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USER MANUAL OF UNF CODE

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Contents

Introduction

The UNF code (2001 version) written in FORTRAN-90 is developed for calculating fast neutron reaction data of structure materials with incident energies from about 1 keV up to 20 MeV. There are 87 subroutines and 15 functions in UNF code.

The code consists of the spherical optical model, the unified Hauser-Feshbach and exciton model. The angular momentum dependent exciton model is established to describe the emissions from compound nucleus to the discrete levels of the residual nuclei in pre-equilibrium processes, while the equilibrium processes are described by the Hauser-Feshbach model with width fluctuation correction. The emissions to the discrete level in the multi-particle emissions for all opened channels are included. The double-differential cross sections of neutron and proton are calculated by the linear momentum dependent exciton state density. Since the improved pickup mechanism has been employed based on the Iwamoto-Harada model, the double-differential cross sections of alpha-particle, ^{3}He, deuteron and triton can be calculated by using a new method based on the Fermi gas model. The recoil effects in multi-particle emissions from continuum state to discrete level as well as from continuum to continuum state are taken into account strictly, so the energy balance is held accurately in every reaction channels. If the calculated direct inelastic scattering data and the calculated direct reaction data of the outgoing charged particles are available from other codes, one can input them, so that the calculated results will included the effects of the direct reaction processes. To keep the energy balance, the recoil effects are taken into account for all of the reaction processes. The gamma-production data are also calculated. The calculated neutron reaction data can be output in the ENDF/B-6 format.

All formulation used in UNF code can be found in the book entitled

"NEUTRON PHYSICS——Principle, Method and Application" published by China Atomic Energy Press in 2001.

The code can handle a decay sequence up to (n,3n) reaction channel.

The total reaction channels are 14 (0:13) as shown in the Table 1.

In fact the reaction channels (n,np) and (n,pn) as well as (n,nα) and (n,αn) should be treated as one channel, respectively. Thus the total reaction channels are 12 (0:11).

Table 1 14 reaction channels considered in UNF code

No.	Channels	No.	Channels	No.	Channels
0	n,γ	5	(n,d)	10	(n,pn)
1	(n,n')	6	(n,t)	11	(n,2p)
2	(n,p)	7	(n,2n)	12	(n,αn)
3	(n,α)	8	(n,np)	13	(n,3n)
4	(n,^{3}He)	9	(n,nα)		

The physical quantities calculated by using UNF code contain:

(1) Cross sections of total, elastic scattering, non-elastic scattering, and all reaction channels in which the discrete level emissions and continuum emissions are included.

(2) Angular distributions of elastic scattering both in CMS and LS.

(3) The energy spectra of the particle emitted in all reaction channels.

(4) Double-differential cross sections of all kinds of particle emissions (neutron, proton, alpha-particle, deuteron, triton and ^{3}He, as well as the recoil nuclei.

(5) Partial kerma factors of every reaction channel and the total kerma factor.

(6) Gamma production data (gamma spectra, gamma production cross sections and multiplicity), including the gamma production cross sections from level to level.

(7) Total double-differential cross sections of each kind outgoing particles from all reaction channels.

(8) Cross sections of isomeric states, if the level is a isomeric state of the residual nucleus.

(9) dpa cross sections used in radiation damage.

UNF code can also handle the calculations for a single element or for natural nucleus, and the target can be in ground state or in its isomeric state. Besides the output file, the outputting in ENDF/B-6 format is also included (files3, 4, 6, 12, 13, 14, 15 or files-3, 4, 5, which are controlled by a flag).

Meanwhile, some self-checking functions are designed for checking the errors in the input parameter data, if it exist. Users can correct them according to the indicating information in advance.

1 Spherical Optical Potential

In UNF code the spherical optical potential is employed to calculate total cross section, shape elastic scattering cross section and its angular distribution, absorption cross section, as well as the transmission coefficients and inverse cross section of the reaction channels No: 1-6 for (n,p, α, ^{3}He, d, t).

For the reaction channels (n,2n) and (n,3n) the transmission coefficients are taken from (n,n) channel. The calculated transmission coefficients for the second emitted particles of the reaction channels (n,pn), (n,pp), and (n,αn) with the same parameters as that for these particles in the channels No: 1-2, but with different mass number and charge number, accordingly. The transmission coefficients of p and α in the reaction channels (n,np) and (n,nα) are taken from (n,p) and (n,α) channels, respectively. Therefore 9 sets of the transmission coefficients are needed to be calculated. Some conversion arrays are used in the UNF code to mark the data. The conversion array KOP (0:13) denotes the corresponding

number (1:9) of the transmission coefficients for each reaction channel (0:13). The type of the emitted particle from every reaction channel is denoted by the conversion array KTYP1 (0:13) and conversion array KTYP2 (0:13) for the first and second emitted particles, respectively. The reaction channel number (0:11) are marked by the conversion array KCH (0:13) (See Table 2).

Table 2 14 conversion arrays

No.	Channels	KOP	KTYP1	KTYP2	KGD	KCH
0	(n,γ)		0	0	0	0
1	(n,n')	1	1	1	1	1
2	(n,p)	2	2	2	2	2
3	(n,α)	3	3	3	3	3
4	(n,^{3}He)	4	4	4	4	4
5	(n,d)	5	5	5	5	5
6	(n,t)	6	6	6	6	6
7	(n,2n)	1	1	1	7	7
8	(n,np)	2	1	2	5	8
9	(n,nα)	3	1	3	8	9
10	(n,pn)	7	2	1	5	8
11	(n,2p)	8	2	2	9	10
12	(n,αn)	9	3	1	8	9
13	(n,3n)	1	1	1	10	11

The construction of the discrete levels of the residual nuclei for the 14 reaction channels has only 11 sets of independent nuclei, of which the (n,np) and (n,pn) reaction channels have the identical residual nuclei as same as that of the (n,d) reaction channel, while that of the reaction channels (n,nα) and (n,αn) have the same one. Thus, only 11 sets of the discrete level schemes are needed in the input parameters including level energy, spin and parity. As the same reason, the data of the pair corrections and the level density parameters are also needed as the same as the afore-mentioned 11 sets input parameters. The conversion array KGD (0:13) is used for denoting the 11 sets parameters with the order number (0:10).

All the conversion arrays are listed in the Table 2 .

The phenomenological optical potential includes the following parts;

(a): Real part

$$V_{\mathrm{r}}(r)=\frac{-V_{\mathrm{r}}(\varepsilon)}{1+\exp[(R-r_{\mathrm{r}})/a_{\mathrm{r}}]}$$

(b): Imaginary part of surface absorption

$$W_{\mathrm{s}}(r)=-4W_{\mathrm{s}}(\varepsilon)\frac{\exp[(r-R_{\mathrm{s}})/a_{\mathrm{s}}]}{(1+\exp[(r-R_{\mathrm{s}})/a_{\mathrm{s}}])^2}$$

(c): Imaginary part of volume absorption

$$W_{\mathrm{v}}(r)=\frac{-U_{\mathrm{v}}(\varepsilon)}{1+\exp[(r-R_{\mathrm{v}})/a_{\mathrm{v}}]}$$

(d): Spin-orbit potential

$$V_{\mathrm{so}}(r)=-\frac{2V_{\mathrm{so}}}{a_{\mathrm{so}}r}\frac{\exp[(r-R_{\mathrm{so}})/a_{\mathrm{so}}]}{(1+\exp[(r-R_{\mathrm{so}})/a_{\mathrm{so}}])^2}$$

(e): Coulomb potential

$$V_{\mathrm{c}}(r)=\begin{cases}0.7720448\dfrac{Z_{\mathrm{b}}Z}{R_{\mathrm{c}}}(3-\dfrac{r^2}{R_{\mathrm{c}}^2}) & \text{if} \quad r\le R_{\mathrm{c}}\\[2ex] 1.440975\dfrac{Z_{\mathrm{b}}Z}{r} & \text{if} \quad r>R_{\mathrm{c}}\end{cases}$$

where A, Z stand for the mass and charge numbers of target nucleus, s_{b} and Z_{b} are the spin and charge number of particle b and ε is the energy of particle b in the center of mass system.

The total optical potential reads

$$V_{\mathrm{b}}(r)=V_{\mathrm{r}}(r)+\mathrm{i}[W_{\mathrm{s}}(r)+W_{\mathrm{v}}(r)]+V_{\mathrm{so}}(r)+V_{\mathrm{c}}(r)$$

The energy dependence of potential depths are given by

$$V_{\mathrm{r}}(\varepsilon)=V_0+V_1\varepsilon+V_2\varepsilon^2+V_3(A\text{-}2Z)/A+V_4(Z/A^{1/3})$$

$$W_{\mathrm{s}}(\varepsilon)=W_0+W_1\varepsilon+W_2(A\text{-}2Z)/A$$

$$U_{\mathrm{v}}(\varepsilon)=\max\{0.,U_0+U_1\varepsilon+U_2\varepsilon^2\}$$

All kinds of radius are given by

$$R_i = r_i A^{1/3} \quad (i=r, s, v, so, c)$$

In particular the diffusion widths of imaginary potential for proton take the form

$$a_s = a_{s0} + a_{s1}\frac{A-2Z}{A}$$

$$a_v = a_{v0} + a_{v1}\frac{A-2Z}{A}$$

Thus, altogether there are 12 parameters for potential depth, 5 parameters for radiuses and 4 (or 6 for proton) for diffusion widths in the phenomenological optical potential.

2 Parameters of UNF Code

There are three parameters in UNF code to control the storage size.

NEL: (integer) is the permitted maximum number of incident energy points.

NLV: (integer) is the permitted maximum number of the discrete levels including the ground state of the compound nucleus and the residual nuclei of the reaction channel No:1-6. The permitted maximum number is fixed 20 for the residual nuclei of the reaction channels No:7-11.

NGS: (integer) is the permitted maximum bin number of the γ production spectra.

So far the values of the three parameters in UNF code are set NEL=250, NLV=40, and NGS=300, respectively. If the users want to increase the size, then change the value accordingly, and compile the code again.

3 Flags

In UNF code several flags were set for different calculation purpose, so that the users should understand the functions of these flags in advance.

(1) KTEST: if users want to study some medium results for physical analysis, then set KTEST=1, when doing the calculation of multi-incident energy points users would be better to set KTEST=0, otherwise the output size may be too large.

(2) KOPP: if users want to output the optical potential parameters then set KOPP=1, otherwise set KOPP=0.

(3) KDDCS: It is used to control the double-differential cross section calculations. When user only want to calculate the data of the reaction cross sections, then set KDDCS=0, while user needs the data of the double-differential cross sections, then set KDDCS=1.

(4) KGYD: It is used to control the γ-production calculation. When users do not need them, then set KGYD=0, otherwise set KGYD=1.

(5) KENDF: It is used to control the ENDF/B-6 format output. In general the physical results are output in the file "UNF.OUT". When users need the ENDF/B-6 format outputting, then set KENDF=1 for the files-3, 4, 6, 12, 13, 14, 15 outputting, and set KENDF=2 for only the files 3, 4, 5, otherwise set KENDF=0 without ENDF/B-6 format outputting.

4 Input Files

Three input files are set up in UNF code.

4.1 File “UNF.DAT”

(A) For the common used parameters. The sequence of the input data is illustrated as below:

Card 1: The 5 flags are input with the sequence as same as that mentioned

above, which are KTEST, KOPP, KDDCS, KGYD, KENDF.

Card 2: The status of target KS0 (Integer) KS0=1 for ground state, KS0>1 for isomeric state (the number is the level order number, here the ground state is 1)

Card 3: NAB (Integer) is the number of isotopes, NAB=1 only for one isotope, while NAB>1 for natural nucleus. So far NAB≤10 is limited in UNF code.

Card 4: IZT(Integer) Charge number of target

Card 5: IAT(1:NAB) (Integer) The mass numbers of each isotope

Card 6: FONG(1:NAB) (Real) The abundance of each isotope

Card 7: MAT (Integer) Material number to mark the element in ENDF/B-6 format file

Card 8: MEL: (Integer) Number of incident energies and NOE: (Integer)

(notation: NOE=0 Doing the calculation for all incident energies; NOE≠0 Only doing the calculation for single incident energies with the order number NOE (1≤NOE≤MEL))

EL(I), I=1, MEL(real) incident energies in unit of MeV

MET(I), I=1, MEL(integer) energy point type

MET(I)=1 only output cross sections

MET(I)=2 output cross sections and angular distributions

MET(I)=3 besides outputting cross sections and angular distributions, the outputting double-differential cross section and γ production data is also issued in ENDF/B-6 format.

Card 9: The 5 angels for the neutron double-differential cross sections outputting to fit the measured data in laboratory system.

Card 10: DLH (real) Bin size of γ spectra.

(B) For each isotope the input data are as follows:

The sequence of the input data is illustrated as below

Card 1:

AMT (real) mass of the target in unit of a.m.u

CK (real) Kulbach parameter in exciton model

EF (real) Fermi energy (MeV)

CE1 (real) adjustable factor in γ radiation

Card 2:

EHF: (real) The energy bound between the Hauser-Feshbach model and the unified Hauser-Feshbach and exciton model.

If EL(LE) < EHF the Hauser-Feshbach model is used;

If EL(LE) > EHF the pre-equilibrium reaction model is performed.

Card 3:

BIND(0:13) (real) Binding energies of the last emitted particle of the reaction channels (0:13) (Notation: BIND(0)=0. for gamma emission)

ALD(0:10) (real) Level density parameters of the 11 residual nuclei (Gilbert-Cammeron formula is employed in UNF code)

DELT(0:10) (real) Pair correction values of 11 residual nuclei

Card 4: Two peak giant resonance parameter used for Gamma emissions CSGA (0:10,1:2) absorption cross sections of photo-nuclear reactions for 11 residual nuclei (in b)

EG(0:10,1:2) Energies of two peak giant dipole-resonance for 11 residual nuclei.(in MeV)

GG(0:10,1:2) Widths of giant dipole-resonance peaks (in MeV). The input sequence is CSGA(I,1), CSGA(I,2), EG(I,1), EG(I,2), GG(I,1), GG(I,2), I=0:10

Card 5: DGM (real) The parameter of the direct gamma emission

Card 6: Data of the discrete levels

NDL(0,10) (integer) Number of discrete levels of residual nuclei

EDL(0:10,K) (real) K=1, NDL(I) Level energies in unit of MeV

SDL(0:10,K) (real) K=1, NDL(I) Spins of levels

IPD (0:10,K) (integer) K=1, NDL(I) Parities of levels (+1 or -1). The input sequence is NDL(I), I=0,10

J=0:10 for (n,γ), (n,n'), (n,p), (n,α), (n,^{3}He), (n,d), (n,t), (n,2n), (n,nα), (n,2p), and (n,3n) reaction channels.

EDL(J,K), K=1, NDL(J)

SDL(J,K), K=1, NDL(J)

IPD(J,K), K=1, NDL(J)

(Notation: the order number of the ground state is 1, the order number of the first excitation level is 2 and so on. If NDL(I)=0, then the content of the J=I term is empty)

Notations 1: for calculation of natural nucleus, limited by ENDF/B-6 format, the total number of the discrete levels included in all isotopes of the inelastic scattering channel could no be over 40, if user want to set up the data file in ENDF/B-6 format.

