - geometric progression, ratio of two near-by points of the grid is $10^{\mathbf{Step}}$.
- **Arbitrary** - each point should be preset separately.

While selecting first two options the left panel will be active involving 4 windows for editing:

- **Initial value**
- **Final value**
- **Step**
- **Number of points**
- and button **Execute**.

The desired values should be input in the edit windows. The input is completed either after the button **Enter** is pressed, or when the windows lose the input focus, i.e. moving the cursor to another element.

Any three values from four should be input for grid definition. When it happens the fourth value is calculated automatically. Pressing the button with the legend “**if the grid suits you**, **press this button”** the grid points will be calculated. These points will be reflected in the right window.

The process of grid creation could be continued as much as you like, moreover the grids will combine. It can be used, for example, for presetting different grid steps in various areas of the argument range. Before presetting new parameters of the grid it is necessary first to clean all edit windows - an effort of changing their values one by one will not give a result.

While choosing the third option for setting the grid the panel with the window for parameters input becomes unable. In this case the right panel with the title **“Enter the required points”** activates. The window in this panel opens for editing (when using two first options this window was used only for displaying the grid elements, editing was impossible). In this window the desired editing can be made, including not only insertion of new points, but also deleting the old ones. That could be used if it is needed to correct grids set by two

first options. After the editing is finished press the indicated button "**to finish the input press this button"**.

While defining the grid points verification occurs, whether the point goes out of the limits indicated in the first window's line. If so, the dialogue window is output with a question, whether the point should remain in the grid (press button **Yes**) or refuse it (button **No**). For calculation of grids of progression type button **Cancel** can be also used in order to stop the grid calculation.

For calculation of progression due to round off errors the point laying on the boundary can be defined as being out of the limits. This point should be remained in the grid since inconsiderable going out of the boundaries is not taken into account.

Block with title **"Order"** involves switches:

- **increasing**
- **decreasing**
- **none**

Selection among them defines how the grid points will be sorted. When selecting **"none"** the grid points will be arranged in the order of their creation.

5.2.2 Functions of the "Field of tables"

This field involves the tables themselves and the control panel.

A small window for editing, titled **"Table number"** involves the table number displayed in the field at the present moment. Tables are numerated in order of their creation. If the tables are created as a result of selection from the **selection field** in the **"Menu of data selection"**, they are numerated according to the order of their appearance in this list from top to bottom. Any number can be input to this window according to a common procedure, finishing input by pressing **Enter** or using the up-down control.

The following buttons manipulate the table:

 - delete the table. As usual, a dialogue window with a requirement of deleting confirmation is output. If the table is displayed on the plot in the working field, the dialogue is supplied with request **"Do you really wish to delete the table with its curve?"** and three responses are proposed: **Yes** - delete both the table and graphic; **No** - delete only the table; **Cancel** - think over and don't delete anything.

 and  - the button can have one of these two images depending on whether the table is displayed or not on the graphic in the working field, and indicates, appropriately, whether to eliminate or insert the table in it. The tables created outside the menu for data selection, for example, the tables of evaluation or comparison are not placed on the graphic automatically, to achieve it press the right button. For tables, which couldn't be presented on the graphic this button is invisible.

 - change the format of numerical output. A dialogue panel will appear to change a number of output digits and presentation form (always with an exponent, with a fixed point, with an exponent and a fixed point depending on the value magnitude). Two various default formats of tables are available: for data - with a small number of digits, and for the spline coefficients - with a great number of digits. The format will be changed for all tables of the same type as a displayed table has.

 - close the current field and go over to **"Menu of data selection"**.

5.3 Editing data at the "Working field"

This field involves a plot, which will be illustrated in the report, and control buttons.

 - the output window contains the graphic legend. It can be moved, as any other windows in order to find the most suitable place for it. It should be taken into account that on the screen it can be located in any place including that outside the **working field**, but on the report's graphic it is displayed only when found inside the field. Besides, if the list is too large and can not be enclosed by the window, the window will have a scroll bar with which one can access any line of the list on the screen, but it will be usefulness on the paper. In this case one should thought over the splitting of the overall plot in several smaller ones. Clicking twice on the line will allow to edit the legend. A special window will be output with which the **"Text"** of subscription could be changed, **"Marker"** and **"Color"** for illustrating a point on the curve could be selected. The switch **"The same color for all curves"** allows to draw all curves with the same color, chosen for specific curve. Two more settings will influence all images of the curve, but not only that referring to the current editing. One can change the **"Size of the marker"**. Pressing **"Font"** will start the system dialogue in font selecting for displaying subscriptions for all curves. Button **legend** is invisible when the output window is opened. It becomes visible when closing the **legend** window by system menu.

 - editing of axis X.

 - editing of axis Y.

 - deleting of the whole report and starting the new one without closing the window. A report prepared preliminary should be printed by addressing to the command from menu **"Report"**.

Axes are edited in the relevant window, which will be called by pressing the button. The window is split into several fields and includes control buttons. There are the fields with the following buttons:

- **Name** - inputting it to the editing field can change the axis name.
- **Scale** - the scale can be either **linear** or **logarithmic** - the desired value is selected from the list. If a window with subscription **"scale"** is inactive, it means that there is at least one non-positive value in the data, and selection of logarithmic scale is impossible. Three buttons combined in a group with title **"Grid"** control the image of the coordinate grid. One of three options could be chosen:
- **Absent** - reject the coordinate grid;
- **Far-between** - the grid will be drawn only over the major tick labels of the axis;
- **Dense** - the grid will be drawn over all tick labels of the axis.
- Button ***FONT***, if visible, causes system dialogue for selecting the font with which subscriptions on the axes will be done. For both axes the only one font exists, therefore its selection for one of axes will lead to the change of images on another axis. This button is invisible when addressing to the graphic window of the data change, which is not intended for outputting data for printing, and therefore, it doesn't matter what font is used for subscriptions.
- **Ok -** exit with the changes saved.
- **Cancel -** cancel the changes made.

The following buttons allow to enlarge some plot areas, that is to work in the "magnifier" mode:

 - start performing a mode of a magnifier creation. The shape of the cursor is changed. Click of the left mouse button fixes the left top corner of a magnifier section. Its right bottom corner is defined by moving the cursor to right and down without releasing of the button. Borders of the magnifier are plotted as the dotted lines. Initially a scale in the magnifier is the same as the scale of the whole plot.

 - clicking this button ends the performance of the mode of a magnifier creating, if the previous button was clicked by mistake. Using this button the existing magnifier may be deleted. To delete a magnifier it is necessary to ***mark*** it by double clicking. Borders of the marked magnifier change their color.

 - hitting the upper arrow increases the image, hitting the lower arrow decreases it. Limits of increasing are from 1 to 1000. (One can not decrease the initial image as the decreasing arrow works only in the case the image was prior increased).

 - ends a work with the marked magnifier. Its border becomes black again. One can work with another magnifier.

 - moving the magnifier. The shape of the cursor is changed. The cursor should be placed within the magnifier, the left mouse button should be pressed, and then the magnifier is moved by cursor moving without releasing the button.

6. EDITING AND EVALUATING OF DATA

It is possible to edit experimental data, insert spline from the file, delete sets of data, perform new evaluation.

Data are evaluated by polynomial splines. For coefficients of Legendre polynomials coefficients themselves are approximated, for total cross-sections values of S-factor are approximated. For the user of evaluated data it does not matter how the evaluation is developed since the evaluation results in a cross-section. S-factor is displayed on the explicit request. During data processing they are displayed as a graphic in the **"Graphic window"**. At the top there is a control panel and at the left there is a panel with the buttons for plot viewing in the mode of "magnifier". (The functions of these buttons were described above in 5.3).

Initially parameters of graphic axes - subscriptions and scale (linear or logarithmic) are obtained from the data.

To start data editing one should click twice at any data point in a plot. Table with the indicated line including the coordinates of the point selected will be displayed at the left part of the screen.

The window involves menu. Not all of menu commands are always active. It depends on the processing status. Commands of menu are listed below:

- **Edit** - update of data sets including the author's list and the reference. Correction of spline coefficients.
- **Fit** - selection of approximation function. After the selection of this item one can use the command **Spline** that provides going over to a new menu for carrying out a new evaluation by splines. Now only spline approximation is realized in SaBa. There is possible to obtain spline approximation for the total cross-section (without using S-factor

representation). In this case new evaluation is not written and the result is saved using the **NewSpline** command.

- **Write** - write a new evaluation to a file;
- **ViewData -** selection of data representation;
- **SetErrors** - update of errors given in previous data evaluation;
- **InputSpline** - input from file either spline coefficients or experimental data;
- **Help** - obtaining specific information on the program;
- **Exit** - come back to the main menu.

6.1 Editing of the data (Command "Edit")

There are the following items for this command:

- **Data** - it should be addressed to review all the data of particular experiments and their systematic errors, and for the data change - deleting, addition of sets and/or single points, change values and subscriptions, i.e. editing experimental data.
- **Spline correction** - unable if panel **"Spline"** is not opened. This action is rarely used, it is intended mainly for input of splines in polynomial presentation into SaBa. For transformation of this presentation to the basic one used in SaBa, it is difficult to define defect, since one should compare derivatives calculated with final precision for two polynomials. Therefore, polynomial presentation is transformed to the basic one assuming that in all inner knots defect is equal to the maximal possible one, i.e. a order of spline *+1*. Coefficients of the basic splines of large defects (actually usefulness in expansion) turn small, as compared to the rest ones. This procedure proposes to indicate what coefficients should be canceled. A list of coefficients is displayed where the canceled ones should be indicated. The basic spline with lower defect couldn't be canceled keeping that with the bigger one. After correction there is no need to address the spline building - the desired spline has been already obtained by canceling negligible components. ***It is not recommended to perform this operation in other cases, as well as in misunderstanding of the basic presentation.***

Command "Data"

Editing is made in the window involving primarily a list of authors of data sets and their systematic errors. The following commands are available:

- **SetEdit -** editing of experimental data. A command set described below is provided for this purpose.
- **PointsEdit -** editing of point coordinates. Selection of this command is possible only after the selection of the **Points** command from the "**SetEdit"** menu was made.
- **Help -** obtaining specific information on the program.
- **Exit -** finish work with a current window and come back to a previous one.

To edit some data set click the left button of the mouse on the relevant line, and then select command **SetEdit** from menu.

Except experimental the list involves subscriptions for approximating curves: **"Spline #1"** for a spline and **"Estimate #1"** for evaluation. (Except #1, in the future other numbers

will be possible, when it will be possible to work simultaneously with several curves). Curves couldn't be edited, therefore, selecting the appropriate line **SetEdit** becomes passive.

6.1.1 Editing of the data sets (Command "SetEdit")

For experimental data the following editing capabilities are proposed.

