

JAERI - M
86-074

MONTE CARLO ALGORITHMS FOR SIMULATING
PARTICLE EMISSIONS FROM PREEQUILIBRIUM
STATES DURING NUCLEAR SPALLATION REACTIONS

May 1986

Yasuaki NAKAHARA and Takahiko NISHIDA

日 本 原 子 力 研 究 所
Japan Atomic Energy Research Institute

JAERI-Mレポートは、日本原子力研究所が不定期に公刊している研究報告書です。
入手の問い合わせは、日本原子力研究所技術情報部情報資料課（〒319-11茨城県那珂郡東海村）あて、お申しこしください。なお、このほかに財団法人原子力弘済会資料センター（〒319-11茨城県那珂郡東海村日本原子力研究所内）で複写による実費頒布をおこなっております。

JAERI-M reports are issued irregularly.

Inquiries about availability of the reports should be addressed to Information Division
Department of Technical Information, Japan Atomic Energy Research Institute, Tokai-
mura, Naka-gun, Ibaraki-ken 319-11, Japan.

©Japan Atomic Energy Research Institute, 1986

編集兼発行 日本原子力研究所
印刷 (株)高野高速印刷

Monte Carlo Algorithms for Simulating
Particle Emissions from Preequilibrium
States during Nuclear Spallation
Reactions

Yasuaki NAKAHARA and Takahiko NISHIDA

Department of Reactor Engineering
Tokai Research Establishment
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken

(Received April 15, 1986)

Investigations have been made on the method how to incorporate the process of particle emissions from the preequilibrium states into the simulation calculations of nuclear spallation reactions.

The spallation reactions have been treated usually as the two step processes. The first step is the intra-nuclear cascade of nucleons initiated by a sufficiently energetic particle, such as a proton with the energy of hundreds to thousands MeV. The second step is the competing decay of the residual nucleus in highly excited states by fissions and/or particle evaporations from the compound state. The two step model is generalized to a three step model, in which the preequilibrium decay step is inserted in between the two steps mentioned above. The treatment of preequilibrium decay is based on the Griffin's exciton model.

A proposal is made of the conditions for making transitions from Step 1 to Step 2 and Step 2 to Step 3 in simulation calculations of the entire process of spallation. The first condition is defined by the number of particles trapped in the nucleus during the intra-nuclear cascade and the second one by the number of excitons reaching the effectively equilibrium state.

Monte Carlo algorithms have been formulated for simulating the spallation reaction on the basis of the three step model.

Keywords: Nuclear Reaction, Spallation, Preequilibrium Decay, Exciton Model, Fission, Evaporation, Proton, Nucleon, Monte Carlo Method, Simulation, Two Step Model, Three Step Model

核破碎反応過程における前平衡状態からの粒子放出
シミュレーションのモンテカルロ・アルゴリズム

日本原子力研究所東海研究所原子炉工学部

中原 康明・西田 雄彦

(1986年4月15日受理)

核破碎反応に前平衡状態からの粒子放出過程を組み込む方法についての研究を行った。

一般に核破碎反応は二段階過程として取扱われている。第一段階は、数百乃至数千MeVのエネルギーの陽子のような高エネルギー入射粒子によって引き起こされる核内核子カスケードである。第二段階は、高励起状態にある残留核の複合核状態からの核分裂と粒子蒸発の競争過程による崩壊である。この二段階モデルを三段階モデルに拡張する。新モデルにおいては、前平衡状態崩壊過程は上記二つの段階の中間に組み込まれる。前平衡崩壊はGriffinの励起子モデルに基づいて扱われる。

核破碎全過程のシミュレーション計算において第一から第二段階、第二から第三段階への移行を決める条件を提案する。第一条件は核内カスケード時に核内に封じ込められたままのカスケード粒子の数によって決められ、第二条件は実効的に平衡状態に達する励起子の数によって与えられる。

三段階モデルを用いて核破碎反応のシミュレーションを行うためのモンテカルロ・アルゴリズムを定式化した。

Contents

1. Introduction	1
2. Exciton Model of Preequilibrium Decay	2
2.1 Exciton State Density	2
2.2 Particle Emission Rate	4
3. Preequilibrium Decay during the Nuclear Spallation Process	5
3.1 Exciton State at the End of the Intra-nuclear Cascade	5
3.2 Transition from the Preequilibrium State to the Compound State	6
4. Monte Carlo Algorithms for Simulating the Process of Particle Emissions from the Preequilibrium State	7
4.1 Particle Emission Rates and Probabilities	8
4.2 Residual Interaction Transition Probabilities	10
5. Summary and Discussions	11
References	12
Appendix: State Densities for the Two Body Interactions	17

目 次

1. 序 論	1
2. 前平衡崩壊の励起子モデル	2
2.1 励起子状態密度	2
2.2 粒子放出率	4
3. 核破碎過程における前平衡崩壊	5
3.1 核内カスケード終了時の励起子状態	5
3.2 前平衡状態から複合核状態への移行	6
4. 前平衡状態からの粒子放出過程シミュレーションのためのモンテカルロ・アルゴリズム	7
4.1 粒子放出率と粒子放出確率	8
4.2 残留相互作用転移確率	10
5. まとめと検討	11
参考文献	12
付録： 二体相互作用に対する状態密度	17

1. Introduction

A nucleus bombarded by a sufficiently energetic particle, such as a proton with the energy of hundreds to thousands MeV, undergoes a complicated destruction process, i.e., the so called spallation. Usually the nuclear spallation has been modelled as a two step process.⁽¹⁾⁻⁽⁶⁾ The first step is the intra-nuclear cascade of nucleons initiated by an incident particle, during which several neutrons, protons and pions are knocked out of the nucleus. The second step is the competing decay of the residual nucleus in highly excited state by fission and/or particle evaporations from the compound state.

In the two step model of spallation two important reaction processes are not taken into consideration. One is the fragmentation of nucleus which could occur during and/or immediately after the intra-nuclear cascade. Many models and ideas have been proposed to explain the mechanism of fragmentation.⁽⁷⁾⁻⁽¹⁰⁾ But the actual process of fragmentation is so complicated that none of them has succeeded in offering a convincing explanation. The other is the preequilibrium decay of the residual nucleus after the intra-nuclear cascade. Contrary to the fragmentation, the preequilibrium decay processes have been successfully analyzed both qualitatively and quantitatively by the exciton model proposed by Griffin,⁽¹¹⁾ which has been improved extensively by many physicists.⁽¹²⁾⁻⁽¹⁴⁾

The spallation neutron spectra calculated by the two step model show remarkable underestimates in comparison with measured ones in the range of neutron energy of above 10 MeV.⁽⁵⁾ Tsukada and Nakahara showed that it is possible to narrow the discrepancy by effectively stretching the mean free paths of nucleons in the nucleus. The idea is based on the physical intuition that some collective effects other than the Pauli blocking effect will exist and reduce further the nucleon-nucleon collision probabilities.⁽¹⁵⁾ But due to the difficulty in formulating fundamental criteria to determine the effective mean free paths from the general point of view their idea is not suited to be used in the systematic simulation calculations of spallation processes. The exciton model is another candidate for explaining the discrepancy. It is well known that neutrons emitted from the preequilibrium state have the spectra harder than those evaporated from the compound state.⁽¹¹⁾⁻⁽¹⁴⁾ The exciton model has the advantage in its generality of formulation, which is very useful in incorporating it into the systematic simulation flow.

