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# MEND—A Code for Calculating Nuclear Data of Medium-heavy Nuclei below 250 MeV*

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**Abstract**: Based on the spherical optical model, pre-equilibrium statistical theory, and Hauser-Feshbach theory, etc., the code MEND (Medium Energy Nuclear Data) is written for calculating the complete set of nuclear data of medium-heavy nuclei in medium-low energy region (≤250 MeV). For the reactions induced by neutron and proton below 250 MeV, the total cross sections, reaction cross sections, elastic scattering differential cross sections, double differential cross sections and energy spectra, etc. calculated by the code MEND, generally agree with those corresponding experimental data. MEND is a foundational program for nuclear reaction in medium-low energy region and is wildely used for nuclear data calculation and establishing ENDF/B6 format files of medium-low energy region in China.

**Key words**: MEND program; nuclear reaction; nuclear data; calculation

**CLC number**: O571.42$^+$1; O571.42$^+$2 **Document code**: A

## 1 Introduction

The code MEND (Medium Energy Nuclear Data)[1−2] is developed from our former code CCRMN[3−4], and it can calculate the complete set of nuclear data of medium-heavy nuclei in medium-low energy region, namely, the incident particles energy is bellow 250 MeV. The MEND considers six kinds of light particles as the incident and emission particles, and these particles are: n, p, α, d, t and $^3$He. There are eighteen emission processes included in MEND. With input parameters, MEND can calculate the total cross section, elastic scattering cross section and its angular distribution, reaction cross section, radiative capture cross section, inclusive cross sections and their energy spectra, etc..

Actually, compared with the code MEND, several programs TALYS[5], GNASH[6], ALICE/ASH[7], etc., which are written by foreign experts, have the similar calculation functions. All these programs have basically the same theoretical frame and similar functions, but there are also some differences among them. Since the improved Iwamoto-Harada pick-up reaction mechanism[8] has been included in the exciton model for the light composite particle emissions, the code MEND can provide better description of the shapes and magnitude of the energy spectra and the double differential cross section of emitting d, t, $^3$He and α than TALYS, GNASH, and ALICE/ASH.

Up to now, the program MEND has been used by some users in China to calculate the complete set of nuclear data below 200 MeV for many target nuclei with neutron and proton as projectile, good results and ENDF/B6 format library are obtained for the project ADS (Accelerator Driven

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sub-critical System).

This paper is arranged as follows. In section 2, we introduce the functions and structure of MEND briefly; the theoretical frames of MEND are listed in section 3; in Section 4, the calculation methods are given; Section 5 is the input and output files, and Section 6 is some calculation results. The calculation formula and corresponding parameters of optical model and cascade nucleon emission etc. are listed in appendix.

## 2 Functions and Structures

The calculation and output quantities are as following: total cross section; elastic scattering cross section and its angular distribution; total reaction (non-elastic) cross section; radiative capture cross section; every kind of reaction cross sections in first and second emission processes; the inclusive cross sections and their energy spectra as well as double differential cross sections (calculated with Kalbach Systematics[9]) of the six emitting particles; the production cross sections and energy spectra of total γ photons producing in all kinds of reactions; the production cross sections and energy spectra of all kinds of recoil( residual) nuclei.

For the calculation of radiative capture cross section and its γ spectra, besides the usual evaporation mechanism, the direct and pre-equilibrium (PE). emission γ photons are also considered in MEND. The theory approach and calculation formula are due to Akkermans and Gruppelaar[10]. We get the direct γ photons by letting $n=1$ in their equation (8).

All output quantities from the eighteen emission processes are obtained. The emission particles can be n, p, α, d, t and $^3$He in first to fourth emission processes; n, p, α and d in fifth to seventh emission processes; n, p and α in eighth to tenth emission processes; only n and p in eleventh to eighteenth emission processes.

MEND contains a main program, a block data, 67 subroutines and 42 functions. And there are four source code files: mend. for, peg. for, hf. for and common. for. User should put them in a same subdirectory for compiling them. User can also put peg. for and hf. for together with mend. for to form a much larger file, meanwhile, the two statements 'include peg. for' and 'include hf. for' at the end of mend. for should be deleted. However, user cannot put common. for together with other files because the statement 'include common. for' appears in many subroutines. The source code files include about 28500 lines totally.

## 3 Theoretical Frames

The theoretical frames of MEND are spherical optical model, 'direct' reactions in continuous levels and intranuclear cascade nucleons emission based on empirical formula, PE statistical theory based on exciton model, evaporation model and Hauser-Feshbach (HF) theory with width fluctuation correction.

Four kinds of spherical optical potential can be employed to calculate the total cross section, shape elastic scattering cross section and its angular distribution, absorption cross section, as well as transmission coefficients used in HF theory and 'inverse cross sections' used in PE theory. Usually, the phenomenological optical potential of Becchetti and Greenlees[11] (BG form) or those of Koning and Delaroche[12] (KD form) are used. MEND can also do the phenomenological optical potential calculation with CH89 parameters[13] and microscopic optical potential calculation based on Skyrme force[14] for n and p channels. The microscopic potential and the later two global phenomenological potential are very useful for those nuclides without experimental data for adjusting optical potential parameters.

The cascade emissions of one to four nucleons with certain fractions before PE and evaporation are considered in MEND. The cascade yields of nucleons and the energy spectra of cascade nucleons are calculated with empirical formula[15].

The PE emission mechanism is included exactly in first, second and third emission processes, it is also exactly (for nucleon emissions) or approximately (for emissions of composite particles) considered in fourth and fifth emission processes. Combining the cascade emission of nucleons and the PE mechanism, there are some fractions for both PE emission and evaporation in first to fifth emission process, and there is only evaporation (without PE emission) in sixth to eighteenth emission process.