- **Bias** - in the field of systematic error on selected line one should click on the mouse, afterwards the number will be edited in this cell in a common way. The panel will remind that editing can be completed only by pressing button **Enter**. Afterwards buttons **OK** and **Cancel** become active. Pressing one of them confirms the necessity to accept the inserted number, or return to the previous value.
- **Authors** and
- **References** - all these values are edited in accordance with the same scheme in the field of authors of the selected line: after clicking on the mouse on this field a text defining, accordingly, authors or the reference, appears in the selected line. Let's edit this text pressing **Enter** to complete the editing. Afterwards buttons **OK** and **Cancel** become active. Pressing one of them we are confirming the necessity to accept the inserted text, or return to the previous value. In contrast to the systematic error editing, editing of these fields is used to correct errors of data input, while systematic errors can be changed for obtaining the best evaluation.
- **Delete** - request will be made to confirm, and in the case of the positive response a set will be excluded from consideration. It hasn't been excluded from SaBa yet, the set will be canceled finally while addressing to command **Write** and its command **Changed data**.
- **Points** - for reviewing data of indicated set in a numerical form, as well as editing of this set. Content of the window is changed. The **PointsEdit** command becomes enable and the **SetEdit** command becomes unable. At the top of the window author's name of the first edited data set is displayed. The window is a table of sets of data for the chosen author with three columns titled: **X** - argument, **Y** - function, **DY** - error of evaluation. Each number can be changed directly in the table. To achieve it the desired cell of the table should be clicked on by the left button of the mouse, and then the right button of the mouse should be clicked on. Afterwards the cell will transform to the editing window, and below the table there will be a notation: **"to complete input press Enter"**. Following this procedure on the completion of editing **Enter** should be pressed. Then notation will change into: **"Make change - OK**, **refuse - Cancel"**, and two appropriate buttons become active, being inaccessible before. Pressing one of them completes operation with the cell, pressing **OK** changes the meaning for input, and **Cancel** - remains as previously. The made changes are active only with operations in the graphic window, in order to store them in SaBa it will be necessary to address command **Write**.

- **Order** - usually experimental data arrange in the order of increasing of the argument value. There is no need, except some convenience in reviewing, in this order for any processing, excluding the definition of the knot positions, in the algorithm of which this order is foreseen to reduce the calculation time. In the absence of this order the knots are not fit and the message is displayed about disorder in points. It is frequently a follow-up of the error in setting the data (which are usually preset as ordered), therefore, they should be, first, verified, and then use this command. The data will be arranged in the order of

argument increasing, but to store this arrangement for ever the changed data should be written in the command of menu named **Write**.

6.1.2 Editing of the points (Command "PointsEdit")

Other changes of data are possible while addressing command **PointsEdit**. The command involves the following:

- **Insert after** and
- **Insert before**

a new point of data will be inserted in the mentioned place relative to the selected line. An algorithm of insertion is simple: a new line appears with three numbers entered in it - 99999. These numbers should be replaced for desired ones, as described in the **PointsEdit** command. Cancel of insertion is not foreseen, since to delete the inserted line it is suffice to address the **Delete** command.

- **Delete** - the selected line is deleted from data. A dialogue window is displayed preliminary to confirm that the desire of exclusion is needed.
- **Error as in experiment** - evaluation errors are set the same, as experimental ones. After the data are input evaluation errors are set similarly. However as a result of evaluator's activities it may happen that these errors turned inapplicable.
- **Set errors** - it makes possible to change evaluation errors. The same error is set for all points. An editing window is displayed, in which the desired value is to be set. It can be expressed in percentage, and symbol % is set after the number.
- **Multiply** - allows multiplying all points of set of data by coefficients. A window will be opened where the following fields are available:
  - **Arguments by** - entering coefficient value for an argument.
  - **Functions by** - entering coefficient value for a function.
  - **Evaluation errors by** - entering coefficient value. Your own coefficient can be set, but coefficients for errors array are automatically set the same as those for functions, if there is no evident input of mentioned coefficients.
    Experimental errors in the graphic window are not displayed, their changes could be noticed only in window **"Review and output of tables and plots"**.
  - **Error of evaluation by** - entering coefficient value for evaluation error.
  - **Keep for the following sets** - using set coefficients while editing the other data sets. Having made a mark in window **"Keep for the following sets"** the set coefficients are stored in order to enter the window for the next time.
    The following standard buttons are used in this window:
  - **Help** - obtaining specific information on the program;
  - **Ok** - exit to menu **PointsEdit** with the changes saved;
  - **Cancel** - exit to menu **PointsEdit** with the changes canceled;
  - **Exit** - come back to the previous window **DataEdit,** where operations with other sets of data can be continued.

6.2 Spline fitting of the data (Command "Fit")

Now only the **Spline** command is available in this menu. Selecting this command the button of axes editing and the "magnifier" mode become unable. An additional menu line is

displayed. Knots of the spline on axis OX are displayed as symbol  , located one above another as many times as the defect is. For example, knot of defect 2 is imaged as  .

It is possible to manipulate directly with spline knots using their images on axis OX. In this case their locations can be changed, and defects, as well.

To change the spline knot the user should first *select* it, i.e. click on it image by the left button of the mouse. The selected knot will be imaged in the dotty frame. Clearing the selection is achieved by pressing the left button of the mouse once more.

The selected knot can be removed to another place on axis OX. To achieve it doesn't release the pressed button of the mouse after the knot is selected, move it to the desired place and then release it. The obtained spline will be displayed on the screen.

To set a precise numerical value to the selected knot or to change its defect one should call a pop-up menu by pressing the right button of the mouse. This menu involves two commands:

- **Delete** - the selected knot is deleted;
- **Change** - a new panel is displayed, where another location and defect can be set. If a logarithmic scale is used along axis OX, then with switch **Lin/Ln** an option may be chosen for setting the knot location - either by its true value, or by natural logarithm of this value.

With the buttons of this panel spline parameters can be changed: its knots, defect and a order.

The spline is not changed immediately after the change of some of these parameters. Setting the required parameters the user should address either the building of the spline with preset fixed knots, or begin fitting knots using preset ones as initial approximation. The only one exeption is for moving the knot with the mouse. The obtained spline is built immediately after the moving is completed.

On the additional panel the following buttons are:

- **FixNodes** - a spline is built with fixed knots displayed on the graphic. This spline should be built if it is necessary to evaluate spline errors. An algorithm of a spline building with fixed knots is described in Appendix C.
- **FitNodes** - a spline is built with defined knot positions.
- **OldSpline** - this button is active if a new spline was built by pressing one of buttons **FixNodes** or **FitNodes**. The previous spline is inserted in the list with old splines, and it could be extracted from it by pressing this button. In this case the spline displayed on the screen is lost forever.
- **NewKnots** - deleting the spline from the screen and inserting it in the list with old splines. This procedure is useful in the case, when crucial current arrangement of knots is required, it is necessary for changing the scale - linear for logarithmic or reverse along either axes, or one of the axes. In this case a series of operations should be as follows.
  1. Set the desired scale by calling the window for axes editing;
  2. Start setting new spline by pressing this button. The change of this order will lead to the situation that after setting knots the spline will be built in the previous order - its status at the moment of the button pressing will be "remembered" in it. After the button is pressed the window "**Initial setting of knots"** will be displayed.
- **Order=3** - changing the spline order. Number 3 is set on initiation of the window but in principle it is a variable equal to the spline order, for the change of which this button is

intended. By pressing this button a window will be displayed, in which a new order should be defined. For completion button **OK** should be pressed in this window. The window is modal, i.e. until it is not closed no other operations are possible. After closing defects are corrected, since defects shouldn't exceed the spline order.

- **Ins.Knot** - entering the knot. When this button is pressed cursor of the mouse become an arrow directed upward. The user should indicate a place on axis *OX* by this arrow where the knot should be placed, and press the left button of the mouse as many time as the defect is. It couldn't exceed the spline order, therefore, at some moment pressing on the button becomes usefulness. To exit the mode of "insert knot" this button should be pressed again (during all this time the button looks like as pressed and fixed).
- **a=0** - entering a regulation parameter**.** "0" is set during initiation of the window but in principle it identifies a regulation parameter. By pressing this button the window is displayed, in which a new parameter should be defined. For completion button **OK** should be pressed in this window. The window is modal, i.e. until it is not closed no other activities are possible.
- **Bound** - setting boundary conditions of the spline. The spline with these conditions can be build only on the basis of already existing spline, which should be obtained from the data base, or built by pressing buttons **Fix.Knots** or **Fit.Knots**.
- **Close** - complete operation with the spline. Images of spline knots are removed from the screen, the list with old splines is cleaned, therefore after going out of *editing* all intermediate results will be lost. No changes will occur in the data base itself, therefore the user can return to the spline presented in the base, by closing and opening once more the graphic window, not executing command **Write** for the spline.

6.2.1Definition of the knot positions (Command "FitKnots")

The control panel for definition of the knot positions involves three buttons and editing window (see Fig. 2).

An algorithm of fitting is described in Appendix D.

Control panel for definition of the knot positions

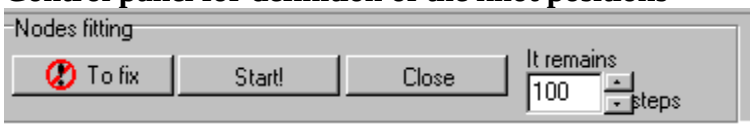

Fig. 2

- **To fix** - fix the knot. After pressing cursor of the mouse transforms in a cross. Pointing out some of spline's knot with this cursor makes it *fixed*, i.e. not participating in the definition of the knot positions. The fixed knot is colored with black. Fixation of some knots can ease the definition of the knot positions for a great number of knots under fitting, when it is difficult to reach the minimum over all knots. Any number of knots can be fixed. To exit the fixation mode press on the button once more.
- **Start!** - start fitting. The process course will be displayed in editing window subscribed **"It remains ... steps"**. Before pressing this button in the window a desired number of acceptable iterations can be set. If the fitting continues for a long time, one can notice

that this button will change its name for **Stop,** and pressing it will allow exiting from the procedure of fitting.

- **Close** - stops operations with this panel and return to panel **"Spline"**.

If this procedure is successful there will be no any message, only the obtained spline is displayed.

In other cases both a message and the spline is displayed, but the spline will be not optimal, it is only that achieved by the moment of fitting termination.