The difficulty in incorporating the preequilibrium decay process into the spallation reaction lies in the difficulty to define definite stages of transitions from the intra-nuclear cascade to the preequilibrium decay and from the preequilibrium to compound decay. In the cascade-exciton model due to Gudima et al.,⁽¹⁶⁾ the initial exciton state is chosen parametrically. No attempt has been reported at performing the full scale simulation calculations of spallation with preequilibrium decay taken into consideration.

In this report we propose Monte Carlo algorithms in a form suitable for the incorporation of the preequilibrium decay process into a simulation code system: NMTC/JAERI⁽⁴⁾ for high energy nuclear reactions and nucleon-meson transport.

2. Exciton Model of the Preequilibrium Decay

In our simulation scheme, we use the exciton model proposed by Griffin.⁽¹¹⁾ It is a simple statistical model which neglects nuclear angular momenta and shell structures. Simplicity of the model is a very important factor in the Monte Carlo simulation, because the event probabilities must be calculated repeatedly on the basis of the model. Neglect of the angular momenta will not be a crude approximation when the incident particle is a proton and the shell structures will have little effects on the particle emission processes because the excitation energy of the residual nucleus at the end of intra-nuclear cascades is sufficiently large, i.e., of the order of 100 MeV for sufficiently energetic incident protons with the energy of the order of 1 GeV. The Griffin's model was programmed by Kalbach for calculating preequilibrium and direct reaction double differential cross sections.⁽¹⁷⁾ For its use in the Monte Carlo simulation we need different formulations and algorithms.

2.1 Exciton State Density

The excited state of a nucleus can be defined by the numbers, p and h , of excited particle and hole degrees of freedom, respectively, above and below the Fermi surface. The sum $n=p+h$ is referred to as the exciton

The difficulty in incorporating the preequilibrium decay process into the spallation reaction lies in the difficulty to define definite stages of transitions from the intra-nuclear cascade to the preequilibrium decay and from the preequilibrium to compound decay. In the cascade-exciton model due to Gudima et al.,⁽¹⁶⁾ the initial exciton state is chosen parametrically. No attempt has been reported at performing the full scale simulation calculations of spallation with preequilibrium decay taken into consideration.

In this report we propose Monte Carlo algorithms in a form suitable for the incorporation of the preequilibrium decay process into a simulation code system: NMTC/JAERI⁽⁴⁾ for high energy nuclear reactions and nucleon-meson transport.

2. Exciton Model of the Preequilibrium Decay

In our simulation scheme, we use the exciton model proposed by Griffin.⁽¹¹⁾ It is a simple statistical model which neglects nuclear angular momenta and shell structures. Simplicity of the model is a very important factor in the Monte Carlo simulation, because the event probabilities must be calculated repeatedly on the basis of the model. Neglect of the angular momenta will not be a crude approximation when the incident particle is a proton and the shell structures will have little effects on the particle emission processes because the excitation energy of the residual nucleus at the end of intra-nuclear cascades is sufficiently large, i.e., of the order of 100 MeV for sufficiently energetic incident protons with the energy of the order of 1 GeV. The Griffin's model was programmed by Kalbach for calculating preequilibrium and direct reaction double differential cross sections.⁽¹⁷⁾ For its use in the Monte Carlo simulation we need different formulations and algorithms.

2.1 Exciton State Density

The excited state of a nucleus can be defined by the numbers, p and h , of excited particle and hole degrees of freedom, respectively, above and below the Fermi surface. The sum $n=p+h$ is referred to as the exciton

number. The nuclear state is assumed to be formed initially by (p_0, h_0) and the difference $p-h$ remains constant during the decay so that $p-h=p_0-h_0$. This assumption does not hold near the equilibrium but may be said to be adequate for preequilibrium calculations.⁽¹⁷⁾ It is assumed also that a nuclear state is described by equally spaced single particle states with the density g_0 .

For a nucleus with the excitation energy E , the exciton state density is given by⁽¹⁷⁾

$$\omega(p, h, E) = \frac{g_0^n g^n(p) [E - A(p, h)]^{n-1}}{p! h! (n-1)!} f(p), \quad (1)$$

where

$$A(p, h) = E_p(p, h) - [p(p+1) + h(h+1)] / (4g_0) \quad (2)$$

$$E_p(p, h) = p_m^2 / g_0: \text{ Pauli energy} \quad (3)$$

$$p_m = \text{Max}(p, h) . \quad (4)$$

The factor $g(p)$ is the correction to g_0 derived on the assumption that the single particle state density varies as the square root of the energy in the nuclear potential well and g_0 is the average near the Fermi surface, i.e.,

$$g(p) = \begin{cases} \frac{p}{n} \left(\frac{V+E/n}{V} \right)^{\frac{1}{2}} + \frac{h}{n} \left(\frac{V-E/n}{V} \right)^{\frac{1}{2}}, & \text{for } h \leq 2, \\ 1 & h > 2. \end{cases} \quad (5)$$

In Eq. (5) V is the potential well depth. The factor $f(p)$ is the correction to the state density due to the finite depth of the potential well;

$$f(p) = \begin{cases} 1 - \left[h \left(\frac{E-V}{V} \right)^{n-1} - \frac{h(h-1)}{2} \left(\frac{E-2V}{V} \right)^{n-1} \right] \Theta(E-V), & \text{for } h \leq 2, \\ 1, & \text{for } h > 2, \end{cases} \quad (6)$$

where Θ is the Heaviside function:

$$\begin{aligned} \Theta(x) &= 1, \text{ when } x \geq 0, \\ &= 0, \text{ when } x < 0. \end{aligned}$$

2.2 Particle Emission Rate

The average rate of emitting an unbound particle of type b and kinetic energy ϵ from the unbound state specified by (p,h) is given by⁽¹⁷⁾

$$W_b^{(u)}(p,h,\epsilon)d\epsilon = \frac{(2s_b+1)A_b Q_b(p)}{\pi^2 \hbar^3 \omega^{(u)}(p,h,E)} \epsilon \sigma_b(\epsilon) \omega(p-A_b, h, U) d\epsilon, \quad (7)$$

where

- s_b = the spin of the emitted particle b,
- A_b = the mass of the emitted particle,
- σ_b = the inverse cross section for the composite nucleus formation,
- U = the excitation energy of the nucleus after the emission of a particle b,
- $\omega^{(u)}$ = the density of unbound states.

The factor $Q_b(p)$ takes into account of the difference between the proton and neutron degrees of freedom and depends on the proton and neutron numbers of a projectile, a target nucleus and an emitted particle. Because it is difficult to derive a definite expression of $Q_b(p)$ at the end of the intra-nuclear cascade, we assume that $Q_b(p)=1$ in our algorithm.

As for the inverse cross section σ_b , we use the same expressions as those used in the NMTC/JAERI code⁽⁴⁾, which were derived by Dostrovsky et al.

For neutrons,

$$\sigma_b(\epsilon) = \alpha(1+\beta/\epsilon)\pi R^2, \quad (8)$$

where

$$\begin{aligned} \alpha &= 0.76 + 1.93A \\ \alpha\beta &= 1.66A^{-2/3} - 0.050, \\ R &= 1.70 \times 10^{-13} A^{1/3} \text{ [cm]: nuclear radius,} \\ A &= \text{the mass of the nucleus.} \end{aligned}$$

For charged particles,

$$\begin{aligned} \sigma_b(\epsilon) &= (1+C_b)(1-k_b V_b/\epsilon)\pi R^2, \quad \text{for } \epsilon \geq k_b V_b, \\ &= 0, \quad \text{for } \epsilon < k_b V_b. \end{aligned} \quad (9)$$

where C_b and k_b are constants tabulated in a data file for the use with NMTC/JAERI and V_b is the Coulomb barrier height for the particle b.

