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# A Computer Program for Analyses of Light and Intermediate-Mass Fragment Emission in Heavy Ion Reactions by an Extended Sum-rule Model

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# LIMES: A COMPUTER PROGRAM FOR ANALYSES OF LIGHT AND INTERMEDIATE-MASS FRAGMENT EMISSION IN HEAVY ION REACTIONS BY AN EXTENDED SUM-RULE MODEL

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## ABSTRACT

### LIMES : A COMPUTER PROGRAM FOR ANALYSES OF LIGHT AND INTERMEDIATE-MASS FRAGMENT EMISSION IN HEAVY ION REACTIONS BY AN EXTENDED SUM-RULE MODEL

The computer program LIMES is based on an improved version of the extended sum-rule model for light and intermediate-mass fragment emission in heavy ion reactions. It includes a code for dynamical calculations of the critical angular momentum for fusion following the suggestions of C. Ngô (Prog. Part. Physics **16** (1986) 139). The report briefly describes the use of this program, the necessary input for the calculations of the element distribution and partial cross sections and gives a Fortran listing. Using the fitting routine FITEX the program provides an option for fast parameter adjustments. The use is demonstrated by an application to a specific example.

## ZUSAMMENFASSUNG

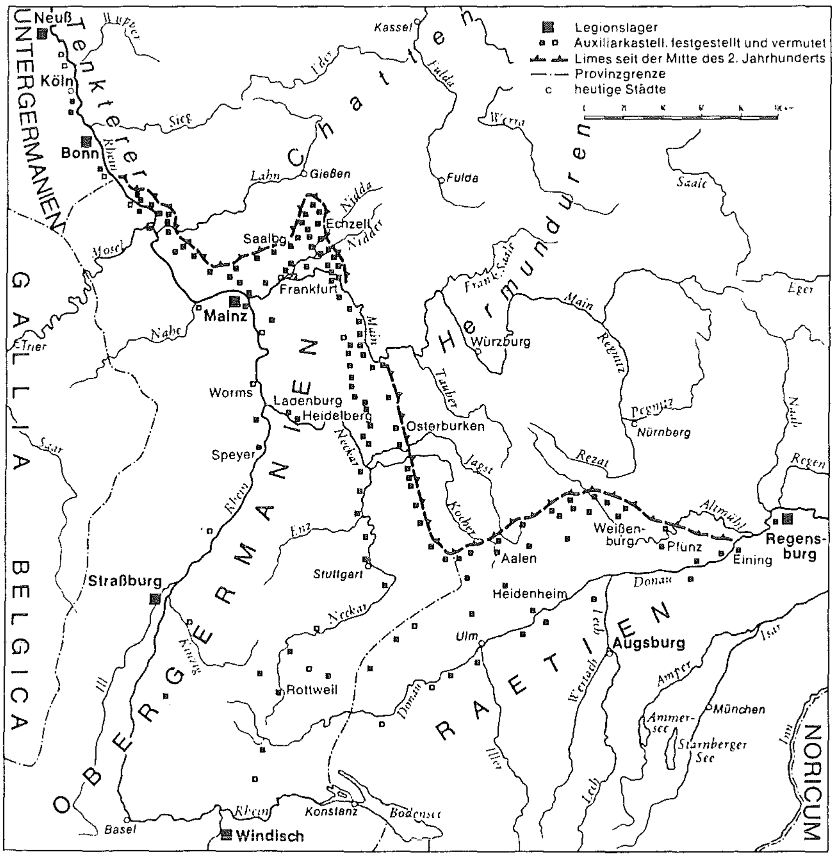
### LIMES : EIN RECHENPROGRAMM ZUR ANALYSE DER LEICHTEN UND INTERMEDIATE-MASS FRAGMENT EMISSION IN SCHWERIONEN-REAKTIONEN IM RAHMEN EINES ERWEITERTEN SUMMENREGEL-MODELLS

Das Rechenprogramm LIMES basiert auf einer verbesserten Version eines Modells einer erweiterten Summen-Regel für die Emission von leichten Teilchen und Fragmenten mittlerer Masse in Schwerionen-Reaktionen. Es umfaßt auch eine Routine zur dynamischen Berechnung des kritischen Drehimpulses für die Fusion (nach C. Ngô, Prog. Part. Physics **16** (1986) 139). Die Benutzung des Programms und die notwendige Eingabe für die Berechnungen der Elementverteilungen und partiellen Wirkungsquerschnitte werden ausführlich beschrieben. Die Fortran-Liste ist vollständig mit angegeben. Das Programm benutzt die Fit-Routine FITEX zum Anpassen von Parametern. Die Anwendung wird mit einem Beispiel verdeutlicht.

# Contents

# 1. Introduction

The emission of complex fragments in light and heavy ion interactions at intermediate energies has been found to be a quite general phenomenon where both equilibrium and nonequilibrium reaction mechanism appear to coexist. Generalizing the sum-rule model worked out by Wilczyński et al. [1] for a global description of complete and incomplete fusion processes the extended sum-rule model [2] adopts the view that the nearly equilibrated component of the intermediate mass fragment (IMF) emission arises with the dynamical evolution of the system via partial equilibrated states on the way to fusion.
Following the formulation given in refs [2,3] the present report compiles the basic formulas for the calculation of the element distribution $\sigma(Z)$ of IMF emission and describes the computer code for sum-rule model analyses of measured data.



Limes Germaniae

## 2. Short summary of basic formulas

The basic assumption of the sum-rule models [1,2,3] is a parametrization of the partial cross section $\sigma_l(i)$ for the entrance angular momentum $l$ and the particular channel $i$ (defined by charge and mass of the measured ejectile) by a probability $P(i)$ for the channel and a transmission coefficient $T_l(i)$:

$$\sigma_l(i) = T_l(i)\, P(i)\, N_l \quad .$$

Here $N_l$ is a $l$-dependent normalization factor. The probability for the channel $i$ follows the $Q_{gg}$ systematics

$$P(i) \sim exp \frac{Q_{gg}(i) - Q_c(i)}{\tau}$$

where $\tau$ is a free parameter of the model representing the effective (apparent) temperature and $Q_{gg}$ is the Q-value of the ground state transition. The change of the Coulomb interaction is taken into account by the correction $Q_c$:

$$Q_c = \frac{e^2 (Z_1^f Z_2^f - Z_1^{in} Z_2^{in})}{R_c}$$

where $Z_1{}^f$ and $Z_2{}^f$ are the charges of the ejectile and the residual nucleus, and $Z_1{}^i$, $Z_2{}^i$ the charges of target and projectile, respectively. The Coulomb interaction radius $R_c$ is given by

$$R_c = r_{0c} (A_1^{1/3} + A_2^{1/3})$$

where $r_{0c}$ is believed to be an adjustable parameter of the model. The transmission coefficient $T_l(i)$ in the entrance channel is defined by two components:

$$T_l(i) = T_{1,l}(i) + T_{2,l}$$

The first transmission coefficient describes complete ($i=1$) and incomplete ($i>1$) fusion processes, the latter as fast binary cluster transfers either from the target to the projectile ( IMF - fragment ) or vice versa (light particle) :

$$T_{1,l}(i) = \left\{ 1 + exp \left[ \frac{l - l_{lim}(i)}{\Delta l} \right] \right\}^{-1}$$

The limiting entrance channel angular momentum $l_{lim}$ is calculated with the condition that the transferred cluster enters the attractive region of the catching nucleus. In the system of the absorbing nucleus this critical angular momentum is estimated by

$$l_{cr}(l_{cr}+1) = \frac{\mu(C_1+C_2)}{\hbar^2}\left[2\pi(\gamma_1+\gamma_2)C_1C_2(C_1+C_2) - Z_1Z_2e^2\right]$$

where the half-density radii $C_{1,2}$ are given by

$$C_{1,2} = R_{1,2}\left[1-\left(\frac{b}{R_{1,2}}\right)^2 \pm \dots\right] \qquad b = 1\,fm$$

with

$$R_{1,2} = 1.28\,A_{1,2}^{1/3} - 0.76 + A_{1,2}^{-1/3}$$

and the surface energy coefficients

$$\gamma_{1,2} = .95\left[1-1.78\left(\frac{N_{1,2}-Z_{1,2}}{A_{1,2}}\right)^2\right] \; MeV\ fm^{-2} \quad .$$

For the case that the target $A_2$ takes a cluster with n nucleons the limitation in the entrance channel is given by

$$l_{lim} = \frac{A_1}{n}\, l_{cr}$$

and for the case that the projectile $A_1$ takes a cluster of the mass m

$$l_{lim} = \frac{A_2}{m}\, l_{cr} \quad .$$

The second transmission coefficient $T_{2,l}$ [2,3],

$$T_{2,l} = \left\{1+exp\left[\frac{l-l_{cr}^{dyn}}{\Delta l}\right]\right\}^{-1}$$

is equal for all channels (i>1), i. e. it is independent from the channel. It enables to introduce further reaction types in the sum-rule model without detailed assumptions. By choosing the limitation in angular momentum as $l_{cr}{}^{dyn}$ ( the way to calculate is described in chapter 4. ), dissipative processes at large angular momenta are taken into account. In case of $T_{2,l}$ =0 the model reduces to the original model [1].

The partial cross sections are summed over all channels. In order to normalize the model the resulting cross sections for an angular momentum $l$ in the entrance channel is limited to the reaction cross section:

$$\sum_i \sigma_l(i) = \sum_i N_l\, P(i)\, T_l(i) = N_l \sum_i P(i)\, T_l(i) = \pi\lambda^2(2l+1)(1-|S_l|^2)$$

thus

$$N_l = \frac{\pi \lambda^2 (1 - |S_l|^2)(2l + 1)}{\sum\limits_i P(i)\ T_l(i)}$$

where $S_l$ are the elastic scattering partial amplitudes related to the elastic scattering cross section:

$$\frac{d\sigma_{el}(\theta)}{d\Omega} = |f(\theta)|^2$$

with

$$f(\theta) = f_c(\theta) + \frac{1}{2ik} \sum_{l=0}^{\infty} (2l + 1)(S_l - 1)\, e^{2i\delta_l} P_l(\cos\theta)$$

and the Coulomb scattering amplitudes

$$f_c(\theta) = \frac{\eta\, exp\left(2i\left(2\delta_0 - \eta\, ln(sin^2 \frac{\theta}{2})\right)\right)}{2k\ sin^2 \frac{\theta}{2}} .$$

The Coulomb scattering phase shifts are given by

$$\delta_l = arg\ \Gamma(l + 1 + i\eta)$$

where $\eta$ is the Sommerfeld - parameter. For the use in the sum-rule model the $S_l$

$$S_l = |S_l|\, e^{i\phi}$$

can be parametrized by the smooth cut-off form

$$|S_l| = \frac{1}{1 + exp\left(\frac{L_1 - l}{\Delta L_1}\right)}$$

and

$$\phi = \frac{\Delta_0}{1 + exp\left(\frac{l - L_2}{\Delta L_2}\right)}$$

For an evaluation of this parametrization the following procedures are possible :

- a fit of the parameters $L_1$, $\Delta L_1$, $\Delta_0$, $L_2$ and $\Delta L_2$ to reproduce the elastic scattering cross section.
- the use of an adequate optical potential, to deduce the $S_l$ (for example by the code MODINA [4] ).

- for a first approximation, of course it is possible to use the original sharp cut-off procedure for the $S_l$

$$S_l = \{ \begin{array}{l} 0 \;\; for \;\; l < l_{max} \\ 1 \;\; for \;\; l > l_{max} \end{array}$$

where $l_{max}$ is calculated by :

$$l^2_{max} = \frac{2\,\mu\,R^2_{in}}{\hbar^2}\,(E_0 - B_{in})$$

with

$$B_{in} = \frac{Z_1 Z_2 e^2}{r_0 (A_1^{1/3} + A_2^{1/3})}$$

and

$$R_{in} = 0.5 + 1.36\;(A_1^{1/3} + A_2^{1/3})$$

where μ is the reduced mass.

Thus the cross section for a channel $i$ is given by

$$\sigma\,(i) = \sum_{l=o}^{l_{max}} N_l\;(T_{1,l}(i) + T_{2,l})\;P(i)$$

which may be split in two parts

$$\sigma(i) = \sigma_1(i) + \sigma_2(i)$$

with $\sigma_1(i)$ representing the contribution for the original model.

# 3. Program LIMES

## 3.1 Concept of LIMES

The computer program LIMES for analyzing light and intermediate mass fragment emission in heavy ion induced reactions is written in standard Fortran 77 and uses single precision variables for floating point calculations. The integer variables are defined as signed 32 bit values. A translation into a more powerful language like 'C' should be easy to do, even a number of problems, like the long argument lists would disappear. The program is developed under MS-DOS on a IBM-AT compatible Computer. A transfer to systems with better performance, like an advanced home-computer, workstation or a mainframe should be possible without further problems. Such a transfer would overcome the later discussed problems with the address size of the personal computer.

The program LIMES is a tool to work with the extended sum-rule as well as with the original version of Wilczyński. There are no limitations to special reactions in the code, all necessary changes for other reactions can be done by input. LIMES provides several different options, like calculating the model predictions with a specified set of parameters or adjust the free parameters of a sum-rule with a fit procedure. An output of all calculated partial cross sections $\sigma_l(i)$ as a table is also possible for a fixed parameter set.