For emission of composite particles in PE theory, the improved pick-up reaction mechanism[8] is adopted. In the calculation of state densities for the exciton model, the Pauli principle is accommodated. The angular momentum and parity conservation are not considered in cascade nucleon emissions, PE theory and evaporation model.

The HF theory with width fluctuation correction is used for the first emission process, in which the angular momentum and parity conservation are considered, and the cross section and angular distribution of discrete levels can be given.

Usually, MEND can not calculate the direct reaction contributions in discrete levels, which are calculated with other codes (such as DWUCK4[16] and ECIS94[17]) and treated as input in MEND. However, for n or p as projectile, MEND itself can also calculate the direct reaction contributions of some collective levels in n, p channels with the approach in Ref. [5]. Besides the direct reactions in discrete levels, MEND also calculates the 'direct' reactions in continuous levels with empirical formulae before cascade nucleon emission, PE and evaporation. These empirical formulae include pickup, stripping, exchange and knockout reaction mechanisms[18] as well as the deuteron breakup model[19].

MEND does not calculate fission cross sections. For sub-actinides, user can obtain fission cross sections from experimental data or other way. They are treated as input in MEND.

## 4 Calculation Methods

Methods used in MEND to calculate all kinds of reaction cross sections are the same as in CCRMN[4], in which the basic idea is how to change the multi-fold (more than two) integration into a double-fold integration by using excited energy of residual nucleus instead of emission particle energy as integrate variable and exchanging the integrate order. However, CCRMN can calculate cross sections but energy spectra. The methods for calculating the energy spectra of the emitting particle moving against the residual nucleus are given in the Ref [2], here we give the outlines of the methods as follows:

In the real calculation of numerical integration in the code MEND, the expressions of integrands are of terrible complexity. We substitute the abbreviative notations $f_1(u_1,\ldots)$, $f_2(u_1,u_2,\ldots)$ for the extra-complex expressions in the integrands, and only clearly give the limits of integrations. At the same time, in order to make the symbols clearer and simpler, we also omit the script of channels indicating the kind of emitting particles; with $BV1$, $BV2$, $BV3$ and $BV4$ denoting the binding energies of the emitting light particle and the corresponding residual nucleus, with $Z1$, $Z2$, $Z3$ and $Z4$ denoting the energies at which the 'inverse cross sections' start having obviously nonzero values (for example, being larger than $10^{-6}$), with $E_1$, $E_2$, $E_3$ and $E_4$ denoting the kinetic energies of the emitting particles, with $u_1$, $u_2$, $u_3$ and $u_4$ denoting the excited energies of the corresponding residual nuclei in the first, second, third and fourth emitting process, respectively. Let $E$ denoting the excited energy of compound nucleus consisted of projectile and target, $E_0$ denoting the kinetic energy of the projectile moving against the target nucleus in their center of mass frame.

For the first emitting process, the reaction cross section can be expressed as:

$$\sigma_1 = (\int_0^{BZ2} + \int_{BZ2}^{B1}) f_1(u_1, \cdots) \mathrm{d}u_1, \qquad (1)$$

where $BZ2 = BV2 + Z2$, $B1 = E - BV1 - Z1$. The reason that the integration for $u_1$ is divided into two parts is the second emitting process won't open if $u_1 \leqslant BZ2$. In the following calculation of $\sigma_2$, $\sigma_3$, $\cdots$, the integrations for $u_2$, $u_3$, $\cdots$, are also divided into two parts, the reasons are the same, we won't explain anymore. When we calculate $\sigma_1$, we save the values of $f_1(u_1, \cdots)$ at all integral base points in the higher excited energy region $[BZ2, B1]$ to supply to calculation of the second emitting process by linear interpolation. Because $E_1 = E - BV1 - u_1$ and $u_1$ have the relation corresponding to each other one by one ($E$ and $BV1$ with non-varying value in the integration), the values of $f_1(u_1, \ldots)$ at various base points of the integration for $u_1$ is also the values of $f_1(E - BV1 - E_1, \ldots)$ at various base points of the integration for $E_1$, i. e. the non-normalized energy spectrum values of outgoing particle moving against its residual nucleus at various base points $E_1$.

For second emitting process, let

$$FF2(u_2) = \int_{u_2+BV2+Z2}^{B1} f_2(u_1, u_2, \cdots) f_1(u_1, \cdots) \mathrm{d}u_1, \qquad (2)$$

where the integral base points for $u_1$ are not the same as in Eq. (1), the values of $f_1(u_1, \ldots)$ should be gotten from above saved value by linear interpolation. The reaction cross section can be denoted as

$$\sigma_2 = (\int_0^{BZ3} + \int_{BZ3}^{B2}) FF2(u_2, \cdots) \mathrm{d}u_2, \qquad (3)$$

where $BZ3 = BV3 + Z3$, $B2 = B1 - BV2 - Z2$. When we calculate $\sigma_2$, we should save the values of $FF2(u_2)$ at all integral base points in the energy region $[BZ3, B2]$ to supply to calculation of the third emitting process by linear interpolation. Because $E_2 = u_1 - BV2 - u_2$ and $u_2$ have not anymore the relation corresponding to each other one by one ($u_1$ is a varying integral variable although the value of $BV2$ is still non-varying), the energy spectra in second emitting process have to be recalculated instead of directly getting from the saved values of $FF2(u_2)$ in calculation of cross section $\sigma_2$. Let

$$sp_2(E_2) = \int_{E_2+BV2}^{B1} fe_2(u_1, E_2, \cdots) f_1(u_1, \cdots) \mathrm{d}u_1, \qquad (4)$$

where $fe_2(u_1, E_2, \cdots)$ is a function of $u_1$ and $E_2$ obtained from $f_2(u_1, u_2, \cdots)$ in which $u_2$ should be changed to $u_1 - BV2 - E_2$. The reaction cross section can also be denoted as

$$\sigma_2 = \int_{Z2}^{B2+Z2} sp_2(E_2) \mathrm{d}E_2. \qquad (5)$$

We can check the precision of numerical calculation by comparing the value of $\sigma_2$ calculated from Eq. (5) with that from Eq. (3). The values of $sp_2(E_2)$ in Eq. (4) at various integral base points for $E_2$ are just the non-normalized energy spectra of the emitting light particle moving against its residual (recoil) nucleus for second emitting process.