Notations 2: for the reaction channels of multi-particle emissions, such as (n,np), (n,pn), (n,nα), (n,αn), (n,2p) and (n,3n), the number of discrete levels could not be over 20 in the calculation limited by UNF code. Since the number of reaction channel (n,d) has identical residual nucleus with (n,np) and (n,pn), so the number of discrete levels could also not be over 20.

Card 7: Branching ratio in γ de-excitation process. The branching ratio from I_{th} level to J_{th} level is written in the format (I3, I3, F5.2). The number of the lines of the input branching ratios for each residual nucleus is denoted by NUL (integer). Thus, the input order for each residual nucleus is NUL (integer) 6(I3, I3, F5.2)....

NUL lines.

There are 6 set data in one line. If the branching ratio between two levels is 0, then it does not need in the input file.

The input sequence is J=0:10 for (n,γ), (n,n'), (n,p), (n,^{3}He), (n,d), (n,t), (n,2n), (n,nα), (n,2p) and (n,3n) reaction channels.

Card 8: Optical potential parameters

AR Array (1:6). Diffusivities parameters of real potentials

AS Array (1:6). Diffusivities of sur. abs. ima. potentials

AVV Array (1:6). Diffusivities of volume absor. imag. potentials

AS0 Array (1:6). Diffusivities of L-S coupling potentials

XR Array (1:6). Radius parameters of real potentials

XS Array (1:6). Radiuses of sur. abs. ima. potentials

XV Array (1:6). Radiuses of volume absor. imag. potentials

XS0 Array (1:6). Radiuses of L-S coupling potentials

XC Array (1:6). Coulomb potentials Radius parameters

U0 Array (1:6). Constant terms of volume absorption imaginary potentials

U1 Array (1:6). Energy-linear term factors of volume absorption imaginary potentials

U2 Array (1:6). Energy-square term factors of volume absorption imaginary potentials

V0 Array (1:6). Constant factors in real potential for x particle of (n,x) reactions, with x=n,p, ^{3}He, d, t.

V1 Array (1:6). Energy-linear term factors in real potentials

V2 Array (1:6). Energy-square term factors in real potentials

V3 Array (1:6). Charge-symmetry term factors in real potentials

V4 Array (1:6). Charge-linear term factors in real potentials

VS0 Array (1:6). Constant factors of L-S coupling potentials

W0 Array (1:6). Constant terms of surface absorption imaginary potentials

W1 Array (1:6). Energy-linear term factors of surface absorption imaginary potentials

W2 Array (1:6). Charge-symmetry term factors of surface absorption imaginary potentials

A2S AS(proton) =AS(2) + A2S. (N-Z)/A only for proton

A2V AVV(proton) =AVV(2) + A2V. (N-Z)/A only for proton

In the case of natural nucleus the more isotopes (NAB>1) are needed to be calculated, the input parameters of the second isotope should be given in the same format as the first isotope. Then the ENDF/B-6 outputting is given for the natural nucleus.

4.2 File "DIR.DAT": This file is used for inputting the data of direct inelastic scattering and direct reactions, the input sequence is

I=1 direct inelastic scattering

I=2 direct reaction of (n,p)

I=3 direct reaction of (n,α)

I=4 direct reaction of (n,^{3}He)

I=5 direct reaction of (n,d)

I=6 direct reaction of (n,t)

In I_{th} term the input order is that the first line is the channel explanatory note, the second line gives the values of NPE (the number of incident energies, so far NPE≤40 is limited in UNF code) and LDM (the maximum value of the angular momentum in Legendre expansion form, LDM≤20 is limited in UNF code), the third line gives NDL(I) integers with 1 or 0, while "1" or "0" means the direct process is taken or is not taken into account for the level. In each incident energy input the cross section CSDIR(K) and the Legendre coefficients FL(0:LDM, K) of the level with the integer "1" in the array NDL.

4.3 File “OTH.DAT”

Card 1: If the user wants to observe the γ production data between levels, then set this file as follows:

For each kind of residual nuclei (0:10), at first input a integer NGM, which implies the number of the observed γ ray production between levels by user. Then input NGM pair integer of the level order numbers in this residual nucleus. For each integer pair (k1, k2) implies the γ ray is emitted from k1 level to k2 level, (so k1>k2). If the user does not want to observe this term, then set a “0” in this residual nuclei.

Card 2: If the user wants to calculate the reaction cross sections of the isomeric level within the 11 kind of residual nuclei (0:10), then set the isomeric level number in this residual nucleus, otherwise only set “0” in it.

Card 3: If set KDPA=1 the dpa cross sections will be calculated, otherwise set KDPA=0.

Card 4: Input the threshold energy E_d of PKA in unit of MeV.

This file only used for NAB=1 for one element calculation. But in the case of NAB>1 the NAB elements data for OTH.DAT are needed since different element may have different status of isomeric level.

5 Output Files

Five files are opened in UNF code for outputting

(1) File “UNF.OUT” This file is used for the output of calculated quantities

(2) File “PLO.OUT” This file is used for the DDCS outputting of all kinds outgoing particles, as well as the angular-energy spectra of 5 angles for

outgoing neutron in laboratory system when NOE>0.

(3) File “B6.OUT” This file is used for outputting the file in ENDF/B-6 format if KENDF=1 or 2.

(4) File “KMA.OUT” This file is used for outputting kerma factors.

(5) File “DPA.OUT” This file is used for outputting the dpa cross sections if KDPA=1 in the ODH.DAT file.

6 Guide for Running UNF Code

In order to calculate the fast neutron data, some preparations need to be set down in advance.

(1) At first set the UNF.DAT file.

(2) If the data of the direct inelastic scattering and direct reaction are available from other codes, then input the data in the file “DIR.DAT” with the proper format (See 4.2). If I_{th} direct reaction data are not taken into account, the user must put a “0” in this channel of file “DIR.DAT”.

(3) Set the OTH.DAT in advance. After set down the preparations mentioned above, the users can start the neutron data calculation.

(4) After adjustment procedure of parameters, users set KENDF=1 (in general KTEST=0) and run UNF code. The physical results output in file “UNF.OUT” and the ENDF/B-6 output in file “B6.OUT”.

(5) If the running is stop, and some information occurs on the screen, which informs the user there are some errors in the input data file, then the user needs to correct them accordingly.

(6) When set KTST=1 and NOE>0 for performing one incident neutron energy calculation, the threshold energies of every reaction channels, as well as that of inelastic scattering of the discrete levels are given in

"UNF.OUT" file, which are useful for the calculation to set up the ENDF/B-6 outputting file. Meanwhile, checking the normalization of the de-excitation ratios, some other information will be given to make sure that the input data file are (or not) correct.

(7) Only in the case of NOE>0 for one incident energy point calculation, the 5 set of double-differential cross sections will be output in "PLO.OUT" file for fitting the measured data.

Notations: In the input files "UNF.DAT" and "DIR.DAT" there are some one-line-annotations to indicate the data contents. UNF code reads them as a character. So the users must pay attention to "do not leaving any space lines ahead these characters" when writing at the input data. Otherwise all of the reading must be out of order.

An interface "PRE-UNF" based on RIPL has been established to set up the UNF.DAT and OTH.DAT files mentioned above automatically. If NAB>1 the NAB elements for each element with the charged number of Z can be set up simultaneously for both UNF.DAT file and OTH.DAT file, so the user needs to pay attention to whether any isomeric level is involved in a element.

Appendix A

UNF.DAT FILE

```
KTEST KOPP KDDCS KGYD KENDF
  0       0       1       1       1
THE STATUS OF TARGET 1: GROUND STATE   >1: ISOMERIC STATE
1
THE NUMVER OF ISOTOPES
2
THE CHARGE NUMBER OF THE NUECLEUS
29
MASS NUMBERS OF EACH ISOTOPES
  63      65
ABUNDANCE OF EACH ISOTOPES
0.6917   0.3083
MATERIAL NUMBER
3290
NUMBER OF INCIDENT ENERGIES, 'NOE','EL(I),I=1,MEL AND MET(I),I=1,MEL
29                  0
0.001   0.01   0.05   0.1   0.5    0.75    1.0   1.5   2.0   2.5
3.0     3.5    4.0    4.5   5.0    6.0     7.0   7.5   8.0   9.0
10.0   12.0   14.0   14.5   15.0   16.0   17.5   18.0   20.0
3 1 1 2 1   1 3 1 2 2
2 1 3 1 2   3 2 1 3 1
3 3 3 1 2   3 1 3 3
ANGLES IN LS FOR FITTING DDCS OF NEUTRON
30.   60.   90.   120.   150.
BIN SIZE IN GAMMA PRODUCTION
0.10
============= THE INPUT DAT OF ELEMENT No:1 ==================
  M(T)              CK         EF        CE1
  62.9295898      500.0       32.0       1.0
ENERGY BOUND BETWEEN HF AND MULTI-STEP REACTION MODEL
```

6.5

BINDING ENERGIES(0:13)

0.0 7.9160919 7.1995635 6.2011445 17.444110 11.816096 16.155116

10.854230 6.1246310 5.7765668 6.8411410 11.275454 7.4915142 8.8941669

LEVEL DENSITY PARAMETERS(0:10)

7.765, 7.161, 7.455, 7.754, 8.195, 7.336, 7.857, 6.731, 7.199, 8.804, 6.182,

PAIR CORRECTION VALUES(0:10)

−0.18, 1.3, 2.5, −0.25, 1.2, 2.5, 1.05, −0.15, 1.22, −0.28, 1.32,

PARAMETERS OF GIANT RESONANSE MODEL(CSE EE GG) (0:10)

0.075, 0.075, 0.034, 0.026, 0.026, 0.034, 0.034, 0.075, 0.026, 0.026, 0.075,

0.0, 0.0, 0.050, 0.040, 0.040, 0.050, 0.050, 0.0, 0.040, 0.040, 0.0,

16.70,16.70, 16.30, 16.37, 16.37, 16.30, 16.30, 16.70, 16.37, 16.37,16.70,

16.70,16.70, 16.30, 16.37, 16.37, 16.30, 16.30, 16.70, 16.37, 16.37,16.70,

0.0, 0.0, 18.51, 18.90, 18.90, 18.51, 18.51, 0.0, 18.90, 18.90, 0.0,

6.89, 6.89, 2.44, 2.56, 2.56, 2.44, 2.44, 6.89, 2.56, 2.56, 6.89,

PARAMETER OF DIRRECT GAMMA (DGAM)

0.25

DISCRETE LEVEL NUMBER FOR ALL RESIDUAL NUCLEI No:1

11, 18, 0, 0, 0, 0, 8, 9, 0, 9,

FOR(N,G) 64-CU

0.0, 0.1593, 0.2783, 0.3439, 0.3622, 0.5746, 0.6088, 0.6630, 0.7391, 0.7462, 0.8783,