The program is a mixture of batch processing and interactive programming. It is split into these two modes by a choice which part of the input is often changed and which stays stable. The calculation is defined by three different input files each for one logical block of input, but the name of the used input file is asked interactively from the program. This enables the user to keep ready several inputs for different reactions. The control flags can be set interactively, so the user can perform different modes like calculating the original model, fitting or output of the partial cross sections without leaving LIMES. The interactive mode allows an effective control of the calculations.

Fig. 1 gives a flow diagram which describes the logical structure of LIMES. The subroutine FITEX [5] solves the nonlinear least-squares problem.

The run time of LIMES depends directly on the number of used channels and angular momenta. For the example discussed in sect. 3.2. the time is less than 20 seconds for a fixed parameter calculation and some minutes for fitting on the described machine. The required memory to run LIMES can be roughly estimated

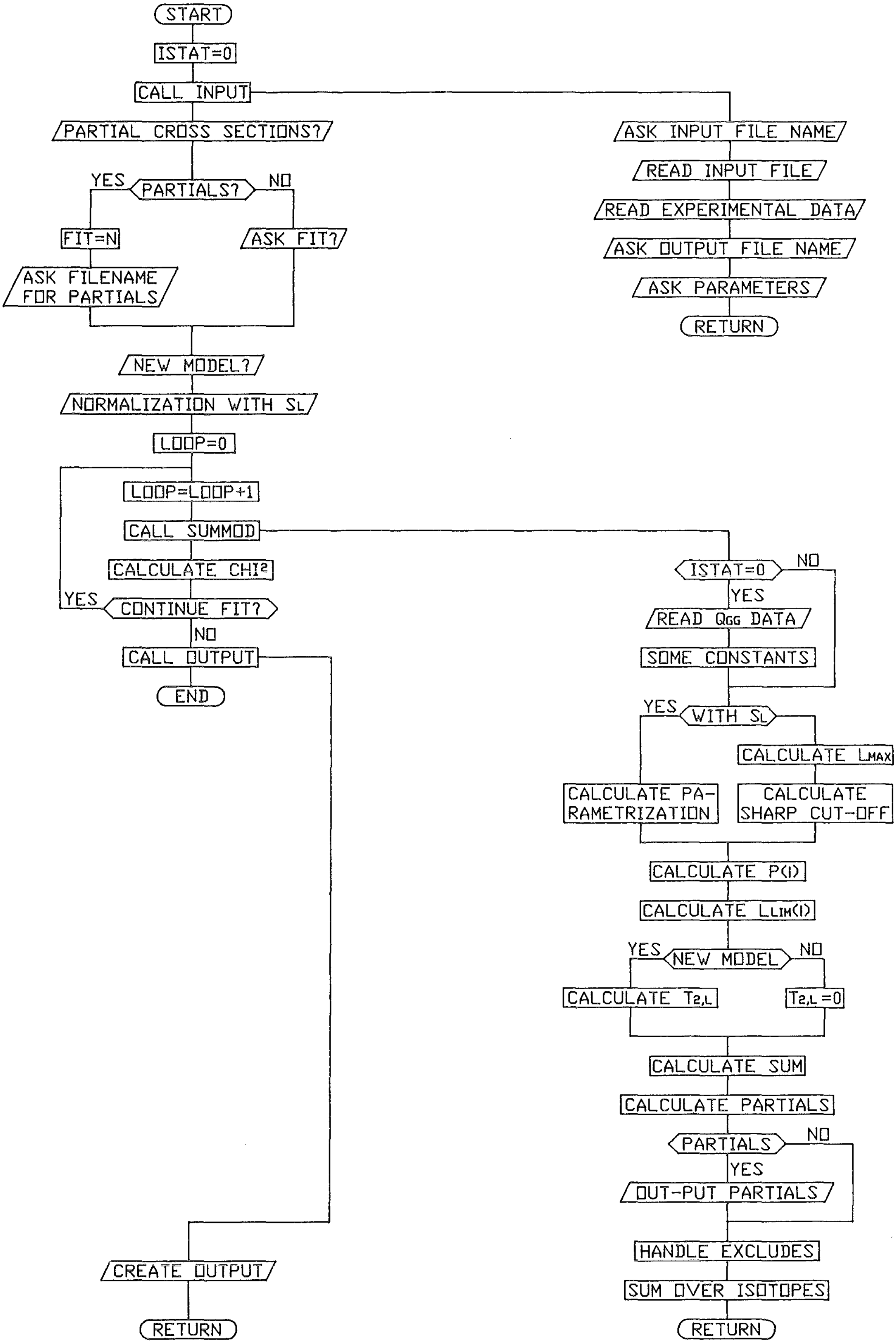


Fig. 1 Flow diagram of LIMES.

by an offset for the code by itself depending on the used compiler, the size of the small arrays and mainly by the two two-dimensional arrays. The limit of the arrays is defined in the third line of the program by a parameter statement to 100 channels and 100 angular momenta. If larger arrays are necessary only this line has to be modified. The program performs a runtime boundary check, to inform the user, if by accident more channels or angular momenta are used as defined before.

The used array size of 100 * 100 results in a total size of 40 kB. For a state of the art machine it is no problem to increase the size over the 64 kB border, but at the Personal Computer most compilers are **not** able to do this. Even the IBM professional FORTRAN compiler V1.00 handles the array, but the rest of the program is crashing or doing some other funny things. In any case on the Personal Computer the maximum memory size of 640 kB is the limit.

### 3.2 Example describing the use of LIMES

This chapter gives an example of the use of LIMES with a calculation for the reaction of 156 MeV $^{6}$Li + $^{nat}$Ag. The experimental data are taken from refs [7,8]. LIMES requires several input files. The first is the $Q_{gg}$ table of the different reaction channels. All channels included there are taken into account for the normalization of the sum-rule.

The file LIAG.QGG has the following format:

```
156 MeV 6-Li + nat-Ag   Qgg - Table
95
   Z      A        Qgg
   0.,    0.,      14.674
   0.,    1.,      7.022
   1.,    1.,      6.509
   .
   .
   .
   23.,   52.,     40.01
   24.,   54.,     43.27
   25.,   56.,     40.074
```

The first line of the table is the header of the calculation, the next is an integer representing the number of channels. The third line is a dummy text as header of the table. Each of the following lines defines a particular channel. For example, the first line of the table 0., 0., 14.674 denotes an ejectile with mass and charge zero (complete fusion of the projectile with the target). The third value is the corresponding Q - value of the ground states. The line number in the table is equivalent to the channel number in program and of the output. The complete table is given in appendix A.

The experimental σ(Z) data necessary for the fit procedure are provided in the second input file LIAG.EXP. The format of the file is :

```
156 MeV 6-Li + nat-Ag   experimental data
   14
   Z       value          relative error
   1.,     1088.3,        .2
   2.,     236.,          .2
   4.,     2.1,           .2
   5.,     1.23,          .2
   6.,     1.,            .2
   7.,     0.26,          .2
   8.,     0.153,         .2
   9.,     0.05,          .2
   10.,    0.048,         .2
   11.,    0.025,         .2
   12.,    0.025,         .2
   13.,    0.026,         .2
   14.,    0.015,         .2
   15.,    0.013,         .2
```

Again the first line is the header of the calculation. The second consists of an integer value for the total number of the following data points. The third line is a dummy header for the table. The line 1. 1088.3 .2 means, that the integrated cross section for $Z=1$ ejectiles (proton,deuteron and triton) is 1088.3 mbarn, with a relative error of 20%. The experimental input file is necessary, if no fit is required a dummy file can be used.

The third input file LIAG.IN defines the reaction parameters. The lines starting with dashes are just comments:

```
--- TITLE OF THE CALCULATION
 156 MeV 6-Li + nat-Ag
--- MASS OF THE PROJECTIL                             REAL
6.
--- CHARGE OF THE PROJECTILE                          REAL
3.
--- MASS OF THE TARGET                                REAL
108.
--- CHARGE OF THE TARGET                              REAL
47.
--- LAB ENERGY  (MeV)                                 REAL
156.
--- DEL                                               REAL
 3.
--- RL1, DELTAL                                 2 *   REAL
 48.84   3.3
--- LCRDYN                                            INT
51
--- FILE NAME OF Qgg-DATA                             TEXT
LIAG.QGG
--- FILE NAME OF THE EXPERIMENTAL DATA                TEXT
LIAG.EXP
--- NUMBER OF THE CHANNELS TO BE EXCLUDED             INT
 1
--- EXCLUDED CHANNELS BY THE OUTPUT OF THE CROSS SECTIONS
 4.  8.
```

Up to the line DEL, which stands for the diffuseness in $l$-space the input is obligatory. The next line RL1 and DELTAL requests parameters describing the partial scattering amplitudes $S_l$ (see chapter 2). These values can be given as dummy, if by executing the program the normalizing option is set to NO. The dynamical limiting angular momentum $l_{cr}{}^{dyn}$ is the result of a calculation by the program DYNFUS (see chapter 4) and is dummy if the original model [1] is used. The last two input lines, called 'EXCLUDED CHANNELS' give the possibility to exclude channels which are needed by normalizing, but not for the fit procedure. The excluded channels are completely calculated in the sum-rule but ignored when fitting the cross sections. The user has the possibility to exclude several channels by specifying their number and one line for each with charge and mass. With this three input files it is possible to start LIMES. All further parameters and controls are requested during the run.

The following example performs a fit for the case of the reaction of 156 MeV $^6$Li + $^{nat}$Ag. By normal letters the output of the program is indicated, **bold** letters show the input given by the user. Some explanations are added in *italics*:

```
    L     ight and                      Iliana Brancus
    I     ntermediate                   Juergen Wentz
    M     ass fragment emission              and
    E     xtended                      Hans-Ulrich Hohn
    S     um-rule                        July 1989

INPUTFILE FOR INITIALIZING DATA              : LIAG.IN
156 MeV 6-Li + nat-Ag
NUMBER OF EXPERIMENTAL POINTS                :   14

OUTPUTFILE-NAME                              : LIAG1.OUT
TEMP, R0C                                    :  3.          1.5
TEMP =     3.00000000  R0C =     1.50000000  DEL =     3.00000000

PARTIAL CROSS-SECTIONS ?          Y(es), N(o)   : N
FIT ?                             Y(es), N(o)   : Y
NEW MODEL ?                       Y(es), N(o)   : Y
```

*Y means that the extended sum-rule model is used, N the original model of Wilczyński is used.*

```
NORMALIZATION WITH SL ?           Y(es), N(o)   : Y
```

*Y means that the parametrization for the $S_l$ is used, N implies a sharp cut-off at $l_{max}$.*

```
   A1            Z1            A2            Z2            ELAB
   0.600E+01     0.300E+01     0.108E+03     0.470E+02     0.156E+03

LMAX =  96       IPMAX =  95       LCRF =  51
```

```
LOOP =     1    CHI**2 =   27.01646610
                    TEMP  =     3.00000000   R0C =     1.50000000

LOOP =     2    CHI**2 =   27.27686880
                    TEMP  =     4.00000000   R0C =     1.50000000

LOOP =     3    CHI**2 = 587786.06200000
                    TEMP  =     3.00000000   R0C =     2.50000000

LOOP =     4    CHI**2 =   13.62654020
                    TEMP  =     3.49781394   R0C =     1.50001121
```

*at this point some loops of the fit are skipped*

```
LOOP =    18    CHI**2 =    6.23329115
                    TEMP  =     3.89492798   R0C =     1.45762455

LOOP =    19    CHI**2 =    6.23309946
                    TEMP  =     3.88908100   R0C =     1.45912027

LOOP =    20    CHI**2 =    6.23308372
                    TEMP  =     3.88781190   R0C =     1.45962882

FIT ENDS WITH CODE =       0  THIS MEANS
FIT ENDS WITHOUT ERROR

NEW CALCULATION ?            Y(es), N(o)       : N
```

By requiring a new calculation the program restarts at the very beginning. The output of the results can be found in the file LIAG1.OUT, where the elemental and isotopical cross sections [mbarn] are given in tables. This file reports also on the whole control input and the used input file names:

```
     TEMPERATURE       R0C              CHI2
     3.88781190        1.45962882       6.23308372
  14
  Z                 S1                S1+S2
```

```
0.10000E+01     0.13215E+02     0.24932E+03
.
.
.
0.14000E+02     0.42667E-02     0.12867E-01
0.15000E+02     0.91436E-03     0.29729E-02

156 MeV 6-Li + nat-Ag
PARTIAL CROSS SECTIONS        N
F I T - PROCEDURE             Y
NEW MODEL                     Y
NORMALIZATION WITH SL         Y

INPUT FILE WAS                    LIAG.IN
QGG FILE WAS                      LIAG.QGG
EXPERIMENTAL DATA FILE WAS        LIAG.EXP

THE FIT ENDS WITHOUT ERRORS

 THE TOTAL CROSS SECTION FOR THE SINGLE CHANNELS

I     1. Term          2. Term          Sum
1     0.4052E+03       0.0000E+00       0.4052E+03
2     0.5529E+02       0.1307E+04       0.1363E+04
.
.
.
93    0.4864E-04       0.2509E-03       0.2996E-03
94    0.9273E-04       0.5170E-03       0.6097E-03
95    0.3637E-04       0.2186E-03       0.2550E-03
```

The calculated elemental cross sections compared with the experimental data are shown in fig. 2, a complete listing of the file is given in appendix B.