Messages can be the following:

- **A number of iterations was exceeded** - one can set a new number in the editing window **"It remains … steps"** and continue by pressing button **Start!**
- **Linear system is degenerated. The user can try to eliminate one of the knots** - it happens, when there are more knots, than data, in some interval. Just from this interval the knots should be eliminated.
- **The fitting was obligatory terminated** - button **Stop** was pressed.
- **The Newton method does not converge. The user may try to eliminate one of the knots** – reasons can be different, including that there are too many knots in the interval of smooth change of data. There are sufficiently many points, therefore, the *linear system was not degenerated*, but there are no univocal optimal positions of knots. Just from this interval knots should be eliminated.
- **There was an unpredicted error** – according to the fitting algorithm there shouldn't be such an error. Hence, it is either the system failure, or there is an error in the algorithm. The user may try to reset SaBa.
- **It is required to increase defect in the shaded knot. Do it**? – in this case one of knots is displayed in the shaded rectangular. Actually, there are two knots, not one, almost merged in the process of fitting. The fitting can be continued only if these knots will be changed for one with the defect equal to sum of the changed defects. If the response is **Yes**, the procedure will be fulfilled, afterwards the fitting will be continued. If **No** the obtained spline can be also used, but it could be not optimal since the process hasn't been yet completed. Besides, in the interval between two merged knots coefficients of polynomial presentation will be high that may cause difficulties in calculations.

While building the spline the error of obtained spline parameters is not evaluated, since the obtained nonlinear task is two complicated. Covariant matrix of coefficients is evaluated (according to which approximation error can be evaluated) only for linear task, when defined knot locations are fixed, and only spline coefficients are considered as parameters under definition. Therefore, after fitting knots button ***Fix.Knots*** should be pressed – the ready-made spline will be the same as it was, but it will have a corridor of errors defined in accordance with the algorithm described below.

Evaluation of spline errors

The evaluation of obtained approximation error is carried out basing on the linear model of approximation: $S(x)=\sum_i c_i B_i(x)$, where $B_i(x)$-basic splines, c_i- coefficients under search.

Then, $\sigma^2 S(x) = \sum_{i,j} \mathrm{cov}(c_i, c_j) B_i(x) B_j(x)$,

where $cov(c_i, c_j)$ - covariant matrix equal to reverse matrix of linear system for deriving c_j.

The obtained value depends on a priori evaluations of the experiment error and corresponds to reality so, as these errors do.

More particularly see Appendix E.

6.2.2 Entering of the new knots (Command "NewKnots")

Selecting this command a panel **“Initial setting of knots”** is displayed. The following commands are available:

- **Uniform** Selecting **"uniform"** a number of inner knots enclosed between boundary
- **Arbitrary** knots, which are define automatically, should be set.
- **Automatic** Selection of **"arbitrary"** will demand in the future to locate all knots explicitly including the boundary ones. Therefore, in most cases it is more convenient to choose **"uniform"**, perhaps with zero number of intermediate knots in order to locate intermediate knots later by button **Ins.Knot** at the panel **"Spline"**. **"Automatic"** is most convenient. In this case the program tries to search a number of knots, with which after increasing their amount by 1, evaluation of average dispersion $\bar{s}$ will increase. It will take place in the case if addition of a new knot will lead to inconsiderable change of error, and evaluation of dispersion will increase at the expense of denominator decrease in the formula shown below.
- **Limiting number of knots** - setting the maximum number of knots. Knots are selected from the grid composed from values of experimental points. They are selected so that the distance between two near-by ones will be not less than the length of the interval for spline building divided by the limiting number of knots, the value of which can be set in the editing window.
- **Limiting defect** - setting the limiting defect. In the case when it differs from 1 the program will select not only knots, but also a defect in each knot not exceeding the preset value.
- **Initial number of parameters** - setting the number of parameters from which the search should begin. The matter is that evaluation of average dispersion as N_p function, can have not only one maximum. For example, if the approximating function has many extremums, the spline with a small number of parameters will always smooth them, and give out the same residual value for this number increased by 1. For a cubic spline the initial number of parameters is proposed to be 4 as default, that corresponds to one cubic polynomial.

Average dispersion is calculated by the following formula:

$$\bar{s} = \frac{\sum (y_i - S(x_i))^2 w_i}{N_e - N_p},$$

where

S(x) -spline;

x_i , y_i , w_i - experimental point and its weight;

N_e - a number of experimental points;

N_p - a number of free spline’s parameters.

After pressing **OK** the process of knot searching starts. It is accompanied with display of information window, in which pressing button **Cancel** will make possible to stop the process. But usually everything happens so quickly that there is no such a need.

6.2.3 Setting of the boundary conditions (*Command "Bound"*)

Similarly to evaluation of errors the spline building with boundary conditions is possible only for linear task. Therefore, an order of operations should be the following: first, spline is built with definition of the knot positions, and only then the boundary conditions are set for this spline. If these conditions don't contradict with data, then the execution of these conditions will not change considerably the spline.

On the spline boundaries conditions can be set in the form of equality of values of function and derivatives to preset values. These conditions will be observed, but nevertheless the spline error can be evaluated if errors of preset values will be known.

Usually, boundaries of interval, where data are approximated, serve as points, in which conditions are set, but in this version of the program these points can be moved within some limits. These limits depend on spline's knot position.

Conditions can be set on both or one end of the spline. Conditions may be set on both ends only if there is a sufficient number of spline's knots between these ends – full intervals between knots should be not less than the spline order +1. For setting conditions use the panel showed on Fig. 3.

This panel consists of two identical parts for the **Left** and **Right bounds**. Button subscribed **"set/do not set"** turns on or turns off the condition on the boundary. Being turned off all elements of the relevant half-panel become passive, despite they conserve their values if set.

In the editing window designated **"X="** the argument value, with which function values and its derivatives will be set, can be defined. On default this value is assumed to be equal to the corresponding boundary of the area of approximated data. The preset value of **X** should be within mentioned limits.

Panel for setting boundary conditions

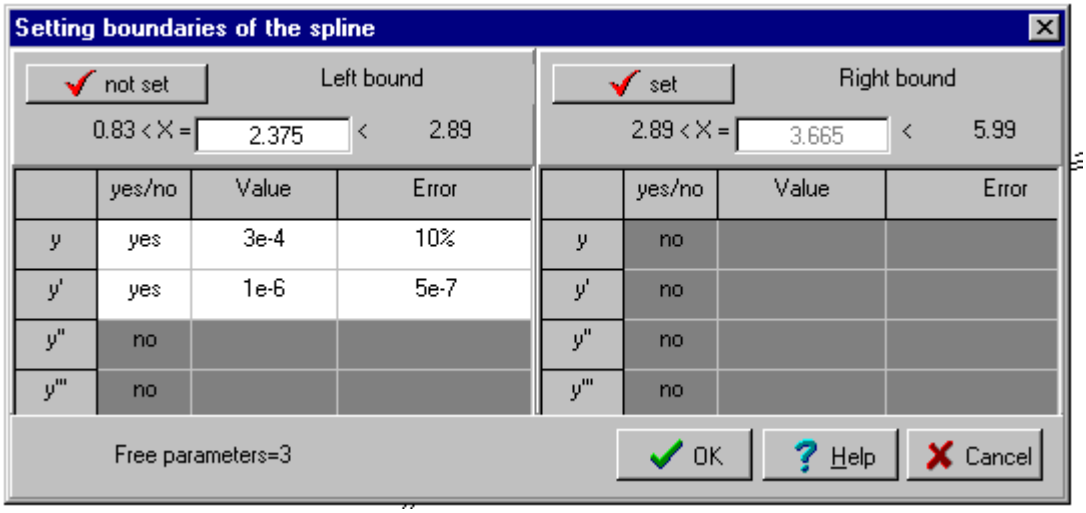

Fig. 3

Clicking on the column-titled **"yes/no"** the user will indicate whether the appropriate derivative will be set. With linear scales along both axes a set of these values may be arbitrary, for example, only values of the first and third derivatives may be set. With logarithmic scales there should be no gaps in setting derivatives: these values should be set beginning with the function and ending with the last derivative of interest, besides, true values, not logarithms should be set (i.e. *dy/dx* should be set instead of *d*ln*y/d*ln*x*).

Either the absolute error should be preset, or the relative one in percentage (see Fig.3).

In the line with subscription **"Free parameters ="** there is given a number of free parameters, which is reduced by 1 when setting the next condition, and increased by 1 when canceling the condition. This number couldn't be negative.

More particularly see Appendix F.

6.2.4 *Selection of the regularization parameter (Command "a=0")*

For building spline with fixed knots it is possible to effect the behavior of the approximating function externally, i.e. independently on the approximated data.

For building spline with fixed knots no objective function $F(a)$ is minimized, which was obtained from the maximum likelihood method, but a sum of $F(a)$ and regularization addition: $F(a) + a\int_{x_0}^{x_n} (S''(x,a))^2\,dx$,

where $S(x)$ - the approximating spline;

$[x_0, x_n]$ - approximation interval;

$a \geq 0$ - regularization parameter.

Introducing an addition will allow suppressing unwanted spline oscillations. The higher a the less is the spline curvature, in the limit for $a \to \infty$ the spline tends to a straight line. Along with this the precision of data approximation worsens, and the statistic theory, which allows evaluating the approximation error, fails.

Using the definition of the knot positions allows to get along without addition ($a=0$). It should be used only in extreme cases. More particularly see Appendix F.

6.3 Writing of the new spline coefficients to the Database (Command "Write")

Data and evaluations changed in the course of operations may be written to the database. Before closing the graphic window verification is performed whether all the changes are written, i.e. a message is sent that changes will be lost upon the window closing.

There are the following commands:

- **Changed data**
- **New spline**
- **New evaluation**
- **Spline to a text file**

Each command is active only if there are changes in relevant data. If there are no changes command **Write** is unable. Therefore it is impossible to write spline from SaBa to a text file at this window having made no changes. To perform this action use the

window ***"Review and output of tables and plots"***. Format description for writing spline to a text file is given in the section ***"Output of spline coefficients (Command "AdditionalTables")"***.

6.4 Selection of the data presentation (Command "ViewData")

This menu command is active only in the processing of total cross-sections, since for their operations with the Legendre polynomial expansion the S-factor presentation is not used.

There are two forms of data representation:

- **S-factor** - representation in a form of astrophysical factor. All data are recalculated with regard to S-factor presentation. Energies are transformed in the system of center of mass.
- **Cross-section -** representation in a form of total cross-section.

Experimental data may be also edited in the form of S-factors. For going over to cross-sections the required recalculation will be performed automatically.

6.5 Assigning of the uncertainties (command "SetErrors")

After the evaluation is built evaluated errors can be defined for each set: systematic and statistic. The systematic error for each ***j*** set is defined as follows:

$$b^j = \frac{\sum_{i=1}^{n} y_i^j - S\left(x_i^j\right)}{n^j},$$

where x_i^j, y_i^j - points of data in amounts of n^j,

$S(x)$ - evaluation function.

