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An improved numerical method to compute neutron/gamma deexcitation cascades starting from a high spin state

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ABSTRACT

Numerous nuclear processes involve the deexcitation of a compound nucleus through the emission of several neutrons, gamma-rays and/or conversion electrons. The characteristics of such a deexcitation are commonly derived from a total statistical framework often called "Hauser–Feshbach" method. In this work, we highlight a numerical limitation of this kind of method in the case of the deexcitation of a high spin initial state. To circumvent this issue, an improved technique called the Fluctuating Structure Properties (FSP) method is presented. Two FSP algorithms are derived and benchmarked on the calculation of the total radiative width for a thermal neutron capture on ^{238}U. We compare the standard method with these FSP algorithms for the prediction of particle multiplicities in the deexcitation of a high spin level of ^{143}Ba. The gamma multiplicity turns out to be very sensitive to the numerical method. The bias between the two techniques can reach 1.5 γ/cascade. Finally, the uncertainty of these calculations coming from the lack of knowledge on nuclear structure is estimated via the FSP method.

1. Introduction

Numerous nuclear reactions involve the formation of an excited compound nucleus. These nuclei may then lose their energy through the emission of several neutrons, gamma-rays and possibly conversion electrons. Given the initial bounded or virtual level $(EJ^{\pi})_i$ of such a nucleus, a standard problem resides in the determination of a few average observables characterizing the deexcitation process. Such calculations have a broad field of applications including namely the prediction of:

- The gamma multiplicities and spectra in capture reactions at low incident neutron energy [1,2]. Beyond the prediction of gamma observables, these calculations are also required to infer indirectly the spin of the resonances [3,4], or the branching ratio of some isomeric states [5].
- The prompt neutron and gamma emissions from fission fragments [6–8], as well as their spin distribution [9–14].
- The spin distribution of the compound nuclei involved in surrogate reaction studies [15].

These phenomena have been widely calculated using one statistical technique. For every nuclei involved in the deexcitation cascade, experimental data provides the decay structure at low energies. The high part of the excitation energy scale is discretized in small intervals (bins). Inside these intervals, all the structure properties are considered constant equal to an averaged value. The probability of a transition between two bins can then be determined. Based on these probabilities, a deterministic or Monte Carlo technique is applied to compute an average observable over all possible deexcitation cascades. This statistical technique is often referred as a Hauser–Feshbach method [16]. However, in this particular context, no entry channel is involved in the calculation. Therefore this method does not take into account any correlations between channels. In this paper, we refer to this method as the Average Structure Properties (ASP) method. Indeed, the structure properties of the nuclei involved are averaged over small energy bins.

The ASP method has been successfully used in many applications. However, we discovered that a numerical issue rises in the case of a specific application: the calculation of the neutron/gamma deexcitation from nuclei with high spin values. To circumvent this drawback, we propose another method that will be referred as the Fluctuating Structure Properties (FSP) method. This method consists in a generalization of the work of Becvar [17] on gamma/electron cascades calculation. We will show that this FSP

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method yields a more physical behavior when applied to nuclei with high spin values. Moreover, it also estimates the uncertainties coming from our lack of knowledge on the nuclear structure.

The present article is organized as follows. First of all, the Section 2 presents briefly the standard ASP deexcitation algorithm. We emphasize the numerical issue of the ASP method by calculating the neutron emission probability P_n for a range of initial excited levels in a ^{143}Ba compound nucleus. This last isotope was chosen because it is a highly yielded primary fragment in the spontaneous fission of ^{252}Cf (sf) [18]. The Section 3 is devoted to the new FSP method. After a complete description of the principle, two algorithms are derived. The neutron emission probability P_n obtained with these algorithms for ^{143}Ba are highlighted in perspective of the results coming from the ASP method. Finally, the Section 4 compares the three algorithms (one for ASP and two for FSP). We test the consistency of our implementation by calculating the total radiative width of an excited state of ^{238}U (a standard in nuclear data evaluations). Then we discuss the neutron and gamma multiplicities computed with the three algorithms for a ^{143}Ba deexcitation process.

2. The average structure properties (ASP) method

2.1. Description and notations

Let us consider a nucleus in an initial level $(E, J, \pi)_i$, where E stands for the excitation energy, and J^π are the quantum numbers associated with the total angular momentum and the parity. We assume that this initial level is not stable and that the nucleus will deexcite through the emission of several neutrons, gamma-rays and/or conversion electrons. Our goal is to calculate the average of an observable Q (*e.g.* a particle multiplicity) over all the possible cascades:

$$Q_{\mathrm{ASP}} = \sum_c Q(c)p(c) \tag{1}$$

where $Q(c)$ is the value of Q given the cascade c and $p(c)$ is the probability that the cascade c happens. Given the probabilities $p(c)$, both a deterministic or a Monte Carlo numerical method can compute Q_{ASP}. In this work, a large amount of cascade events are sampled according to the distribution $p(c)$. Each event increments an estimator of Q_{ASP}.