The next example demonstrates the way to get a table of the partial cross sections. For the free parameters of the sum-rule model the result of the previous fit is used. The three input files LIAG.QGG, LIAG.EXP and LIAG.IN are unchanged. Only the interactive input has to be changed in the following way:

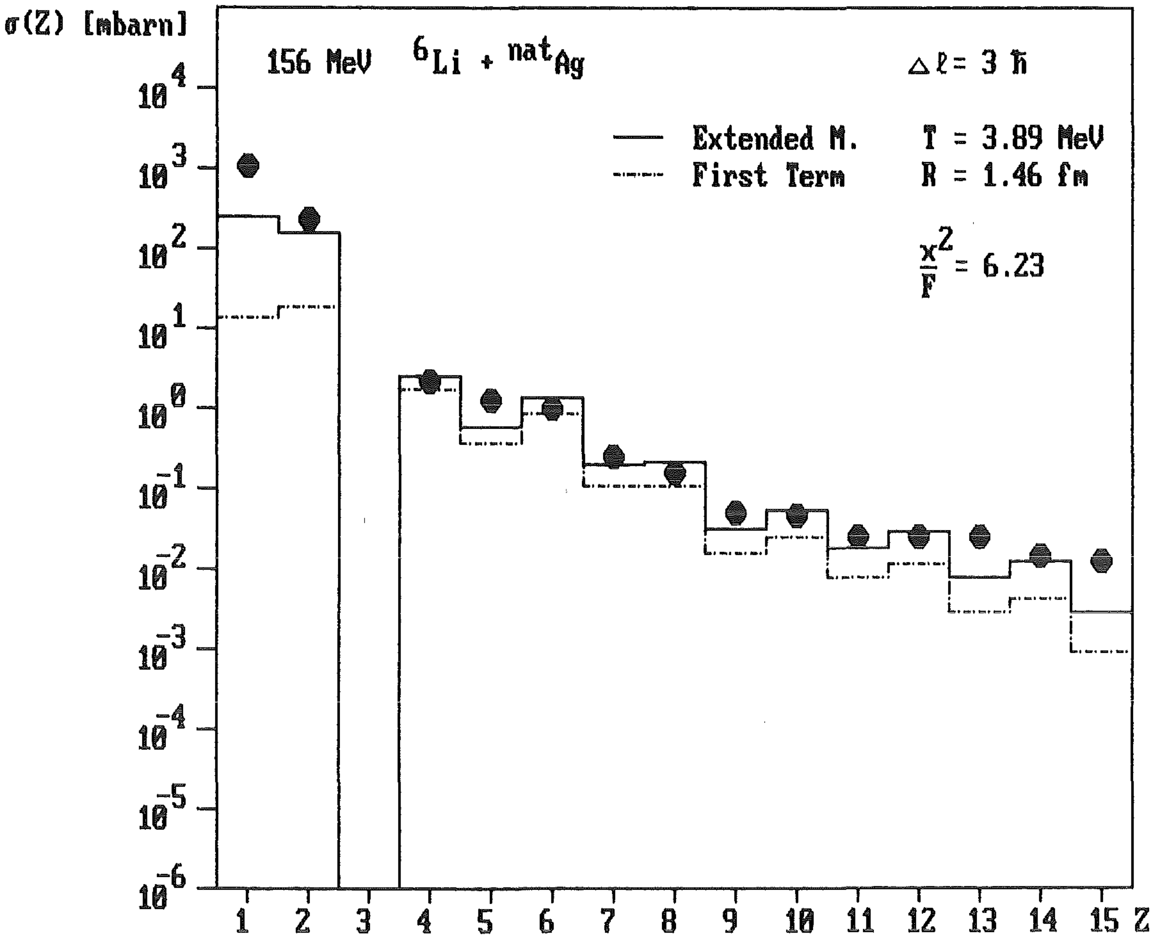


Fig. 2 Elemental distribution of complex fragment emission in the reaction of 156 MeV $^6$Li + $^{nat}$Ag. The full line is the result of the extended sum-rule model. The experimental data points are taken from refs [7,8]. The contribution of the first term $\sigma_{1,l}(i)$ is indicated by the dashed line.

| | | |
|---|---|---|
| L | ight and | Iliana Brancus |
| I | ntermediate | Juergen Wentz |
| M | ass fragment emission | and |
| E | xtended | Hans-Ulrich Hohn |
| S | um-rule | July 1989 |

INPUTFILE FOR INITIALIZING DATA : LIAG.IN
156 MeV 6-Li + nat-Ag
NUMBER OF EXPERIMENTAL POINTS : 14

OUTPUTFILE-NAME : LIAG2.OUT

```
TEMP, R0C                                          :  3.89       1.46
TEMP =      3.89000010  R0C =      1.46000004  DEL =      3.00000000

PARTIAL CROSS-SECTIONS ?           Y(es), N(o)   : Y
FILENAME FOR THE PARTIAL CROSS SECTIONS : LIAG3.OUT
NEW MODEL ?                        Y(es), N(o)   : Y
NORMALIZATION WITH SL ?            Y(es), N(o)   : Y

   A1            Z1            A2            Z2            ELAB
   0.600E+01     0.300E+01     0.108E+03     0.470E+02     0.156E+03

LMAX =  96       IPMAX =  95      LCRF =  51

LOOP =       1   CHI**2 =     6.23534060
                      TEMP  =     3.89000010   R0C =     1.46000004


NEW CALCULATION ?                  Y(es), N(o)   : N
```

The output file LIAG2.OUT contains except of the controls the same information as LIAG1.OUT. The table of the partial cross sections $\sigma_l(i)$ is in the file LIAG3.OUT. Because this file has a size of over 300 kB only the first and last lines are printed. The format for each line contains the full information, so by using the table as input to other programs the sorting routine can be created simply. After some control information the $\sigma_l(i)$ [mbarn] are given in lines by $i$, $l$ , $\sigma_{1,l}(i)$  $\sigma_{2,l}(i)$ :

```
   PARTIAL CROSS SECTIONS
   156 MeV 6-Li + nat-Ag
   THE INPUT FILE WAS            liag.in
   THE FIRST OUTPUT FILE IS      liag2.out

   I     L     S1(I,L)            S2(I,L)
   1     0     0.574260E+00       0.000000E+00
   1     1     0.172263E+01       0.000000E+00
   1     2     0.287072E+01       0.000000E+00
   1     3     0.401834E+01       0.000000E+00
   1     4     0.516526E+01       0.000000E+00
```

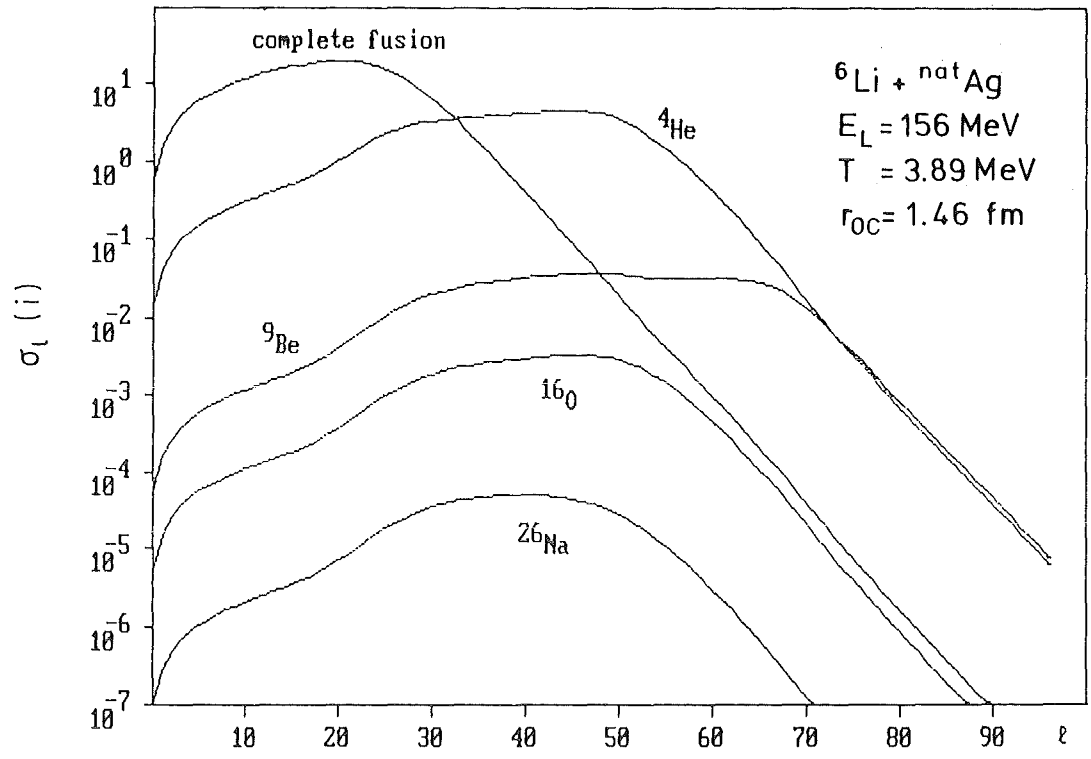


Fig. 3 Partial cross section $\sigma_l(i)$ for some channels of the reaction 156 MeV $^{6}$Li + $^{nat}$Ag calculated with the extended sum-rule model as shown in the second example.

```
 1    5    0.631107E+01     0.000000E+00
 1    6    0.745520E+01     0.000000E+00
 1    7    0.859680E+01     0.000000E+00
 1    8    0.973457E+01     0.000000E+00
 1    9    0.108666E+02     0.000000E+00
 1   10    0.119902E+02     0.000000E+00
 .
 .
 .
95   84    0.274471E-12     0.407651E-09
95   85    0.204742E-12     0.304089E-09
95   86    0.152785E-12     0.226921E-09
```

|  |  |  |  |
|---|---|---|---|
| 95 | 87 | 0.114039E-12 | 0.169376E-09 |
| 95 | 88 | 0.851315E-13 | 0.126441E-09 |
| 95 | 89 | 0.635555E-13 | 0.943953E-10 |
| 95 | 90 | 0.474483E-13 | 0.704724E-10 |
| 95 | 91 | 0.354226E-13 | 0.526112E-10 |
| 95 | 92 | 0.264435E-13 | 0.392750E-10 |
| 95 | 93 | 0.197391E-13 | 0.293174E-10 |
| 95 | 94 | 0.147334E-13 | 0.218828E-10 |
| 95 | 95 | 0.109962E-13 | 0.163320E-10 |
| 95 | 96 | 0.820617E-14 | 0.121882E-10 |

In fig. 3 the partial cross sections $\sigma_l(i)$ for some representative channels are plotted.

### 3.3 List of the error codes of LIMES

The following list gives a brief description of the error codes which may appear during execution. Additional some information about user action is provided.

Error codes with numbers between 10 and 19 belong to errors which are detected in the subroutine SUMMOD:

**error 11** **Number of channels is greater than the dimension of the array**

By reading the input file with the $Q_{gg}$ values, the program found more channels defined therein as the parameter IPMAXP gives as maximum possible value. The user can reduce the number of channels or increase the maximum number in line 3 of the program.

**12** **The LMAX resulting from the SL is greater than the dimension of the arrays**

By the use of the smooth cut-off normalization the program calculates the limit for the angular momenta LMAX = 2*RL1. The error indicates that the parameter for the maximum array size LMAXP is smaller than LMAX. To overcome this error the user can increase the parameter LMAXP in line 3 of the program or reduce the factor 2 in the term LMAX = 2*RL1.

13 **The sharp cut-off LMAX is greater than the l-depending arrays.**
In case that the sharp cut-off model is selected the program calculates LMAX by the expressions given in chapter 2. This error appears if the LMAX is larger than LMAXP. The user should increase LMAXP in line 3 of the program.

The errors detected in Subroutine INPUT lead to code numbers between 21 and 29.

error 21 **Number of excluded channels is greater than the dimension of the array.**
By reading the standard input file the program found more excluded channels than the maximum channel number given by the parameter IPMAXP at line 3 of the program.

22 **Number of experimental points is greater than the dimension of the array**
The input file with the experimental data contains more data points as allowed by the maximum channel number IPMAXP. The parameter IPMAXP in line 3 of the program should be increased.

A second type of error code may result from the use of the subroutine FITEX, the error codes of the fit are less than 10:

fit error 0 The fit ends without errors

1 The fit is in process

3 The maximum number of loops defined by the variable IW(2) is reached.

4 Rounding error in FITEX

5 The results of the sum-rule model are independent from the free parameters.

6,7 Unidentified error in FITEX.

No fit procedure is perfect, in the case that FITEX is not able to find a minimum within the specified start values, most times a variation of the start values solves the problem.

