Extending ENDF Procedures to Handle Photon Channels and Light Charged Particles Using Relativistic Kinematics

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1 Introduction

The current ENDF procedure for computing the energy of a primary photon from capture uses the following approximation:

$$E'_\gamma = E_\gamma + \frac{A}{A+1} E \tag{1}$$

where E_γ is given in File 12 and the option LP=2 is used. Normally, a section of File 14 is also present that states that the photon is emitted isotropically in the lab frame.

However, our new evaluation for neutrons incident on ^{1}H proposed for ENDF/B-VII gives an anisotropic center of mass angular distribution for the capture photon in File 6, and it specifies that the deuteron produced by the capture is to be handled as a discrete recoil particle from the photon emission. This case cannot be handled using the current ENDF description of primary photon production, and the kinematics of the reaction cannot be described using the formulas in Appendix E. Proper relativistic methods must be used.

The reverse of this capture reaction is the photon induced breakup of the deuteron. This process should also be described using proper relativistic methods.

Similar problems will occur in the future for the capture reactions on ^{2}H and ^{3}He, and for the photo breakup of ^{3}H and ^{4}He. Things get a little more complicated starting with ^{6}Li, because there will be more than one primary photon. An extension to the File 6 format would be required in those cases. We anticipate that the kind of data now being proposed for ^{1}H will also become available for targets up to ^{9}Be over the next few years.

For these reasons, we have derived a set of relativistic kinematics formulas to describe reactions with photons in either the entry or exit channel. These formulas can also be used to add relativistic effects for reactions among light particles. We propose that these relativistic formulas be added to Appendix E and that the language in the manual be revised in several places to explain how to the relativistic methods. We also propose an extension to the File 6 format to handle angular distributions and recoil behavior for multiple primary photons. See below for the details.

2 The Relativistic Effects for Photon Channels

Our normal procedures for a primary capture photon like the 2.224 MeV event for n+^{1}H capture emits the photon as a discrete line with the energy given by Eq.1 isotropically in the lab frame. The recoil deuteron moves straight ahead in the lab frame with energy $E/(A+1)$. The following table shows what happens when the relativistic formulas are used:

E(MeV)	μ	ω_γ	E_γ(MeV)	ω_r	E_r(MeV)
.100	-1.0	-1.0000	2.256	1.0000	.0679
	0.0	.0073	2.273	.9865	.0513
	1.0	1.0000	2.289	1.0000	.0348
2	-1.0	-1.0000	3.117	1.0000	1.107
	0.0	.0326	3.222	.9986	1.002
	+1.0	+1.0000	3.327	1.0000	.897
10	-1.0	-1.0000	6.695	1.0000	5.529
	0.0	.0729	7.221	.9986	5.003
	1.0	1.0000	7.746	1.0000	4.478
100	-1.0	-1.0000	40.464	1.0000	61.760
	0.0	.2249	52.203	.9932	50.021
	1.0	1.0000	63.942	1.0000	38.282

Note that the discrete photon line broadens, and that its angular distribution shifts slightly forward. Similarly, there is now a spread in the recoil energies, although the recoil direction remains very close to forward.

The relativistic broadening effect decreases with increasing target mass. Here is a table for the more energetic of the two primary photons in ^{7}Li:

E(MeV)	μ	ω_γ	E_γ(MeV)	ω_r	E_r(MeV)
.100	-1.0	-1.0000	2.116	1.0000	.012
	0.0	.0018	2.120	.9883	.013
	+1.0	1.0000	2.124	1.0000	.009
10	-1.0	-1.0000	10.567	1.0000	1.466
	0.0	.0184	10.765	.9969	1.268
	+1.0	1.0000	10.962	1.0000	1.070
100	-1.0	-1.0000	83.385	1.0000	18.648
	0.0	.0587	88.587	.9804	13.445
	+1.0	1.0000	93.790	1.0000	8.243

3 Format Extensions to Support Multiple Primary Photons

For ^{6}Li, ^{7}Li, and ^{9}Be, the current ENDF evaluations provide for two primary photons, one to the ground state, and one to the first level, which is followed by a second photon going the rest of the way to the ground state. Projected new evaluations for these nuclides will provide different center-of-mass angular distributions for these two primary photons. These will result in two different energy-angle distributions for the recoil nucleus also.

We propose to handle this in File 6. The first subsection would give the angular distribution for the most energetic primary photon (the one going to the ground state) with ZAP=0 and AWP equal to the photon energy. The second subsection would describe the recoil from this photon emission as a discrete two-body event. The next subsection would describe the angular distribution for the primary photon going to the first level, including giving its energy in the AWP field. The next subsection would be another recoil description. This would be followed by a subsection giving the spectrum of the gamma cascade from that level. This pattern would continue until all the primary photons have been described. In this way, all the correlations would be preserved.

4 Changes to Chapter 6

change first line on page 6.2...

AWP Product mass in neutron units. When ZAP=0, this field can contain the energy of a primary photon. In that case, this section will contain an angular distribution (LAW=2) for the primary photon.

add before last line on page 6.2...

