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THE FORMULATION OF "UNIFY" CODE FOR THE CALCULATION OF FAST NEUTRON DATA FOR STRUCTURAL MATERIALS

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This work was performed under IAEA Research Contract No. 4324

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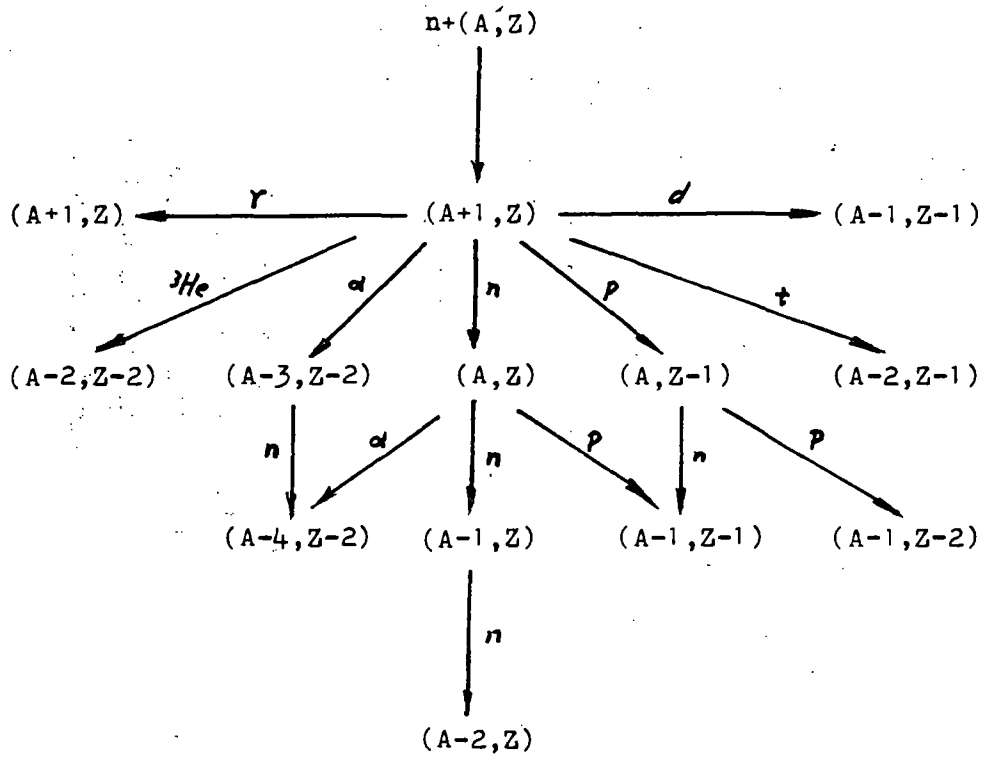

Fig.1 Overall scheme of the reaction chains

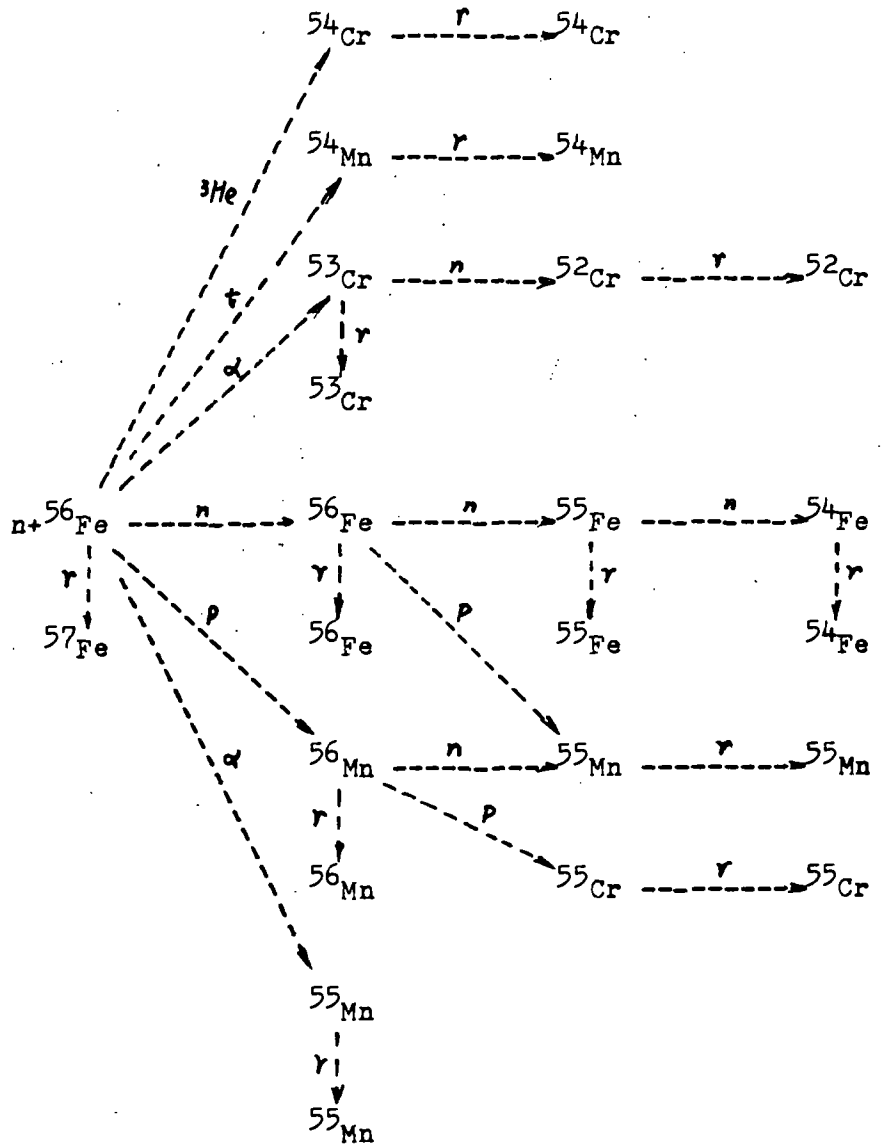

Fig.2 Sample decay chains for n+^{56}Fe

2. Exciton Model

(2.1) Master Euqation and Mean Lifetime

In the theoretical description of pre-equilibrium reaction two models have become widely popular: the hybrid model [1,2,3] and the exciton model [4]. The exciton model has been adopted in the present unified model. The evaluation of particle-hole excitation can be described by the master equation which is first proposed by Cline and Blann [5]. The master equation has the form proposed by Cline [6] and Ribansky [7].

$$\frac{dq(n,t)}{dt} = \lambda^{+}(n-2)q(n-2,t)+\lambda^{-}(n+2)q(n+2,t)$$

$$-[\lambda^{+}(n)+\lambda^{-}(n)+W_t(N)]\ q(n,t). \qquad (2.1.1)$$

Here: n is the exciton number, being equal to the sum over the number of particles p and that of holes h.

q(n,t) stands for the occupation probability in exciton state n at time t.

$\lambda^{+}(n)$ and $\lambda^{-}(n)$ are the internal transition rates from n to n±2, respectively.

$W_t(n)$ stands for the total emission rates from state n, summed over all kinds of outgoing particles and r-ray.

The mean lifetime $\tau(n)$ of the exciton state n is defined by

$$\tau(n)=\int_0^{\infty} q(n,t)dt. \qquad (2.1.2)$$

Carrying out integration of the master equation over time, the mean lifetimes satisfy the equation [8]

$$-q(n,t=0)=\lambda^{+}(n-2)\tau(n-2)+\lambda^{-}(n+2)\tau(n+2)$$

$$-[\lambda^{+}(n)+\lambda^{-}(n)+W_t(n)]\ \tau(n).$$

$$\text{for } n=n_0,n_0+2,\ldots. \qquad (2.1.3)$$

where q(n,t=0) is the initial condition for the process.

The average energy spectrum for the particle b emission at channel energy ε is then given by

$$\frac{d\sigma(ab)}{d\varepsilon}=\sigma_a\sum_b W_b(n,\varepsilon)\tau(n). \qquad (2.1.4)$$

where a denotes the incident particle, σ_a stands for the composite formation cross section, $W_b(n,\varepsilon)$ is the emission rate of particle b at energy ε from the exciton state n.

The solution of mean lifetime is obtained by the closed formula as following

$$\tau(n)=\mathcal{F}_n\eta(n)\prod_{\substack{i=n_0\\ \Delta i=2}}^{n-2}\lambda^+(i)\eta(i)\mathcal{F}_{i+2} \qquad \text{for } n\ n_0 \qquad (2.1.5.a)$$

$$\tau(n_0)=\mathcal{F}_{n_0}\eta(n_0) \qquad \text{for } n=n_0 \qquad (2.1.5.b)$$

where
$$\mathcal{F}_n=\frac{1}{1-}\cdot\frac{F_n}{1-}\cdot\frac{F_{n+2}}{1-}\cdots \qquad (2.1.6)$$

$$F_n=\lambda^+(n)\lambda^-(n+2)\eta(n)\eta(n+2) \qquad (2.1.7)$$

$$\eta(n)=[\lambda^+(n)+\lambda^-(n)+W_t(n)]^{-1}. \qquad (2.1.8)$$

(2.2) Exciton State Densities

The equidistant spacing model has been widely used in the exciton model, mainly because levels near the Fermi surface contribute most of the excited configuration at low excitation energy (E<30 MeV).