Afterwards mean statistic error is defined for each set:

$$\varepsilon^j = \sqrt{\frac{\left(y_i^j - S\left(x_i^j\right) - b^j\right)^2}{n^j}}.$$

While performing evaluation a logarithmic scale was used for the function, and instead of values *y* their natural logarithms are used, and evaluation of errors are assumed as relative.

In many cases the evaluation results can be improved using as systematic errors and evaluation errors the values obtained.

To execute this operation a window with the table is displayed, where all sets are listed and obtained evaluation errors are given (in the column titled **"New"**), and those with which this evaluation was defined (the column is titled **"Previous"**). For each error the column exists titled **"Action"**, the cells of which can take one of the following meanings:

- **replace** - ***previous*** evaluation will be changed for a ***new one***,
- **don't alter** - the ***previous*** error is left,
- **correct** - cell with a ***new*** error becomes the editing window, where the existing value can be changed. The change should be completed by pressing **Enter** (otherwise there will be no a result). This changed value will replace the error.

Meaning of column **"Action"** is changed by clicking the mouse on the cell: the original **"change**" after first clicking will transform to **"don't alter"**, after second - to **"correct"**, and then again - to **"change"**.

6.6 Input of the new data from the file (Command "Input")

For input the dialogue will be proposed to choose the file of coefficients. If the file structure is correct the input will be accomplished without additional efforts, and the result will be displayed on the screen. Otherwise a message will be displayed in which file's line the error has been found, and the line itself.

After input the spline should be corrected.

The following commands are provided for data inputting by two ways:

- **Data -** input of a new set of experimental data. This input is described in section 5.1.3. While specifying a table title it is supposed that at the first line the author's names are given and at the second one there is a reference.
- **Spline** - input of coefficients of a new spline. This capability should be used only in case when there is a higher approximation performed outside SaBa, and it is required to use it. Only cubic splines can be input. Preliminary a file with spline coefficients in polynomial presentation should be prepared using the following format:

  - **1-st line** - three integers: *N* -a number of subsequent lines, *LX=0*, if there is a linear scale along *X*, and *=1*, if there is a logarithmic one. *LY* - the same for axis *Y*. These numbers should be delimited from each other only by spaces, no other delimiters are acceptable.
  - The **next *N* lines** - 6 numbers on each line delimited only by spaces, no other delimiters are acceptable. The first number - knot X_i, then 4 coefficients of polynomial A_0, A_1, A_2, A_3 over degrees $X - X_i$, and the last number - error of the spline in the knot. It should be noted that values of spline coefficients in the last line are inconsiderable (significant is only the location of the last knot and error in it), but in spite of it arbitrary numbers should present.

    For the logarithmic scale natural logarithms of true values should be set as knots along *X*.
  - For the logarithmic scale relative errors are set along *Y*.
  - Before inputting the spline for S-factor approximation the user should select the relevant representation (see **ViewData**).

7. CREATION OF THE ENDF FILE

Files are created in format ENDF-B/VI /4/ from all data referring to the indicated knot. Several files may exist, since for each isotope and every incident particle a separate file is created.

Writing process begins with opening the window **"Creation of the ENDF/B-VI file"** that includes control buttons and fields.

A dialogue panel is displayed where the selection in the group of switches titled **"Define the file location"** should be made. There are two possibilities:

- **Write to the existing file** – it hasn't been realized yet.
- **Create a new file**.

There are the following control buttons in the window:

- **Ok** - selection is considered executed after pressing button **OK**, afterwards this button is changed for **Retry**, which will allow repeating selection of the switch.
- **Close** - pressing this button will lead to refuse to create the ENDF file.
- **Help** - obtaining specific information on the program.
- **Execute** - is unable when opening the window.

After the selection is made the field **"The available data"** is displayed.

A list of all available reactions (in the selected knot) is displayed. With this list reactions are chosen, which should be written to the ENDF file. To achieve it use the line with the text ***"Write to the file"*** or ***"Don't write to the file"*** before description of each reaction. The text is changed upon clicking on the left button of the mouse. Reactions not included to the file will be dark in the list.

Having selected the reaction, button **Execute** should be pressed.

Afterwards, the beginning of the file will be displayed. It will be output to the window **"Editor of ENDF file"**.

Editor of ENDF file

A window **"Editor of ENDF file"** includes control buttons and a field where data presented in the ENDF format are displayed.

For each reaction a part of file will be output, corresponding to that reaction. In the displayed text changes could be made, but thoroughly, in order not to damage the ENDF file structure.

After the file formation is completed zero record of the file is displayed for verification. This record doesn't refer to the ENDF file structure and can be used for various identification goals.

The following buttons are available:

- **Ok -** write to the file. Writing procedure is performed only after viewing of the whole file content. The **OK** button should be pressed until the end of file is displayed. Exit from the window **"Editor of ENDF file"** is executed. A standard panel requiring the file name and the directory is displayed. File name suggested by SaBa is formed using the designation of isotope and incident particle.
- **Cancel -** cancels the work in the window **"Editor of ENDF file"** and provides for going over to a previous window.
- **Lab.Authors, reference -** is displayed only after opening the window **"Editor of ENDF file".** This button is used for special change of the ENDF title. A panel will be displayed with standard control buttons (**OK, Cancel, Help**) and fields, in which it is proposed to enter the following information:
  - **Laboratory** – laboratory, in which the work has been done. Corresponds to **ALAB** (see /2/, p.1.5). Not more than 11 symbols.
  - **Authors** – authors of the work. Corresponds to **AUTH** (see /2/, p.1.5). Not more than 33 symbols.
  - **Main reference** – corresponds to **REF** (see /2/, p.1.5). Not more than 21 symbol.

The introduced values are stored and will be used for creation of all subsequent files. Closing the panel by button **Cancel** will lead to restoration of all values existing earlier for all fields.

In the file title there are no references to works used for evaluation – there is only line REFERENCES – it shouldn't be taken into account since this piece of information will be filled in after processing of all reactions from the file.

If a set of reactions is not over the process of file creation is repeated.

CONCLUSION

The library of evaluated and experimental data on charged particles is intended, first of all, for scientists engaged in the activities related with nuclear data obtaining with regard to thermonuclear power, astrophysics, medicine, and etc. It may be also useful for researches studying physics of nucleus.

In the opinion of the developers this product can serve as a good basis for creation of specific applications. In particular, it is assumed that the evaluated data presented in this version should be added with calculations on nuclear physics models in order to extrapolate them into the area of low energies. It will allow obtaining values of velocities of nuclear reactions, which are important for astrophysical applications, and obtain a computerized presentation.

The developers of the library will be grateful to users for their remarks on the proposed product.

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APPENDIX A. Statistical Model

An approximation is made on the base of the statistical model proposed in /3/. According to this model a cross-section evaluation can be obtained by the sets of experimental data of various authors, the data may be shifted relative to each other. We propose a description of the model.

Assume that there are the data of $R \geq 1$ authors. The data of one author will be called a set of data. Assume that r-set contains n_r points $\{x_j^r, y_j^r, \sigma_j^{r2}\}$, $j = 1, 2, \ldots n_r$, where x_j^r - an independent variable (of energy), y_j^r - function (of a cross-section), σ_j^{r2} - dispersion of y_j^r (measurement error squared, further it will be called a statistic error). Except the statistic error there is a systematic error in measurements, it is accepted to be equal for all points and having zero mathematical expectation and known dispersion Σ_r^2.

The evaluation is sought for in the form of function $f(x,a)$, where a - parameters defined from the viewpoint of maximum of likelihood, i.e. giving the most probable evaluation curve.

The condition derivation for α is given in /3/, we won't present it and we'll only write out the final expression: parameters $\boldsymbol{a}$ should carry the minimum of the function

$$\Phi(a) = \frac{1}{2}\sum_{r=1}^{R}\left\{\sum_{j=1}^{n_r}\frac{\left(f(x_j^r,a)-y_j^r\right)^2}{\sigma_j^{r2}} - W_r\left(\sum_{j=1}^{n_r}\frac{f(x_j^r,a)-y_j^r}{\sigma_j^{r2}}\right)^2\right\},$$

where $W_r = \dfrac{\Sigma_r^2}{1+\sum_{j=1}^{n_r} 1/\sigma_j^{r2}}$. (1)

When using the model actually the difficulties appear dealing with presetting systematic error dispersions Σ_r^2, since they are not given by authors of experiment and their availability is usually revealed by comparison of the results of different authors. Despite all mentioned the use of the model is helpful when evaluating nuclear cross-sections and experimental results in general when they are obtained in various conditions and, hence, are shifted relative to each other. Values Σ_r^2 regulate the shift of data sets as regards the evaluation curve which is defined by statistic errors σ_j^{r2}. For example, let's assume that there are two sets of data. One of them consists of a great number of points measured with small statistic errors, but it contains a considerable systematic error and, therefore, it is shifted explicitly relative to the true values. In the second set there are few points having significant statistic errors, so, it is difficult to define the evaluation curve shape according to them. With the model one can simply obtain a curve with either a proper shape and disposed in a proper place presetting Σ^2 as zero for the second set and as a high value for the first one.

It should be noted that if all Σ^2 are zeroes then the model corresponds simply to a statistic model of the least squares method.

To realize the model it is important to choose the form of the evaluating function $f(x,a)$. We shall speak about it later and now we are presenting some more formulae independent on a specific type. As it will be seen further not all parameters a linearly appear in $f(x\ a)$, therefore, a method should be chosen for approximate search of the minimum. We shall use the Newton method. For this method we should to calculate the first and second

derivative functions $Q(a)$ over $a = \{a_s,\ s = 1, n\}$. Let's designate j point weight as $w_j^r = 1/\sigma_j^{r2}$ and $\Delta_j^r = f(x_j^r, a) - y_j^r$ - deviation of the given value from the evaluation function. We shall obtain:

$$\frac{\partial \Phi}{\partial a_k} = \sum_{r=1}^{R} \left\{ \sum_{j=1}^{n_r} \frac{\partial f(x_j^r, a)}{\partial a_k} \Delta_j^r - W_r \sum_{j=1}^{n_r} w_j^r \frac{\partial f(x_j^r, a)}{\partial a_k} \sum_{j=1}^{n_r} w_j^r \Delta_j^r \right\}, \tag{2}$$

$$\frac{\partial^2 \Phi}{\partial a_k \partial a_l} = \sum_{r=1}^{R} \left\{ \sum_{j=1}^{n_r} \left(\frac{\partial^2 f\left(x_j^r, a\right)}{\partial a_k \partial a_l} \Delta_j^r + \frac{\partial f\left(x_j^r, a\right)}{\partial a_k} \frac{\partial f\left(x_j^r, a\right)}{\partial a_l} \right) w_j^r - W_r \left(\sum_{j=1}^{n_r} \frac{\partial^2 f\left(x_j^r, a\right)}{\partial a_k \partial a_l} w_j^r \sum_{j=1}^{n_r} \Delta_j^r w_j^r + \sum_{j=1}^{n_r} \frac{\partial f\left(x_j^r, a\right)}{\partial a_k} w_j^r \sum_{j=1}^{n_r} \frac{\partial f\left(x_j^r, a\right)}{\partial a_l} w_j^r \right) \right\}. \tag{3}$$

APPENDIX B. Presentation of the Evaluation Function by Splines

As approximation function $f(x,a)$ splines are taken. In the most of the known approximation programs only cubic splines of defect 1 are used, i.e. piece-wise polynomial functions of third degree with continuous second derivative. At the same time it isn't difficult to extend the approximation space employing the splines of any order and arbitrary defect. For the neutron cross-section approximation the possibility of the use of another order could be useful for solving the approximation tasks requiring certain conditions. Most often such requirement is linearity or presentation by a quadratic parable, as well as in the cases when the continuity of more than two derivatives is demanded.

