RADIATIVE NUCLEON CAPTURE AND THE OPTICAL POTENTIAL

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Abstract.
Two approaches to the description of radiative nucleon capture on medium and heavy nuclei in the MeV region, the (consistent) direct-semidirect model (CDSD/DSD) and the pre-equilibrium single-particle radiative mechanism, are compared one with another and against the available data at incident energies below 20 MeV, both in the continuum region and when leading to discrete states of essentially single-particle configurations. The role of the optical potential, important for the CDSD approach, is re-investigated and some modifications are suggested. The significance of several model parameters entering the pre-equilibrium calculations is also addressed. Also some cross section trends important for possible production of therapeutic radioisotopes are extracted.

Keywords: gamma emission, cross sections, pre-equilibrium decay, computer codes
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Introduction

Reactions of radiative capture of nucleons — even though very difficult to be measured due to their low cross sections — serve as a challenge for different gamma emission mechanisms already for decades. The pre-equilibrium model (see, e.g., [1]) appeared to be rather successful to describe the gamma energy spectra in the continuum region in 14 MeV neutron-induced reactions [2, 3, 4]. The study of excitation functions extended the applicability of the model to energies starting from few MeV to about 30 MeV. Significant improvement was the incorporation of spin into the formalism of the pre-equilibrium exciton model [5, 6], which enabled also pre-equilibrium calculations leading to discrete states and the comparison to the direct-semidirect model calculations.

Both models have some common features, even though they are strictly complementary in their underlying physics. Whereas the direct-semidirect model deals with wavefunctions and specific interactions of nucleons, while completely ignoring competing processes, the pre-equilibrium models are of statistical nature and they deeply involve quantities like the level densities etc. The competition — e.g. of the nucleon emission — is naturally contained there. What is common to both models is that they both are capable to reproduce (more-or-less) the data corresponding to hard gamma emission [7] observed in radiative nucleon capture at energies above few MeV.

The available experimental data are not frequent due to low cross sections and — at the same time — low detector efficiency for these hard gammas.
EMPIRE and TALYS computer codes

Whereas one can use simple exciton-model based codes at nucleon energies exceeding 10 MeV and sufficiently far from the closed shells, like non-spin code PEQAG [8] or its spin-dependent successor DEGAS [9], it is advisable to incorporate sophisticated nuclear reaction codes which include whole range of approaches and are also coupled to extensive libraries of parameters, if one needs some estimate for a reaction not just tailored to use of simple statistical pre-equilibrium code only. Two codes of this family have been recently released, namely EMPIRE-II (version 2.18 in 2002 [10] and version 2.19 in 2005 [11]) and TALYS in the same year [12, 13].

They are very close as for their underlying physics at the pre-equilibrium stage (e.g., the same single-nucleon radiative mechanism formula for the $\gamma$ emission is used both in EMPIRE and in TALYS), and similarly both of them use very extensive tables of various recommended parameters.

The main differences important for the pre-equilibrium stage of the reaction may be summarized as follows: i) The basic approach to the pre-equilibrium stage is the two-component one (i.e. distinguishing between the neutrons and the protons) in TALYS, whereas one-component formulation with a charge factor is used in EMPIRE; ii) One-particle radiation mechanism for the $\gamma$ emission is used in EMPIRE, but TALYS adds the quasideuteron (two-particle) $^2$, what may cause some differences (however, very small ones) at excitation energies above about 30 MeV; iii) Though the level densities (using the default option) are the same in both codes (with parameters taken from RIPL [14]), different (semi-)microscopic approaches are available for the advanced user; iv) Classical optical model enabling the use of the deformed potential is used to calculate the particle transmission coefficients $T_l$ in EMPIRE with parameters from libraries, and the local and global parameterization of [15] for the spherical optical model is employed in TALYS. This difference influences the $\gamma$ emission only via the competition with that of the particles, but may be significant at lower energies.

Reactions ($n, \gamma$) leading to therapeutic isotopes

The need to produce isotopes for diagnostic and therapeutic purposes stimulated also calls for further measurements and evaluations of the ($n,\gamma$) reactions at energies below 20 MeV. Within the IAEA Coordinated Research Program, some very desirable isotopes for therapeutic needs have been identified and are studied [16]. With opening two excellent codes to community earlier this year, one has got a chance to predict the excitation curves with much better reliability than before. Generally, there are not many data on such ($n,\gamma$) reactions [17] in the continuum region. As an example of the correspondence between the experiment and the calculations, we present the data together with the calculations.

$^1$ The main differences between two versions of EMPIRE-II may be characterized as replacing data libraries by their more recent versions, adding of further subroutines and also replacing some minor bugs.

$^2$ The quasideuteron mechanism is also included in EMPIRE-II v. 2.19, but it is considered for the photonuclear reactions only, and not for the $\gamma$ emission.
of TALYS [12, 13] and two versions of EMPIRE-II (v. 2.18 [10] and v. 2.19 [11]) in Fig. 1. Essentially, we kept the default parameters in EMPIRE, just with allowance for full inclusion of pre-equilibrium emission and γ cascades. Details of the form of the Giant Dipole Resonance (which enters the calculations of the γ emission via the detailed balance principle) and of other parameters did not show much influence on the resulting excitation functions calculated using EMPIRE-II v. 2.18 [16, 18], and we therefore applied this approach also to version 2.19 and TALYS.

