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Recent developments in the modeling of (n,γ) reactions with FIFRELIN

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Recent developments in the modeling of (n,γ) reactions with FIFRELIN

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Abstract   Nowadays, the accuracy of experimental results relies more and more on detailed simulations. In the STEREO experiment, the interaction of neutrinos in the liquid scintillator is signed by a n-capture on a Gd atom. The FIFRELIN predictions of the Gd γ-cascades were shown to significantly improve the Data/MC agreement. In the CRAB method, lately proposed to calibrate cryogenic particle detectors at low energy (100 eV), the FIFRELIN cascades of the W and Ge isotopes played a central role in the feasibility study of the method. The FIFRELIN code employs a Monte Carlo Hauser-Feshbach framework based on Bečvár's algorithm. A sample of nuclear level schemes is generated for a specific isotope of interest, taking into account the uncertainties from nuclear structure. In this work, new improvements on the FIRELIN de-excitation process are reported. Angular correlations of γ-rays in the de-excitation process have been implemented in order to provide a more accurate description of the γ-ray cascades. The anisotropy of the γ-rays with respect to the axis of a previously emitted γ-ray is modeled using the angular correlation formalism, which requires as input the spins and multipolarities of the states involved in the FIFRELIN cascade. Furthermore, the simulation of the primary γ-rays emitted from (n,γ) reactions has been updated using the EGAF database.

Keywords   gamma directional correlations, FIFRELIN, neutron-capture

INTRODUCTION

The FIFRELIN [1,2] code has been developed for the evaluation of fission data providing an accurate description of the neutron and gamma properties of the fission process. Recent studies for the STEREO experiment [3], where the modeling of the detector response relies on the de-excitation of ^{156,158}Gd after neutron capture have demonstrated an improved agreement of FIFRELIN with the data, compared to GEANT4 [4]. Furthermore, the FIFRELIN code had a central role in the feasibility study of the CRAB method, which can be used to calibrate cryogenic detectors at the energy scale of 100 eV, a region interesting for light dark matter and neutrino studies [5].

FIFRELIN employs a Monte Carlo Hauser-Feshbach framework based on Bečvár's algorithm devoted to gamma emission [6] and extended to coupled neutron/gamma emission [7]. A sample of nuclear level schemes is generated taking into account the uncertainties from nuclear structure. FIFRELIN accounts for the lower energy part of the level scheme from the RIPL-3 database [8]. For the higher energy part, a combination between known levels and theoretical nuclear models (level densities, spin/parity distributions) is used to account for the unknown part of the true level scheme of the nucleus of interest.

In the present work, we report on the recent developments on the modeling of the de-excitation process in FIFRELIN. The angular correlations between an arbitrary number of subsequent gamma rays have been added, enabling a complete description of the spatial distribution of the emitted gamma-rays. The formal theory of angular correlations is employed, using the statistical tensor formalism [9]. Within this framework, higher order angular correlations, like triple-gamma correlations, are also reproduced. Furthermore, the EGAF database [10] has been used to provide a

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better description of the higher energy part of the de-excitation process. A comparison with the ENSDF [11] shows a remarkable agreement in the high energy part of the spectrum (>4 MeV).
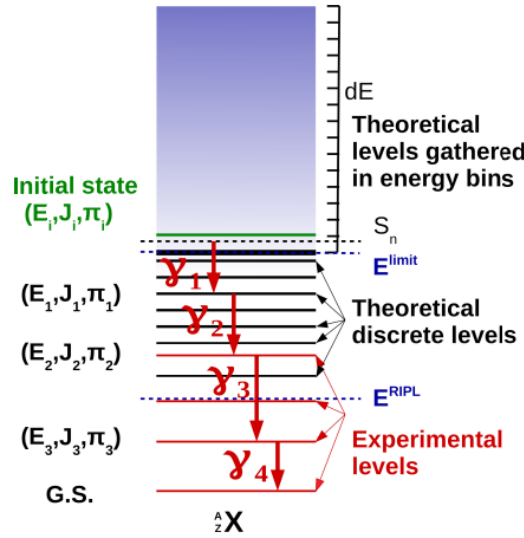

