DE LA RECHERCHE À L'INDUSTRIE

Modeling nuclear de-excitation with FIFRELIN and applications to neutrino studies

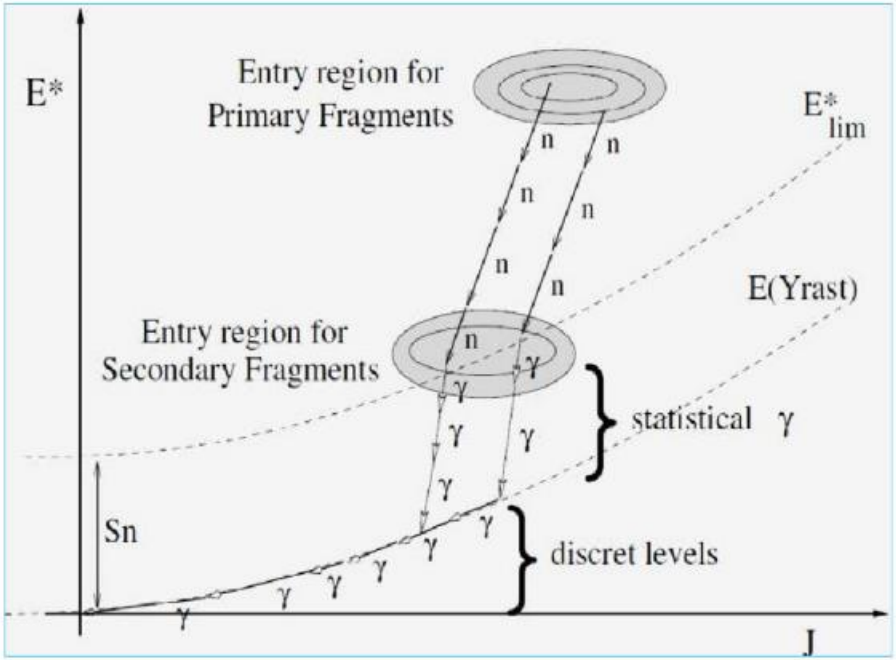
Achment Chalil[1,2]

[1]DRF, IRFU, DPhN, LEARN, CEA Saclay
[2]DES, IRESNE, DER, SPRC, LEPh, CEA Cadarache

IRN Neutrino Meeting - 17 November 2022

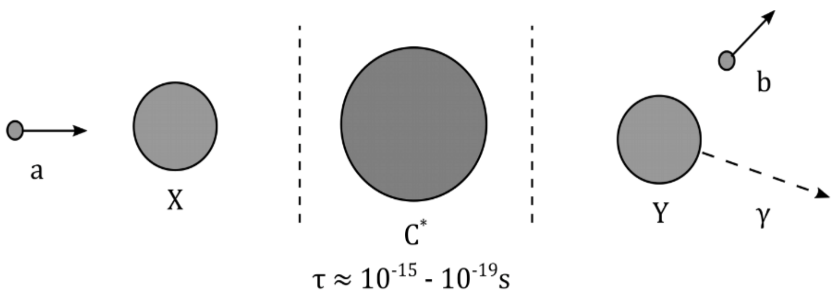
FIssion FRagment Evaporation Leading to an Investigation of Nuclear data (FIFRELIN)

- Developed at CEA Cadarache (LEPh)
- Modeling of fission process
- Reactor Application and Nuclear Data Evaluations
- The latter part of fission can be used to model the de-excitation of every nucleus (decay mode)
- Accurate de-excitation modeling is important for various applications



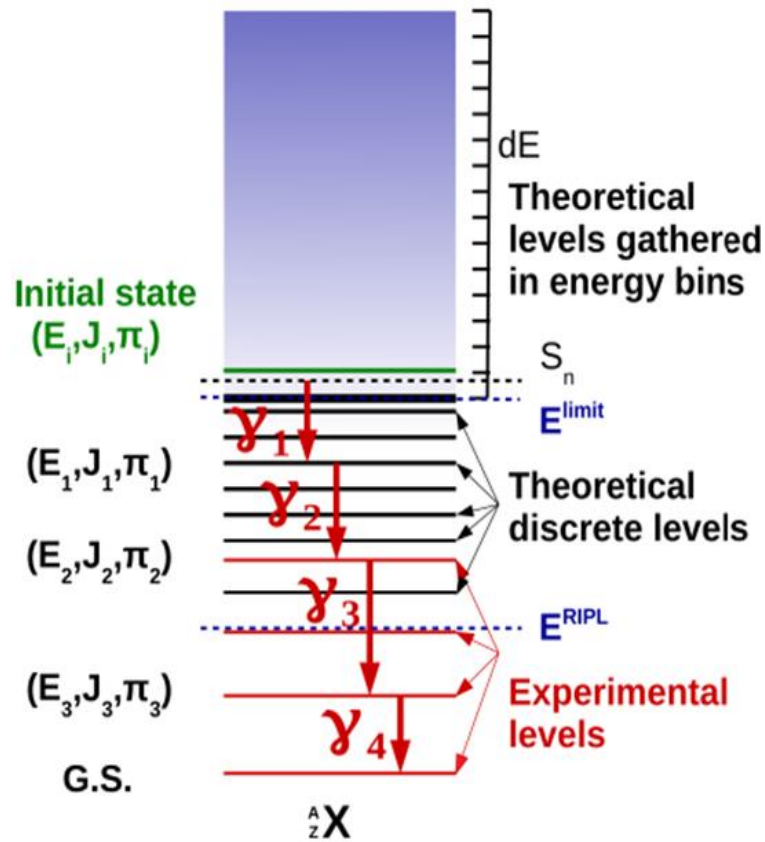
O. Litaize et al. EPJ. A ***51*** *177 (2015)*

Nuclear de-excitation modeling using FIFRELIN



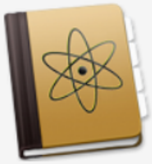
- Nucleus in excited state
  (e.g. after a capture reaction)
- Gamma de-excitation (+conversion electrons)
- Problem: Level schemes are not fully known
- Low-energy part from RIPL3 database
  (evaluated levels from data)
- Theoretical models are used for the higher energy

<u>Focus on missing ingredients:</u>
- Updates on nuclear data
- Accurate description of the directions of the emitted particles



*H. Almazán et al. (STEREO Collaboration) EPJ. A **55** 183 (2019)*

RIPL-3 (Nuclear Reactions)



Reference Input Parameter Library (RIPL-3)

R. Capote, M. Herman, P. Oblozinsky, P.G. Young, S. Goriely, T. Belgya, A.V. Ignatyuk, A.J. Koning, S. Hilaire, V.A. Plujko, M. Avrigeanu, O. Bersillon, M.B. Chadwick, T. Fukahori, Zhigang Ge, Yinlu Han, S. Kailas, J. Kopecky, V.M. Maslov, G. Reffo, M. Sin, E.Sh. Soukhovitskii and P. Talou

Nuclear Data Sheets - Volume 110, Issue 12, December 2009, Pages 3107-3214

RIPL discrete levels database updated in **September 2020** - it contains the correction for +X,.. levels

ENSDF (Nuclear Structure)

Evaluated Nuclear Structure Data File (ENSDF)

ENSDF contains recommended nuclear structure and decay data for all the known nuclides, which are obtained following a critical review of all available experimental data, supplemented with systematic trend studies and theoretical models. ENSDF data include (i) nuclear level properties, such as observation source, energy, half-life, decay modes, spin and parity; (ii) gamma ray energies, intensities, multipolarities, mixing ratios and conversion coefficients; (iii) nuclear radiation energy and intensity as well as radiation-specific data for different radiation types, such as such as gammas, alphas, betas and neutrons. Data for about 220 nuclides are fully evaluated each year; additionally, many datasets are partially updated each year.

Nearly all the evaluation work is supported by the US Nuclear Data Program. The National Nuclear Data Center at Brookhaven National Laboratory is responsible for coordinating the evaluation effort as well as its web and journal dissemination. Most of the recently completed evaluations are published in *Nuclear Data Sheets*, a monthly journal published by Academic Press, a division of Elsevier Science.