> An exception to this ordering is made when capture primary photons are being described. Then the ordering is (1) angular distribution of primary photon to ground state (LAW=2), (2) corresponding recoil (LAW=4), (3) angular distribuiton of primary photon to first excited state, (4) corresponding recoil, (5) energy distribution of cascade photons from first excited state (LAW=1 delta function), and so on, until all primary photons have been described.

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> In addition, LAW=2 can be used to give the angular distributions for primary photons in sections with MT=102.

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> , or when detailed angular distributions are given for primary photons.

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> A special represention of primary capture photons for light isotopes is allowed using MT=102. The first subsection gives the angular distribution in the center of mass for the primary photon to the ground state using LAW=2. The next subsection gives the two-body recoil for this event using LAW=4. This is followed by a subsection giving the angular distribution for the primary photon to the first excited state and a subsection giving the corresponding recoil. The next subsection gives the energy spectrum of the gamma cascade from deexciting this level using LAW=1, NA=0, and ND=NEP discrete photon lines. This pattern is continued until all the primary photons have been described. In each section with LAW=2, ZA=0 and the AWP field

contains the energy of the primary photon. The laboratory energies and cosines for the primary gamma and its corresponding recoil particle must be computed using relativistic kinematics as described in Appendix E.

5 Changes to Appendix E

add after Figure E.2....

When the masses are small and the energies large, or when either m_1 or m_2 is a photon, it is appropriate to use relativistic kinematics. A good example of the this is calculating the energy and emission angle for the photon from neutron capture on ^{1}H as the center of mass cosine μ varies over its range. Another example is the distributions for the products of the photo breakup of the deuteron. Define

$$\begin{aligned}
\mathrm{AWR} &= \text{target mass ratio to the neutron,} && (2)\\
\mathrm{AWRI} &= \text{projectile mass ratio to the neutron,} && (3)\\
\mathrm{AWRP} &= \text{product mass ratio to the neutron, and} && (4)\\
Q &= \text{reaction Q value.} && (5)
\end{aligned}$$

The following equations can be used to compute the quantities shown in Figure E.2:

$$\begin{aligned}
m &= m_{\mathrm{neutron}}c^2 = 939565.6\,\mathrm{eV} && (6)\\
m_1 &= \mathrm{AWRI}\,m && (7)\\
m_2 &= \mathrm{AWR}\,m && (8)\\
m_3 &= \mathrm{AWRP}\,m && (9)\\
m_4 &= m_1 + m_2 - m_3 - Q && (10)\\
s_i &= m_1 + m_2 && (11)\\
d_i &= m_1 - m_2 && (12)\\
s_f &= m_3 + m_4 && (13)\\
d_f &= m_3 - m_4 && (14)\\
s &= s_i^2 + 2m_2E_1 && (15)\\
k_i^2 &= \frac{(s - s_i^2)(s - d_i^2)}{4s} && (16)
\end{aligned}$$

$$k_f^2 = \frac{(s-s_f^2)(s-d_f^2)}{4s} \tag{17}$$

$$z_2 = \sqrt{k_i^2 + m_2^2} \tag{18}$$

$$z_3 = \sqrt{k_f^2 + m_3^2} \tag{19}$$

$$z_4 = \sqrt{k_f^2 + m_4^2} \tag{20}$$

$$E_3 = \frac{z_2 z_3 + \sqrt{k_i^2 k_f^2}\mu}{m_2} - m_3 \tag{21}$$

$$E_4 = \frac{z_2 z_4 - \sqrt{k_i^2 k_f^2}\mu}{m_2} - m_4 \tag{22}$$

$$p_1^2 = E_1^2 + 2m_1 E_1 \tag{23}$$

$$p_3^2 = E_3^2 + 2m_3 E_3 \tag{24}$$

$$p_4^2 = E_4 + 2m_4 E_4 \tag{25}$$

$$\omega_3 = \frac{(E_1+s_i)(E_3+m_3) - z_3\sqrt{s}}{\sqrt{p_1^2 p_3^2}} \tag{26}$$

$$\omega_4 = \frac{(E_1+s_i)(E_4+m_4) - z_4\sqrt{s}}{\sqrt{p_1^2 p_4^2}} \tag{27}$$

where the k quantities are center-of-mass momenta, and the p quantities are lab momenta. The symbol z is used instead of the more conventional ω because of the conflict with the symbol used for laboratory cosines in Figure E.2.

6 Conclusions

It should be noted that the capture cross sections are very small at the energies where the relativistic effects become interesting, so these improvements in the ENDF representation may not have striking practical results. However, the physics models that produce these evaluations do evaluate these effects, and we feel that it is important not to throw away the physics when we format the data.

The new formats and kinematics formulas will impact both processing codes and Monte Carlo transport codes. At Los Alamos, NJOY will require changes in the HEATR module for heating and damage calculations, in the GROUPR module for producing nγ and photonuclear matrices, and in the

ACER module for providing libraries for the MCNP Monte Carlo transport code. MCNP will require changes to implement the relativistic kinematics.

For people only interested in fairly low energies, it would be easy to write a filtering routine that would strip out the MT=102 section of File 6 and write corresponding sections of MF=12 and 14 (approximated as isotropic) in its place. Then the old methods could be used from there on.