III.B.3. High-Energy Gaussian Approximation to Doppler Broadening

The high-energy Gaussian approximation (HEGA) to the free-gas model (FGM) for Doppler broadening has been used successfully for many years [WV12, AF71, FF80], and is the original option available within SAMMY. Its use, however, is now discouraged [NL98]: It is unusable at low energies, inaccurate at all energies, and requires the same amount of computer time and memory as does the FGM. Nevertheless, it is still included in the code for comparison purposes.

The Doppler-broadened cross section may be approximated by convoluting the unbroadened cross section with a Gaussian function of energy as

$$\sigma_D\left(E\right) = \frac{1}{\Delta_D \sqrt{\pi}} \int_{Emin}^{Emax} \exp\left\{ \frac{\left(E-E'\right)^2}{\Delta_D^2} \right\} \sigma\left(E'\right) dE' \quad , \tag{III B3.1}$$

where the Doppler width Δ_D is again given by

$$\Delta_D = \sqrt{\frac{4mE\ kT}{M}} \quad . \tag{III B3.2}$$

In this equation, m represents the mass of the neutron, M is the target mass, k is Boltzmann's constant, and T is the effective temperature of the sample material. SAMMY evaluates the Doppler width directly from this formula (i.e., without using heavy-mass approximations). The integration limits in Eq. (III B3.1) are actually infinite but are approximated by $Emax = E + 5\Delta_D$ and $Emin = E - 5\Delta_D$.

For Doppler broadening via the high-energy Gaussian approximation, the only input quantity that the user must provide to SAMMY is the effective temperature *T*. See Table VI A.1, card set 5, variable TEMP, or Table VI B.2, card set 4, variable TEMP.

Caveat: For very low energies, the integration limits may fall below zero. In this case, SAMMY will issue a warning and switch to the FGM. To circumvent this problem, either use the FGM directly (see Section III.B.1), use the Leal-Hwang Doppler broadening (Section III.B.2), or invoke the option "NO LOW-ENERGY BROADEning is to be used" in the INPut file (see Table VI A1.2).

Again, the *recommended* method of Doppler broadening is the FGM, described in Section III.B.1. Use of the high-energy Gaussian approximation described in this section is not encouraged.