For each nuclide, all known experimental data used to deduce nuclear structure information are included. Each type of experiment is presented as a separate dataset. In addition, there is a dataset of "adopted" level and gamma-ray transition properties, which represent the evaluator's determination of the best values for these properties, based on all available experimental data.

As of the most recent update on November 9, 2022, the ENSDF database contains 19683 datasets for 3416 nuclides.

EGAF (Neutron capture)

Evaluated Gamma-ray Activation File (EGAF)

The Evaluated Gamma-ray Activation File (EGAF) has been developed as part of a Coordinated Research Project for the Development of a Database for Prompt Gamma-ray Neutron Activation Analysis sponsored by the International Atomic Energy Agency (IAEA). A file is provided for each isotope containing ENSDF datasets for the Adopted and Budapest PGAA data and the Reedy and Frankle neutron capture data. These data can be viewed with the Isotope Explorer 2.2 ENSDF Viewer.

Development of ENSDF functionality for FIFRELIN

- Not all nuclear data are implemented in RIPL-3 (e.g. multipolarity mixing ratios)
- Need for access ENSDF database and extract the relevant information
- Complicated format but a lot of useful information can be extracted

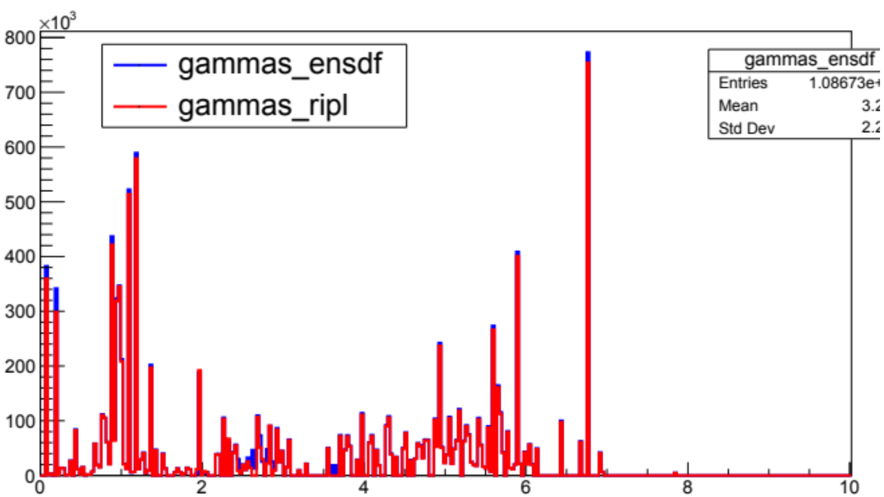
```
235U    L 46.103     8 9/2-              14 PS     AP                        a
235U 2 L FLAG=Z
235U X L XREF=ADFJKN
235U  cL T$from B(E2)=6.7, average of B(E2)=4.834 {I16} in muonic atom,
235U 2cL B(E2)=7.4 {I7} in Coulomb excitation (1957Ne07), and B(E2)=8.0 {I12}
235U 3cL in (d,d'). The approximate value of the half-life is due to the large
235U 4cL uncertainty in the E2 |g-ray mixing ratio (|d=0.14 {I14}).
235U    G 46.21      5  100       M1+E2     0.14     14    5.E1    3
235U 2 G FL=0.0
235U S G LC=40 19$MC=10 6$NC+=3.5 19
235U S G NC=2.7 15$OC=0.6 4$PC=0.12 6$QC=0.0081 4
235U  cG $B(E2)(W.u.)= 839, B(M1)(W.u.)=0.31 18
235U    L 51.6968    11 5/2+             191 PS    5                         B
235U X L XREF=ABDFGIL
235U  cL T$from {+239}Pu |a decay (1970Ho02,1970ToZZ)
235U    G 38.661     2     38.0 8 M1+E2     0.48     3     298     24
235U 2 G FL=13.0339
235U S G LC=219 17$MC=59 5$NC+=20.2 16
235U S G NC=15.9 13$OC=3.7 3$PC=0.62 5$QC=0.01231 24
235U  cG          B(E2)(W.u.)={ 65 {I7}}, B(M1)(W.u.)={ 0.00141 {I7}}
235U    G 51.624     1     100  2 E2                       310
235U 2 G FL=0.0760
235U S G LC=226 4$MC=62.6 9$NC+=21.5 3
235U S G NC=16.97 24$OC=3.89 6$PC=0.630 9$QC=0.001600 23
235U  cG          B(E2)(W.u.)={ 215 {I10}}
235U    L 81.724     4 7/2+                                                  b
```

Part of ENSDF file for ^{235}U

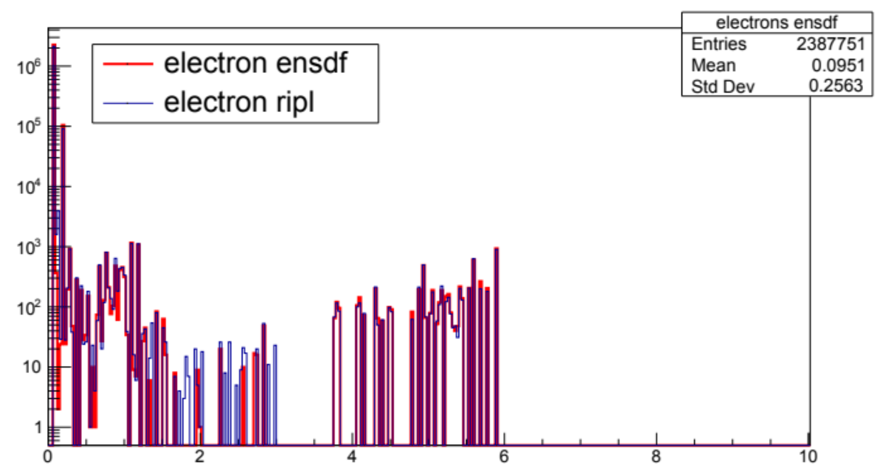
Comparison ENSDF-RIPL3

- Tests on the de-excitation of ^{158}Gd using only experimental levels
- Minor differences between databases but may be needed to be taken into account

Gamma and electron spectra using ENSDF and RIPL3-2021



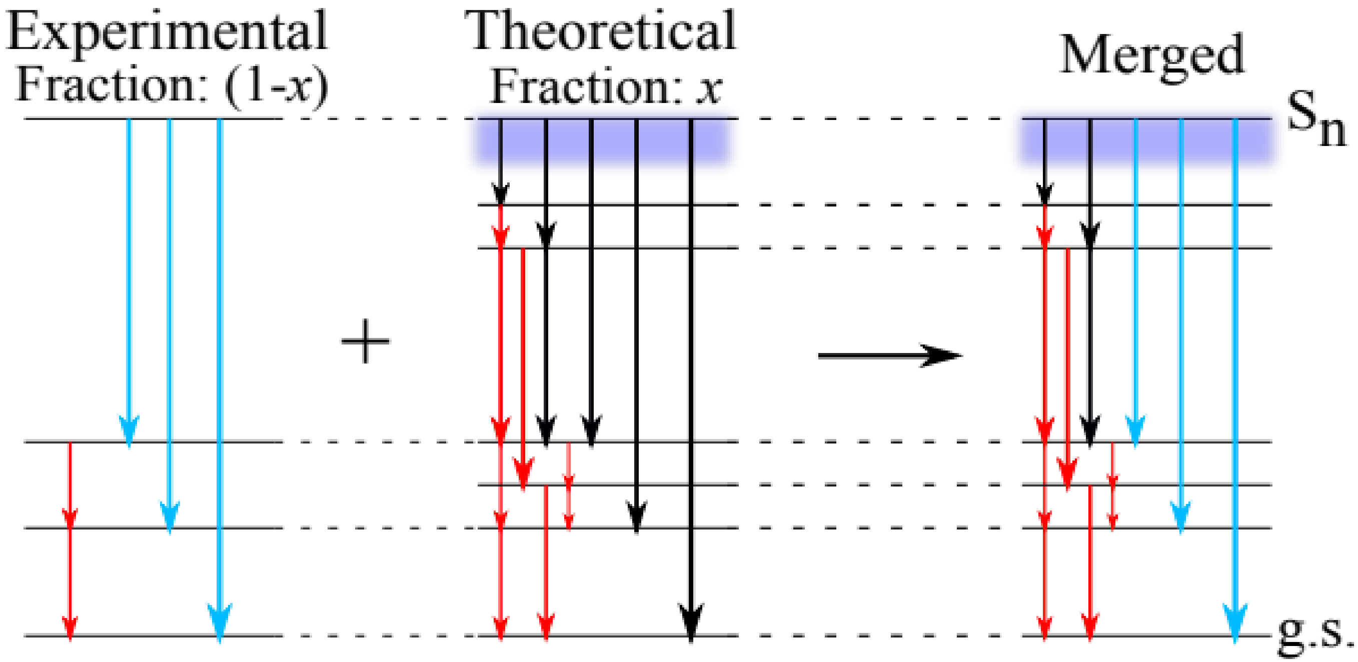
Gamma energy [MeV]



