Annals of Nuclear Energy 96 (2016) 170–175

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Relativistic kinematics for photoneutron production in Monte Carlo transport calculations

Edmund Caro

Bechtel Marine Propulsion Corporation – Knolls Atomic Power Laboratory, P.O. Box 1072, Schenectady, NY 12301, United States

ARTICLE INFO

Article history:
Received 1 February 2016
Received in revised form 25 April 2016
Accepted 29 April 2016
Available online 1 July 2016

Keywords:
Photon
Neutron
Photonuclear
Photoneutron
Gamma

ABSTRACT

MC21 is a continuous-energy Monte Carlo radiation transport code for the calculation of the steady-state spatial distributions of reaction rates in three-dimensional models. The code supports neutron and photon transport in fixed source problems, as well as iterated-fission source (eigenvalue) neutron problems. The capability to simulate the production of photon-induced neutrons has been added to the code. In this paper, relativistic two-body kinematics are used to derive exact expressions for the secondary energy and angle distribution of photoneutrons. This treatment, implemented in MC21, is important in cases where the evaluated photonuclear data does not give an explicit energy distribution. Comparisons of the relativistic relations were made to approximations in MCNP5 and TRIPOLI-4, highlighting the magnitude of the error of those approximations.

1. Introduction

MC21 is a Monte Carlo neutron and photon transport code under joint development by Bechtel Marine Propulsion Corporation at the Knolls Atomic Power Laboratory and the Bettis Atomic Power Laboratory (Griesheimer et al., 2013). MC21 is the Monte Carlo transport kernel of a system of codes that provides an automated, computer-aided modeling and post-processing environment. In photon transport calculations, typically, the reactions simulated are the photoatomic reactions such as photoelectric, incoherent (Compton) scattering, coherent scattering, and pair production. In cases where the energy of the source photons are high, in the MeV range, photonuclear interactions need to be taken into account in transport simulations. These photons can interact with nuclides above the threshold of a photoneutron reaction and induce the production of neutrons. Sources of high energy photons include the decay of fission products and activation nuclides in a nuclear reactor or from spent fuel. These photons can subsequently interact with deuterium in heavy water or with a beryllium reflector, for example, thus producing neutrons from a photoneutron reaction. The production of photoneutrons can be an important source of neutrons in a reactor or in certain reactor component scenarios, depending on the gamma sources present and the material composition. For a full description of the photoatomic interaction physics as implemented in MC21, the reader is referred to Griesheimer et al. (2013). As a brief summary, MC21 uses continuous energy transport of photons and treats all common photon interaction mechanisms, including Compton scattering, coherent scattering, pair production, and photoelectric interactions. It also employs a thick-target bremsstrahlung approximation. Electron transport is not explicitly treated.

For each nuclide having photonuclear data, the ENDF file (Herman et al., 2012) specifies both the cross sections and secondary angle and energy distributions for outgoing neutrons from photoneutron reactions. In many cases, the evaluators have chosen to represent the outgoing energy and angle distributions as tabulated or parameterized functions. When this occurs, NJOY is able to produce secondary distribution data in the usual ACE-format laws (MacFarlane et al., 2012); consequently MC21 uses the same sampling routines as it would use for incident neutron reactions that have a neutron in the exit channel. There is one particular ENDF product energy-angle distribution that requires further efforts in order to faithfully represent the collision physics. When the distribution is specified as a discrete two-body scattering distribution (MF = 6, LAW = 2), NJOY processes the data to provide a tabulated angle distribution in the ACE-format data, but it is left to the Monte Carlo code to decide how to calculate the exiting neutron energy. In ENDF/B-VII.1 data, two-body scattering is specified for photoneutron reactions in ^{2}H, ^{12}C, ^{16}O, ^{51}V, ^{180}W, and ^{183}W. As will be discussed later, Monte Carlo codes have adopted different methods for how to calculate the exiting photoneutron energy for two-body events. This paper describes the photonuclear reaction for a (γ,n) event or the photon-induced production of a neutron in the exit channel. Section 2 describes how the energy

E-mail address: edmund.caro@unnpp.gov

http://dx.doi.org/10.1016/j.anucene.2016.04.049
0306-4549/

and direction for a particle emerging from a two-body collision of a (γ,n) reaction can be determined rigorously using relativistic kinematic relations. Sections 2.2 and 2.3 applies these relations to describe the two-body kinematics used for obtaining the exiting neutron energy and direction from the photoneutron reaction $X(\gamma,$ n)Y. Section 3 describe the comparisons with photoneutron kinematics approximations used in other Monte Carlo codes.

2. Two-body interaction applied to photoneutron reactions

In MC21, the exiting neutron energy and direction for photoneutron reactions are obtained from relativistic two-body kinematics. The relations used for calculating the kinematic quantities are exact and are not specific to any particular reaction.

2.1. Overview of relativistic kinematics

A four-vector is defined as a line segment with direction in four-dimensional spacetime in the same way as a three-dimensional vector (to be referred to as a three-vector) can be defined as a line segment with direction in three-dimensional Euclidean space. This quantity contains a time component and three spatial components. Four-vectors can be added, subtracted, and multiplied by numbers in agreement to the standard rules for vectors. The length of a four-vector is the absolute value of the spacetime distance between its tail and its tip, and is not specific to any inertial frame. The length of four-vectors are invariant (the quantity does not change) in all inertial frames, and that is the usefulness and importance of four-vectors (Landau and Lifshitz, 1971; Hartle, 2003).