1.0, 2.0, 2.0, 1.0, 3.0, 4.0, 2.0, 1.0, 2.0, 3.0, 0.0,

11*1,

FOR (N,N) 63-CU

0.0, 0.6697, 0.9621, 1.3270, 1.4120, 1.5470, 1.8612, 2.0112, 2.0622, 2.0814,

2.0926, 2.2079, 2.3366, 2.3380, 2.4048, 2.4972, 2.5064, 2.5120,

1.5, 0.5, 2.5, 3.5, 2.5, 1.5, 3.5, 1.5, 0.5, 2.5,

3.5, 0.5, 2.5, 1.5, 3.5, 1.5, 4.5, 0.5,

13*-1, 1, −1, −1, 1, −1,

FOR (N,P) 63-Ni

FOR (N,A) 60-Co

FOR (N,He) 61-Co

FOR (N,D) 62-Ni

FOR (N,T) 61-Ni

18

FOR (N,2N)) 62-CU

0.0, 0.0408, 0.2435, 0.2878, 0.3902, 0.4261, 0.5483, 0.6375,

1.0, 2.0, 2.0, 2.0, 4.0, 3.0, 1.0, 1.0,

8*1,

FOR (N,NA) 59-Co

0.0, 1.0993, 1.1905, 1.2916, 1.4343, 1.4595, 1.4817, 1.7447, 2.0618,

3.5, 1.5, 4.5, 1.5, 0.5, 5.5, 2.5, 3.5, 3.5,

9*-1,

FOR (N,2P) 62-Co

FOR (N,3N) 61-CU

0.0, 0.4751, 0.9701, 1.3106, 1.3942, 1.6605, 1.7326, 1.9042, 1.9327,

1.5, 0.5, 2.5, 3.5, 2.5, 1.5, 3.5, 2.5, 1.5,

9*-1,

BRANCHING RATIO(0:10)---FORNAT(6(2I3,F5.2))--N0:1

FOR (N.G)64-CU

5

2 1 1.00 3 1 1.00 4 1 0.96 4 2 0.04 5 1 0.02 5 2 0.98

6 2 0.06 6 5 0.94 7 1 0.82 7 2 0.08 7 3 0.04 7 4 0.06

8 1 0.32 8 2 0.27 8 3 0.35 8 4 0.06 9 1 0.07 9 2 0.63

9 3 0.10 9 4 0.03 9 5 0.17 10 3 0.70 10 5 0.21 10 7 0.09

11 1 0.57 11 2 0.03 11 4 0.40 0 0 0.00 0 0 0.00 0 0 0.00

FOR (N,N)63-CU

10

2 1 1.00 3 1 1.00 4 1 0.84 4 3 0.16 5 1 0.72 5 2 0.06

5 3 0.22 6 1 0.76 6 2 0.02 6 3 0.22 7 1 0.55 7 3 0.45

8 1 0.48 8 2 0.22 8 3 0.26 8 5 0.02 8 6 0.02 9 1 0.16

9 2 0.48 9 6 0.36 10 1 0.38 10 3 0.24 10 4 0.26 10 6 0.10

10 7 0.02 11 1 0.08 11 3 0.49 11 4 0.38 11 5 0.05 12 3 0.43

12 4 0.57 13 1 0.65 13 2 0.03 13 3 0.20 13 5 0.07 13 7 0.05

14 1 1.00 15 1 0.07 15 2 0.04 15 3 0.30 15 4 0.24 15 5 0.15

15 6 0.04 15 7 0.04 15 8 0.04 15 9 0.04 15 10 0.04 16 1 0.82

16 2 0.14 16 3 0.02 16 5 0.02 17 4 0.27 17 7 0.40 17 11 0.33

18 1 0.93 18 2 0.07 0 0 0.00 0 0 0.00 0 0 0.00 0 0 0.00

FOR (N,P)63-Ni

0

FOR (N,A)Co-60

0

FOR (N,He)Co-61

0

FOR (N,D)Ni-62

0

FOR (N,T)Ni-61

0

FOR(N,2N)62-CU

3

2 1 1.00 3 1 0.99 3 2 0.01 4 2 1.00 5 2 0.96 5 3 0.04

6 2 1.00 7 1 0.48 7 2 0.47 7 3 0.01 7 4 0.04 8 1 0.01

8 2 0.90 8 3 0.08 8 4 0.01 0 0 0.00 0 0 0.00 0 0 0.00

FOR(N,NA)59-Co

3

2 1 1.00 3 1 1.00 4 1 0.93 4 2 0.07 5 2 0.21 5 4 0.79

6 1 0.93 6 3 0.07 7 1 0.76 7 2 0.23 7 4 0.01 8 1 0.55

8 2 0.34 8 7 0.11 9 1 0.08 9 3 0.47 9 7 0.41 9 8 0.04

FOR(N,2P)62-Co

0

FOR (N,3N)61-CU

4

2 1 1.00 3 1 0.99 3 2 0.01 4 1 0.94 4 3 0.06 5 1 0.85

5 2 0.12 5 3 0.03 6 1 0.65 6 2 0.16 6 3 0.14 6 5 0.05

7 1 0.62 7 3 0.14 7 4 0.22 7 5 0.02 8 1 0.36 8 3 0.42

8 4 0.22 9 1 0.67 9 2 0.25 9 3 0.08 0 0 0.00 0 0 0.00

OPTICAL MODEL PARAMETERS

0.7457460, 0.580, 0.900, 0.7200, 0.5000, 0.410,

0.2568850, 0.360, 0.8800, 0.8800, 0.800, 0.500,

0.2568850, 0.360, 1.0000, 1.0000, 0.800, 0.500,

0.7457460, 0.650, 0.7200, 0.7200, 0.5000, 1.0000,

1.1855790, 1.250, 1.2000, 1.2000, 1.0500, 1.6400,

1.4129900, 1.250, 1.4000, 1.4000, 1.4300, 1.0000,

20

1.4129900, 1.250, 1.0000, 1.0000, 1.0000, 1.6400,

1.1855790, 1.250, 1.2000, 1.2000, 0.7500, 1.0000,

1.0000000, 1.2500, 1.3000, 1.3000, 1.3000, 1.3000,

−0.845861, −2.700, 0.0000, 0.0000, 0.0000, 1.3500,

0.2384280, 0.2200, 0.0000, 0.0000, 0.0000, 0.0000,

0.0000000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,

55.563385, 55.38500,151.90, 151.90, 91.130, 45.00,

−0.457278, −0.3200, −0.1700, −0.1700, 0.00, 0.00,

0.0017920, 0.000, 0.000, 0.000, 0.000, 0.000,

−27.03870, 14.00, 50.00, 50.00, 0.000, 0.000,

0.0000000,0.40000, 0.0000, 0.0000, 2.2000, 0.4000,

3.4130000,3.1000, 1.2500, 1.2500, 3.500, 0.000,

16.076340,11.8000,41.7000, 41.7000, 10.6200, 0.0000,

−0.352875,−0.2500,−0.3300, −0.3300, 0.000, 0.0000,

−35.46683,12.000, 44.000, 44.000, 0.000, 0.000,

0.700, 0.700,

========== THE INPUT DAT OF ELEMENT No:2 ==========

M(T)	CK	EF	CE1
64.9277890	500.0	32.0	1.0

ENERGY BOUND BETWEEN HF AND MULTI-STEP REACTION MODEL

6.5

BINDING ENERGIES(0:13)

0.0 7.0666570 8.4154700 7.1495978 19.320060 12.286783 15.688714

9.9046581 7.444753 6.7703842 6.0959410 12.312772 6.6874434 7.9160919

LEVEL DENSITY PARAMETERS(0:10)

8.472, 8.057, 8.361, 8.804, 9.112, 8.232, 7.937, 7.765, 8.195, 9.539, 7.161,

PAIR CORRECTION VALUES

−0.10, 1.5, 1.4, −0.28, 1.4, 2.7, 1.02, −0.18, 1.20, −0.20, 1.30,

PARAMETERS OF GIANT RESONANSE MODEL(CSE EE GG)

0.075, 0.075, 0.034, 0.026, 0.026, 0.034, 0.034, 0.075, 0.026, 0.026, 0.075,

0.0, 0.0, 0.05, 0.04, 0.04, 0.05, 0.05, 0.0, 0.04, 0.04, 0.0,

16.7, 16.7, 16.3, 16.37, 16.37, 16.3, 16.3, 16.7, 16.37, 16.37, 16.7,

0.0, 0.0, 18.51, 18.9, 18.9, 18.51,18.51, 0.0, 18.9, 18.9, 0.0,

6.89, 6.89, 2.44, 2.56, 2.56, 2.44, 2.44, 6.89, 2.56, 2.56, 6.89,

0.0, 0.0, 6.37, 7.61, 7.61, 6.37, 6.37, 0.0, 7.61,7.61, 0.0,

PARAMETER OF DIRRECT GAMMA (DGAM)

0.25

DISCRETE LEVEL NUMBER FOR ALL RESIDUAL NUCLEI No:2

9, 13, 0, 0, 0, 0, 0, 9, 5, 0, 18,

FOR(N,G) 66-CU

0.0, 0.1859, 0.2378, 0.2750, 0.3858, 0.4652, 0.5908, 0.7298, 0.8227,

1.0, 2.0, 2.0, 3.0, 1.0, 2.0, 4.0, 3.0, 2.0,

9*1,

FOR (N,N) 65-CU

0.0, 0.7706, 1.1156, 1.4818, 1.6234, 1.7250, 2.0943, 2.1074, 2.2128,

2.2785, 2.3290, 2.4066, 2.5257,

1.5, 0.5, 2.5, 3.5, 2.5, 1.5, 3.5, 2.5, 0.5,

3.5, 1.5, 4.5, 4.5,

12*-1,1,

FOR (N,P) 65-Ni

FOR (N,A) 62-Co

FOR (n,He) 63-Co

FOR (N,D) 64-Co

FOR (N,T) 63-Co

FOR (N,2N) 64-CU

0.0, 0.1593, 0.2783, 0.3439, 0.3622, 0.5746, 0.6088, 0.6630, 0.7391,

1.0, 2.0, 2.0, 1.0, 3.0, 4.0, 2.0, 1.0, 2.0,

9*1,

FOR (N,NA) 61-Co

0.0, 1.0275, 1.2051, 1.2858, 1.6189,

3.5, 1.5, 1.5, 2.5, 3.5,

5*-1,

FOR (N,2P) 64-Co

FOR (N,3N) 63-Cu

0.0, 0.6697, 0.9621, 1.3270, 1.4120, 1.5470, 1.8612, 2.0112, 2.0622, 2.0814, 2.0926,

2.2079, 2.3366, 2.3380, 2.4048, 2.4972, 2.5064, 2.5120,

1.5, 0.5, 2.5, 3.5, 2.5, 1.5, 3.5, 1.5, 0.5, 2.5, 3.5,

0.5, 2.5, 1.5, 3.5, 1.5, 4.5, 0.5,

22

13*-1,1,-1,-1,1,-1,

BRANCHING RATIO(0:10)---FORNAT(6(2I3,F5.2))--N0:2

FOR (N,G)66-CU

3

2 1 1.00 3 1 1.00 4 1 0.01 4 2 0.99 5 1 0.97 5 2 0.03

6 1 0.95 6 2 0.01 6 4 0.04 7 4 1.00 8 2 0.91 8 4 0.09

9 1 0.61 9 2 0.04 9 5 0.28 9 6 0.07 0 0 0.0 0 0 0.0

FOR (N,N)65-CU

6

2 1 1.00 3 1 1.00 4 1 0.83 4 3 0.17 5 1 0.56 5 2 0.11

5 3 0.33 6 1 0.71 6 2 0.01 6 3 0.28 7 1 0.29 7 3 0.53

7 4 0.13 7 5 0.05 8 1 0.16 8 2 0.10 8 3 0.36 8 4 0.32

8 6 0.06 9 1 0.37 9 2 0.55 9 6 0.08 10 1 0.02 10 3 0.98

11 1 0.48 11 2 0.29 11 3 0.23 12 3 0.27 12 4 0.56 12 7 0.17

13 4 1.00 0 0 0.00 0 0 0.00 0 0 0.00 0 0 0.00 0 0 0.00

FOR (N,P)65-Ni

0

FOR(N,A)62-Co

0

FOR(N,He)63-Co

0

FOR(N,D)64-Ni

0

FOR (N,T)63-Co

0

FOR (N.2N)64-CU

5

2 1 1.00 3 1 1.00 4 1 0.96 4 2 0.04 5 1 0.02 5 2 0.98

6 2 0.06 6 5 0.94 7 1 0.82 7 2 0.08 7 3 0.04 7 4 0.06

8 1 0.32 8 2 0.27 8 3 0.35 8 4 0.06 9 1 0.07 9 2 0.63

9 3 0.10 9 4 0.03 9 5 0.17 10 3 0.70 10 5 0.21 10 7 0.09

11 1 0.57 11 2 0.03 11 4 0.40 0 0 0.00 0 0 0.00 0 0 0.00

FOR (N,NA)61-Co

1

2 1 1.00 3 1 0.96 3 2 0.04 4 1 1.00 5 1 0.62 5 4 0.38
FOR (N,2P)64-Ni
0
FOR (N,3N)63-CU
10
2 1 1.00 3 1 1.00 4 1 0.84 4 3 0.16 5 1 0.72 5 2 0.06
5 3 0.22 6 1 0.76 6 2 0.02 6 3 0.22 7 1 0.55 7 3 0.45
8 1 0.48 8 2 0.22 8 3 0.26 8 5 0.02 8 6 0.02 9 1 0.16
9 2 0.48 9 6 0.36 10 1 0.38 10 3 0.24 10 4 0.26 10 6 0.10
10 7 0.02 11 1 0.08 11 3 0.49 11 4 0.38 11 5 0.05 12 3 0.43
12 4 0.57 13 1 0.65 13 2 0.03 13 3 0.20 13 5 0.07 13 7 0.05
14 1 1.00 15 1 0.07 15 2 0.04 15 3 0.30 15 4 0.24 15 5 0.15
15 6 0.04 15 7 0.04 15 8 0.04 15 9 0.04 15 10 0.04 16 1 0.82
16 2 0.14 16 3 0.02 16 5 0.02 17 4 0.27 17 7 0.40 17 11 0.33
18 1 0.93 18 2 0.07 0 0 0.00 0 0 0.00 0 0 0.00 0 0 0.00
OPTICAL MODEL PARAMETERS
0.7457460, 0.580, 0.900, 0.7200, 0.5000, 0.410,
0.2568850, 0.360, 0.8800, 0.8800, 0.800, 0.500,
0.2568850, 0.360, 1.0000, 1.0000, 0.800, 0.500,
0.7457460, 0.650, 0.7200, 0.7200, 0.5000, 1.0000,
1.1855790, 1.250, 1.2000, 1.2000, 1.0500, 1.6400,
1.4129900, 1.250, 1.4000, 1.4000, 1.4300, 1.0000,
1.4129900, 1.250, 1.0000, 1.0000, 1.0000, 1.6400,
1.1855790, 1.250, 1.2000, 1.2000, 0.7500, 1.0000,
1.0000000, 1.2500, 1.3000, 1.3000, 1.3000, 1.3000,
−0.845861, −2.700, 0.0000, 0.0000, 0.0000, 1.3500,
0.2384280, 0.2200, 0.0000, 0.0000, 0.0000, 0.0000,
0.0000000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
55.563385, 55.38500, 151.90, 151.90, 91.130, 45.00,
−0.457278, −0.3200, −0.1700, −0.1700, 0.00, 0.00,
0.0017920, 0.000, 0.000, 0.000, 0.000, 0.000,
−27.03870, 14.00, 50.00, 50.00, 0.000, 0.000,
0.0000000, 0.40000, 0.0000, 0.0000, 2.2000, 0.4000,
3.4130000, 3.1000, 1.2500, 1.2500, 3.500, 0.000,
16.076340, 11.8000, 41.7000, 41.7000, 10.6200, 0.0000,
−0.352875, −0.2500,−0.3300, −0.3300, 0.000, 0.0000,
−35.46683, 12.000, 44.000, 44.000, 0.000, 0.000,
0.700, 0.700,
24

DIR.DAT FILE

```
FOR (N,N') 63cu
18    20                 (notation: 18 incident neutron energies, and Lmax=20)
0  1  1  1  1  0  1  0  0  0  0  0  0  0  0  0  0  0
 1.0000                  (notation: the first incident energy)
 0.8623E-02    1.00000  0.2656345  −0.0468745 −0.0090906  0.0035008 −0.0002518
                        0.0000129   0.0000003  0.0000007  0.0000008  0.0000011
                        0.0000012   0.0000016  0.0000017  0.0000021  0.0000023
                        0.0000028   0.0000029  0.0000036  0.0000037  0.0000045
 0.9840E-03    1.00000  0.1790060  −0.0104250 −0.0006112  0.0000498 −0.0000007
                        0.0000005   0.0000004  0.0000009  0.0000006  0.0000013
                        0.0000009   0.0000019  0.0000013  0.0000026  0.0000017
                        0.0000034   0.0000022  0.0000043  0.0000027  0.0000053
 0.0000E+00    0.00000  0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
 0.0000E+00    0.00000  0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
 0.0000E+00    0.00000  0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
                        0.0000000   0.0000000  0.0000000  0.0000000  0.0000000
  2.0000                 (notation: the second incident energy)
              .
              .
              .
20.0000                  (notation: the 18th incident energy)
 0.2199E-01    1.00000  0.4345621   0.2013494  0.0768496  0.0207795 −0.0133181
                       −0.0420165  −0.0287509 −0.0141307 −0.0196234 −0.0112449
                        0.0163561   0.0204165  0.0095513  0.0046556  0.0019304
                        0.0008028   0.0003285  0.0001342  0.0000556  0.0000280
```

0.2169E-01 1.00000 0.4306029 0.2000085 0.0741151 0.0199395 −0.0135000
−0.0425118 −0.0268081 −0.0137639 −0.0193177 −0.0104380
0.0162710 0.0201069 0.0092726 0.0044589 0.0018423
0.0007628 0.0003107 0.0001266 0.0000525 0.0000267
0.2126E-01 1.00000 0.4249518 0.1980161 0.0702780 0.0188224 −0.0138332
−0.0431027 −0.0242241 −0.0132231 −0.0188408 −0.0093874
0.0160966 0.0196675 0.0089323 0.0042217 0.0017375
0.0007153 0.0002897 0.0001175 0.0000487 0.0000252
0.2116E-01 1.00000 0.4235179 0.1974981 0.0693169 0.0185524 −0.0139286
−0.0432347 −0.0235960 −0.0130850 −0.0187152 −0.0091341
0.0160463 0.0195564 0.0088540 0.0041676 0.0017138
0.0007046 0.0002849 0.0001155 0.0000479 0.0000249
0.2056E-01 1.00000 0.4151993 0.1944040 0.0638418 0.0170790 −0.0145536
−0.0438827 −0.0201276 −0.0122988 −0.0179715 −0.0077347
0.0157299 0.0189160 0.0084443 0.0038888 0.0015928
0.0006501 0.0002609 0.0001053 0.0000437 0.0000232
FOR (N,P)
0 0
FOR (N,A)
0 0
FOR (N,HE3)
0 0
FOR (N,D)
0 0
FOR (N,T)
0 0
for (n,n') 65cu
19 20 (notation: 19 incident neutron energies, and Lmax=20)
0 1 1 1 1 0 1 1 1 1 0 0 0
0.9000 (notation: the first incident energy)
0.0000E+00 1.00000 0.2768671 −0.0430051 −0.0071451 0.0021647 −0.0001294
0.0000057 0.0000005 0.0000007 0.0000009 0.0000011
0.0000013 0.0000016 0.0000018 0.0000022 0.0000024
0.0000028 0.0000031 0.0000036 0.0000040 0.0000045
26

0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
1.0000	(notation: the second incident energy)					
0.6254E-02	1.00000	0.2768671	−0.0430051	−0.0071451	0.0021647	−0.0001294
		0.0000057	0.0000005	0.0000007	0.0000009	0.0000011
		0.0000013	0.0000016	0.0000018	0.0000022	0.0000024
		0.0000028	0.0000031	0.0000036	0.0000040	0.0000045
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000

		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000E+00	0.00000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
		0.0000000	0.0000000	0.0000000	0.0000000	0.0000000

.