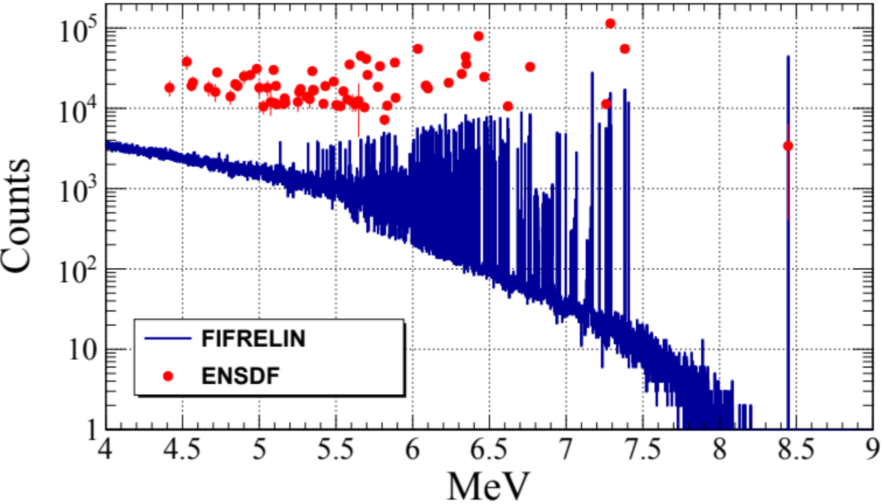
Electron energy [MeV]

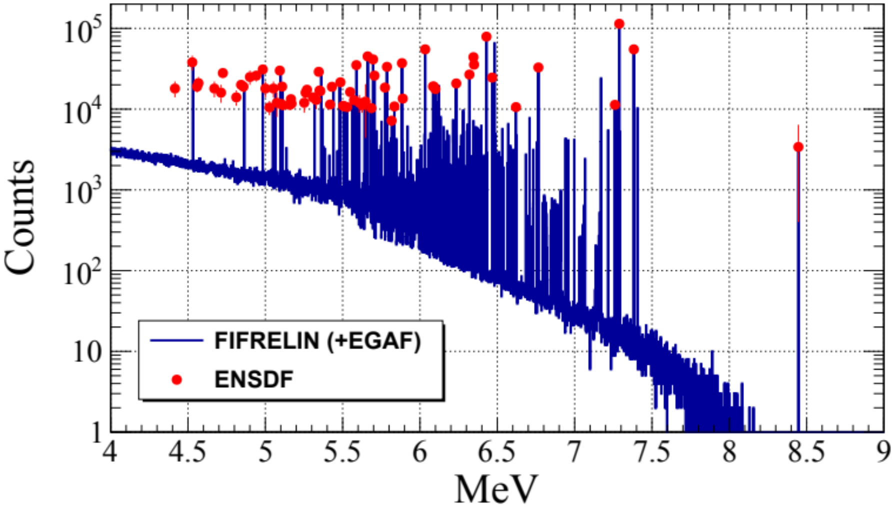
Merging RIPL-3 and EGAF

- RIPL-3 for discrete part
- EGAF for primary transitions
- Theoretical models for the continuous part of the spectrum



Example on de-excitation of ^{156}Gd after neutron capture

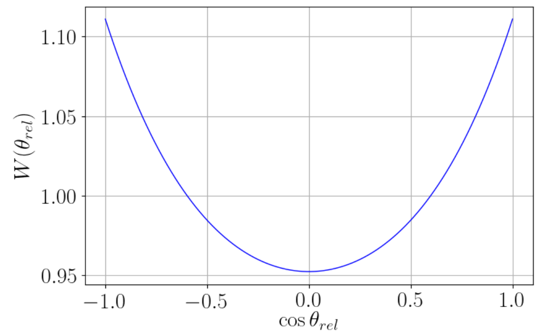


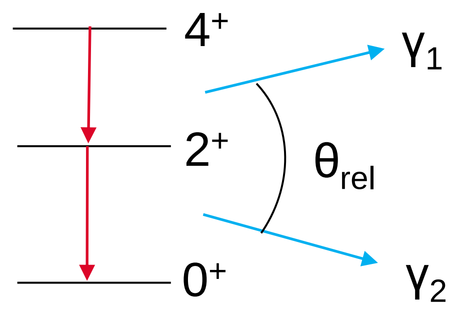


Improved description on the high energy part of the spectrum

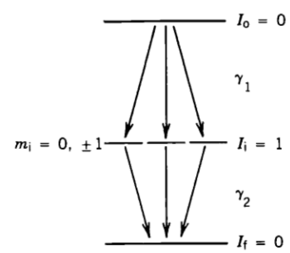
Gamma directional correlations-Physics description

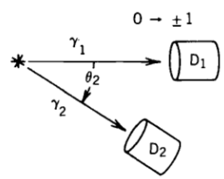
- The second is emitted anisotropically with respect to the first
- Reason: unequal population of the m-substates





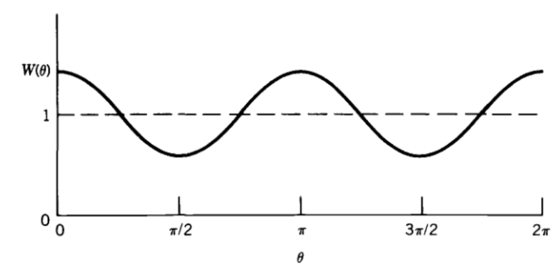
$$W(\theta) = \sum_{m_i} p(m_i) W_{m_i \to m_f}(\theta)$$





- $W(0\to 1)=W(0\to -1) \sim ½ (1+\cos^2(\theta))$
- $W(0\to 0) \sim \sin^2(\theta)$

- The transition $m_0=0\to m_i=0$ gives zero probability in the direction of the first gamma
- Anisotropic emission of the second gamma with respect to the first

