Accuracy of the Pulse Height Weighting Technique for Capture Cross Section Measurements

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The accuracy of the pulse height weighting technique for the measurement of neutron capture (n,γ) cross sections is investigated. Detailed Monte Carlo simulations of capture measurements are compared to experimental data. Several causes of systematic deviation are investigated and their effect is quantified.

KEYWORDS: pulse height weighting technique, C_6D_6 detectors, Monte Carlo simulations, nuclear statistical model, neutron capture cross section

I. Introduction

In recent times there has been a renewed interest in high accuracy neutron cross section data. The sources of this interest are in the field of nuclear technology, in particular in relation to the concept of Accelerator Driven Systems, and the field of Nuclear Astrophysics. The n_TOF facility at CERN,[1)] presently in its commissioning phase, has been constructed with the aim of obtaining high quality data relevant to both fields of research. Radiative capture measurements with improved accuracy are an important part of the planned experimental programme. In a first phase such measurements will be carried out using a set of C_6D_6 liquid scintillator detectors applying the Pulse Height Weighting Technique (PHWT). The goal of a few percent accuracy on the (n,γ) cross sections can only be achieved when all the sources of systematic uncertainties are well under control. We have therefore carried out a detailed investigation of the sources of error associated with the principles of the PHWT itself.

The PHWT is based[2)] on the use of a small efficiency γ-ray detector, such that essentially only one γ-ray out of the capture cascade is registered at a time, but whose detection efficiency is proportional to the photon energy: $\varepsilon_\gamma = kE_\gamma$. Under these conditions the efficiency for detecting a cascade will be proportional to the known cascade energy and independent of the actual cascade path: $\varepsilon_c \approx \sum_j \varepsilon_{\gamma_j} = kE_c$. The proportionality of the efficiency with the γ-ray energy is achieved through the manipulation of the detector energy response distribution $R(E)$ (or its energy binned equivalent R_i) by the introduction of a "pulse height" (deposited energy) dependent weighting factor $W(E)$, which is to be applied to each registered count. The smooth (in practice polynomial) behaviour of the weighting factor is determined by least squares fit for a number of γ-ray responses in the energy range of interest (up to 10 MeV)

$$min\left(\sum_j \sum_i W_i R_i^j - kE_{\gamma_j}\right)^2 \qquad (1)$$

Apart from the detection of background counts (i.e. counts not related to capture γ-rays) other sources of error related to the working principle of the PHWT can be identified: a) the detection of more than one γ-ray per cascade, b) the loss of cascade γ-rays due to the electron conversion process and most importantly, c) the adequacy of the weighting function employed. It will be shown in the following sections that the use of detailed Monte Carlo simulations allows one to quantify these systematic uncertainties.

II. Simulation of γ-ray detector response

Historically, due to the difficulty of obtaining monoenergetic γ-ray sources in the energy range of interest, the detector response distributions needed to calculate the weighting factors were obtained from Monte Carlo simulations. At one point a serious discrepancy was found between the neutron width Γ_n obtained by the PHWT and the one obtained from transmission measurements for the well known 1.15 keV resonance in ^{56}Fe. After thorough investigations it became clear that the problem had its origins in the Monte Carlo simulated response distributions.

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This conclusion was mainly supported by measurements at Geel[3,4] of mono-energetic γ-ray responses. The method employed was the coincidence technique for two-gamma cascades populated in (p,γ) resonance reactions in light nuclei. The measurements were performed with a detector arrangement similar to that employed in the (n,γ) measurements. The extracted experimental weighting function giving a cross section in agreement with the standard transmission value for the 1.15 keV resonance in ^{56}Fe, was proposed for the capture measurements. However it was also recognized that the cause of the discrepancy between the Monte Carlo simulated response and the measurement was due to the large influence of the materials surrounding the source which produce secondary radiation. This includes the sample under study itself, casting some doubts on the universality of the weighting function so determined. In order properly to take into account the systematic differences of the various sample/detector set-ups only the Monte Carlo method is practicable. Indeed, at Oak Ridge[5] the Monte Carlo method was further investigated and it was found that the EGS4 code[6] gave a satisfactory result for the 1.15 keV resonance in ^{56}Fe measured with their experimental capture set-up. They were not able, however,[3] to produce the same result for the Geel set-up.