Since in Monte Carlo calculations only ratios of the expressions like Eq. (7) are used, the explicit expressions for $\omega^{(u)}(p,h,E)$ are immaterial.

3. Preequilibrium Decay during the Nuclear Spallation Process

As was mentioned in Chapt. 1, it is necessary to define two definite conditions for incorporating the preequilibrium decay into the spallation process. The one is for determining the starting conditions of the preequilibrium decay at the end of the intra-nuclear cascades. The other is for timing the transition from the preequilibrium state to the compound state. With these conditions we can complete a computational flow scheme of the three step method, which is described in Fig. 1.

3.1 Exciton State at the End of the Intra-nuclear Cascade

All the nucleon-meson transport codes such as NMTC and HETC⁽¹⁾ and NMTC/JAERI⁽⁴⁾ use an intra-nuclear cascade code developed by Bertini⁽¹⁸⁾ for performing the Step 1 calculations. The Monte Carlo history of a particle participating in the cascade is no longer traced when its energy measured with respect to the outside of the nucleus falls below a certain cutoff energy, which is taken to be one-half of the Coulomb potential at the surface of the nucleus and is assumed to be the same for all particles.⁽¹⁸⁾ The Coulomb potential for the particle b is given by

$$V_b = \frac{Z_b Z e^2}{R + R_b} \quad (10)$$

where Z_b and Z are the charge numbers of the particle b and the nucleus, respectively, e is the charge of a proton and R_b is the correction constant.⁽¹⁹⁾

The implication of the treatment described above is that the particles whose histories have been terminated have wave lengths too long for subsequent reactions to be represented as particle-particle two body collisions. Their energies are still well above the Fermi surface and contribute to the excitation of the residual nucleus. It follows naturally from these arguments that we can use the number of particles whose histories have been terminated during the cascades as the particle

Since in Monte Carlo calculations only ratios of the expressions like Eq. (7) are used, the explicit expressions for $\omega^{(u)}(p,h,E)$ are immaterial.

3. Preequilibrium Decay during the Nuclear Spallation Process

As was mentioned in Chapt. 1, it is necessary to define two definite conditions for incorporating the preequilibrium decay into the spallation process. The one is for determining the starting conditions of the preequilibrium decay at the end of the intra-nuclear cascades. The other is for timing the transition from the preequilibrium state to the compound state. With these conditions we can complete a computational flow scheme of the three step method, which is described in Fig. 1.

3.1 Exciton State at the End of the Intra-nuclear Cascade

All the nucleon-meson transport codes such as NMTC and HETC⁽¹⁾ and NMTC/JAERI⁽⁴⁾ use an intra-nuclear cascade code developed by Bertini⁽¹⁸⁾ for performing the Step 1 calculations. The Monte Carlo history of a particle participating in the cascade is no longer traced when its energy measured with respect to the outside of the nucleus falls below a certain cutoff energy, which is taken to be one-half of the Coulomb potential at the surface of the nucleus and is assumed to be the same for all particles.⁽¹⁸⁾ The Coulomb potential for the particle b is given by

$$V_b = \frac{Z_b Z e^2}{R + R_b} \quad (10)$$

where Z_b and Z are the charge numbers of the particle b and the nucleus, respectively, e is the charge of a proton and R_b is the correction constant.⁽¹⁹⁾

The implication of the treatment described above is that the particles whose histories have been terminated have wave lengths too long for subsequent reactions to be represented as particle-particle two body collisions. Their energies are still well above the Fermi surface and contribute to the excitation of the residual nucleus. It follows naturally from these arguments that we can use the number of particles whose histories have been terminated during the cascades as the particle

number p_0 of the exciton state.

The next problem is how to determine the hole number h_0 of the exciton state. In the usual preequilibrium calculations the initial exciton state (p_0, h_0) are assumed a priori. Kalbach says that in most cases we can assume that $(p_0, h_0) = (A_a + 1, 1)$, where A_a is the mass of the incident particle.⁽¹⁷⁾ For the preequilibrium decays following the intra-nuclear cascades, however, this assumption is not appropriate, because it does not reflect the preceding histories. But in most calculations of nucleon induced preequilibrium reactions good results have been obtained by making summations over the exciton states $(p, p-1)$ with p changing from 2 up to some large number for which the contribution from each state becomes negligible.⁽²⁰⁾ Hence an assumption acceptable in our Monte Carlo scheme would be $h_0 = p_0 - 1$.

Summarizing the arguments, we have the following. The number of particles in the exciton state at the end of the intra-nuclear cascade, p_0 , can be considered to be equal to the number of particles whose histories have been terminated during the cascade because of the energy decrease below one-half of the Coulomb barrier. The corresponding number of holes, h_0 , can be assumed to be given by the relation $h_0 = p_0 - 1$.

3.2 Transition from the Preequilibrium State to the Compound State

In a picture of exciton representation of nuclear states the number of excitons increases stepwise with $\Delta n = 2$ as the internal transitions continue⁽¹²⁾ and the compound state is considered to be the state with infinite number of excitons, i.e., the continuum particle state. This can be seen as follows. For simplicity we rewrite Eq. (1) as

$$\omega(n, E) = \frac{g_0 (g_0 E)^{n-1}}{p! h! (n-1)!} \quad (11)$$

assuming that $g(p) = 1$, $A(p, h) = 1$ and $f(p) = 1$. By making summation of Eq. (1) over n , we get

$$\omega(E) = \sum_n \omega(n, E) \simeq \exp(2\sqrt{g_0 E}) \quad (12)$$

which is nothing but the energy level density for compound nucleus with

the level density parameter α replaced by g_0 . The relation between the parameters g_0 and α are given by $\alpha = \pi^2 g_0 / 6$.⁽¹⁶⁾ Thus, for sufficiently large n , larger than some n_{eq} , we can use the conventional evaporation model instead of the preequilibrium model. The exciton number n_{eq} can be used as a key factor to determine the switching from the preequilibrium model to the compound model in our computational flow.

The problem to be settled next is about the value of n_{eq} , i.e., how large is large enough. In the PRECO-D2 code the maximum exciton number is set to be 20.⁽¹⁷⁾ Of course, this value will depend on the excitation energy at the end of the intra-nuclear cascade. But the value of 20 may be large enough or even the smaller number may be sufficiently large as the value of n_{eq} , because contributions from the exciton states decrease rapidly in the log scale with the increase of n , as is seen in the paper of Iwamoto and Harada.⁽²⁰⁾ On the other hand, Gudima et al. derived an approximate relation:

$$n_{eq} \approx \frac{1}{\pi} \sqrt{\frac{6}{5}AE} \quad (13)$$

from a balance condition between the $+$ and $-\Delta n$ transitions.⁽¹⁶⁾ For example, when $A=200$, the value of n given by Eq. (13) is larger than 20 for $E \geq 20$ MeV.

Although the optimum value of n_{eq} is not fixed yet, the following condition can be employed in our scheme. When the number of excitons becomes greater than a certain critical number n_{eq} , the Step 2 calculation is to be terminated and the computational flow is carried on to the Step 3.

4. Monte Carlo Algorithms for Simulating the Process of Particle Emission from the Preequilibrium State

Monte Carlo simulation of the process of particle emissions from the preequilibrium state requires statistical algorithms, which are quite different from those used in calculating double differential cross sections.⁽¹⁷⁾ Details of the algorithms for each stage of the Monte Carlo simulation are described following the flow shown in Fig. 2

the level density parameter α replaced by g_0 . The relation between the parameters g_0 and α are given by $\alpha = \pi^2 g_0 / 6$.⁽¹⁶⁾ Thus, for sufficiently large n , larger than some n_{eq} , we can use the conventional evaporation model instead of the preequilibrium model. The exciton number n_{eq} can be used as a key factor to determine the switching from the preequilibrium model to the compound model in our computational flow.