### 3.4 Listing of LIMES

The following is the standard FORTRAN 77 listing of the program LIMES. The used subroutine FITEX can be found in [4,5].

```
      PROGRAM LIMES
C
      PARAMETER (LMAXP=100,IPMAXP=100,IWMAXP=1000)
C
C**********************************************************************
C
C                          L I  M E S
C
C LIMES    is a program for analysis of light and IMF fragment emission
C          in heavy ion reactions
C
C The calculations are based on an Extended Sum-Rule Model ( I.M. Brâncuş
C KfK 4453, Kernforschungszentrum Karlsruhe 1988 ) ISSN 0303-4003
C
C The program, is described in I.M. Brâncuş, J. Wentz and  H.U. Hohn
C KfK 4610B, Kernforschungszentrum Karlsruhe 1989. ISSN 0303-4003
C
C The subroutine FITEX for adjusting the free parameters is from
C G W. Schweimer 1974 and linked as module. The source code of the
C fit-procedure can be found in
C I.M. Brâncuş, J. Oehlschläger, J. Wentz KfK 4454B, Kernforschungszentrum
C Karlsruhe 1988 ISSN 0303-4003
C
C                                   Jürgen Wentz        July 1989
C
C*******************************************************************
```

```
C
      INTEGER IW(IWMAXP)
C
      REAL E(IWMAXP),F(IWMAXP),W(IWMAXP),X(IWMAXP),
     &     Y(IPMAXP),FEHL(IPMAXP),XCLD1(IPMAXP),XCLD2(IPMAXP)
C
      DIMENSION P(IPMAXP),QGG(IPMAXP),ALCR(IPMAXP),
     &          ALIM(IPMAXP),A3P(IPMAXP),Z3P(IPMAXP),
     &          SUM(0:LMAXP),SIGZ1(0:IPMAXP),SIGZ2(0:IPMAXP),
     &          SIGMA1(IPMAXP),SIGMA2(IPMAXP),
     &          SIG1(0:LMAXP,IPMAXP),SIG2(0:LMAXP,IPMAXP),
     &          ZC(IPMAXP),SECTO(IPMAXP),STREU(0:LMAXP),
     &          SECTE(IPMAXP))
C
      CHARACTER*20 CFIL1,CFIL2,CFIL3,CFIL4,CFILEN
      CHARACTER*20 CFIT,CPART,CIN,CMOD,CSL
      CHARACTER*80 CHEAD
C
 100  KE = 0
      N  = 2
C
      W(1) = 1000.
      W(2) = 0.
      W(3) = 0.
C
      IW(1) = 3
      IW(2) = 100
      IW(3) = 0
C
C --- ABSOLUTE SEARCH ACCURACIES FOR THE VARIABLES
C
      E(1) = .001
      E(2) = .001
C
      ISTAT = 0
C
C --- CALL THE INPUT SUBROUTINE
C
```

```
      CALL INPUT (CHEAD,A1,A2,Z1,Z2,CFIL1,ELAB,RL1,DELTAL,LCRF,
     &            CFIL2,CFIL3,CFIL4,IZXCLD,XCLD1,XCLD2,TEMP,R0C,
     &            ZC,Y,FEHL,M,NPT,CFILEN,IWMAXP,IPMAXP,DEL)
C
      WRITE (*,*)' PARTIAL CROSS-SECTIONS ?          Y(es), N(o)  : '
      READ (*,'(A20)') CPART
C
      IF (INDEX(CPART,'N').NE.0.OR.INDEX(CPART,'n').NE.0) THEN
C
        WRITE (*,*)' FIT ?                               Y(es), N(o)  : '
        READ (*,'(A20)') CFIT
C
      ELSE
C
        CFIT = 'N'
        WRITE(*,*) ' FILENAME FOR THE PARTIAL CROSS SECTIONS : '
        READ (*,'(A20)') CFIL4
C
      ENDIF
C
      WRITE (*,*)' NEW MODEL ?             Y(es), N(o)  : '
      READ (*,'(A20)') CMOD
C
      WRITE (*,*)' NORMALIZATION WITH SL ?   Y(es), N(o)  : '
      READ (*,'(A20)') CSL
C
C ---  LOOP FOR THE FIT - PROCEDURE
C
      LOOP = 0
C
      X(1) = TEMP
      X(2) = R0C
C
 200  LOOP    = LOOP + 1
      TEMP    = X(1)
      R0C     = X(2)
C
C ---  CALCULATE THE SUM-RULE MODEL WITH THE GIVEN
```

```
C ---  PARAMETERS
C
       CALL SUMMOD (TEMP,R0C,DEL,NPT,ISTAT,P,QGG,ALCR,ALIM,
      &             RL1,A3P,Z3P,SUM,SIGZ1,SIGZ2,SIGMA1,SIGMA2,SIG1,
      &             SIG2,ZC,SECTO,STREU,SECTE,LMAXP,IPMAXP,CPART,
      &             A1,Z1,A2,Z2,ELAB,LMAX,DELTAL,LCRF,CFIL2,CFIL4,
      &             CMOD,XCLD1,XCLD2,IZXCLD,CSL,CFILEN,CHEAD,
      &             CFIL1,IPMAX)
C
C ---  CALCULATE THE CHI**2 OF THE THEORETICAL AND
C ---  EXPERIMENTAL DATA
C
       W(4) = 0.
       DO 300 I=1,NPT
         F(I) = (Y(I)-SECTO(I))/(FEHL(I)*Y(I))
         W(4) = W(4)+F(I)*F(I)
 300   CONTINUE
C
       CHI2 = W(4)/(M-N-1)
C
       WRITE (*,*) ' LOOP =',LOOP,'  CHI**2 = ',CHI2
       WRITE (*,*) '           TEMP   = ',X(1),'   R0C = ',X(2)
       WRITE (*,*) ' '
C
       IF (INDEX(CFIT,'y').NE.0.OR.INDEX(CFIT,'Y').NE.0)
      & CALL FITEX (KE,M,N,F,X,E,W,IW)
C
       IF (KE.EQ.1) GOTO 200
C
C ---  ERRORS OR MISRUNNING OF THE FIT
C
       IF (INDEX(CFIT,'y').NE.0.OR.INDEX(CFIT,'Y').NE.0) THEN
C
         WRITE(*,*) ' FIT ENDS WITH CODE = ',KE,'  THIS MEANS'
         IF(KE.EQ.0)WRITE(*,*)' FIT ENDS WITHOUT ERROR'
         IF(KE.EQ.3)WRITE(*,*)' MAXIMUM NUMBER OF LOOPS IS
      &     REACHED'
         IF(KE.EQ.4)WRITE(*,*)' ROUNDING ERROR IN FITEX'
```

```
        IF(KE.EQ.5)WRITE(*,*)' THE SUM-RULE IS NOT DEPENDING ON
     &     ONE OF THE PARAMETERS'
        IF(KE.GE.6)WRITE(*,*)' UNIDENTIFIED ERROR IN FITEX'
C
      ENDIF
C
C---  CREATE THE OUTPUT FILE
C
      CALL OUTPUT(CFIL1,CFIL2,CFIL3,CFIL4,CFILEN,X,ZC,SECTE,
     &        SECTO,CFIT,CPART,CMOD,CSL,X(1),X(2),CHI2,NPT,
     &        CHEAD,IPMAXP,IPMAX,SIGMA1,SIGMA2)
C
C---  NEW CALCULATION ?
C
      WRITE (*,*)' '
      WRITE (*,*)' NEW CALCULATION ?        Y(es), N(o)  : '
      READ (*,'(A20)') CIN
      IF (INDEX(CIN,'y').NE.0 .OR. INDEX(CIN,'Y').NE.0) GOTO 100
C
      STOP
      END
C
C*****************************************************************
C
C---  SUBROUTINE FOR CALCULATING THE SUM-RULE MODEL
C
      SUBROUTINE SUMMOD (TEMP,R0C,DEL,NPT,ISTAT,P,QGG,ALCR,
     &                  ALIM,RL1,A3P,Z3P,SUM,SIGZ1,SIGZ2,SIGMA1,
     &                  SIGMA2,SIG1,SIG2,ZC,SECTO,STREU,SECTE,
     &                  LMAXP,IPMAXP,CPART,A1,Z1,A2,Z2,ELAB,LMAX,
     &                  DELTAL,LCRF,CFIL2,CFIL4,CMOD,XCLD1,
     &                  XCLD2,IZXCLD,CSL,CFILEN,CHEAD,CFIL1,
     &                  IPMAX)
C
      DIMENSION P(IPMAXP),QGG(IPMAXP),ALCR(IPMAXP),
     &          ALIM(IPMAXP),A3P(IPMAXP),Z3P(IPMAXP),
     &          SUM(0:LMAXP),SIGZ1(0:IPMAXP),SIGZ2(0:IPMAXP),
     &          SIGMA1(IPMAXP),SIGMA2(IPMAXP),
     &         SIG1(0:LMAXP,IPMAXP),SIG2(0:LMAXP,IPMAXP),
     &         ZC(IPMAXP),SECTO(IPMAXP),STREU(0:LMAXP),
     &         SECTE(IPMAXP),XCLD1(IPMAXP),XCLD2(IPMAXP)
C
      CHARACTER*20 CFIL1,CFIL2,CFIL4,CFILEN,CPART,CMOD,CSL
      CHARACTER*80 DUMMY,CHEAD
C
      IF (ISTAT.EQ.0) THEN
C
        WRITE(*,*) '   A1     Z1     A2     Z2     ELAB'
        WRITE(*,'(5E12.3)') A1,Z1,A2,Z2,ELAB
        WRITE(*,*) ' '
C
C --- INPUT OF THE QGG VALUES
C
        OPEN(UNIT=3,FILE=CFIL2)
C
        READ (3,'(A80)') DUMMY
        READ (3,*) IPMAX
        READ (3,'(A80)') DUMMY
C
        IF (IPMAX.GT.IPMAXP) THEN
           MIST = 1
           GOTO 9000
        ENDIF
C
        DO 100 IP=1,IPMAX
           READ (3,*) Z3P(IP),A3P(IP),QGG(IP)
 100  CONTINUE
C
        CLOSE(UNIT=3)
C
C --- KINEMATICS AND CONSTANTS
C
        PI    = 4.*ATAN(1.)
        PI4   = 4.*PI
        P1    = 1./3.
        PM1   = -P1
```

```
C
         A  = A1+A2
         Z  = Z1+Z2
         N  = A-Z
         AI = (N-Z)/A
C
         GAM      = .95*(1.-1.78*AI*AI)
         E1       = 1.44
         HC2      = 197.32**2
         AMU      = 931.478
         ARED     = A1*A2/(A1+A2)
         CL       = AMU/HC2
         ECM      = ELAB*A2/(A1+A2)
         ALAM2    = 0.5/CL/ARED/ECM
         ALAM     = SQRT(ALAM2)
         PILAM    = PI*ALAM2
         R0T      = 0.764
C
         ISTAT = 1
C
C ---  NORMALIZATION CONDITION
C
C ---  SHARP CUT-OFF    -  ALL SL = 1
C
C ---  SMOOTH CUT-OFF   -  NL = CL * (1-ABS(SL**2))
C
C        WITH   SL FROM THE PARAMETRIZATION
C
C        ABS(SL) = 1./(1.+EXP((RL1-L)/DELTAL))
C
       IF (INDEX(CSL,'Y').NE.0.OR.INDEX(CSL,'y').NE.0) THEN
C
         LMAX = 2 * INT (RL1)
C
         IF (LMAX.GT.LMAXP) THEN
            MIST = 2
            GOTO 9000
         ENDIF
```

```
C
      DO 200 L=0,LMAX
C
        EXP1 = (RL1-L)/DELTAL
C
        IF (EXP1 .LT. -87.) THEN
          STREU(L) = 0.
        ELSE IF (EXP1 .GT. 87.) THEN
          STREU(L) = 1.
        ELSE
          STR1 = 1./(1.+EXP(EXP1))
          STREU(L) = 1.-STR1*STR1
        ENDIF
C
 200  CONTINUE
C
     ELSE
C
C ---  CALCULATE THE SHARP CUT-OFF
C
      RC      = 1.5*(A1**P1+A2**P1)
      BIN     = E1*Z1*Z2/RC
      LMAX    = INT(SQRT(2*AMU/HC2*ARED*RC**2*(ECM-BIN)))
C
      IF (LMAX.GT.LMAXP) THEN
        MIST = 3
        GOTO 9000
      ENDIF
C
      DO 300 L=0,LMAX
        STREU(L) = 1.
 300 CONTINUE
C
     END IF
C
      WRITE (*,'(1X," LMAX = ",I3,5X,
    &          "IPMAX = ",I3,5X,"LCRF = ",I3)') LMAX,IPMAX,LCRF
      WRITE(*,*) ''
```

```
C
      ENDIF
C
C ---  START OF THE SUM-RULE MODEL
C
       RC = R0C*(A1**P1+A2**P1)
C
       DO 400 IP=1,IPMAX
C
C ---  REACTION PROBABILITIES
C
          A3 = A3P(IP)
          A4 = A-A3
          Z3 = Z3P(IP)
          Z4 = Z-Z3
          QC = (Z3*Z4-Z1*Z2)*E1/RC
C
          EXP1 = (QGG(IP)-QC)/TEMP
C
          IF (EXP1 .LT. -87.) THEN
             P(IP) = 0.
          ELSE IF (EXP1 .GT. 87.) THEN
             P(IP) = 3.4E+38
          ELSE
             P(IP) = EXP(EXP1)
          ENDIF
C
C ---  LIMITATION OF ANGULAR MOMENTA
C
          AT = ABS(A4-A2)
          ZT = ABS(Z2-Z4)
C
          R1 = 1.28*A1**P1-0.76+0.8*A1**PM1
          C1 = R1-1./R1
          R2 = 1.28*A2**P1-0.76+0.8*A2**PM1
          C2 = R2-1./R2
C
          IF (AT.LT.4.) THEN
```

```
            CT = R0T*AT**P1
         ELSE
            RT = 1.28*AT**P1-0.76+0.8*AT**PM1
            CT = RT-1./RT
         END IF
C
         IF (A2.GT.A4) THEN
            AREDI = A1*AT/(A1+AT)
            C0 = C1+CT
            ALCR(IP) = SQRT(CL*AREDI*C0*C0*(PI4*GAM*C1*CT
     &                     -E1*Z1*ZT/C0))-.5
            ALIM(IP) = A2/AT*(ALCR(IP))
         ELSE
            AREDI = A2*AT/(A2+AT)
            C0 = C2+CT
            ALCR(IP) = SQRT(CL*AREDI*C0*C0*(PI4*GAM*C2*CT
     &                     -E1*Z2*ZT/C0))-.5
            ALIM(IP) = A1/AT*(ALCR(IP))
         END IF
C
 400   CONTINUE
C
C ---  THE RELATIVE CROSS SECTIONS FIRST TERM
C
       DO 600 IP = 1,IPMAX
C
         DO 500 LL=0,LMAX
C
            EXP1 = (LL-ALIM(IP))/DEL
            IF (EXP1 .LT. -87.) THEN
               SIG1(LL,IP) = P(IP)
            ELSE IF (EXP1 .GT. 87.) THEN
               SIG1(LL,IP) = 0.
            ELSE