For third emitting process, let

$$FF3(u_3) = \int_{u_3+BV3+Z3}^{B2} f_3(u_2, u_3, \cdots) FF2(u_2) \mathrm{d}u_2, \qquad (6)$$

where the integral base points for $u_2$ are not the same as in Eq. (3), the values of $FF2(u_2)$ should be gotten from above saved value by linear interpolation. The reaction cross section can be denoted as

$$\sigma_3 = (\int_0^{BZ4} + \int_{BZ4}^{B3}) FF3(u_3, \cdots) \mathrm{d}u_3, \qquad (7)$$

where $BZ4 = BV4 + Z4$, $B3 = B2 - BV3 - Z3$. When we calculate $\sigma_3$, we should save the values of $FF3(u_3)$ at all integral base points in the energy region $[BZ4, B3]$ to supply to calculation of the forth emitting process by linear interpolation. Because $E_3 = u_2 - BV3 - u_3$ and $u_3$ also have not the relation corresponding to each other one by one ($u_2$ is a varying integral variable although the value of $BV3$ is non-varying), the energy spectra in third emitting process have to be recalculated instead of directly getting from the saved values of $FF3(u_3)$ in calculation of cross section $\sigma_3$. Let

$$sp_3(E_3)=\int_{E_3+BV3}^{B2} fe_3(u_2,E_3,\cdots)FF2(u_2)\mathrm{d}u_2. \tag{8}$$

The reaction cross section can also be denoted as:

$$\sigma_3=\int_{Z3}^{B3+Z3} sp_3(E_3)\mathrm{d}E_3. \tag{9}$$

We can check the precision of numerical calculation by comparing the value of $\sigma_3$ calculated from Eq. (9) with that from Eq. (7). The values of $sp_3(E_3)$ in Eq. (8) at various integral base points for $E_3$ are just the non-normalized energy spectra of the emitting light particle moving against its residual (recoil) nucleus for third emitting process.

Following the approaches in third emitting process, we can deduce the formulae to calculate the cross sections and energy spectra for any $k$-th ($k\geqslant 4$) emitting process.

Based on the energy spectra of relative motion, the energy spectra of six emitting light particles and of all kinds of recoil nuclei in Lab-frame can be calculated with Chadwick's approach (see the appendix of the Ref. [20]). From the energy spectra of six emitting light particles in Lab-frame and the corresponding PE fraction given in the output file 'specp. dat', the double differential cross sections of six emitting light particles in Lab-frame can also be calculated with Kalbach systematics[9]. We have already written a small code Kalbah to do this work.

## 5 Input and Output Files

In MEND, the input files include mendi. dat and mdir. dat; the output files include mendo. dat (general output), CStabl. out (tables of cross sections), specp. dat (normalized energy spectra of six emission particles and total γ-ray, as well as the pre-equilibrium fractions for six emission particles), specr. dat (normalized energy spectra of all kinds of recoil nuclei), sptabl. out (tables of differential cross sections $\mathrm{d}\sigma/\mathrm{d}E$ of six emission particles and total γ-ray) and B6out. dat (ENDF/B6 format output file); besides, mendv. dat ('inverse cross sections' table) is an output file if $INCS=0$ and an input file if $INCS>0$; aaDLTA. dat (tables of level density parameters and pair energy corrections) is an output file calculated with GCCI formula and parameters[21] if $IaDL=0$ and an input file if $IaDL=1$. In this way, user can adjust some parameters in aaDLTA. dat to make corresponding reaction cross sections in better accordance with experimental data.

User can find the explanation of the meaning of all the quantities in the input files from the comment lines in source files of MEND. Part calculation formule directly referred the input quantities are given in appendix. Here we do not give the example of input files, users can contact us if they need the example and the explanation.

## 6 Calculation Results

Using MEND, with neutron as projectile, all kind of cross sections, angular distributions, energy spectra and double differential cross sections are consistently calculated and evaluated for $^{24-26}$Mg, $^{27}$Al, $^{28-30}$Si, $^{40,42-44,46,48}$Ca, $^{50,52-54}$Cr, $^{54,56-58}$Fe, $^{59}$Co, $^{58,60-62,64}$Ni, $^{63,65}$Cu, $^{90-92,94,96}$Zr, $^{93}$Nb, $^{92,94-98,100}$Mo, $^{180,182-184,186}$W, $^{204,206-208}$Pb, $^{209}$Bi; and with proton as projectile, all kind of cross sections, angular distributions,

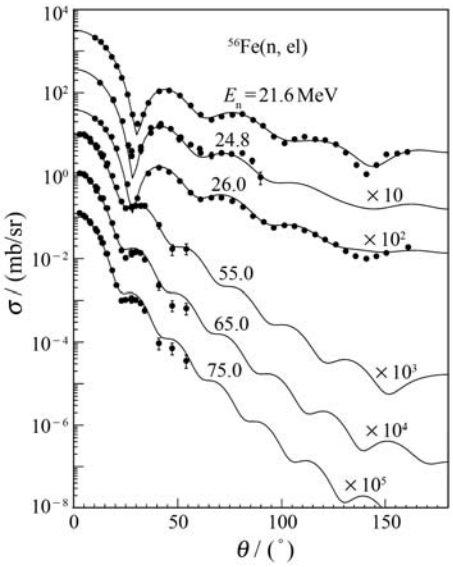


Fig. 1 Calculated neutron elastic scattering differential cross sections (solid line) compared with experimental data for n+$^{56}$Fe.