The problem to be settled next is about the value of n_{eq} , i.e., how large is large enough. In the PRECO-D2 code the maximum exciton number is set to be 20.⁽¹⁷⁾ Of course, this value will depend on the excitation energy at the end of the intra-nuclear cascade. But the value of 20 may be large enough or even the smaller number may be sufficiently large as the value of n_{eq} , because contributions from the exciton states decrease rapidly in the log scale with the increase of n , as is seen in the paper of Iwamoto and Harada.⁽²⁰⁾ On the other hand, Gudima et al. derived an approximate relation:

$$n_{eq} \approx \frac{1}{\pi} \sqrt{\frac{6}{5} AE} \quad (13)$$

from a balance condition between the $+$ and $-\Delta n$ transitions.⁽¹⁶⁾ For example, when $A=200$, the value of n given by Eq. (13) is larger than 20 for $E \geq 20$ MeV.

Although the optimum value of n_{eq} is not fixed yet, the following condition can be employed in our scheme. When the number of excitons becomes greater than a certain critical number n_{eq} , the Step 2 calculation is to be terminated and the computational flow is carried on to the Step 3.

4. Monte Carlo Algorithms for Simulating the Process of Particle Emission from the Preequilibrium State

Monte Carlo simulation of the process of particle emissions from the preequilibrium state requires statistical algorithms, which are quite different from those used in calculating double differential cross sections.⁽¹⁷⁾ Details of the algorithms for each stage of the Monte Carlo simulation are described following the flow shown in Fig. 2

4.1 Particle Emission Rates and Probabilities

The emission rate of a particle b for a nucleus at the (p, h, E) state, where p and h are the numbers of particles and holes at the excitation energy E , is obtained by integrating Eq. (7) over the kinetic energy ϵ of the particle to be emitted. We define the unnormalized emission rate by the relation:

$$R_b(p, h, E) = (2s_b + 1) A_b \int_{k_b V_b}^{E - B_b - \delta} \epsilon \sigma_b(\epsilon) \omega(p - A_b, h, E - B_b - \epsilon) d\epsilon, \quad (14)$$

where the approximation $Q(p) = 1$ is made and the factor $\pi^2 \hbar^3 \omega^{(u)}(p, h, E)$ in Eq. (7) is omitted, because only the ratios of R_b are used later. In Eq. (14) B_b is the binding energy of the particle b , δ is the pairing energy and $k_b V_b$ is the effective Coulomb barrier height. These quantities are calculated in a subroutine DRES⁽¹⁹⁾ of the NMTC code. Spins of neutron, proton, deuteron, triton, He and α particle are given as follows;

$$s_n = 1/2, s_p = 1/2, s_d = 1, s_t = 1/2, s_{\text{He}} = 1/2, s_\alpha = 0.$$

If $\sum_b R_b(p, h, E) > 0$, particle emissions are possible. The calculation is continued to the selection of the particle to be emitted. The type of the particle to be emitted from the (p, h, E) state is selected according to the emission probability:

$$P_b(p, h, E) = R_b(p, h, E) / \sum_b R_b(p, h, E) \quad (15)$$

After the emission of the particle b the exciton state is changed to $(p - A_b, h, E - B_b - \epsilon)$. The kinetic energy ϵ of the emitted particle b is determined by the probability function:

$$P(\epsilon) = \frac{\epsilon \sigma_b(\epsilon) \omega(p - A_b, h, E - B_b - \epsilon)}{\int_{k_b V_b}^{E - B_b - \delta} \epsilon \sigma_b(\epsilon) \omega(p - A_b, h, E - B_b - \epsilon) d\epsilon} \quad (16)$$

The directional cosine $\mu = \cos\theta$ of the particle emitted with the kinetic energy ϵ is selected according to the probability distribution:

$$PA(\mu) = \frac{P(\mu)}{\int_{-1}^1 P(\mu) d\mu} \quad (17)$$

where $P(\mu)$ is given phenomenologically in terms of Legendre polynomials as (21)

$$P(\mu) = \sum_{l=0,2,4,6} b_l(\epsilon) P_l(\mu) , \quad (18)$$

where

$$\begin{aligned} b_0 &= 1, \\ b_l &= (2l+1) / \{1 + \exp[A_l(B_l - \epsilon)]\}, \\ A_l &= 0.036 + 0.0039 / [l(l+1)], \\ B_l &= 92 - 90 / l(l+1). \end{aligned}$$

The integration of the denominator in Eq. (17) can be performed analytically, giving the expression:

$$PA(\mu) = (C_1 + C_2\mu^2 + C_3\mu^4 + C_4\mu^6) / B , \quad (19)$$

where

$$\begin{aligned} C_1 &= b_0(\epsilon) - \frac{1}{2}b_2(\epsilon) + \frac{3}{8}b_4(\epsilon) - \frac{5}{16}b_6(\epsilon) , \\ C_2 &= \frac{3}{2}b_2(\epsilon) - \frac{30}{8}b_4(\epsilon) + \frac{105}{16}b_6(\epsilon) , \\ C_3 &= \frac{35}{8}b_2(\epsilon) - \frac{315}{16}b_6(\epsilon) , \\ C_4 &= \frac{231}{16}b_6(\epsilon) , \\ B &= 2b_0(\epsilon) - \frac{1}{2}b_4(\epsilon) . \end{aligned}$$

We neglected factors containing an angular momentum of nucleus, the effect of which is expected to be minor. (21)

The angle θ in μ is the value determined with respect to the direction $\vec{\Omega}$ of the incident particle, as shown in Fig. 3, i.e., $\mu = \vec{\Omega} \cdot \vec{\Omega}'$. In a coordinate system with the z axis chosen in the direction of $\vec{\Omega}$, $\vec{\Omega}'$ can be expressed as follows;

$$\vec{\Omega}' = \alpha \vec{l} + \beta \vec{m} + \mu \vec{n} , \quad (20)$$

where \vec{l} , \vec{m} and \vec{n} are unit vectors such as

$$\vec{n} // \vec{\Omega}, \vec{l} \perp \vec{m} \perp \vec{n}$$

and α and β are given by

$$\alpha = \cos 2\pi r, \quad r = \text{uniform random number in } [0,1],$$

$$\beta = \sqrt{1 - \alpha^2 - \mu^2}$$

on the assumption of azimuthal symmetry. In order to carry the calculation on to the inter-nuclear cascades of the emitted particles we need the components of $\vec{\Omega}'$ in the (x,y,z) coordinate system, which is expressed as

$$\vec{\Omega}' = \alpha' \vec{i} + \beta' \vec{j} + \mu' \vec{k}, \quad (21)$$

where \vec{i} , \vec{j} and \vec{k} are unit vectors in the directions of x, y and z axes, respectively. The transformation from (α, β, μ) to (α', β', μ') can be done by utilizing the algorithms used in the subroutines such as DATAO, DATAHI, PCOL and GETRIG in the NMTC code.