To the contrary, the use of the defect exceeding 1 may be rather useful since cross-sections change so sharply that they couldn't be presented as a very smooth function and one is to be satisfied only with the first derivative or only one function. A method for definition of knot positions given below allows specifying automatically the knots where the defect is to be increased. Let's introduce the following agreement:

> **further the defect means a value that is one unit less than the commonly accepted defect,** i.e. a usual "spline" possessing defect equal to 1 in our presentation is 0. This redesignation gives a convenience in writing down formula for the splines with various defects.

Actually, let's recall the basic presentation of the spline. Assume that $X = \{x_0 < x_1 < \ldots x_{n-1}, x_n\}$ - the spline grid. Let $l_i \geq 0,\ i = 1,\ldots n-1$ be the defects of the internal knots (for boundary knots x_0 and x_n the definition of the defect isn't applicable since out the $[x_0, x_n]$ the spline is not specified and, hence, we can't speak about the continuity of the derivatives in the knots). All the splines with such a set of defects form a linear space. The basis in it could be chosen by various methods but for calculations the most suitable is that with elements having the most limited carrier, i.e. each element isn't zero on a small number of intervals of the grid and is identically zero within the rest intervals.

Assume that the spline order is $p \geq 0$. We would like to remind the known designation:

$$f_+ = \begin{cases} f, & f \geq 0 \\ 0, & f < 0 \end{cases}$$

Then the spline having defect d (in our understanding) in knot x_i and identically equal to zero at $x \le x_i$ (we shall state that "the spline begins in x_i") and, additionally, with the minimal carrier is expressed with precision of a factor

$$B_{i,d} = \sum_{j=i+1}^{i+p+1-l} \frac{(x_j - x)_+^p}{(x_j - x_i)^d \prod_{s=i,\, s\neq j}^{i+p+1-d} (x_j - x_s)} \qquad (4)$$

To make sure that it is really the spline with necessary properties we are to verify that $B_{i,\,d}$ in point x_i is zero up to p–1–d derivative. We won't give a detailed proof since it is reduced to rather elementary but complicated algebraical transformations. We shall outline the way: at first we are to demonstrate the required smoothness in x_i for $d = 0$. It could be achieved by induction over p . After this the spline derivatives of any defect can be presented by suitable values of the spline of zero defect but with lower power.

To define the basis of the linear space one is to expand the original grid by p knots to the left and p to the right. The following knots will be obtained $x_{-p},...x_{-1}$ and x_{n+1}, ... x_{n+p}. Certain locations of these knots are insignificant since their changes will be compensated by changes of the factors before the basic splines in the approximation function. For definiteness we shall choose:

$x_{-p} - x_{-p+1} = x_{-p+1} - x_{-p+2} = ... = x_1 - x_0$,

$x_{n+1} - x_n = x_{n+2} - x_{n+1} = ... = x_n - x_{n-1}$.

The basis of the spline linear space under consideration consists of all $B_{i,d}$ for $i = -p$, ..., $n-1$ and for every i all d not higher than l_i should be taken. (For $i<0$ it is accepted $l_i = 0$). The linear independence of such a set of basic splines could be demonstrated from the fact that either carriers of different elements aren't included one in another, or in the initial knot there is a spline having non-zero derivative which couldn't be expressed through zero derivatives of the rest. The basis completeness, i.e. a possibility to present any spline with a preset set of defects in the form of decomposition by its elements can be obtained comparing the number of its elements and the dimension of given linear space which could be defined, for example, by subtracting a number of conditions of the function continuity and its derivatives from a number of coefficients of all polynomials with p-degree in all intervals of the grid.

We'd like to stress an important property that will be required further:

basis spline $B_{i,d}$ of defect d is obtained from basis spline $B_{i,d-1}$ of $d-1$ as a result of transition to the limit at $x_i \Rightarrow x_{i+1}$. In this case it should be considered that the spline begins with x_{i+1} and the first term in sum (4) disappears since the corresponding interval disappears, too.

Basing on this property conclusion is made in the process of the definition of the knot positions, it is the following: if the minimum of the efficiency function is at the merger of two knots then it is necessary to go over to a single spline knot with a greater defect.

Besides, this property will be employed to obtain a presentation of the basis spline not by powers $(x_j - x)_+$ as in (4) but by powers $(x - x_j)_+$. The necessity to have such a presentation will be revealed in the analysis of formula (4):

assume that $d = 0$. At x approaching x_i, $B_{i,d}$ as the spline of defect 0 and power p has order $(x - x_i)^p$, i.e. it is a small value which at the same time is to be expressed through a great number of terms of $(x_j - x)^p$ type being rather higher. As a result, $B_{i,d}$ near x_i is calculated with bad accuracy and working only with formula (4) it is possible to obtain actually not only a nonsmooth spline but also with explicit breaks. For $d>0$ the accuracy of presentation (4) is

somewhat higher since both order $(x - x_i)^{p-d}$ is lower and a number of terms is less but, nevertheless, it could be insufficient.

To avoid these obstacles one is to present the basis spline by powers $(x-x_j)_+$. One half of the spline can be calculated by this presentation, another - by formula (4).

For $d = 0$ formula (4) will have the form:

$$B_{i,0} = \sum_{j=i}^{i+p} \frac{(x - x_j)_+^p}{\prod_{s=i, s\neq j}^{i+p+1} (x_s - x_j)} \tag{5}$$

and this conversion possesses good accuracy in the vicinity of x_i and, subsequently, a bad one in the vicinity of x_{i+p+1}.

It is not so simple to obtain the expressions with nonzero defect from (4) since they are to contain powers $(x-x_i)_+$ less than p, and such powers are absent in (4). Therefore, we shall employ the property mentioned above and seek for the limits of expression (5) at $x_i \Rightarrow x_{i+1}$, as well as limiting expressions.

The limits mentioned were calculated and the following formula was obtained:

$$B_{i,d} = \sum_{q=0}^{d} (-1)^q C_p^{d-q} \frac{(x - x_i)_+^{p-d+q}}{\prod_{j=i+1}^{i+p-d+1} (x_j - x_i)} \sum_{j_1=i+1}^{i+p-d+1} \frac{1}{x_{j_1} - x_i} \sum_{j_2=j_1}^{i+p-d+1} \frac{1}{x_{j_2} - x_i} \cdots$$

$$\sum_{j_l=j_{l-1}}^{i+p-d+1} \frac{1}{x_{j_l} - x_i} + \sum_{j=i+1}^{i+p-d+1} \frac{(x - x_j)_+^p}{(x_i - x_j)^l \prod_{q=i, q\neq j}^{i+d-l+1} (x_q - x_j)}, \tag{6}$$

where C_p^{l-q} - binomial coefficients.

To prove (6) giving actually the values of the limits required we are introducing the functions:

$S_m^{(n)}(a_1, \ldots a_n)$ = sum of single terms from a_i with power m and

$T_m^{(n)}(a_1, \ldots a_n)$ = sum of all terms from a_i with power m where every a_i enters in with power not exceeding 1.

$B_{i,d}$ is expressed through function $S_m^{(n)}$ in the following way:

$$B_{i,d} = \sum_{q=0}^{d} (-1)^q C_p^{d-q} \frac{(x - x_i)_+^{i+p+q-d}}{\prod_{j=i}^{i+p-d+1} (x_j - x_i)} S_q^{(p-d+1)}\left(\frac{1}{x_{i+1} - x_i}, \ldots \frac{1}{x_{i+p-d+1} - x_i}\right) +$$

$$\sum_{j=i+1}^{i+p-d+1} \frac{(x - x_j)_+^p}{(x_i - x_j) \prod_{q=i, q\neq j}^{i+p-d+1} (x_q - x_j)}$$

The relations are obvious:

$$S_m^{(n+1)}(a_1, \ldots a_n, a_{n+1}) = S_m^{(n)}(a_1, \ldots a_n) + a_{n+1} S_{m-1}^{(n+1)}(a_1, \ldots a_n, a_{n+1})$$

$$T_m^{(n+1)}(a_1, \ldots a_n, a_{n+1}) = T_m^{(n)}(a_1, \ldots a_n) + a_{n+1} T_{m-1}^{(n)}(a_1, \ldots a_n). \tag{7}$$

Using them the following relation could be proved with the induction by n :

$S_m^{(n)} - S_{m-1}^{(n)} T_1^{(n)} + S_{m-2}^{(n)} T_2^{(n)} - \ldots (-1)^m T_m^{(n)} = 0,$

then with the help of it and the L'Hospital rule transition from $B_{i,d}$ to $B_{i,d+1}$ can be obtained.

Expression (6) is seemed to be complicated but it can be calculated rather efficiently since all coefficients may be calculated beforehand (analogously as for (4)), therefore, the speed of the spline calculation will not suffer from the more complicated form of the basis spline. To calculate coefficient relation (7) can be employed. If the programming language is used accepting the recursing, then the coefficient calculation program will be very simple.

APPENDIX C. Linear Task

In the task it is assumed that a fixed grid of the spline is given with mentioning the defect in every knot, the basis of the spline space $\{B_i, i=1, \ldots m\}$ is built and coefficients of the spline decomposition are being sought for

$$f(x,a) = \sum_{i=1}^{m} a_i B_i(x) \qquad (8)$$

with this basis satisfying the condition of minimum (1). In decomposition (8) the basis splines are enumerated by a common index without indicating an initial point of the grid and defect, since a certain form of the basis spline in the consideration given is insignificant.