Several authors have given formula for the density of excited particle-hole states without incorporating the Pauli exclusion principle [9,10], or they have given approximations [11,12] based on statistical methods. The exact expression of exciton state density has been obtained by Zhang [13], which has the approximate formula

$$\omega(p,h,E)=\frac{g(gU)^{h'}(gU-A(p,h))^{p'-1}}{p!\,h!\,(p+h-1)!}. \qquad (2.2.1)$$

where
$$p'=\max(p,h) \text{ and } h'=\min(p,h). \qquad (2.2.2)$$

and g stands for the single particle level density, being approximately equal to $g=\frac{6}{\pi^2}a$, here a is the level density parameter.

In Eq.(2.2.1) U is the effective excitation energy which is given by the excitation energy subtracted by the pairing energy D [14] (to see Table 1), A(p,h) is the correction value from

Table 1 Pairing Energy Correction Values

For proton

Z	D	Z	D	Z	D	Z	D	Z	D	Z	D
12	2.46	13	2.09	14	1.62	15	1.62	16	1.83	17	1.73
18	1.35	19	1.54	20	1.20	21	1.06	22	1.36	23	1.43
24	1.17	25	1.24	26	1.20	27	1.28	28	1.28	29	1.35
30	1.36	31	1.19	32	1.14	33	1.12	34	1.58	35	1.17
36	1.18	37	1.22	38	0.97	39	0.92	40	0.62	41	0.68
42	0.64	43	0.72	44	0.75	45	0.71	46	0.87	47	0.88
48	0.89	49	0.79	50	0.89	51	0.78	52	0.69	53	0.61
54	0.72	55	0.77								

For neutron

N	D	N	D	N	D	N	D	N	D	N	D
12	2.67	13	1.80	14	1.67	15	1.86	16	2.04	17	1.64
18	1.44	19	1.54	20	1.30	21	1.27	22	1.29	23	1.41
24	1.50	25	1.50	26	1.43	27	1.88	28	1.47	29	1.57
30	1.46	31	0.93	32	0.72	33	1.12	34	1.29	35	0.94
36	1.24	37	1.25	38	1.14	39	1.32	40	1.15	41	1.24
42	1.43	43	1.09	44	1.20	45	1.04	46	0.70	47	0.85
48	0.76	49	0.92	50	0.99	51	1.10	52	0.92	53	0.73
54	0.70	55	0.87	56	0.61	57	0.69	58	0.55	59	0.40
60	0.73	61	0.58	62	0.86	63	1.13	64	0.84	65	0.79

Table 2. The ratios of the exact Pauli exclusion correction values and Kalbach's values

h\p	2	3	4	5	6	7
0	1.0	1.638	1.886	1.987	2.029	2.050
1	2.0	2.187	2.215	2.200	2.179	2.164
2	2.366	2.407	2.355	2.294	2.252	2.228
3		2.429	2.375	2.316	2.279	2.257
4			2.339	2.300	2.280	2.261
5				2.283	2.272	2.254
6					2.262	2.244
7						2.227

(continued)

h\p	8	9	10	11	12
0	2.062	2.070	2.075	2.077	2.078
1	2.155	2.148	2.140	2.133	2.126
2	2.211	2.194	2.178	2.166	2.156
3	2.235	2.212	2.194	2.181	2.170
4	2.236	2.213	2.199	2.188	2.176
5	2.230	2.212	2.202	2.190	2.174
6	2.223	2.211	2.201	2.186	2.168
7	2.213	2.206	2.196	2.179	2.167
8	2.206	2.200	2.189	2.174	2.167
9		2.194	2.182	2.171	2.166
10			2.172	2.165	2.163
11				2.163	2.160
12					2.155

$$A^k(p,h) = \tfrac{1}{4}p(p-1)+\tfrac{1}{4}h(h-1)$$

the Pauli exclusion principle being approximately equal to

$$A(p,h)=\frac{1}{2}p(p-1)+\frac{1}{2}h(h-1) \qquad (2.2.3)$$

The exact Pauli exclusion correction values are given in Ref. [13]. The ratios between the exact Pauli exclusion correction values and the Kalbach's values [12] are shown in Table 2. Summing over the exciton number (p=h), the exciton state densities should be normalized to the Fermi-gas formula for one -fermion gas. The normalized factor f(U) for the exciton state densities (2.2.1) is obtained numerically

$$f(U)=0.06*\pi^2/(aU)**0.125 \qquad (2.2.4)$$

in order to coincide with the following back-shifted Fermi gas formula [14]

$$\rho_{B-S}(E)=\sqrt{\frac{\pi}{3}}\ \frac{e^{2\sqrt{aU}}}{48a^{1/4}(U+t)^{5/4}}. \qquad (2.2.5)$$

$$\text{with } a=\frac{\pi^2}{6}g. \qquad (2.2.6)$$

Here the nuclear temperature t is given by

$$U=at^2-t. \qquad (2.2.7)$$

Thus, the renormalized exciton state densities have the following form

$$\omega^R(p,h,E)=f(U)*\omega(p,h,E). \qquad (2.2.8)$$

(2.3) J and π Dependent Exciton State Densities

As the assumption in the Weisskopf-Ewing model the spin distribution of levels in continuum is proportional to 2J+1, where J denotes the level spin [15]. For more realistic spin distribution as in Hauser-Feshbach theory the J-dependent factor is in the form

$$R(J)=\frac{2J+1}{\sqrt{2\pi}\,2\sigma^3}\exp(-(J+1/2)^2/2\sigma^2). \qquad (2.3.1)$$

For an equilibrium excited nuclear system, the spin cut-off parameter has an energy dependent form [16]

$$\sigma^2_{eq}(E)=0.146atA^{2/3}. \qquad (2.3.2)$$

In the spin-dependent exciton model, the expression of the spin cut-off parameter is exciton number dependent [17]

$$\sigma^2_{pre-eq}(n)=0.24nA^{2/3}. \qquad (2.3.3)$$

Here, we assume the maximum value being equal to the value for standard Hauser-Feshbach model, i.e., $\sigma^2_{eq}(E)$. Accordingly, we may use the minimum value within Eqs.(2.3.2) and (2.3.3) for $\sigma^2(n,E)$.

The value of $\sigma^2_{pre-eq}(n)$ is relatively small at low exciton states, this means that for precompound emission there is a limitation of angular momentum from spin cut-off in the emission state.

Thus, the J-π dependent exciton state densities are given by

$$\rho(p,h,I,\pi,E)=\tfrac{1}{2}R(I)\omega^{k}(p.h.E). \qquad (2.3.4)$$

where the parity factor is assumed to be a factor of 1/2 for continuum states.

(2.4) Internal Transition Rates

Since binary collisions occur in excited nuclear system as the description in exciton model, therefore only transitions with $\Delta n=0$ and $\Delta n=\pm 2$ are allowed. The internal transition rates with the Pauli exclusion principle are given by

$$\lambda^{+}(n)=\frac{2\pi}{\hbar}\langle M^2\rangle\, g\,\frac{(gu-A(p,h))^2}{(p+h-1)}, \qquad (2.4.1)$$

$$\lambda^{0}(n)=\frac{2\pi}{\hbar}\langle M^2\rangle\, g(gU-A(p,h))*(A(p,h)-2ph)/(p+h), \qquad (2.4.2)$$

$$\lambda^{-}(n)=\frac{2\pi}{\hbar}\langle M^2\rangle\, g(p+h-2)ph/2. \qquad (2.4.3)$$

The average squared matrix element $\langle M^2\rangle$ for residual interaction has been parameterized which is practically very successful [18].

$$\langle M^2\rangle=K/EA^3. \qquad (2.4.4)$$

where K is a constant as a parameter in exciton model.

(2.5) Equilibrium Exciton Number

The equilibrium exciton number $\bar{n}$ defined by $\lambda^{+}(\bar{n})=\lambda^{-}(\bar{n})$ is a physical quantity. The equilibrium distribution of the exciton occupation probability has a peak at $n=\bar{n}$. From Eqs.(2.4.1) and (2.4.3) one can get [13].

$$\bar{n}=\sqrt{1.4gU}. \qquad (2.5.1)$$

If the Williams value of A(p,h) were used instead, the equilibrium exciton number would be

$$\bar{n}=\sqrt{1.6gU}. \qquad (2.5.2)$$

Setting A(p,h)=0 to neglect the Pauli exclusion correction as in the Ericson formula, it yields

$$\bar{n}=\sqrt{2gU}. \qquad (2.5.3)$$

The comparison of Eq.(2.5.1) with Eqs.(2.5.2) and (2.5.3) indicates that the Pauli exclusion correction reduces the equilibrium exciton number. In our calculations Eq.(2.5.1) is adopted.