               SIG1(LL,IP) = P(IP)/(1.+EXP(EXP1))
            END IF
C
 500     CONTINUE
```

```
C
 600     CONTINUE
C
C ---    THE RELATIVE CROSS SECTIONS SECOND TERM
C
         IF (INDEX(CMOD,'n').NE.0 .OR. INDEX(CMOD,'N').NE.0) THEN
C
C ---    SECOND TERM = 0 , THE ORIGINAL SUM-RULE IS CALCULATED
C
           DO 800 IP = 1,IPMAX
              DO 700 LL=0,LMAX
                 SIG2(LL,IP) = 0.
 700          CONTINUE
 800       CONTINUE
C
         ELSE
C
C ---    FOR CHANNEL 1 THE SECOND TERM IS 0.
C
           DO 900 LL = 0,LMAX
              SIG2(LL,1) = 0.
 900     CONTINUE
C
C ---    SECOND TERM FOR I = 2,3, ... IPMAX
C
           DO 1100 IP = 2,IPMAX
C
              DO 1000 LL=0,LMAX
C
                 EXP1 = (LL-LCRF)/DEL
                 IF (EXP1 .LT. -87.) THEN
                    SIG2(LL,IP) = P(IP)
                 ELSE IF (EXP1 .GT. 87.) THEN
                    SIG2(LL,IP) = 0.
                 ELSE
                    SIG2(LL,IP) = P(IP) / (1.+EXP(EXP1))
                 END IF
C
```

```
1000      CONTINUE
C
1100  CONTINUE
C
        ENDIF
C
C ---    THE SUM - RULE CONDITION
C
        DO 1300 LL=0,LMAX
C
           SUM(LL) = 0.
C
           DO 1200 IP=1,IPMAX
              SUM(LL) = SUM(LL)+SIG1(LL,IP)+SIG2(LL,IP)
1200       CONTINUE
C
1300  CONTINUE
C
C ---    PARTIAL CROSS SECTIONS
C
        DO 1500 IP=1,IPMAX
C
           SIGMA1(IP) = 0.
           SIGMA2(IP) = 0.
C
           DO 1400 LL=0,LMAX
C
C ---          FOR THE FIRST TERM
C
              SIG1(LL,IP) = 10.*PILAM*(2.*LL+1)*STREU(LL)*SIG1(LL,IP)
     &                        /SUM(LL)
C
              SIGMA1(IP) = SIGMA1(IP) + SIG1(LL,IP)
C
C ---          FOR THE SECOND TERM
C
              SIG2(LL,IP) = 10.*PILAM*(2.*LL+1)*STREU(LL)*SIG2(LL,IP)
     &                        /SUM(LL)
```

```
C
           SIGMA2(IP) = SIGMA2(IP) + SIG2(LL,IP)
C
 1400   CONTINUE
C
 1500 CONTINUE
C
C ---  PRINT THE PARTIAL CROSS SECTIONS TO THE OUTPUT
C
      IF (INDEX(CPART,'y').NE.0 .OR. INDEX(CPART,'Y').NE.0) THEN
C
        OPEN (UNIT = 2,FILE = CFIL4)
C
        WRITE(2,*) ' PARTIAL CROSS SECTIONS'
        WRITE(2,*) CHEAD
        WRITE(2,*) 'THE INPUT FILE WAS        ',CFIL1
        WRITE(2,*) 'THE FIRST OUTPUT FILE IS  ',CFILEN
        WRITE(2,*) ' '
        WRITE(2,*) '  I   L     S1(I,L)      S2(I,L)'
C
        DO 1700 IP=1,IPMAX
           DO 1600 LL=0,LMAX
              WRITE (2,'(2I5,2E14.6)')IP,LL,SIG1(LL,IP),SIG2(LL,IP)
 1600      CONTINUE
 1700   CONTINUE
C
        CLOSE(2)
C
      ENDIF
C
C ---  SUM OF ISOTOPES
C
      DO 1800 IP=0,INT(Z3P(IPMAX))
        SIGZ1(IP) = 0.
        SIGZ2(IP) = 0.
 1800 CONTINUE
C
C ---  EXCLUDED CHANNELS
```

```
C
      DO 2000 IXCLD = 1,IZXCLD
C
        DO 1900 IP=1,IPMAX
C
           IF (Z3P(IP).EQ.(XCLD1(IXCLD)).AND.
     &        A3P(IP).EQ.(XCLD2(IXCLD))) THEN
           SIGMA1(IP) = 0.
              SIGMA2(IP) = 0.
           ENDIF
C
 1900   CONTINUE
C
 2000 CONTINUE
C
C ---  SUM THE ISOTOPES WITHOUT EXCLUDED CHANNELS
C
      DO 2100 IP=1,IPMAX
        SIGZ1(INT(Z3P(IP))) = SIGZ1(INT(Z3P(IP)))+SIGMA1(IP)
        SIGZ2(INT(Z3P(IP))) = SIGZ2(INT(Z3P(IP)))+SIGMA2(IP)
 2100 CONTINUE
C
C ---  PREPARATION FOR FIT AND OUTPUT (TAKE ONLY POINTS
C ---  WHERE AN EXPERIMENTAL POINT IS AVAIABLE )
C
      DO 2200 IN=1,NPT
        IZ = ZC(IN)
        SECTE(IN) = SIGZ1(IZ)
        SECTO(IN) = SIGZ1(IZ) + SIGZ2(IZ)
 2200 CONTINUE
C
C ---  END OF THE SUM-RULE MODEL
C
      RETURN
C
C ---  ERROR DESCRIPTIONS
C
 9000 WRITE(*,*) 'PROGRAM ABORTED WITH ERROR CODE = ',MIST+10
```

```
      WRITE(*,*)' '
      GOTO (9001,9002,9003),MIST
C
 9001 WRITE(*,*)'NUMBER OF CHANNELS IS GREATER
     &THAN THE DIMENSION OF THE ARRAY'
      WRITE(*,*)'PLEASE INCREASE   IPMAXP'
      STOP
C
 9002 WRITE(*,*)'THE LMAX RESULTING FROM THE SL -
     &PARAMETRIZATION IS'
      WRITE(*,*)'GREATER THAN THE DIMENSION OF THE L-
     &DEPENDING ARRAYS'
      WRITE(*,*)'PLEASE INCREASE   LMAXP'
      STOP
C
 9003 WRITE(*,*)'THE SHARP CUT-OFF LMAX IS GREATER THAN THE'
      WRITE(*,*)'L-DEPENDING ARRAYS'
      WRITE(*,*)'PLEASE INCREASE   LMAXP'
      STOP
C
      END
C
C*******************************************************************
C
C ---   SUBROUTINE FOR PROGRAM INPUT
C
      SUBROUTINE INPUT (CHEAD,A1,A2,Z1,Z2,CFIL1,ELAB,RL1,
     &                  DELTAL,LCRF,CFIL2,CFIL3,CFIL4,IZXCLD,
     &                  XCLD1,XCLD2,TEMP,R0C,ZC,Y,FEHL,M,NPT,
     &                  CFILEN,IWMAXP,IPMAXP,DEL)
C
      DIMENSION XCLD1(IPMAXP),XCLD2(IPMAXP),ZC(IWMAXP),
     &            Y(IWMAXP),FEHL(IPMAXP)
C
      CHARACTER*20 CFIL1,CFIL2,CFIL3,CFIL4,CFILEN
      CHARACTER*80 CHEAD,DUMMY
C
C ---   SHOW TITLE
```

```
C
      WRITE(*,*)' '
      WRITE(*,*)'     L     ight and                      Iliana Brancus'
      WRITE(*,*)'     I     ntermediate                   Juergen Wentz'
      WRITE(*,*)'     M     ass fragment emission             and'
      WRITE(*,*)'     E     xtended                     Hans-Ulrich Hohn'
      WRITE(*,*)'     S     um-rule                          July 1989'
      WRITE(*,*)' '
C
      WRITE (*,*)' INPUTFILE FOR INITIALIZING DATA       : '
      READ (*,'(A20)') CFIL1
C
      OPEN(UNIT=4,FILE=CFIL1)
C
C --- TITLE OF THE ACTUAL CALCULATION
C
      READ (4,'(A80)') DUMMY
      READ (4,'(A80)') CHEAD
      WRITE(*,*) CHEAD
C
C --- PROJECTILE    MASS    AND    CHARGE
C
      READ (4,'(A80)') DUMMY
      READ (4,*) A1
      READ (4,'(A80)') DUMMY
      READ (4,*) Z1
C
C --- TARGET        MASS    AND    CHARGE
C
      READ (4,'(A80)') DUMMY
      READ (4,*) A2
      READ (4,'(A80)') DUMMY
      READ (4,*) Z2
      READ (4,'(A80)') DUMMY
C
C --- ENERGY IN THE LAB-SYSTEM
C
      READ (4,*) ELAB
```

```
C
C ---  DIFFUSENESS IN L-SPACE OF THE TRANSMISSION
C      COEFFICIENTS
C
       READ (4,'(A80)') DUMMY
       READ (4,*) DEL
C
C ---  PARAMETRIZATION OF THE SL
C
       READ (4,'(A80)') DUMMY
       READ (4,*) RL1,DELTAL
C
C ---  L CR DYN   CALCULATED BY   D Y N F U S
C
       READ (4,'(A80)')DUMMY
       READ (4,*) LCRF
C
C ---  FILE WITH THE QGG TABLE
C
       READ (4,'(A80)') DUMMY
       READ (4,'(A20)') CFIL2
C
C ---  FILE NAME OF THE EXPERIMENTAL DATA
C
       READ (4,'(A80)') DUMMY
       READ (4,'(A20)') CFIL3
C
C ---  READ THE EXCLUDED CHANNELS
C
       READ (4,'(A80)') DUMMY
       READ (4,*) IZXCLD
C
       IF (IZXCLD.GT.IPMAXP) THEN
         MIST = 1
         GOTO 9000
       ENDIF
C
      READ (4,'(A80)') DUMMY
```

```
C
      DO 100 I = 1,IZXCLD
        READ (4,*) XCLD1(I),XCLD2(I)
 100  CONTINUE
C
      CLOSE(4)
C
C --- INPUT OF THE EXPERIMENTAL CROSS SECTIONS
C
      OPEN(UNIT=11,FILE=CFIL3)
C
      READ (11,'(A80)') DUMMY
      READ (11,*) NPT
      M = NPT
      WRITE (*,*)' NUMBER OF EXPERIMENTAL POINTS          : ',NPT
      WRITE (*,*)' '
C
      IF (NPT.GT.IPMAXP) THEN
        MIST = 2
        GOTO 9000
      END IF
C
      READ (11,'(A80)') DUMMY
      DO 200 I=1,NPT
        READ (11,*) ZC(I),Y(I),FEHL(I)
 200  CONTINUE
C
      CLOSE(11)
C
      WRITE (*,*)' OUTPUTFILE-NAME                    : '
      READ (*,'(A20)') CFILEN
C
      WRITE (*,*)' TEMP, R0C                     : '
      READ (*,*) TEMP,R0C
      WRITE (*,*)' TEMP = ',TEMP,'  R0C = ',R0C,'  DEL = ',DEL
      WRITE(*,*) ' '
C
      RETURN
```

```
C
C ---   ERROR DESCRIPTIONS
C
 9000  WRITE(*,*) 'PROGRAM ABORTED WITH ERROR CODE = ',MIST+20
       WRITE(*,*) ' '
       GOTO (9001,9002),MIST
C
 9001  WRITE(*,*)'NUMBER OF EXCLUDED CHANNEL IS GREATER THAN
      &THE DIMENSION OF THE ARRAY'
        STOP
C
 9002  WRITE(*,*)'NUMBER OF EXPERIMENTAL POINTS IS GREATER
      &THAN THE DIMENSION OF THE ARRAY'
       WRITE(*,*)'PLEASE INCREASE   IPMAXP'
       STOP
C
       END
C
C***************************************************************
C
C ---   SUBROUTINE FOR PROGRAM OUTPUT
C
       SUBROUTINE OUTPUT(CFIL1,CFIL2,CFIL3,CFIL4,CFILEN,X,ZC,
      &                   SECTE,SECTO,CFIT,CPART,CMOD,CSL,TEMP,
      &                   R0C,CHI2,NPT,CHEAD,IPMAXP,IPMAX,
      &                   SIGMA1,SIGMA2)
C
       DIMENSION ZC(IPMAXP),SECTO(IPMAXP),SECTE(IPMAXP),
      &          SIGMA1(IPMAXP),SIGMA2(IPMAXP)
C
       CHARACTER*20 CFIL1,CFIL2,CFIL3,CFIL4,CFILEN
       CHARACTER*20 CFIT,CPART,CMOD,CSL
       CHARACTER*80 CHEAD
C
       OPEN(UNIT=10,FILE=CFILEN)
C
       WRITE (10,*) '    TEMPERATURE       R0C        CHI2'
       WRITE (10,*) TEMP,R0C,CHI2
       WRITE (10,*) NPT
       WRITE (10,*) '    Z        S1        S1+S2'
       DO 400 I = 1,NPT
         WRITE (10,'(3E13.5)') ZC(I),SECTE(I),SECTO(I)
 400   CONTINUE
C
       WRITE(10,*)' '
       WRITE(10,*)'    ', CHEAD
       WRITE(10,*)' PARTIAL CROSS SECTIONS             ',CPART
       WRITE(10,*)' F I T - PROCEDURE                  ',CFIT
       WRITE(10,*)' NEW MODEL                          ',CMOD
       WRITE(10,*)' NORMALIZATION WITH SL              ',CSL
       WRITE(10,*)' '
       WRITE(10,*)' INPUT FILE WAS                     ',CFIL1
       WRITE(10,*)' QGG FILE WAS              ',CFIL2
       WRITE(10,*)' EXPERIMENTAL DATA FILE WAS   ',CFIL3
       WRITE(10,*)' '
C
       IF (INDEX(CFIT,'y').NE.0.OR.INDEX(CFIT,'Y').NE.0) THEN
         IF (KE.EQ.0) THEN
            WRITE(10,*) ' THE FIT ENDS WITHOUT ERRORS'
         ELSE
            WRITE(10,*) ' THE FIT ENDS WITH ERROR ',KE
         ENDIF
       ENDIF
C
       IF (INDEX(CPART,'Y').NE.0.OR.INDEX(CPART,'y').NE.0)
      &WRITE(10,*)' OUTPUT FOR THE PARTIAL CROSS SECTIONS IN
      &',CFIL4
C
C ---  RESULT FOR EACH CHANNEL
C
       WRITE(10,*) ' '
       WRITE(10,*) ' THE TOTAL CROSS SECTION FOR THE SINGLE
      &CHANNELS'
       WRITE(10,*) ' '
       WRITE(10,*) ' I     1. Term      2. Term       Sum'
C
```

```
      DO 500 I = 1,IPMAX
         WRITE(10,'(I4,3E15.4)')I,SIGMA1(I),SIGMA2(I),SIGMA1(I)
     &       +SIGMA2(I)
 500  CONTINUE
C
      CLOSE(10)
C
      RETURN
      END
C
C ****************** END OF LIMES *******************************
```

