Available online at www.sciencedirect.com
ScienceDirect
Nuclear Data Sheets 118 (2014) 276–279
Nuclear Data Sheets
www.elsevier.com/locate/nds

Exclusive Multiple Emission Cross Sections in the Hybrid Monte Carlo Pre-equilibrium Model and in EMPIRE-3.1

B.V. Carlson,[1,*] L. Brito,[1] D.F. Mega,[1] R. Capote,[2] M. Herman,[3] and M.E. Rego[4]
[1] *Instituto Tecnológico de Aeronáutica, São José dos Campos SP, Brazil*
[2] *International Atomic Energy Agency, PO Box 100, Vienna-A-1400, Austria*
[3] *National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
[4] *Instituto de Pesquisas Energéticas (IPEN), São Paulo SP, Brazil*

We discuss the general concept of exclusive emission cross sections and spectra and the exclusive spectra of the ENDF library. We briefly review the exclusive hybrid Monte Carlo simulation model and show how its exclusive cross sections can be integrated into the reaction code EMPIRE-3.1. We close by discussing several examples.

I. INTRODUCTION

Exclusive emission spectra and angular distributions provide detailed information about a reaction. Such information can be provided for certain multiple emission spectra and angular distributions in the ENDF library and are of some interest, at least at low energies. Exclusive quantities are trivial to calculate in Monte Carlo codes where all emissions can be tracked. They are slightly more difficult to calculate in conventional statistical equilibrium codes. Here we show how this calculation can be performed and how the pre-equilibrium stage of the reaction can be easily integrated into the subsequent decay chain, as is done in the EMPIRE-3.1 reaction code.

II. EXCLUSIVE CROSS SECTIONS

A completely exclusive cross section can be defined as one in which all observables of the final state are well defined (uncertainty permitting). As an example, consider nucleon-nucleus scattering. The observables of the completely exclusive cross section would be the neutron spin projection and linear momentum, and the total nuclear spin, spin projection, linear momentum, excitation energy, charge and mass number.

Conservation laws make some observables redundant. In general, one final momentum is redundant if the momenta of all other emitted particles and that of the residual nucleus are known. The residual nucleus excitation energy is redundant if all momenta and any other excitation energies are known. The charge and mass number of the residual nucleus is determined by the charge and mass numbers of the emitted particles.

However, what is usually of interest to us, in particular, in the case of ENDF files, is a more 'inclusive' exclusive cross section. This is the emission cross section associated with the production of a particular residual nucleus. It can obtained by summing all contributions to the particle bound states of the nucleus of interest that involve emission of the desired particle. As an example, consider the exclusive two-neutron emission cross section for the decay $Z,\ A \to Z,\ A-2$. This cross section sums both of any two neutron emissions that leave the nucleus Z, A-2 with excitation energy E* below the particle emission threshold. It also includes the contributions of two neutron emissions above the threshold that are followed by by photon emission that lowers the residual excitation energy below the threshold.

Exclusive emission cross sections are actually simply related to the production cross sections of residual nuclei. Of more interest are exclusive emission spectra and angular distributions, which are not. Exclusive multi-particle spectra and angular distributions cannot be transformed between the lab and CM frames and must be calculated in the desired frame, which is usually the laboratory one.

Let us consider several examples:

- For the exclusive one neutron emission cross section, the occupations of states below particle emission threshold in the residual nucleus contribute. As one neutron is emitted fo form each residual nucleus, the exclusive emission cross section is identical to the production cross section,

$$\sigma_{x,n}(Z, A-1) = \sigma_{prod}(Z, A-1). \tag{1}$$

---

[*] Corresponding author: brett@ita.br

http://dx.doi.org/10.1016/j.nds.2014.04.057

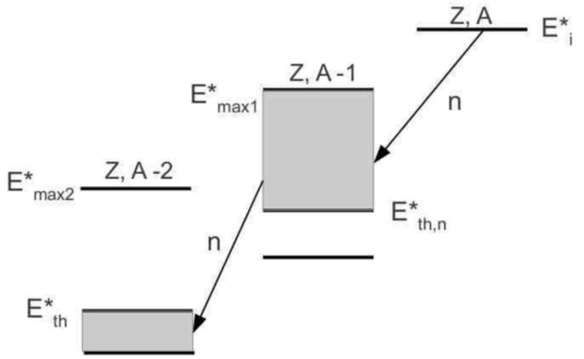

FIG. 1. Level graph of exclusive two-nucleon transition.