The task is solved simply: the derivatives over parameters a_i (see (2)) are equated with zero and the linear system is obtained:

$$\sum_{i=1}^{m} a_i \left(\sum_{r=1}^{R} T_{rik} - W_r S_{ri} S_{rk} \right) = \sum_{r=1}^{R} \sum_{j=1}^{n_r} y_j^r w_j^r \left(B_k\left(x_j^r\right) - W_r S_{rk} \right), k = 1,\ldots m$$
$$\text{where} \quad T_{rik} = \sum_{j=1}^{n_r} w_j^r B_i\left(x_j^r\right) B_k\left(x_j^r\right), \quad S_{ri} = \sum_{j=1}^{n_r} w_j^r B_i\left(x_j^r\right). \qquad (9)$$

The matrix of system (9) is symmetrical and defined positively. The positive definition is determined by the way of its obtaining by the maximum likelihood method. Actually, the definiteness isn't always obtained since when a number of parameters exceeds a number of assigned points the system will degenerate, i.e. the matrix is semidefined positively. Although, solution could be always found out when applying a somewhat complicated method of Cholesky wherein for the next decomposition step the line with the maximum diagonal element is selected. On the one hand, this choice improves the solution accuracy, on the other hand, it allows to seek for some solution in the case of degeneration. The latter takes place unless the greatest diagonal element is not more than zero. From theoretically known semidefiniteness and necessity of existing at least one solution it follows that the rest composed matrix part is merely zero, although, in the process of calculations it could happen otherwise (due to rounding-off errors). Therefore, any values (in the program zeroes are assigned) can be assigned to corresponding unknown terms with the rest expressed through them and, finally, the spline will be obtained giving one of the minimum values (1). (From the properties of quadratic function it's obvious that all its minimal values are, actually, equal to each other).

For the linear case some more tasks of interest could be solved additionally to the main one, namely building approximation.

APPENDIX D. Nonlinear Task

When solving the linear task it was assumed that the spline knot positions were preset, it proceeded from some considerations. At the same time in the most cases there are no any "considerations" and the spline knots are selected intuitively. A lot of examples could be introduced when the knot positions seemed to be suitable lead to the results far from good. Therefore, the most reasonable way is the knot inclusion in the number of parameters over which the minimization (1) is conducted. The only difficulty is nonlinearity of the task appeared, however it may be overcome.

For solution we shall employ the Newton method which demands the derivative calculations. The Newton method will be used only for nonlinear parameters. A set of parameters ***a*** in (1) will be divided in two sets ***a1*** - the spline coefficients with minimization already considered and ***a2*** - the spline knots. Then the nonlinear task formulation will be the following: find out the minimum by ***a2*** for function $\Phi_1(a2)$, defined as $\Phi_1(a2) = \min_{a1} \Phi(a)$.

Partial derivatives Φ_1 can be expressed through those Φ, with regard to $\frac{\partial \Phi}{\partial a1} = 0$. Let's write out them in details denoting the nonlinear parameters (the knots) through x and linear ones, as earlier, through a.

$$\frac{\partial \Phi_1}{\partial x_l} = \frac{\partial \Phi}{\partial x_l} + \sum_i \frac{\partial \Phi}{\partial a_i}\frac{\partial a_i}{\partial x_l} = \frac{\partial \Phi}{\partial x_l} \tag{10}$$

$$\frac{\partial^2 \Phi_1}{\partial x_l \partial x_k} = \frac{\partial^2 \Phi}{\partial x_l \partial x_k} + \sum_i \frac{\partial^2 \Phi}{\partial x_l \partial a_i}\frac{\partial a_i}{\partial x_k} + \sum_i \frac{\partial^2 \Phi}{\partial x_k \partial a_i}\frac{\partial a_i}{\partial x_l} + \sum_{i,j} \frac{\partial^2 \Phi}{\partial a_i \partial a_j}\frac{\partial a_i}{\partial x_l}\frac{\partial a_j}{\partial x_k} \tag{11}$$

Differentiating equality $\frac{\partial \Phi}{\partial a_i} = 0$ over x_k we shall obtain relations

$$\frac{\partial^2 \Phi}{\partial a_i \partial x_k} + \sum_j \frac{\partial^2 \Phi}{\partial a_i \partial a_j}\frac{\partial a_j}{\partial x_k} = 0$$

showing that the two latest terms in (11) give zero. Equations for calculation of $\frac{\partial a_i}{\partial x_k}$ was derived from the last equation. Substituting it in (11) one get the expression for second derivatives Φ_1 written for convenience in the matrix form: $H_1 = H - X^T A^{-1} X$

where $H_1 = \left(\frac{\partial^2 \Phi_1}{\partial x_i \partial x_j} \right)$,

$H = \left(\frac{\partial^2 \Phi}{\partial x_i \partial x_j} \right)$,

$$X = \left(\frac{\partial^2 \Phi_1}{\partial a_i \partial x_j} \right),$$

$$A = \left(\frac{\partial^2 \Phi_1}{\partial a_i \partial a_j} \right).$$

A coincides with the matrix for linear task (9) and the reverse one is found in the process of the task solution. Thus, it is clear that in the case of the linear task degeneration the nonlinear task can't be solved.

The formulae for derivatives $\Phi(\boldsymbol{a})$ are presented above, it remains only to deduce those for partial basis spline derivatives. To simplify the expression the "local" numeration will be introduced for the spline knots when the initial knot of the basis spline under consideration will obtain number 0. It is assumed that all summations in the formulae given below without indicating the upper limit are carried out over all spline knots contained in its carrier, except those contradicting the condition written down under the sum sign. We shall also assume that $p > 0$.

Let's introduce preliminary two values:

$$S_{1k} = \sum_{i \neq k} \frac{1}{x_i - x_k} \text{ and } S_{2k} = \sum_{i \neq k} \frac{1}{(x_i - x_k)^2}.$$

At first, we are considering expression (4). It is written down in the form $B = \sum_i L_i P_i$,

where $P_i = (x_i - x)_+^p$, L_i - coefficient defined in (4).

Partial derivatives will be calculated in the following way:

$$\frac{\partial B}{\partial x_k} = \sum_{i \neq k} P_i \frac{\partial L_i}{\partial x_k} + P_k L_k \left(\frac{p}{x_k - x} + S_{1k} - \frac{d}{x_k - x_0} \right). \qquad (12)$$

The case with $k = 0$ isn't selected, although there could have happened the division by $x_0 - x_0$. But P_0 is zero at the whole basis spline carrier, therefore, it is assumed that this term will not be calculated. The similar situation will take place in further formulae and won't be explained. It should be also reminded that *d* is the basis spline defect.

$$\frac{\partial L_i}{\partial x_0} = L_i \frac{d+1}{x_i - x_0},$$

$$\frac{\partial L_k}{\partial x_k} = L_k \left(S_{1k} - \frac{d}{x_k - x_0} \right),$$

$$\frac{\partial L_i}{\partial x_k} = \frac{L_i}{x_i - x_k} \text{ in all the rest cases.}$$

To calculate second derivatives there are several formulae depending on the knot number relations over which differentiation is conducted:

$$\frac{\partial^2 B}{\partial x_0} = (d+1)(d+2) \sum_i \frac{P_i L_i}{(x_i - x_0)^2}, \qquad (13)$$

$$\frac{\partial^2 B}{\partial x_0 \partial x_k} = \sum_{i \neq k} \frac{P_i L_i}{(x_i - x_0)(x_i - x_k)} + \frac{P_k L_k}{x_k - x_0} \left(\frac{p}{x_k - x} + S_{1k} - \frac{d+1}{x_k - x_0} \right), \qquad (14)$$

$$\frac{\partial^2 B}{\partial x_k} = 2\sum_{i\neq k}\frac{P_i L_i}{(x_i - x_k)^2} + P_k L_k\left(\frac{p}{x_k - x}\left(\frac{p}{x_k - x} + 2S_{1k} - \frac{2d}{x_k - x_0}\right) + \right.$$
$$\left. + \frac{d}{x_k - x_0}\left(\frac{d+1}{x_k - x_0} - 2S_{1k}\right) + S_{2k} + S_{1k}^2\right), \qquad (15)$$

$$\frac{\partial^2 B}{\partial x_k \partial x_l} = \sum_{i\neq k, i\neq l}\frac{P_i L_i}{(x_i - x_k)(x_i - x_l)} +$$
$$+ \frac{P_l L_l}{x_l - x_k}\left(\frac{p}{x_l - x} + S_{1l} - \frac{d}{x_l - x_0} - \frac{1}{x_l - x_k}\right) + \qquad (16)$$
$$+ \frac{P_k L_k}{x_k - x_l}\left(\frac{p}{x_k - x} + S_{1k} - \frac{d}{x_k - x_0} - \frac{1}{x_k - x_l}\right).$$

To express the basis spline by (6) more complicated formulae were obtained. Let's present (6) in the form

$$B = \sum_{j=0}^{d} D_j \frac{P_0}{(x - x_0)^{d-j}} + \sum_{i>0} L_i P_i,$$

where $P_i = (x - x_i)_+^p$,

D_j and L_i - coefficients defined in (6).

D_j will be expressed in the form

$$D_j = G_j S_j^{(p-d+1)}\left(\frac{1}{x_1 - x_0}, \ldots \frac{1}{x_{p-d+1} - x_0}\right),$$

where $S_j^{(p-d+1)}$ - function specified in Appendix B.

Derivatives are calculated by formulae:

$$\frac{\partial B}{\partial x_0} = \sum_{j=0}^{d}\frac{P_0}{(x - x_0)^{d-j}}\left(\frac{\partial D_j}{\partial x_0} - \frac{p - d + j}{x - x_0}\right) + (d+1)\sum_{i>0}\frac{P_i L_i}{x_i - x_0}, \qquad (17)$$

$$\frac{\partial D_j}{\partial x_O} = G_i R_O(j,1) = D_j S_{1O},$$

where R_0 is calculated by the recurrent formula:

$R_0(j,m) = \sum_{i\geq m}\left\{\frac{T(j-1,i)}{(x_i - x_0)^2} + \frac{R(j-1,i)}{x_i - x_0}\right\}$ being the derivative over x_0 of the function $S_j^{(p-d+1)}$ calculated, in turn, by the recurrent relation:

$$T(j,m)=\sum_{i\ge m}\frac{T(j-1,i)}{x_i-x_0},$$
$$T(0,m)=1,$$
$$R_0(0,m)=0.$$

The $S_j^{(p-d+1)}$ is equal to $T(j, 1)$.

$$\frac{\partial^2 B}{\partial x_0^2}=\sum_{j=0}^{d}\frac{P_0}{(x-x_0)^{d-j}}\left(\frac{(p-d+j)(p-d+j-1)}{(x-x_0)^2}D_j-2\frac{p-d+j}{x-x_0}\frac{\partial D_j}{\partial x_0}+\frac{\partial^2 D_j}{\partial x_0^2}\right)+ \tag{18}$$
$$+(d+1)(d+2)\sum_{i>0}\frac{P_iL_i}{(x_i-x_0)^2}$$
$$\frac{\partial^2 D_j}{\partial x_0}=G_iS_1R_0(j,1)+G_iR_{02}(j,1)+\frac{\partial D_j}{\partial x_0}S_{10}+D_jS_{20},$$

where R_{02} is recurrently calculated by the relation :

$$R_{02}(j,m)=\sum_{i\le m}\left\{\frac{2T(j-1,i)}{(x-x_0)^3}+\frac{2R_1(j-1,i)}{(x-x_0)^2}+\frac{R_{02}(j-1,i)}{x-x_0}\right\},$$
$$R_{02}(0,m)=0$$

and serves for the second derivative calculation over x_0 from $S_j^{(p-d+1)}$.