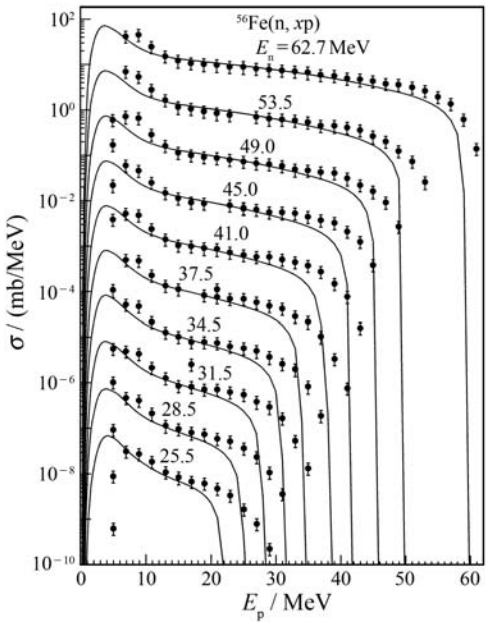


Fig. 2 Calculated energy spectra of proton emission (solid line) compared with experimental data for n+$^{56}$Fe.

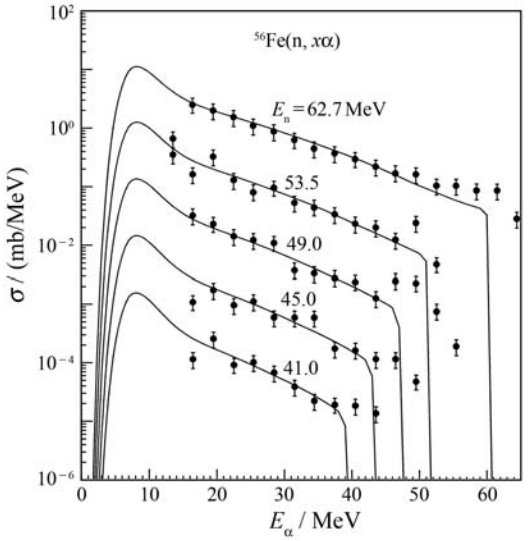


Fig. 3 Calculated energy spectra of α emission (solid line) compared with experimental data for n+$^{56}$Fe.

energy spectra and double differential cross sections are consistently calculated and evaluated for $^{27}$Al, $^{28-30}$Si, $^{40,42-44,46,48}$Ca, $^{54,56-58}$Fe, $^{59}$Co, $^{58,60-62,64}$Ni, $^{63,65}$Cu, $^{90-92,94,96}$Zr, $^{92,94-98,100}$Mo, $^{180,182-184,186}$W, $^{204,206-208}$Pb, $^{209}$Bi as target nucleus. Generally speaking, good agreement is generally observed between the calculated results and the experimental data. For some nuclei as examples, theoretical calculated results are compared with existing experimental data as shown in Figs. 1 to 7. Parts of above results calculated with MEND have been published[22-36].

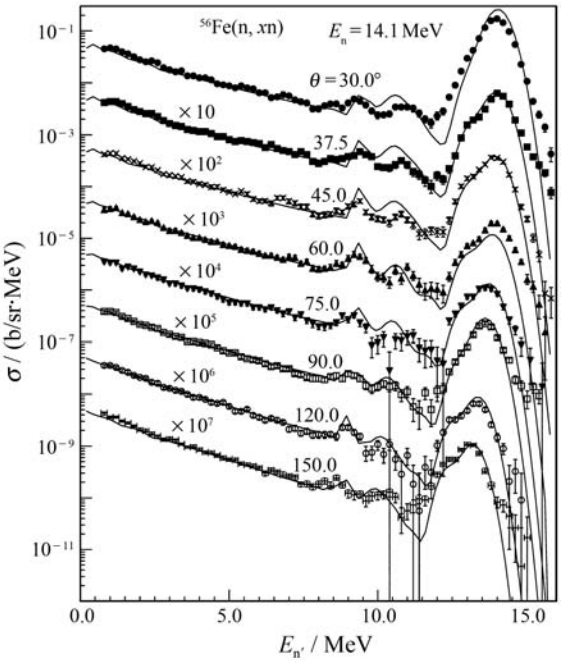


Fig. 4 Calculated double differential cross sections of neutron emission (solid line) compared with experimental data for n+$^{56}$Fe.

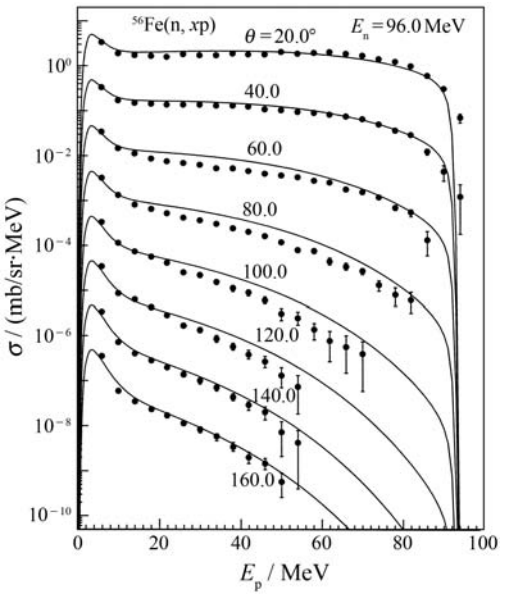


Fig. 5 Calculated double differential cross sections of proton emission (solid line) compared with experimental data for n+$^{56}$Fe.