## 3.5 List of variables used in LIMES

The following gives a list in alphabetic order of all variables used in LIMES. The dimension of a variable is given by scalar (SCAL) or an array of the dimension n (ARR nD) and the type by integer (INT), character*n (CH*n) or real (REAL). The column REF gives a reference list through the single modules of LIMES :

| | | |
|---|---|---|
| M | - | MAIN program |
| S | - | SUMMOD subroutine |
| I | - | INPUT subroutine |
| O | - | OUTPUT subroutine |
| A | - | the variable is not local |

The last column gives the meaning of the variable, the italics terms are defined in chapter 2.

| Variable | Dim | Type | Ref | | Meaning |
|---|---|---|---|---|---|
| A | SCAL | REAL | S | | total mass ( $A_1 + A_2$ ) |
| A1 | SCAL | REAL | MSI | A | mass of the projectile |
| A2 | SCAL | REAL | MSI | A | mass of the target |
| A3 | SCAL | REAL | S | | mass of the ejectile |
| A3 | ARR 1D | REAL | MS | A | masses of the ejectiles |
| A4 | SCAL | REAL | S | | remaining mass ( A - $A_3$ ) |

| | | | | | |
|---|---|---|---|---|---|
| AI | SCAL | REAL | S | | $(N-Z)/A$ |
| ALAM | SCAL | REAL | S | | wave length $\lambda$ |
| ALAM2 | SCAL | REAL | S | | $\lambda^2$ |
| ALCR | ARR 1D | REAL | MS | A | critical angular momenta $l_{cr}(i)$ |
| ALIM | ARR 1D | REAL | MS | A | limiting angular momenta $l_{lim}(i\ )$ |
| AMU | SCAL | REAL | S | | atomic mass unit |
| ARED | SCAL | REAL | S | | reduced mass |
| AREDI | SCAL | REAL | S | | reduced mass of $A_1$ and A |
| AT | SCAL | REAL | S | | $\|A4 - A_2\|$ |
| BIN | SCAL | REAL | S | | Coulomb wall $B_{in}$ |
| C0 | SCAL | REAL | S | | $C_1$ + CT |
| C1 | SCAL | REAL | S | | half density radius of the projectile $C_1$ |
| C2 | SCAL | REAL | S | | half density radius of the target $C_2$ |
| CFIL1 | SCAL | CH*20 | MSIO | A | input file name |
| CFIL2 | SCAL | CH*20 | MSIO | A | $Q_{gg}$ file name |
| CFIL3 | SCAL | CH*20 | MIO | A | experimental data file name |
| CFIL4 | SCAL | CH*20 | MSIO | A | partial cross section file name |
| CFILEN | SCAL | CH*20 | MSIO | A | output file name |
| CFIT | SCAL | CH*20 | MO | A | flag, fit? (yes / no ) |
| CHEAD | SCAL | CH*80 | MSIO | A | title of the calculation |
| CIN | SCAL | CH*20 | M | A | flag, new calculation ? (yes / no ) |
| CL | SCAL | REAL | S | | AMU / $\hbar^2$ |
| CMOD | SCAL | CH*20 | MSO | A | flag, new model ( yes / no ) |
| CPART | SCAL | CH*20 | MSO | A | flag, partial cross sections ( yes / no ) |
| CSL | SCAL | CH*20 | MSO | A | flag, normalization with $S_l$ ( yes / no ) |
| CT | SCAL | REAL | S | | half density radius of AT |
| DEL | SCAL | REAL | MSI | A | diffuseness in $l$-space $\Delta l$ |
| DELTAL | SCAL | REAL | MSI | A | diffuseness in $l$-space $\Delta L$ |
| DUMMY | SCAL | CH*80 | SI | A | dummy |
| E | ARR 1D | REAL | M | | search accuracies |
| E1 | SCAL | REAL | S | | elementary charge |
| ECM | SCAL | REAL | S | | center of mass energy |
| ELAB | SCAL | REAL | MSI | A | laboratory energy |
| EXP1 | SCAL | REAL | S | | help variable |
| F | ARR 1D | REAL | M | | parameter functions |
| FEHL | ARR 1D | REAL | MI | | relative errors of experimental data points |
| GAM | SCAL | REAL | S | | surface energy coefficient |

| | | | | | |
|---|---|---|---|---|---|
| HC2 | SCAL | REAL | S | | $\hbar^2$ |
| I | SCAL | INT*4 | MIO | | loop counter |
| IN | SCAL | INT*4 | S | | loop counter |
| IP | SCAL | INT*4 | S | | loop counter for the channels |
| IPMAX | SCAL | INT*4 | MSIO | A | number of channels |
| IPMAXP | SCAL | INT*4 | MSIO | A | parameter for the dimension of the arrays which depend on the channels |
| ISTAT | SCAL | INT*4 | MS | A | flag which is 0 in the first fit loop |
| IW | ARR 1D | INT*4 | M | | control values of FITEX |
| IWMAXP | SCAL | INT*4 | MI | A | parameter for the dimension of the arrays in the fit procedure |
| IXCLD | SCAL | INT*4 | MIS | A | excluded channels |
| IZ | SCAL | INT*4 | S | | loop counter |
| IZXCLD | SCAL | INT*4 | MIS | A | number of excluded channels |
| KE | SCAL | INT*4 | M | | error variable of the fit procedure |
| L | SCAL | INT*4 | S | | loop counter for the angular momenta $l$ |
| LCRF | SCAL | INT*4 | MSIO | A | $l_{cr}{}^{dyn}$ |
| LL | SCAL | INT*4 | S | | loop counter for the angular momenta $l$ |
| LMAX | SCAL | INT*4 | S | | limit of the angular momenta |
| LMAXP | SCAL | INT*4 | MS | A | parameter for the arrays depending on the angular momentum |
| LOOP | SCAL | INT*4 | M | | loop counter |
| M | SCAL | INT*4 | M | | number of experimental points |
| MIST | SCAL | INT*4 | MSI | | error variable |
| N | SCAL | INT*4 | MSI | | number of free parameters |
| N | SCAL | INT*4 | S | | total neutron number |
| NPT | SCAL | INT*4 | MSIO | A | number of experimental points |
| P | ARR 1D | REAL | S | | probabilities $P( i )$ |
| P1 | SCAL | REAL | S | | 1./3. |
| PI | SCAL | REAL | S | | $\pi$ |
| PI4 | SCAL | REAL | S | | $4 * \pi$ |
| PILAM | SCAL | REAL | S | | $\pi * \lambda^2$ |
| PM1 | SCAL | REAL | S | | - 1./3. |
| QC | SCAL | REAL | S | | Coulomb correction |
| QGG | ARR 1D | REAL | MS | A | Q-values of the ground states |
| R0C | SCAL | REAL | MSIO | A | Coulomb interaction radius constant |

| | | | | | |
|---|---|---|---|---|---|
| R0T | SCAL | REAL | S | | 0.764 |
| R1 | SCAL | REAL | S | | $R_1$ |
| R2 | SCAL | REAL | S | | $R_2$ |
| RC | SCAL | REAL | S | | Coulomb interaction radius |
| RL1 | SCAL | REAL | MSI | | cut-off angular momentum $L_1$ |
| RT | SCAL | REAL | S | | $R_t$ |
| SECTE | ARR 1D | REAL | MSO | A | elemental cross sections (1. term). |
| SECTO | ARR 1D | REAL | MSO | A | elemental cross sections |
| SIG1 | ARR 2D | REAL | MS | A | general working array for the $\sigma_{1,l}(i)$ |
| SIG2 | ARR 2D | REAL | MS | A | general working array for the $\sigma_{2,l}(i)$ |
| SIGMA1 | ARR 1D | REAL | MSO | A | $\sigma_1(i)$ |
| SIGMA2 | ARR 1D | REAL | MSO | A | $\sigma_2(i)$ |
| SIGZ1 | ARR 1D | REAL | MS | A | $\sigma_1(Z)$ |
| SIGZ2 | ARR 1D | REAL | MS | A | $\sigma_2(Z)$ |
| STR1 | SCAL | REAL | S | A | dummy by calculating $S_l$ |
| STREU | ARR 1D | REAL | MS | A | $1 - \| S_l \|^2$ |
| SUM | ARR 1D | REAL | MS | A | sum over all unnormalized $\sigma_l(i)$ |
| TEMP | SCAL | REAL | MSIO | A | effective temperature |
| W | ARR 1D | REAL | M | | control array of FITEX |
| X | ARR 1D | REAL | M | | parameter array of FITEX |
| XCLD1 | ARR 1D | REAL | MSI | A | charge of the ejectiles of the excluded channels |
| XCLD2 | ARR 1D | REAL | MSI | A | mass of the ejctiles of the excluded channels |
| Y | ARR 1D | REAL | MI | A | experimental data points |
| Z | SCAL | REAL | S | | total charge |
| Z1 | SCAL | REAL | S | | charge of the projectile |
| Z2 | SCAL | REAL | S | | charge of the target |
| Z3 | SCAL | REAL | S | | charge of the ejectile |
| Z3P | ARR 1D | REAL | MS | A | charges of the ejectiles |
| Z4 | SCAL | REAL | S | | remaining charge |
| ZC | ARR 1D | REAL | MSIO | | ejectile charges associated to the experimental points |
| ZT | SCAL | REAL | S | | $\| Z_2 - Z4 \|$ |

# 4. The program DYNFUS

## 4.1 The critical angular momentum $l_{cr}^{dyn}$ for dissipative interaction processes in ion-ion collisions

While the formation of a completely equilibrated compound nucleus of the two interacting partners and the fast incomplete fusion processes can be assumed to be limited by a critical angular momentum value corresponding to a static fusion barrier (sudden approximation interaction potential), the cluster emission accompaning dissipative phenomena are limited by a l-value in the entrance channel angular momentum space which takes into account (energy and) orbital momentum dissipation due to tangential friction. C. Ngô et al. [8] have described a simple dynamical model for fusion and have worked out a computational procedure to determine the dynamical limit. Following this procedure the program DYNFUS calculates $l_{cr}^{dyn}$ for a given colliding system and incident energy.