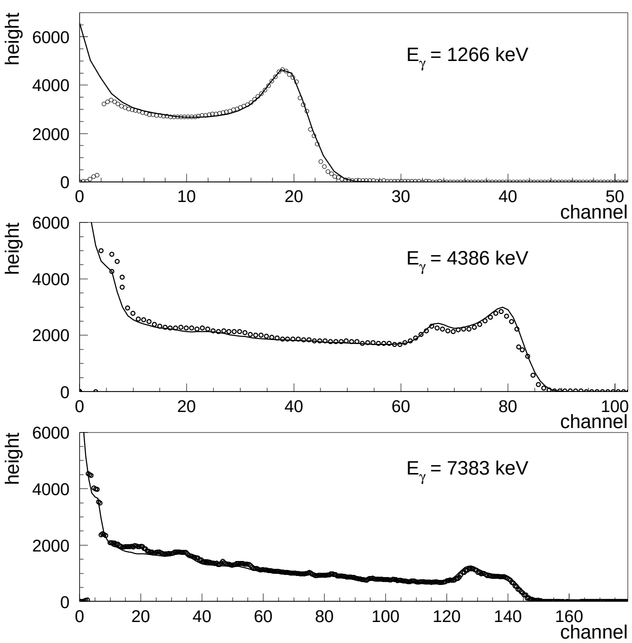

Fig. 1 Comparison of measured (circles, from Ref. 3) and GEANT3 simulated (continuous line) C_6D_6 detector γ-ray response distributions. Both the 4.386 and 7.383 MeV simulations include the known contaminants

We have re-investigated the issue of the accuracy of the Monte Carlo simulations; in particular whether the differences between simulation and measurement could be due to insufficient detail in the description of the measuring set-up or rather due to a poor implementation in the Monte Carlo code of the relevant physical processes in the generation and interaction of the secondary radiation. The simulation package GEANT3[7] was chosen based on our previous successful experience and its capability of defining complex geometries. The code was used to investigate extensively the response of the (p,γ) experimental set-up described in Ref. 3 in the photon energy range 1.2-8.4 MeV. The detailed geometric description of the beam line, target and detectors was reproduced in the simulation. The main results of this study can be summarized as follows:

1) The shape of the measured response distribution is well reproduced by the simulation (see **Fig. 1**) throughout the whole γ-ray energy range. The absolute value of the efficiency is well reproduced at the higher energies but there is a tendency to overestimate it at low energies (up to 18 % at 1.2 MeV, see **Fig. 2**).

2) At high γ-ray energies the contribution to the detection efficiency of the secondary radiation produced in the dead materials is very large: close to 40 % around 8 MeV. The contribution of the detector dead material itself is negligible compared with the contribution of the (p,γ) target backing (0.3 mm thick Ta plate) of this set-up.

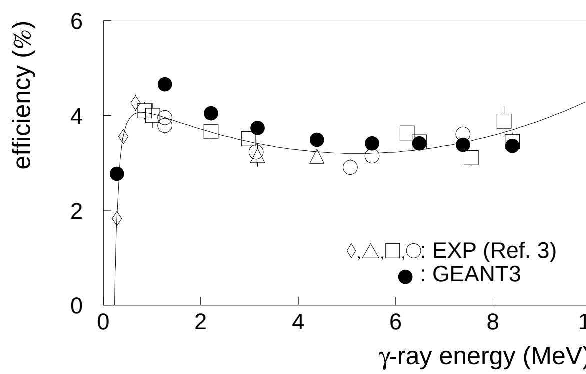

Fig. 2 Comparison of measured (open symbols, from Ref. 3) and GEANT3 simulated (bold circle) C_6D_6 detector γ-ray efficiencies. The line represents a fit to the experimental data

