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The Short-Collision-Time Approximation in ENDF

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Summary I

- The short-collision-time approximation (SCTA) is used in ENDF to extend the range of tabulated values of the incoherent inelastic cross section to higher values of α and β than can be calculated from the tabulated thermal neutron scattering law S(α,β,T).
- It’s usually attributed to Lamb (PR 55, 190, 1939) and paraphrased “at high values of energy and momentum transfer, the neutron scatters from a bound-atom as it would from a free gas at an effective temperature.”
- However, the formula introduced by the General Atomics team in the late sixties when they developed the ENDF files differs from that description, a fact which has led to considerable “discussion”.

Summary II

- We will display the GA formula, and for the record, five "alternative" forms which appear in ENDF-related documents:
  - "The NJOY Nuclear Data Processing System", LA-9303-M, Vol II (ENDF-324), May 1982 (currently available from RSIC)
  - "New Thermal Neutron Scattering Files for ENDF/B-VI Release 2", LA-12639-MS (ENDF 356), March 1994 (currently available from LANL)
  - "ENDF- 6 Formats Manual, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII", ENDF-102, BNL-NCS-44945-05-Rev June 2005 (currently available from NNDC)
  - Two "corrected" versions from the Formats Committee which have not yet been issued.

Introduction I

- The double-differential cross section in terms of the symmetrized Scattering Law, S(α,β,T), is (in ENDF notation)

$$\boldsymbol{d^2\sigma(E\rightarrow E',\mu,T)/dE'd\Omega = (\sigma_b/4\pi T)\,\sqrt{(E'/E)}\,\exp\text{-}(\beta/2)\,S(\alpha,\beta,T)}$$

in barns/steradian-eV with $\boldsymbol{\alpha=[E+E'-2\mu\sqrt{(EE')}]/AT}$ and $\boldsymbol{\beta=(E'-E)/T}$ the dimensionless momentum-squared and energy transfers. T is the temperature in eV and A=M/m.

- Detailed balance “DB” is defined (for our purposes) by:

$$\boldsymbol{M(E,T)\sigma(E\rightarrow E') = M(E',T)\sigma(E'\rightarrow E)}$$

where

$$\boldsymbol{M(E,T)=(E/T^2)\,\exp\text{-}(E/T)}$$

Introduction II

- DB is necessary and sufficient for the neutrons to achieve thermal equiibrium with the moderator. It is required of all ordinary moderators.
- Symmetry of ***$S(\alpha,\beta,T)$*** in beta is necessary and sufficient for the ***cross section*** to obey DB. That is what the factor ***$\exp-(\beta/2)$*** accomplishes on the preceding slide.
- DB is a thermodynamic statement about media in thermodynamic equilibrium. As such, it involves the ambient, thermodynamic temperature, regardless of what pseudo-temperatures may occur inside of $S(\alpha,\beta,T)$.

Introduction III

- The monatomic ideal gas Scattering Law is

$$S_{MIG}(\alpha,\beta,T) = [1/\sqrt{(4\pi\alpha)}]\ \exp-\{(\alpha^2+\beta^2)/4\alpha\}$$

- It is symmetric in β, so the cross section satisfies DB at the temperature T. The cross section is

$$d^2\sigma_{MIG}(E\rightarrow E',\mu,T)/dE'd\Omega = (\sigma_b/4\pi T)\ \sqrt{(E'/4\pi\alpha E)}\ \exp-\{(\alpha+\beta)^2/4\alpha\}$$

- If it is integrated over angles, the "total" cross section is

$$\sigma_{MIG}\ (E\rightarrow E') = (\sigma_b/E)\mathrm{erf}(\sqrt{(E'/T)}) \quad E'<E \quad \textit{downscatter}$$

$$\sigma_{MIG}\ (E\rightarrow E') = (\sigma_b/E)\mathrm{erf}(\sqrt{(E/T)})\ \exp-\{(E'-E)/T\} \quad E'>E \quad \textit{upscatter}$$