Further it will be assumed that $k\neq l$ is more than zero.

$$\frac{\partial B}{\partial x_k}=\sum_{j=0}^{d}\frac{P_0}{(x-x_0)^{d-j}}\frac{\partial D_j}{\partial x_k}+\sum_{i>0,i\neq k}\frac{P_iL_i}{x_i-x_k}+ \tag{19}$$
$$+P_kL_k\left(\frac{d}{x_0-x_k}+S_{1k}-\frac{p}{x-x_k}\right),$$
$$\frac{\partial D_j}{\partial x_k}=G_jK(j,1,k)-\frac{D_j}{x_k-x_0},$$

where K is defined by the recurrent relation

$$K(j,m,k)=\sum_{i\ge m}\frac{K(j-1,i,k)}{x_i-x_0}-\underbrace{\frac{T(j-1,k)}{(x_k-x_0)^2}}_{k\ge m}$$

and serves to calculate the first derivative over x_k for function $S_j^{(p-d+1)}$. The condition under the second term means that it is added only under the condition observation.

$$\frac{\partial^2 B}{\partial x_k^2}=\sum_{j=0}^{d}\frac{P_0}{(x-x_0)^{d-j}}\frac{\partial^2 D_j}{\partial x_k^2}+2\sum_{i>0,i\neq k}\frac{P_iL_i}{(x_i-x_k)^2}+ \tag{20}$$
$$P_kL_k\left(\frac{d(d+1)}{(x_0-x_k)^2}+S_{1k}^2+\frac{p(p-1)}{(x-x_k)^2}+S_{2k}+\frac{2d}{x_0-x_k}\left(S_{1k}-\frac{p}{x-x_k}\right)-\frac{2pS_{1k}}{x-x_k}\right),$$

$$\frac{\partial^2 D_j}{\partial x_k^2} = G_j\left(U(j,1,k) - \frac{K(j,1,k)}{x_k - x_0}\right) - \frac{1}{x_k - x_0}\frac{\partial D_j}{\partial x_k} + \frac{D_j}{(x_k - x_0)^2},$$

where U is defined by the recurrent relation

$$U(j,m,k) = \sum_{i \geq m} \frac{U(j-1,i,k)}{x_i - x_0} + \underbrace{\frac{2T(j-1,k)}{(x_k - x_0)^3} - \frac{2K(j-1,k,k)}{(x_k - x_0)^2}}_{k \geq m}$$

and is used to calculate the second derivative over x_k for function $S_j^{(p-d+1)}$.

$$\begin{aligned}\frac{\partial^2 B}{\partial x_0 \partial x_k} &= \sum_{j=0}^{d} \frac{P_0}{(x - x_0)^{d-i}}\left(\frac{\partial^2 D_j}{\partial x_0 \partial x_k} - \frac{p - d + j}{x - x_0}\frac{\partial D_j}{\partial x_k}\right) + \\ &+ (d+1)\sum_{i>0, i \neq k} \frac{P_i L_i}{(x_i - x_0)(x_i - x_k)} + \frac{P_k L_k}{x_k - x_0}\left(\frac{p}{x - x_k} + \frac{1}{x_k - x_0}\right),\end{aligned} \tag{21}$$

$$\frac{\partial^2 D_j}{\partial x_0 \partial x_k} = G_j\left(S_{10}K(j,1,k) + V(j,1,k)\right) - \frac{1}{x_k - x_0}\frac{\partial D_j}{\partial x_0} - \frac{D_j}{(x_k - x_0)^2},$$

where V is defined by the recurrent relation:

$$\begin{aligned}V(j,m,k) = &\sum_{i \geq m}\left\{\frac{K(j-1,i,k)}{(x_i - x_0)^2} + \frac{V(j-1,m,k)}{x_i - x_0}\right\} - \\ &\underbrace{-\frac{2T(j-1,k)}{(x_k - x_0)^3} - \frac{R_0(j-1,k)}{(x_k - x_0)^2}}_{k \geq m}\end{aligned}$$

and is used to calculate the mixed derivative over x_0 and x_k for function $S_j^{(p-d+1)}$.

$$\begin{aligned}\frac{\partial^2 B}{\partial x_k \partial x_l} = &\sum_{j=0}^{d} \frac{P_0}{(x - x_0)^{d-j}}\frac{\partial^2 D_j}{\partial x_k \partial x_l} + \sum_{\substack{i>0 \\ i \neq k \\ i \neq l}} \frac{P_i L_i}{(x_i - x_k)(x_i - x_l)} + \\ &+ \frac{P_l L_l}{x_l - x_k}\left(S_{1l} + \frac{d}{x_0 - x_l} - \frac{1}{x_l - x_k} - \frac{p}{x - x_l}\right) + \\ &+ \frac{P_k L_k}{x_k - x_l}\left(S_{1k} + \frac{d}{x_0 - x_k} - \frac{1}{x_k - x_l} - \frac{p}{x - x_k}\right)\end{aligned} \tag{22}$$

where W is defined by the recurrent relation:

$$W(j,m,k,l) = \sum_{i \geq m} \frac{W(j-1,i,k,l)}{x_i - x_0} - \underbrace{\frac{K(j-1,k,l)}{(x_k - x_0)^2}}_{m \leq k} - \underbrace{\frac{K(j-1,l,k)}{(x_l - x_0)^2}}_{m \leq l}$$

and is used to calculate the mixed derivative over x_k and x_l for function $S_j^{(p-d+1)}$. In the case of nonlinear task only an approximation is carried out.

To specify the error of the approximation built it is necessary after the definition of the knot positions to build the spline with these fixed knots and to define the error. Thus, in the approximation error the knot specification inaccuracy will not be taken into account. Most likely its contribution is insignificant as compared to that of spline coefficient errors. Actually, having preset any (except very degenerated) knot positions and defined with them the coefficients, we shall obtain the approximation looking like the truth. While presetting arbitrary coefficients we would certainly obtain nothing reasonable, no matter how the knots were selected. Besides, the problem arises: if we were satisfied with the spline error evaluation with the knots fixed and given basing on some considerations then why it became worse under the optimized knots?

Boundary conditions also can't be given since the task obtained will be too complicated and the conditions will become nonlinear, because they contain the spline knot values. It is not obligatory to solve this task for practice. In reasonable tasks the boundary conditions should correspond to experimental points and are set only to improve the accuracy. Therefore, when defining the knot positions without giving the conditions one can look forward to the situation that the subsequent transfer to the spline building with the fixed knots and conditions will not cause a considerable change of the spline.

APPENDIX E. Covariance matrix for spline coefficients

If the matrix of system (9) isn't degenerated then the covariance matrix for coefficients $cov(a_i, a_j)$ can be found out with subsequent definition of dispersion for the approximation built in any point x

$$\sigma^2 f(x) = \sum_{i=1}^{m} \sum_{j=1}^{m} cov(a_i, a_j) B_i(x) B_j(x). \qquad (23)$$

It is known that for the common method of the least squares the covariance matrix coincides with the reverse matrix for the usual set of equations. Let's show that for the given statistical model the same relation is valid.

At first we shall find out the condition for which the linear system matrix should satisfy to in order the reverse one would coincide with the covariance matrix for coefficients. The general linear system for coefficient $\boldsymbol{a}$ definition along observation vector $\boldsymbol{y}$ may be written as

$$A\boldsymbol{a} = B\boldsymbol{y},$$

where A - the system matrix,

B - matrix by which free system terms are expressed through the observation vector.

It follows $\boldsymbol{a} = A^{-1} B\boldsymbol{y}$. (24)

Let's designate covariance matrix $\boldsymbol{a}$ through C_a, covariance matrix $\boldsymbol{y}$ through C_y . Since covariance is bilinear function from (24) it follows:

$C_a = A^{-1} B\, C_y\, (A^{-1} B)^T = A^{-1} B\, C_y\, B^T\, (A^{-1})^T$, (25)

where symbol T means transposition. Since matrix (9) is symmetrical this symbol in A will be omitted further.

As desired, $C_a = A^{-1}$,therefore, from (25) it follows:

$A = B\, C_y\, B^T$. (26)

This condition is required and sufficient since all transformations from (24) to (26) are reversible and can be done in the reverse order.

Thus, we are to define preliminary the covariance matrix for observation vector. Any observation y_i^r is presented in the form

$$y_i^r = M\, y_i^r + \varepsilon_i^r + b_r,$$

where symbol M is the expectation, ε_i^r and b_r - random values with zero expectation and dispersions, subsequently, σ_j^{r2} and Σ_r^2. Therefore, we obtain

$$cov(y_i^r, y_i^r) = \sigma_j^{r2} + \Sigma_r^2,$$
$$cov(y_i^r, y_j^r) = \Sigma_r^2, \text{ if } i \neq j,$$
$$cov(y_i^r, y_j^s) = 0, \text{ if } r \neq s.$$

Now (i, j) element for composition $B\, C_y\, B^T$ is calculated:

$$P_{ij} = \sum_{r=1}^{R}\sum_{l=1}^{n_r}\sum_{s=1}^{R}\sum_{k=1}^{n_s} cov\left(y_l^r, y_k^s\right) b_{il}^r b_{jk}^s = \sum_{r=1}^{R}\sum_{l=1}^{n_r}\sum_{k=1}^{n_r} cov\left(y_l^r, y_k^r\right) b_{il}^r b_{jk}^r =$$
$$= \sum_{r=1}^{R}\left(\sum_{l=1}^{n_r}\left(\sigma_l^{r2} + \Sigma_r^2\right) b_{il}^r b_{jl}^r + \Sigma_r^2 \sum_{k\neq l}^{n_r} b_{il}^r b_{jk}^r \right) =$$
$$= \sum_{r=1}^{R}\left(\sum_{l=1}^{n_r} \sigma_l^{r2} b_{il}^r b_{jl}^r + \Sigma_r^2 \sum_{k=1}^{n_r}\sum_{l=1}^{n_r} b_{il}^r b_{jk}^r \right)$$

since the elements from matrix A are also the sums over the set number we shall compare only the sum components, index r is omitted:

$$\sum_{l=1}^{n} \sigma_l^2 b_{il} b_{jl} = \sum_{l=1}^{n} \sigma_l^2 \frac{B_i(x_l) - WS_i}{\sigma_l^2} \frac{B_j(x_l) - WS_j}{\sigma_l^2} =$$
$$= \sum_{l=1}^{n} \frac{B_i(x_l) B_j(x_l)}{\sigma_l^2} - 2WS_iS_j + W^2 S_i S_j \sum_{l=1}^{n} 1/\sigma_l^2 =$$
$$= \sum_{l=1}^{n} \frac{B_i(x_l) B_j(x_l)}{\sigma_l^2} - WS_iS_j - S_iS_j \frac{W^2}{\Sigma^2},$$

since $S_i = \sum_{l=1}^{n} \frac{B_i(x_l)}{\sigma_l^2}$, and $W = \frac{\Sigma^2}{1 + \Sigma^2 \sum_{l=1}^{n} 1/\sigma_l^2}$.