It is hard to understand point 1) since one expects the Monte Carlo simulation to perform better at low energies: the secondary radiation generated in dead materials plays a very small role so that the detection efficiency is essentially given by the probability that the γ-ray penetrates the sensitive volume and interacts with it, which should be accurately reproduced by the Monte Carlo code. A normalization problem in the data should not therefore be excluded. On the other hand from 2) one concludes that even with a similar detector arrangement the validity of the experimental (p,γ) weighting function when applied to (n,γ) measurements of samples of different composition and size is questionable. In fact this point was experimentally investigated by G. Fioni[4] by comparing the PHWT result for the 1.15 resonance in ^{56}Fe obtained for samples of different thickness and composition: 0.5 mm, 1.0 mm, and 1.5 mm metallic Fe samples, a 4.1 mm

Fe_2O_3 sample, and a sandwich of five Fe samples with four Au samples totalling a thickness of 2.2 mm and 0.6 mm respectively. All samples were 8 cm in diameter. The measurements for the single metallic and oxide samples were normalized to the measurement of the 4.9 eV resonance in ^{197}Au performed with a 0.1 mm thick Au sample, while the sandwich sample provides self calibration. The neutron width Γ_n extracted in Ref. 4 from the capture measurement, normalized to the standard transmission value, is shown in **Fig. 3** (triangles). This figure clearly illustrates the complex dependency of the extracted result on sample thickness and composition: the thick sandwich sample (2.2 mm Fe) gives a result in agreement with the transmission value as well as the thinner metallic samples (0.5 mm and 1.0 mm), while the 1.5 mm metallic sample and the Fe_2O_3 sample clearly deviate.

These measurements would have constituted an excellent test of our Monte Carlo simulated weighting functions, but this requires us to re-analyze the original data and unfortunately they were not accessible. Accordingly we adopted an alternative way to test the Monte Carlo simulation namely, to make a realistic simulation of the measurement and analyze the simulated data with the experimental (p,γ) weighting function in order to compare with the true data result. This requires a procedure to generate capture cascades with the appropriate γ-ray energy and multiplicity distribution for each resonant state of interest. The statistical model of the nucleus provides such a possibility through the application of the Monte Carlo method as will be explained in the following section.

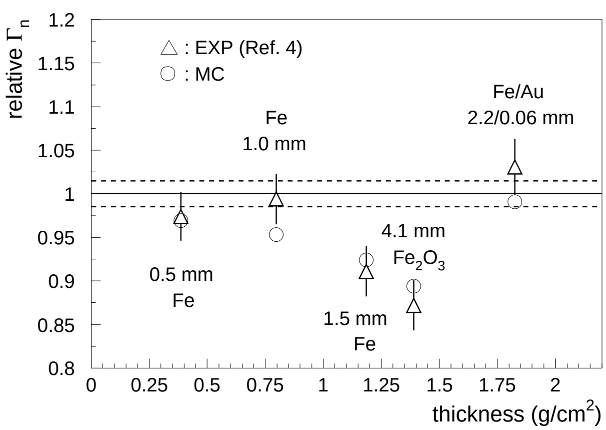

Fig. 3 Comparison of the neutron widths for the 1.15 keV resonance in ^{56}Fe obtained for several samples. Values are normalized to $\Gamma_n = 61.7(9)$ meV. Triangles: from experiment (Ref. 4), circles: from Monte Carlo simulation

III. Simulation of capture cascades

A computer program was written in order to generate realistic cascade events by the Monte Carlo method. For each capture nucleus a known low excitation energy level scheme is defined consisting of a complete set of levels with known spin-parity and branching-ratios. At higher energies and up to the resonant state, the statistical model of the nucleus is used to generate a level scheme. Levels of appropriate spin and parity are generated from a level density formula (giving the average level spacings) by introducing fluctuations of the Wigner type. The E1, M1 and E2 electromagnetic transition intensities are generated from the Giant Resonance (GR) model (Axel-Brink hypothesis) by introducing fluctuations of the Porter-Thomas type. As we will explain later the electron conversion process is also taken into account. With this code a list of capture events is generated, which is subsequently used as input to the GEANT3 simulation code. Each event consists of a list of γ-ray energies, and eventually electron and X-ray energies.