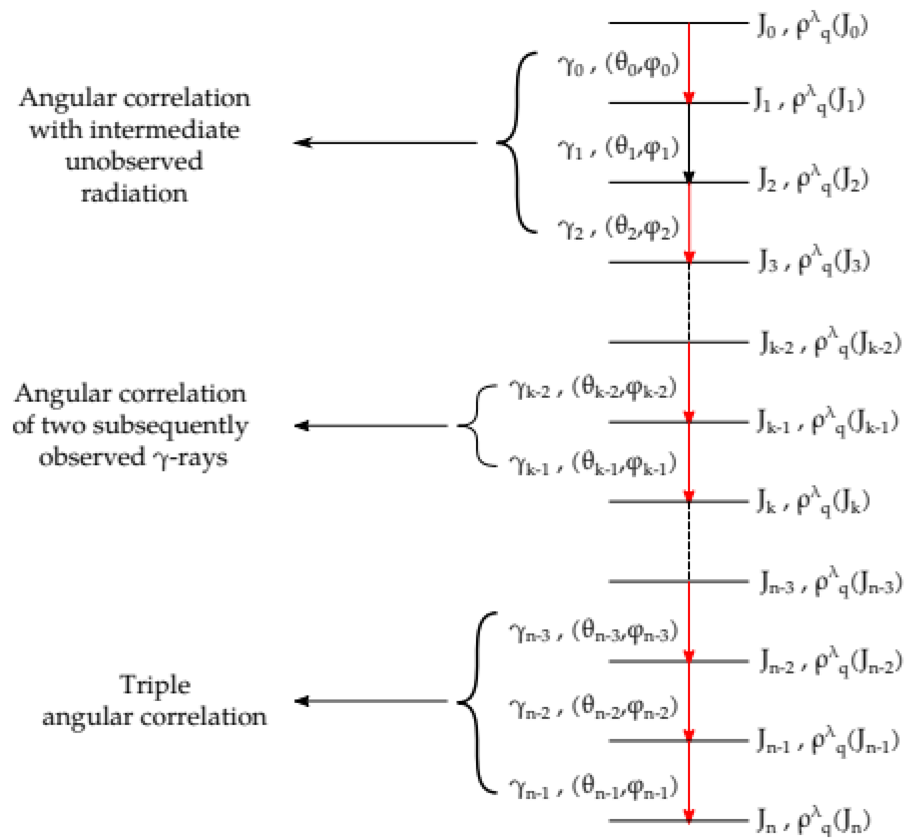


$$W(\theta_{rel}) = 1 + a_2 P_2(\cos\theta_{rel}) + a_4 P_4(\cos\theta_{rel})$$

Gamma-directional correlations – Physics description

- The effect does not concern only two consecutive gamma-rays
- There are higher order angular correlations (triple correlations)
- There are correlations between two non-consecutive gamma rays

$$W(\theta_i,\phi_i) = \sum_{\lambda_f, q_f} (-1)^{\lambda_f + q_f} \sqrt{2\lambda_f + 1}\rho_{q_f}^{\lambda_f}(J_f) \times A_{\lambda_f}(L, L', J_i, J_f, \delta)\mathscr{D}_{q_f 0}^{\lambda_f *}(\phi_i, \theta_i, 0)$$



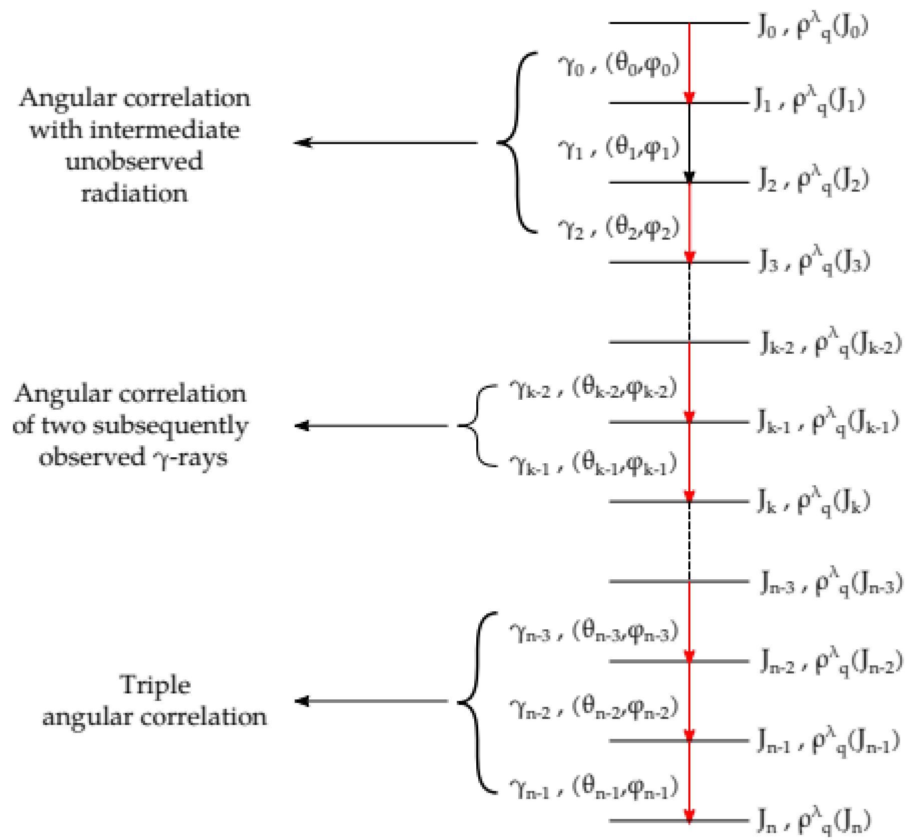
L. C. Biedenharn and M. E. Rose Rev. Mod. Phys. 25, 729 (1953)
R. Steffen, K. Adler, W. Hamilton (Ed.), The electromagnetic interaction in nuclear spectroscopy, North-Holland, Amsterdam (1975)
A. Chalil et al., EPJ A 58 30 (2022) and references therein

Gamma-directional correlations – Physics description

- The effect does not concern only two consecutive gamma-rays
- There are higher order angular correlations (triple correlations)
- There are correlations between two non-consecutive gamma rays

$$W(\theta_i,\phi_i) = \sum_{\lambda_f,q_f} (-1)^{\lambda_f+q_f}\sqrt{2\lambda_f+1}\,\rho^{\lambda_f}_{q_f}(J_f)$$
$$\times A_{\lambda_f}(L,L',J_i,J_f,\delta)\mathscr{D}^{\lambda_f *}_{q_f 0}(\phi_i,\theta_i,0)$$

Statistical tensor



L. C. Biedenharn and M. E. Rose Rev. Mod. Phys. 25, 729 (1953)
R. Steffen, K. Adler, W. Hamilton (Ed.), The electromagnetic interaction in nuclear spectroscopy, North-Holland, Amsterdam (1975)
A. Chalil et al., EPJ A 58 30 (2022) and references therein

DIRECTIONS OF GAMMA-RAYS (ANGULAR CORRELATIONS)

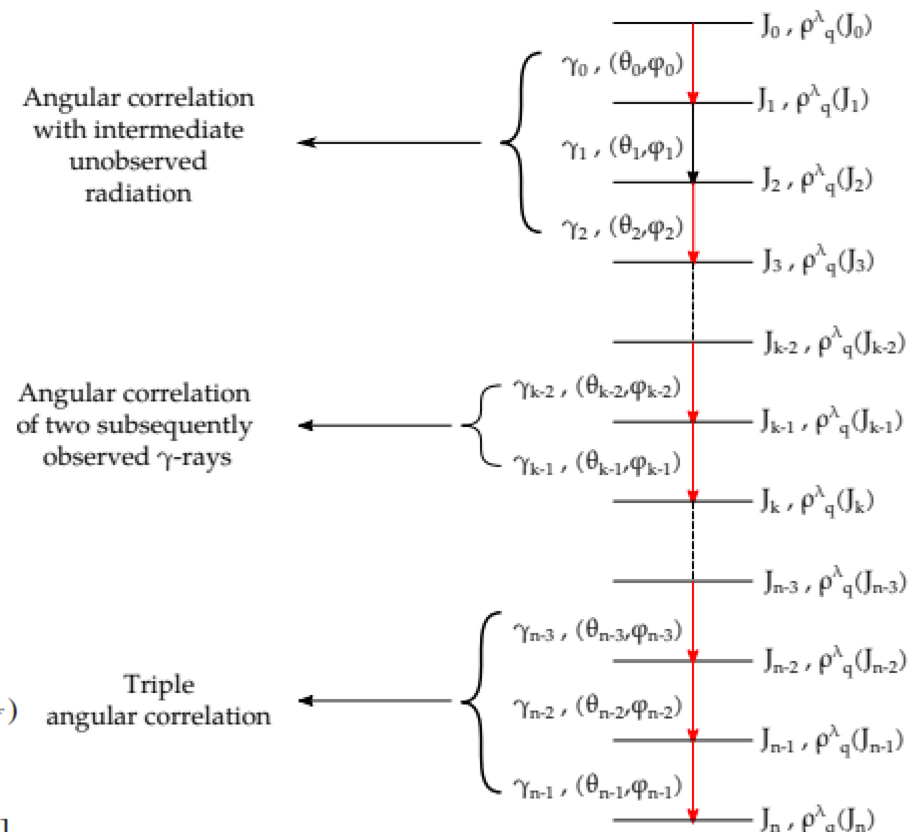
Gamma-directional correlations – Physics description

