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The Temperature of Coherent Scattering Cross Sections

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Summary

- The 2200 m/s cross sections tabulated in Mughabghab's "Atlas of Neutron Resonances" for capture, fission, and other ***non-elastic*** reactions, are ***room-temperature quantities***, although not explicitly stated.
- For 1/v isotopes, those values are invariant under Doppler-broadening.
- For non-1/v materials, ***room-temperature*** Westcott g-factors are provided, and their temperature-dependence is discussed. The cross sections which define the g-factors are ***not*** broadened, but this small effect is masked by the larger effect of the Maxwellian flux temperature.
- However, the tabulated 2200 m/s ***scattering*** cross sections are at ***absolute zero***, and can differ ***significantly*** from their ***room-temperature*** values.

Discussion I

- ENDF cross sections (except File 7 moderators) are free-atom, target-at-rest, laboratory c.s. values. They are Doppler-broadened with a classical free-gas model, so target-at-rest and absolute zero Kelvin are synonymous.
- Sometimes forgotten is that ***constant cross sections “Doppler-broaden” at low energy.*** Here are some representative values for the 2200 m/s scattering cross sections of a few light nuclei, whose low masses make the effect large:

	Atlas	ENDF/B-VII.0 (NJOY 99.81)		
Name		0 K	~300 K	~550 K
H1	20.491	20.436	30.064 (1.471)	36.765 (1.799)
Li6	0.75	0.718	0.778 (1.084)	0.829 (1.155)
C12	4.746	4.739	4.938 (1.042)	5.108 (1.078)
O16	3.761	3.852	3.973 (1.031)	4.077 (1.058)

Discussion II

- The fact that constant cross sections Doppler-broaden at low energy is not something that gets treated in textbooks. If the cross section is averaged, or if the “small term” in the formula is omitted, it doesn’t broaden, but if the reaction rate is averaged with the full formula, the effective cross section is not constant.

- Here is the formula as derived in ORNL/TM-13525 “Doppler Broadening Revisited”, N. M. Larson, M. C. Moxon, L. C. Leal, and H. Derrien, 1998:

$$\sigma_D(E)/\sigma_0 = [1/\sqrt{(\pi)}x]\exp-(x^2) + (1 + 1/2x^2)\mathrm{erf}(x)$$

with $x=\sqrt{(EA/T)}$ [neutron energy, mass ratio, temperature in eV]

At low energy, $\sigma_D(E)$ => “1/v”. At T = room temperature and E = 2200 m/s, E = T = .0253 eV and x= $\sqrt{A}$. Even for low A, the exponential is small and the error function is ~1.0, so that

$$\sigma_{D2200}(E)/\sigma_0 \approx 1+1/2A$$

Discussion III

- ENDF cross sections are frequently associated with Standards work. Here are three excerpts from ENDF-351, NISTIR 5177 “The ENDF/B-VI Neutron Cross Section Measurement Standards”, A. D. Carlson, et al, May 1993:

Table 1. H(n,n) Cross Section ENDF/B-VI Mat 0125
Recommended as a Standard from 10 eV to 20 MeV

E(eV)	σ(b)
1.00-5	2.0478+1
2.53-2	2.0478+1
2.00+7	4.8227-1

Being smooth, hydrogen is not something for which Doppler-broadening would be expected, so the fact that the 2200 m/s value is off by 50% could possibly escape notice. Temperature is not mentioned.

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Discussion IV

- Here are excerpts from the Li6 and carbon listings:

Appendix D. Li6(n,n) Cross Section

E(MeV)	σ(b)
0.10-12	------
0.253-7	0.6717
0.280+1	1.5072

Table 4. C(n,n) Cross Section ENDF/B-VI Mat 600
Recommended as a Standard below 1.8 MeV

E(eV)	σ(b)
1.00-5	4.7392+0
2.53-2	4.7392+0
1.80+6	1.7980+0

Same comment as for H1, but the much smaller differences make the possibility of overlooking the problem more plausible.

Why is σ_{coh} a Zero-Kelvin Quantity?

- The reason is that ***coherent scattering*** cross sections are obtained from neutron-optics measurements of the ***coherent scattering amplitude***, as described in the Atlas, or in Sears "Neutron Optics". The point which is not universally recognized is that such experiments measure the ***target-at-rest*** value of the coherent scattering amplitude, ***regardless of the temperature at which the experiment itself is carried out, and regardless of the target atom's state of motion or binding.***

- The underlying physical point is that there is no momentum or energy transfer at zero degrees, so f(0) can not "sense" the target's state, and hence is the same as if the target were at rest, i.e., at zero kelvin from the standpoint of "ENDF cross sections".

What about $\sigma_{incoherent}$?

- In the context of the present discussion, the term ***incoherent*** is something of a red herring, although it is important experimentally.

- σ_{inc} is “***manufactured”*** from the ***coherent*** scattering lengths corresponding to the different isotopes in the target, plus the two s-wave channels for the non-zero-spin isotopes, I±½. The amplitudes from the different isotopes and the different J-values will not interfere with each other, so their contribution to the total scattering has to be split into each one’s contribution to the total coherent amplitude and an incoherent part.

- However, the scattering lengths which are combined are all similar forward-scattering quantities which, as described on the previous slide, are zero-kelvin quantities whose corresponding ***cross sections*** must be doppler-broadened if they are to be “combined” with other measured cross sections.

Final Comments I

- Because of their unique ability to measure the “nuclear” quantity f(0), and the related low-energy ***scattering length***, the cross sections are much more accurate than anything that can be done by conventional neutron-beam setups. Evaluators should therefore “pin” their scattering cross sections to those values. And not forget to broaden them appropriately.

- Cross section fitting codes, like EDA, REFIT, and SAMMY, work from resonance parameters and are well-positioned to use coherent cross sections because the resonance parameters are also zero-Kelvin quantities, and Doppler- and resolution-broadening of the input data sets is an integral part of the procedure. But if a cross section is believed to be at room-temperature, but is not, the chance for error still exists.

Final Comments II

- The point made earlier, demonstrated in the ORNL paper, that the approximate form of the Doppler formula fails to get the effect, is another path for error if the user is not aware of the fact that the coherent scattering cross sections he got from some tabulation are not what he should be "seeing" at room temperature.
- What's the next-to-worst-case scenario?

An evaluator includes a zero-kelvin, unbroadened 2200 m/s scattering cross section with other measurements and fails to correctly broaden it before combining it.

- The worst-case is if he is working on a neutron Standard.

End of Slides

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