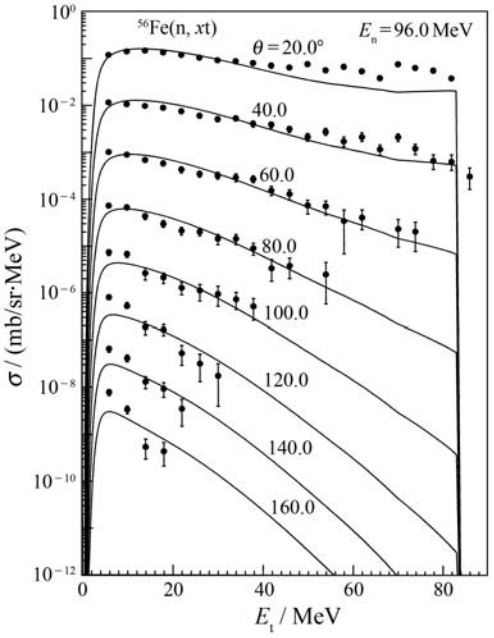


Fig. 6 Calculated double differential cross sections of triton emission (solid line) compared with experimental data for n+$^{56}$Fe.

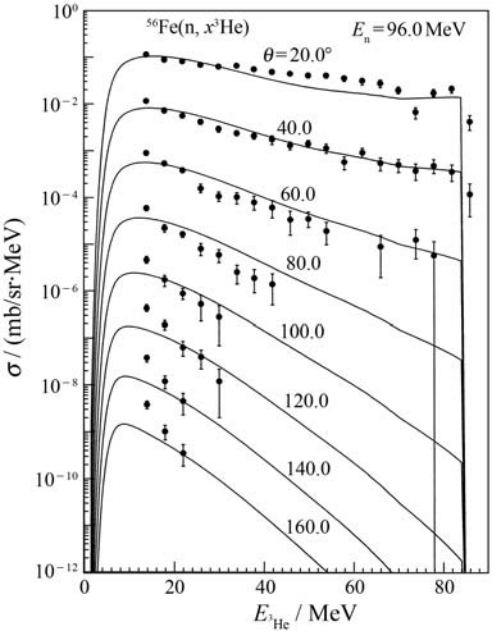


Fig. 7 Calculated double differential cross sections of $^3$He emission (solid line) compared with experimental data for n+$^{56}$Fe.

# Appendix: Part Calculation Formulae

## 1 Optical Model

### 1.1 Optical potential of BG form

The optical potential[11] considered here are Woods-Saxon form for the real part, Woods-Saxon and derivative Woods-Saxon form for the imaginary parts corresponding to the volume and surface absorption respectively, and the Thomas form for the spin-orbit part. Their potential parameters are presented as:

$$V_b(r, E_L) = -V_r(E_L) f_r(r) + i[4a_s W_s(E_L) \times \frac{df_s(r)}{dr} - W_v(E_L) f_v(r)] - V_{SO}(r) + V_C(r), \tag{1}$$

where $V_b(r, E_L)$ stands for the total potential of incoming or outgoing particle b.

The Woods-Saxon form factor

$$f_i(r) = \left[1 + \exp\left(\frac{r - R_i}{a_i}\right)\right]^{-1},$$

with i = r, v, s. (2)

Spin-orbit potential

$$V_{SO}(r) = \frac{\lambda_\pi^2 (V_{SO} + iW_{SO})}{a_{SO} r} \times \frac{\exp[(r - R_{SO})/a_{SO}]}{(1 + \exp[(r - R_{SO})/a_{SO}])^2} \times [j(j+1) - l(l+1) - S_b(S_b+1)]. \tag{3}$$

Coulomb potential

$$V_C(r) = \begin{cases} 0.7720448 \dfrac{Z_b Z}{R_C}\left(3 - \dfrac{r^2}{R_C^2}\right), & \text{if} \quad r \leqslant R_C \\ 1.440975 \dfrac{Z_b Z}{r}, & \text{if} \quad r > R_C . \end{cases} \tag{4}$$

The energy dependence of potential depths are given by

$$V_r(E_L) = V_0 + V_1 E_L + V_2 E_L^2 + \frac{V_3 (N - Z)}{A} + \frac{V_4 Z}{A^{1/3}} \tag{5}$$

$$W_s(E_L) = W_{s0} + W_{s1}E_L + \frac{W_{s2}(N-Z)}{A}, \quad (6)$$

or

$$W_s(E_L) = W_{s0} + W_{s1}E_L + \frac{W_{s2}(N-Z)}{A}, \quad \text{when } E_L \leqslant E_{ws} \quad (6a)$$

$$W_s(E_L) = W_{s0h} + W_{s1h}E_L + \frac{W_{s2}(N-Z)}{A}, \quad \text{when } E_L \geqslant E_{ws} \quad (6b)$$

$$W_{s0h} = W_{s0} + (W_{s1} - W_{s1h})E_{ws}, \quad (6c)$$

$$W_v = W_{v0} + W_{v1}E_L + W_{v2}E_L^2, \quad (7)$$

$$a_j = a_{j0} + \frac{a_{j1}(N-Z)}{A}, \quad j = v, s, \quad (8)$$

and $a_{j1}=0.7$ for proton channel, $a_{j1}=0.0$ for other 5 emitting channels. Where $E_L$ is the incident particle energy in laboratory system and in $E_L<250$ MeV energy region; $Z$, $N$ and $A$ are the proton, neutron and mass number of the target nucleus, respectively. In order to improve the agreement between the theoretical and experimental values at the higher energy part, the $E_L^2$ term is introduced in the volume absorption potential $W_v$, and the express of surface absorption potential is divided into two parts at energy $E_{ws}$. Usually, for optical potential of BG form, there are altogether 23 adjustable parameters: $V_0$, $V_1$, $V_2$, $V_3$, $V_4$, $W_{SO}$, $W_{s1}$, $W_{s2}$, $E_{ws}$, $W_{s1h}$, $W_{v1}$, $W_{v2}$, $V_{SO}$, $W_{SO}$, $a_r$, $a_{SO}$, $a_{v0}$, $a_{SO}$, $r_r$, $r_s$, $r_v$, $r_{SO}$, $r_c$, which can be automatically obtained for a given nucleus with the code APMN[21] based on its experimental data of $\sigma_{tot}$, $\sigma_{non}$ and elastic scattering angular distributions.