Fig. 1. *[Color Online] Illustration of the γ de-excitation scheme in a cascade with FIFRELIN [3].*

MONTE CARLO SIMULATIONS OF GAMMA DIRECTIONAL CORRELATIONS

A general method of simulating angular distributions and correlations from decaying particles with spin using the density matrix formalism has been presented in [12]. The event generator DECAY4 [13] as well as GEANT4 [4,14] can simulate the effect of directional angular correlations, but there is no detailed documentation or step-by-step mathematical description. Furthermore, they are restricted to radioactive sources [15]. Simulations for double gamma angular correlations have also been made as extensions to GEANT4 [16].

For this work, the cascade of γ-rays starting from an initial state J_0 and ending to a state J_n:

$$J_0 \xrightarrow{\gamma_0} J_1 \xrightarrow{\gamma_1} \dots J_{n-1} \xrightarrow{\gamma_{n-1}} J_n$$

a set of statistical tensors can be calculated, depending on the orientation of the initial state J_0. The set of transitions $\gamma_0, \gamma_1 \dots \gamma_{n-1}$ can be either all observed, or partly unobserved by a detector. If the initial state is randomly oriented, then its statistical tensor is simply given by $\rho_{\lambda q}(J_0) = \delta_{\lambda 0} \delta_{q 0}$ where δ_{ij} is the Kronecker delta, λ is the rank of the statistical tensor and q takes integer values between $-\lambda$ and λ. By knowing the initial-state statistical tensor, all the statistical tensors can subsequently be calculated from a recursive master equation [9, 17]:

$$\rho_{q_f}^{\lambda_f}(J_f) = \sum_{\lambda_i, q_i, \lambda, q} (-1)^{\lambda_i + q_i} \sqrt{2\lambda + 1} \, \rho_{q_i}^{\lambda_i}(J_i) \begin{pmatrix} \lambda_f & \lambda & \lambda_i \\ -q_f & q & q_i \end{pmatrix} A_\lambda^{\lambda_i \lambda_f} \mathfrak{D}_{q_f 0}^{\lambda_f}(\varphi_i, \theta_i, 0)$$

where $\begin{pmatrix} \lambda_f & \lambda & \lambda_i \\ -q_f & q & q_i \end{pmatrix}$ is a Wigner 3j symbol, $A_\lambda^{\lambda_i \lambda_f}$ is a generalized angular distribution coefficient

and $\mathfrak{D}^{\lambda_f}_{q_f 0}(\varphi_i, \theta_i, 0)$ is the Winger D-matrix. The generation of events can now be performed using the probability distribution functions for each gamma ray, going from an initial state J_i to a final state J_f:

$$W(\theta_i, \varphi_i) = \sum (-1)^{\lambda_f + q_f} \sqrt{2\lambda_f + 1} \, \rho^{\lambda_f}_{q_f} A_\lambda \left(L, L', J_i, J_f, \delta\right) \mathfrak{D}^{\lambda_f}_{q_f 0}(\varphi_i, \theta_i, 0)$$

