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USER'S MANUAL FOR THE CODE SIAPRE AS  
IMPLEMENTED AT LAWRENCE LIVERMORE NATIONAL  
LABORATORY

H. Vonach

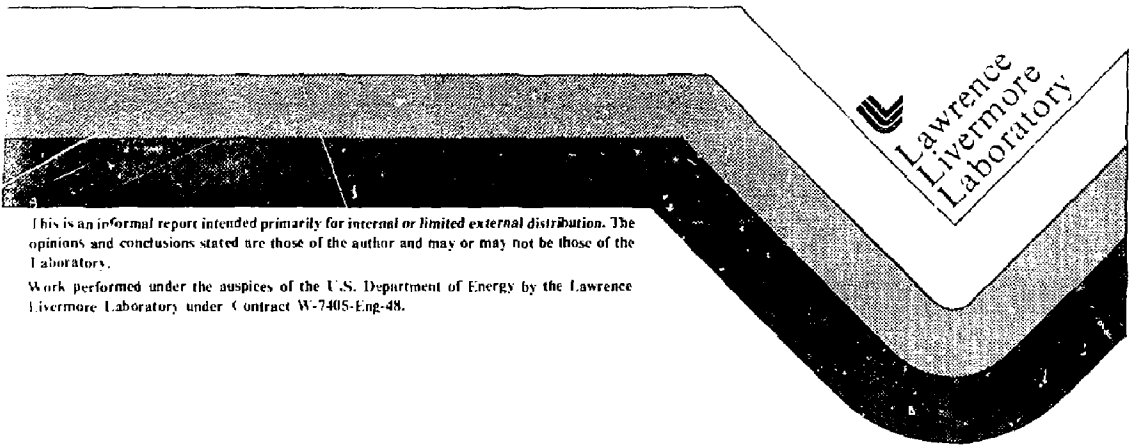
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**MASTER**

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1. ABSTRACT

This report gives a detailed description of the input and output of the statistical model code STAPRE including a special section on the various level density options of the code.

It is to be used in conjunction with the report IRK 76/01 + Add 76 + Add 78 by B. Strohmaier and M. Uhl which describes in detail the physical models on which the code is based and its general organization and structure.

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## 2. INTRODUCTION

The statistical model code STAPRE has been described in detail by B. Strohmaier and M. Uhl.<sup>1,2</sup> In Ref. 1 the authors give a general description of the models used in the code, the structure of the code, the required input parameters and the output which can be obtained by the program. In addition Ref. 1 gives some recommendations on the choice of the input parameters, and examples on the influence of various model parameters on the calculated cross-sections. Reference 2, written as a manual for use of the code at Vienna, gives a complete description of the models used in the code including all equations used for all program options and detailed instructions for preparing the input for the code as implemented in Vienna.

This report is meant as an amendment to Ref. 2, in order to make it easier to use the code as implemented at present at Lawrence Livermore National Laboratory.

It contains the following information:

- 1) A description of the input to STAPRE for the slightly modified Livermore version of STAPRE.
- 2) A detailed description of both the basic program output and the various additional output options.
- 3) A detailed description on the various level density options possible in STAPRE. This section summarizes the information given at different location in IRK 76/01 and its Addendum 1978 and gives detailed instructions on how to use the most important level density models with STAPRE.
- 4) A description of the STAPRE energy grid which is essential for understanding many details of the STAPRE output.

As already discussed this report is essentially an amendment to IRK 76/01. It therefore can only be used effectively in conjunction with that report.

### 3. INPUT FOR THE STATISTICAL MODEL CODE STAPRE AS IMPLEMENTED AT THE LLNL COMPUTER

#### 3.1) General Organization of Input:

Two input files have to be provided:

- a) a transmission coefficient file containing all particle transmission coefficients needed in the calculations, except those for non-standard particles.
- b) an input file containing all other information.

#### 3.2) Transmission Coefficient File:

The transmission coefficient file has to provide sets of transmission coefficients  $T_{\ell}$  for at least 4 energies for each kind of particle used in the calculation. The transmission coefficients have to be listed in the sequence: neutrons, protons,  $\alpha$ -particles, deuterons but only for those particles to be actually used as specified in card 3 of input file.

For each particle the  $T_{\ell}$  sets have to be listed in order of increasing energy. The transmission coefficients have to be provided as function of c.m. (channel) energy. A maximum of 104 energies and corresponding transmission coefficient sets is accepted by the program.

A file of this kind can be generated by means of the program OPTLN (see description of that program by F.S. Dietrich). To do this, optical potentials have to be provided in the order n, p, d,  $\alpha$  to OPTLN and a list of increasing energies for each potential for which the transmission coefficients are to be calculated.

Before the output file produced by OPTLN can be used by STAPRE, one line of title has to be added to it. (Most useful is some information on the potentials used.)

The program uses the transmission coefficient file to calculate transmission coefficients for all particle energies needed by 3rd order interpolation of  $\ln T_{\ell}(E_p)$  versus particle energies  $E_p$ . Therefore, the number of energies (at least 4!) and their distribution has to be chosen to allow this interpolation to be done with sufficient accuracy.

For neutrons calculations should be done for rather closely spaced energies (e.g., .01, .03, .05, .07, .1, .3, .5, .7 and 1.0) below one MeV, for higher energies the spacings can be increased to 1-2 MeV; for charged

particles energy spacing varying from 0.5 MeV at the coulomb barrier to about 2 MeV well above the barrier have proved to be adequate. In general the change of the total reaction cross-section with energy can be used as a good basis for deciding on the input energies for OPTLN.

If a particle other than n, p, d, or  $\alpha$  (a so-called non-standard particle), is used as projectile, the transmission coefficients for that particle are not contained in the transmission coefficient file but have to be supplied as a block of cards 12 in the input file.

### 3.3) Input File

#### 1) Title

FORMAT (8A10)

Title of the problem

Note: The first column must contain a # as indicator of the beginning of a new problem.

#### 2) Information on kind of projectile and emitted particles

NLAUF (I), I = 1,7

FORMAT (7I2)

NLAUF (1) ---code for the projectile

NLAUF (I)  $I \geq 2$  ---code for the particle emitted from the (I-1)<sup>th</sup> CN

Note: Code numbers for the particles are:

- 1 ...neutron
- 2 ...proton
- 3 ...alpha particle
- 4 ...deuteron
- 99 ...non-standard particle (only allowed as projectile)

Therefore:  $1 \leq \text{NLAUF (I)} \leq 4$  or  $\text{NLAUF (I)} = 99$  for  $I = 1$ ,

$1 \leq \text{NLAUF (I)} \leq 4$  for  $I \geq 2$ .

Examples: ( $\alpha, p$ )                   ...b3b2  
 (n,  $\gamma$ )                         ...b1  
 ( $^{16}_0, 3n\alpha$ )                   ...99b1b1b1b3

3) General information on options to be used in calculations.

N, NGACOM, NPAR, LLMAX, DU, NFISS, NPHI

Col 1-2 (I2) N ...total number of compound nuclei  $1 \leq N \leq 6$

Col 3-4 (I2) NGACOM...number of the compound nucleus for which gamma-ray cascades are taken into account for the first time.

$1 \leq \text{NGACOM} \leq N$  that is at least the last compound nucleus must be allowed to emit photons. Examples:  $N = 3$ ,  $\text{NGACOM} = 2$ : only particle emission from CN 1, in addition photon emission by 2. and 3. CN.

Col 5-6 (I2) NPAR...types of particles whose emission is accounted for in the Hauser-Feshbach denominator

- 1 ...neutrons only
- 2 ...neutrons, protons
- 3 ...neutrons, protons, alpha particles
- 4 ...neutrons, protons, alpha particles, deuterons

Therefore,  $1 \leq \text{NPAR} \leq 4$ . In addition NPAR must be chosen large enough to contain the incident particle (if n, p,  $\alpha$  or d) and all particles needed for the reaction chain specified in card 2.

Col 7-8 (I2) LLMAX ...maximum multipolarity of  $\gamma$ -rays

- 1 ...E1 and M1 radiation
- 2 ...E1, M1, E2, M2 radiation
- 3 ...E1, ..., M3 radiation

Therefore,  $1 \leq \text{LLMAX} \leq 3$ .