The residual nucleus after the emission of particle b is defined by

$$A' = A - A_b, \quad Z' = Z - Z_b, \quad E' = E - B_b - \epsilon. \quad (22)$$

4.2 Residual Interaction Transition Probabilities

When no particle emissions occur but the preequilibrium state has not relaxed to the compound state yet, the exciton state changes through residual interaction transitions characterized by the phenomenologically assumed conditions: (12), (17)

$$P_0 - h_0 = p - h = \text{const.}, \quad (23)$$

$$\Delta p = \Delta h = -1 \text{ or } 0 \text{ or } 1.$$

Transition probabilities corresponding to these condition are given as follows;

$$\begin{aligned} P(p, h \rightarrow p-1, h-1) &= \lambda_- / \lambda, \\ P(p, h \rightarrow p, h) &= \lambda_0 / \lambda, \\ P(p, h \rightarrow p+1, h+1) &= \lambda_+ / \lambda, \end{aligned} \quad (24)$$

where $\lambda = \lambda_- + \lambda_0 + \lambda_+$.

All of the transition rates have the general form, for example, ⁽¹⁷⁾

$$\lambda_+ = \lambda_+(p,h,E) = (2\pi/\hbar)M(p)\omega_+(p,h,E) , \quad (25)$$

where M^2 is the mean square of two body interaction matrix element and ω_+ is the density of accessible states.

The nucleus is imagined to pass sequentially through exciton configuration of increasing complexity with the probability λ_+/λ dominant over the probability λ_-/λ until the compound state specified by $n=n_{eq}$ is reached, when λ_+/λ becomes nearly equal to λ_-/λ . Speaking in more detail, there are several kinds of transitions. For example, $\lambda_+^{(ub)}$ (p,h,E) is the average rate for creating a particle-hole pair in the transition from an unbound state specified by (p,h) to a bound state (p+1,h+1). Similarly, the rates $\lambda_+^{(uu)}$, $\lambda_+^{(bu)}$, $\lambda_+^{(bb)}$, $\lambda_0^{(ub)}$, $\lambda_0^{(bu)}$, $\lambda_-^{(ub)}$ and $\lambda_-^{(bu)}$ can be defined, ⁽¹⁷⁾ which have also the general form given by Eq. (25). As easily seen, the $\lambda_0^{(bb)}$ and $\lambda_0^{(uu)}$ are meaningless physically. The rates $\lambda_-^{(bb)}$ and $\lambda_-^{(uu)}$ are assumed to be negligible.

Since the rates are used only as the ratios, as shown in Eq. (24) and the factor $2\pi M^2(p)/h$ is common to all of them, it is not used in the later calculations. We need only the state densities in evaluating the probabilities given by Eq. (24). Thus we use the relations:

$$\begin{aligned} \lambda_- &\propto \omega_-^{(ub)} + \omega_-^{(bu)} , \\ \lambda_0 &\propto \omega_0^{(ub)} + \omega_0^{(bu)} , \\ \lambda &\propto \omega_+^{(uu)} + \omega_+^{(ub)} + \omega_+^{(bu)} + \omega_+^{(bb)} . \end{aligned} \quad (26)$$

The detailed expressions of ω 's are given in Appendix.

5. Summary and discussions

A proposal has been made on the method of incorporating the process of particle emissions from the preequilibrium state into the Monte Carlo simulation calculations of nuclear spallation reactions. Two conditions have been presented for making transitions from the intranuclear cascade stage to the preequilibrium decay stage and from the preequilibrium to compound decay stage. The one is determined by the number of particles, histories of which have been terminated during the cascade. The other is

All of the transition rates have the general form, for example, ⁽¹⁷⁾

$$\lambda_+ = \lambda_+(p, h, E) = (2\pi/\hbar)M(p)\omega_+(p, h, E) , \quad (25)$$

where M^2 is the mean square of two body interaction matrix element and ω_+ is the density of accessible states.

The nucleus is imagined to pass sequentially through exciton configuration of increasing complexity with the probability λ_+/λ dominant over the probability λ_-/λ until the compound state specified by $n=n_{eq}$ is reached, when λ_+/λ becomes nearly equal to λ_-/λ . Speaking in more detail, there are several kinds of transitions. For example, $\lambda_+^{(ub)}(p, h, E)$ is the average rate for creating a particle-hole pair in the transition from an unbound state specified by (p, h) to a bound state $(p+1, h+1)$. Similarly, the rates $\lambda_+^{(uu)}$, $\lambda_+^{(bu)}$, $\lambda_+^{(bb)}$, $\lambda_0^{(ub)}$, $\lambda_0^{(bu)}$, $\lambda_-^{(ub)}$ and $\lambda_-^{(bu)}$ can be defined, ⁽¹⁷⁾ which have also the general form given by Eq. (25). As easily seen, the $\lambda_0^{(bb)}$ and $\lambda_0^{(uu)}$ are meaningless physically. The rates $\lambda_-^{(bb)}$ and $\lambda_-^{(uu)}$ are assumed to be negligible.

Since the rates are used only as the ratios, as shown in Eq. (24) and the factor $2\pi M^2(p)/h$ is common to all of them, it is not used in the later calculations. We need only the state densities in evaluating the probabilities given by Eq. (24). Thus we use the relations:

$$\begin{aligned} \lambda_- &\propto \omega_-^{(ub)} + \omega_-^{(bu)} , \\ \lambda_0 &\propto \omega_0^{(ub)} + \omega_0^{(bu)} , \\ \lambda_+ &\propto \omega_+^{(uu)} + \omega_+^{(ub)} + \omega_+^{(bu)} + \omega_+^{(bb)} . \end{aligned} \quad (26)$$

The detailed expressions of ω 's are given in Appendix.

5. Summary and discussions

A proposal has been made on the method of incorporating the process of particle emissions from the preequilibrium state into the Monte Carlo simulation calculations of nuclear spallation reactions. Two conditions have been presented for making transitions from the intranuclear cascade stage to the preequilibrium decay stage and from the preequilibrium to compound decay stage. The one is determined by the number of particles, histories of which have been terminated during the cascade. The other is

the effective number of excitons reaching equilibrium. Applicability of the present algorithm should be checked by performing the extensive numerical calculations and making careful comparisons between their results and available experimental data. These are our next work.

A problem remains not having mentioned yet, which is the integral in Eq. (14). It is possible to perform its integration analytically, but it is very tedious. Moreover, final expressions are not only complicated but very lengthy. Hence it seems better to use a numerical integration method in order to avoid any undesired errors apt to sneak in during the analytical integration and programming.

References

- (1) Coleman, W.A., Armstrong, T.W.: "The Nucleon-Meson Transport Code NMTC," ORNL-4606 (1970).
Chandler, K.C., Armstrong, T.W.: "Operating Instructions for the High Energy Nucleon-Meson Transport Code HETC," ORNL-4744 (1972).
Fission processes are not incorporated in these original versions.
- (2) Takahashi, T.: "Fission Reaction in High Energy Cascade," BNL-NCS-51245 (1984); Nucl. Sci. Eng., 87, 432 (1984).
- (3) Atchison, F.: "Spallation and Fission in Heavy Metal Nuclei under Medium Energy Proton Bombardment," Jü1-Conf-34 (1980);
"A Theoretical Study of a Target Reflector and Moderator Assembly for SNS," RL-81-006 (1981).
- (4) Nakahara, Y.: "Studies on High Energy Spallation and Fission Reactions," Proc. ICANS-IV, KENS-Report (1981).
- (5) Nakahara, Y., Tsutsui, T.: NMTC/JAERI: "A Simulation Code System for High Energy Nuclear Reactions and Nucleon-Meson Transport Processes," JAERI-M 82-198 (1982) (in Japanese).
- (6) Armstrong, T.W., Cloth, P., Filges, D., Neef, R.D.: "Theoretical Target Physics Studies for the SNQ Spallation Neutron Source," Jü1-Spez-196 (1983).
- (7) Moeller, E., Nemes, M.C., Gross, D.H.E.: Nucl. Phys., A433, 671 (1985).
- (8) Campi, X., Desbois, J., Lipparini, E.: Nucl. Phys., A428, 327c (1984).

the effective number of excitons reaching equilibrium. Applicability of the present algorithm should be checked by performing the extensive numerical calculations and making careful comparisons between their results and available experimental data. These are our next work.