Introduction IV

- Since we are interested in high E and E'-values, the erf's are flat and the interesting thing is the upscattering tail ***exp-{E'-E)/T}*** that "drops off"more slowly as the temperature increases.
- For example, at a higher T*, the MIG cross section would be

$$d^2\sigma(E\rightarrow E',\mu,T^*)/dE'd\Omega = (\sigma_b/4\pi T^*)\ \sqrt{(E'/4\pi\alpha^* E)}\ \exp-\{(\alpha^*+\beta^*)^2/4\alpha^*\}$$

and would upscatter more, ***exp-{(E'-E)/T*}***

The GA Formula I

- The reference for this formula is “Neutron Scattering Kernels Calculations at Epithermal Energies”, GA-9950, UC-80, Reactor Technology, March 17, 1970, G. M. Borgonovi, Gulf General Atomic, Inc.
- In that report, equation (1) defines the double-differential cross section, and is the same definition as the one shown previously. It has a typographical error, in that the cross section is differential in dE although there is no E in the formula.
- Equation (2) has a typographical error. The symbol κ is used where β should be.
- Equation (3) has a typographical error. The symbol $S(\kappa,\omega)$ is used where “S-bar” should be.

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The GA Formula II

- To derive the SCTA, the following assumptions were made:
  - incoherent scattering
  - Gaussian approximation for the intermediate scattering function
  - Cubic Bravais crystal, harmonic motion

- The SCTA itself is "sin ωt = ωt; cos ωt = 1 – $(\omega t)^2/2$"

- The result is that the Scattering Law can be written as their Equation (13):

$$S_{SC}(\alpha,\beta,T) = [1/\sqrt{(4\pi\alpha T^*/T)}]\ \exp-\{((\alpha+\beta)^2)T/4\alpha T^* - \beta/2\},$$

- Although this does not have the free-gas form shown on the preceding slide, when substituted into the cross section formula, it produces a free-gas-at-T*, which was shown on Slide 3.

The GA Formula III

- That has two problems:
  - Since it satisfies DB at T*, it doesn’t satisfy it at T, where we want it.
  - It has an unphysically long upscatter tail, as shown on the following slide.

- Both of these defects can be remedied by re-defining the Scattering Law, which they did as follows:

$$S_{SC}(\alpha, \beta, T) \Longrightarrow$$

$$S_{SC}(\alpha, -|\beta|, T) = [1/\sqrt{(4\pi\alpha T^*/T)}]\ \exp-\{((\alpha + |\beta|)^2)T/4\alpha T^* -|\beta|/2\}$$

- This is the GA formula for the SCTA. It is currently coded that way in THERMR. It is written that way in only one document that I have seen, namely "Thermal Neutron Scattering Data, etc.“, INDC(NDS)-0470, M. Mattes and J Keinert, April 2005. However, Andrej and Mike assure me that it is OK in the unpublished forthcoming revision to ENDF-102.

