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A METHOD FOR PROCESSING ENDF/B PHOTON FORM FACTOR DATA†

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In many reactor and shielding applications, the transport of low energy photons is of little consequence; hence, methods[1,2] are widely employed which use the Klein-Nishina formalism as the basis of multigroup photon cross section calculations. The Klein-Nishina expression neglects the coherent scattering effects which exist at energies comparable to the binding energies of atomic electrons and can lead to calculational errors for those few applications which have important low energy contributions.

The DINT[3] code was written at Sandia to produce multigroup matrices which have proper treatments of low energy transport. DINT is characterized by double numerical integrations in energy and by its very complete evaluated library. In this library, all important photon cross sections have been parameterized in a manner to minimize the amount of data required to represent cross sections from very low energies to 20 MeV and above.

In response to the needs of the ENDF/B user community for low energy data, a new ENDF/B evaluation[4] has been recently released. This library uses the normal schemes for representing energy and angular distributions; viz., Legendre fits and tabulated arrays are employed. Form factor data is given in "File 27".

This paper describes a method for processing the ENDF/B photon data

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to generate group-to-group scattering matrices. The method has the following salient features:

1. It is tailored toward treating the full energy and angular detail with which the cross sections are represented in ENDF/B.
2. It is simple to program.
3. It closely parallels a treatment[5] developed for producing multigroup neutron matrices.
4. The time required to execute the method on a computer varies linearly with the number of energy groups as opposed to double numerical integration schemes which tend to vary as the square of the number of groups.

A group-to-group transfer term for photon incoherent or coherent scattering can be written:

$$\sigma_\ell(g\to g') = \frac{\int_{E\epsilon g}^{dE} \phi_\ell(E) \int_{E'\epsilon g'} dE'\ \sigma_\ell(E\to E')}{\int_{E\epsilon g} dE\ \phi_\ell(E)} \tag{1}$$

where $\sigma_\ell(E\to E')$ is the ℓth term of a Legendre fit to the cross section. This term can be written:

$$\sigma_\ell(E\to E') = \frac{2\ell+1}{4\pi} \int_{-1}^{1} d\mu\ P_\ell(\mu)\sigma(E,\mu)F(E,\mu)\delta(E\to E',\mu) \tag{2}$$

where $P_\ell(\mu)$ is the Legendre Polynomial at μ, $\sigma(E,\mu)$ is the coherent or the incoherent cross section at E for scattering through μ, $F(E,\mu)$ is the atomic form factor for coherent scattering or is the incoherent scattering function for Compton scattering, and $\delta(E\to E',\mu)$ is the "delta function" which serves to conserve energy and momentum.

When (2) is substituted into (1), a rather formidable expression is obtained. Consider what happens when the order of the integrals is changed so that the angular integration is outermost. For a single angle, μ_m, the δ-function determines what portion of group g can scatter to group g'. If a mechanical quadrature in angle is taken, the group-to-group terms can be written:

$$\sigma_\ell(g\to g') = \frac{\frac{2\ell+1}{4\pi} \sum_{m=1}^{M} W_m P_\ell(\mu_m) \int_{E_{low}(\mu_m,g')}^{E_{high}(\mu_m,g')} dE\ \sigma(E,\mu_m)F(E,\mu_m)\ \phi_\ell(E)}{\int_{E\varepsilon g} dE\ \phi_\ell(E)} \quad (3)$$

This expression contains no complicated "physics" except for the determination of the limits on the dE integral in the numerator, and these, of course, are determined through the δ-function.

The method lends itself to investigating a variety of numerical quadratures (trapezoidal, Simpson's, Gaussian, etc.) in angle. Presently, a 15th order Lobatto quadrature is employed with good results. The inner integral over energy is solved analytically for all possible products of the five functional representations allowed by ENDF/B with the exception of the product of interpolation types 4 and 5, which suffers from limited machine precision.

The principal advantages of using equation (3) are:

- its simplicity,
- its treats coherent and incoherent scattering, and
- any of the ENDF/B formalisms to present $\sigma(E,\mu)$ are easily accommodated in a manner which treats the full detail used to represent the energy variation.

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