A problem remains not having mentioned yet, which is the integral in Eq. (14). It is possible to perform its integration analytically, but it is very tedious. Moreover, final expressions are not only complicated but very lengthy. Hence it seems better to use a numerical integration method in order to avoid any undesired errors apt to sneak in during the analytical integration and programming.

References

- (1) Coleman, W.A., Armstrong, T.W.: "The Nucleon-Meson Transport Code NMTC," ORNL-4606 (1970).
Chandler, K.C., Armstrong, T.W.: "Operating Instructions for the High Energy Nucleon-Meson Transport Code HETC," ORNL-4744 (1972).
Fission processes are not incorporated in these original versions.
- (2) Takahashi, T.: "Fission Reaction in High Energy Cascade," BNL-NCS-51245 (1984); Nucl. Sci. Eng., 87, 432 (1984).
- (3) Atchison, F.: "Spallation and Fission in Heavy Metal Nuclei under Medium Energy Proton Bombardment," Jü1-Conf-34 (1980);
"A Theoretical Study of a Target Reflector and Moderator Assembly for SNS," RL-81-006 (1981).
- (4) Nakahara, Y.: "Studies on High Energy Spallation and Fission Reactions," Proc. ICANS-IV, KENS-Report (1981).
- (5) Nakahara, Y., Tsutsui, T.: NMTC/JAERI: "A Simulation Code System for High Energy Nuclear Reactions and Nucleon-Meson Transport Processes," JAERI-M 82-198 (1982) (in Japanese).
- (6) Armstrong, T.W., Cloth, P., Filges, D., Neef, R.D.: "Theoretical Target Physics Studies for the SNQ Spallation Neutron Source," Jü1-Spez-196 (1983).
- (7) Moeller, E., Nemes, M.C., Gross, D.H.E.: Nucl. Phys., A433, 671 (1985).
- (8) Campi, X., Desbois, J., Lipparini, E.: Nucl. Phys., A428, 327c (1984).

- (9) Lopez, J.A., Siemens, P.J.: Nucl. Phys., A431, 728 (1984).
- (10) Aichelin, J., Huefner, J.: Phys. Lett., 136B, 15 (1984).
- (11) Griffin, J.J.: Phys. Rev. Lett., 17, 4-8 (19866).
- (12) Blann, M.: "Preequilibrium Decay," Ann. Rev. Nucl. Sci. vol. 25, 123-166 (1975).
- (13) Hodgson, P.E.: "Pre-equilibrium Processes in Nuclear Reactions," Heavy Ion Collisions, p.220-247, Springer (1982).
- (14) Iwamoto, A., Harada, K.: Nucl. Phys., A417, 472 (1984).
- (15) Tsukada, K., Nakahara, Y.: Atomkernenergie Kerntech., 44, 186 (1984).
- (16) Gudima, K.K., Mashnik, S.G., Toneev, V.D.: Nucl. Phys. A401, 329 (1983).
- (17) Kalbach, C.: PRECO-D2: "Program for Calculating Preequilibrium and Direct Reaction Double Differential Cross Sections," LA-10248-MS (1985).
- (18) Bertini, H.W.: "Monte Carlo Calculations on Intranuclear Cascade," ORNL-3383 (1963).
- (19) Dresner, L.: "EVAP-A Fortran Program for Calculating the Evaporation of Various Particles from Excited Compound Nuclei," ORNL-TM-196 (1962).
- (20) For example; Iwamoto, A., Harada, K.: Phys. Rev. C, 26, 1821 (1982).
- (21) Kalbach, C.: Phys. Rev. C, 23, 112 (1981).