- The effect does not concern only two consecutive gamma-rays
- There are higher order angular correlations (triple correlations)
- There are correlations between two non-consecutive gamma rays

$$W(\theta_i,\phi_i) = \sum_{\lambda_f,q_f} (-1)^{\lambda_f+q_f}\sqrt{2\lambda_f+1}\,\rho^{\lambda_f}_{q_f}(J_f) \times A_{\lambda_f}(L,L',J_i,J_f,\delta)\,\mathscr{D}^{\lambda_f *}_{q_f 0}(\phi_i,\theta_i,0)$$

Angular correlation coefficient

$$A_\lambda(L,L',J_i,J_f,\delta) = \frac{1}{1+\delta^2}[F_\lambda(L,L,J_i,J_f) + 2\delta F_\lambda(L,L',J_i,J_f) + \delta^2 F_\lambda(L',L',J_i,J_f)].$$



L. C. Biedenharn and M. E. Rose Rev. Mod. Phys. 25, 729 (1953)
R. Steffen, K. Adler, W. Hamilton (Ed.), The electromagnetic interaction in nuclear spectroscopy, North-Holland, Amsterdam (1975)
A. Chalil et al., EPJ A 58 30 (2022) and references therein

DIRECTIONS OF GAMMA-RAYS (ANGULAR CORRELATIONS)

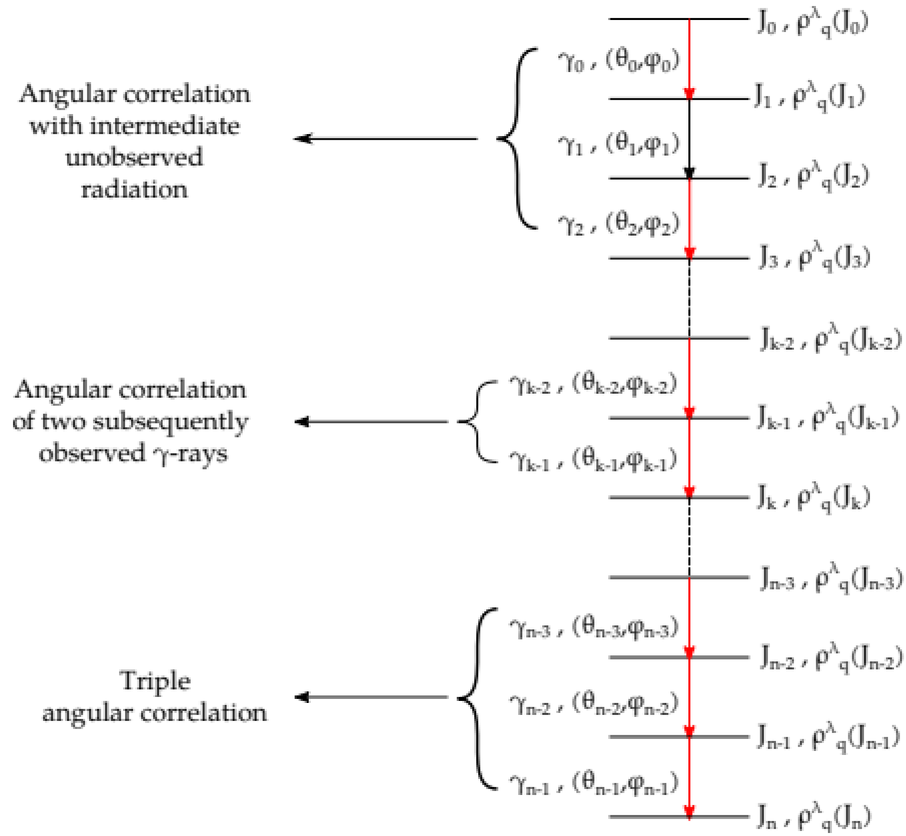
Gamma-directional correlations – Physics description

- The effect does not concern only two consecutive gamma-rays
- There are higher order angular correlations (triple correlations)
- There are correlations between two non-consecutive gamma rays

$$W(\theta_i,\phi_i) = \sum_{\lambda_f,q_f} (-1)^{\lambda_f+q_f}\sqrt{2\lambda_f+1}\,\rho^{\lambda_f}_{q_f}(J_f) \times A_{\lambda_f}(L,L',J_i,J_f,\delta)\mathscr{D}^{\lambda_f *}_{q_f 0}(\phi_i,\theta_i,0)$$

$$\mathscr{D}^{\lambda *}_{q0}(\phi,\theta,0) = (-1)^q\sqrt{\frac{4\pi}{2\lambda+1}}Y^{\lambda}_{-q}(\theta,\phi) = (-1)^{(q+|q|)/2}\sqrt{\frac{(\lambda-|q|)!}{(\lambda+|q|)!}} \times P^{|q|}_{\lambda}(\cos\theta)e^{-iq\phi}.$$

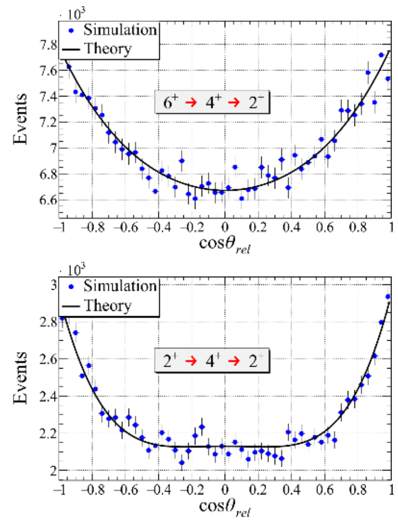
Wigner D-matrix

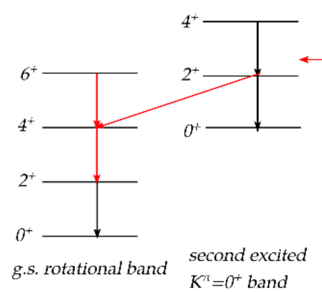


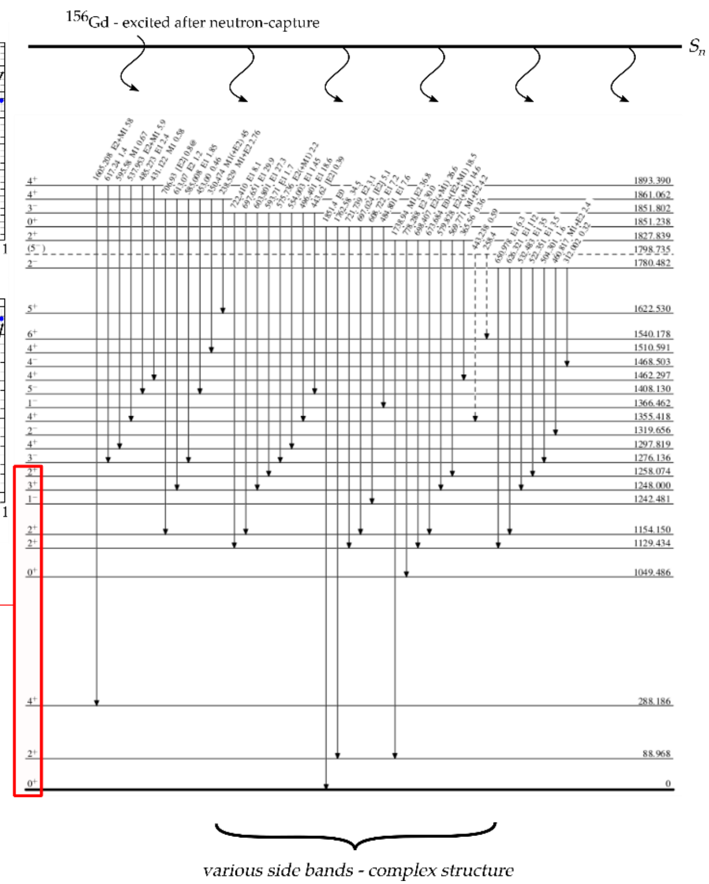
L. C. Biedenharn and M. E. Rose Rev. Mod. Phys. 25, 729 (1953)
R. Steffen, K. Adler, W. Hamilton (Ed.), The electromagnetic interaction in nuclear spectroscopy, North-Holland, Amsterdam (1975)
A. Chalil et al., EPJ A 58 30 (2022) and references therein