(2.6) Formation Factor of Composite Particle

The formation factor $F^{b}_{LM}(\varepsilon)$ for light composite particle b in compound nucleus has been proposed by Iwamoto and Harada [19, 20] and simplified by Zhang [21]. The model contains two new points. One is the calculation of the formation factor $F^{b}_{LM}(\varepsilon)$ which stands for the probability of composite particle b with outgoing energy ε composed by L particles above the Fermi surface and M particles below. The intrinsic wave function of the composite particle is taken by its ground state of an harmonic oscillator potential with the oscillator parameter $\hbar w$ which is determined by the experimental rms radius of the particle b (to see Table 3). The other new point is the inclusion of the pickup type contribution in the particle emission mechanism, in which some nucleons of the emitted composite particle come from levels below the Fermi surface.

In order to obtain the formation factor of composite particle with A_b nucleons, we need to calculate the integral

$$F^{b}_{LM}(\varepsilon)=\frac{1}{(2\pi\hbar)^{Ab-1}}\int_{P\ \text{fixed}}\prod_{i=1,\,[LM]}^{Ab-1} d\eta_i\, d\xi_i \qquad (2.6.1)$$

Table 3. Parameters of composite particles

cluster	r (fm)	hw (Mev)
d	1.96	8.1
t	1.7	14.4
^{3}He	1.88	11.7
Alpha	1.6	18.2

Here η_i and ξ_i are the relative momentum and the relative coordinate of the nucleons of the composite particle b. [LM] stands for the constraint condition as

$$|\vec{p}_i| > p_f \qquad \text{for } i=1,2,\ldots L,$$

$$|\vec{p}_i| < p_f \qquad \text{for } i=L+1,\ldots A_b. \qquad (2.6.2)$$

where $\vec{p}_i$ is the momentum of the i-th nucleon, p_f is the Fermi momentum.

From the energy conservation, the physical observable energy ε_b of the emitted composite particle b is related to other quantities by the relation

$$\varepsilon_b = \frac{P^2}{2mA_b} + \frac{3}{4}\hbar w_b(A_b-1) - A_b E_f + B_b. \qquad (2.6.3)$$

where E_f is the Fermi energy (E_f=33 MeV) and $P_f^2=2mE_f$,

B_b is the binding energy of particle b in the compound nucleus.

Two functions Q_1 and Q_2 are introduced as below

$$Q_1(x,D_b) = \frac{2}{3\pi}\left\{3\sin^{-1}(Y) - 8y*(1-y^2)^{5/2} + 2y(1-y^2)^{3/2} + 3y(1-y^2)^{1/2}\right\}$$

$$Q_2(x,D_b) = \frac{32\sqrt{mD_b}}{\pi P}\left[\frac{1}{5}\left(\frac{P^2}{4mD_b} - \frac{2E_f}{D_b}+1\right)(1-y^2)^{5/2} - \frac{1}{7}(1-y^2)^{7/2}\right] \qquad (2.6.4)$$

with the denoting

$$D_b = \frac{3}{2}\hbar w_b, \qquad (2.6.5.a)$$

and

$$y = x/\sqrt{mD_b}\ . \qquad (2.6.5.b)$$

The explicit expression of $F_{LM}(P)$ are given as below

(1) For deutron $(D_b=D_2)$

$$F_{20}(P)=\begin{cases}1 & 2(P_f+\sqrt{mD_2})<P\\ Q_1(\frac{1}{2}P-P_f)+Q_2(\frac{1}{2}P-P_f) & 2P_f<P\leqslant 2(P_f+\sqrt{mD_2})\\ Q_2(\sqrt{P_f^2-\frac{1}{4}P^2}) & 2\sqrt{P_f^2-mD_2}<P\leqslant 2P_f\\ 0 & P\leqslant 2\sqrt{P_f^2-mD_2}\end{cases}\qquad(2.6.6.a)$$

$$F_{11}(P)=\begin{cases}0 & 2(P_f+\sqrt{mD_2})<P\\ 1-Q_1(\frac{1}{2}P-P_f)-Q_2(\frac{1}{2}P-P_f) & 2P_f<P\leqslant 2(P_f+\sqrt{mD_2})\\ 1-2Q_2(\sqrt{P_f^2-\frac{1}{4}P^2})+Q_2(P_f-\frac{1}{2}P)-Q_1(P_f-\frac{1}{2}P) & 2\sqrt{P_f^2-mD_2}<P\leqslant 2P_f\\ 1+Q_2(P_f-\frac{1}{2}P)-Q_1(P_f-\frac{1}{2}P) & 2(P_f-\sqrt{mD_2})<P\leqslant 2\sqrt{P_f^2-mD_2}\\ 0 & P\leqslant 2(P_f-\sqrt{mD_2})\end{cases}\qquad(2.6.6.b)$$

$$F_{02}(P)=\begin{cases}0 & 2P_f<P\\ Q_1(P_f-\frac{1}{2}P)+Q_2(\sqrt{P_f^2-\frac{1}{4}P^2})-Q_2(P_f-\frac{1}{2}) & 2\sqrt{P_f^2-mD_2}<P\leqslant 2P\\ Q_1(P_f-\frac{1}{2}P)-Q_2(P_f-\frac{1}{2}P) & 2(P_f-mD_2)<P\leqslant 2\sqrt{P_f^2-mD_2}\\ 1 & P\leqslant 2(P_f-\sqrt{mD_2})\end{cases}\qquad(2.6.6.c)$$

(2) For triton or ^3He $(D_3=\frac{3}{2}\hbar w_t$ or $\frac{3}{2}\hbar w_{^3He})$

$$F_{30}(P)=A\left\{\int_0^a dP'B\int_{-1}^{1}d\cos\beta\, F_{20}(\tilde{P})+\int_a^b dP'B\int_{-1}^{c}d\cos\beta\, F_{20}(\tilde{P})\right\}\qquad(2.6.7.a)$$

$$F_{21}(P)=A\left\{\int_0^a dP'B\int_{-1}^{1}d\cos\beta\, F_{11}(\tilde{P})+\int_a^b dP'B\left[\int_{-1}^{c}d\cos\beta F_{11}(\tilde{P})+\int_c^1 d\cos\beta\, F_{20}(\tilde{P})\right]\right\}\qquad(2.6.7.b)$$

$$F_{12}(P)=A\left\{\int_0^a dP'B\int_{-1}^{1}d\cos\beta F_{02}(\tilde{P})+\int_a^b dP'B\left[\int_{-1}^{c}d\cos\beta F_{02}(\tilde{P})+\int_c^1 d\cos\beta F_{11}(\tilde{P})\right]\right\}\qquad(2.6.7.c)$$

$$F_{03}(P)=A\left\{\int_a^b dP'B\int_c^1 d\cos\beta F_{02}(\tilde{P})\right\}\qquad(2.6.7.d)$$

where

$$\tilde{P}=\left[\frac{4}{9}P^2+\frac{4}{3}Pp'\cos\beta+P'^2\right]^{1/2}$$

$$a=\frac{1}{3}P-P_f,$$

$$b=\sqrt{\frac{4}{3}mD_3},$$

$$c=\left(\frac{1}{9}P^2+p'^2-P_f^2\right)/\frac{2}{3}Pp'$$

and $$A=\frac{27}{4\pi(mD_3)^3} \qquad B=P'^2\left(\frac{4}{3}mD_3-P'^2\right)^{3/2}. \qquad (2.6.8)$$

β is the angle between P and p'.