### 1.2 Optical potential of KD form

The phenomenological optical model potential (OMP) $u$ for nucleon-nucleus is usually determined as[12]:

$$u(r, E) = -V_V(r, E) - iW_V(r, E) - iW_D(r, E) + [V_{SO}(r, E) + iW_{SO}(r, E)]L \cdot \sigma + V_C(r), \quad (9)$$

where $V_i$ and $W_i$ are the real and imaginary components of the volume-central ($i$=v), surface-central ($i$=D) and spin-orbit ($i$=SO) potentials, respectively. $E$ is the laboratory energy of the incident particle in MeV. All components are separated into $E$-dependent well depth, $V_V$, $W_V$, $W_D$, $V_{SO}$, and $W_{SO}$, and energy-independent radial parts $f$, namely

$$V_V(r, E) = V_V(E)f(r, R_V, a_V), \quad (10)$$

$$W_V(r, E) = W_V(E)f(r, R_V, a_V), \quad (11)$$

$$W_D(r, E) = -4a_D W_D(E)\frac{d}{dr}f(r, R_D, a_D), \quad (12)$$

$$V_{SO}(r, E) = V_{SO}(E)\left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\frac{d}{dr}f(r, R_{SO}, a_{SO}), \quad (13)$$

$$W_{SO}(r, E) = W_{SO}(E)\left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\frac{d}{dr}f(r, R_{SO}, a_{SO}). \quad (14)$$

As usual, the form factor $f(r, R_i, a_i)$ is a Woods-Saxon shape

$$f(r, R_i, a_i) = \left[1 + \exp\left(\frac{r - R_i}{a_i}\right)\right]^{-1}. \quad (15)$$

The geometry parameters are the radius $R_i = r_i A^{1/3}$ and the diffuseness parameters $a_i$. For charged projectiles, the Coulomb term $V_C$, as usual, is given by that of a uniformly charged sphere:

$$V_C(r) \begin{cases} = \dfrac{Zze^2}{2R_C}\left(3 - \dfrac{r^2}{R_C^2}\right), & \text{for } r \leqslant R_C \\ = \dfrac{Zze^2}{r}, & \text{for } r \leqslant R_C \end{cases} \quad (16)$$

with $Z$ and $z$ are the charge of the target and projectile respectively, and $R_C = r_C A^{1/3}$ the Coulomb radius.

The global neutron and proton OMP for $0.001 < E < 200$ MeV and $24 < A < 209$ are given in Ref. [12], we will not list them here.

## 2 Cascade Nucleon Emission

The weight of cascade nucleon emission is read as

$$casc = \frac{(a_{10} + a_{11}\sqrt{E_0} + a_{12}E_0)Y(E_0)}{Y(E_0^*)}, \quad (17)$$

where $E_0^*$ is a large energy (usually taken as 2000.0), $E_0$ is the incoming energy in center of mass system.

The total yields of cascade nucleons[15]

$$Y(E_0)=\frac{3-(E_0/1500)^{0.5}}{1+(E_0/50)^{0.27}}\times\left[(2.905-0.0092Z)\left(\frac{E_0}{300}\right)^{0.252Z^{0.263}}-0.1\right], \tag{18}$$

$$\left(\frac{Y_n}{Y_p}\right)_p=1.5+2.1\left(\frac{A-2Z}{Z}\right), \quad \text{(for proton as projectile)} \tag{18a}$$

$$\left(\frac{Y_n}{Y_p}\right)_n=2\left(\frac{Y_n}{Y_p}\right)_p, \quad \text{(for neutron as projectile)}. \tag{18b}$$

It is supposed that at most, 3 neutrons and 2 protons can be emitted in cascade progress. Let $casc=0.0$ if it is less than 1%, and let $casn=1-casc$. So $casc$ is divided to 12 residual nuclei according to the weights $wnp(0:3,0:2)$ which are inversely proportion to $[(n-Y_n)^2+(p-Y_p)^2+0.1]^2$ (The total weight of 12 $wnp(0:3,0:2)$ should be 1). Then, $casc * wnp(n,p)$ are calculated for each residual nucleus, let $wnp(n,p)=0$ if it is less than 0.4%, then renormalization is made. At last add $wnp(0,0)$ into casc which is the weight in PE emission and evaporation.

## 3 Lever Density

### 3.1 The GCCI (Gilbert-Cameron-Cook-Ignatyuk) level density parameter[37]

$$a=a_c\frac{1-e^{-u}}{u}+a_1\left(1-\frac{1-e^{-u}}{u}\right), \tag{19}$$

where $u=\mathrm{fued}(U-\Delta)$

$$a_c=\begin{cases}A/8.0, & \text{if } Z<9 \text{ or } N<9,\\ A(A_{ss}\cdot S+Q_b), & \text{for other nuclei},\end{cases} \tag{20}$$

$$a_1=(aif1-aif2\cdot A)A, \tag{21}$$

$$\text{or}\quad a_1=(aif1\cdot A+aif2\cdot A^{2/3}), \tag{22}$$

$Z$, $N$ and $A$ are the number of charge, neutron and mass of the compound nucleus, respectively; $U$, $\Delta$ and $S$ are the excited energy, pair energy and shell correction, respectively. $Fued$, $aif1$, $aif2$ can be taken as adjustable parameters in some range, usually $fued=0.05$; for Eq. (21), $aif1=0.1375$, $aif2=8.36\times10^{-5}$[37]; for Eq. (22), $aif1=0.073$, $aif2=0.115$[40], or $aif1=0.0666$, $aif2=0.2587$[41].