The method was applied to simulate the capture experiment[3,4] on different iron and gold samples mentioned in the previous section. One million cascades were generated for the 1.15 keV p-wave capture resonance in ^{56}Fe ($J^\pi = 1/2^-$, $E_c = 7.647$ MeV) and the 4.9 eV s-wave capture resonance in ^{197}Au ($J^\pi = 2^+$, $E_c = 6.512$ MeV). The number of levels generated was around 1.3×10^3 and 7.8×10^5 respectively.The experimentally known levels and transitions below 2.0 MeV in ^{57}Fe and below 1.12 MeV in ^{198}Au were taken into account. The back-shifted Fermi gas model level density formula parameters and the gamma strength function parameters were taken from standard compilations.[8)]

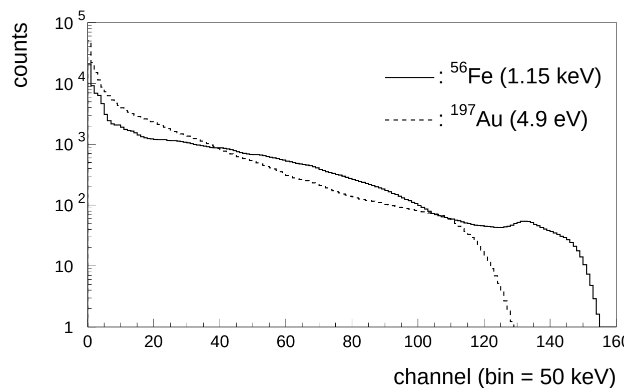

Fig. 4 Monte Carlo simulated C_6D_6 spectra for the 1.15 keV resonance in ^{56}Fe obtained with the 1.0 mm sample (solid line) and for the 4.9 eV resonance in ^{197}Au obtained with the 0.1 mm sample (dashed line)

GEANT3 simulations were then performed with the proper cascade events and geometrical description for each of the sample measurements. The energy deposited in the C_6D_6 detectors for each event was histogramed (see **Fig. 4** for examples). GEANT3 simulations were also performed with mono-energetic γ-rays for each sample and the corresponding weighting function calculated using **Eq. 1**. From each histogram the weighted sum $S_W = \sum_i W_i N_i$ was calculated. According to the principle of the PHWT this sum should be equal (for $k = 1$ in **Eq. 1**) to the cascade energy times the number of cascades $E_c N_c$, for the correct weighting function. In fact, it was verified that the ratio $r = S_W / E_c N_c$ differs from unity by less than 0.5 % for all the simulated cases. This can also be interpreted as a measure of the *precision* of the calculated weighting functions.

An erroneous weighting function produces in general different values of r for different samples due to the differences in the deposited energy spectra (see **Fig. 4**). In practice the capture measurements are normalized to some standard such as the 4.9 eV resonance in ^{197}Au. Therefore it is the relative difference of the respective ratios r which provides the systematic deviations of the extracted cross sections for a wrong weighting function. In **Fig. 3** we have plotted (circles) the ratios r_{Fe}/r_{Au} calculated for each sample combination from the simulated spectra using the experimental (p,γ) weighting function obtained in Ref. 3. As can be observed these values follow the experimental result very closely. In other words the simulated data are reproducing accurately the experimental data, which is itself a remarkable result. From the observation of **Fig. 3** it can be anticipated that it will be possible to obtain an accuracy of the order of 2-3 % when the weighting function deduced from the Monte Carlo simulated γ-ray response distribution is used to analyze PHWT capture measurements, in concordance with the required goal.