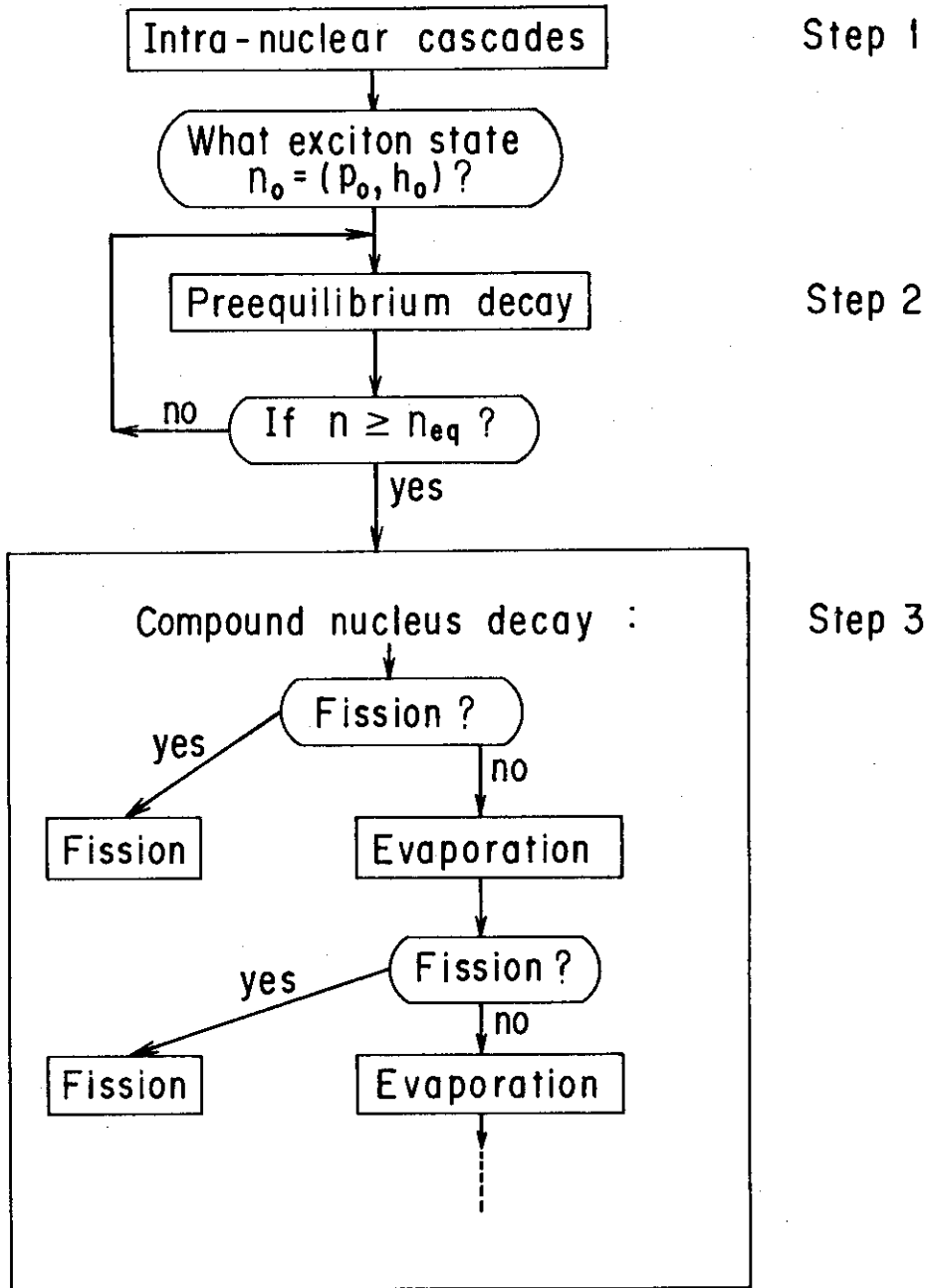


Fig. 1 Scheme of the three step method

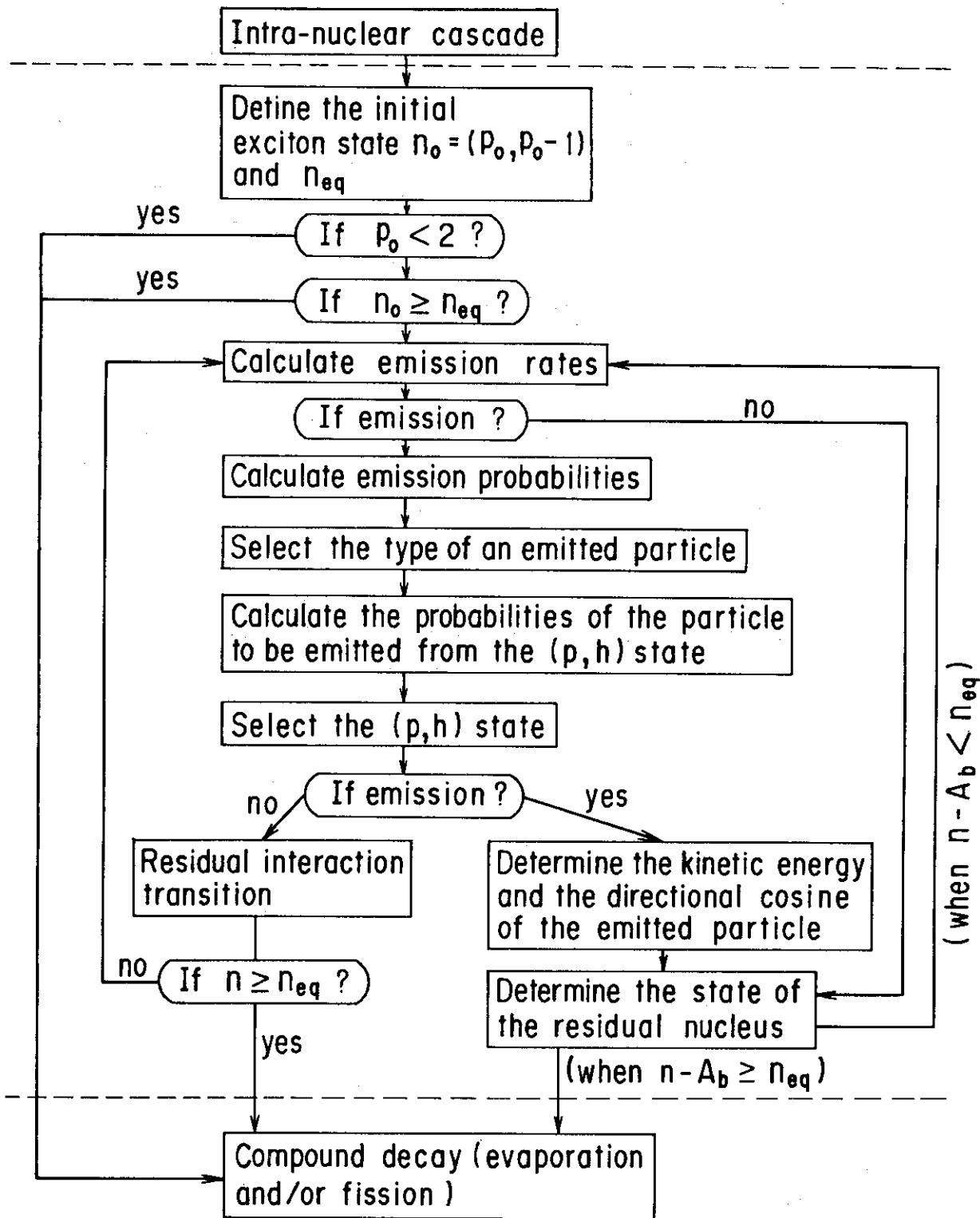


Fig. 2 Flow of the preequilibrium decay calculation

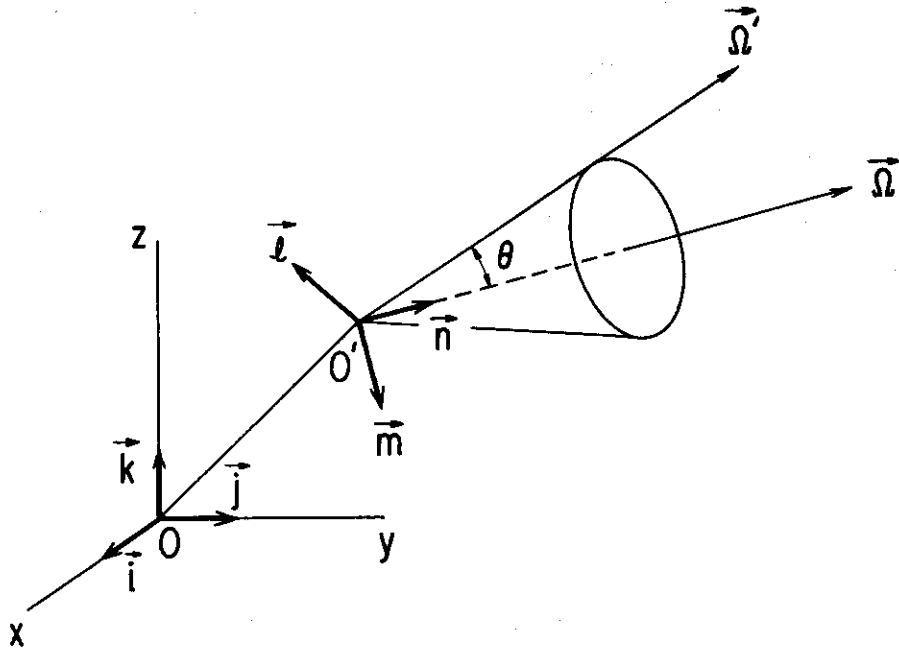


Fig. 3 Angle of particle emission

APPENDIX: STATE DENSITIES FOR THE TWO BODY INTERACTIONS

We use the same expressions of state densities as those used by Kalbach⁽¹⁷⁾. Before writing them, it seems better to make definitions of some quantities to be used in them.

Effective single particle state densities, g_u and g_p , for the unbound particle and the remaining degrees of freedom:

$$g_u(p) = \begin{cases} g_0 \left\{ \frac{p-1}{n-1} \left[\frac{V+(E-S)/n}{V} \right]^{\frac{1}{2}} + \frac{h}{n-1} \left[\frac{V-(E-S)/n}{V} \right]^{\frac{1}{2}} \right\} & \text{for } h \leq 2, \\ g_0, & \text{for } h > 2 \end{cases} \quad (\text{A1})$$

$$g_p(p) = \begin{cases} g_0 \left[\frac{V+S+(E-S)/n}{V} \right]^{\frac{1}{2}}, & \text{for } h \leq 2, \\ \frac{1}{g_0} \left[\frac{V+S}{V} \right]^{\frac{1}{2}}, & \text{for } h > 2, \end{cases} \quad (\text{A2})$$

where S is the separation energy equal to the binding energy for neutrons and the binding energy plus the Coulomb barrier for charged particles.