(3) For α -particle ($D_b=D_4$)

$$F_{40}(P)=R\left\{\int_0^d dp'\,W\int_{-1}^{1}d\cos\beta\,F_{20}(p_+)F_{20}(p_-)\right\} \qquad (2.6.9.a)$$

$$F_{31}(P)=R\left\{\int_0^d dp'\,W\int_{-1}^{1}d\cos\beta\,(F_{20}(p_+)F_{11}(p_-)+F_{11}(p_+)F_{20}(p_-))\right\} \qquad (2.6.9.b)$$

$$F_{22}(P)=R\left\{\int_0^d dp'\,W\int_{-1}^{1}d\cos\beta\right.$$

$$\left.(F_{20}(p_+)F_{02}(p_-)+F_{11}(p_+)F_{11}(p_-)+F_{02}(p_+)F_{20}(p_-))\right\} \qquad (2.6.9.c)$$

$$F_{13}(P)=R\left\{\int_0^d dp'\,W\int_{-1}^{1}d\cos\beta\,(F_{11}(p_+)F_{02}(p_-)+F_{02}(p_+)F_{11}(p_-))\right\} \qquad (2.6.9.d)$$

$$F_{04}(P)=R\left\{\int_0^d dp'\,W\int_{-1}^{1}d\cos\beta\,F_{02}(p_+)F_{02}(p_-)\right\} \qquad (2.6.9.e)$$

where

$$p_+=\left(\frac{1}{4}P^2+p'^2+Pp'\cos\beta\right),$$

$$p_-=\left(\frac{1}{4}P^2+p'^2-Pp'\cos\beta\right),$$

$$R=\frac{2}{\pi(mD_4)^3},$$

$$W=p'^2(2mD_4-p'^2)^{3/2},$$

$$d=\sqrt{2mD_4}. \qquad (2.6.10)$$

The normalization condition is

$$\sum_{LM} F^{b}_{LM}(\varepsilon)=1 \qquad \text{with } L+M=A_b \qquad (2.6.11)$$

From study on the pickup type emissions, if the excitation energy is not so high ($E<30$ MeV), it turns out that the configurations of L=1,2 for light composite particles (like α ,d,t,He) always give the dominate contribution [19,20,21,22]. Therefore only F^{b}_{1M} and F^{b}_{2M} are included in the calculation.

(2.7) Q-Factor

The factor Q^{b}_{LM} (p,h) accounts for the memory by the system in the first stages of the reaction of the projectile type when emitting the particle b. The Q-factor is the exciton number dependent. The Q-factor was obtained by Kalbach [22] for the case in which all constructing nucleons of emitted composite particles are above the Fermi surface. It reads

$$Q^{b}(p,h)=\left(\frac{A}{Z}\right)^{Z_b}\left(\frac{A}{N}\right)^{N_b}\binom{A_b}{Z_b}^{-1}\binom{P}{A_b}^{-1}$$

$$\sum_{i=0}^{h}\left[\binom{h}{i}\left(\frac{Z}{4}\right)^{i}\left(\frac{N}{A}\right)^{h-i}\right]\binom{Z_a+i}{Z_b}\binom{P-Z_a-i}{N_b} \quad \text{for } n<\bar{n} \qquad (2.7.1)$$

where A,Z are the mass number and the proton number of the target nucleus, respectively. $A_b,Z_b,N_b(A_a,Z_a,N_a)$ are the nucleon, proton and neutron numbers of the ejectile (projectile).

At equilibrium, the correlation between projectile and ejectile should be vanished and the Q-factor becomes unity.

For pickup type composite particle emissions, the configurations [LM] become complex. With the same approach but for the configuration [LM] mentioned above, the combination factor Q has been obtained

$$Q^{b}_{LM}(p,h)=\left(\frac{A}{Z}\right)^{Z_b}\left(\frac{A}{N}\right)^{N_b}\binom{A_b}{Z_b}^{-1}\binom{P}{L}^{-1}\binom{A-h}{M}^{-1}$$

$$\sum_{i=0}^{h}\left[\binom{h}{i}\left(\frac{Z}{A}\right)^{i}\left(\frac{N}{A}\right)^{h-i}\right]\sum_{j}\binom{Z_a+i}{j}\binom{N_a+h-i}{L-j}\binom{Z-i}{Z_b-j}\binom{N-h+i}{N_b-L+j}$$

$$\text{for } n<\bar{n} \qquad (2.7.2)$$

When M=0 the Eq.(2.7.2) is reduced to the Kalbach formula (2.7.1). In the case of neutron projectile, $Z_a=0$, $N_a=1$, $A_a=1$, the Eq.(2.7.2) is simplified in the form

$$Q^b_{LM}(p,h)=\binom{A}{Z}^{Z_b}\binom{A}{N}^{N_b}\binom{A_b}{Z_b}^{-1}\binom{P}{L}^{-1}\binom{A-h}{M}^{-1}$$

$$\sum_{i=0}^{h}\left[\binom{h}{i}\left(\frac{Z}{A}\right)^{i}\left(\frac{N}{A}\right)^{h-i}\right]\sum_{j}\binom{i}{j}\binom{h+1-i}{L-j}\binom{Z-i}{Z_b-j}\binom{N-h+i}{N_b-L+j}$$

$$\text{for} \quad n<\bar{n}. \qquad (2.7.3)$$

For neutron and proton emissions, Eq.(2.7.3) has the property

$$\frac{N}{A}Q^n_{10}(p,h)+\frac{Z}{A}Q^p_{10}(p,h)=1. \qquad (2.7.4)$$

At equilibrium

$$Q^b_{LM}(p,h)=1 \qquad \text{for} \quad n\geqslant\bar{n} \qquad (2.7.5)$$

is set in the calculation. This is the asymptotical limit of Eq.(2.7.2) for high number of p and h. In particular, r-emission corresponds $Z_b=N_b=0$ and Eq.(2.7.3) yields $Q^r_{00}=1$ consistently.

(2.8) Discrete Level Excitation

An option has been introduced to account for discrete level excitation in the calculation. The discrete nuclear levels must be given as input by users up to an energy ED, which is the highest energy of discrete levels. For residual energies above $(U-B-ED)/(1+A_b/A)$ (B is the binding energy), the usual procedure for the continuum is followed. Based on the renormalized exciton state densities, the level density of residual nucleus now is rewritten into

$$\sum_n \rho(n,I,\pi,E)=\begin{cases}\rho_{B-S}(I,\pi,E) & \text{for } E>ED\\ \sum_k \delta_{I_k,I}\,\delta_{\pi_k,\pi}\,\delta(E-E_k) & \text{for } E\leqslant ED\end{cases} \qquad (2.8.1)$$

Here I_k, π_k and E_k are the spin, parity and energy of the k-th discrete level.

From Eq.(2.8.1) one can see that the parity factor 1/2 in Eq.(2.3.4) is not held yet, which is dependent on the structure

of discrete levels. If there are no knowledge on discrete level structure for some residual nuclei, ED=0 is set in the calculation.

Because the contribution of the state densities are mainly from n=3 state at very low excitation energy, we assume that discrete levels are only accounted in the exciton state n=3. With this assumption, the level density with $E \leqslant ED$ is expressed by

$$\rho(n,I,\pi,E)=\sum_k \delta_{I_k,I}\,\delta_{\pi_k\pi}\,\delta(E-E_k)\,\delta_{n,3} \qquad (2.8.2)$$

In the UNIFY code, this is adopted for the calculation of the effect from discrete levels.

(2.9) Emission Rates

All kinds of light particle emissions with $A \leqslant 4$ have been considered in the calculation.

The emission rates can be obtained by the method proposed by Kalbach-Cline [5,6,22] based on the detailed balance or microscopic reversibility.

(2.9.1) Emission Rates of r-ray

For exciton state $n \geqslant 3$, the two terms $\Delta n=0$ and $\Delta n=-2$ are included.

$$W_r(n,E,\varepsilon)=\frac{\varepsilon^2}{\pi^2\hbar^3c^2}\,\frac{1}{\omega^R(n,E)}\,\sigma_{abs}^{r}(\varepsilon)\,*$$

$$\frac{w^R(1,1,\varepsilon)\,w^R(p-1,h-1,E-\varepsilon)}{g(n-2)+w^R(1,1,\varepsilon)}\;\frac{gn\,w^R(p,h,E-\varepsilon)}{gn+w^R(1,1,\varepsilon)} \qquad (2.9.1)$$

while for the "direct" r-ray emission, the first term in Eq. (2.9.1) is vanished.

The r-ray absorbtion cross section takes the giant dipole resonance form

$$\sigma_{abs}^{r}(\varepsilon)=\sum_{i=1}^{2}\sigma_{0i}\,\frac{\Gamma_i^2\varepsilon^2}{(\varepsilon-E_i^2)^2+(\Gamma_i\varepsilon)^2} \qquad (2.9.2)$$

where the giant dipole resonance parameter Γ_i, E_i are nucleus dependent.