$$Q_b=\begin{cases}0.142 & \text{for spherical nuclei}\\ 0.12 & \text{for deformed nuclei}\end{cases}, \tag{23}$$

$$A_{ss}=\begin{cases}0.00917, & \text{for Cameron-Cook}[38]\\ 0.0088, & \text{for Su Zongdi}[39]\end{cases}. \tag{24}$$

### 3.2 The level density formula

$$\rho(Z,A,U)=\begin{cases}\dfrac{\exp[(U-U_0)/T]}{T}, & \text{for } U\leqslant U_x+\Delta\\ \text{(constant temperature form)}\\ \dfrac{\exp(2\sqrt{aU_e})}{12\sqrt{2}\sigma U_e(aU_e)^{1/4}}, & \text{for } U>U_x+\Delta\\ \text{(high temperature form)}\end{cases}, \tag{25}$$

where

$$\begin{cases}U_x=U_c+\dfrac{U_a}{A},\\ U_e=U-\Delta,\\ T=\left[\sqrt{\dfrac{a}{U_x}}-\dfrac{1.5}{U_x}\right]^{-1},\\ \sigma^2=\begin{cases}\sigma_0^2=0.0888(aU_x)^{1/2}A^{2/3}, & \text{if } U\leqslant U_x+\Delta\\ 0.0888(aU_e)^{1/2}A^{2/3}, & \text{if } U>U_x+\Delta\end{cases},\end{cases} \tag{26}$$

$$\begin{cases}U_c=2.5, & U_a=150.0, \quad \text{for Cameron-Cook}\\ U_c=1.4, & U_a=263.0, \quad \text{for Su Zongdi.}\end{cases} \tag{27}$$

In real calculation, we find the level density for low excited energy is often some larger than that it should be, so we introduce two adjustable parameters uxxd and fasud. Let the level density $\rho$ for 2nd to 6th emission process change to $\rho\times\exp(fasud\times(u-uxxd))$ when $u<uxxd$, usually, $5<uxxd$ $0\leqslant fasud\leqslant0.5$. If $fasud=0$, there are no change for all $\rho$.

# 4 The State Density Parameter of Single Particle

$$g=\begin{cases} g_0=A/13.0, \text{ if } uecg\leqslant 0.01 \\ g_0\times fact, \text{ if } uecg>0.01 \end{cases} \tag{28}$$

$$fact=\frac{1-\mathrm{e}^{-uecg}}{uecg},\quad uecg=ccg1(v)\times(U-\Delta)\ . \tag{28a}$$

$ccg1(v)$ ($v=0, 1, 2, \cdots, 6$) are 7 adjustable parameters for 7 emitting channels (channel 0 corresponds to $\gamma$ photon emission). Usually, $0\leqslant ccg1(v)<0.05$. And $fact=1$ if $ccg1(v)\to 0$.

# 5 Calculation of γ Photons Emission

## 5.1 The evaporation rate of photons for compound system $\Gamma_r(Z, A, U)$

$$\Gamma_r(Z, A, U)=\int_0^U \frac{1}{\pi(c\hbar)^2}E_r^2\sigma_A(E_r, Z, A)\rho(Z, A, U-E_r)\mathrm{d}E_r, \tag{29}$$

$$\sigma_A(E_r, Z, A)=\sum_{j=1}^{2}\sigma_{Aj}^0(Z, A)E_r\times\left\{\frac{E_r\Gamma_{gj}(Z, A)\Gamma_{gj}(Z, A, E_r)}{[E_{gj}^2(Z, A)-E_r^2]^2+E_r^2\Gamma_{gj}^2(Z, A, E_r)}+\frac{27.63489\Gamma_{gj}(Z, A)(U-E_r)}{E_{gj}^2(Z, A)a}\right\}, \tag{30}$$

$$\Gamma_{gj}(Z, A, E_r)=\Gamma_{gj}(Z, A)\frac{E_r^2+4\pi^2(U-E_r)/a}{E_{gj}^2(Z, A)}, \tag{31}$$

where

$$\begin{cases} E_{g1}=E_0\left(1-\dfrac{\beta}{3.0}\right)^2, \\ \Gamma_{g1}=0.232E_{g1}, \\ \sigma_{A1}^0=\alpha*0.0145\dfrac{A}{E_{g1}}, \end{cases} \quad \begin{cases} E_{g2}=E_0(1-0.16\beta), \\ \Gamma_{g2}=0.275E_{g2}, \\ \sigma_{A2}^0=\alpha*0.0235\dfrac{A}{E_{g2}}. \end{cases} \tag{32}$$

$\alpha$, $\beta$ are two adjustable parameters. At first, user can take $\alpha=1.0$, $\beta=0$ (for single peak huge dipole resonance). As another choice, $(U-E_r)$ in second term inside the braces of Eqs. (30) and (31) can be replaced with $B_n-E_r$ (if $B_n$ is larger than $E_r$) or zero (if $B_n$ is less than $E_r$). Here $B_n$ is the binding energy of neutron with the corresponding residual nucleus, $U$ is the excited energy of the compound nucleus.