.

.

20.0000 (notation: the 19_{th} incident energy)

0.2270E-01	1.00000	0.4375999	0.2021357	0.0807721	0.0221367	−0.0119846
		−0.0403190	−0.0308124	−0.0136942	−0.0186576	−0.0125273
		0.0156058	0.0207292	0.0099966	0.0049840	0.0020706
		0.0008582	0.0003499	0.0001426	0.0000589	0.0000294
0.2231E-01	1.00000	0.4333668	0.2001342	0.0777346	0.0210633	−0.0120059
		−0.0409454	−0.0285432	−0.0131504	−0.0184715	−0.0116601

		0.0155722	0.0204185	0.0096659	0.0047348	0.0019584
		0.0008074	0.0003275	0.0001329	0.0000549	0.0000278
0.2184E-01	1.00000	0.4280819	0.1976483	0.0740087	0.0198466	−0.0121352
		−0.0415829	−0.0259373	−0.0124646	−0.0181689	−0.0106863
		0.0154548	0.0200238	0.0093231	0.0044802	0.0018456
		0.0007564	0.0003051	0.0001233	0.0000510	0.0000261
0.2165E-01	1.00000	0.4258114	0.1965816	0.0724323	0.0193576	−0.0122169
		−0.0418192	-0.0248752	−0.0121726	−0.0180247	−0.0102917
		0.0153894	0.0198528	0.0091922	0.0043842	0.0018034
		0.0007374	0.0002967	0.0001197	0.0000495	0.0000255
0.2097E-01	1.00000	0.4173139	0.1925760	0.0666574	0.0176713	−0.0126283
		−0.0425481	−0.0211277	−0.0111132	−0.0174476	−0.0088923
		0.0151066	0.0192106	0.0087612	0.0040738	0.0016686
		0.0006770	0.0002702	0.0001085	0.0000449	0.0000237
0.2095E-01	1.00000	0.4170552	0.1924539	0.0664851	0.0176233	−0.0126430
		−0.0425668	−0.0210188	−0.0110821	−0.0174295	−0.0088513
		0.0150973	0.0191909	0.0087491	0.0040653	0.0016649
		0.0006754	0.0002695	0.0001082	0.0000448	0.0000236
0.2079E-01	1.00000	0.4149379	0.1914496	0.0650769	0.0172355	−0.0127682
		−0.0427137	−0.0201333	−0.0108295	−0.0172811	−0.0085164
		0.0150222	0.0190310	0.0086532	0.0039975	0.0016357
		0.0006624	0.0002639	0.0001058	0.0000438	0.0000232
0.2068E-01	1.00000	0.4135808	0.1908043	0.0641802	0.0169929	−0.0128523
		−0.0428014	−0.0195739	−0.0106701	−0.0171858	−0.0083038
		0.0149738	0.0189285	0.0085934	0.0039556	0.0016178
		0.0006544	0.0002604	0.0001044	0.0000432	0.0000230

for (n,p)

0 0

for (n,a)

0 0

for (n,He3)

0 0

for (n,d)

0 0

for (n,t)

0 0

OTH.DAT FILE

```
========================= INPUT FOR THE ELEMENT No: 1 ========================
FOR LEVELS OF GAMMA PRODUCTION CROSS SECTION BETWEEN DISCRETE LEVELS
(N,G)
0
(N,N)
0
(N,P)
0
(N,A)
0
(N,HE)
0
(N,D)
0
(N,T)
0
(N,2N)
0
(N,NP)
0
(N,NA)
0
(N,2P)
0
(N,3N)
0
FOR ISOMERIC LEVELS NUMBER OF IV=0,10 FOR 11 RESIDUAL NUCLEI
0   0 0 0 0 0   0 0 0 0 0
IF THE DPA DATA ARE NEEDED SET KDPA=1, OTHERWISE KDPA=0
0
INPUT THE THRESHOULD ENERGY Ed OF PKA IN UNIT OF MeV
0.000060
========================= INPUT FOR THE ELEMENT No: 2 ========================
========================= INPUT FOR THE ELEMENT No: 3 ========================
========================= INPUT FOR THE ELEMENT No: 4 ========================
```

Appendix B

UNF Code for Fast Neutron Reaction Data Calculations

Abstract

The theoretical improvements have been made in the unified Hauser-Feshbach and exciton model. The angular momentum conservation is considered in whole reaction processes for both equilibrium and pre-equilibrium mechanism. The recoil effects in varied emission processes are taken into account strictly, so the energy balance can be held exactly. A method for calculating double-differential cross sections of composite particles is proposed. Based on this theoretical frame, the UNF code (2001 version) for calculating neutron induced reaction data of structure materials below 20 MeV was issued. The functions of the UNF code are introduced.

Introduction

For fast neutron reaction data calculations, there are several widely used computer code, such as GNASH (Refs.[1] and [2]) and TNG (Ref.[3]), which are useful for fast neutron evaluation. The equilibrium and the pre-equilibrium statistical mechanism are employed in both codes, but in different approach. In the theoretical description of the model there are still some thing could be improved. The first point is about the emissions of the first outgoing particles, there should be three types of emission mechanisms, i.e. direct emission, pre-equilibrium emission and equilibrium emission. In particular, the emission from compound nucleus to the discrete levels of the residual nuclei, each of which has

its individual spin and parity. Therefore the angular momentary conservation and parity conservation should be taken into account properly. These three types of emission mechanisms have been taken into account in both GNASH code and TNG code. But GNASH code does consider the angular momentum conservation in the pre-equilibrium part of the calculations. The TNG code is based on a unified model, in which the lifetime of particle-hole states are independent of spin, which imply that the angular momentum conservation in the pre-equilibrium process is not included. So locating a proper approach to describe the pre-equilibrium emissions from compound nucleus to the discrete levels is required, which needs to develop an angular momentum dependent exciton model. It is introduced in Sec.B1. Combining with the Hauser-Feshbach model, this kind of reaction mechanism can be described based on the unified Hauser-Feshbach and exciton model[4]. In this model the formula of the energy spectrum reads as follows:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon}=\sum_{J\pi}\sigma_{\mathrm{a}}^{J\pi}\sum_{n}P^{J\pi}(n)\frac{W_{\mathrm{b}}^{J\pi}(n,E^{*},\varepsilon)}{W_{\mathrm{T}}^{J\pi}(n,E^{*})} \tag{B1}$$

where $\sigma_{\mathrm{a}}^{J\pi}$ stands for the absorption cross section, $P^{J\pi}(n)$ refers to the occupation probability of the n exciton state in the $j\pi$ channel, which can be obtained by solving the j-dependent exciton master equation to conserve the angular momentum in the pre-equilibrium reaction processes, $W_{\mathrm{b}}^{J\pi}(n,E^{*},\varepsilon)$ is the emission rates of particle b at exciton state n with outgoing energy ε. Obviously, if we do not consider the parity and angular momentum effects, Eq.(B1) is reduced to the exciton model, while if the pre-equilibrium effect is omitted, Eq.B1 is reduced to the Hauser-Feshbach model. In the case of low incident energies ($E_{\mathrm{n}}\leq 20$ MeV), only n=3 is taken into account for the pre-equilibrium mechanism. Therefore, the formula of the energy spectrum in practical calculation reads

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon}=\sum_{j\pi}\sigma_{\mathrm{a}}^{j\pi}\left\{P^{j\pi}(3)\frac{W_{\mathrm{b}}^{j\pi}(3,E^{*},\varepsilon)}{W_{\mathrm{T}}^{j\pi}(3,E^{*})}+Q^{j\pi}(3)\frac{W_{\mathrm{b}}^{j\pi}(E^{*},\varepsilon)}{W_{\mathrm{T}}^{j\pi}(E^{*})}\right\} \tag{B2}$$

where $Q^{j\pi}(3)=1-P^{j\pi}(3)$ is the occupation probability of equilibrium state in the $j\pi$ channel and $W_{\mathrm{b}}^{J\pi}(E^{*},\varepsilon)$ is the emission rate in the Hauser-Feshbach model, in which the width fluctuation correction is included.

Based on the unified Hauser-Feshbach and exciton model the emissions of the first particle emissions from compound nucleus can be described with pre-equilibrium mechanism and equilibrium mechanism as well as direct reaction process. In this model the angular momentum depended exciton model is used for conserving angular momentum in the pre-equilibrium emission processes. At low incident energies (E_{n}≤20 MeV), the secondary particle emissions are described by multi-step Hauser-Feshbach model. To do so in this way the angular momentum conservation and the parity conservation can be carried through the whole reaction processes up to (n,3n) reaction channel.

The second point is the energy balance for each reaction channel, since it is quite important in the application of the nuclear engineering. To meet the needs of energy balance the recoil effects should be taken into account strictly. This kind of accurate kinematics is introduced in Sec B2.

The semi-empirical model for double-differential cross sections of the complex particles emissions is used in GNASH code, while in UNF code, a method to calculate double-differential cross sections of the complex particles with the pickup mechanism is used. This method is introduced in Sec.B3. This is the third point on the improvements of the theoretical model.

The functions of UNF code (2001 version) are elaborated in Sec.B4 and some typical calculated results are shown in Sec.B5 with some discussions. A summary is given in Sec. B6.

B1 Angular Momentum Coupling Effect in Pre-Equilibrium Particle Emission

To consider the angular momentum and parity conservation the angular momentum (J) and parity (π) should be addressed in the master equation of exciton model, so the master equation of $j\pi$ channel reads

$$\frac{\mathrm{d}q^{J\pi}(n,t)}{\mathrm{d}t} = \lambda_{+}^{J\pi}(n-2)q^{J\pi}(n-2,t) + \lambda_{-}^{J\pi}(n+2)q^{J\pi}(n+2,t)$$

$$-[\lambda_{+}^{J\pi}(n) + \lambda_{-}^{J\pi}(n) + W_{\mathrm{t}}^{J\pi}(n)]q^{J\pi}(n,t) \qquad \text{(B3)}$$

where $\lambda_{\pm}^{J\pi}$ is the internal transition rate and $W_{\mathrm{t}}^{J\pi}$ is the total emission rate of the exciton state in $j\pi$ channel. The $j\pi$ dependent internal transition rate can be written in the form

$$\lambda_{\mathrm{v}}^{J\pi} = \lambda_{\mathrm{v}}(n)\chi^{J}(n), \qquad \mathrm{v} = +,0,- \qquad \text{(B4)}$$

Where $\lambda_{\mathrm{v}}(n)$ is the internal transition used in the usual $j\pi$ independent exciton model, while $\chi^{J}(n)$ stands for the angular momentum factor. In FKK model[5] the angular momentum conservation was considered properly. Following the approach of FKK model the angular momentum factor can be constructed. But in FKK model only spin-zero nucleon was used. In this paper the spin-1/2 nucleon is used to provide the angular momentum factor.

The δ type residual two-body interaction is used for the particle-hole excitation, which can be expanded in the form as follows:

$$\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) = \frac{\delta(r_1 - r_2)}{r_1 r_2}\sum_{Km} \mathrm{Y}_{Km}^{*}(\hat{r}_1)\mathrm{Y}_{Km}(\hat{r}_2) \qquad \text{(B5)}$$

Applying the basic formula, the reduced matrix elements are defined by

$$\left\langle j'm'\left|T_{LM}\right|jm\right\rangle = C^{j'\ m'}_{LM\ jm}\left\langle j''\left\|T_L\right\|j\right\rangle \tag{B6}$$

and:

$$\left\langle j'\left\|T_L\right\|j\right\rangle = \sum_{Mm} C^{J'\ m'}_{LM\ jm}\left\langle j'm'\left|T_{LM}\right|jm\right\rangle \tag{B7}$$

Where C is the Clebsch-Gordon coefficient. The tenser product of T^p and T^q satisfies the equation as

$$[T^p U^q]^r_{m_r} = \sum C^{\ r\ \ m_r}_{pm_p qm_g} T^p_{m_p} T^q_{m_q} \tag{B8}$$

Thus the reduced matrix element is obtained by

$$\left\langle j_a, j_b, j\left\|[T^p\cdot U^q]^r\right\|j_c, j_d, j'\right\rangle = \sum_{m_r m'} C^{j\ \ m}_{rm_r j'm'}\left\langle j_a j_b, jm\left|[T^p\times U^q]^r_{m_r}\right|j_c j_d, j'm'\right\rangle$$

$$= \sum C^{j\ \ m}_{rm_r j'm'} C^{j\ \ m}_{j_a m_a j_b m_b} C^{j'\ \ m'}_{j_c m_c j_d m_d} C^{r\ \ m_r}_{pm_p qm_g} C^{j_a\ \ m_a}_{pm_p j_c m_c} C^{j_b\ \ m_b}_{qm_q j_d m_d}\left\langle j_a\left|T^p_{m_p}\right|j_c\right\rangle\left\langle j_b\left|U^q_{m_q}\right|j_d\right\rangle$$

$$= (-1)^{j+j'+p+q+r}\hat{j}_a\hat{j}_b\frac{\hat{j'}}{\hat{r}}(2j+1)\begin{Bmatrix} j_a & j_b & j \\ j_c & j_d & j' \\ p & q & r\end{Bmatrix}\left\langle j_a\left\|T^p\right\|j_c\right\rangle\left\langle j_b\left\|U^q\right\|j_d\right\rangle \tag{B9}$$

where $\hat{j}\equiv\sqrt{2j+1}$ and $\{\ \}$ is the 9-*j* coefficient.

Using

$$T^p\cdot U^p = (-1)^p\hat{p}[T^p\times U^p]^0_0$$

and

$$\begin{Bmatrix} j_a & j_b & j \\ j_c & j_d & j' \\ p & p & 0\end{Bmatrix} = \frac{(-1)^{j+p-j_a-j_d}}{\hat{j}\hat{p}} W(j_a j_c j_b j_d, p\ j)\delta_{jj'} \tag{B10}$$

we have

$$\left\langle j_a j_b j\left\|T^p\cdot U^p\right\|j_c j_d j'\right\rangle = \hat{j}_a\hat{j}_b\hat{j}\hat{j}'(-1)^{j-j_a-j_d}\ \delta_{jj'}W(j_a j_c j_b j_d, j_p)$$

$$\left\langle j_{\mathrm{a}}\left\|T^{p}\right\|j_{\mathrm{c}}\right\rangle\left\langle j_{\mathrm{b}}\left\|U^{p}\right\|j_{\mathrm{d}}\right\rangle \tag{B11}$$

In our case, $T^{p}=\mathrm{Y}^{p}$ and $U^{p}=\mathrm{Y}^{p}$, where Y^{p} stands for the spherical harmonics function. The derivation procedure can be found in Ref.[6] in detail. For the nucleon with spin=1/2, the antisymmetrization needs to be taken into account.