The integrated r-ray emission rate is

$$W_r(n,E)=\int_0^E d\varepsilon\, W_r(n,E,\varepsilon). \qquad (2.9.3)$$

(2.9.2) Emission Rates of Particles

(1) In the initial exciton state $n_o=1$

Since the "direct" r-ray emission is included in the unified model, the initial exciton state should start at $n_o=1$ ($p_o=1$, $h_o=0$). At this stage only r-ray emission is happend. The total emission rate should be

$$W_t(n_o)=W_r(n_o). \qquad (2.9.4)$$

(2) In the doorway state n=3

The discrete levels have been taken into account in the state n=3 as assumed in(2.1.2). The emission rate of particle b of the k-th level has the form

$$W_b^k(n=3,E)=\frac{(2S_b+1)\mu_b}{\pi^2\hbar^3}\varepsilon_b^k\,\sigma_a(\varepsilon_b^k)/w(n=3,E)$$

$$\sum_{L=1}^{2}F_{LM}^b(\varepsilon_b^k)Q_{LM}^b(n=3). \qquad (2.9.5)$$

where S_b is the spin of particle b, μ_b is the reduced mass, E_b^k is the k-th level energy of the residual nucleus, ε_b^k is the energy of emitted particle b.

$$\varepsilon_b^k=(E-B_b-E_b^k)/(1+A_b/A). \qquad (2.9.6)$$

For the continuum particle emission

$$W_b(n=3,E)=\frac{2S_b+1}{\pi^2\hbar^3}\frac{\mu_b}{w(n=3,E)}\int_0^{\varepsilon_m}d\varepsilon\,\varepsilon\,\sigma_a(\varepsilon)$$

$$\sum_{L=1}^{2}F_{LM}^b(\varepsilon)Q_{LM}^b(n=3)w^R(p-L,h,E-B_b-\varepsilon(1+A_b/A)) \qquad (2.9.7)$$

with $$\varepsilon_m=(E-B_b-ED)/(1+A_b/A) \qquad (2.9.8)$$

(3) In the exciton states $n\geq 5$

The emission rates from exciton state $n\geq 5$ of particle b has a similar form with Eq.(2.9.7), but only $n\geq 5$ instead. As mentioned above, the discrete levels are not taken into account for $n\geq 5$ states.

Thus, the sum over all kinds of reaction channels yields the total emission rate

$$W_t(n,E)=\sum_b W_b(n,E)+W_r(n,E) \qquad (2.9.9)$$

(3) Unified Model

Semi-phenomenological models for pre-equilibrium decay, notably the exciton and hybrid models, are globally successful in predicting emission cross section and spectra at bombarding energies above 10 MeV [1,23]. These models do not consider, however, the spin and parity conservation laws and disregard information concerning angular momentum altogether. There exist more basic quantum-statistical theories of precompound reaction [24,25,26,27], but those are hardly amenable for practical use. A unified pre-equilibrium and equilibrium reaction model has been proposed by SHI et al[28], which is an attempt to address the question of the introduction and assessment of angular-momentum effects in pre-equilibrium reaction models.

(3.1) Emission Rates

(3.1.1) Emission Rates of r-ray Emission

Analogous to the particle emission rates, the r-ray emission rates may be derived from the principle of detailed balance or microscopic reversibility [29,30,31].

$$W_\gamma(n,E,\varepsilon)=\frac{\varepsilon^2}{\pi^2\hbar^3c^2}\sigma_{\gamma,abs}(\varepsilon)\frac{\sum_k b(k\to n,\varepsilon)\,\omega(k,E')}{\omega(n,E)} \qquad (3.1.1)$$

The coefficients $b(k-n,\varepsilon)$ are the branching ratios. To obtain consistency with the Brink-Axil hypothesis as applied in current equilibrium statistical model, we must impose the condition

$$\sum_k b(k\to n,\varepsilon)=1 \qquad \text{for all allowed } k \quad (k=n, k=n-2). \qquad (3.1.2)$$

The phono-absorbtion cross section has the formula as same as Eq.(2.9.2). Recently, Oblozinsky [32] proposed the formulas for r-ray emission in which the angular momentum conservation is taken into account properly. The r-ray emission rate is written by the form

$$W_\gamma(p,h,E,J\xrightarrow{\lambda\varepsilon}U,S)=\frac{\varepsilon^2\sigma_{\gamma,abs}(\varepsilon)}{3\pi^2\hbar^3c^2}$$

$$\frac{b^{n\ J}_{n-2\ S}\,\rho(p-1,h-1,S,\pi,U)+b^{n\ J}_{n\ S}\,\rho(p,h,S,\pi,U)}{\rho(p,h,J,\pi,E)} \qquad (3.1.3)$$

where ε=E-U gives the r-ray energy. The branching ratios are given by

$$b^{n\ J}_{n-2\ S}=\frac{Y^n_{n-2}\,X^{n\ J}_{n-2\ S}}{Y^{n-2}_{n-2}\,X^{n-2\ J}_{n-2\ S}+Y^n_{n-2}\,X^{n\ J}_{n-2\ S}} \qquad (3.1.4)$$

and $$b_{n\,s}^{n\,J} = \frac{Y_n^n X_{n\,s}^{n\,J}}{Y_n^{n+2} X_{n\,s}^{n+2\,J} + Y_n^n X_{n\,s}^{n\,J}}.$$

J,π,E (S,π,U) are the spin, parity and the excitation energy of compound nucleus (residual necleus), respectively.

$$Y_n^n = ng \quad \text{and} \quad Y_n^{n+2} = g\varepsilon^2. \tag{3.1.5}$$

Only E1 $(\lambda=1)$ transition contributions are considered in the calculation. The angular momentum factor $X_{n\,S}^{n+2\,T}$ have been obtained.

$$X_{n\,s}^{n\,T} = \frac{2J+1}{R_n(S)} \sum_{j_1 j_2 j_3} (2j_1+1)R1(j_1)(2j_2+1)R1(j_2)R_{n-1}(j_3)$$

$$\left(C^{\lambda\;\;0}_{j2\,\frac{1}{2},\,j1\,-\frac{1}{2}}\right)^2 \left\{\begin{matrix} j_2 & j_3 & S \\ J & \lambda & j_1 \end{matrix}\right\}^2 . \tag{3.1.6.a}$$

$$X_{n\,s}^{n+2\,J} = \frac{2J+1}{(2S+1)(2\;\;+1)} \sum_{j_1 j_2} (2j_1+1)R1(j_1)(2j_2+1)R_1(j_2)$$

$$\left[C^{\lambda\;\;0}_{j2\frac{1}{2},\,j1\,-\frac{1}{2}}\right]^2 \Delta(S,\lambda,J) \tag{3.1.6.b}$$

where

$$\Delta(S,\lambda,J) = \begin{cases} 1 & \text{for} \quad |S-\lambda| < J < S+\lambda \\ 0 & \text{for} \quad \text{otherwise.} \end{cases} \tag{3.1.6.c}$$

For "direct" r-ray emission only the $\Delta n=0$ exists and $n_0=1$ is the initial exciton number. Eq.(3.1.6.a) is substantially simplified since the core spin j_3 is now fixed. Assuming $j_3=0$ one gets $j_2=S$, $j_1=J$. Therefore

$$X_{1\;\;S}^{1\;\;J} = (2\lambda+1)(2J+1)R1(J)\begin{pmatrix} S & \lambda & J \\ 1/2 & 0 & 1/2 \end{pmatrix}^2 \tag{3.1.7}$$

The "semi-direct" r-ray emission (n=3) and the pre-equilibrium r-ray emission consist of two terms ($\Delta n=0$ and $\Delta n=-2$).

Thus the r-ray emission rate for E1 decay is expressed by

$$W_\gamma^{J\pi}(p,h,E,\varepsilon) = \sum_{s=|J-1|}^{J+1} W_\gamma(p,h,E,J \xrightarrow{\lambda=1,\,\varepsilon} U,S) \tag{3.1.8}$$

and

$$W_\gamma^{J\pi}(p,h,E) = \int d\varepsilon\, W_\gamma^{J\pi}(p,h,E,\varepsilon). \tag{3.1.9}$$

(3.1.2) Emission rates of particles

The J-π-dependent emission rates of particles in the unified model can be extended to

$$W_b^{J\pi}(n,\varepsilon)=\frac{1}{2\pi\hbar}\sum_{l'j'}\sum_{I'\pi'} T^b_{l'j'}(\varepsilon)/\rho_c(p,h,I,\pi,E)$$

$$\sum_{L=1}^{2}\rho_b(p-L,hI',\pi',E')F^b_{LM}(\varepsilon)Q^b_{LM}(p,h). \quad (3.1.10)$$

where $T^b_{l'j'}(\varepsilon)$ is the transmission coefficient of particle b in l'J' channel, I',π',E' are the spin, parity, excitation energy of residual nucleus, ρ_b and ρ_c are the J-π dependent state densities of residual and compound nuclei, respectively.

$$E'=E-B_b-\varepsilon(1+A_b/A). \quad (3.1.11)$$

(1) For $n_o=1$

only (n,r) channels open

$$W_t^{J\pi}(n_o)=W_r^{J\pi}(n_o). \quad (3.1.12)$$

(2) For n=3

The emission rate to k-th level of residual nucleus is

$$W_b^{J\pi,K}(n=3,E)=\frac{1}{2\pi\hbar}\sum_{lj} T^b_{lj}(\varepsilon^k_b)\sum_{L=1}^{2}F^b_{LM}(\varepsilon^k_b)Q^b_{LM}(n=3)/\rho_c(n=3,J,\pi,E).$$

(3.1.13)

and for the continuum region

$$W_b^{J\pi}(n=3,E)=\frac{1}{2\pi\hbar}\int_0^{\varepsilon_m} d\varepsilon\, W_b^{J\pi}(n=3,E,\varepsilon)$$

with $\varepsilon_m=(E-B_b-ED)/(1+A_b/A)$. (3.1.14)

here

$$W_b^{J\pi}(n=3,E)=\frac{1}{2\pi\hbar}\sum_{lj}\sum_{I'\pi'} T^b_{lj}(\varepsilon_b)/\rho_c(n=3,I,\pi,E)*$$

$$\sum_{L=1}^{2}F^b_{LM}(\varepsilon_b)Q^b_{LM}(n=3)\rho_b(p-L,h,I',\pi',E'). \quad (3.1.15)$$

The relations

$$\vec{j}+\vec{I}=\vec{J}, \qquad \vec{j}=\vec{S}_b+\vec{l} \quad (3.1.16)$$

and

$$(-1)^{\ell}\pi'=\pi \qquad (3.1.17)$$

must be held

(3) For $n>3$

There is no discrete levels as the assumption in (2.8), The expression of emission rates are as same as Eq.(3.1.15), except for $n>3$ instead of $n=3$.