## 4.2 Example describing the use DYNFUS

This chapter gives an example in evaluating the critical dynamical angular momentum for the reaction of 156 MeV $^{6}$Li + $^{nat}$Ag with the program DYNFUS. The use of the program is simple because only a minimum of input is required and the main output is $l_{cr}^{dyn}$. The following gives a listing of the interactive input and output of DYNFUS. By normal letters the output is indicated, bold letters show the input requested from the user:

```
CHARGE OF PROJECTILE          3.
MASS OF PROJECTILE            6.
CHARGE OF TARGET              47.
MASS OF THE TARGERT           108.
LAB ENERGY                    156.
ECM =                         147.78947449
   CA1,CA2 =     1.81712067   4.76220322
```

```
    CA     =     6.57932377
    R1,R2 =      2.10785985          5.52415562
    C1,C2 =      1.63344514          5.34313250
    C,CB  =      6.97657776          1.25100219
XK,FSTIXK =  6.35037231          0.19944586

BARRIER FOR L        =  0.000
POSITION  S          =  2.715   R =  9.692
HEIGHT  V =  19.597

 FOR L =      59          = = > NO FUSION
 FOR L =      29          = = > FUSION
 FOR L =      44          = = > FUSION
 FOR L =      51          = = > FUSION
 FOR L =      55          = = > NO FUSION
 FOR L =      53          = = > NO FUSION
 FOR L =      52          = = > NO FUSION

BARRIER FOR L =  52.000
 POSITION  S =   3.000   R =  9.977
   HEIGHT  V = 119.061

 END OF CALCULATION PROGRAM DYNFUS

CRITICAL L =  51

FUSION CROSS SECTION      =  2106.5  MB
DYNAMICAL ENERGY SURPLUS  =    28.73 MEV
```

This result of 51 $\hbar$ for the critical dynamical angular momentum was used in the example of sect. 3.2.

### 4.3 Listing of DYNFUS

The following is the standard FORTRAN 77 listing of the program DYNFUS:

```
      PROGRAM DYNFUS
C
C**********************************************************************
C
C     DYNAMICAL CALCULATION OF FUSION CROSS SECTIONS
C
C        SIMPLIFIED VERSION OF THE ORIGINAL PROGRAM
C        FROM THE PAPER "THE ROLE OF FUSION IN H. I. REACTIONS",
C        T.SUOMIJARVI, R.LUCAS, C.Ngô, E.TOMASI, D.DALILI AND
C        J. MATUSZEK, NUVO. CIM. 82A (1984) 56
C
C
C              Juergen Wentz      August 1989
C
C**********************************************************************
C
      COMMON /AREA/ C,CBAR,Z,XMU,XL,CR,CT,XLST,G,DL
      COMMON /CNTS/ IS
C
      DATA SI,SU,EPS/0.,6.,0.001/
      DATA PI/3.141592654/
C
C --- STATEMENT-FUNCTIONS
C
      VN(S)   = CBAR*EXP(-(S+1.6)**2/5.4)
      V(S)    = VN(S)+Z/(C+S)+XL*XL*DL/(C+S)**2
      DV(S)   = -(S+1.6)/2.7*VN(S)-Z/(C+S)**2-2.*DL*XL*XL/(C+S)**3
      D2V(S)  = VN(S)/2.7*(-1.+(S+1.6)**2/2.7)+
     &  2.*Z/(C+S)**3+6.*DL*XL*XL/(C+S)**4
      F1(S)   = Z/2./(C+S)+VN(S)*(1.-(S+1.6)*(C+S)/5.4)-E
C
      WRITE(*,*)' CHARGE OF PROJECTILE       '
      READ(*,*) Z1
      WRITE(*,*)' MASS OF PROJECTILE         '
      READ(*,*) A1
      WRITE(*,*)' CHARGE OF TARGET           '
      READ(*,*) Z2
      WRITE(*,*)' MASS  OF THE TARGET        '
      READ(*,*) A2
      WRITE(*,*)' LAB ENERGY                    '
      READ(*,*) ELAB
      ECM=ELAB*A2/(A1+A2)
      WRITE(*,*)' ECM =                      ',ECM
C
C---  INITIALIZING
C
      XMU    = A1*A2 / (A1+A2)
      DL     = 20.83 / XMU
      Z1Z2   = Z1 * Z2
      Z      = 1.44 * Z1Z2
      EE     = 1. / 3.
      CR     = 31000.
      CT     = CR * 0.5
      CA1    = A1**EE
      CA2    = A2**EE
      CA     = CA1 + CA2
      R1     = 1.16 * CA1
      R2     = 1.16 * CA2
      C1     = R1 - 1./R1
      C2     = R2 - 1./R2
      C      = C1 + C2
      CB     = C1 * C2/C
      CBAR   = -34. * CB
      XK     = 0.2191 * SQRT(ECM*XMU)
      FSTICK= 1./(1.+(A1*CA1*CA1+A2*CA2*CA2)/(2.5*XMU*CA*CA))
C
      WRITE(*,*)' CA1,CA2  = ',CA1,CA2
      WRITE(*,*)'    CA    = ',CA
      WRITE(*,*)'  R1,R2   = ',R1,R2
      WRITE(*,*)'  C1,C2   = ',C1,C2
      WRITE(*,*)'  C,CB    = ',C,CB
      WRITE(*,*) 'XK,FSTIXK = ',XK,FSTICK
C
C---  ALGORITHM
C
      XL   = 0.
      XX1  =  SI
      XX2  =  SU
      Y1   =  DV(SI)
      Y2   =  DV(SU)
C
 101  CONTINUE
C
      X=(XX1+XX2)*0.5
      Y=DV(X)
      IF (Y*Y1.GT.0.) XX1=X
      IF (Y*Y2.GT.0.) XX2=X
      IF (ABS(XX1-XX2).GE.EPS) GOTO 101
      S0   =  X
      R12  =  C+S0
      V12  =  V(S0)
      D2   =  D2V(S0)
C
      IF (ECM .LE. V12) THEN
        WRITE(*,'(" INPUT ENERGY LOWER THEN THE BARRIER!")')
        GOTO 9999
      ENDIF
C
      IF (D2 .GE. 0.) THEN
        WRITE(*,'(" NO POCKET IN THE POTENTIAL FOR L = ",F4.1)') XL
        WRITE(*,'(" ***** NO FUSION *****")')
        GOTO 9999
      ENDIF
C
      WRITE(*,'(/" BARRIER FOR L = ",F7.3/"  POSITION  S = ",F7.3,
     &  "   R =",F7.3/"    HEIGHT  V = ",F7.3/)') XL,S0,R12,V12
      E     =ECM
      XX1   =SI
      XX2   =SU
      Y1    =F1(SI)
      Y2    =F1(SU)
C
 102  CONTINUE
C
```

```
      X    = (XX1+XX2)*0.5
      Y    = F1(X)
      IF (Y*Y1.GT.0.) XX1=X
      IF (Y*Y2.GT.0.) XX2=X
      IF (ABS(XX1-XX2).GE.EPS) GOTO 102
      S1   = X
      R1   = S1+C
      XL1  = (ECM-VN(S1)-Z/R1)/DL*R1*R1
C
      IF (XL1.LE.0.) THEN
        WRITE(*,'(" BE CAREFUL: ECM < BARRIER")')
        GOTO 9999
   ENDIF
C
      XL1  = SQRT(XL1)
      L1   = INT(XL1+0.5)
      XL1  = L1
      T0   = 0.
      TF   = 1000.
      H    = .1
      N    = TF/H
      NF   = 0
      XLA  = 0.
      XLB  = 2.*XL1
C
 105 CONTINUE
C
      XLI    = (XLA+XLB)*0.5
      XLI    = AINT(XLI)
      XLST   = XLI*FSTICK
      R0     = 20.
      XL     = XLI
      S0     = R0-C
      DR0    = -3.*SQRT((ECM-V(S0))/(XMU*465.75))
      CALL RK(T0,R0,DR0,XLI,TF,RF,DRF,XLF,H,EPS,N,NF)
      LI=INT(XLI)
C
      IF (NF.EQ.2) THEN
```

```
         WRITE(*,*)' FOR L =',LI,' = = > FUSION'
         IF (XLI.NE.XL1) XLA=XLI
       ELSE
         WRITE(*,*)' FOR L =',LI,' = = > NO FUSION'
         XLB=XLI
       ENDIF
C
       IF (ABS(XLB-XLA).GT.1.) GOTO 105
       LCR  =XLI+0.5
       IF (NF.NE.2) LCR=XLI-1.+0.5
       SEC  =10.*PI/(XK*XK)*(LCR+1)**2
       XL   =XLI
C
 109   CONTINUE
C
       XX1  =  SI
       XX2  =  SU
       Y1   =  DV(SI)
       Y2   =  DV(SU)
C
 112   CONTINUE
C
       X =  (XX1+XX2)*0.5
       Y =  DV(X)
       IF (Y*Y1.GT.0.) XX1=X
       IF (Y*Y2.GT.0.) XX2=X
       IF (ABS(XX1-XX2).GE.EPS) GOTO 112
       SF=X
       D2=D2V(SF)
C
       IF (D2.GE.0.) THEN
         XL=XL-1.
         GOTO 109
       ENDIF
C
       XL   =XLI
       R12  =C+SF
       V12  =V(SF)
```

```
      DE    =ECM-V12
C
      WRITE(*,'(/" BARRIER FOR L = ",F7.3/"  POSITION  S = ",F7.3,
     &  "   R =",F7.3/"    HEIGHT  V = ",F7.3/)') XLI,SF,R12,V12
      WRITE(*,*)' END OF CALCULATION PROGRAM DYNFUS '
      WRITE(*,'(/" CRITICAL L = ",I4//
     &   " FUSION CROSS SECTION      =",F8.1," MB"/
     &   " DYNAMICAL ENERGY SURPLUS  =",F9.2," MEV"/)')
     &   LCR,XLF,SEC,DE
C
 9999 CONTINUE
      STOP
      END
C
C ***************************************************************
C
      SUBROUTINE RK(T1,R1,DR1,FL1,TF,RF,DRF,FLF,H,EPS,N,NF)
C
      COMMON /CNTS/ IS
C
      ANS1=10000.
      ANS2=10000.
      ANS3=10000.
C
      NF=0
C
      DO 10 J=1,10
        T=T1
        R=R1
        DR=DR1
        FL=FL1
        DO 20 I=1,N
           A1=H*DR
           B1=H*RKV(T,R,DR)
           C1=H*RKL(T,R,FL)
           A2=H*DR
           B2=H*RKV(T+H*0.5,R+A1*0.5,DR+B1*0.5)
           C2=H*RKL(T+H*0.5,R+A1*0.5,FL+C1*0.5)
```

```
          A3=H*DR
          B3=H*RKV(T+H*0.5,R+A2*0.5,DR+B2*0.5)
          C3=H*RKL(T+H*0.5,R+A2*0.5,FL+C2*0.5)
          A4=H*DR
          B4=H*RKV(T+H,R+A3,DR+B3)
          C4=H*RKL(T+H,R+A3,FL+C3)
C
          A=(A1+A2+A2+A3+A3+A4)/6.
          B=(B1+B2+B2+B3+B3+B4)/6.
          C=(C1+C2+C2+C3+C3+C4)/6.
 1      IF (R.LT.3.) THEN
            T=808.
          ELSE
            T=T+H
            R=R+A
            DR=DR+B
            FL=FL+C
          ENDIF
          IF (R.GT.20..AND.DR.GT.0.) GOTO 30
          IF (T.GT.800.) NF=2
          IF (NF.EQ.2) GOTO 30
 20     CONTINUE
C
        IF (ABS(R-ANS1).LT.EPS.AND.ABS(DR-ANS2).LT.EPS.AND
     &     ABS(FL-ANS3).LT.EPS) GOTO 30
        H=H*0.5
        N=N*2
        ANS1=R
        ANS2=DR
        ANS3=FL
 10    CONTINUE
C
       IF (J.LT.10) GOTO 30
       WRITE(*,'(" BE CAREFUL: J =",I3,
     &   " DIVERGENCE OF THE INTEGRATION ROUTINE")') J
       RETURN
C
 30    CONTINUE
```

```
C
      RF   =R
      DRF  =DR
      FLF  =FL
C
      RETURN
      END
C
C ************************************************************
C
      FUNCTION RKL(T,R,FL)
C
      COMMON /AREA/ C,CBAR,Z,XMU,XL,CR,CT,XLST,G,DL
      COMMON /CNTS/ IS
C
      RKL=-CT*G*(FL-XLST)/(103.5*XMU)
      XL=FL
C
      RETURN
      END
C
C***************************************************************
C
      FUNCTION RKV(T,R,DR)
C
      COMMON /AREA/ C,CBAR,Z,XMU,XL,CR,CT,XLST,G,DL
      COMMON /CNTS/ IS
C
      S=R-C
      IS=IS+1
      GH=(S+1.6)**2/5.4
C
      IF (ABS(GH).GT.38.) THEN
        GH=0.
      ELSE
        GH=EXP(-GH)
      ENDIF
C
```

```
      P1=CBAR*GH
      P3=-(S+1.6)/2.7*P1-Z/(C+S)**2-2.*DL*XL*XL/(C+S)**3
      G=0.
C
     IF (S.LT.2.5) THEN
        GH=(S-0.75)*5.
        G=1.
      IF (ABS(GH).LT.38.) G=1./(1.+EXP(GH))
      ENDIF
C
      RKV=(-P3-CR*G*DR)/(103.5*XMU)
C
      RETURN
      END
```

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# Appendix A:$Q_{gg}$ table of the reaction of 156 MeV $^{6}$Li + $^{nat}$Ag