The probabilities $p(c)$ are drastically dependent on the structure properties of every nuclei involved in the deexcitation process. An exact computation of these probabilities would require:

1. The exact level scheme of every nuclei involved. This level scheme has to be known up to an energy $E_{top}(A)$. For the initial nucleus $E_{top}(A)$ is the initial excitation energy. After each neutron emission, it decreases by the corresponding binding energy:

   $$E_{top}(A-1) = E_{top}(A) - S_n(A).$$

2. The partial widths of every possible transitions from any initial to any final level. These levels may not belong to the same nucleus.

Whereas these properties are not known in such detail for masses $A > 50$, some statistical information is available (e.g. the level density). This incomplete knowledge can be used to approximate the probabilities $p(c)$.

In the ASP method, the level scheme of any nucleus is divided into two energy regions separated by an energy denoted $E_{cut\text{-}off}$. In the low energy range ($E < E_{cut\text{-}off}$), the level scheme consists in the discrete levels provided by an experimental or evaluated data base. In the high energy range ($E > E_{cut\text{-}off}$), the excitation energy scale is divided into bins of an arbitrary width dE. In that region, the nucleus is no more characterized by its excited level but only by its energy bin and its J^π value. In order to clarify the discussion, it is convenient to define a level set noted $[EJ^\pi]$. It corresponds either to the set of J^π levels with an energy in $[E-dE/2; E+dE/2]$, either to a discrete level (E, J, π). We also note $N([EJ^\pi])$ the number of levels contained in the set $[EJ^\pi]$. If the level set actually corresponds to a discrete level, this quantity is equal to one. The ASP method estimates the number of levels $N([EJ^\pi])$ as an average value given by:

$$N([EJ^\pi]) = \begin{cases} \rho(E, J, \pi) \cdot dE & \text{for an energy bin} \\ 1 & \text{for one discrete level} \end{cases} \tag{2}$$

where $\rho(E, J, \pi)$ designates the level density of the nucleus.

The average partial width for a transition $[EJ^\pi]_i$ to $[EJ^\pi]_f$ with the emission of a particle p of energy E_p and characterized by a set α of quantum numbers is expressed as:

$$\Gamma_p([EJ^\pi]_i \to [EJ^\pi]_f, \alpha) = \left\langle \sum_{n_f \in [EJ^\pi]_f} \Gamma_p(n_i \to n_f, \alpha) \right\rangle_{n_i \in [EJ^\pi]_i}. \tag{3}$$

It is obtained by summing the level to level partial widths over final levels and averaging over initial levels. Such a partial width can also be written:

$$\Gamma_p([EJ^\pi]_i \to [EJ^\pi]_f, \alpha) = \bar{\Gamma}_p(E_p, \alpha) \cdot \delta(\alpha, J_i^\pi, J_f^\pi) \cdot N([EJ^\pi]_f). \tag{4}$$

The Kronecker's symbol δ accounts for the selection rules and is evaluated to 1 if the transition is possible and 0 otherwise. The factor $\bar{\Gamma}_p(E_p, \alpha)$ is the average width of the possible transitions. In this model, it is assumed to be independent of $J\pi_i$ and $J\pi_f$. This quantity can be derived from several advanced analytic models [19–21] or as a result of a microscopic calculation [22].

Once all the widths $\Gamma_p([EJ^\pi]_i \to [EJ^\pi]_f, \alpha)$ are determined, the probability of a specific emission from an initial set $[EJ^\pi]_i$ is given by the ratio:

$$p([EJ^\pi]_i \to [EJ^\pi]_f, p, \alpha) = \frac{\Gamma_p([EJ^\pi]_i \to [EJ^\pi]_f, \alpha)}{\Gamma^{\mathrm{tot}}} \tag{5}$$

where Γ^{tot} is the sum of the partial widths over all possible deexcitations from $[EJ^\pi]_i$. The probability $p(c)$ of a deexcitation cascade c can then be written as a product of probabilities calculated with Eq. (5). Eventually, injecting the probability of every possible cascade in Eq. (1) provides the targeted observable Q_{ASP}.

2.2. Implementation details

A Monte Carlo resolution of Eq. (1) based on the ASP method has been implemented in the code FIFRELIN, dedicated to the simulation of the fission fragment deexcitation [23,24]. The description of the structure of the nuclei relies on the RIPL-3 [25] database. In particular, both the energy cutoff ($E_{cut\text{-}off}$) and the discrete levels below this energy are directly taken from RIPL-3. Above $E_{cut\text{-}off}$, the energy scale is divided into bins of 10 keV width. We checked that calculations performed with 5 keV bins lead to the same conclusions.

The total level density used in Eq. (2) is a Composite Gilbert Cameron Model [26]. For each nucleus, three constraints determine the parametrization of the level density:

- The level density is continuous at the matching energy, *i.e.* between the Constant Temperature part (low energies) and the Fermi Gas model part (high energies).
- The derivative of the level density is continuous at the matching energy.
- The number of levels in an energy range $[E_{min}; E_{max}]$ matches the RIPL-3 database. The energies E_{min} and E_{max} are themselves provided by RIPL-3.