(3.2) Ansatz on Mean Lifetime

In the unified model, the average energy spectra should be written in $J-\pi$ dependent form

$$\frac{d\sigma}{d\varepsilon}(a,b)=\sigma_a\sum_{J\pi}\sum_{n}W_b^{J\pi}(n,E,\varepsilon)\tau^{J\pi}(n,E). \qquad (3.2.1)$$

where σ_a stands for absorption cross section with $\sigma_a=\sum_{J\pi}\sigma_a^{J\pi}$
In order to solve the equation of mean lifetime $\tau^{J\pi}(n,E)$, the expression for the initial condition is evidently given by [28]

$$q^{J\pi}(n,t=0)=\frac{\sigma_a^{J\pi}}{\sigma_a}q(n,t=0). \qquad (3.2.2)$$

where $q(n,t=0)$ is identical to the initial condition for the standard master equation, being equal to δ_{n,n_0} . Summing over all exciton numbers and inserting Eq.(3.2.2), it follows that

$$\sum_{n}W_t^{J\pi}(n,E)\tau^{J\pi}(n,E)=\frac{\sigma_a^{J\pi}}{\sigma_a}. \qquad (3.2.3)$$

Assuming that the transition rates and emission rates do not depend strongly on J, one may look for approximation expression for mean lifetime $\tau^{J\pi}(n)$. As a physically plausible and numerically convenient approximation a mean lifetime ansatz has been suggested [28].

$$\tau^{J\pi}(n)=\frac{\sigma_a^{J\pi}}{\sigma_a}\frac{W_t(n)}{W_t^{J\pi}(n)}\tau(n). \qquad (3.2.4)$$

When the quantities $\sigma_a^{J\pi}$, σ_a, $W_t^{J\pi}(n)$, $W_t(n)$ are known, we can solve the $\tau(n)$ of standard exciton master equation to get $\tau^{J\pi}(n)$ with the ansatz (3.2.4)

(3.3). Energy Spectra

Combining Eqs.(3.2.1) and (3.2.2), one gets

$$\frac{d\sigma}{d\varepsilon}(a,b)=\sum_{J\pi}\sigma_a^{J\pi}\frac{\sum_n W_b^{J\pi}(n,E,\varepsilon)\tau^{J\pi}(n)}{\sum_{n'} W_t^{J\pi}(n',E)\tau^{J\pi}(n')}. \quad (3.3.1)$$

Under the ansatz (3.2.4), Eq.(3.3.1) becomes

$$\frac{d\sigma}{d\varepsilon}(a,b)=\sum_{J\pi}\sigma_a^{J\pi}\sum_n\frac{W_b^{J\pi}(n,\varepsilon)}{W_t^{J\pi}(n)}W_t(n)\tau(n) \quad (3.3.2)$$

with
$$\sigma_a^{J\pi}=\pi\lambda_a^2\frac{(2J+1)}{(2S_a+1)(2I+1)}\sum_{lj}T_{lj}^a(\varepsilon_a) \quad (3.3.3)$$

and
$$\vec{j}=\vec{l}+\vec{S}_a. \quad (3.3.4)$$

The total emission rate $W_t^{J\pi}(n)$ in Eq.(3.3.2) is given by

$$W_t^{J\pi}(n)=\sum_b\int d\varepsilon W_b^{J\pi}(n,\varepsilon). \quad (3.3.5)$$

The expression of $W_b^{J\pi}(n,\varepsilon)$ can be found in Eq.(3.1.10).

(4) Simplification Approaches

(4.1) Hauser-Feshbach Approximation

In principle the exciton number n which appears in the summation of Eq.(3.3.2) would be large enough to account the contributions from each exciton stage. Such that the calculation would become very time consuming. As the matter of fact, when exciton number becomes large, the behaviour of the emission processes become similar to that from equilibrium stage. We know the probability conservation condition as follows

$$\sum_n W_t(n)\tau(n)=1. \quad (4.1.1)$$

The spin cut-off factor is exciton number dependent (to see 2.3.3). With n increasing the value of σ^2 increases. When

$$\sigma^2_{pre-eq}(n)=\sigma^2_{eq}(E),$$

the critical exciton number n_c is obtained by the formula

$$n_c=[0.78\sqrt{gU}]_{odd} \quad (4.1.2)$$

where $[\quad]_{odd}$ means taking the odd integer number nearest the value inside branket.

The Hauser-Feshbach approximation for $n > n_c$ is used. Eq. (3.3.2) becomes

$$\frac{d\sigma}{d\varepsilon}(a,b)=\sum_{J\pi}\sigma_a^{J\pi}\left\{\sum_{n=1}^{n_c} W_t(n)\tau(n)\frac{W_b^{J\pi}(n,\varepsilon)}{W_t^{J\pi}(n)}\right.$$

$$\left.\left(1-\sum_{n=1}^{n_c} W_t(n)\tau(n)\right)\frac{W_b^{J\pi}(\varepsilon)}{W_t^{J\pi}}\right\}. \qquad (4.1.3)$$

where $W_b^{J\pi}(\varepsilon)$ and $W_t^{J\pi}$ in the second term are exciton number independent and calculated by the Hauser-Feshbach model.

(4.2) An Economizing Method for Calculation of Particle Emission Rates

To provide particle transmission coefficients, external optical model routines or code must be used. UNIFY code accepts transmission coefficients in the form as a function of total and orbital angular momenta j,l and converts them to T_ℓ using the following expression

$$T_\ell(\varepsilon)=\frac{1}{2\ell+1}\left[(\ell+1)T_{\ell,\ell+\frac{1}{2}}+\ell T_{\ell,\ell-\frac{1}{2}}\right],$$

for s=1/2. (4.2.1)

$$T_\ell(\varepsilon)=\frac{1}{6\ell+3}\left[(2\ell+3)T_{\ell,\ell+1}+(2\ell+1)T_{\ell,\ell}+(2\ell-1)T_{\ell,\ell-1}\right],$$

for s=1 (4.2.2)

and $T_\ell(\varepsilon)=T_{\ell,\ell}(\varepsilon)$ for s=0. (4.2.3)

In the formula of particle emmision rates $W_b^{J\pi}(n,\varepsilon)$ (in the unified model) or $W_b^{J\pi}(\varepsilon)$ (in the Hauser-Feshbach theory), the following factor has to be computed

$$\left[\sum_{l'j'} T^b_{l'j'}(\varepsilon)\sum_{I'\pi'}\rho(I',\pi',E')\right]^{J\pi} \qquad (4.2.4)$$

When the transmission coefficiets $T_{\ell',j'}$ are turned into j'-dependent form as described in Eqs.(4.2.1-4.2.3), the calculation of factor (4.2.4) can be properly simplified to speed up computations [33].