- For the exclusive two neutron emission cross section, the states above the neutron emission threshold in the the first residual nucleus and below the particle emission threshold in the second residual nucleus contribute, as shown in Fig. 1. As two neutrons are emitted for each residual nucleus formed, we have

$$\sigma_{x,n}(Z,A-2) = 2\sigma_{prod}(Z,A-2). \tag{2}$$

- Finally, consider the exclusive neutron (proton) cross section in the reaction $Z,\, A \rightarrow Z-1,\, A-2$. Here, there are two contributions to the exclusive neutron cross section:
  - Neutron emission to the states above the proton emission threshold in $Z,\, A-1$ followed by proton emission to the particle bound states of $Z-1,\, A-2$;
  - Proton emission to the states above the neutron emission threshold in $Z-1, A-1$ followed by neutron emission to the particle bound states of $Z-1,\, A-2$.

  Here, one neutron and one proton are emitted for each residual nucleus, except for those formed by deuteron emission, so that

$$\begin{aligned} \sigma_{x,n}(Z-1,A-2) &= \sigma_{x,p}(Z-1,A-2) \\ &= \sigma_{prod}(Z-1,A-2) \qquad (3) \\ &\quad -\sigma_{x,d}(Z-1,A-2)\,. \end{aligned}$$

III. THE HMS MODEL

The hybrid Monte Carlo simulation (HMS) model was proposed by Blann [1] and later extended by Blann and Chadwick[2] to produce double differential cross sections. The HMS model provides a more physically consistent description of the early stages of a nucleon-induced reaction than the exciton and hybrid models provide[3, 4]. It uses only the densities of available states for creation and decay of single particle-hole pairs. It considers holes and particles as independent modes of excitation and neglects interactions among the excited particles and holes. Holes and particles can scatter with other particles below the Fermi energy to form more particle-hole pairs and particles with sufficient energy can be emitted. An additional advantage of the HMS model compared to earlier ones is that it easily permits the calculation of multiple emissions from the precompound nucleus.

The Monte Carlo decay algorithm used by Blann and Chadwick does not permit the calculation of exclusive cross sections because it does not take into account the relative rate of decay of the particle-hole pairs produced in the excitation process. This is easily remedied. In the exclusive HMS, holes and particles decay and particles are emitted in accord with the partial widths for each process[7]. For particles, the partial widths for decay and escape are taken to be, respectively,

$$\Gamma^{\downarrow}(\vec{p}) = \frac{1}{2}\frac{p}{m}\sigma_{NN}\,\rho_0\,P_{pauli}(p), \tag{4}$$

$$\Gamma^{\uparrow}(\vec{p}) = \frac{(2m+e)\,e\,\sigma\,(e)}{2\pi^2\hbar^2 g_{lev}\,(\varepsilon)}\,, \tag{5}$$

At each step of the simulation, either

1. a particle is emitted; or

2. a particle or hole scatters to a 2p-1h or 1p-2h state. Unlike Blann, we immediately determine the momenta of the new particles and holes and subsequently consider them as independent modes.

The simulation of a HMS event is stopped when the remaining particles and holes each have insufficient energy for further particle emission.

IV. EXCLUSIVE CROSS SECTIONS IN THE HMS MODEL AND IN EMPIRE-3.1

Exclusive cross sections are easily obtained from a Monte Carlo simulation such as the HMS. One needs only to keep track of the particles emitted and the residual nucleus in each event. When an HMS event is stopped, however, although the remaining particles and holes each have insufficient energy to be emitted, the total excitation energy is still often sufficient for further particle emission. Further emissions are accounted for using an equilibrium statistical emission model. In EMPIRE-3.1[8], statistical particle emission is calculated using the Hauser-Feshbach model.