Gamma-directional correlations - Results

- This method was applied to the de-excitation of $^{156,158}Gd$
- All angular correlations are reproduced in a complex level scheme







Eur. Phys. J. A (2022) 58:30
https://doi.org/10.1140/epja/s10050-022-00683-0
THE EUROPEAN PHYSICAL JOURNAL A
Special Article - New Tools and Techniques

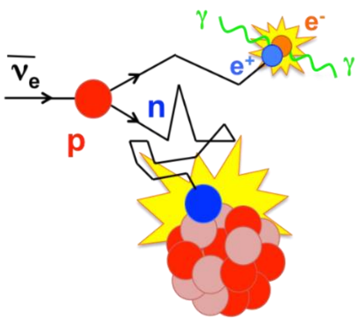
Monte Carlo simulations of γ-directional correlations and their application on FIFRELIN cascades

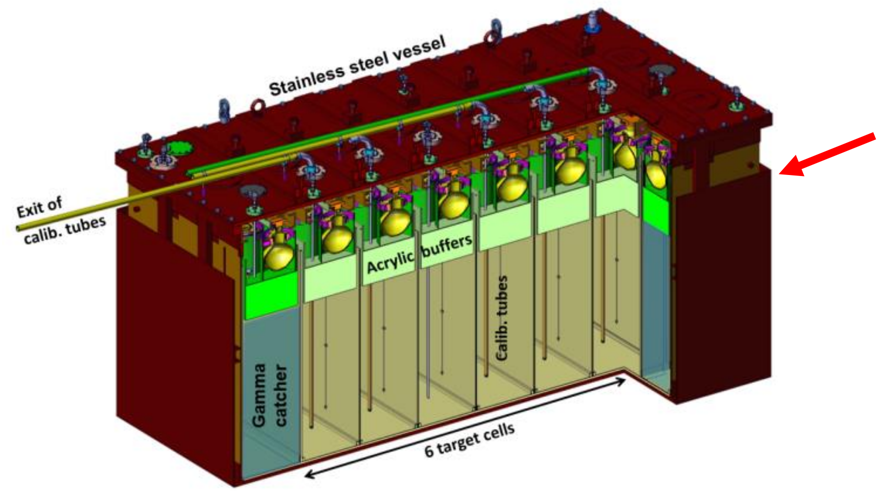
A. Chalil[1,a], T. Materna[1], O. Litaize[2], A. Chebboubi[2], F. Gunsing[1]
[1] IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France
[2] CEA, DES, IRESNE, DER, Cadarache, 13108 Saint-Paul-Lez-Durance, France

The STEREO Detector

- Organic liquid scintillator 3 x 1.5 x 1.5 m
- 6 cells – Gd loaded
- Neutrino detection via Inverse Beta Decay (IBD)

$$\overline{\nu}_e + p \rightarrow e^+ + n$$





Cut view of the STEREO detector

N. Allemandou et al. (STEREO Collaboration) JINST 13 P07009 (2018)

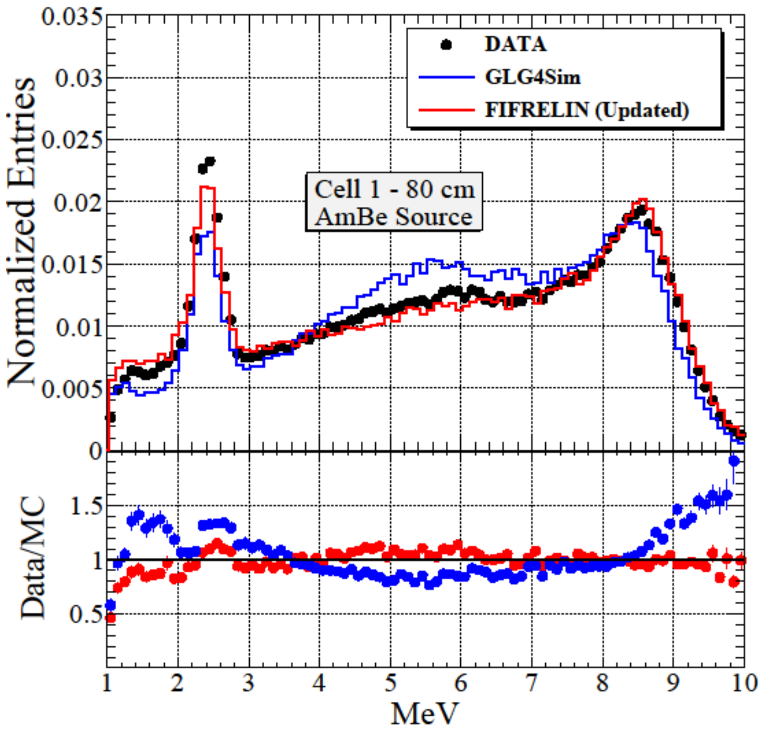
- The positron e^+ interacts with the electrons of the detector → prompt signal
- The neutron diffuses and thermalizes in the detector and after ~10 µs, a second signal (delayed signal) is produced from the reaction: $n + {}^{nat}Gd$
- The coincidence of the two signals is an experimental signature of the detection of the anti-neutrino

The precise modeling of the de-excitation of Gd is important for the determination of the detector response

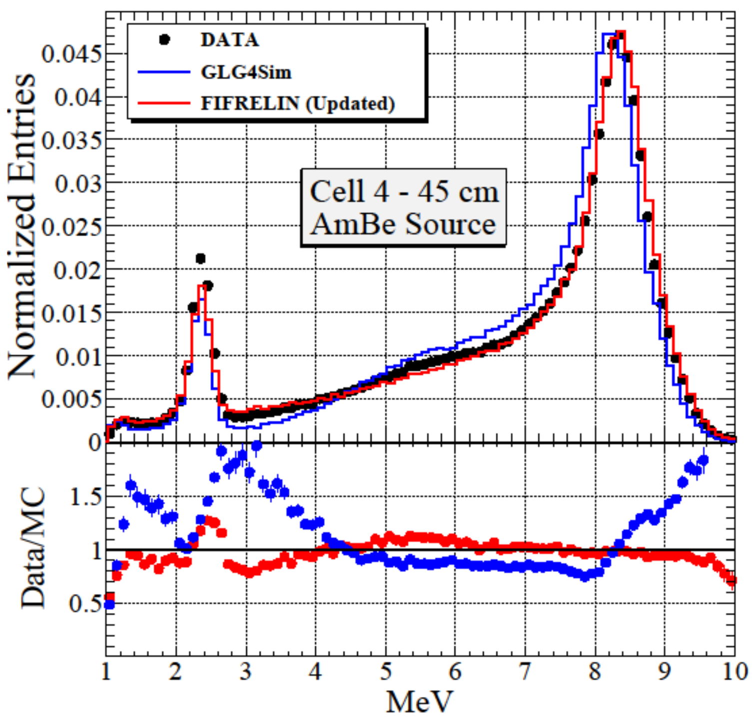
Talk by Rudolph Rogly (STEREO)

Results for the STEREO experiment

- Updated FIFRELIN cascades $^{156,158}Gd$ used in the latest version of STEREO simulation
- Comparison with experimental data (AmBe)
- Improved Data/MC agreement