## 5.2 Emission rate of photons in exciton model[10]

The emission rate is $\int_0^U W_r(n, E_r)\mathrm{d}E_r$,

where

$$W_r(n, E_r)=\frac{1}{\pi\hbar\pi(c\hbar)^2}\frac{E_r^2\sigma_A(E_r, Z, A)}{\omega(Z, A, U, p, h)}\times\left[\frac{\bar{\omega}(Z, A, U-E_r, p-1, h-1)g^2E_r}{(n-2)g+g^2E_r}+\frac{\bar{\omega}(Z, A, U-E_r, p, h)ng}{ng+g^2E_r}\right], \tag{33}$$

where $n=p+h$, $n$, $p$, $h$ are the numbers of exciton, particle, hole, respectively.

$$\bar{\omega}(Z, A, U, p, h)=\frac{g(gU_e)^{h'}(gU_e-A(p, h))^{p'-1}}{p!\ h!\ (p+h-1)!}\times f(U_e) \tag{34}$$

is the exciton state density. If $gU_e\leqslant A(p, h)$ or one of factorial variables becomes negative, let $\bar{\omega}(Z, A, U, p, h)=0$.

$$\begin{cases} h'=\min(p, h),\ p'=\max(p, h), \\ A(p, h)=\dfrac{1}{2}p(p-1)+\dfrac{1}{2}h(h-1), \\ f(U_e)=\dfrac{0.06\pi^2}{(aU_e)^{1/8}}. \end{cases} \tag{35}$$

The transition rate of compound system ($Z$, $A$, $U$) from $n=1$ to $n=3$ is

$$\lambda_+(Z, A, U, 1)=2.3864334DK\left(\frac{g}{A}\right)^3\frac{U_e^2}{U}. \tag{36}$$

The cross section of direct emission gamma photons is

$$\sigma_{r,d}(U)=\frac{\sigma_a Y_{1,r}}{Y_{1,r}+2.3864334DK\ (g/A)^3(U_e^2/U)*DGAM}, \tag{37}$$

where $DK$ is the adjustable Kalbach parameter and

$DGAM$(< or =1.0) is an adjustable parameter for direct gamma photons emission.

## 6 The Preformed Factor $Fl_v(Z_v, A_v, E_v)$ of the Compound Particle Emission

The emission rate of particle v (v=1, 2, 3, 4, 5, 6 corresponding to n, p, α, d, t, $^3$He) in exciton model is

$$W_v(Z, A, U, p, h; Z_v, E_v) = \sum_{l_v=1}^{L_{vm}} W_v^{L_v}(Z, A, U, p, h; Z_v, A_v, E_v), \quad (38)$$

$$W_v^{L_v}(Z, A, U, p, h; Z_v, A_v, E_v) = \frac{2S_v+1}{\pi^2\hbar^3} m_v E_v \sigma_v(E_v) r_v R^{l_v}(Z, A, p, h; Z_v, A_v) \times Fl_v(Z_v, A_v, E_v) \times \frac{\bar{\omega}(Z-Z_v, A-A_v, U-B_v-E_v, p-l_v, h)}{\bar{\omega}(Z, A, U, p, h)}, \quad (39)$$

where $Z$, $A$, $U$, $p$, $h$ are the charge number, mass number, excited energy, particle and hole number of compound system, respectively. $Z_v$, $A_v$, $E_v$ are the charge number, mass number and energy of emitting particle v, respectively. $Fl_v(Z_v, A_v, E_v)=1.0$ for v=1, 2 (n, p emission). For v=3, 4, 5, 6, the compound particle (α, d, t, $^3$He) emission, the calculation of the $Fl_v(Z_v, A_v, E_v)$ factors in pick up mechanism is given in Ref.[8]. $l_v=1$ to $L_{vm}=\max(A_v, 3)$.

If we calculate completely with the formula in Ref.[8], the $Fl_v$ factor for $l_v=1$ or 2 will become zero when $E_v > 90$ MeV, the emission of particles α, t and $^3$He will have no PE fraction, the cross section and emission spectra of α, t, $^3$He will be much smaller and softer than the experimental data. So, for high emission energy $E_v \geqslant EFLM2$, we let $Fl_v = 0$ for $l_v = 3$, renormalization $Fl_v$ for $l_v=1$ and 2 to $RFLM(v)$; for low emission energy $E_v \leqslant EFLM1$, we calculate $Fl_v$ exactly with formula in Ref.[8]; for $EFLM1 < E_v < EFLM2$, we make smoothly connection of above $Fl_v$ in low and high emission energy regions. $EFLM1$, $EFLM2$, $RFLM(v)$ (v=3, 5, 6) corresponding to α, t, and $^3$He are adjustable parameters. Usually, $RFLM(4)=1.0$, $0.15 \leqslant RFLM(v)(v=3,5,6) \leqslant 0.3$; $50 \leqslant EFLM1 \leqslant 80$, $120 \leqslant EFLM2 \leqslant 150$.

## 7 'Direct' Reactions in Continuous Levels

Besides the direct inelastic scattering and direct reaction in discrete levels calculated with DWUCK4[16] and ECIS94[17], MEND also can calculate the direct inelastic scattering and direct reactions in continuous levels with the Kalbach's formulae[18-19]. Several kinds of reaction mechanism are considered here, which include nucleon transfer (pickup, stripping, or nucleon exchange) reaction and knockout reaction[18-19].

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# MEND——一个计算 250 MeV 以下中重核数据的程序*

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**摘　要**: 基于球型光学模型、预平衡发射和 Hauser-Feshbach 统计等理论, 编制了 MEND 程序(Medium Energy Nuclear Data), 该程序适用于中重原子核在入射粒子能量低于 250 MeV 的中低能区的全套核数据计算。对于中子和质子在 250 MeV 以下诱发的核反应, 其全截面、反应截面、弹性散射微分截面、双微分截面和能谱等理论计算值与相应的实验值基本一致。MEND 是计算中低能核反应的基础程序, 在我国已被广泛用于核数据计算及建立中能核数据库。

**关 键 词**: MEND 程序; 核反应; 核数据; 计算

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