In the case of λ_{+}, a particle (j_{a}) creates a particle-hole $(j_{\mathrm{b}}, j_{\mathrm{d}})$. Besides the particle a and the particle-hole b and d, the residual part of the compound nucleus is called observer, which has the spin *S*. The angular momentum coupling triangle relations $\Delta(J, j_{\mathrm{a}}, S), \Delta(j_{\mathrm{b}}, j_{\mathrm{d}}, j_{3}), \Delta(j_{3}, j_{\mathrm{c}}, j_{\mathrm{a}})$ must be held to keep the angular momentum conservation in the pre-equilibrium process. The final result of the angular momentum factor of χ_{+}^{J} is obtained by

$$\chi_{+}^{J}(n)=\frac{1}{32\pi^{2}R_{n}(J)}\sum_{sj_{\mathrm{a}}}R_{n-1}(s)R_{1}(j_{\mathrm{a}})F_{+}(j_{\mathrm{a}})\Delta(j_{\mathrm{a}}JS) \tag{B12}$$

$$F_{+}(j_{\mathrm{a}})=\sum_{j_{3}j_{\mathrm{c}}}\frac{1}{2j_{3}+1}(2j_{\mathrm{c}}+1)R_{1}(j_{\mathrm{c}})G_{+}(j_{\mathrm{a}}j_{\mathrm{c}}j_{3}) \tag{B13}$$

$$G_{+}(j_{\mathrm{a}}j_{\mathrm{c}}j_{3})=\sum_{j_{\mathrm{b}}j_{\mathrm{d}}}(2j_{\mathrm{b}}+1)(2j_{\mathrm{d}}+1)R_{1}(j_{\mathrm{b}})R_{1}(j_{\mathrm{d}})$$

$$[C^{j_{3}\ 0}_{j_{\mathrm{a}}\frac{1}{2}j_{\mathrm{c}}-\frac{1}{2}}C^{j_{3}\ 0}_{j_{\mathrm{b}}\frac{1}{2}j_{\mathrm{d}}-\frac{1}{2}}+(-1)^{j_{\mathrm{c}}+j_{\mathrm{d}}}C^{j_{3}\ 0}_{j_{\mathrm{a}}\frac{1}{2}j_{\mathrm{d}}-\frac{1}{2}}C^{j_{3}\ 0}_{j_{\mathrm{b}}\frac{1}{2}j_{\mathrm{c}}-\frac{1}{2}}]^{2} \tag{B14}$$

For the case of χ_{-}^{J}, a particle (j_{a}) annihilates a particle-hole pair $(j_{\mathrm{b}}j_{\mathrm{d}}, j_{3})$, the derivation procedure is as the same as that of χ_{+}^{J}. In this case only the weight $R_{n-3}(s)$ is used instead of $R_{n-1}(s)$ in Eq.(B12).

Being consistent with the independent exciton model, the angular momentum factors satisfy the normalization condition

$$\sum_J (2J+1) R_n(J) \chi_{\nu}^{J} = 1, \quad \nu = +,0- \tag{B15}$$

where $R_n(J)$ is the spin distribution factor of angular momentum in n exciton state

$$R_n(J) = \frac{2J+1}{\sqrt{2\pi}\, 2\sigma_n^3} \exp[\frac{-(J+\frac{1}{2})^2}{2\sigma_n^2}] \tag{B16}$$

where $\sigma_n = 0.24 n A^{\frac{2}{3}}$ refers to the spin cut-off factor of the n exciton state for the nucleus with the mass number A, σ_n is independent of energy.

Table B1 The occupation probabilities of $Q^{j\pi}(n=3)$, $P^{j\pi}(n=3)$ and the absorption cross section $\sigma_a^{j\pi}$ of ^{54}Fe at E_n=12 MeV

j	$Q^{j\pi}(3)$	$P^{j\pi}(3)$	σ_a^{j+} (b)	σ_a^{j-} (b)
0.5	0.4371	0.5629	3.586E-02	3.871E-02
1.5	0.5928	0.4072	7.173E-02	7.412E-02
2.5	0.6722	0.3278	1.263E-01	1.112E-01
3.5	0.7236	0.2764	1.684E-01	1.191E-01
4.5	0.7620	0.2380	1.711E-01	1.489E-01
5.5	0.7929	0.2071	2.053E-01	4.345E-02
6.5	0.8175	0.1825	5.649E-03	5.070E-02
7.5	0.8372	0.1628	6.456E-03	7.689E-04
8.5	0.8519	0.1481	1.032E-04	8.651E-04
9.5	0.8623	0.1377	1.146E-04	1.347E-05
10.5	0.8676	0.1324	1.721E-06	1.482E-05
11.5	0.8681	0.1319	1.877E-06	2.160E-07
12.5	0.8611	0.1389	0.000E+00	2.340E-07

As an example, the occupation probabilities at incident neutron energy E_n=12 MeV for different j are given in Table B1 to show the angular momentum conservation effect. For low j region the pre-equilibrium state is dominant part, while for high j region the equilibrium contributions become important, which

means that the components with high j in compound nucleus need multi-step intrinsic-collision processes. Averaged by the absorption cross section, the pre-equilibrium emission occupies the percentage of 28.86%, while the equilibrium emission occupies 71.14 %.

B2 Recoil Effect and Energy Balance

The energy balance for whole reaction processes must be taken into account to set up neutron data file for application. For each reaction channel with a reaction Q value, the released total energy includes the energies of the outgoing particles E_{p}, the recoil nucleus E_{R}, and the gamma decay energy E_{γ}. The energy balance needs

$$E_{\mathrm{R}} + E_{\mathrm{p}} + E_{\gamma} = E_{\mathrm{n}} + Q \tag{B17}$$

where E_{n} stands for the incident neutron energy in laboratory system (LS). If the recoil nucleus is assumed static in the center of mass system (CMS) after sequential particle emission, in this way neither the accurate shape of outgoing particle spectra nor the energy balance could be obtained. This paper will give the formulation of the energy balance of the secondary particle emissions, which is employed in the UNF code. In UNF code only the sequential particle emissions are taken into account.

The particle emissions have three cases, (1) from continuum states to continuum states, (2) from continuum states to discrete levels, (3) from discrete levels to discrete levels, of which the formulation has been given in Ref. [7].

Beside the laboratory system (LS) and the center of mass system (CMS), the recoil nucleus system (RNS) is also needed, which is a moving system along with the recoil residual nucleus. The physical quantities are labeled by subscripts l,c,r, respectively for the three motion systems. At low incident energies (<20

MeV), the pre-equilibrium mechanism is taken into account only for the first particle emissions, while the isotropic distribution is employed for the second emission particles in RNS. In this case the double-differential cross sections of the secondary particle emissions in CMS can be easily obtained.

The physical quantities used in this paper are defined as following :

$E^{*}=\frac{M_{\mathrm{T}}}{M_{\mathrm{C}}}E_{\mathrm{n}}+B_{\mathrm{n}}$: excitation energy;

B_{n}: binding energy of incident neutron in compound nucleus;

M_{T}, M_{C} : masses of target and compound nucleus, respectively ;

m_1, m_2: mass of the first and the second emitted particle, respectively;

ε_1, ε_2: energy of the first and the second emitted particle, respectively;

M_1, M_2: mass of residual nucleus after the first and the second emitted particle, respectively;

E_1,E_2: energies of residual nuclei after the first and the second particle emissions, respectively,

B_1, B_2: binding energy of the first and the second emitted particle in its compound nucleus, respectively;

E_{k_1} , E_{k_2} : level energy with the level order number k_1, k_2 reached by the first and the second emitted particle, respectively;

$f_l(\varepsilon_{m_1}^{\mathrm{c}})$: Legendre expansion coefficient of the first emitted particle in CMS.;

$f_l(\varepsilon_{m_2}^{\mathrm{c}})$: Legendre expansion coefficient of the second emitted particle in CMS;

B2.1 Double Differential Cross Section from Continuum State to Continuum State

Based on the relation of the double differential cross sections between CMS

and RNS

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega^{\mathrm{c}}\mathrm{d}\varepsilon^{\mathrm{c}}}\mathrm{d}\Omega^{\mathrm{c}}\mathrm{d}\varepsilon^{\mathrm{c}} = \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega^{\mathrm{r}}\mathrm{d}\varepsilon^{\mathrm{r}}}\mathrm{d}\Omega^{\mathrm{r}}\mathrm{d}\varepsilon^{\mathrm{r}} \tag{B18}$$

The Jacobian is given by

$$\mathrm{d}\varepsilon'^{\mathrm{r}}\mathrm{d}\Omega^{\mathrm{r}} = \sqrt{\frac{\varepsilon^{\mathrm{c}}}{\varepsilon^{\mathrm{r}}}}\mathrm{d}\varepsilon^{\mathrm{c}}\mathrm{d}\Omega^{\mathrm{c}} \tag{B19}$$

The normalized double differential cross section in the standard form reads

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon\mathrm{d}\Omega} = \sum_l \frac{2l+1}{4\pi} f_l(\varepsilon)\mathrm{P}_l(\cos\theta) \tag{B20}$$

where $\mathrm{P}_l(\cos\theta)$ refers to the Legendre polynomial. Averaged by the double-differential cross section of the residual nucleus after the first particle emission, the double-differential cross section of the second particle emission can be obtained by

$$\begin{aligned}\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon^{\mathrm{c}}_{m_2}\mathrm{d}\Omega^{\mathrm{c}}_{m_2}} &= \int \frac{\mathrm{d}^2\sigma}{\mathrm{d}E^{\mathrm{c}}_{M_1}\mathrm{d}\Omega^{\mathrm{c}}_{M_1}}\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}\mathrm{d}\Omega^{\mathrm{r}}_{m_2}}\sqrt{\frac{\varepsilon^{\mathrm{c}}_{m_2}}{\varepsilon^{\mathrm{r}}_{m_1}}}\mathrm{d}E^{\mathrm{c}}_{M_1}\mathrm{d}\Omega^{\mathrm{c}}_{M_1} \\ &\equiv \sum_l \frac{2l+1}{4\pi} f_l(\varepsilon^{\mathrm{c}}_{m_2})\mathrm{P}_l(\cos\theta^{\mathrm{c}}_{m_2})\end{aligned} \tag{B21}$$

where the double-differential cross section of the residual nucleus of M_1 has the form

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E^{\mathrm{c}}_{M_1}\mathrm{d}\Omega^{\mathrm{c}}_{M_1}} = \sum_l \frac{2l+1}{4\pi} f_l(E^{\mathrm{c}}_{M_1})\mathrm{P}_l(\cos\theta^{\mathrm{c}}_{M_1}) \tag{B22}$$

The isotropic distribution of the second particle emission in RNS reads

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}\mathrm{d}\Omega^{\mathrm{r}}_{m_2}}=\frac{1}{4\pi}\frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \tag{B23}$$

In terms of the orthogonal property of the Legendre polynomial, the Legendre coefficient of the second emitted particle is obtained by

$$f_l(\varepsilon^{\mathrm{c}}_{m_2})=\frac{1}{4\pi}\int \mathrm{d}\Omega^{\mathrm{c}}_{m_2}\,\frac{\mathrm{d}^2\sigma}{\mathrm{d}E^{\mathrm{c}}_{M_1}\mathrm{d}\Omega^{\mathrm{c}}_{M_1}}\frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}}\sqrt{\frac{\varepsilon^{\mathrm{c}}_{m_2}}{\varepsilon^{\mathrm{r}}_{m_2}}}\mathrm{P}_l(\cos\theta^{\mathrm{c}}_{m_2})\mathrm{d}E^{\mathrm{c}}_{M_1}\mathrm{d}\Omega^{\mathrm{c}}_{M_1} \tag{B24}$$

Denoting Θ as the angle between $\Omega^{\mathrm{c}}_{M_1}$ and $\Omega^{\mathrm{c}}_{m_2}$, then the integration over $\mathrm{d}\Omega^{\mathrm{c}}_{m_2}$ can be replaced by $\mathrm{d}\cos\Theta\,\mathrm{d}\Phi$, and using the relation

$$\mathrm{P}_L(\cos\theta^{\mathrm{c}}_{m_2})=\frac{4\pi}{2L+1}\sum_m \mathrm{Y}^*_{Lm}(\Theta,\Phi)\mathrm{Y}_{Lm}(\Omega^{\mathrm{c}}_{M_1}) \tag{B25}$$

Then carrying out the integration over $\mathrm{d}\cos\Theta\,\mathrm{d}\Phi$ we have

$$f_l(\varepsilon^{\mathrm{c}}_{m_2})=\frac{1}{2}\int f_l(E^{\mathrm{c}}_{M_1})\frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}}\sqrt{\frac{\varepsilon^{\mathrm{c}}_{m_2}}{\varepsilon^{\mathrm{r}}_{m_2}}}\mathrm{P}_l(\cos\Theta)\mathrm{d}E^{\mathrm{c}}_{M_1}\mathrm{d}\cos\Theta \tag{B26}$$

From the energy relation between RNS and CMS

$$\varepsilon^{\mathrm{r}}_{m_2}=\varepsilon^{\mathrm{c}}_{m_2}+\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}-2\sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}\varepsilon^{\mathrm{c}}_{m_2}}\cos\Theta \tag{B27}$$

and substituting $\cos\Theta$ in Eq.(B26) by $\varepsilon^{\mathrm{r}}_{m_2}$, then Eq.(B26) becomes into the following form

$$f_l(\varepsilon^{\mathrm{c}}_{m_2})=\frac{1}{4}\sqrt{\frac{M_1}{m_2}}\int_A^B \mathrm{d}E^{\mathrm{c}}_{M_1}\frac{f_l(E^{\mathrm{c}}_{M_1})}{\sqrt{E^{\mathrm{c}}_{M_1}}}\int_a^b \frac{\mathrm{d}\varepsilon^{\mathrm{c}}_{m_2}}{\sqrt{\varepsilon^{\mathrm{r}}_{m_2}}}\frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}}\mathrm{P}_l\left(\frac{\varepsilon^{\mathrm{c}}_{m_2}+\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}-\varepsilon^{\mathrm{r}}_{m_2}}{2\sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}\varepsilon^{\mathrm{c}}_{m_2}}}\right) \tag{B28}$$

For the given values of $\varepsilon^{\mathrm{c}}_{m_2}$ and $E^{\mathrm{c}}_{M_1}$, by means of the condition $-1 \le x \le 1$ for the Legendre polynomial of $\mathrm{P}_l(x)$, the integration limits of *a* and *b* in Eq.(B28) are given by

$$\begin{aligned} a &= \max\left\{\varepsilon^{\mathrm{r}}_{m_2,\min}, \left(\sqrt{\varepsilon^{\mathrm{c}}_{m_2}} - \sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}}\right)^2\right\} \\ b &= \min\left\{\varepsilon^{\mathrm{r}}_{m_2,\max}, \left(\sqrt{\varepsilon^{\mathrm{c}}_{m_2}} + \sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}}\right)^2\right\} \end{aligned} \tag{B29}$$