Col 9-13(F5.3) DU...binsize (MeV) of the energy grid

Note: DU must be larger than the maximum number of bins the program can handle (at present 80 or 200 in the Livermore versions of STAPRE) divided by the excitation energy of the first CN.

Col 14-15(I2) NFISS...code for the calculation of fission cross sections

- 0... fission decay is ignored
- 1... fission decay is taken into account as described in section 1 of Add 1978 of IRK 76/01
- 2... fission decay is taken into account. For the WF-corrected first chance fission cross section, however, all continuum fission channels are treated as one single channel. The fluctuation index of this channel is derived from MNFRI (see card 4.) and a generalized  $\chi^2$  distribution equivalent to the actual distribution up to the second moment.

Col 16-17(I2) NPHI...code for the treatment of the averaging of the WF-corrected first chance fission cross section with respect to intermediate class II structure; leave blank if fission is ignored.

0... Eq. (11') is used  
>0... Eq. (11 of Add 1978 to IRK 76/01) is used. In this case the maximum number of meshpoints for the integration with respect to E is  $2^{NPHI} + 1$ . Recommended values for NPHI are 5 or 6. If the prescribed accuracy DDEL (cf. record 4.) is not achieved a message is printed out ("PHI INTEGRATION ACCURACY DEL= NOT ACHIEVED..."). In this case NPHI should be increased. The computation time which is considerable for NPHI > 0 can be reduced by putting NFISS equal to 2.

4) Input parameters for width fluctuation correction

NNWFC, GRE, NNFREI, DDEL, NNINT

Col 1-2(I2) NNWFC... switch for the width fluctuation correction

0...on  
1...off

Col 3-8(F6.2) GRE ... limit for the Hauser-Feshbach denominator above which the width fluctuation correction factor is put equal to unity (cf. section 4. of IRK 76/01)  
Note: If columns 3 to 8 are left blank, GRE = 50 is assumed.

Col 9-10(I2) NNFREI... fluctuation index for the width fluctuation correction (cf. section 2.2. of IRK 76/01)  
Note: If columns 9 and 1 are left blank, NNFREI = 1 is assumed.

Col 11-16(F6.3) DDEL... prescribed relative accuracy for the integration in the width fluctuation correction (cf. section 4. of IRK 76/01).

Note: If columns 11 to 16 are left blank, DDEL = .01 is assumed.

Col 17-20(I4) NNINT... maximum number of mesh-points for the calculation of the integral in the width fluctuation correction.

Note 1: NNINT must be a power of 2.

Note 2: If NNINT = 0 the program assumes NNINT= 64.

Note 3: If NNINT > 64 the program assumes NNINT= 64.



In general it is sufficient to leave card 4 blank and leave it to the program to decide on the amount of WFC needed in the calculation.

If it is obvious that no WFC is necessary because of sufficient exit channels for the first CN some time can be saved by switching the WFC off (NNWFC = 1).

5) Chemicals symbols and charge numbers of compound nuclei

(PARC (I,1), PARC (I,2)), I = 1, N

Col 1-2(A2)	PARC (1,1) ... chemical symbol	} of 1 <sup>st</sup> CN
Col 3-5(F3.0)	PARC (1,2) ... charge number	
Col 5-6(A2)	PARC (2,1) ... chemical symbol	} of 2 <sup>nd</sup> CN
Col 8-10(F3.0)	PARC (2,2) ... charge number	

and so on until last CN.

6) Information on target nucleus

ATAR, STAR, KPTAR, Q

Col 1-4(F4.1)	ATAR ... mass number	} of the target nucleus
Col 5-8(F4.1)	STAR ... spin	
Col 9-10(I2)	KPTAR... parity (+1 or -1)	
Col 11-16(F6.2)	Q ..... separation energy (MeV) of the projectile from the 1 <sup>st</sup> CN	

Note 1: If the projectile is n, p,  $\alpha$  or d, columns 11 - 16 may be left blank, because Q is determined by other input data.

Note 2: If the projectile has negative parity, KPTAR has to be replaced by its opposite. This may be the case for non-standard projectiles.

7) Information on projectile

Col 1-4(F4.0)	AGESCH... mass number	} of projectile
Col 5-8(F4.1)	SGESCH... spin	

This card is needed for non-standard projectiles and has to be omitted if projectile is n, p,  $\alpha$  or d.

8) Information on incident energies

- Col 1-6(F6.2) EEINL... L.S. bombarding energy (MeV). The program alters the incident energy in such a way as to adjust the excitation energy of the first CN to the nearest upper edge of a bin of the energy grid defined by DU.
- Col 7-8(I2) KDE... the incident energy can be varied stepwise in such a way that the excitation energy of the first CN is reduced by  $KDE * DU$  by each step. ( $KDE > 0$ ).
- Col 9-11(I3) KKZMM... number of incident energies - generated from EEINL as described above - for which the calculations are done. For  $KKZMM = 0$  the program assumes  $KKZMM = 1$ .

9) Parameters for precompound particle emission from 1st CN.

FM, NPI, NHI, IPAULI, KTESTP, MILANO, PHIMIL

- Col 1-8(F8.1) FM ..... the constant ( $\text{MeV}^3$ ) which by Eq. (7) of IRK 76/0) defines the matrix element for internal transitions competing with pre-equilibrium decay. For  $FM = 0$ , pre-equilibrium decay is not taken into account.
- Col 9-10(I2) NPI ..... initial particle number
- Col 11-12(I2) NHI ..... initial hole number
- Col 13-14(I2) IPAULI... switch for inclusion of the Pauli principle in the calculation of internal transition rates.
- 0 ... off  
1 ... on
- Col 15-16(I2) KTESTP... code for the parameters  $g$  and  $D\Delta$  in Eq. (10') of Addenda, Sept. 1976.
- 0 or 1...  $g = \frac{6 A}{\pi^{28}}$ ,  $D\Delta = 0$
- 2 or 3...  $g = \frac{6 A}{\pi^{28}}$ ,  $D\Delta = 12 A^{-1/2} * \begin{cases} 0 \text{ for odd} \\ 1 \text{ for odd mass} \\ 2 \text{ for even} \end{cases}$  nuclei
- 4 or 5...  $g = \frac{6 A}{\pi^{28}}$ ,  $D\Delta = \Delta$
- 6 or 7...  $g = \frac{6}{\pi^2} a$ ,  $D\Delta = 0$
- 8 or 9...  $g = \frac{6}{\pi^2} a$ ,  $D\Delta = \Delta$

Col 17-18(12) MILANO... switch for the calculation of the emission rates for nucleon-induced reactions.  
0...Eq. (9) of IRK 76/01 is used for  $\lambda(n, \nu)_{dev}$   
1...Eqs. (9') and (9'') of Addenda, Sept. 1976 are used for the emission rates of nucleons and alpha particles, respectively.

Col 19-24(F6.2) PHIMIL... the probability  $\phi$  in Eq. (9'') of Addenda, Sept. 1976

Note 1: For odd values of KTESTP internal transition rates and some other quantities related to preequilibrium decay are printed out.

Note 2: For PHIMIL  $< 0$  for alpha particle emission rates Eq. (9) of IRK 76/01 is used instead of Eq. (9'') of Addenda, Sept. 1976.

Note 3: For MILANO = 1 the program assumes the following values for the initial numbers of particles and holes: NPI = 2, NHI = 1.

#### 10) Output Options

##### KTEST1, KTEST2, KTEST3, KTESTW, KGAPR

Col 1-2(12) KTEST1... switch for printing level densities, the contributions to the Hauser-Feshbach denominator of the different particles and of photons, the fission probabilities, the total decay widths and gamma strength functions and gamma transmission coefficients.

0 ... off  
1 ... on

Col 3-4(12) KTEST2... switch for printing the quantities  $WB(E, I, \pi)$  DU and  $\overline{WB}(E, I, \pi)$  DU (cf. section 2. of IRK 76/01)

0 ... off  
1 ... on

Col 5-6(12) KTEST3... switch for printing particle and, if calculated, gamma-ray spectra resulting from the decay of the different compound nuclei.

0 ... off  
1 ... on

Col 7-8(12) KTESTW... key for the extension of the protocol of the calculation of the width fluctuation correction

0 ... very short  
1 ... very detailed and long

Col 9-10(I2)      KGAPR... key for printing production cross sections for gamma-rays from discrete levels

0 or 1 ... none  
 $\geq 2$  ...for the levels 2, ..., J ( $J = \min(\text{number of discrete levels, KGAPR})$ )

11) Separation energies for all particles evaporated from each CN.