Effective total single particle state density g_a :

$$g_a(p+1) = \begin{cases} \frac{n-1}{n} g_u(p+1) + \frac{1}{n} g_p(p+1), & \text{for } h \leq 1, \\ g_0 & \text{for } h > 1. \end{cases} \quad (\text{A3})$$

The fraction of unbound states which have more than one unbound particle $m(p)$:

$$m(p) = \frac{\sum_{i=2}^p \sum_{j=0}^h (-1)^{i+j} \binom{p}{i} \binom{h}{j} \mathbb{H} (E-iS-jV) (E-iS-jV)^{n-1}}{\sum_{i=1}^p \sum_{j=0}^h (-1)^{i+j+1} \binom{p}{i} \binom{h}{j} \mathbb{H} (E-iS-jV) (E-iS-jV)^{n-1}}, \quad (\text{A4})$$

for $h \leq 2$, while for $h > 2$ only $j=0$ is to be considered.

The correction factor $f_1(p)$ for taking into consideration of the finite well depth:

$$f_1(p) = \frac{1}{p} \sum_{i=1}^p \sum_{j=0}^h (-1)^{i+j+1} \binom{p}{i} \binom{h}{j} \left(\frac{E-iS-jV}{E-S} \right)^{n-1} \mathbb{H}(E-iS-jV) \quad (\text{A5})$$

Miscellaneous quantities:

$$A_{i,o}(p,h) = \frac{1}{2g_o} [p_m^2 + (p_m - i)^2] - \frac{1}{4g_o} [p - i]^2 + h^2 + n - i, \quad (\text{A6})$$

$$X_i(p) = [E - A_{i,o}(p,h) - iS] \mathbb{H}[E - A_{i,o}(p,h) - iS], \quad (\text{A7})$$

$$f_+(p) = \begin{cases} 1 - \left(\frac{E-S-V}{E-S} \right)^{n-1} \mathbb{H}(E-S-V) - \frac{1}{2} \left(\frac{E-2S}{E-S} \right)^{n-1} \mathbb{H}(E-2S) \\ \quad + \frac{1}{2} \left(\frac{E-2S-V}{E-S} \right)^{n-1} \mathbb{H}(E-2S-V), \\ \quad \text{for } h \leq 2, \\ \\ 1 - \frac{1}{2} \left(\frac{E-2S}{E-S} \right)^{n-1} \mathbb{H}(E-2S), \\ \quad \text{for } h > 2. \end{cases} \quad (\text{A8})$$

$$f_o(p) = 1 - \frac{1}{2} \left(\frac{E-2S}{E-S} \right)^{n-1} \mathbb{H}(E-2S). \quad (\text{A9})$$

$$f_u(p) = \frac{2f_1(p) m(p)}{p-1} \left(\frac{E-S}{E-2S} \right)^{n-1} \mathbb{H}(E-2S). \quad (\text{A10})$$

$$G_1 = \text{Max}(E-V, 0). \quad (\text{A11})$$

$$G_2 = \text{Max}(E-V-S, 0). \quad (\text{A12})$$

$$g_h = g_o [(V-S)/V]^{\frac{1}{2}}. \quad (\text{A13})$$

In equations given above, \mathbb{H} is the Heaviside function.

In terms of these quantities, the state densities for the two body interactions are given as follows;

$$\omega_+^{(uu)}(p, h, E) = \frac{g_a(p+1)g_u^2(p+1)}{2n} \frac{X_1^{n+1}(p+1) \left[\frac{1}{n} f_+(p+1) + \frac{n-1}{n} f(p+1) \right]}{X_1^{n-1}(p)} + \frac{m(p)}{1-m(p)} \omega_+^{(ub)}(p, h, E), \quad (A14)$$

$$\omega_+^{(ub)}(p, h, E) = \frac{1-m(p)}{2n(n+1)} \left\{ g^3(p+1)f(p+1) \left[\frac{n^2}{2} [X_0(p+1) - X(p)]^2 + \frac{n}{2} [X_0^2(p+1) - X_1^2(p)] + X_0(p+1)X_1(p) \right] 2g_p(p+1)g_u^2(p+1)f_+(p+1) \frac{X_1^{n+1}(p+1)}{X_1^{n-1}(p)} \right\}, \quad (A15)$$

$$\omega_+^{(bu)}(p, h, E) = \frac{g_p(p+1)g_u^2(p+1)h}{X_0^{n-1}(p)f(p) - pX_1^{n-1}(p)f_1(p)} \left\{ \frac{X_1^{n+1}(p+1) - pX_2^{n+1}(p+1)}{2n(n+1)} - \frac{1}{4n(n+1)} \left[G_1^{n-1} [n(n-1)G_1^2 - 2(n+1)(n-1)G_1X_1(p+1) + n(n+1)X_1^2(p+1)] - pG_2^{n-1} [n(n-1)G_2^2 - 2(n+1)(n-1)G_2X_2(p+1) + n(n+1)X_2^2(p+1)] \right] \right\}, \quad (A16)$$

$$\omega_+^{(bb)}(p, h, E) = \frac{1}{2n(n+1)} \frac{1}{X_0^{n-1}(p)f(p) - pX_1^{n-1}(p)f_1(p)} \left\{ ng^3(p+1)X_0^{n+1}(p+1)f(p+1) - p(n-1)g_u^3(p+1)X_1^{n+1}(p+1)f_1(p+1) - pg^3(p+1)X_1^{n-1}(p)f_1(p) \left[\frac{n^2}{2} [X_0(p+1) - X_1(p)]^2 + \frac{n}{2} [X_0^2(p+1) - X_1^2(p)] + X_0(p+1)X_1(p) \right] \right\} - \omega_+^{(bu)}(p, h, E), \quad (A17)$$

$$\omega_0^{(ub)}(p, h, E) = \frac{[1-m(p)]g^2}{n} \left[\frac{p+2h-1}{2} n[X_0(p) - X_1(p)] f(p) + (p-1) X_1(p)] f(p) - 2f_0(p) \right], \quad (A18)$$

$$\omega_0^{(bu)}(p, h, E) = \frac{g_u(p) g_p(p)}{2n} \frac{1}{X_0^{n-1}(p) f(p) - pX_1^{n-1}(p) f_1(p)} \left[(p+2h-1)\{2X_1^n(p) + n[X_1(p) - X_2(p)]X_1^{n-1}(p)\} f(p) - (p-1)(p+2h-1)\{2X_2^n(p) + n[X_1(p) - X_2(p)] X_2^{n-1}(p)\} f_1(p) - 4(n-1) X_1^n(p) f_1(p) + 4(p-1)(n-2) X_2^n(p) f_2(p) \right] \quad (A19)$$

$$\omega_-^{(ub)}(p, h, E) = [1-m(p)] g_h h(h-1)/2, \quad (A20)$$

$$\omega_-^{(bu)}(p, h, E) = \frac{g_q(p-1) hp(p-1)}{4} \frac{1}{X_0^{n-1}(p) f(p) - pX_1^{n-1}(p) f_1(p)} \left\{ X_1^{n-3}(p-1) [(n-2)(n-3)X_1^2(p-1) - 2(n-1)(n-3)X_1(p-1) X_0(p) + (n-1)(n-2)X_1^2(p)] f(p) - (p-2)X_2^{n-3}(p-1) [(n-2)(n-3)X_2^2(p-1) - 2(n-1)(n-3)X_2(p-1) X_1(p) + (n-1)(n-2)X_1^2(p)] f_1(p) - 4[X_1^{n-1}(p) f_1(p) - (p-2)X_2^{n-1}(p) f_u(p)] \right\}. \quad (A21)$$

In equations given above, $g(p)$ and $f(p)$ are those defined by Eqs. (5) and (6), respectively.