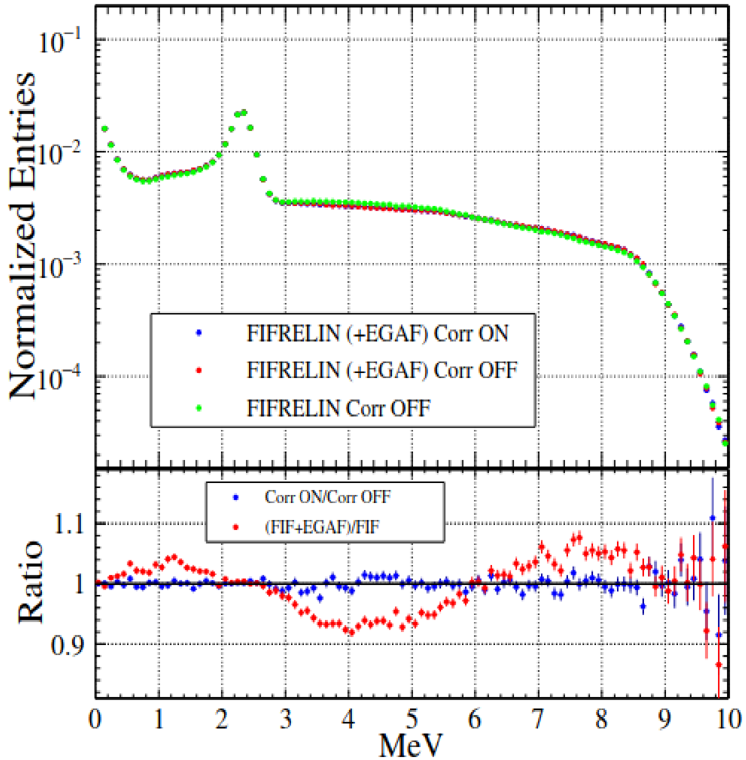
Top of detector cell

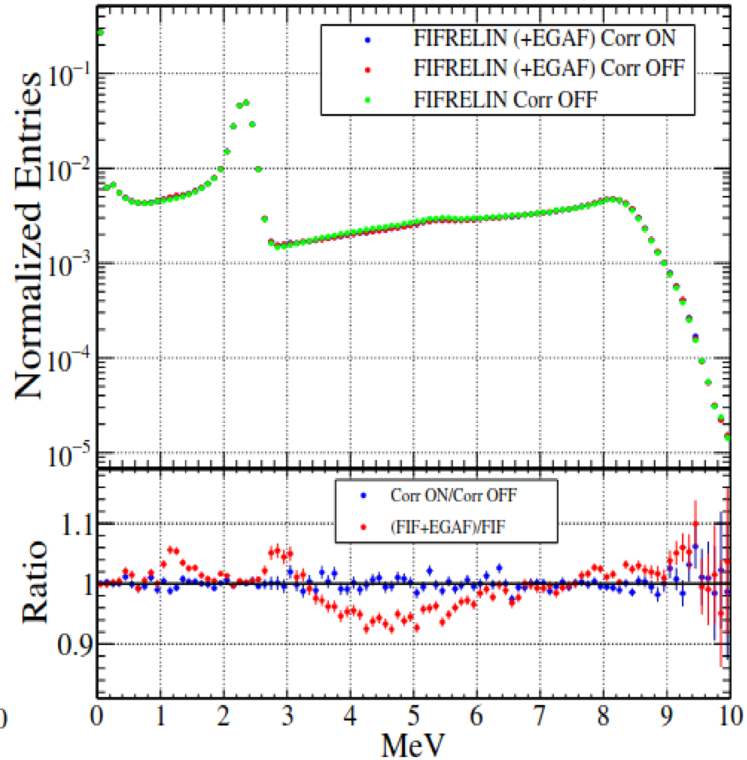


Center of detector cell

Results for the STEREO experiment

- Impact on the border of the detector when adding EGAF transitions
- Angular correlations have negligible impact





Updated Repository

- ~10 million of cascades are distributed to the community via an updated repository: DOI: 10.5281/zenodo.6861341

Improved FIFRELIN de-excitation model for neutrino applications

H. Almazán[a,1], L. Bernard[b,2], A. Blanchet[c,3], A. Bonhomme[1,3], C. Buck[1], A. Chalil[d,3], A. Chebboubi[4], P. del Amo Sanchez[5], I. El Atmani[e,3], L. Labit[5], J. Lamblin[2], A. Letourneau[3], D. Lhuillier[3], M. Licciardi[2], M. Lindner[1], O. Litaize[4], T. Materna[3], H. Pessard[5], J.-S. Réal[2], J.-S. Ricol[2], C. Roca[1], R. Rogly[3], T. Salagnac[f,2], V. Savu[3], S. Schoppmann[g,1], T. Soldner[6], A. Stutz[2], L. Thulliez[3], M. Vialat[6]

arXiv:2207.10918 [hep-ex]

- Possibility to be used for Super-Kamiokande (?)

ELSEVIER

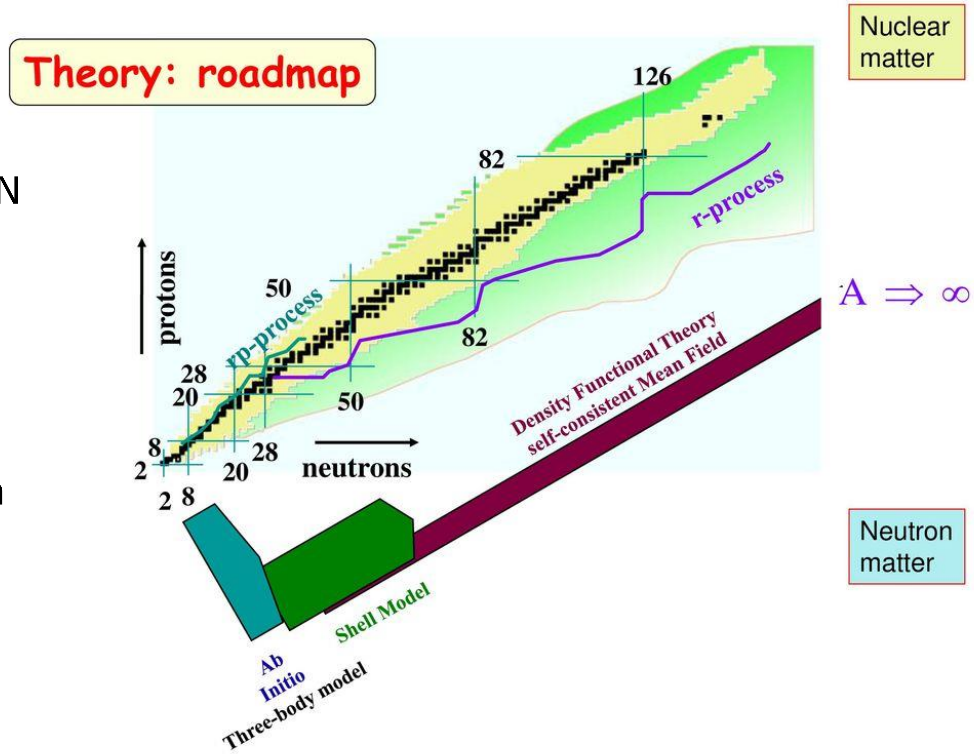
Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Volume 1027, 11 March 2022, 166248

First gadolinium loading to Super-Kamiokande

WHAT ABOUT TIMING IN FIFRELIN?

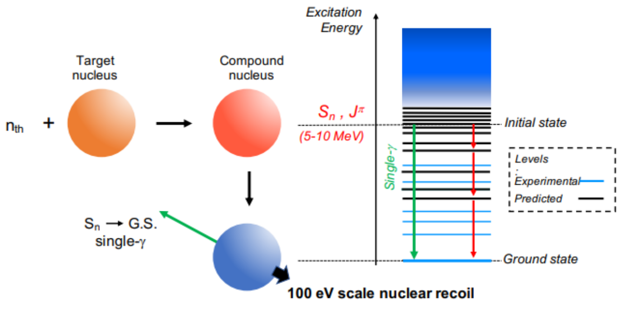
- If a lifetime of a state is known, FIFRELIN considers the experimental value from RIPL3 database
- If not, Weisskopf estimates
- Weisskopf estimates → Not good approximation for most transitions (assume the transitions comes only from a single nucleon)
- Use of Nuclear Models depending on the isotope of interest



H. Sagawa, *Lectures in Istanbul*, 2008

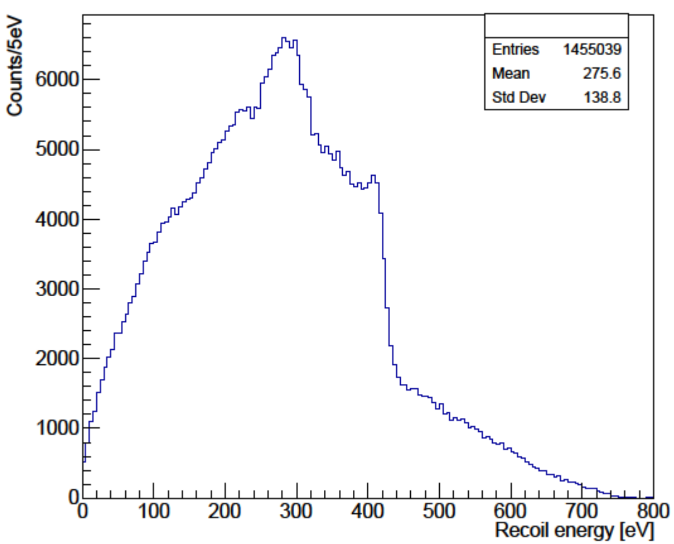
TIMING AND CRAB

- Calibration by Recoils for Accurate Bolometry
- Method for calibrating bolometers – important for dark matter, neutrino studies
- Timing sensitivity can be important in certain elements