The following cards have to be supplied for all compound nuclei ( $I = 1, N$ ).

11.1)      PARR (I,K) K = 1, NPAR (as defined in card 3)

Col 1-6(F6.2)	Separation Energy (MeV) for n	}      from 1st CN
Col 7-12(F6.2)	Separation Energy (MeV) for p	
Col 13-18(F6.2)	Separation Energy (MeV) for $\alpha$	
Col 19-24(F6.2)	Separation Energy (MeV) for d	

11.2)      Same information for CN2

...etc.

Note:      Only separation energies for particles to be considered according to choice of NPAR (card 3) have to be given.

12) Data regarding transmission coefficients for non-standard incoming particles

12.1)

Col 1-2(I2)      LMAX ... number of partial waves

12.2)

Col 1-80(8A10)      TEXT ... alpha numerical text

The following blocks of data (12.3) and (12.4) must be supplied for the LMAX partial waves with ascending orbital angular momentum 0, 1, 2, ..., LMAX-1.

12.3)

Col 1-2(I2)      NN      number of energy values for which transmission coefficients of the orbital angular momentum considered are prepared. Restriction:  $4 < NN < 104$ .

12.4) X(II), Y(II), II = 1, NN, 8 pairs of energies and transmission coefficients per card, in order of increasing energy.

FORMAT (8(F4.2, E5.3))

X(II) ... energy (MeV)

Y(II) ... transmission coefficient for energy X(II)

Note: The block of data 12.) must be omitted for standard incoming particles (n, p, d,  $\alpha$ ).

13) Control parameter for choice of transmission coefficient sets

Col 1-2(I2) NTRAN

Note: NTRAN can assume two values only: 1 or N:

1... a single set of transmission coefficients is used for all CN.

N... number of compound nuclei, each CN has its own set of transmission coefficients.

Note: A single set of transmission coefficients will be sufficient in most cases (NTRAN = 1).

Version NTRAN = N has not yet been tested with the slightly modified Livermore STAPRE version using the transmission coefficient file!

14) Information on the level density, of the first compound nucleus

	DC	(L)...	level density parameters for the first compound nucleus.	
Col 1-6(F6.0)	DC	(1)...	a (MeV <sup>-1</sup> )	Fermi-Gas level density parameters
Col 7-12(F6.0)	DC	(2)...	$\theta_{\text{eff}}/\theta_{\text{rigid}}$	$\theta_{\text{rigid}} \approx$ rigid body moment of inertia with $r_0=1.25$ fm
Col 13-18(F6.0)	DC	(3)...	$\Delta$ (MeV)	Ground-state energy shift for Fermi-Gas
Col 19-24(F6.0)	DC	(4)...	$\delta W$ (MeV)	Parameter in Ignatyuk model.

Col 25-30(F6.0)	DC	(5)...	$E_1^t$ (MeV)	} Parameters for 1st constant temperature part of level density
Col 31-36(F6.0)	DC	(6)...	$C_1$ (MeV <sup>-1</sup> )	
Col 37-42(F6.0)	DC	(7)...	$T_1$ (MeV)	
Col 43-48(F6.0)	DC	(8)...	$\sigma_1$	
Col 49-54(F6.0)	DC	(9)...	$E_2^t$ (MeV)	} Parameters for 2nd constant temperature part of level density
Col 55-60(F6.0)	DC	(10)...	$C_2$ (MeV <sup>-1</sup> )	
Col 61-66(F6.0)	DC	(11)...	$T_2$ (MeV)	
Col 67-72(F6.0)	DC	(12)...	$\sigma_2$	
Col 73-78(F6.0)	DC	(13)...	$\theta_1 / \theta_{rigid}$	

Note: If an energy dependent a-parameter is used (cf. Eq. (16) of Add. 1978 to IRK 76/01), that is, if  $\delta W \neq 0$  the input datum a represents the asymptotic a-parameter a.

Col 79-80(I2) ISYMC... code for the angular momentum dependence of the level density

- 0... Eq. (14) standard Fermi-Gas formula
- 1... Eq. (17) with  $G_{ax} = 1/2$
- 2... Eq. (17) with  $G_{ax} = 1$
- 3... Eq. (18) with  $G_{ns} = 1/4$
- 4... Eq. (18) with  $G_{ns} = 1/2$
- 5... Eq. (18) with  $G_{ns} = 1$
- 1... the level density is calculated by means of Eq. (29) if IRK 76/01 = Lang's form of Fermi-Gas formula

The above Symbols are explained in more detail in IRK 76/01 and Add. 1978 to IRK 76/01. For Fermi-gas model use just D(1)-DC(3), ignore DC(4)-DC(13) and choose desired form of Fermi-Gas model by means of quantity ISYMC as explained in Section 5 of this report. Concerning use of Gilbert-Cameron model see also Section 5 of this report.

15) Information on level scheme and gamma-decay properties of first CN

This information is only to be given if gamma-emission from first CN is allowed (NGACOM = 1 in card 3).

15.1)

Col 1-2(I2) NDISK = number of discrete levels to be used in calculation  $1 \leq \text{NDISK} \leq 50$

15.2(I) Properties of discrete levels, 6 levels per card, as many cards as needed for all NDISK levels.

15.2(1)

Col 1-6(F6.2)	ED	(1)	Excitation energy	} of ground state
Col 7-10(F4.1)	SD	(1)	Spin	
Col 11-12(F2)	KPD	(1)	Parity	
			.	
Col 61-66(F6.2)	ED	(6)	Excitation energy	} of fifth excited level
Col 67-70(F4.1)	SD	(6)	Spin	
Col 71-72(I2)	KPD	(6)	Parity	

15.2(2)

Col 1-6(F6.2)	ED	(7)	Excitation energy	} of sixth excited level
Col 7-10(F6.1)	SD	(7)	Spin	
Col 11-12(I2)	KPD	(7)	Parity	

and so on until ED, SD and KPD are listed for all NDISK levels. The levels have to be listed in order of ascending energy.

15.3) Information on continuum gamma-decay properties

15.3(1)

Col 1-6(F6.2)	UB	Neutron separation energy of CN1		
Col 7-10(F4.1)	S1	Lower spin of s-wave resonances in CN1		
Col 11-14(F4.1)	S2	Higher spin of s-wave resonances in CN1		
Col 15-16(I2)	KP	Parity of s-wave resonances in CN1		

Note 1: UB is already given in record 11.1, but needed by the program a second time at this stage.

Note 2: S1 and S2 are equal to  $I + 1/2$  and  $I - 1/2$ , I being the ground state spin of the nucleus reached from CN1 by emission of one neutron, KP is the parity of that ground state. If  $I = 0$ , both S1 and S2 have to be given the value 0.5.

Col 17-23(F7.3)	GR:	average radiation width in meV at the neutron binding energy in CN1.		
-----------------	-----	--	--	--

Note: For GR = 0 the total radiation width is calculated according to D.G. Gardner.<sup>3</sup>

Col 24-25(I2) NF: number of subsequent cards to specify the E1 strength functions.

Note 1: At present only values of  $N_F = 0$  and  $N_F = 1$  are allowed.

Note 2: For  $N_F = 0$  all  $\gamma$ -ray strength functions are derived from the Weisskopf model.

For  $N_F = 1$  the E1 strength function is derived from the giant resonance model (with optional addition of a Weisskopf contribution), all other strength functions are Weisskopf.

Col 26-34(E9.3) PG(1): normalization factor for E1 strength function  $f_{\gamma E1}(E_\gamma)$

Note: For PG(1) = 0 the normalization is carried out by fitting the total radiation width to GR. For PG(1) = 1, the strength function is given the values predicted by either the Weisskopf model or the giant resonance parameters, as given in the following card 15.3 depending on the value of  $N_F$ . For other values of PG(1) the strength functions are obtained by multiplication of the above mentioned predictions with the numerical value of PG(1).

Col 35-43(F9.3) PG(2) =  $f_{\gamma M1}(E_\gamma = UB) / f_{\gamma E1}(E_\gamma = UB)$

Col 44-52(F9.3) PG(3) =  $f_{\gamma E2}(E_\gamma = UB) / f_{\gamma E1}(E_\gamma = UB)$

Col 53-61(F9.3) .