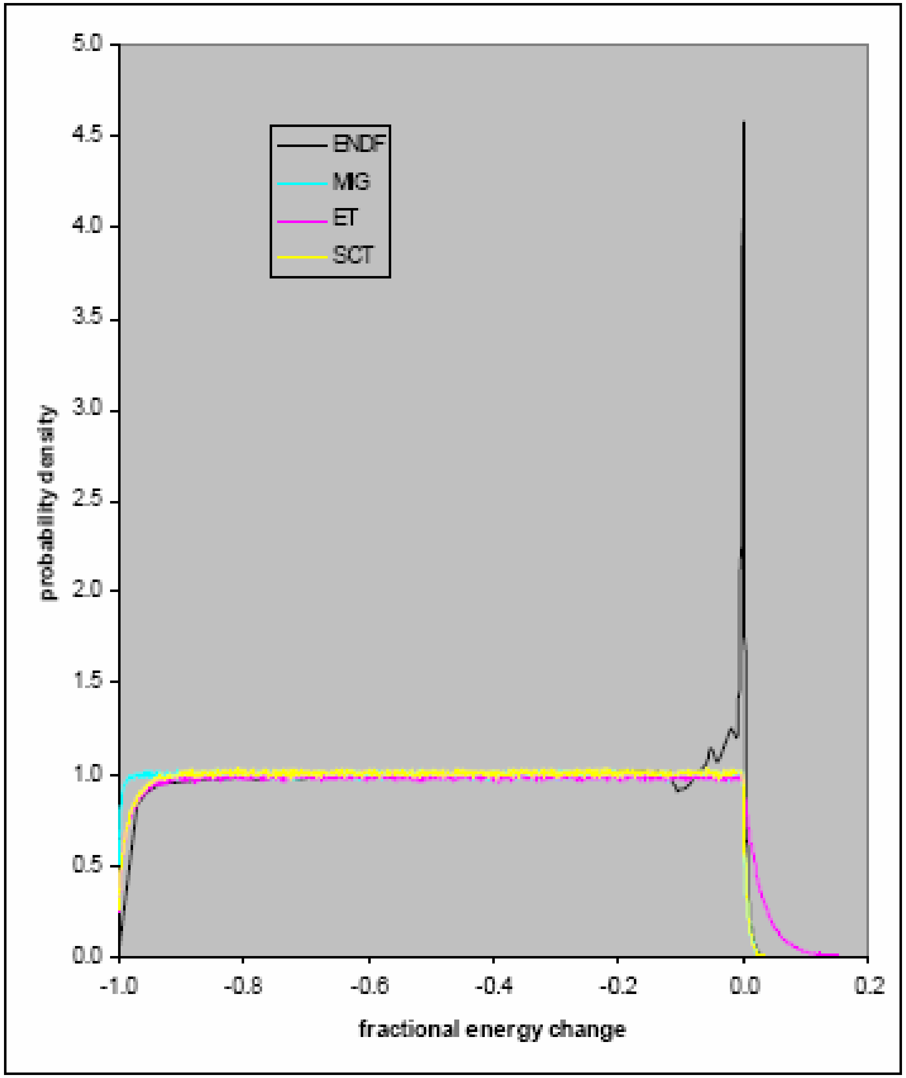

Figure 1. Fractional Energy Change PDF for 4.09 eV Neutrons on ^1H in Water at 293.6 K

- ENDF is LEAPR + GA SCTA.
- MIG is FREE GAS at T-ambient
- ET is FREE GAS at T-effective
- SCT is GA SCTA

Some “Alternative” Forms I

- The reason for displaying these is to provide a definitive statement of what GA intended, and to identify known misprinted versions unambiguously.

- The square root in front is usually OK so here are just the exponents without the minus sign:

1. “The NJOY Nuclear Data Processing System”, LA-9303-M, Vol II (ENDF324), May 1982 (currently available from RSIC)

$$(|\alpha| - \beta)^2 T/4|\alpha|T^* + |\beta|/2)$$

Missing absolute-value signs on first β; unnecessary absolute-value signs on α.

Some "Alternative" Forms II

2. "New Thermal Neutron Scattering Files for ENDF/B-VI Release 2", LA-12639-MS (ENDF 356), March 1994 (currently available from LANL)

$$(\alpha - |\beta|)^2 T/\alpha T^* + |\beta|/2$$

Missing factor of 4 in denominator.

3. "ENDF- 6 Formats Manual, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII", ENDF-102, BNL-NCS-44945-05-Rev June 2005 (currently available from NNDC)

$$(\alpha - \beta)^2 T/4\alpha T^* + |\beta|/2$$

Missing absolute-value signs on first β

Some “Alternative” Forms III

4. A “corrected” version from the (former) Formats Committee which has not yet been issued.

$$(\alpha-\beta)^2 T/4\alpha T^* + (\beta + |\beta|)/2$$

Missing absvals on the first β; an extra β probably from the cross section.

5. A “corrected” version of the above, which has not yet been issued.

$$(\alpha-|\beta|)^2 T/4\alpha T^* + (\beta + |\beta|)/2$$

An extra β probably from the cross section.

Acknowledgement

Material on the GA formula was taken from a paper submitted to the International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009) Saratoga Springs, NY, May 3 – 7, 2009, entitled “Comparison of Some Monte Carlo Models for Bound Hydrogen Scattering”, by TM Sutton, TH Trumbull, and CR Lubitz.