where $A_\lambda\left(L, L', J_i, J_f, \delta\right)$ is the angular distribution coefficient. More details about this method can be found in [18].
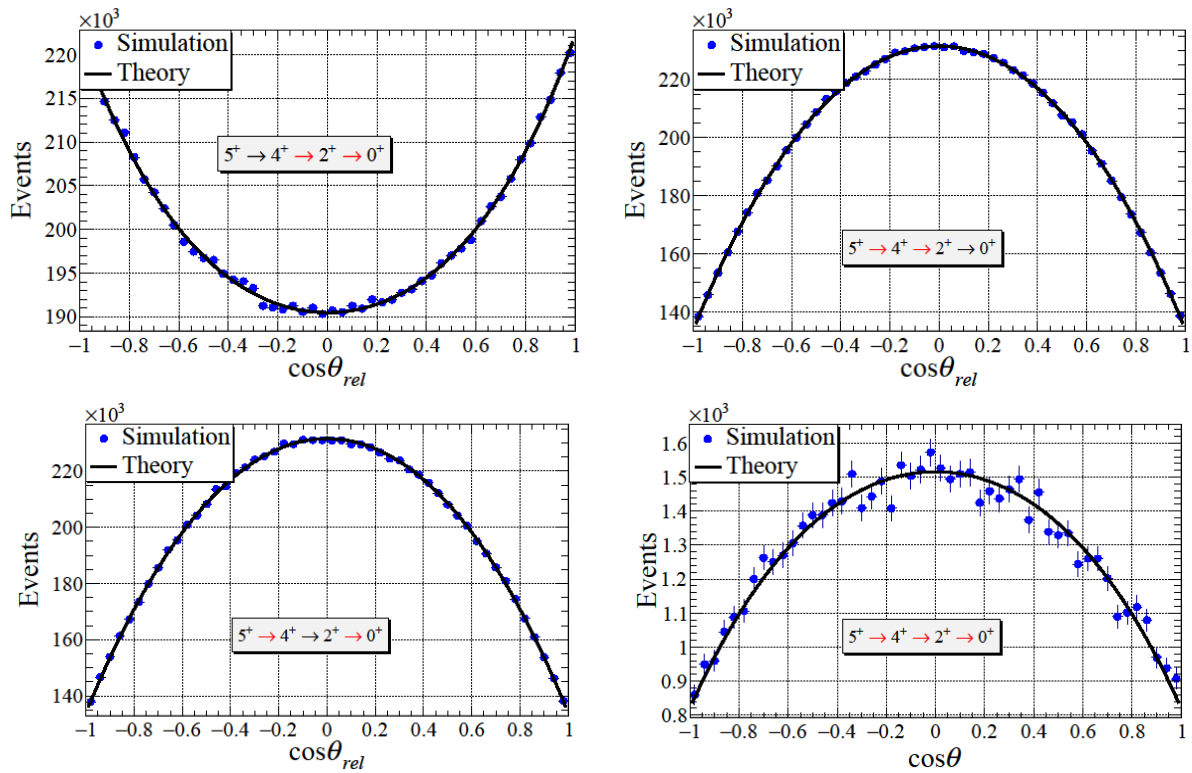

Fig. 2 *Simulation of the triple gamma cascade $5^+ \to 4^+ \to 2^+ \to 0^+$ of ^{110}Cd. The transition $5^+ \to 4^+$ is mixed, with a multipolarity mixing ratio $\delta = -0.42$. The arrows in red indicate the observed transitions.*
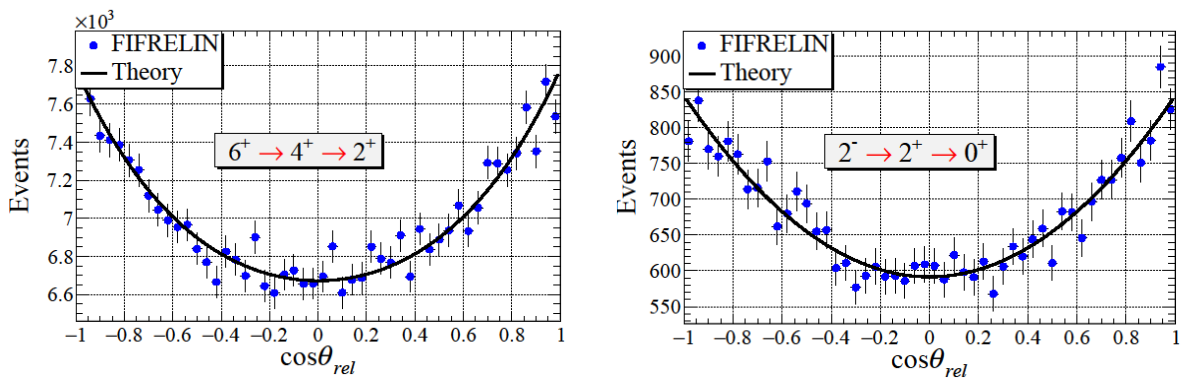