In terms of the velocity composition relation of $\boldsymbol{v}^{\mathrm{r}}_{m_2}$ and $\boldsymbol{v}^{\mathrm{c}}_{M_1}$, the energy region of the second particle emission is obtained by

$$\varepsilon^{\mathrm{c}}_{m_2,\max} = \left(\sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1,\max}} + \sqrt{\varepsilon^{\mathrm{r}}_{m_2,\max}}\right)^2 \tag{B30}$$

$$\varepsilon^{\mathrm{c}}_{m_2,\min} = \begin{cases} \left(\sqrt{\varepsilon^{\mathrm{r}}_{m_2,\max}} - \sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1,\min}}\right)^2 & \text{if } \varepsilon^{\mathrm{r}}_{m_2,\max} < \frac{m_2}{M_1}E^{\mathrm{c}}_{M_1,\min} \\ \left(\sqrt{\varepsilon^{\mathrm{r}}_{m_2,\min}} - \sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1,\max}}\right)^2 & \text{if } \frac{m_2}{M_1}E^{\mathrm{c}}_{M_1,\max} < \varepsilon^{\mathrm{r}}_{m_2,\min} \\ 0 & \text{othewise} \end{cases} \tag{B31}$$

When $f_0(E^{\mathrm{c}}_{M_1})$ is normalized, the $f_0(\varepsilon^{\mathrm{c}}_{m_2})$ is also normalized. By means of exchanging the integration order, the integration limits of $\varepsilon^{\mathrm{c}}_{m_2}$ are $(\sqrt{\varepsilon^{\mathrm{r}}_{m_2}} \pm \sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}})^2$ for every values of $\varepsilon^{\mathrm{r}}_{m_2}$ and $E^{\mathrm{c}}_{M_1}$. By using Eq.(B28)

$$\int_{\varepsilon^{\mathrm{c}}_{m_2,\min}}^{\varepsilon^{\mathrm{c}}_{m_2,\max}} f_0(\varepsilon^{\mathrm{c}}_{m_2})\mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} = \int f_0(E^{\mathrm{c}}_{M_1})\mathrm{d}E^{\mathrm{c}}_{M_1}\int \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}}\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2} = 1 \tag{B32}$$

It is easy to see from Eq.(B30) that the scope of the outgoing energy spectrum is broadened, when the recoil effect is taken into account. The lighter of the nucleus, the stronger of recoil effect and the broad effect even more

obviously.

When the value of $\varepsilon^{\mathrm{c}}_{m_2}$ is given, and $\varepsilon^{\mathrm{c}}_{m_2,\min} \le \varepsilon^{\mathrm{c}}_{m_2} \le \varepsilon^{\mathrm{c}}_{m_2,\max}$ the integration area of $E^{\mathrm{c}}_{M_1}$ is given by the existing condition of the integration over $\varepsilon^{\mathrm{r}}_{m_2}$ (a<b) as follows:

$$A = \begin{cases} \max\{E^{\mathrm{c}}_{M_1,\min}, \dfrac{M_1}{m_2}\left(\sqrt{\varepsilon^{\mathrm{c}}_{m_2}} - \sqrt{\varepsilon^{\mathrm{r}}_{m_2,\max}}\right)^2\} & \text{if } \varepsilon^{\mathrm{c}}_{m_2} > \varepsilon^{\mathrm{r}}_{m_2,\max} \\ \max\{E^{\mathrm{c}}_{M_1,\min}, \dfrac{M_1}{m_2}\left(\sqrt{\varepsilon^{\mathrm{r}}_{m_2.\min}} - \sqrt{\varepsilon^{\mathrm{c}}_{m_2}}\right)^2\} & \text{if } \varepsilon^{\mathrm{c}}_{m_2} < \varepsilon^{\mathrm{r}}_{m_2,\min} \\ E^{\mathrm{c}}_{M_1,\min} & \text{othewise} \end{cases}$$

$$B = \min\left\{E^{\mathrm{c}}_{M_1,\max}, \frac{M_1}{m_2}\left(\sqrt{\varepsilon^{\mathrm{c}}_{m_2}} + \sqrt{\varepsilon^{\mathrm{r}}_{m_2,\max}}\right)\right\} \tag{B33}$$

The double-differential cross section and the energy region of the recoil residual nucleus after the second particle emission can be obtained by replacing m_2 and $\varepsilon^{\mathrm{r}}_{m_2}$ with M_2 and $E^{\mathrm{r}}_{M_2}$ in Eq.(B28), respectively.

On the other hand, one can prove the energy balance is held in an analytical way. By means of the velocity $\boldsymbol{v}^{1}_{m_1} = \boldsymbol{V}_{\mathrm{C}} + \boldsymbol{v}^{\mathrm{c}}_{m_1}$, where $\boldsymbol{V}_{\mathrm{C}}$ is the motion velocity of the center of the mass; the energy carried by the first emitted particle from compound nucleus to the continuum states can be given by

$$E^{1}_{m_1} = \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_1}\{(\frac{m_{\mathrm{n}}m_1}{M^2_{\mathrm{C}}}E_{\mathrm{n}} + \varepsilon^{\mathrm{c}}_{m_1})f_0(\varepsilon^{\mathrm{c}}_{m_1}) + \frac{2\sqrt{m_{\mathrm{n}}m_1}}{M_{\mathrm{C}}}\sqrt{E_{\mathrm{n}}\varepsilon^{\mathrm{c}}_{m_1}}f_1(\varepsilon^{\mathrm{c}}_{m_1})\} \tag{B34}$$

By using the following formula, the energy carried for the second emitted particle m in LS can be given by

$$E^{1} = \frac{m}{2}\int (v^{1})^2 \frac{\mathrm{d}^2\sigma}{\mathrm{d}E^{\mathrm{c}}_{M_1}\mathrm{d}\Omega^{\mathrm{c}}_{M_1}}\mathrm{d}E^{\mathrm{c}}_{M_1}\mathrm{d}\Omega^{\mathrm{c}}_{M_1} \tag{B35}$$

The energy carried by the second emitted particle in LS is given by

$$E^{1}_{m_2} = \int \mathrm{d}\varepsilon^{\mathrm{c}}_{\mathrm{m}_2} \left\{ \frac{m_{\mathrm{n}} m_2}{M^2_{\mathrm{C}}} E_{\mathrm{n}} f_0(\varepsilon^{\mathrm{c}}_{m_2}) + \varepsilon^{\mathrm{c}}_{m_2} f_0(\varepsilon^{\mathrm{c}}_{m_2}) + 2\frac{\sqrt{m_{\mathrm{n}} m_2}}{M_{\mathrm{C}}} \sqrt{E_{\mathrm{n}} \varepsilon^{\mathrm{c}}_{m_2}} f_1(\varepsilon^{\mathrm{c}}_{m_2}) \right\} \quad \text{(B36)}$$

From Eq.(B28), $f_1(\varepsilon^{\mathrm{c}}_{m_2})$ in the third term in Eq.(B36) has the explicit form

$$f_{l=1}(\varepsilon^{\mathrm{c}}_{m_2}) = \frac{1}{4}\sqrt{\frac{M_1}{m_2}} \int_A^B \mathrm{d}E^{\mathrm{c}}_{M_1} \frac{f_1(E^{\mathrm{c}}_{M_1})}{\sqrt{E^{\mathrm{c}}_{M_1}}} \int_a^b \frac{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}}{\sqrt{\varepsilon^{\mathrm{r}}_{m_2}}} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_1}} \left(\frac{\varepsilon^{\mathrm{c}}_{m_2} + \frac{m_2}{M_1} E^{\mathrm{c}}_{M_1} - \varepsilon^{\mathrm{r}}_{m_2}}{2\sqrt{\frac{m_2}{M_1} E^{\mathrm{c}}_{M_1} \varepsilon^{\mathrm{c}}_{m_2}}} \right) \quad \text{(B37)}$$

Substituting Eq.(B37) into Eq.(B36), and by exchanging the integration order as the same as in Eq.(B32), the third term in Eq.(B36) becomes

$$\frac{1}{4}\frac{M_1}{M_{\mathrm{C}}}\sqrt{\frac{m_{\mathrm{n}} E_{\mathrm{n}}}{m_2}} \int \mathrm{d}E^{\mathrm{c}}_{M_1} \frac{f_1(E^{\mathrm{c}}_{M_1})}{E^{\mathrm{c}}_{M_1}} \int \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \frac{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}}{\sqrt{\varepsilon^{\mathrm{r}}_{m_2}}} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} \{\varepsilon^{\mathrm{c}}_{m_2} + \frac{m_2}{M_1} E^{\mathrm{c}}_{M_1} - \varepsilon^{\mathrm{r}}_{m_2}\} \quad \text{(B38)}$$

Carrying out the integration over $\varepsilon^{\mathrm{c}}_{m_2}$ with the integration limits as the same as that in Eq.(B32), this part becomes into $8\frac{m_2}{M_1}\sqrt{\frac{m_2}{M_1} E^{M_1}_{\mathrm{c}} \varepsilon^{m_2}_{\mathrm{r}}} E^{M_1}_{\mathrm{c}}$. By using $\int \mathrm{d}\varepsilon^{\mathrm{r}}_{m_2} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} = 1, E^{\mathrm{c}}_{M_1} = \frac{m_1}{M_1}\varepsilon^{\mathrm{c}}_{m_1}$, and $f_1(E^{\mathrm{c}}_{M_1}) = -\frac{M_1}{m_1} f_1(\varepsilon^{\mathrm{c}}_{m_1})$, the third term in Eq.(B36) is reduced into

$$-2\frac{\sqrt{m_{\mathrm{n}} m_1}}{M_{\mathrm{C}}} \frac{m_2}{M_1} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_1} \sqrt{E_{\mathrm{n}} \varepsilon^{\mathrm{c}}_{m_1}} f_1(\varepsilon^{\mathrm{c}}_{m_1})$$

The second term in Eq.(B36) can be reduced by

$$\int \varepsilon^{\mathrm{c}}_{m_2} f_0(\varepsilon^{\mathrm{c}}_{m_2}) \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} = \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} \frac{1}{4}\sqrt{\frac{M_1}{m_2}} \int \frac{f_0(E^{\mathrm{c}}_{M_1})}{\sqrt{E^{\mathrm{c}}_{M_1}}} \mathrm{d}E^{\mathrm{c}}_{M_1} \int \frac{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}}{\sqrt{\varepsilon^{\mathrm{r}}_{m_2}}} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \varepsilon^{\mathrm{c}}_{m_2}$$

$$= \int \mathrm{d}E^{\mathrm{c}}_{M_1} \frac{1}{4}\sqrt{\frac{M_1}{m_2}} \frac{f_0(E^{\mathrm{c}}_{M_1})}{\sqrt{E^{\mathrm{c}}_{M_1}}} \int \frac{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}}{\sqrt{\varepsilon^{\mathrm{r}}_{m_2}}} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \frac{1}{2} (\varepsilon^{\mathrm{c}}_{m_2})^2 \Big|_{(\sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}} - \sqrt{\varepsilon^{\mathrm{r}}_{m_2}})^2}^{(\sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}} + \sqrt{\varepsilon^{\mathrm{r}}_{m_2}})^2}$$

$$= \int \mathrm{d}E^{\mathrm{c}}_{M_1} f_0(E^{\mathrm{c}}_{M_1}) \int \mathrm{d}\varepsilon^{\mathrm{r}}_{m_2} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} (\frac{m_2}{M_1} E^{\mathrm{c}}_{M_1} + \varepsilon^{\mathrm{r}}_{m_2})$$

$$= \frac{m_1 m_2}{M_1^2} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} f_0(\varepsilon^{\mathrm{c}}_{m_2}) \varepsilon^{\mathrm{c}}_{m_2} + \int \mathrm{d}\varepsilon^{\mathrm{r}}_{m_2} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \varepsilon^{\mathrm{r}}_{m_2} \tag{B39}$$

Thus, the energies carried by the second emitted particle is obtained by

$$\begin{aligned} E^{1}_{m_2} = & \frac{m_{\mathrm{n}} m_2}{M_{\mathrm{C}}^2} E_{\mathrm{n}} + \frac{m_1 m_2}{M_1^2} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} f_0(\varepsilon^{\mathrm{c}}_{m_2}) \varepsilon^{\mathrm{c}}_{m_2} + \int \mathrm{d}\varepsilon^{\mathrm{r}}_{m_2} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \varepsilon^{\mathrm{r}}_{m_2} \\ & - 2 \frac{\sqrt{m_{\mathrm{n}} m_1}}{M_{\mathrm{C}}} \frac{m_2}{M_1} \sqrt{E_{\mathrm{n}}} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_1} f_1(\varepsilon^{\mathrm{c}}_{m_1}) \sqrt{\varepsilon^{\mathrm{c}}_{m_1}} \end{aligned} \tag{B40}$$

In terms of the same procedure for m_2 the energy carried by its residual nucleus M_2 can be obtained by

$$\begin{aligned} E^{1}_{M_2} = & \frac{m_{\mathrm{n}} M_2}{M_{\mathrm{C}}^2} E_{\mathrm{n}} + \frac{m_1 M_2}{M_1^2} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} f_0(\varepsilon^{\mathrm{c}}_{m_2}) \varepsilon^{\mathrm{c}}_{m_2} + \frac{m_2}{M_2} \int \mathrm{d}\varepsilon^{\mathrm{r}}_{m_2} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \varepsilon^{\mathrm{r}}_{m_2} \\ & - 2 \frac{\sqrt{m_{\mathrm{n}} m_1}}{M_{\mathrm{C}}} \frac{M_2}{M_1} \sqrt{E_{\mathrm{n}}} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_1} f_1(\varepsilon^{\mathrm{c}}_{m_1}) \sqrt{\varepsilon^{\mathrm{c}}_{m_1}} \end{aligned} \tag{B41}$$

The γ de-excitement energy is obtained by the averaged residual excitation energy

$$\begin{aligned} E^{1}_{\gamma} &= \int \frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} \mathrm{d}\Omega^{\mathrm{c}}_{m_2}} \frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon^{\mathrm{c}}_{m_1} \mathrm{d}\Omega^{\mathrm{c}}_{m_1}} \left[E^* - B_1 - B_2 - \varepsilon^{\mathrm{c}}_{m_1} - \varepsilon^{\mathrm{c}}_{m_2} - E^{\mathrm{c}}_{M_1} \right] \mathrm{d}\varepsilon^{\mathrm{c}}_{m_1} \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} \mathrm{d}\Omega^{\mathrm{c}}_{m_1} \mathrm{d}\Omega^{\mathrm{c}}_{m_2} \\ &= E^* - B_1 - B_2 - \int \varepsilon^{\mathrm{c}}_{m_1} f_0(\varepsilon^{\mathrm{c}}_{m_1}) \mathrm{d}\varepsilon^{\mathrm{c}}_{m_1} - \int \varepsilon^{\mathrm{c}}_{m_2} f_0(\varepsilon^{\mathrm{c}}_{m_2}) \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} - \int f_0(E^{\mathrm{c}}_{M_1}) E^{\mathrm{c}}_{M_1} \mathrm{d}E^{\mathrm{c}}_{M_1} \end{aligned} \tag{B42}$$

where

$$\int \varepsilon^{\mathrm{c}}_{m_2} f_0(\varepsilon^{\mathrm{c}}_{m_2}) \mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} = \frac{m_1 m_2}{M_1^2} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_1} f_0(\varepsilon^{\mathrm{c}}_{m_1}) \varepsilon^{\mathrm{c}}_{m_1} + \int \mathrm{d}\varepsilon^{\mathrm{r}}_{m_2} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \varepsilon^{\mathrm{r}}_{m_2} \tag{B43}$$

$$\int E^{\mathrm{c}}_{M_2} f_0(E^{\mathrm{c}}_{M_2}) \mathrm{d}E^{\mathrm{c}}_{M_2} = \frac{m_1 M_2}{M_1^2} \int \mathrm{d}\varepsilon^{\mathrm{c}}_{m_1} f_0(\varepsilon^{\mathrm{c}}_{m_1}) \varepsilon^{\mathrm{c}}_{m_1} + \frac{m_2}{M_2} \int \mathrm{d}\varepsilon^{\mathrm{r}}_{m_2} \frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}} \varepsilon^{\mathrm{r}}_{m_2} \tag{B44}$$

Therefore,

$$E_{\gamma}^{1}=E^{*}-B_{1}-B_{2}-\frac{M_{\mathrm{C}}}{M_{1}}\int \mathrm{d}\varepsilon_{m_1}^{\mathrm{c}} f_{0}(\varepsilon_{m_1}^{\mathrm{c}})\varepsilon_{m_1}^{\mathrm{c}}-\frac{M_{1}}{M_{2}}\int \mathrm{d}\varepsilon_{m_2}^{\mathrm{r}}\frac{\mathrm{d}\sigma}{\mathrm{d}\varepsilon_{m_2}^{\mathrm{r}}}\varepsilon_{m_2}^{\mathrm{r}} \qquad \text{(B45)}$$

It is easy to see that if the recoil effect is not taken into account, the residual nucleus is static in CMS, in this way the energy carried by the second emitted particle only has the second term in Eq.(B43), while the first term is the energy gain by recoil effect. From Eq.(B43) one can see that the recoil effect increases with the decreasing of the mass of residual nucleus, and with the increasing of the mass of emitted particles.