The relations used for calculating the kinematic quantities are exact and are not specific to any particular reaction. While a full derivation of the relations used in MC21 for relativistic kinematics is beyond the scope of this paper, the most important points and formulas are highlighted.

The contravariant components of the four-momentum vector for a particle of mass m and velocity $\vec{v}$ are defined as

$$\boldsymbol{P}^{\mu} = (\gamma mc, \gamma m\vec{v}). \tag{1}$$

where the Lorentz factor, γ, is

$$\gamma = \frac{1}{\sqrt{1-\left(\frac{d\vec{r}}{dt}\right)^2/c^2}} = \frac{1}{\sqrt{1-\left(\frac{\vec{v}}{c}\right)^2}} = \frac{1}{\sqrt{1-\beta^2}}. \tag{2}$$

The first term on the right-hand side of Eq. (1) is related to the total energy of the particle, $E=\gamma mc^2$. The second term on the right-hand side of the equation is the momentum of the particle, $\vec{p} = \gamma m\vec{v}$. Eq. (1) is therefore equivalent to the following expression.

$$\boldsymbol{P}^{\mu} = \left(\frac{E}{c}, \vec{p}\right). \tag{3}$$

The covariant components of the four-momentum vector are

$$\boldsymbol{P}_{\mu} = \left(\frac{E}{c}, -\vec{p}\right). \tag{4}$$

The term E in Eqs. (3) and (4) is the sum of the kinetic energy and the rest-mass equivalent energy of the particle

$$E = T + mc^2. \tag{5}$$

From Eqs. (3) and (4), we have the square of the four-momentum of a free particle

$$\boldsymbol{P}_{\mu}\boldsymbol{P}^{\mu} = \frac{E^2}{c^2} - p^2, \tag{6}$$

where $p = \|\vec{p}\|$. From Eqs. (3) and (4),

$$\boldsymbol{P}_{\mu}\boldsymbol{P}^{\mu} = m^2c^2. \tag{7}$$

This result is an invariant since it does not change under a rotation or a Lorentz transformation of the four-dimensional coordinate system. Equating Eqs. (6) and (7) yields the energy, mass, momentum relation

$$E^2 = p^2c^2 + \left(mc^2\right)^2. \tag{8}$$

2.2. Two-body interaction applied to photoneutron reactions

In this section we describe the general two-body interaction mechanics and its application to a photon interacting with a nuclide where a neutron and a residual nuclide are produced, represented by $X(\gamma,\text{n})Y$. We solve for the exiting neutron energy and direction using relations described in the previous section and applying techniques used at high energy physics laboratories for solving kinematics problems (Hagerdorn, 1980; Olive, 2014).

Let us represent the interaction $X(\gamma,\text{n})Y$ in terms of particle masses as $m_1(m_2,m_3)m_4$, where m_1 is the target nucleus mass, m_2 is the incident particle mass, m_3 is the emergent particle mass, and m_4 is the residual nucleus mass. It is assumed that the particles and nuclei are not excited (ground state). Consider a reaction in the laboratory frame of reference where a particle m_2 that collides with particle m_1, initially at rest, results in two exiting particles, m_3 and m_4.

The four-momentum contravariant vector for the reacting particles is

$$\boldsymbol{P} = \left(\frac{E_1+E_2}{c}, \vec{p}_1 + \vec{p}_2\right). \tag{9}$$

Since the target nucleus (m_1) is at rest, $\vec{p}_1 = 0$, $T_1 = 0$, and $E_1 = m_1c^2$ resulting in

$$\boldsymbol{P} = \left(\frac{m_1c^2+E_2}{c}, \vec{p}_2\right). \tag{10}$$

The four-momentum squared is invariant, and applying this to the reacting particles one obtains

$$s = \boldsymbol{P}\cdot\boldsymbol{P} = \boldsymbol{P}_{\mu}\boldsymbol{P}^{\mu}. \tag{11}$$

Applying Eq. (8) to Eq. (11) for particle 2, the invariant quantity is now expressed as

$$s = m_1^2c^2 + m_2^2c^2 + 2m_1E_2. \tag{12}$$

E_2 can be substituted with the rest-mass equivalent energy plus the kinetic energy to yield

$$s = (m_1c + m_2c)^2 + 2m_1T_2 \tag{13}$$

In this paper an apostrophe is used to denote a particle quantity in the center-of-mass (COM) frame of reference. In the center-of-mass frame of reference the momenta of m_1 and m_2 are equal and opposite. Therefore the total momentum is equal to zero. The momenta of m_3 and m_4 are also equal and opposite. The four-momentum vector in the center-of-mass frame of reference for the pre-collisions system is

$$\boldsymbol{P}_{cm} = \boldsymbol{P}'_1 + \boldsymbol{P}'_2 = \left(\frac{E'_1+E'_2}{c}, 0\right). \tag{14}$$

The Lorentz invariant s does not change from one frame of reference to another, as it is the scalar product of a four-vector. In the center-of-mass reference frame one obtains

$$s = \boldsymbol{P}_{cm}\cdot\boldsymbol{P}_{cm} = \left(\frac{E\prime_1+E\prime_2}{c}\right)^2 = \frac{E_{cm}^2}{c^2}, \tag{15}$$