The detailed simulation of the experiment constitutes the appropriate tool to evaluate other sources of systematic deviation as well. One such possible error is that introduced by the non negligible probability of detecting more than one cascade γ-ray. The effect depends on the detector efficiency, the cascade multiplicity and to a lesser extent on the cascade energy distribution. The comparison of a simulation where all the cascade radiation is emitted simultaneously with one where the radiation is emitted sequentially measures this effect. For instance, in the previous cases it was verified that the differences were less than 1 %. Another systematic effect is related to the electronic threshold which has to be applied in order to eliminate excessive noise in the measurement of the C_6D_6 spectra. The threshold affects the ratios r differently due to the differences in spectrum shape for different samples (see **Fig. 4**). For example, if instead of a 100 keV threshold as was used in the measurements, a threshold of 200 keV is employed, the Monte Carlo results shown in **Fig. 3** increase by about 2.5 % (the same increase is expected for the experimental result).

The last issue we will discuss is the possible loss of counts due to the substitution in the cascade of γ-rays by less penetrating electrons caused by the conversion electron emission process. Conversion can be very important for some nuclei. For instance ^{198}Au has very strongly converted low lying transitions, with potentially disastrous consequences since gold is usually employed for normalization as was already mentioned. In order to study this effect a somewhat simplified model of the conversion process was included in the cascade generation code. A brief description of the method follows. The experimental or theoretical conversion coefficients for a given transition give the relative probabilities for K, L or M conversion electron emission. For K conversion the fluorescence yield ω_K gives the probability for X-ray or Auger e^- emission followed respectively by one or two X-rays. To obtain the energy of these secondary emissions an average value for the L shell binding energy is assumed while the M shell binding energy is taken as zero. To be consistent with this simplification, for L conversion only an X-ray or an Auger e^- are emitted with probability given by the average fluorescence yield $\overline{\omega}_L$, while for M conversion no secondary radiation is generated at all. Cascades were generated for capture in the 4.9 eV resonance in ^{197}Au including and not including the conversion process for the experimentally known converted transitions. When these were used in the GEANT3 code to simulate the measurement with the 0.1 mm gold sample, it was found that the difference of ratios r was less than the 0.5 % estimated precision, indicating that at least in this case the effect is small.

IV. Conclusions

Several systematic effects related to the PHWT have been investigated by means of Monte Carlo simulations. The overall conclusion of this study is that an accuracy of the order of 2-3 % can be achieved when the weighting functions are calculated from Monte Carlo simulated γ-ray response distributions and other systematic effects are corrected for, based on detailed simulations of the measurement. We expect to have an experimental confirmation of this result from the initial measurements which will be carried out at n_TOF, just after the commissioning phase.

References

1) The n_TOF Collaboration, "European collaboration for high-resolution measurements of neutron cross sections between 1 eV and 250 MeV," CERN-SPSC-99-8/SPSC-P-310, CERN (1999).
2) R.L. Macklin, J.H. Gibbons, "Capture cross section studies for 30-220 keV neutrons using a new technique," *Phys. Rev.*, **159**, 1007 (1967).
3) F. Corvi, G. Fioni, F. Gasperini, P.B. Smith, "The weighting function of a neutron capture detection system," *Nucl. Sci. Eng.*, **107**, 272 (1991).
4) G. Fioni, "Resonance neutron capture in ^{56}Fe and ^{60}Ni below 300 keV" Ph.D. Thesis, Gent University, Belgium (1991).
5) F.G. Perey, J.O. Johnson, T.A. Gabriel, R.L. Macklin, R.R. Winters, J.H. Todd, N.W. Hill "Responses of C_6D_6 and C_6F_6 gamma-ray detectors and the capture in the 1.15 keV resonance of ^{56}Fe," *Proc. Int. Conf. Nuclear Data for Science and Technology,* Mito, Japan, 30 May - 3 June 1988, p.379 (1988).
6) W.R. Nelson, H. Hirayama, D.W.O. Rogers, "The EGS4 code system," SLAC-265, Stanford Linear Accelerator Center (1985).
7) "GEANT: Detector description and simulation tool," CERN Program Library W5013 (1994).
8) "Reference input parameter library for theoretical calculations and nuclear reactions (RIPL)," Nuclear Data Center, International Atomic Energy Agency (1998).