Col 62-70(F9.3) .

Col 71-79(F9.3) PG(6) =  $f_{\gamma M3}(E_\gamma = UB) / f_{\gamma E1}(E_\gamma = UB)$

Note: For PG(I) = 0, ( $2 \leq I \leq 6$ ) the quantities PG(I) are put equal to the ratios of the Weisskopf units.

Note: PG(I), I = 2,5 are absolute strength function ratios at the neutron binding energy, not Weisskopf enhancement factors!

15.3(2) Information on the E1 giant resonance parameters. Photo-absorption cross sections may be calculated as sum of up to 3 different resonances.

Col 1-6(F6.2) ERR (1)...position (MeV)

Col 7-12(F6.2) GRR (1)...width (MeV)

Col 13-18(F6.2) SRR (1)...peak cross section (mb)

} for the 1<sup>st</sup> giant resonance of the photo absorption cross section.



Col 19-24(F6.2)	ERR (2)...position	}	of 2 <sup>nd</sup> resonance
Col 25-30(F6.2)	GRR (2)...width		
Col 31-36(F6.2)	SRR (2)...peak cross section		
Col 37-42(F6.2)	ERR (3)...position	}	of 3 <sup>rd</sup> resonance.
Col 43-48(F6.2)	GRR (3)...width		
Col 49-54(F6.2)	SRR (3)...peak cross section		

Note 1: For ERR (L) = 0. (L ≥ 2) the L<sup>th</sup> resonance will not be taken into account.

Note 2: For ERR (1) = 0, a single E1 giant resonance defined by the Brink-Axel parameters (ERR (1) = 80 · A<sup>-1/3</sup>, GRR (1) = 5, SRR (1) = 13 · A/5) will be assumed.

Col 55-60(F6.2)	ES1...lower limit (MeV) of the step	}	mentioned in Eq. (28) of IRK 76/01,
Col 61-66(F6.2)	ES2...upper limit (MeV) of the step		
Col 67-72(F6.2)	FRS...reduction factor (0 ≤ FRS ≤ 1)		

Note: If columns 55 to 78 are left blank, no step is taken into consideration.

Col 73-78(F6.2) QSP...fraction of the Weisskopf contribution

$f_{\gamma E1}^{\text{Weisskopf}}$  to the strength function  $f_{\gamma E1}^{\text{photo abs.}}(\epsilon_{\gamma})$ :

$$f_{\gamma E1}^{\text{Weisskopf}} = \text{QSP} * f_{\gamma E1}^{\text{photo abs.}}(\epsilon_{\gamma} = \text{UB}) .$$

Note: If NF = 0 (see 15.3.1) the card 15.3.2 has to be omitted.

15.4(I) Information on  $\gamma$ -branching ratios for transitions between discrete levels. One card is needed for each of the NDISK discrete levels.

(VZD (L,M), M = 1, L), L = 1, NDISKC

FORMAT (25 F3.0)

VZD (L,M) branching ratio for the gamma transitions from the L<sup>th</sup> to the M<sup>th</sup> level of the 1<sup>st</sup> CN.

Note 1: NDISKC is the number of discrete levels which are in order of ascending energy, of the 1<sup>st</sup> CN.

Note 2: The VZD (L,M) need not be normalized.

Note 3: For a stable or isomeric level VZD (L,M) = 0. for all M.

Thus the set of branching ratio cards looks as follows:

15.4(1) blank

15.4(2)

Col 1-3(F3.0) VZD(2,1) = "Branching Ratio" for transition from the first excited to the ground state.

15.4(3)

Col 1-3(F3.0) VZD (3,1) Br.R. from 2<sup>nd</sup> excited level to ground state.

Col 4-6(F3.0) VZD (3,2) Br.R. from 2<sup>nd</sup> excited level to 1. excited level.

15.4 (NDISK)

Col 1-3(F3.0) VZD(NDISK+1)

Col 3(NDISK-1) - 3(NDISK1) VZD(NDISK+(NDISK-1))

Note 1: Up to 50 discrete levels may be used by the program in general, however branching ratios can be included only for transitions ending at levels 1-25. Transitions to higher levels cannot be specified in the program and must be ignored.

Note 2: If no information on branching ratios is available or no information on the  $\gamma$ -cascades is needed all branching ratio cards should have a 1. in column 1-3, otherwise blank. In this case the program will assume ground-state gamma-decay for all discrete levels and correctly calculate the ground-state population.

16) Information on level densities and discrete levels of residual nuclei reached in decay of 1<sup>st</sup> CN.

16.1) Level density of residual nucleus in format of card 14.

16.2) Number of discrete levels NDISK in format of card 15.1.

16.3(I) Energies, spin and parities of discrete levels in format of cards 15.2(I).

Information 16.1-16.3 has to be provided for all residual nuclei taken into account according to choice of NPAR in card 3 in the order:

1. Residual Nucleus reached by n-emission
2. " " " by p-emission
3. " " " by  $\gamma$ -emission
4. " " " by d-emission

17) Information on the gamma-decay properties of second compound nucleus.

17.1) Information on continuum gamma-decay.  
Properties in format of cards 15.3.1 and 15.3.2.

17.2(1) Gamma decay-branching ratios in format of cards 15.4(1).

Cards 17.1-17.2(1) have to be omitted if no- $\gamma$ -emission is allowed from that compound nucleus according to choice of NGACOM in card 3.

Note: No level density and discrete level information is needed for the second and any further compound nuclei as this is already contained in the information for the preceding residual nuclei.

18) Information on residual nuclei formed by decay of second compound nucleus identical to that described in 16.

19) For each further compound nucleus a block of information 17 + 18 (18 only, if no  $\gamma$ -emission is taken into account) has to be provided.

Note 1: At least for the last compound nucleus  $\gamma$ -decay must be taken into account and information 17.1-17.2(1) has to be provided.

Note 2: In many cases the last compound nucleus will not have enough energy to emit any particles. However even in this case information 18) on level densities and discrete levels of the possible (but inaccessible) residual nuclei is needed. Dummy values e.g., just one level with  $E = 0$ ,  $I = 0$ ,  $P = +1$  may be used.

The following blocks 20 and 21.NB.1 to 21.NB.3 refer to fission. They have to be omitted if in card 3.)-NFISS is specified as zero.

20) BARR (L), L = 1, 12), NSTEP

	BARR (L) ...	parameters of the deformation potential described in section 1.3.1. and illustrated in Fig.1. of Add. 1978 to IRK 76/01.
Col 1-6 (F6.2)	BARR (1) ...	$E_A$
Col 7-12 (F6.2)	BARR (2) ...	$\hbar\omega_A$
Col 13-18 (F6.2)	BARR (3) ...	$E_B$
Col 19-24 (F6.2)	BARR (4) ...	$\hbar\omega_B$
Col 25-30 (F6.2)	BARR (5) ...	$E_{II}$
Col 31-36 (F6.2)	BARR (6) ...	$\hbar\omega_{II}$
Col 37-42 (F6.2)	BARR (7) ...	$W_D$
Col 43-48 (F6.2)	BARR (8) ...	$W_I$
Col 49-54 (F6.2)	BARR (9) ...	$QQ_I$
Col 55-60 (F6.2)	BARR (10) ...	$QQ$
Col 61-66 (F6.2)	BARR (11) ...	$\rho$
Col 67-72 (F6.2)	BARR (12) ...	unassigned
Col 73-76 (14)	NSTEP ...	number of meshpoints for integration of Eq. (13 of ADD. 1978 to IRK 76/01).

(MeV)

(MeV)

Note 1: From the quantities BARR (L) the control parameter NBARR is derived as follows:

- i. NBARR = 1 if BARR (L) = 0 for L > 3 indicating that a single humped fission barrier is assumed.
- ii. NBARR = 2 if BARR (L) = 0 for L > 5 indicating that a double humped barrier and complete damping in the secondary minimum is assumed.
- iii. NBARR = 3 if BARR (5) > 0 and BARR (6) > 0 indicating that a double humped barrier and partial damping in the secondary minimum is assumed. Only in this case Eq. (13 of Add. 1978 to IRK 76/01) is solved.

Note 2: If columns 61 to 66 are left blank,  $\rho = 2$  is assumed.