Denoting the observables of the initial and final nucleus of a H-F statistical emission as α' and α and those of the emitted particle as β, the branching ratio for the corresponding transition is

$$\Pi(\alpha,\alpha';\beta) = \frac{\tau(\alpha,\alpha';\beta)}{\sum_{\tilde{\beta},\tilde{\alpha}}\int de_{\tilde{\beta}}\,\tau(\tilde{\alpha},\alpha';\tilde{\beta})}, \qquad (6)$$

where

$$\tau(\alpha,\alpha';\beta) = \qquad (7)$$
$$\frac{(1+(-1)^{l_\beta}\pi_\alpha\pi_{\alpha'})}{2}\rho(E^*_\alpha, I_\alpha, \pi_\alpha)T_\beta^{j_\beta l_\beta}(\varepsilon_\beta).$$

The production cross sections $d\sigma_{prod}(\alpha)$ of the daughter nucleus in the state α are calculated using the branching ratios as

$$d\sigma_{prod}(\alpha) = \sum_{\alpha',\beta}\Pi(\alpha,\alpha';\beta)\,d\sigma_{prod}(\alpha') \qquad (8)$$
$$+d\sigma_{prod,0}(\alpha),$$

The contribution from CN formation, direct or pre-equilibrium processes, denoted by $d\sigma_{prod,0}$ is the only contribution to the population of the initial compound nucleus. Daughter nuclei in the chain have a contribution (or contributions) from particle emission, as well as a possible contribution from $d\sigma_{prod,0}$, when direct or pre-equilibrium processes occur.

Completely exclusive cross sections $d\sigma_x(\beta,\alpha)$, in which the emission of the particle β furnishes a daughter nucleus in the state α, can be calculated similarly as

$$d\sigma_x(\beta,\alpha) = \sum_{\alpha'}\Pi(\alpha,\alpha';\beta)\,d\sigma_{prod}(\alpha') \qquad (9)$$
$$+\sum_{\alpha',\beta'}\Pi(\alpha,\alpha';\beta')\,d\sigma_x(\beta,\alpha')$$
$$+d\sigma_{x0}(\beta,\alpha).$$

Here there are three contributions:

1. One in which the final emission is of a particle β;
2. Another taking into account all earlier emissions of β and a final emission of any possible particle; and
3. Finally, a possible direct / pre-equilibrium contribution $d\sigma_{x0}$.

In EMPIRE-3.1, the production cross sections $d\sigma_{prod}(\alpha)$ are calculated using the Hauser-Feshbach branching ratios. To reduce storage requirements, the completely exclusive cross sections $d\sigma_x(\beta,\alpha)$ are calculated using the Weisskopf approximation. They thus keep track of excitation and emission energies but not angular momenta and parities.

Here we give two examples, showing the typical behavior of the 2-neutron and 3-neutron exclusive emission spectra obtained from HMS simulations followed by equilibrium statistical emission. In Fig. 2, we display the two-neutron exclusive emission spectrum of the reaction ^{59}Co(p,3n)^{58}Ni at proton energies of 50, 100 and 200 MeV, while in Fig. 3, we display the three-neutron exclusive emission spectrum of the reaction ^{59}Co(p,3n)^{57}Ni at the same proton energies.

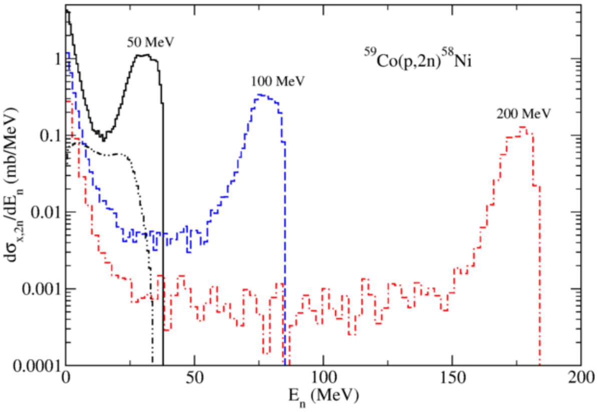

FIG. 2. The exclusive two-nucleon emission spectrum of the reaction ^{59}Co(p,2n)^{58}Ni at three different bombarding energies.