The expression for the level density $\rho(I',\pi',E')$ factorized into a spin-and parity-dependent part and a part which solely depends on the energy

$$\rho(I',\pi',E')=f(I',E')P(\pi')\rho_0(E'), \qquad (4.2.5)$$

where $\rho_0(E')$ is the nuclear state density and $P(\pi')$ is the parity factor (mostly assumed to be 1/2), while the spin distribution factor $f(I',E')$ has a more realistic assumption

$$f(I',E')=\frac{2I'+1}{\sqrt{2\pi}\,2\sigma^3}\exp(-(I'+1/2)^2/2\sigma^2). \qquad (4.2.6)$$

If the transmission coefficients $T^a_{\ell'j'}$ are replaced by $T^a_{j'}$ like in Eqs.(4.2.1-3), the remaining summation over j' in Eq.(4.2.4) can be treated through an appropriate transformation from summation to integration [33]. Let

$$S(J,\ell',s',E')=\sum_{J'I'} f(I',E)=\sum_{j'=|J-l'|}^{J+l'}\ \sum_{I'=|j'-s'|}^{j'+s'} f(I',E') \qquad (4.2.7)$$

For the case of s'=0 or s'=1/2

$$S(J,l',s',E')=\int_{|J-l'|-1/2}^{J+l'+1/2} dj' \sum_{I'=|j'-s'|}^{j'+s'} f(I',E')$$

$$=\frac{1}{\sqrt{2\pi}\,\sigma}\Big\{\exp[-(|J-l'|-s')^2/2\sigma^2]-\exp[-(J+I'-s'+1)^2/2\sigma^2]$$

$$+\delta_{s',\frac{1}{2}}\exp[-(|J-l'|+s')^2/2\sigma^2-\delta_{s',\frac{1}{2}}\exp[-(J+I'+s'+1)^2/2\sigma^2]\Big\}. \qquad (4.2.8)$$

In the case of arbitrary values of the ejectile spin s' (e.g for deutron emission), both summations in Eq.(4.2.7) are obtained through a change to integrals

$$S(j,l',s',E') = \int_{|J-l'|-1/2}^{J+l'+1/2} dj' \int_{|j'-s'|-1/2}^{j'+s'+1/2} dI' \; f(I',E')$$

$$= 1/2\left\{ \mathrm{erf}\left[\frac{J+l'-s'+1/2}{\sqrt{2}\sigma}\right] - \mathrm{erf}\left[\frac{|J-l'|-s'-1/2}{\sqrt{2}\sigma}\right] \right.$$

$$\left. + \mathrm{erf}\left[\frac{|J-l'|-s'+1/2}{\sqrt{2}\sigma}\right] - \mathrm{erf}\left[\frac{J+l'+s'+3/2}{\sqrt{2}\sigma}\right] \right\} \qquad (4.2.9)$$

where erf denotes the error function.

(5) Angular Distribution

(5.1) Generilized Master Equation

In our code only the angular distribution of multi-neutron emission is included based on the generilized master equation proposed by Mantzouranis et. al [34,35]. The generilized master equation of the exciton model yields the double-differential cross section as

$$\frac{d^2\sigma(a,b)}{d\varepsilon\, d\Omega} = \sigma_a \sum_n W_b(n,\varepsilon)\tau(n,\Omega). \qquad (5.1.1)$$

where $\tau(n,\Omega)$ is the mean lifetime of state n at emission angle Ω. It is possible to transform it to a Legendre polynomial representation [36-45].

$$\tau(n,\Omega) = \int_0^\infty q(n,\Omega,t)dt = \sum_\ell \zeta_\ell(n) P_\ell(\cos\theta), \qquad (5.1.2)$$

$$q(n,\Omega,t) = \sum_\ell \eta_\ell(n,t) P_\ell(\cos\theta), \qquad (5.1.3)$$

$$\int d\Omega' G(\varepsilon\Omega, \varepsilon'\Omega') P_\ell(\cos\theta') = \mu_\ell(\varepsilon,\varepsilon') P_\ell(\cos\theta) \qquad (5.1.4)$$

with $\theta = \Omega - \Omega'$,

and

$$\mu_\ell(\varepsilon) = \int \mu_\ell(\varepsilon,\varepsilon')d\varepsilon'. \qquad (5.1.5)$$

where $G(\varepsilon\Omega, \varepsilon'\Omega')$ is the intra-nuclear scattering kernel. The Legendre coefficients $\zeta_\ell(n)$ of the mean lifetime satisfy a set of time-integrated master equations for each ℓ

$$-\eta_\ell(n,t=0)=\mu_\ell(\varepsilon)\lambda^+(n-2)\xi_\ell(n-2)+\mu_\ell(\varepsilon)\lambda^-(n+2)\xi_\ell(n+2)$$
$$-[\lambda^+(n)+\lambda^-(n)+(1-\mu_\ell(\varepsilon))\lambda^0(n)+W_t(n)]\xi_\ell(n). \qquad (5.1.6)$$

The closed solution of Eq.(5.1.6) can be got by the following formula

$$\xi(n\geq 3)=\mathcal{F}_{n_0}\xi_\ell(n)\frac{2l+1}{4\pi}\mu_\ell(\varepsilon)\prod_{\substack{k=n_0\\ \Delta k=2}}^{n-2}\mu_\ell(\varepsilon)\lambda^+(k)\xi_\ell(k)\mathcal{F}_{k+2} \qquad (5.1.7.a)$$

$$\xi_\ell(no)=\xi_\ell(no)\frac{2l+1}{4\pi}\mu_\ell(\varepsilon)\mathcal{F}_{n_0}, \qquad (5.1.7.b)$$

where
$$\mathcal{F}_n=\frac{1}{1-}\,\frac{F_n}{1-}\,\frac{F_{n+2}}{1-}\cdots \qquad (5.1.7.c)$$

with
$$F_n=\mu_\ell^2(\varepsilon)\lambda^+(n)\lambda^-(n+2)\xi_\ell(n)\xi_\ell(n+2), \qquad (5.1.7.d)$$

and
$$\xi_\ell=[\lambda^+(n)+\lambda^-(n)+(1-\mu_\ell(\varepsilon))\lambda^0(n)+W_t(n)]^{-1}. \qquad (5.1.7.e)$$

(5.2) Intra-Nuclear Scattering Kernel $G(\varepsilon'\Omega'\rightarrow\varepsilon\Omega)$

The important quantity in the double differential cross section is the scattering kernel $G(\varepsilon'\Omega'\rightarrow\varepsilon\Omega)$. At the beginning, the free nucleon-nucleon scattering which is assumed to be isotropic in the c.m system was used [36,45].

$$G^{free}(\varepsilon'\Omega'\rightarrow\varepsilon\Omega)=\frac{1}{\pi}\cos(\alpha)\Theta(\frac{\pi}{2}-\alpha). \qquad (5.2.1)$$

Based on the Fermi gas model, the influence of the Fermi motion and the Pauli exclusion principle has been taken into account. The Kikuchi-Kawai energy-angle correlation kernel provided the start point to set up the formulas of μ_ℓ. The most singnificant improvement of this approach is the rise of backward direction of the double differential cross section for the higher energy neutron [47]. The expression for $\mu_\ell(\varepsilon,\varepsilon')$ is given by

$$\mu_\ell(\varepsilon,\varepsilon')=\frac{1}{\sigma}\int\frac{d^2\sigma}{d\varepsilon' d\Omega'}P(\cos\alpha')d\Omega' \qquad (5.2.2)$$

$$\frac{d^2\sigma^2}{d\varepsilon'\, d\Omega'} = \begin{cases} A = \dfrac{3\bar{\sigma}}{8\pi E_f}\sqrt{\dfrac{EL'}{E_f}}\;\dfrac{EL-EL'}{Q*EL} & \text{(A-area)} \\ B = \dfrac{3\bar{\sigma}}{8\pi E}\sqrt{\dfrac{EL'}{E_f}}\;\dfrac{EL*EL'\sin^2\theta-(EL'-E_f)Q}{Q\sqrt{Q*EL}} & \text{(B-area)} \end{cases} \qquad (5.2.3)$$

$$\bar{\sigma} = \int d\varepsilon' \int d\Omega' \frac{d^2\sigma}{d\varepsilon' d\Omega'} = \sigma\left[1-\frac{7}{5}\frac{E_f}{EL}+\frac{2}{5}\frac{E_f}{EL}\left(2-\frac{EL}{E_f}\right)\Theta(2E_f-EL)\right] \qquad (5.2.4)$$

with $$Q=EL+EL'-2\sqrt{EL*EL'}\cos\theta \qquad (5.2.5)$$

and
$$\left.\begin{matrix}\alpha_1\\ \beta_1\end{matrix}\right\} = \frac{1}{\sqrt{EL*EL'}}\left[EL-E_f\mp\sqrt{E_f(E_f-EL+EL')}\right]$$
$$\left.\begin{matrix}\alpha_2\\ \beta_2\end{matrix}\right\} = \frac{1}{\sqrt{EL*EL'}}\left[EL'-E_f\mp\sqrt{E_f(E_f+EL-EL')}\right] \qquad (5.2.6)$$

The relations of EL and EL' with the observable energies are

$$EL=\varepsilon+E_f+B,$$
$$EL'=\varepsilon'+E_f+B. \qquad (5.2.7)$$

where E_f is Fermi energy and B is the binding energy of neutron.