Note 3: NSTEP < INDE \* INDJ (see IRK 76/01 for INDE and INDJ); if columns 73 to 76 are left blank, NSTEP is determined by an internal criterion.

The following blocks 21.NB.1 to 21.NB.3 refer to the barrier transition states which are discussed in sec. 1.3.2. of addendum 1978 to IRK 76/01. Depending on the value assigned to NBARR (cf. Note 1 to card 20) they have to be supplied for NB = 1, NBARR; that is, for the single humped barrier if NBARR = 1, for barrier A (NB = 1) and barrier B (NB = 2) if NBARR = 2 and for barrier A (NB = 1), barrier B (NB = 2) and the combined barrier AB (NB = 3) if NBARR = 3.

21.NB.1 Level density parameters for the continuum of the transition states in form of card 14.

21.NB.2 Parameters related to the discrete transition states (cf. sec. 1.3.2. of addendum 1978 to IRK 76/01).

Col 1-2(I2)	NFISSD (NB) ...	number of bandheads ( $\leq 10$ )
Col 3-8(F6.0)	DFISS (1, NB)...	rotational constant $A_r$ (keV)
Col 9-14(F6.0)	DFISS (2, NB)...	decoupling parameter $c$
Col 15-20(F6.0)	DFISS (3, NB)...	unassigned
Col 21-26(F6.0)	DFISS (4, NB)...	the continuum of transition states starts at the lower edge of the first bin (binsize DU) above DFISS (4, NB).

Note 1: DFISS (4, NB) is given in MeV

Note 2: For DFISS (4, NB) = 0 all transition states are treated as continuum and the following cards 21.NB.3 have to be omitted

21.NB.3 Information on heads of rotational bands in order of increasing excitation energy, 6 bandheads on first card, if number of bandheads NFISSD (NB) larger use second card.

FORMAT (6(F6.2, F4.1, I2))

Col 1-6 (F6.2)	EB (1, NB)...	excitation energy (MeV)	} of the 1st bandhead
Col 7-10(F4.1)	KB (1, NB)...	K quantum number	
Col 11-12(I2)	PB (1, NB)...	parity (+1 or -1)	

and so on until EB (NFISSD,NB), KB(NFISSD,NB) and PB(NFISSD,NB).

Note 1: For  $K = 0$  bands and axial symmetric shapes with R-symmetry the spin sequence is:

$I = 0, 2, 4, \dots$  if  $ISYM(NB) = 0$  or  $1$  and  $KB(L,NB) = 0$ ;

$I = 1, 3, 5, \dots$  if  $ISYM(NB) = 0$  or  $1$  and  $KB(L,NB) = 0.1$ .

Note 2:  $EB(L,NB)$  is referred to the lowest transition state

Note 3: For  $PB(L, NB) = 2$  it is assumed that there are two bandheads with  $EB(L, NB)$  and  $KB(L, NB)$  one with positive and one with negative parity.

#### 4 STAPRE OUTPUT

##### 4.1) Summary

The STAPRE code produces a short basic output containing the main results of the calculation, as cross sections for formation of the ground and isomeric states of all compound nuclei involved in the reaction chain and the particle and photon production cross section summed over the whole reaction chain.

In addition the program will produce more detailed output depending on the choice of the various output control parameters in card 10 of input. In this way 5 kinds of additional output may be provided.

- 1) Level densities, contributions to Hauser-Feshbach denominator by the different kinds of particles and photons, total decay widths, fission probabilities, gamma-ray strength functions, and transmission coefficients.
- 2) Continuum populations of the various compound nuclei both before and after  $\gamma$ -decay from higher lying levels.
- 3) Particle and gamma-spectra resulting from the decay of the different compound nuclei.
- 4) Detailed protocol on width fluctuation correction.
- 5) Gamma-ray production cross-sections for transitions between the discrete levels of all CN.

A detailed description of both the basic and optional output is given in the following sections.

4.2) Basic Output

- 1) Title of problem.
- 2) Information on how many CN may be formed at the maximum excitation energy specified in input.
- 3) Title line of transmission coefficients file.
- 4) (N) Input parameters used in calculations of the decay of the various CN:
 

4(N)1	Continuum $\gamma$ -decay parameters of CN	
4(N)2	Level density parameters of CN	
4(N)3(NPAR)1	Particle Separation Energy	}
4(N)3(NPAR)2	Level density parameters	
4(N)3(NPAR)3	Energies spins, parities of discrete levels	

of residual nuclei reached by n, p,  $\alpha$ , d emission in that order.

Particle separation energy is the energy needed to separate the evaporated particle from CN to reach ground-state of the respective residual nucleus.

Note 1: Information 4(N)1 is given only for those compound nuclei, which are allowed to emit  $\gamma$ -rays according to the choice of NGACOM.

Note 2: Information on residual nuclei is given only for those actually used in the calculation according to the choice of NPAR in card 3.

- 5) Adjusted input energy actually used in the calculations.
- 6) Total reaction cross section for projectile at the adjusted input energy.
- 7) Information on pre-equilibrium decay:
  - 7.1) Internal transition rates (in  $\text{sec}^{-1}$ ) for transition between  $n$ ,  $n-2$ , and  $n+2$  excites states, starting with  $n_i = NP + NH$  the sum of initial particle and hole numbers specified in input card 9 up to  $n_{\text{max}}$  where equilibrium is reached.
  - 7.2) Continuum decay rates ( $\text{sec}^{-1}$ ) for the  $n$ -exciton states from  $n_i$  to  $n_{\text{max}}$ .
  - 7.3) Branching ratios between continuum emission and the three kinds of allowed internal transitions for all steps of the pre-equilibrium decay.
  - 7.4) Table showing how much particle emission occurs during the various steps of the pre-equilibrium decay.

- 7.5) Excitation energy of the composite system = excitation energy of CN1.
- 7.6)  $|\text{Matrix element}|^2$  for internal transitions used in the calculation according to the choice of quantity FM in input card 9.
- 7.7) Pre-equilibrium fraction = fraction of composite nuclei decaying by particle emission of any kind during pre-equilibrium decay. Thus fraction = 1 minus the pre-equilibrium fraction that gets equilibrated to CN1.
- 7.8) Sum over pre-equilibrium spectrum = total cross-section for emission of the particle leading to CN2 during pre-equilibrium decay.

Note: Pre-equilibrium fraction refers to emission of all kinds of particles; sum over pre-equilibrium spectrum only to emission of one kind of particle (leading to CN2); therefore in general, sum over pre-equilibrium spectrum < pre-equilibrium fraction x total reaction cross section.

- 8) Spin and parity distribution for the levels in CN1 formed by absorption of projectile in target at the chosen bombardment energy (population cross section in b).
- 9) Information on use of width-fluctuation correction (WFC).  
Table showing the effective number of open channels for decay of CN1 for all possible J and  $\pi$  values, information for which of these decays a WFC has been applied.
- 10) Information whether photon decay of CN1 is permitted.
- 11) "Sum over primary spectrum" which is total cross section for primary photon emission from CN1.
- 12) Cross sections for primary gamma transitions from initial state in CN1 to discrete levels in CN1.
- 13) Total population cross sections for discrete levels of CN1 by either primary  $\gamma$ -transitions or gamma cascades.
- 14) Total production cross sections for ground state and possible isomeric levels in CN1.
- 15) Activation (total production) cross sections for CN1.  
Note: Information 11-15 is obviously only given if CN1 is allowed to emit photons (NGACOM = 1 in card 3).
- 16) Second printout of sum over primary spectra which then means total emission cross section for particle leading from CN1 to CN2.