Fig. 3. *Angular correlations in the de-excitation of ^{156}Gd, simulated by FIFRELIN. (a) The angular correlation of the g.s. band cascade $6^+_1 \to 4^+_1 \to 2^+_1$. (b) The angular correlation for the cascade $2^-_2 \to 2^+_3 \to 0^+_{g.s.}$.*
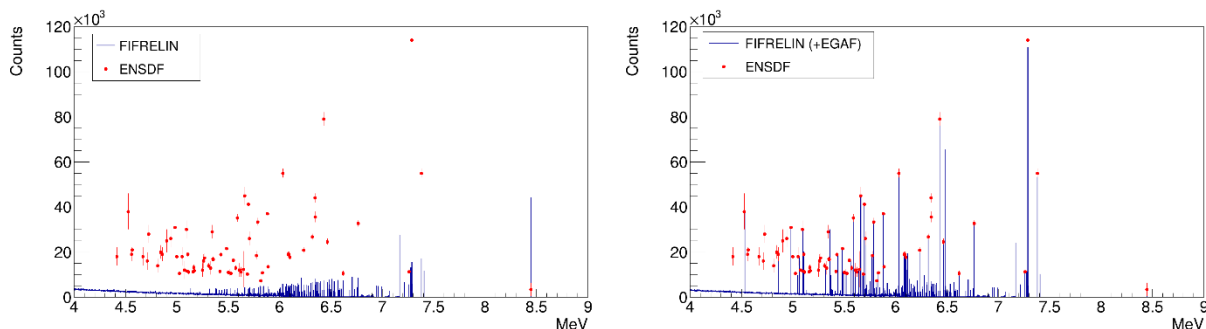
Fig. 4. Comparison of a FIFRELIN simulation using only theoretical models for the description of the primary gamma rays (left) and of a FIFRELIN simulation coupled with the EGAF [database (right). The agreement with ENSDF is significantly improved with the inclusion of transitions from EGAF.

Within the framework of this method, the complete effect of gamma directional correlations is reproduced. Examples of double correlations are shown in Fig. 2 for the case of a triple gamma cascade from the decay of ^{110m}Ag [19]. The correlation between the first and the third gamma is shown on the bottom right panel and, most importantly, a triple gamma angular correlation simulation is demonstrated on the bottom right panel.

This approach was coupled with the FIFRELIN output for the case of the de-excitation of ^{156}Gd after thermal neutron capture. Angular correlations are reproduced in complete agreement with the theoretical calculations. Two cases for this nucleus are shown in Fig. 3.

UTILIZATION OF THE EGAF DATABASE

EGAF (Evaluated Gamma Activation File) [10] is a database of prompt and delayed neutron capture gamma-ray cross sections. The database consists of data acquired from measurements performed with the guided neutron beam at the Budapest reactor, in combination with data from literature.

The implementation of the EGAF database in FIFRELIN for the primary gamma rays has yielded a much better description in the higher energy part of the gamma spectrum. In Fig. 4, a comparison with the ENSDF data is shown among two simulations of FIFRELIN. As illustrated, the inclusion of EGAF database describes very well the transitions at higher excitation energies, in comparison with the use of only theoretical models.

DISCUSSION AND CONCLUSIONS

Recent additions have been applied to the FIFRELIN Monte Carlo Code, improving on the modeling of the nuclear de-excitation after thermal neutron capture. The full effect of angular correlations has been implemented for gamma-rays. The possibility of implementing other types of angular correlations, e.g. conversion electron directional correlations, is under investigation. The present approach, coupled with GEANT4 simulations of detector arrays, could potentially eliminate the need for geometrical corrections, as a direct comparison between the simulation and the data can be made.

The addition of the EGAF database provides a very good description of the higher energy part of the de-excitation spectrum of nuclei, the precise modeling of which can be highly important for

both low- and high-energy physics studies, while highlighting the connection between the two fields in search of new physics.

Acknowledgements

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