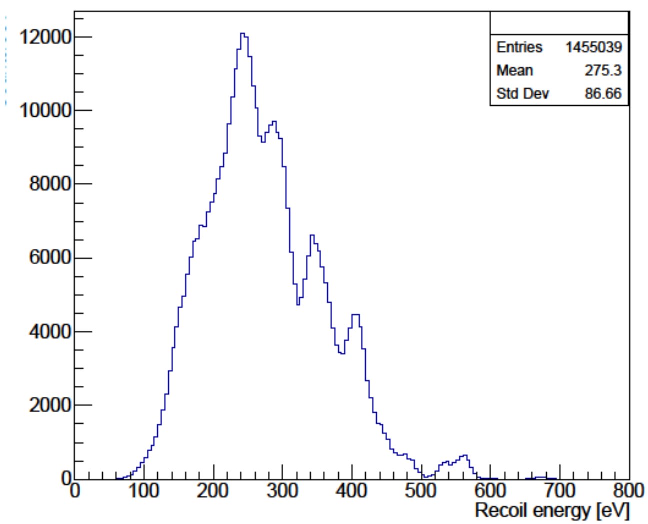


L. Thulliez et al 2021 JINST 16 P07032

t(collision) > t(gamma)



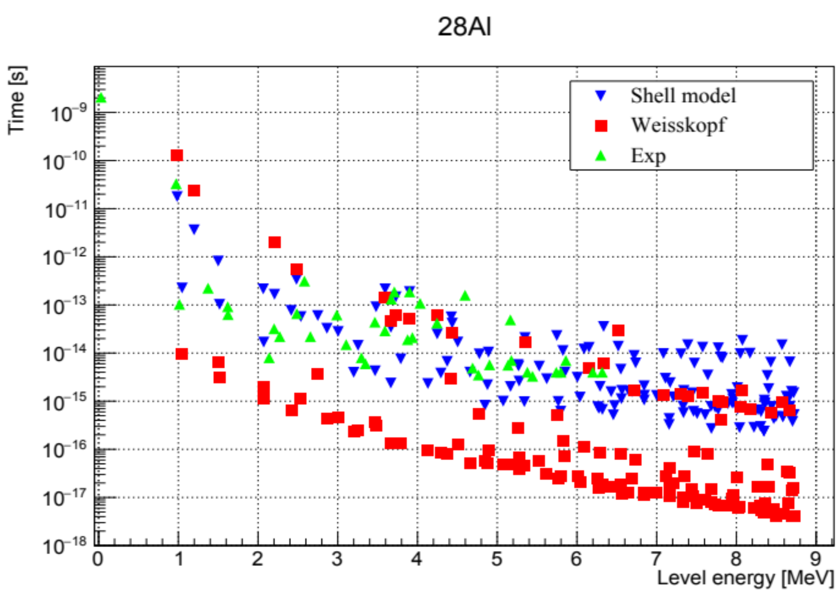
t(collision) < t(gamma)

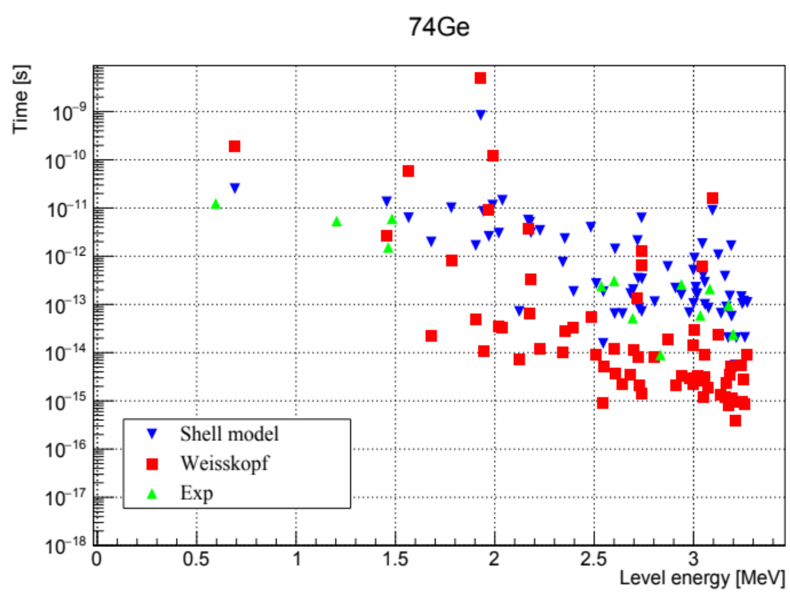


Talk by Gabrielle Soum

SHELL MODEL CALCULATIONS

- Shell model calculations for isotopes Si, Al (usdb interaction) and Ge (jun45 interaction)
- Calculations were performed with the KShell code
  - *Comp. Phys. Comm. 244, 372 (2019)*





Conclusions and future prespectives

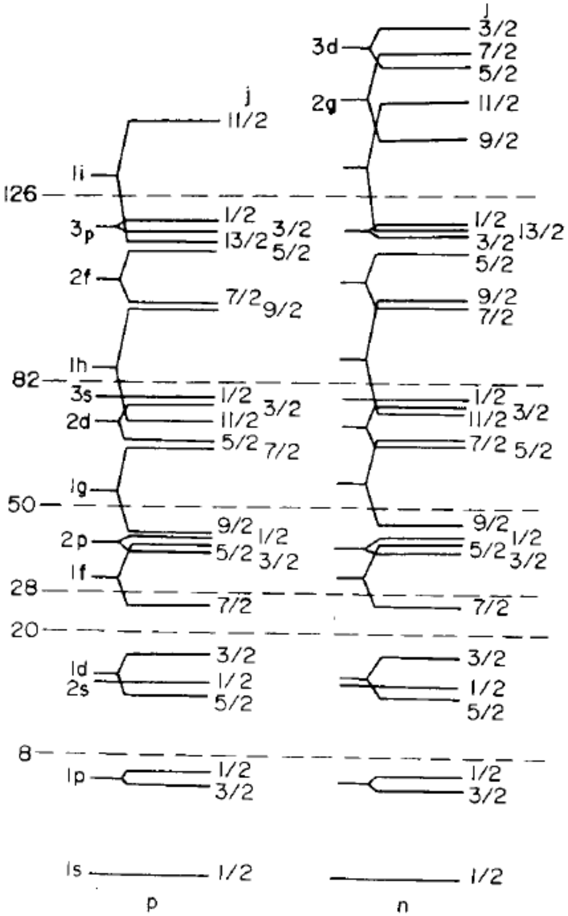
- Implementation of different databases (EGAF + RIPL3)
- Implementation of γ-angular correlations
- ENSDF implementation under works
- Results for the STEREO experiment with improved the Data/MC agreement
- Timing improvements under works
- Updated repository of ~ 10 million of cascades for Gd
  doi: 10.5281/zenodo.6861341

We acknowledge the financial support of the Cross-Disciplinary Program on Numerical Simulation of CEA, the French Alternative Energies and Atomic Energy Commission.

THANK YOU FOR YOU ATTENTION!

WHAT ABOUT TIMING IN FIFRELIN?

- If a lifetime of a state is known, FIFRELIN considers the experimental value from RIPL3 database
- If not, Weisskopf estimates
- Weisskopf estimates → Not always accurate
  (assume the transitions comes only from a single nucleon)
- Use of Nuclear Models depending on the isotope of interest



Single-particle states (Nuclear shell model)

A. Sitenko, *Lectures on the Theory of Nucleus*, Pergamon Press 1975