At 100 and 200 MeV, both emission spectra have two peaks - a high-energy one corresponding to pre-equilibrium emission and a low-energy one corresponding to equilibrium emission. The contribution from pure equilibrium emission is negligible at these energies. The pure pre-equilibrium emission spectrum is flat and is of the same magnitude as the flat middle section of the shown spectra. Thus, the dominant physical process contributing to these cross sections is an initial pre-equilibrium emission followed by one (two-neutron spectra) or two (three-neutron spectra) equilibrum emissions.

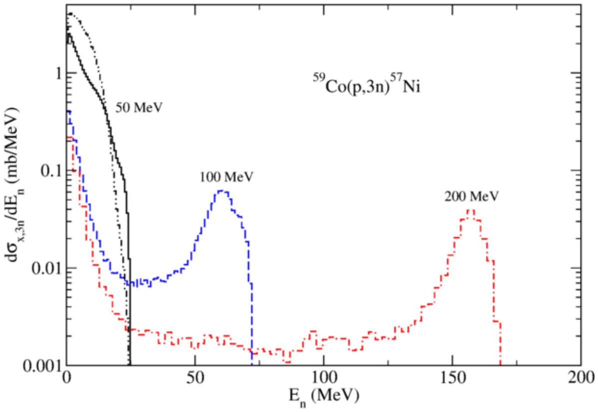

FIG. 3. The exclusive three-nucleon emission spectrum of the reaction ^{59}Co(p,3n)^{57}Ni at three different bombarding energies.

At 50 MeV, the two-neutron emission spectrum displays two peaks while the three-neutron spectrum does not. For this energy, the pure equilibrium spectra are also displayed as dashed-double-dotted lines in the figures. As this energy is near the peak energy of the pure equilibrium three-neutron emission cross section, the equilibrium spectrum is of the same order of magnitude as pre-equilibrium + equilibrium one. This two-neutron emission cross section, on the other hand, has its maximum at a much lower energy. It already displays the typical high energy structure of equilibrium and pre-equilibrium peaks.

V. CONCLUSIONS

We have modified the HMS model in order to obtain exclusive multiple emission cross sections. These have been integrated into the statistical decay chain in EMPIRE-3.1 to allow the calculation of exclusive spectra and angular distributions. At energies far above their evaporation peaks, single emission exclusive cross sections are determined by pre-equilibrium/direct contributions alone. In contrast, at energies far above their evaporation peaks, multiple emission exclusive cross sections are dominated by the combination of a pre-equilibrium / direct emission followed by equilibrium emissions. Exclusive multiple emission spectra are characterized by a low-energy evaporation peak and a high-energy equilibrium / direct emission peak.

Acknowledgements: BVC acknowledges partial support from the Brazilian research funding agencies FAPESP, the CNPq and CAPES. DFM and LB acknowledge support from CAPES. MER acknowledges partial support from the CNPq.

[1] M. Blann, Phys. Rev. C **54**, 1341 (1996).
[2] M. Blann, M.B. Chadwick, Phys. Rev. C **57**, 233 (1998).
[3] J. Bisplinghoff, Phys. Rev. C **33**, 1569 (1986).
[4] C.A. Soares Pompéia, B.V. Carlson, Phys. Rev. C **74**, 054609 (2006).
[5] J.J. Griffin, Phys. Rev. Lett. **17**, 57 (1966).
[6] M. Blann, Phys. Rev. **21**, 1357 (1968).
[7] B.V. Carlson, D.F. Mega, EPJ Web of Conferences **21**, 09001 (2012).
[8] M. Herman *et al.*, Nucl. Data Sheets **108**, 108 (1997); EMPIRE-3.1, available online at http://www.nndc.bnl.gov/empire/.