Then

$$\Sigma^2 \sum_{l=1}^{n} b_{il} \sum_{k=1}^{n} b_{jk} = \Sigma^2 \sum_{l=1}^{n} \frac{B_i(x_l) - WS_i}{\sigma_l^2} \sum_{k=1}^{n} \frac{B_j(x_k) - WS_j}{\sigma_k^2} =$$
$$= \Sigma^2 S_i S_j \frac{W^2}{\Sigma^4} = S_i S_j \frac{W^2}{\Sigma^2}.$$

Comparison with (9) demonstrates that condition (26) is really fulfilled and the reverse matrix for the set of equations to define the spline coefficients gives the covariance matrix for these coefficients.

The reverse matrix is obtained in the process of the system solution by the Cholesky method. For the degenerated matrix it's not specified and in this case it's impossible to calculate the approximation error because in this case the coefficients are not simply defined.

APPENDIX F. Boundary Conditions

The linear task is easy to solve analytically also additionally taking into account any linear conditions. In program Saba these conditions are realized for only one significant case: setting conditions on the spline boundaries requiring that the approximating function and/or its derivative will be equal to the values given. For the convenience of application the condition setting is accepted not precisely on the boundaries of the spline specification region, i.e. in the grid points x_0 and/or x_n but also close to these points. "Close" has the following meaning: let's designate as x_l the point in which the condition is valid on the left and as x_r - on the right. These points should satisfy inequalities:

$$x_{-p} < x_l \le x_1,$$
$$x_{n-1} < x_r \le x_{n+p}.$$

There are no difficulties in solving the task with linear conditions except the question: is it possible to define the error of the approximation built? We assume that along with the function values and/or their derivatives their errors (mean square deviation) are also preset. The evaluation curve even if accurately passing through the preset values will possess the definite error.

It is suggested that the preset values are statistically independent. In most cases it will be not quite so, for example, if the function and its derivatives are calculated according to the expression with coefficients containing the statistical error. Then the correlation coefficient between the function and derivative will be almost obligatory not zero. For the algorithm described below the independence of the preset values is insignificant, we could also have demanded to preset the total covariance matrix for them, but will the user be eager to calculate and preset it? Therefore, a simplified formulation of the task was excepted, moreover, the experience shows the preset derivative error doesn't influence considerably the evaluation function error.

The main task is solved by successive exclusion of variables expressed in accordance with conditions from function (1). Simultaneously the system covariance matrix is transformed, correspondingly. It is sufficient to define the covariance matrix for coefficients being the task solution. Actually, assume that $\boldsymbol{a}$ is found out as solution of system $A\boldsymbol{a} = \boldsymbol{b}$ i.e. $\boldsymbol{a} = A^{-1}\boldsymbol{b}$. Then the matrix with covariance C_a is related with matrix C_b by the expression

$$C_a = A^{-1}C_b(A^{-1})^T. \qquad (27)$$

The original (without any exclusions) matrix C_b is known - according to all described in the previous section and relation $\boldsymbol{b} = A\boldsymbol{a}$ it is matrix A .

Let's describe the algorithm by steps.

1) Preset conditions are transformed to a three-angular form.

Let them originally have the form

$$\begin{aligned} &\lambda_{11}a_1 + \lambda_{12}a_2 + \ldots + \lambda_{1m}a_m = d_1 \\ &\ldots \quad \ldots \quad \ldots \\ &\lambda_{k1}a_1 + \lambda_{k2}a_2 + \ldots + \lambda_{km}a_m = d_k \end{aligned} \qquad (28)$$

Coefficients λ_{ij} - the basis splines values and their derivatives in the points with presetting conditions which combinations provide fulfillment of tasks; d_i - the preset values.

The basis spline numeration is selected so that the principal minor with order k from system (28) will not be degenerated. Additionally, if conditions are preset at the both spline ends they shouldn't meet, i.e. they won't contain nonzero coefficients λ_{ij} with the same j . (It should be reminded that the basis splines have the minimal carrier, therefore the most coefficients in (28) are zeroes). This condition is accepted to simplify the exclusion algorithm. It doesn't impose high limitations, for example, it is sufficient that the spline grid should contain not less than p internal knots.

At the present stage principal minor (28) leads to a three-angular form with the values *1* on the main diagonal. Simultaneously covariance matrix $cov(d_i, d_j)$ originally given as the diagonal matrix with the dispersion values on the diagonal is exposed to corresponding transformations.

Assume that transformation is accomplished by l line. It is performed in two phases. At first l line divides in λ_{ll}(it is obvious that coefficients λ differ from those specified in (28) since the matrix is imposed to transformation but for simplicity it shouldn't be noted). Then d_l is transformed to $d_l' = d_l/\lambda_{ll}$ and the matrix obtains the form

$$cov(d_s, d_i') = cov(d_s, d_i)/\lambda_{ll},\ s = 1,...k$$
$$cov(d_l', d_s) = cov(d_l, d_s)/\lambda_{ll},\ s = 1, ..., k.$$

During the second phase the lines with numbers greater than l are transformed

$$d_t' = d_t - \lambda_{tl}d_l,\ t = l+1, ..., k.$$

In this case the covariance matrix is transformed by formulae

$$cov(d_s, d_t') = cov(d_s, d_t) - \lambda_{ts}cov(d_s, d_l),\ s = 1, ..., k,$$
$$cov(d_t', d_s) = cov(d_t, d_s) - \lambda_{ts}cov(d_l, d_s),\ s = 1, ..., k.$$

Matrixes are transformed just in the order they are written, therefore, they lead to a correct result and it may be verified.

2) Unknown value exclusions.

To obtain the covariance matrix there will be required matrix $cov(d_i, b_j)$ initially being zero since it is agreed that boundary conditions and free terms of system (9) specified only in observations are statistically independent. In the process of unknown value exclusions this matrix is also transformed.

With i step of exclusion when the relation is used

$$a_i = d_i - \lambda_{ii+1}a_{i+1} - ... - \lambda_{ii+1}a_k,$$

obtained from boundary conditions at the first phase the system matrix is transformed by formula

$$A_{ql}' = A_{ql} - \lambda_{il}s_q - \lambda_{iq}A_{il},$$

and free term by formula

$$b_q' = b_q - \lambda_{iq}b_i - d_is_q \quad \text{for } q, l > i.$$

In this case covariance matrixes are transformed by formulae:

at first

$$cov(b_q', b_l') = cov(b_q, b_l) - \lambda_{iq}cov(b_i, b_l) - \lambda_{il}cov(b_i, b_q) +$$
$$+ \lambda_{il}\lambda_{iq}cov(b_i, b_i) + s_qs_lcov(d_i, d_i) - s_qcov(d_i, b_l) - s_lcov(d_i, b_q) +$$
$$+ (s_q\lambda_{il} + s_l\lambda_{iq})cov(d_i, b_i), \qquad \text{for } l > i,$$

then

$$cov(d_s, b_q') = cov(d_s, b_q) - \lambda_{sq}cov(d_s, b_i) - s_qcov(d_s, d_i), \text{ for } q = 1, ... k,$$

where $s_q = A_{iq} - A_{ii}\lambda_{iq}$,

$s_l = A_{il} - A_{ii}\lambda_{il}.$.

After the second phase competition the task solution can be reproduced as solution of the linear system of the following form

$$\begin{pmatrix} U & P \\ 0 & A \end{pmatrix}\begin{pmatrix} a_{i\le k} \\ a_{i>k} \end{pmatrix}=\begin{pmatrix} d \\ b \end{pmatrix},$$

where U - upper three-angular matrix obtained at the first transformation phase,

P - matrix expressing the first k coefficients through others obtained at the first phase,

A - symmetrical matrix semidefined positively obtained at the first phase,

d - vector obtained when transforming conditions at the first phase,

b - free term vector obtained at the second transformation phase ,

moreover, the covariance matrix for the total vector $\begin{pmatrix} d \\ b \end{pmatrix}$ is known.

Then system $(A)(a_{i>k})=(b)$ is solved by a common method, i.e. by the Cholesky method, in the process reverse matrix A^{-1} is defined. Reverse matrix U is found out trivially, so, we also obtain the reverse matrix for the whole task in the form

$$\begin{pmatrix} U^{-1} & -U^{-1}PA^{-1} \\ 0 & A^{-1} \end{pmatrix},$$

after this using relation (27) the covariance matrix for coefficients is specified.

Appendix G. Spline with Regularization

In our task regularization means that the efficiency function is added with

$$\Delta\Phi(a)=\alpha\int_{x_0}^{x_n}\left(f^{(p-1)}(x,a)\right)^2 dx. \qquad (29)$$

In this case the spline power is to be more than zero. The regularization parameter α also exceeds zero. The significance of the addition is to suppress the spline oscillations in the regions with a lack of experimental points but with many knots. The spline usually oscillates significantly between the points and insertion of $\Delta\Phi$ can suppress it. The most known is the regularization employment for cubic splines when $\Delta\Phi$ being zero corresponds to the straight line and, hence, in the places free of points the spline tries to transform to the straight line that seems to be quite natural.

However seeking for the optimal knot positions (see the previouse section) allows to do away with regularization in difficult cases since the knot positions could be found out in order to suit mostly the certain data. Therefore, in our cross-section evaluations the regularization didn't gain acceptance, especially, because $\Delta\Phi$ insertion can't be explained statistically and that's why it is impossible to calculate the spline errors with regularization.

As for the realization method, it is rather simple: to the system matrix the terms are added corresponding to the basis spline composition contribution to (17). Integrals are calculated as integral sums at separate grid intervals where they, in turn, are calculated by the Simpson formula as a result a precise value is obtained since subintegral function is the second power polynomial.