The total released energy can be obtained by summing over Eqs.(B36, B40, B41 and B45)

$$E_{\mathrm{T}}^{1}=E_{m_1}^{1}+E_{m_2}^{1}+E_{M_2}^{1}+E_{\gamma}^{1}=E_{\mathrm{n}}+Q \qquad \text{(B46)}$$

Here, $Q=B_{\mathrm{b}}-B_{1}-B_{2}$ is the reaction Q-value in the two particle emission process. Therefore, the energy balance is held exactly in the analytical form.

From the afore-mentioned formulation, one can see that the quantity of the Legendre expansion coefficient with l=1 ($f_{1}(\varepsilon_{m_1}^{\mathrm{c}})$>0) plays an important role in the energies carried by different kinds of emitted particles, which is caused by the forward emission of the first emitted particle in the pre-equilibrium process. If $f_{1}(\varepsilon_{m_1}^{\mathrm{c}})$ increases, then the energy carried by the first emitted particle increasing in LS, while the recoil effect reduces the energies of the second particles emitted from the recoil residual nuclei due to the motion of the center of mass system. Meanwhile, the shape of $f_{0}(\varepsilon_{m_1}^{\mathrm{c}})$ can also influence the energy distributions between the emitted particles, the residual nucleus and de-excitation γ energy. The harder of the spectrum, the more energy carried by the emitted particle, while the energies carried by the residual nucleus and de-excitation γ emissions are reduced. But in pure equilibrium emission process, either isotropic approximation or the Hauser-Feshbach theory，the partial wave with l=1 of the Legendre expansion is zero, only the energy distributions for all of kinds of the

emitted particles are influenced by the shapes of the first emitted particle.

B2.2 Double Differential Cross Sections from Continuum State to Discrete Levels

When the residual nucleus is in discrete level states, the double differential cross section has different expression since $\varepsilon^{\mathrm{r}}_{m_2}$ is a single value. In this case

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon^{\mathrm{r}}_{m_2}\mathrm{d}\Omega^{\mathrm{r}}_{m_2}} = \frac{1}{4}\delta(\varepsilon^{\mathrm{r}}_{m_2} - \varepsilon^{\mathrm{r}}_{m_2,k}) \tag{B47}$$

where $\varepsilon^{\mathrm{r}}_{m_{2,k}}$ is the function of $E^{\mathrm{c}}_{M_1}$ and has the value as

$$\varepsilon^{\mathrm{r}}_{m_2,k}(E^{\mathrm{c}}_{M_1}) = \frac{M_2}{M_1}(E^{*} - B_1 - B_2 - E_{k_2} - \frac{M_{\mathrm{C}}}{m_1}E^{\mathrm{c}}_{M_1}) \tag{B48}$$

The Legendre coefficient in Eq.(B38) becomes into the form

$$f_l(\varepsilon^{\mathrm{c}}_{m_2})_k = \frac{1}{4}\sqrt{\frac{M_1}{m_2}}\int_A^B \frac{f_l(E^{\mathrm{c}}_{M_1})}{\sqrt{\varepsilon^{\mathrm{r}}_{m_2,k}}\sqrt{E^{\mathrm{c}}_{M_1}}}\mathrm{P}_l(\cos\Theta)\mathrm{d}E^{\mathrm{c}}_{M_1} \tag{B49}$$

with

$$\cos\Theta = \frac{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1} + \varepsilon^{\mathrm{c}}_{m_2} - \varepsilon^{\mathrm{r}}_{m_2,k}}{2\sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}\varepsilon^{\mathrm{c}}_{m_2}}} \tag{B50}$$

For a value of $E^{\mathrm{c}}_{M_1}$ the maximum energy of the second emitted particle $\varepsilon^{\mathrm{c}}_{m_2,\max}$ should correspond to the direction of the second emitted particle with the same direction of the first outgoing particle.

$$\varepsilon^{\mathrm{c}}_{m_2,\max}(E^{\mathrm{c}}_{M_1}) = \left(\sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}} + \sqrt{\varepsilon^{\mathrm{r}}_{m_2,k}}\right)^2 \tag{B51}$$

There is a maximum value in Eq.(B51) for $E^{c}_{M_1}$, which is given by

$$\hat{E}^{c}_{M_1} = \frac{\frac{m_1}{M_C} E'_k}{1 + \frac{M_C}{m_1}\frac{M_2}{m_2}} \tag{B52}$$

with

$$E'_k = E^* - B_1 - B_2 - E_{k_2}$$

Substituting the maximum value into Eq. (B51), the maximum energy of the second emitted particle is obtained by

$$\varepsilon^{c}_{m_2,\max} = \frac{m_1}{M_C} R E^{'}_k \tag{B53}$$

For a given value of $\varepsilon^{c}_{m_2}$, from the condition of -1 ≤ cosΘ ≤ 1 one can get the integration area of $E^{c}_{M_1}$ as follows

$$A = \{E^{c}_{M_1,\min}, \frac{1}{R^2}(\sqrt{U} - \sqrt{\frac{m_2}{M_1}\varepsilon^{c}_{m_2}})^2\}$$

$$B = \{E^{c}_{M_1,\max}, \frac{1}{R^2}(\sqrt{U} + \sqrt{\frac{m_2}{M_1}\varepsilon^{c}_{m_2}})^2\} \tag{B54}$$

where $R = \frac{m_2}{M_1} + \frac{M_2}{M_1}\frac{M_C}{m_1}$; $U = \frac{M_2}{M_1}(RE'_k - \frac{M_C}{m_1}\varepsilon^{c}_{m_2})$.

The minimum energy of the second emitted particle $\varepsilon^{m_2}_{c,\max}$ corresponds to the opposite direction of the first outgoing particle.

$$\varepsilon^{c}_{m_2,,\min}(E^{c}_{M_1}) = \left(\sqrt{\frac{m_2}{M_1}E^{c}_{M_1}} - \sqrt{\varepsilon^{r}_{m_2,k}}\right)^2 \tag{B55}$$

There is a zero point at

$$\breve{E}^{\mathrm{c}}_{M_1} = \frac{\frac{M_2}{m_2}E'_k}{1+\frac{M_{\mathrm{C}}}{m_1}\frac{M_2}{m_2}} \tag{B56}$$

There are three cases for the maximum values of the second emitted particle

$$\varepsilon^{\mathrm{c}}_{m_2,\min} = \begin{cases} (\sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1,\min}} - \sqrt{\varepsilon^{\mathrm{r}}_{m_2,k}})^2 & \text{if } \breve{E}^{\mathrm{c}}_{M_1} \le E^{\mathrm{c}}_{M_1,\min} \\ 0 & \text{if } E^{\mathrm{c}}_{M_1,\min} < \breve{E}^{\mathrm{c}}_{M_1} < E^{\mathrm{c}}_{M_1,\max} \\ (\sqrt{\varepsilon^{\mathrm{r}}_{m_2,k}} - \sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1,\max}})^2 & \text{if } E^{\mathrm{c}}_{M_1,\max} \le \breve{E}^{\mathrm{c}}_{M_1} \end{cases} \tag{B57}$$

The expression of the double-differential cross section of the residual nucleus can be obtained by replacing m_2 and $\varepsilon^{\mathrm{r}}_{m_2}$ with M_2, and $E^{\mathrm{r}}_{M_2}$ in Eq.(B49), respectively.

One can prove that the $f_0(\varepsilon^{\mathrm{c}}_{m_2})_k$ is also normalized. By means of exchanging the integration order, the integration limits of $\varepsilon^{\mathrm{c}}_{m_2}$ are $(\sqrt{\varepsilon^{\mathrm{r}}_{m_2,k}} \pm \sqrt{\frac{m_2}{M_1}E^{\mathrm{c}}_{M_1}})^2$ for a value of $E^{\mathrm{c}}_{M_1}$. By using Eq.(B49)

$$\int_{\varepsilon^{\mathrm{c}}_{m_2,\min}}^{\varepsilon^{\mathrm{c}}_{m_2,\max}} f_0(\varepsilon^{\mathrm{c}}_{m_2})\mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} = \int f_0(E^{\mathrm{c}}_{M_1})\mathrm{d}E^{\mathrm{c}}_{M_1} = 1 \tag{B58}$$

When the final state is in the discrete level states, with analogy procedure all of the released energies can be obtained. If the residual nucleus is in E_{k_2} level, which is just the energy of gamma de-excitation. The energy carried by the second emitted particle is obtained by

$$E^{1}_{m_2,k} = \int \left\{ \left(\frac{m_{\mathrm{n}}m_2}{M^2_{\mathrm{C}}}E_{\mathrm{n}} + \varepsilon^{\mathrm{c}}_{m_2} \right) f_0(\varepsilon^{\mathrm{c}}_{m_2})_k + 2\frac{\sqrt{m_{\mathrm{n}}m_2}}{M_{\mathrm{C}}}\sqrt{E_{\mathrm{n}}\varepsilon^{\mathrm{c}}_{m_2}}f_1(\varepsilon^{\mathrm{c}}_{m_2})_k \right\}\mathrm{d}\varepsilon^{\mathrm{c}}_{m_2} \tag{B59}$$

$$E^{1}_{M_1,k}=\int\left\{\left(\frac{m_{\rm n}M_2}{M_{\rm C}^2}E_{\rm n}+E^{\rm c}_{M_1}\right)f_0(E^{\rm c}_{M_1})_k+2\frac{\sqrt{m_{\rm n}M_2}}{M_{\rm C}}\sqrt{E_{\rm n}E^{\rm c}_{M_1}}f_1(E^{\rm c}_{M_1})_k\right\}{\rm d}E^{\rm c}_{M_1} \quad \text{(B60)}$$

Substituting Eqs.(B49, B50) into Eqs.(B59, B60) and carrying out the integration with the integration limits of $\varepsilon^{\rm c}_{m_2}$ as the same as that used in Eq.(B58), the energies carried by m_2 and M_2 can be obtained in the case from continuum state to discrete levels, respectively.

The energy carried by the second emitted particle in LS is given by

$$\begin{aligned}E^{1}_{m_2,k}=&\frac{m_{\rm n}m_2}{M_{\rm C}^2}E_{\rm n}+\frac{M_2}{M_1}(E^*-B_1-B_2-E_{k_2})\\&-(\frac{M_{\rm C}M_2}{M_1^2}-\frac{m_1m_2}{M_1^2})\int{\rm d}\varepsilon^{\rm c}_{m_1}f_0(\varepsilon^{\rm c}_{m_1})\varepsilon^{\rm c}_{m_1}\\&-2\frac{\sqrt{m_{\rm n}m_1}}{M_{\rm C}}\sqrt{E_{\rm n}}\frac{m_2}{M_1}\int f_1(\varepsilon^{\rm c}_{m_1})\sqrt{\varepsilon^{\rm c}_{m_1}}{\rm d}\varepsilon^{\rm c}_{m_1}\end{aligned} \quad \text{(B61)}$$

and

$$\begin{aligned}E^{1}_{M_2,k}=&\frac{m_{\rm n}M_2}{M_{\rm C}^2}E_{\rm n}+\frac{m_2}{M_1}(E^*-B_1-B_2-E_{k_2})\\&-(\frac{M_{\rm C}m_2}{M_1^2}-\frac{m_1M_2}{M_1^2})\int{\rm d}\varepsilon^{\rm c}_{m_1}f_0(\varepsilon^{\rm c}_{m_1})\varepsilon^{\rm c}_{m_1}\\&-2\frac{\sqrt{m_{\rm n}m_1}}{M_{\rm C}}\sqrt{E_{\rm n}}\frac{M_2}{M_1}\int f_1(\varepsilon_{\rm c}^{m_1})\sqrt{\varepsilon^{\rm c}_{m_1}}{\rm d}\varepsilon^{\rm c}_{m_1}\end{aligned} \quad \text{(B62)}$$

The energy carried by the first emitted particle in LS is already given in Eq.(B34), the total released energy is given by ($Q=B_{\rm n}-B_1-B_2$),

$$E^{1}_{{\rm T},k}=E^{1}_{m_1}+E^{1}_{m_2,k}+E^{1}_{M_2,k}+E^{1}_{\gamma,k}=E_n+Q \quad \text{(B63)}$$

Obviously, in the case of the second particle emission from continuum state to discrete state, the energy balance is still held exactly in the analytical form.

The formulation given above is employed in UNF code to set up files-6 with full energy balance in the neutron data library. The precision of energy balance, in general, is much less than one percent due to the accurate kinematics.

B3 Double-Differential Cross Section of Composite Particle Emissions

The pickup mechanism should be involved in the composite particle emission to give the pre-formation probability of composite particle in compound nucleus. At first the Iwamoto- Harada model[8] has been employed in UNF code. But the calculated result indicated that this model overestimated the pre-formation probabilities of the composite particles. The study turns out that the integration over momentum space in the phase space integration has the superfluous part, which is the forbidden area restricted by excitation energy. So the E-dependent improved Iwamoto- Harada pickup mechanism was developed[9] to reduce the pre-formation probabilities, and used in UNF code.