- 17) Information on population of subsequent compound nuclei. For all subsequent compound nuclei the following information is printed:
- 17.1) egrc: position of ground-state of CN in energy grid (relative to ground-state of CN1).
  - 17.2) Kgrc: Nr of energy bin, which contains ground-state of CN.
  - 17.3) Cross-sections for population of discrete levels by particle emission from preceding CN.
  - 17.4) Total population cross-sections for discrete levels including gamma-cascades from continuum.
  - 17.5) Remaining continuum population (due to angular momentum restrictions).
  - 17.6) Total population cross-sections for ground-state and all isomeric levels of CN.
  - 17.7) Activation cross-section = total production cross-section for CN = sum of cross-sections for ground-state and all isomeric states.
- Note: Information 17.4 - 17.7 is of course given only for compound nuclei allowed to emit photons.
- 18) Summary of results
- 18.1) Adjusted bombarding energy in lab and c.m.
  - 18.2) Total reaction cross section for projectile at adjusted bombardment energy.
  - 18.3) Some input parameters on  $\gamma$ -decay and pre-equilibrium emission:
    - NGACOM = Nr of first CN allowed to emit photons
    - I<sub>l</sub> max = max. multi-polarity allowed in  $\gamma$ -emission
    - f<sub>m</sub> = quantity FM in input card 9 determining size of matrix element for internal transitions in pre-equilibrium decay
    - npi, nhi = NPI, NPH initial particle and hole numbers specified in input card 9
  - 18.4) Activation (total production) cross sections for all CN allowed to emit photons (and thus being able to reach its ground-state).

18.5) Particle and photon production cross-section for the total evaporation cascade.

Note 1: Angle-integrated cross-sections are given as function of channel energy in the c.m. system. Unit: b/MeV of channel energy.

Note 2: Only those particles are considered, which lead subsequently from CN1 via CN2...to CNN, particle production cross-sections for competing decays are not calculated.

If a certain calculation is done for several incident energies (as specified by quantities KDE and KKZMM in input card 8) information 1-4 is given only once in the beginning of the output followed by information 5-17 given for each incident energy in order of decreasing bombarding energy.

Finally, production cross-section information from all bombarding energies is summarized in output section: Excitation function. In this section the following quantities are listed as function of incident projectile energy (lab).

- a) Total reaction cross-section for inc. particles.
- b) Total emission cross-section for particles leading from CN1 to CN2.
- c) For each CN with allowed  $\gamma$ -emission, total production cross-sections for ground-state and all isomeric states.
- d) For reactions of type (a,ab..) the particle emission cross-section for particles a in the first reaction step is further subdivided into the compound-elastic and inelastic cross-section.

Note: Output, Excitation Functions handles only up to 5 isomeric levels.

Note: The compound elastic cross-section is not included in the ground-state production cross-section given for the respective compound nucleus.

#### 4.3) Optional Output

4.3.1) Level densities, level width and related quantities and gamma strength functions and transmission coefficients.

For KTEST1 = 1 the following additional output is given:

4.3.1.1) Level densities for CN1 and all residual nuclei populated by decay of CN1 to CNN. In detail the following information is given:

- 4.3.1.1.1) Table of state densities ZZST for excitation energies corresponding to centers of all energy bins (not printed for ISYMC = -1).
- 4.3.1.1.2) List of  $\rho(U, I)$  for all I-values used in the program for U-values corresponding to centers of all energy bins starting with highest excitation energy possible for the respective nucleus Fig. 6.1.
- 4.3.1.1.3) Total level density  $\rho(U)$  at the same excitation energies.
- 4.3.1.1.4) Values of  $\sigma^2$ , the square of the spin-cutoff-factor used in the calculation of  $\rho(U, I)$  also for the same set of excitation energies (called sigrot in output).

Note: These quantities are calculated and printed also for those bins for which the level structure is described by discrete levels in order to allow a check on how the used level density formula matches the actual density at levels at low excitation energy. The level density values for these bins are not used in the actual calculations.

- 4.3.1.2) Contributions to the Hauser-Feshbach denominator from the different kinds of particle emission and from photon emission.

For each CN the contributions to the Hauser-Feshbach denominator due to emission of n, p, d,  $\alpha$  and radiative transitions are given as function of excitation energy, spin and parity of the compound nucleus levels.

Values of these contributions are listed for excitation energies corresponding to the energy bin centers (Fig. 6.1) in order of decreasing excitation energy, ranging from the highest energy bin to the lowest bin of the continuum (shaded areas in Fig. 6.1).

For each energy bin a two line table is given describing the dependence on spin and parity of the CN levels. The upper line gives the HF-denominator contributions for positive and the lower line for negative parity levels. Within each line the HF-denominator contributions are given as function of spin starting with the lowest possible value (either 0 or 1/2 as printed in the table heading).

The described tables of the contributions to the HF-denominators for the different kind of emitted particles are given immediately after the tables of the level densities of the residual nuclei populated by the emission of those particles.

#### 4.3.1.3) Total level widths

Total level widths are given for all energy bins in the continuum for all CN (for CN1 only if it is allowed to emit photons).

For each energy bin the level width is given in the form of a two line table as function of spin  $I$  and parity  $\pi$  of the levels within that bin. Line one lists the total width of positive, line two of negative parity levels, starting always with the lowest possible  $I$ -value (0 or  $1/2$  as given in the table heading) and proceeding in order of increasing spin.

#### 4.3.1.4) Both gamma-ray strength-functions and transmission coefficients as function of photon energy for all multiplicities are printed for all CN which are permitted to emit photons. Strength functions and transmission coefficients are listed for values $E_\gamma = N \cdot DU/2$ for $N = 1, 2N_{\max}+5$ , $DU$ being the chosen energy bin size and $N_{\max}$ the maximum number of bins allowed by the program (at Livermore there exist at present 2 versions with $N_{\max} = 80$ and $200$ respectively).

Note: For CN1 both contributions to the HF-denominator and total level width are only given if it is allowed to emit photons (NGACOM = 1).

#### 4.3.2) Population of the continuum in the decay of the various CN.

For KTEST2 = 1 the following additional information is given:

List of continuum populations  $WB(U, I, \pi)$  and  $\overline{WB}(U, I, \pi)$ . (See section 2 of IRK 76/01.).

$WB(U, I, \pi)$  = cross-section for population of levels with spin  $I$ , parity  $\pi$ , by particle emission from preceding compound nucleus.

It is listed for the second and all subsequent compound nuclei for all energy bins in the continuum (see Fig 6.1).

$\overline{WB}$  = cross-section for population of levels with spin  $I$ , parity  $\pi$ , by particle emission from preceding and  $\gamma$ -decay from all high energy bins of same compound nucleus.

It is given for energy bins in the continuum for all CN (including 1) for which  $\gamma$ -decay is allowed

- 4.3.3) Information on the particle and  $\gamma$ -spectra resulting from the different steps of the evaporation cascade.

If KTEST3 = 1 the following additional information is given:

- 4.3.3.1) Gamma and particle spectrum from first reaction step (pre-equilibrium particle emission and decay of CN1).

- 4.3.3.1.1) Gamma production spectrum:

- a) Angle-int. production cross-sections per bin
- b) Angle-int. production cross-sections in b/MeV
- c) Diff. production cross-sections in b/MeV \* sr assuming isotropic emission.

- 4.3.3.1.2) Particle emission spectra

- a) Angle-int. particle production cross-section from pre-equilibrium emission (b/bin)
- b) Angle-int. particle production cross-sections from compound nucleus decay (b/bin)
- c) Sum of contributions a) and b) = total angle-int. particle emission cross-section in first reaction step up to upper edge of corresponding bin (b).
- d) Total angle-int. particle emission cross-sections in b/MeV
- e) Total diff. particle emission cross-sections in b/MeV \* sr assuming isotropic emission

- 4.3.3.1.3) Log plot of quantities a, b and c on log scale

- 4.3.3.2) Information on gamma and particle emission from subsequent compound nuclei. Photon and particle spectra for all subsequent compound nuclei are given in the form described for the gamma production spectrum of CN1 (2.1.1 a-c). No plots of these cross-sections are provided.

Note: All energies given in the cross-sections tables are c.m. (channel) energies for the centers of the corresponding energy bins.

- 4.3.4) Additional information on the width fluctuation correction.

For KTESTW = 1 a very long and detailed protocol on the width fluctuation correction is printed.

4.3.5) Gamma-ray production cross-sections for transitions between discrete levels.

If the control parameter KGAPR in card 10 is set equal to NDISK<sub>max</sub>, the maximum number of discrete levels given to the program for any of the CN,  $\gamma$ -ray production cross-sections will be printed for all transitions between discrete levels for all compound nuclei.

If KGAPR is set to some lower number N, only the cross-section for transitions depopulating levels N and lower will be given e.g., for N = 2 only the cross-sections for gamma transitions from level Nr 2 (1st excited level) to level Nr 1 (ground state will be printed).