FIGURE 1. Excitation function of the \(^{191}\text{Ir}(n,\gamma)\) reaction. Points denote the experimental data [17], full curves the calculations by TALYS, and the dashed one by EMPIRE-II v. 2.19.

Much more complicated is the situation where there are simply no data. Here, we had to rely on the experience and assume that if a reasonable description is achieved for reactions comparable to experimental data, one can expect not bad prediction using the same approach also in the absence of data. In some cases, TALYS and EMPIRE calculations practically coincide (e.g. \(^{124}\text{Xe}(n,\gamma)\)), but there are also reactions (with no available data or with data laying just in-between the calculations), where these two predictions differ nearly by an order of magnitude (e.g. \(^{102}\text{Pd}(n,\gamma)\) and/or \(^{130}\text{Te}(n,\gamma)\)).

**Reaction** \(^{208}\text{Pb}(p,\gamma)\)

Recent measurements of the \((p,\gamma)\) reactions on \(^{208}\text{Pb}\) leading to discrete states [19] is another challenge to check the validity of pre-equilibrium formulation of the γ emission. Unfortunately, the target nucleus is a double magic one, with extremely enhanced individual features and far off typical statistical behaviour of nuclei in its vicinity, what is — in somewhat weakened sense — true also for the final nucleus of the radiative capture,
One has to be therefore extremely careful with the choice of proper parameters used in this calculation. As already shown previously, the systematics of the level density parameters fails for reactions on $^{208}\text{Pb}$, and one has to apply carefully chosen individual ones. Anyway, Refs. [20] and [21] presented calculations of neutron-induced reactions on Pb (integrated and activation cross sections and also continuous $\gamma$ spectra in [20], and cross sections to discrete states in [21]), whereas the proton-induced one has been measured now, and due to the presence of Coulomb barrier, the competing proton channel is more influenced by not optimal choice of parameters than it was in the neutron reactions.

FIGURE 2. Excitation curve of $^{208}\text{Pb}(p,\gamma)$ leading to the $f_{7/2}^{-}$ (896 keV) discrete state. Crosses are the data of Snover [22], circles the recent ones by Lipoglavšek et al. [19, 23], and the calculations by TALYS, EMPIRE-II v. 2.19 and within the CDSD model are drawn by a full, dotted-dashed, and dotted curves, respectively.

FIGURE 3. As in Fig. 2, but for the $h_{9/2}^{-}$ (ground state) (left) and $i_{13/2}^{+}$ (1609 keV) (right). Only one set of pre-equilibrium calculations is depicted for each of the states, as the other one significantly overpredicts the measured data.

$^{209}\text{Bi}$. The single-particle level density of $^{208}\text{Pb}$ is three times less than the average around.
In Figs. 2 and 3, we present the excitation functions leading to discrete states calculated using two pre-equilibrium codes together with the data [22, 19] and the Consistent Direct-Semidirect Model (CDS) [24] calculations [19]. The sharp experimental peaks are due to the analogue states. More details and knowledge than from the excitation functions may be obtained from the γ energy spectra of direct transitions leading to the discrete states. As an example, we present here that obtained from $^{208}$Pb+p at incident energy of 15.7 MeV. The experimental points as well together with the original calculations of Ref. [23] (CDS plus statistical emission), and the pre-equilibrium curve obtained using (modified) EMPIRE-II code (v. 2.19) are drawn here. One should emphasize that the γ spectra drawn here are the coincident ones with the transition to the $f_{7/2}$ state. As was already noted in [20], the use of statistical approaches (including the pre-equilibrium ones) is very dangerous near the closed shells — and the target here is a doubly-magic nucleus. One should be very careful about the level densities used, and even thus we could not reproduce the experimental spectra satisfactorily. Specifically, the continuous part (that close to the GDR energy, i.e. around 13 MeV) comes out from the pre-equilibrium calculations less important than is seen in the experiment. The CDS calculation is much favourable here, as it assumes treating the states as single-particle ones, what is really a very good approximation in the lead region. Anyway, even the CDS description is far from being completely satisfactory here, what is probably caused by the insufficient treatment of the optical potential for this problem (see also preliminary indication of this influence in [21]). That effect — though usually minor as for its influence — calls for a great attention because of its underlying significance.

Conclusions

The pre-equilibrium model of γ emission depicts the same reality which is contained in the direct-semidirect model, but using statistical approach. Two excellent computer codes, EMPIRE v. 2.19 and TALYS, yield similar results far off the closed shells. In their vicinity, their predictive power weakens and discrepancies become large. The direct-semi-direct model (in its CDS version) performs much better here, but even that calls for some updating of the approaches.

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4 The original paper by Snover [22] brings data which differ by a factor of 2 from those used now [19, 25].
5 As the experimental data are only in counts per channel, the theoretical spectra have normalized to the data.
FIGURE 4. High-energy part of the $\gamma$ spectra from $^{208}$Pb+p at 15.7 MeV, normalized to the experimental cross section of the transition leading to the $f_{7/2}$ state in $^{209}$Bi. Experimental points and also the original calculations (CDSD plus statistical) from [23] are also presented here.