The double-differential cross sections of single nucleon can be calculated by generalized master equation[10, 11] to get the angular momentum dependent lifetime $\tau(n,\Omega)$ with the Legendre expansion form as

$$\tau(n,\Omega)=\sum_{l}\zeta_{l}(n)\mathrm{P}_{l}(\cos\theta) \tag{B64}$$

The double-differential cross section of particle b is represented by

$$\frac{\mathrm{d}^{2}\sigma}{\mathrm{d}\Omega_{\mathrm{b}}\mathrm{d}\varepsilon_{\mathrm{b}}}=\sum_{n}\frac{\mathrm{d}\sigma(n)}{\mathrm{d}\varepsilon_{\mathrm{b}}}A(n,\varepsilon_{\mathrm{b}},\Omega_{\mathrm{b}}) \tag{B65}$$

where $\frac{\mathrm{d}\sigma(n)}{\mathrm{d}\varepsilon_{\mathrm{b}}}$ = component of n exciton state in the spectrum.

In the case of composite particle emission, the outgoing nucleon may pickup some nucleons below and above the Fermi surface to form a composite particle to be emitted. According to the studies on pickup mechanism, at low energies (E_{n}≤20 MeV), the dominant configuration is pickup the nucleons below the Fermi surface[12].

The angular distribution factor in Eq.(B65) of *b* particle with emitted energy

$\varepsilon_{\rm b}$ and direction $\Omega_{\rm b}$ at n exciton state is introduced by

$$A(n,\varepsilon_{\rm b},\Omega_{\rm b})=\frac{1}{N}\int {\rm d}\boldsymbol{p}_1,\cdots,{\rm d}\boldsymbol{p}_{A_{\rm b}}\delta(\boldsymbol{p}_{\rm b}-\sum_{i=1}^{A_{\rm b}}\boldsymbol{p}_i)\prod_{j=2}^{A_{\rm b}}D(V_j)\tau(n,\Omega_1) \quad \text{(B66)}$$

with $p_1 > p_{\rm f}$ and $p_j < p_{\rm f}$ for j=2,⋯, $A_{\rm b}$.

where $\tau(n,\Omega_1)$ = lifetime of the outgoing single nucleon marked by 1

$p_{\rm f}$ = Fermi momentum

$p_{\rm b}$ = momentum of outgoing composite particle b with mass number $A_{\rm b}$.

D = momentum distribution of the compound nucleus

N = normalization factor.

The δ function in Eq.(B66) implies momentum conservation. Obviously, if emitted particle b is a nucleon, then Eq.(B66) will return to the case of single nucleon emission. The Fermi gas model is employed to give the momentum distribution of the nucleon below the Fermi surface.

$$D(\boldsymbol{p}){\rm d}\boldsymbol{p}=\frac{3}{4\pi p_{\rm f}^3}\Theta(p_{\rm f}-p){\rm d}\boldsymbol{p} \quad \text{(B67)}$$

The procedure to carry out the integration analytically over the angle and the momentum of Eq.(B66) can be found in Refs.[13] and [14], which is reduced into the following form

$$A_{\rm b}(n,\varepsilon_{\rm b},\Omega)=\frac{1}{4\pi}\sum_l\frac{\zeta_l(n)}{\zeta_0(n)}R_{\rm b}(\varepsilon_{\rm b}){\rm P}_l(\cos\theta_{\rm b}) \quad \text{(B68)}$$

The factor $R_{\rm b}(\varepsilon_{\rm b})$ in Eq.(B68) is defined by

$$R_l(\varepsilon_{\rm b})=\frac{G_l(\varepsilon_{\rm b})}{G_0(\varepsilon_{\rm b})} \quad \text{(B69)}$$

where

$$G_l(\varepsilon_{\rm b})=\int_{\max\{1,x_{\rm b}-A_{\rm b}+1\}}^{\sqrt{1+E/\varepsilon_{\rm f}}}{\rm d}x_1\ x_1\int_{x_{\rm b}-x_1}^{A_{\rm b}-1}Z_{\rm b}(y){\rm P}_l\left(\frac{x_{\rm b}^2+x_1^2-y^2}{2x_{\rm b}x_1}\right)y{\rm d}y \quad \text{(B70)}$$

E = excitation energy

ε_{f} = Fermi energy

$x_{1} = \dfrac{p_{1}}{p_{\mathrm{f}}}$ = dimensionless momentum of particle 1

$x_{\mathrm{b}} = \dfrac{p_{\mathrm{b}}}{p_{\mathrm{f}}}$ = dimensionless momentum of particle b

$y = \sqrt{x_{\mathrm{b}}^{2} + x_{\mathrm{c}}^{2} - 2x_{\mathrm{b}}x_{1}\cos\theta}$

The final result of $Z_{\mathrm{b}}(y)$ in Eq.(B70) is obtained as follows:

$$Z_{\mathrm{b}}(y) = \begin{cases} 1 & \mathrm{b} = \mathrm{d} \\ (1 - \dfrac{1}{2}y)^{2}(4 + y) & \mathrm{b} = \mathrm{t}, {}^{3}\mathrm{He} \\ \dfrac{(3 - \mathrm{y})^{4}}{y}[210 - 120(3 - y) + 21(3 - y)^{2} - (3 - y)^{3}] & \mathrm{b} = \alpha \end{cases} \quad \text{(B71)}$$

In Eq.(B68), the partial wave coefficients $\zeta_{l}(\varepsilon)$ of single nucleon emission are calculated by the linear momentum dependent exciton state density model[15]. This approach is a consistent way to obtain the angular distribution of outgoing nucleons. In this method the leading particle is not assumed; instead, a statistical population of all states compatible with energy and momentum conservation is proposed. The effects of the Fermi motion of the nucleons, as well as the Pauli blocking by the "sea" of nucleons, are included. In particular, the angular distribution from the first pre-equilibrium state in a nucleon-induced reaction is identical to that obtained with the Kicuchi-Kawai scattering kernel[16,11].

There is no any additional free parameter in this method, which should be pointed out emphatically.

B4 Functions of UNF Code

The UNF code (2001 version) was developed for calculating fast neutron reaction data of structural materials with incident energies from a few kilo-electron-volts to 20 MeV. This code can handle a decay sequence up to (n,3n) reaction channel, including 14 reaction channels. The physical quantities calculated by UNF code contain the follows:

(1) Cross sections of total, elastic scattering, non-elastic scattering, and all reaction channels in which the discrete level emissions and continuum emissions are included.

(2) Angular distributions of elastic scattering both in CMS and LS.

(3) The energy spectra of the particle emitted in all reaction channels.

(4) Double-differential cross sections of all kinds of particle emissions (neutron, proton, alpha particle, deuteron, triton and ^{3}He), as well as the recoil nuclei.

(5) Partial kerma factors of every reaction channels, and the total kerma factor.

(6) Gamma production data (gamma spectra, gamma production cross sections, and multiplicity), including the gamma production cross sections from level to level.

(7) Total double-differential cross sections of all kinds outgoing particles from all reaction channels.

(8) Cross sections of isomeric states, if the level is a isomeric state of the residual nucleus.

(9) dpa cross sections used in radiation damage.

UNF code can also handle the calculations for a single element or for natural nucleus, and the target can be in ground state or in isomeric state.

Besides the output file, the outputting in ENDF/B-6 format is also included, (files3, 4, 6, 12, 13, 14, 15 or files-3, 4, 5, which controlled by a flag).

Meanwhile, some self-checking functions are designed for checking the errors in the input parameter data, if it exist.

B5 Calculated Examples and Discussion

Some calculated results have been shown in Ref.[4]. A large number of figures to compare the calculated results with the measured data have been published in "Communication of Nuclear Data Progress" INDC(CRP)-041/L to 053/L as technical reports during the evaluations of the nuclei for CENDL-3. Some typical calculated examples are given below.

The capture radiation cross section of n+^{160}Gd is shown in Fig.B1. In UNF code the gamma de-excitation has three mechanisms; (1) equilibrium gamma emission, (2) pre-equilibrium gamma emission, (3) direct gamma emission. The Oblozinsky's formula[17] is employed for the last two terms. A small peak occurs at about 14 MeV in the capture radiation cross section, which is the contribution from the direct gamma emission.

The (n,2n) reaction cross section of n+^{150}Nd is shown in Fig.B2. The calculated results agree fairly well with the experimental measurements.

All of the measured data used in Fig.B1 and Fig.B2 are retrieved from EXFOR library.

Only few double-differential measurements have been performed for charged outgoing particles. For n+^{56}Fe the double-differential measurements of (n,xα), (n,d) reactions were performed by Grimes[18]. The comparisons of the calculated results with the experimental data of outgoing alpha particle have been given in Refs. [13] and [19], while the comparisons of the calculated results with the measured data of outgoing deuteron are shown in Fig.B3 of the ^{56}Fe(n,d) reaction at E_n=14.8 MeV for outgoing angles 30, 45, 90, and 135 deg. The results are in good agreement with the measured data.

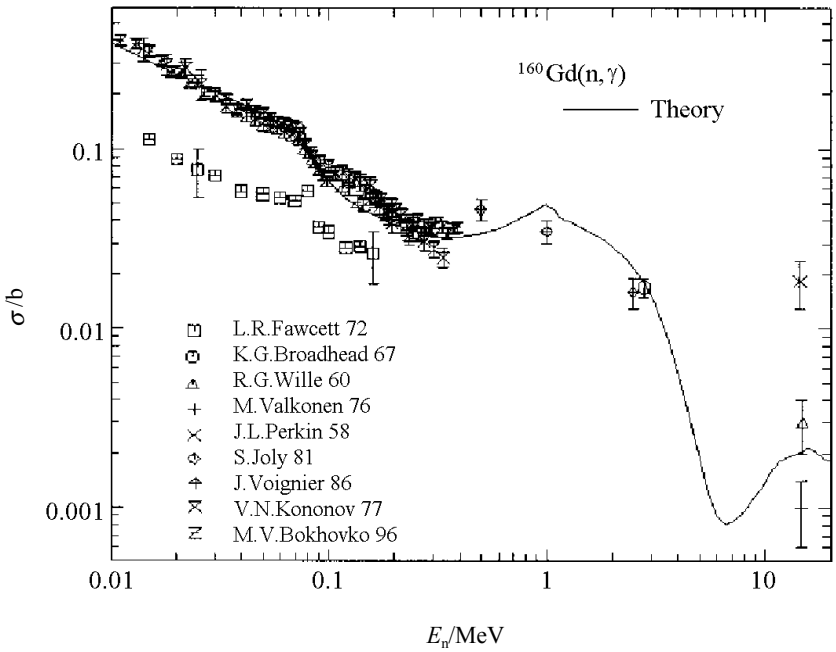

Fig.B1 The (n,γ) cross section of n+^{160}Gd reaction

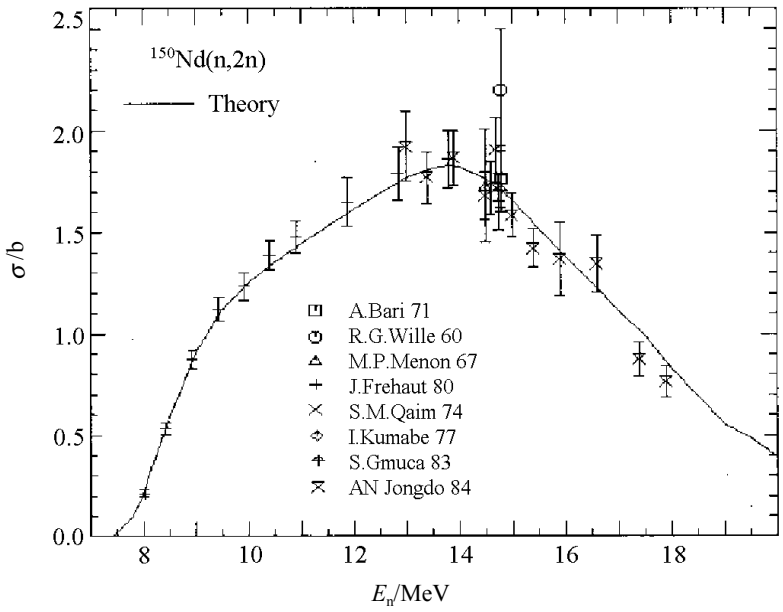

Fig.B2 The reaction cross section of (n,2n) of n+^{150}Nd

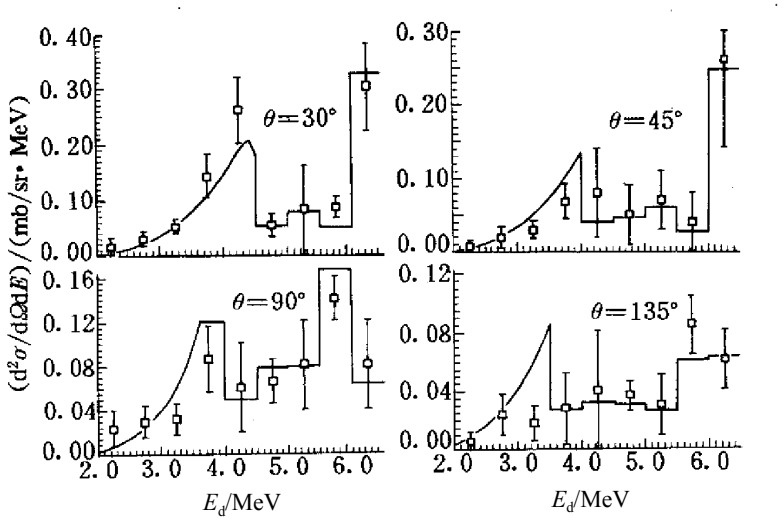

Fig.B3 The deuteron energy-angular spectra of n+^{56}Fe at E_n=14.8 MeV.

The data are taken from Ref.[17]

B6 Summary

The first version of the UNF code was completed in 1992. The code has been developed continually since that time and has often been used as an evaluation tool for setting up CENDL and for analyzing the measurements. During these years many improvements have been made. The Hauser-Feshbach model with the width fluctuation correlation is a very successful theory used for low incident energies. With the increasing of incident energy, the pre-equilibrium mechanism needs to be involved by using angular momentum dependent exciton model.

The frame of the theoretical model used in UNF code has some improvements. Mainly in three aspects as afore-mentioned. Previously, limited by computer condition the UNF code system included three codes, i.e. UNF code used for single element; NUNF used for natural nucleus; SUNF code for fission production nucleus. Now these three codes are unified into one code. Meanwhile,

for the purpose of varied utilization, more functions were added in this code. Thus, the 2001 version of UNF code was issued.

Information on the energies of charged particles produced in the nuclear reactions is needed in several applications. For example, the kerma factor is of specific interest regarding the heat produced in reactors, as well as regarding the calculation of radiation damage in structure materials. Being the accurate kinematics used in the UNF code, the energy-angular spectra of outgoing charged particles, as well as recoil nuclei can be obtained with the accurate kinematics, so the single particle approximation is not needed in the calculations of kerma factor and radiation damage.

Now, the manual of the UNF code is available for users. The format of the input parameter files and the output files, as well as the functions of flag used in UNF code, are introduced in detail, and the examples of the format of input parameters files are given.

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