The above description of STAPRE output is incomplete in two respects:

- 1) Output concerning widths-fluctuation corrections.
- 2) Output concerning fission as the author has not yet worked with these options and is not familiar with those output details.

## 5 LEVEL DENSITY OPTIONS IN STAPRE

### 5.1) General Remarks

Originally the STAPRE Code used only the back-shifted Fermi-Gas model as parameterized in Ref. 4) and 5) for calculating level densities. The relevant formulas are given by M. Uhl and B. Strohmaier in section 3.3) of IRK 76/01. Later on, additional options for level density calculations were added as described in Addendum January 1978. These amendments include constant temperature expressions for the state density, the use of energy dependent a-parameters as proposed by Ignatyuk<sup>7</sup> and various options for introducing collective enhancement for level densities of deformed nuclei.

Thus at present the code allows the use of both Fermi gas-models, a constant temperature model and composite models, e.g., the Gilbert-Cameron model and the Ignatyuk model.

In principle all relevant information on the level density options is given in the mentioned sections of IRK 76/01 and Addendum 1978 to IRK 76/01.

There are however two points which may cause some confusion.

- 1) Depending on the choice of the control ISYM in cards 14 and 16.1 (either  $\geq 0$  or  $-1$ ) the code uses two slightly different Fermi-gas level density formulas.
- 2) Not all of the Gilbert-Cameron parameters can be used directly as input to STAPRE, some of them have to be converted to STAPRE input parameters by some kind of renormalization.

In order to avoid difficulties from these complications, section 2 of this report gives a short discussion on the use of the different forms of the Fermi-Gas level density formula and section 5 provides detailed instruction on how to prepare the STAPRE level density input cards for the Fermi-Gas, Gilbert-Cameron and constant temperature models.

## 5.2) Use of Different Forms of the Fermi-Gas Model

A number of slightly different forms have been used for the state and level density within the Fermi-Gas model by different authors. In the form given by D. W. Lang<sup>6</sup> the density  $\omega(E, M)$  of states of excitation energy  $E$  and  $I_z = M$  is given by:

$$\omega(E, M) = \frac{\exp \left\{ 2 \left[ a(E - \Delta - \hbar^2 M^2 / (2\theta_{\text{eff}})) \right]^{1/2} \right\}}{12 \sqrt{2\theta_{\text{eff}} / \hbar^2} \left[ E - \Delta - \hbar^2 M^2 / (2\theta_{\text{eff}}) + \frac{3}{2} t \right]^{3/2}} \quad (1)$$

$$E - \Delta = at^2 - \frac{3}{2} t + \hbar^2 M^2 / (2\theta_{\text{eff}}) \quad (2)$$

resulting in a total level density.

$$\rho(E) = \frac{\exp \left\{ 2 \left[ a(E - \Delta) \right]^{1/2} \right\}}{12 \sqrt{2\theta_{\text{eff}} / \hbar^2} \left[ E - \Delta + \frac{3}{2} t \right]^{3/2}} \quad (3)$$

On the other hand in most of the recent literature the simpler form is used:

$$\rho(E) = \frac{\exp \left\{ 2[a(E - \Delta)]^{1/2} \right\}}{12 \sqrt{2\theta_{\text{eff}}/\pi^2} [E - \Delta]^{3/2}} \quad (4)$$

The parameters in these equations are level density parameter  $a$ , fictitious ground-state position  $\Delta$  and effective moment of inertia  $\theta_{\text{eff}}$ .

For equal values of parameters  $a$  and  $\Delta$  the level densities predicted by Eq. (3) and (4) are almost equal at high excitation energy but differ considerably at low excitation energies of 2-4 MeV where the level density is normally required to join smoothly to the known density of discrete levels.

If however the level density parameters are determined from a fit to both the density of discrete levels and the average spacing of neutron resonances, fits with either Eq. (3) or (4) will result in considerably different values for the ground-state energy shift  $\Delta$ , but both formulas used with their own parameters will produce almost identical level densities  $\rho(E)$ .

Thus the important point is to find out which formula was used to describe the Fermi-Gas parameters in question from the experimental data and use the same formula in the calculations.

The STAPRE-Code therefore, contains both formulas and allows the use of either Eq. (3) or (4) by means of the control parameter ISYMC in Col 79-80 of the level density card.

ISYMC = 0 use of Eq. (3)  
ISYMC = -1 use of Eq. (4).

5.3) Preparation of level density input cards (see card 14 in input description) for the most common level density models.

5.3.1) Back-shifted Fermi-gas Model

If the backshifted Fermi-Gas model is used in the parameterization of Dilg *et. al.*<sup>5</sup> the following input is supplied:



Card 14 (and all further level density cards):

Col 1-6 (F6.0)  $DC(1) = a \text{ (MeV}^{-1}\text{)}$

Col 7-12(F6.0)  $DC(2) = \theta/\theta_{\text{Rigid}}$

Col 13-18(F6.0)  $DC(3) = \Delta \text{ (MeV)}$

Col 79-80(I2) ISYMC = -1

In Ref. 3 two sets  $a$ - and  $\Delta$  parameters are given for  $\theta/\theta_{\text{Rigid}} = 1$  or .5 for nuclei up to about  $A = 70$  it is definitely better to use  $\theta/\theta_{\text{Rigid}} = 1$ , that is the full rigid body moment of inertia, for heavier nuclei, the choice of  $\theta/\theta_{\text{Rigid}}$  is still an open question.

If Fermi-Gas parameters are used which were derived by fitting Eq. (4) to the exp. data the parameter ISYMC has to be set equal to zero.

### 5.3.2) Gilbert Cameron model (8)

Col 1-6  $DC(1) = a \text{ (MeV}^{-1}\text{)}$

Col 7-12  $DC(2) = \theta/\theta_{\text{Rigid}}$

Col 13-18  $DC(3) = P_n + P_z \text{ (MeV)}$

Col 49-54  $DC(9) = E_x \text{ (MeV)}$

Col 55-60  $DC(10) = C_2 \text{ (MeV}^{-1}\text{)}$

Col 61-66  $DC(11) = T_2 \text{ (MeV)}$

Col 67-72  $DC(12) = \sigma_2$

whereby the parameters  $a$ ,  $P_n + P_z$ ,  $E_x$ ,  $T$  and  $\sigma$  may be directly taken from Ref.(8).

If the quantities  $\theta/\theta_{\text{Rigid}}$  and  $C$  however have to be calculated from the Gilbert-Cameron parameters in the following way:

$$C_1 = \sqrt{2\pi} \cdot \frac{\sigma}{T} \cdot \exp \left[ -E_0/T \right]$$

$$\frac{\theta}{\theta_{\text{Rigid}}} = 5.92 \frac{a}{A} \quad (A = \text{mass number of nucleus})$$

Note: The factor  $\sqrt{2\pi} \cdot \sigma$  arises from the fact that STAPRE uses a constant temperature state density and the G-C model a constant temperature level density.

5.3.3.1) Simple constant temperature, constant model

$$\rho(U, I) = \frac{C}{2\sigma^2} \cdot \exp \left[ \frac{U}{T} - \frac{(I + 1/2)^2}{2\sigma^2} \right]$$

$$\rho(U) = \sum_J \rho(U, I) = C \cdot \exp [U/T]$$

resulting in state density.

$$\begin{aligned} w(U) &= \sum_J (2J + 1) \rho(U, I) \\ &= \sqrt{2\pi} \cdot \sigma C \cdot \exp [U/T] \end{aligned}$$

This model can be implemented by:

$$\text{Col 25-30 DC(5)} = E_1^t \text{ (MeV)}$$

$$\text{Col 31-36 DC(6)} = C_1 \text{ (MeV}^{-1}\text{)}$$

$$\text{Col 37-42 DC(7)} = T_1 \text{ (MeV)}$$

$$\text{Col 43-48 DC(8)} = \sigma_1$$

with the parameters  $T_1 = T$  and  $\sigma_1 = \sigma$  taken directly from the model,  $C_1 = \sqrt{2\pi} \cdot \sigma \cdot C$  and  $E_1^t$  chosen above the highest excitation energy occurring in the calculation.

## 6 THE STAPRE ENERGY GRID

At the beginning of any problem the STAPRE Code establishes an energy grid and performs any subsequent calculation and produces most of its output in the framework of this energy bin structure; thus it is necessary to consider this in some detail.

