III.B.1. Free-Gas Model of Doppler Broadening

A detailed discussion of the "exact" free-gas model (FGM) of Doppler broadening is given in [NL98]; results are summarized in this section. The formula for the FGM of Doppler broadening (see, for example, [FF80, Eq. 102]) takes the form

$$\sigma_D(E) = \frac{1}{\Delta_D\sqrt{\pi}} \int_0^\infty \left[e^{-4\left(E-\sqrt{EE'}\right)^2/\Delta_D^2} - e^{-4\left(E+\sqrt{EE'}\right)^2/\Delta_D^2} \right] \sigma(E')\sqrt{E'/E}\; dE \quad . \qquad \text{(III B1.1)}$$

In this expression, σ_D is the Doppler-broadened cross section and σ is the unbroadened cross section. (Any type of cross section could be represented here: elastic, total, capture, fission, or other reaction, either angle-integrated or angle-differential cross sections.) The Doppler width Δ_D is given by

$$\Delta_D = \sqrt{\frac{4\,m\,E\,k\,T}{M}} \quad . \qquad \text{(III B1.2)}$$

Here, as elsewhere in this section, *m* represents the neutron mass, *M* the target (sample) mass, *k* is Boltzman's constant, and *T* is the effective temperature. (This Doppler width is reported in the SAMMY.LPT file; see Section VII.A.) Alternatively, this equation may be written in terms of "velocity" *v*, where *v* is the square root of energy *E* ($v = \sqrt{E}$), as

$$v\,\sigma_D\left(v^2\right) = \frac{1}{u\sqrt{\pi}} \int_0^\infty \left[e^{-(v-v')^2/u^2} - e^{-(v+v')^2/u^2} \right] v'\sigma\left(v'^2\right)\frac{v'}{v}\; d\,v' \quad , \qquad \text{(III B1.3)}$$

in which we have substituted *v*' for the square root of *E* ' and defined *u* as

$$u = \sqrt{m\,k\,T\,/\,M} \quad . \qquad \text{(III B1.4)}$$

To evaluate this integral, replace *v*' by -*w* in the second term; this gives

$$\begin{aligned} v\,\sigma_D\left(v^2\right) \;&=\; \frac{1}{u\sqrt{\pi}} \int_0^\infty e^{-(v-v')^2/u^2}\, v'\sigma\left(v'^2\right)\frac{v'}{v}\; d\,v' \\ &-\; \frac{1}{u\sqrt{\pi}} \int_0^{-\infty} e^{-(v-w)^2/u^2}\, (-w)\,\sigma\left((-w)^2\right)\frac{(-w)}{v}\; d\,(-w) \quad . \end{aligned} \qquad \text{(III B1.5)}$$

Replacing *v*' by *w* in the first term of Eq. (III B1.5), rearranging the second term, and defining

$$s(w) = \begin{cases} \sigma(w^2) & \text{for } w > 0 \\ 0 & \text{for } w = 0 \\ -\sigma(w^2) & \text{for } w < 0 \end{cases} \tag{III B1.6}$$

puts this equation into the form

$$v\,\sigma_D(v^2) = \frac{1}{u\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-(v-w)^2/u^2}\; w\,s(w)\frac{w}{v}\; d\,w \quad . \tag{III B1.7}$$

In the form of Eq. (III B1.7) with definition (III B1.6), the Doppler-broadening integration can be accomplished readily within SAMMY using the same numerical techniques used for other integrations, without having to give special consideration to “the second term” of Eq. (III B1.1). The integration scheme of Section III A.3 is used directly. The auxiliary energy grid is chosen as described in Section III.A.2, with the exception that the additional low-energy points are equally spaced in *velocity* rather than in energy. Negative velocities are included as needed, in order to properly evaluate the integral at low values of *E*.