(5.3) Legendre Coefficients of Double Differential Cross Section

Based on Eq.(4.1.3) the double differential cross section of neutron emission in the first stage has the explict expression

$$\frac{d\bar{\sigma}(a,b)}{d\varepsilon\, d\Omega} = \sum_{J\pi}\bar{\sigma}^{J\pi}\left\{\sum_{n=3}^{nc} W_t(n)\tau(n,\Omega)\frac{W_b^{J\pi}(n,\varepsilon)}{W_t^{J\pi}(n)} + \frac{1}{4\pi}\left(1-\sum_{n=3}^{nc} W_t(n)4\pi\zeta_{l=0}(n)\right)\frac{W_b^{J\pi}(\varepsilon)}{W_t^{J\pi}}\right\} \qquad (5.3.1)$$

with $$\tau(n,\Omega)=\sum_l \zeta_l(n)P_l(\cos\theta). \qquad (5.3.2)$$

If the double differential cross section is expanded in the Legendre polynomial

$$\sigma(\varepsilon,\Omega)=\sum_{l}\frac{2l+1}{4\pi}\, f_{l}^{cm}(\varepsilon)P_{l}(\cos\Omega). \qquad (5.3.3)$$

Then we have

$$f_{l}^{cm}(\varepsilon)=\sum_{J\pi}\sigma_{a}^{J\pi}\frac{4\pi}{2l+1}\left\{\sum_{n=3}^{nc} W_t(n)\frac{W_b^{J\pi}(n,\varepsilon)}{W_t^{J\pi}(n)}\zeta_{l}(n)\right.$$

$$\left.+\frac{1}{4\pi}\left[1-\sum_{n=3}^{nc} W_t(n)4\pi\zeta_{l=0}(n)\right]\frac{W_b^{J\pi}(\varepsilon)}{W_t^{J\pi}}\delta_{l0}\right\}. \qquad (5.3.4)$$

In particular the partial wave of l=0 gives the energy spectrum.

If the energy-angle correlation is considered in the first step for n=3, one gets

$$\zeta_{l}(n=3)=\frac{\tau(n=3)\mu_{l}(E,\varepsilon)}{\int d\Omega\,\frac{d^2\sigma}{d\varepsilon\, d\Omega}}=\frac{\tau(n=3)\mu_{l}(E,\varepsilon)}{R(E,\varepsilon)}. \qquad (5.3.5)$$

where

$$R(E,\varepsilon)=\begin{cases}1/E & \text{for } EL < E-E_f\\ 1/E\left\{1-\left[(EL+E_f-E)/E_f\right]\right\} & \text{for } EL \geq E-E_f\end{cases} \qquad (5.3.6)$$

(5.4) Transformation Formulas of Legendre Coefficients

In Ref. [48] it is indicated that energy spectra in two system are very close but the angular distributions are different, especially for the low outgoing energy region and not so heavy targets.

The direct numerical transformation method [48,49] is the formula

$$F_{l}(\varepsilon_L)=2\pi\int\frac{d^2\sigma}{d\varepsilon\, d\Omega}(\varepsilon_c,\Omega_c)P_{l}(\cos\Theta_c)\,\|J\|\, d\cos\Theta_L\,. \qquad (5.4.1)$$

where $\|J\|$ is the Jucoby determinant of the transformation of two coordinate system

$$\|J\|=(1+\beta^2-2\beta\mu_L)^{-1/2}. \qquad (5.4.2)$$

with $$\beta=\frac{\sqrt{m\,m'}}{M+m}\sqrt{\frac{E_L}{\varepsilon_L}}\,. \qquad (5.4.3)$$

m,m' and M are the mass of projectile, ejectile and target nucleus, respectively.

$\mathcal{E}_c$, $\mathcal{E}_L$ and E_L are the outgoing energies in the center of mass system (c.m), the loboratory system (l.s) and the incoming energy in (l.s). μ_L and μ_c are the cosine of outgoing angles θ_L in (l.s) and θ_c in (c.m), respectively.

The relations between energies and angles in the two systems are

$$\mathcal{E}_c = \mathcal{E}_L(1+\beta^2-2\beta\mu_L), \tag{5.4.4}$$

and

$$\mu_c = (\mu_L-\beta)(1+\beta^2-2\beta\mu_L)^{-\frac{1}{2}}. \tag{5.4.5}$$

The definitions of $F_\ell(\mathcal{E}_L)$ and $f_\ell(\mathcal{E}_c)$ are given by

$$\frac{d^2\sigma}{d\mathcal{E}\,d\Omega}(\mathcal{E}_L,\Omega_L)=\sum_\ell \frac{2\ell+1}{4\pi}F_\ell(\mathcal{E}_L)P_\ell(\mu_L)$$

$$=\sum_\ell \frac{2\ell+1}{4\pi}f_\ell(\mathcal{E}_c)P_\ell(\mu_c). \tag{5.4.6}$$

An analytical transformation formulas have been developed by SHI, et al [48] . Introducing the transformation matrices $T^{(n)}$ by

$$(2l'+1)\,\|J\|\,\frac{(\mathcal{E}_c-\mathcal{E}_L)^2}{n!}p_{l'}(\cos\theta_c)=\sum_l(2l+1)T^{(n)}_{ll'}(\mathcal{E}_L)p_l(\mu_L).$$

$$n=0,1,\cdots \tag{5.4.7}$$

The recursive relation of $T^{(n)}_{ll'}$ reads

$$T^{(n)}_{l\,l'}(\mathcal{E}_L)=\frac{\beta\mathcal{E}_L}{n}\Big\{\beta T^{(n-1)}_{ll'}(\mathcal{E}_L)-\frac{2(l+1)}{2l+1}T^{(n-1)}_{ll'}(\mathcal{E}_L)$$

$$-\frac{2l}{2l+1}T^{(n-1)}_{l\,l'}(\mathcal{E}_L)\Big\},$$

$$n=1,2\cdots \qquad l,l'=0,1,2,\cdots \tag{5.4.8}$$

with the initial condition

$$T^{(0)}_{l\,l'}(\mathcal{E}_L)=\beta^m S(l,l')\left[1-\beta^2\frac{(l-m)(l+m+1)}{2(m+1)}*\frac{2L^2-2(m-1)L-3m-1}{(2L+3)(2L-2m-1)}\right].$$

$$(5.4.9)$$

with $L=\max\{\ell,\ell'\}$, $m=|l-l'|$ and

$$S(\ell,\ell')=1 \qquad \text{for } \ell=\ell' \qquad (5.4.10.a)$$

$$S(\ell,\ell')=\binom{L}{m}\prod_{i=0}^{m-1}\frac{\ell+m-2i-1}{2L-2i+1} \qquad \text{for } \ell>\ell' \qquad (5.4.10.b)$$

$$S(\ell,\ell')=(-1)^m\binom{L}{m}\prod_{i=0}^{m-1}\frac{\ell+m-2i}{2L-2i-1} \qquad \text{for } \ell<\ell' \qquad (5.4.10.c)$$

Thus the Legendre coefficients in (1.s) can be obtained by the analytical transformation formula

$$F_\ell(\varepsilon_L)=\sum_{n=0}^{N}\sum_{\ell'} T_{\ell\ell'}^{(n)}(\varepsilon_L)f_{\ell'}^{(n)}(\varepsilon_L). \qquad (5.4.11)$$

where $f_{\ell'}^{(n)}(\varepsilon_L)$ stands for the n-th order derivative at $\varepsilon_c=\varepsilon_L$.

(6) Coupling to Hauser-Feshbach Code

(6.1) Energy Bound of H.F and Unified Model

The code to calculate fast neutron data for structural materials is divided into two parts. When the incident neutron energies are lower than ED

$$E_n^{cm} \leq ED \qquad (6.1.1)$$

which implies that all of neutron emission channels are corresponding to the discrete level region of residual nuclei, the Hauser-Feshbach model is employed, while the continuum channels are opened the unified model is used alternatively.

In general the highest energy value of discrete levels ED is smaller than the neutron binding energy $B_n(A)$ of target nucleus. As the bound defined above, (n,2n) reaction channel is not open in H.F model. In case that the inequility $B_n(A)<ED$ is happened for same nuclei, the upper bound of the H.F model becomes to be

$$E_n^{cm} \leq B(A) \qquad (6.1.2)$$

which means that the discrete levels, the energies of which are larger than $B_n(A)$, **have to be cut and treated as continuum.**

(6.2) Mnlti-Particle Emissions

For simplication of the code, the unified model incorporate the multi-particle emissions in a following approach. The pre-equilibrium emissions are taken into account only in the first stage of the neutron induced reaction. Afterwards in the second and the third stages, the H.F model is employed to calculate cross sections and neutron spectra. In other words, if incident energy of neutron is limited below 20 MeV, the equilibration is established after the first particle emission. With this approximation, energy spectra of outgoing particle are calculated by

$$S_{b'}(\varepsilon') = \frac{\sum_{\ell''j''} T^{b\,J''\pi''}_{\ell''j''}(\varepsilon')\,(I'',\pi'',E'')}{T_t^{I'\pi'}}. \qquad (6.2.1)$$

where $\rho(I'',\pi'',E'')$ is the level density instead of the state density. The Fermi-gas formulas [14,49] are used for the level density but the discrete levels must be taken into account.

The angular distributions of the multi-neutron emission in the second and the third stages are always assumed to be isotropic in the code.

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