As starting point the program calculates the excitation energy of the first compound nucleus from the desired bombarding energy and the binding energy supplied by the incident particle. Then it adjusts the incident energy to the nearest multiple of the energy bin size DU.

For example: for the reaction  $^{50}\text{Cr}(n,np)$  at  $E_n = 15$  MeV and  $DU = 1$  MeV the excitation energy of the first CN  $^{51}\text{Cr}$  becomes 23.97 MeV, thus the incident energy is adjusted to 15.03 MeV resulting in an excitation energy of CN1 of 24.0 MeV. The energy grid for this example is shown in Fig. 6.1.

The first compound nucleus always has an excitation energy corresponding to the upper edge of the highest energy bin and equal to an integer multiple of the basic energy bin width.

The ground-states of all other compound and residual nuclei involved are elevated by the respective particle separation energies above the ground state of CN1 and thus they are in general located at some arbitrary position within some energy bin.

The program calculates for each nucleus the position of the highest discrete level given in the input and describes the level structure of all nuclei in the following way:

- 1) For all bins above that containing the highest discrete level the level structure is described by a continuous level density  $\rho(E,I)$ , (shaded area in Fig. 6.1).
- 2) The highest bin containing at least one discrete level and all lower ones are assumed to contain only the levels specified in the input. This may lead to errors if the sequence of levels in the input stops just above a bin border (e.g, bin 12 in  $^{50}\text{V}$  in Fig. 6.1). Then the program assumes that only this one level exists with the bin and will produce a hole in the proton spectrum. To avoid such errors the bin width has to be kept

sufficiently small or the number of discrete levels in the input has to be adjusted to the energy bin structure set up by the program.

Within this bin structure the program follows the decay chain from CN1 to the ground-states of CN1 to CNN (see Fig. 1) and describes the decay process in terms of:

- a) transitions from the starting point (top of highest energy bin in CN1) to discrete levels in all accessible residual nuclei. For these transitions the corresponding transmission coefficients are taken at the exact transition energies.
- b) transitions from the starting point to continuum energy bins in the residual nuclei. For such transitions the transmission coefficients are taken at the energy difference between the initial CN1 excitation energy and the excitation energy corresponding to the center of the populated bin (half-integer multiple of DU).
- c) transitions from an energy bin in the continuum to some other lower energy bin. For such transitions transmission coefficients corresponding to transitions between the centers of the bins are used (transitions energy is an integer multiple of DU).
- d) transitions from continuum bins to discrete residual levels in some lower bin. For these transitions a transition equal to the difference between the center of the continuum bin and the position of the final level is used.

Transitions of type a-d) are taken into account for all kinds of emitted particles and photons. For the neutron channel two additional kinds of transitions are taken into account in order to describe the emission of low-energy neutrons as accurately as possible. These transitions are of the following type:

- e) transitions from a continuum bin to discrete levels in the same bin.
- f) transitions from one continuum bin to another continuum bin with the same energy (corresponding to transitions from the upper part of the  $n$ -emitting bin to the lower parts of the accepting bin).

Examples for transitions of type a-e) are also shown in Fig. 1.

The energy spectrum of all outgoing particles is also described in the framework of the discussed bin structure. All outgoing particles and photons are sorted into energy bins of width DU according to the transition energy ascribed to them as discussed above. Thus the photon and particle spectra do not contain the details on the discrete particle groups and gamma lines, which, however, can be found in the parts of the output describing the population of the discrete levels of the various compound nuclei.

The bin width should in principle be so small that neither the level density nor the transmission coefficients for transitions to any other bin or level change considerably across the bin.

In practice this condition cannot be met for all transitions especially those describing the emission of low energy neutrons. For example, the transitions from the top of CN1 to the highest bin of the compound nucleus reached by neutron emission (Bin Nr 24 in  $^{50}\text{Cr}$  in Fig. 6.1) always contains a neutron energy range from zero to some hundred keV over which neutron transmission coefficients vary enormously. The same is also true for the transitions of type e and f described before. Therefore, for those special cases the program uses a special procedure accounting approximately for the variation of the transmission coefficients with energy across the bin.

In spite of these precautions the finite bin structure may introduce noticeable errors near neutron thresholds and calculations with different bin sizes should be made if cross sections are needed in regions just above neutron thresholds.

Note: The above description of the STAPRE energy grid is valid only if all particle separation energies are positive. For heavy nuclei  $\alpha$ -particle separation energies become negative and the ground-state energy of the residual nucleus reached by  $\alpha$ -particle emission will be lower than that of the compound nucleus. In those cases the STAPRE energy grid will start from the lowest lying ground-state of any of the nuclei occurring in the calculation.

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FIGURE CAPTIONS

Figure 6.1) STAPRE energy grid for the reaction  $^{50}\text{Cr}(n,np)^{49}\text{Cr}$  at incident neutron energy (lab) of 15 MeV and a bin width  $\Delta U = 1$  MeV.

Shaded areas: Level structure of nuclei is described by continuum level density  $\rho(U,J)$ .

$S_n, S_p, S_z$ : Particle separation energies

- - - - - : Bin boundaries

—————: Levels of the various compound and residual nuclei

~~~~~>: Examples of  $\gamma$ -transitions

————->: Examples of particle transitions

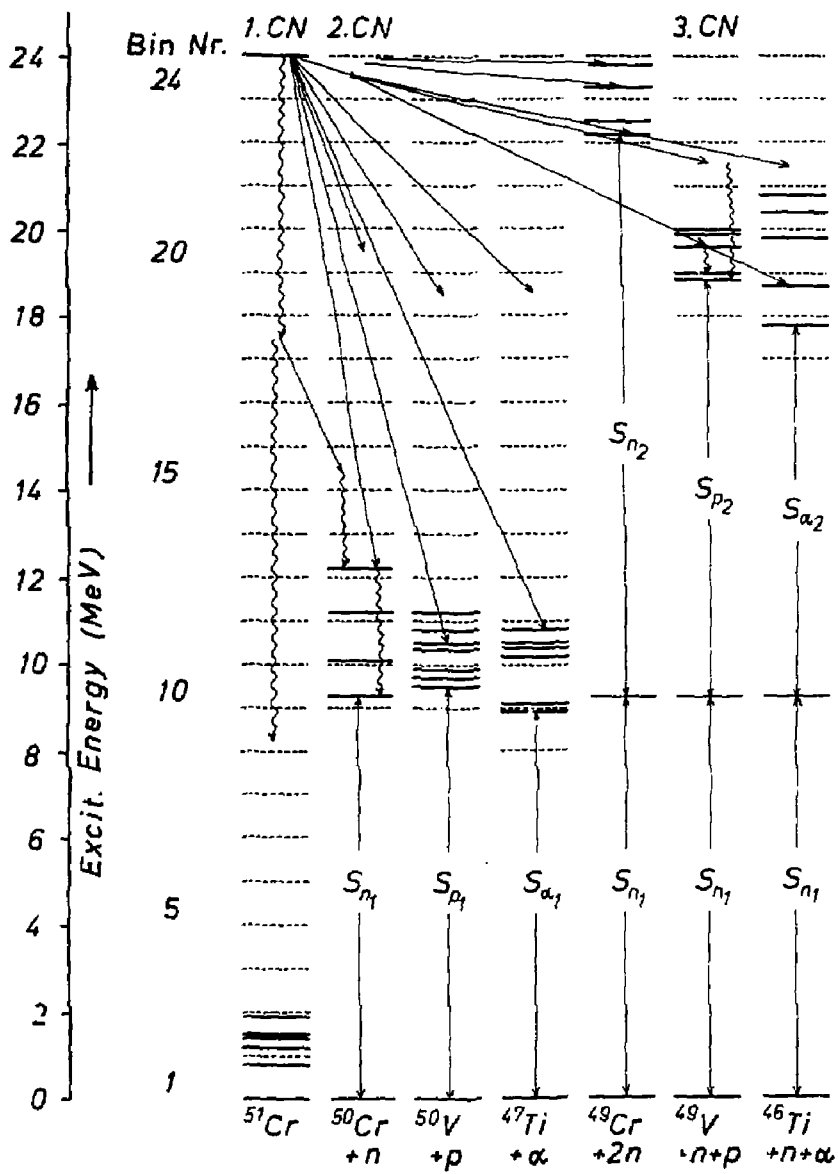


Figure 6.1



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