A complete listing of the $Q_{gg}$-table which was used in the example of sect. 3.2 as input file LIAG.QGG:

```
156 MeV 6-Li + nat-Ag   Qgg - Table
95
   Z      A         Qgg
   0.,    0.,       14.674
   0.,    1.,       7.022
   1.,    1.,       6.509
   1.,    2.,       1.253
   1.,    3.,       -2.251
   2.,    3.,       1.059
   2.,    4.,       11.985
   2.,    5.,       3.937
   3.,    5.,       0.132
   4.,    7.,       -0.516
   4.,    8.,       8.984
   4.,    9.,       3.522
   4.,    10.,      0.838
   5.,    9.,       -0.214
   5.,    10.,      1.421
   5.,    11.,      3.735
   5.,    12.,      -0.134
   6.,    11.,      3.886
   6.,    12.,      13.147
   6.,    13.,      11.59
   6.,    14.,      10.282
   6.,    15.,      4.353
   7.,    13.,      5.507
   7.,    14.,      9.509
   7.,    15.,      11.658
   7.,    16.,      7.117
   7.,    17.,      3.769
   8.,    15.,      9.86
```

| | | |
|---|---|---|
| 8., | 16., | 17.049 |
| 8., | 17., | 14.803 |
| 8., | 18., | 13.939 |
| 8., | 19., | 10.79 |
| 8., | 20., | 8.97 |
| 9., | 17., | 8.182 |
| 9., | 18., | 10.874 |
| 9., | 19., | 13.015 |
| 9., | 20., | 12.55 |
| 9., | 21., | 11.98 |
| 9., | 22., | 9.607 |
| 9., | 23., | 6.61 |
| 10., | 19., | 10.166 |
| 10., | 20., | 18.99 |
| 10., | 21., | 19.143 |
| 10., | 22., | 21.072 |
| 10., | 23., | 19.298 |
| 10., | 24., | 16.394 |
| 11., | 21., | 11.362 |
| 11., | 22., | 16.045 |
| 11., | 23., | 20.759 |
| 11., | 24., | 20.939 |
| 11., | 25., | 20.234 |
| 11., | 26., | 15.458 |
| 11., | 27., | 12.902 |
| 11., | 28., | 7.14 |
| 12., | 24., | 24.442 |
| 12., | 25., | 25.685 |
| 12., | 26., | 27.257 |
| 12., | 27., | 26.262 |
| 12., | 28., | 23.454 |
| 12., | 9., | 18.291 |
| 13., | 25., | 15.483 |
| 13., | 26., | 20.942 |
| 13., | 27., | 25.398 |
| 13., | 28., | 25.707 |
| 13., | 29., | 24.926 |
| 13., | 30., | 21.958 |

| | | |
|---|---|---|
| 13., | 31., | 18.521 |
| 13., | 32., | 14.038 |
| 14., | 28., | 28.124 |
| 14., | 29., | 30.271 |
| 14., | 30., | 30.659 |
| 14., | 31., | 29.952 |
| 14., | 32., | 28.402 |
| 14., | 33., | 25.285 |
| 14., | 34., | 21.542 |
| 15., | 9., | 19.23 |
| 15., | 30., | 24.552 |
| 15., | 31., | 27.601 |
| 15., | 32., | 27.601 |
| 15., | 33., | 28.493 |
| 15., | 34., | 25.09 |
| 15., | 35., | 23.23 |
| 15., | 36., | 21.012 |
| 15., | 37., | 16.592 |
| 16., | 34., | 31.605 |
| 16., | 35., | 31.753 |
| 17., | 37., | 29.832 |
| 18., | 39., | 32.343 |
| 19., | 43., | 31.175 |
| 20., | 47., | 36.919 |
| 21., | 49., | 37.606 |
| 22., | 50., | 42.616 |
| 23., | 52., | 40.01 |
| 24., | 54., | 43.27 |
| 25., | 56., | 40.074 |

# Appendix B:Output of LIMES in the reaction of 156 MeV $^{6}$Li + $^{nat}$Ag

The following is the complete listing of the outputfile LIAG1.OUT of the example in sect. 3.2:

```
    TEMPERATURE        R0C               CHI2
    3.88781190         1.45962882        6.23308372
14
Z                  S1                S1+S2
0.10000E+01        0.13215E+02       0.24932E+03
0.20000E+01        0.18346E+02       0.15544E+03
0.40000E+01        0.17073E+01       0.25236E+01
0.50000E+01        0.37672E+00       0.59500E+00
0.60000E+01        0.83643E+00       0.13971E+01
0.70000E+01        0.11192E+00       0.19891E+00
0.80000E+01        0.11162E+00       0.21282E+00
0.90000E+01        0.15381E-01       0.32005E-01
0.10000E+02        0.25003E-01       0.55866E-01
0.11000E+02        0.76905E-02       0.18564E-01
0.12000E+02        0.11670E-01       0.30312E-01
0.13000E+02        0.28836E-02       0.80661E-02
0.14000E+02        0.42667E-02       0.12867E-01
0.15000E+02        0.91436E-03       0.29729E-02

156 MeV 6-Li + nat-Ag
PARTIAL CROSS SECTIONS       N
F I T - PROCEDURE            Y
NEW MODEL                    Y
NORMALIZATION WITH SL        Y

INPUT FILE WAS                      LIAG.IN
QGG FILE WAS                        LIAG.QGG
EXPERIMENTAL DATA FILE WAS          LIAG.EXP

THE FIT ENDS WITHOUT ERRORS
```

THE TOTAL CROSS SECTION FOR THE SINGLE CHANNELS

| I | 1. Term | 2. Term | Sum |
|---|---|---|---|
| 1 | 0.4052E+03 | 0.0000E+00 | 0.4052E+03 |
| 2 | 0.5529E+02 | 0.1307E+04 | 0.1363E+04 |
| 3 | 0.9562E+01 | 0.1731E+03 | 0.1827E+03 |
| 4 | 0.2471E+01 | 0.4479E+02 | 0.4726E+02 |
| 5 | 0.1182E+01 | 0.1819E+02 | 0.1937E+02 |
| 6 | 0.6477E+00 | 0.6955E+01 | 0.7603E+01 |
| 7 | 0.1472E+02 | 0.1156E+03 | 0.1303E+03 |
| 8 | 0.2976E+01 | 0.1458E+02 | 0.1756E+02 |
| 9 | 0.3277E+00 | 0.9660E+00 | 0.1294E+01 |
| 10 | 0.3049E+00 | 0.1557E+00 | 0.4607E+00 |
| 11 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 12 | 0.9795E+00 | 0.4400E+00 | 0.1419E+01 |
| 13 | 0.4229E+00 | 0.2206E+00 | 0.6435E+00 |
| 14 | 0.6539E-01 | 0.3462E-01 | 0.1000E+00 |
| 15 | 0.8793E-01 | 0.5272E-01 | 0.1407E+00 |
| 16 | 0.1638E+00 | 0.9560E-01 | 0.2594E+00 |
| 17 | 0.5960E-01 | 0.3534E-01 | 0.9494E-01 |
| 18 | 0.3354E-01 | 0.2208E-01 | 0.5562E-01 |
| 19 | 0.3650E+00 | 0.2391E+00 | 0.6041E+00 |
| 20 | 0.2391E+00 | 0.1602E+00 | 0.3993E+00 |
| 21 | 0.1645E+00 | 0.1144E+00 | 0.2790E+00 |
| 22 | 0.3423E-01 | 0.2490E-01 | 0.5913E-01 |
| 23 | 0.1096E-01 | 0.8042E-02 | 0.1900E-01 |
| 24 | 0.2990E-01 | 0.2251E-01 | 0.5241E-01 |
| 25 | 0.5010E-01 | 0.3913E-01 | 0.8923E-01 |
| 26 | 0.1493E-01 | 0.1217E-01 | 0.2710E-01 |
| 27 | 0.6027E-02 | 0.5143E-02 | 0.1117E-01 |
| 28 | 0.7592E-02 | 0.6388E-02 | 0.1398E-01 |
| 29 | 0.4657E-01 | 0.4059E-01 | 0.8717E-01 |
| 30 | 0.2511E-01 | 0.2278E-01 | 0.4789E-01 |
| 31 | 0.1926E-01 | 0.1824E-01 | 0.3750E-01 |
| 32 | 0.8192E-02 | 0.8115E-02 | 0.1631E-01 |
| 33 | 0.4902E-02 | 0.5081E-02 | 0.9983E-02 |
| 34 | 0.1201E-02 | 0.1162E-02 | 0.2363E-02 |
| 35 | 0.2311E-02 | 0.2322E-02 | 0.4633E-02 |

|  |  |  |  |
|---|---|---|---|
| 36 | 0.3849E-02 | 0.4028E-02 | 0.7877E-02 |
| 37 | 0.3275E-02 | 0.3574E-02 | 0.6849E-02 |
| 38 | 0.2710E-02 | 0.3086E-02 | 0.5797E-02 |
| 39 | 0.1410E-02 | 0.1676E-02 | 0.3086E-02 |
| 40 | 0.6247E-03 | 0.7755E-03 | 0.1400E-02 |
| 41 | 0.5284E-03 | 0.5856E-03 | 0.1114E-02 |
| 42 | 0.4922E-02 | 0.5666E-02 | 0.1059E-01 |
| 43 | 0.4921E-02 | 0.5893E-02 | 0.1081E-01 |
| 44 | 0.7762E-02 | 0.9679E-02 | 0.1744E-01 |
| 45 | 0.4722E-02 | 0.6133E-02 | 0.1085E-01 |
| 46 | 0.2148E-02 | 0.2906E-02 | 0.5054E-02 |
| 47 | 0.2062E-03 | 0.2603E-03 | 0.4665E-03 |
| 48 | 0.6625E-03 | 0.8680E-03 | 0.1531E-02 |
| 49 | 0.2144E-02 | 0.2918E-02 | 0.5062E-02 |
| 50 | 0.2160E-02 | 0.3057E-02 | 0.5217E-02 |
| 51 | 0.1733E-02 | 0.2550E-02 | 0.4283E-02 |
| 52 | 0.4880E-03 | 0.7464E-03 | 0.1234E-02 |
| 53 | 0.2433E-03 | 0.3868E-03 | 0.6300E-03 |
| 54 | 0.5317E-04 | 0.8786E-04 | 0.1410E-03 |
| 55 | 0.1792E-02 | 0.2656E-02 | 0.4449E-02 |
| 56 | 0.2378E-02 | 0.3657E-02 | 0.6035E-02 |
| 57 | 0.3434E-02 | 0.5479E-02 | 0.8913E-02 |
| 58 | 0.2561E-02 | 0.4242E-02 | 0.6804E-02 |
| 59 | 0.1199E-02 | 0.2060E-02 | 0.3259E-02 |
| 60 | 0.3061E-03 | 0.5460E-03 | 0.8521E-03 |
| 61 | 0.6279E-04 | 0.1011E-03 | 0.1639E-03 |
| 62 | 0.2469E-03 | 0.4117E-03 | 0.6585E-03 |
| 63 | 0.7496E-03 | 0.1295E-02 | 0.2045E-02 |
| 64 | 0.7832E-03 | 0.1402E-02 | 0.2186E-02 |
| 65 | 0.6183E-03 | 0.1147E-02 | 0.1765E-02 |
| 66 | 0.2781E-03 | 0.5346E-03 | 0.8127E-03 |
| 67 | 0.1109E-03 | 0.2209E-03 | 0.3318E-03 |
| 68 | 0.3379E-04 | 0.6972E-04 | 0.1035E-03 |
| 69 | 0.5759E-03 | 0.1075E-02 | 0.1651E-02 |
| 70 | 0.9668E-03 | 0.1868E-02 | 0.2835E-02 |
| 71 | 0.1032E-02 | 0.2064E-02 | 0.3097E-02 |
| 72 | 0.8318E-03 | 0.1721E-02 | 0.2553E-02 |
| 73 | 0.5396E-03 | 0.1155E-02 | 0.1695E-02 |

| | | | |
|---|---|---|---|
| 74 | 0.2339E-03 | 0.5181E-03 | 0.7521E-03 |
| 75 | 0.8636E-04 | 0.1978E-03 | 0.2842E-03 |
| 76 | 0.2410E-04 | 0.4856E-04 | 0.7266E-04 |
| 77 | 0.9167E-04 | 0.1909E-03 | 0.2826E-03 |
| 78 | 0.1943E-03 | 0.4182E-03 | 0.6126E-03 |
| 79 | 0.1880E-03 | 0.4182E-03 | 0.6063E-03 |
| 80 | 0.2289E-03 | 0.5261E-03 | 0.7549E-03 |
| 81 | 0.9230E-04 | 0.2192E-03 | 0.3115E-03 |
| 82 | 0.5536E-04 | 0.1359E-03 | 0.1912E-03 |
| 83 | 0.3029E-04 | 0.7680E-04 | 0.1071E-03 |
| 84 | 0.9409E-05 | 0.2464E-04 | 0.3405E-04 |
| 85 | 0.2283E-03 | 0.5629E-03 | 0.7912E-03 |
| 86 | 0.2298E-03 | 0.5847E-03 | 0.8145E-03 |
| 87 | 0.6594E-04 | 0.1852E-03 | 0.2511E-03 |
| 88 | 0.6410E-04 | 0.1981E-03 | 0.2622E-03 |
| 89 | 0.2475E-04 | 0.8885E-04 | 0.1136E-03 |
| 90 | 0.6154E-04 | 0.2547E-03 | 0.3162E-03 |
| 91 | 0.4772E-04 | 0.2148E-03 | 0.2625E-03 |
| 92 | 0.1249E-03 | 0.5949E-03 | 0.7198E-03 |
| 93 | 0.4864E-04 | 0.2509E-03 | 0.2996E-03 |
| 94 | 0.9273E-04 | 0.5170E-03 | 0.6097E-03 |
| 95 | 0.3637E-04 | 0.2186E-03 | 0.2550E-03 |