III.B.2. Leal-Hwang Doppler Broadening

The assumption of a free gas model (FGM) for the sample atoms leads to a relatively simple relationship between the cross-section values at different temperatures. Leal and Hwang [LL85] have used this idea to write the Doppler-broadened cross section in the form

$$\sigma_D(E) = F(v)/E \quad , \tag{III B2.1}$$

where "velocity" v is the square root of energy E,

$$v = \sqrt{E} \quad , \tag{III B2.2}$$

and $F(v)$ obeys a partial differential equation having the same form as a one-dimensional time-dependent heat equation. That is, $F(v)$ obeys

$$\left(\frac{\partial^2}{\partial v^2} - \frac{\partial}{\partial \Theta} \right) F(v) = 0 \quad , \tag{III B2.3}$$

in which Θ is given by

$$\Theta = \frac{k\,T}{2\,M} \quad , \tag{III B2.4}$$

where again T is the effective temperature of the sample, k is Boltzmann's constant, and M is the mass of the sample (target) nucleus. This is equivalent to the integral equation in Eq. (III B1.1).

The numerical solution of Eq. (III B2.3) may be readily accomplished by difference techniques. Leal and Hwang have shown that if the step sizes Δv and $\Delta\Theta$ are constant for both velocity v and "temperature" Θ, and if

$$(\Delta v)^2 = 6\,\Delta\Theta \quad , \tag{III B2.5}$$

then the error in the numerical solution is of the order of $(\Delta v)^4$ or $(\Delta\Theta)^2$.

The solution of Eq. (III B2.3) can be written in the form

$$F_i^j \;=\; \frac{1}{6} F_{i-1}^{j-1} \;+\; \frac{2}{3} F_i^{j-1} \;+\; \frac{1}{6} F_{i+1}^{j-1} \quad , \tag{III B2.6}$$

in which the superscript j denotes the value of F evaluated at $\Theta = \Theta_j$, and subscript i denotes the value of F evaluated at $v = v_i$.

By combining Eq. (III B2.6) with the analogous equations for F_i^m, with $m = 1$ to $j - 1$, we find that the $F_i{}^j$ may be written as

$$F_i{}^j = \sum_{k=-j}^{j} a_k^j \, F_{i+k}^0 \quad , \tag{III B2.7}$$

where $F_n^{\,0}$ are the "initial" values of F (i.e., at zero temperature), and where the $a_k^{\,j}$, for negative k, are found from the relationship

$$a_{-k}^{\,j} = a_k^{\,j} \quad . \tag{III B2.8}$$

For positive k, the values of $a_k^{\,j}$ are found from the recursion relationships

$$\begin{aligned} &a_1^1 = 1/6 \qquad a_0^1 = 2/3 \\ &a_2^2 = (1/6)^2 \qquad a_1^2 = 2(1/6)(2/3) \qquad a_0^2 = 2(1/6)^2 + (2/3)^2 \quad , \end{aligned} \tag{III B2.9}$$

and, in general,

$$\begin{aligned} a_n^n &= (1/6)^n \\ a_{n-1}^n &= (1/6)\,a_{n-2}^{n-1} + (2/3)\,a_{n-1}^{n-1} \\ a_{n-2}^n &= (1/6)\,a_{n-3}^{n-1} + (2/3)\,a_{n-2}^{n-1} + (1/6)\,a_{n-1}^{n-1} \\ &\ldots \\ a_k^n &= (1/6)\,a_{k-1}^{n-1} + (2/3)\,a_k^{n-1} + (1/6)\,a_{k+1}^{n-1} \qquad \text{for } 0 < k < n-1 \\ &\ldots \\ a_0^n &= (1/6)\,a_1^{n-1} + (2/3)\,a_0^{n-1} + (1/6)\,a_1^{n-1} = 2(1/6)\,a_1^{n-1} + (2/3)\,a_0^{n-1} \quad . \end{aligned} \tag{III B2.10}$$

The procedure employed in SAMMY is as follows.

(1) Somewhat arbitrarily, choose ΔT = 5 degrees; this number is a user input, so it may be changed if desired. (See Table VI A.1, card set 5, variable DELTTT.) Figure the number of steps required to reach from zero temperature to the effective temperature T, and adjust ΔT so that T can be reached in exactly J steps. Determine the corresponding $\Delta\Theta$ and Δv.

(2) Generate the coefficients a_k^J for $k = 0$ to J. These coefficients will be large for small k and effectively zero for large k. Choose M such that $a_k^J > 0$ for all $k > M$.

(3) Generate the auxiliary energy grid ENERGB, which is uniform in velocity space. M points will be included on each side of the energy region [Emin − Wmin, Emax + Wmax], where Emin and Emax are the experimental energy limits, and Wmin and Wmax are resolution limits at Emin and Emax, respectively.

(4) Generate theoretical cross sections $\sigma(E)$ for all ENERGB points.

(5) Evaluate $F_i^{\,J}$ for all points i in the auxiliary grid, using Eq. (III B2.8), and convert to cross section using Eq. (III B2.1). If needed, the partial derivative of the cross section with respect to the temperature may be generated from

$$\left.\frac{\partial\sigma}{\partial\Theta}\right|_{\Theta=\Theta_J,\, v=v_i} = \frac{1}{\Delta\Theta}\left(F_i^{\,J+1} - F_i^{\,J}\right) \quad . \tag{III B2.11}$$

Using the chain rule with Eq. (III B2.4), combined with Eqs. (III B2.6) and (III B2.11), gives

$$\left.\frac{\partial\sigma}{\partial T}\right|_{\Theta=\Theta_J,\, v=v_i} = \frac{T}{E}\,\frac{\Theta}{\Delta\Theta}\left[\frac{1}{6}F_{i-1}^{J} - \frac{1}{3}F_i^{\,J} + \frac{1}{6}F_{i+1}^{J}\right] \tag{III B2.12}$$

for the derivatives of the cross section with respect to the temperature.

(6) From here on, follow the prescription given in Section III.A, beginning at step 4.

Finally, we recall from the discussion of the free-gas model (Section III.B.1) that the integral equation for Doppler broadening [Eq. (III B1.1) or (III B1.7)] is symmetric with respect to the transformation $v' \rightarrow -v'$, provided $\sigma\left(-\left|v'\right|\right)$ is defined as $-\sigma\left(\left|v'\right|\right)$ as in Eq. (III B1.6). In a similar manner, the Leal-Hwang option permits the direct evaluation of the broadened cross section even for points near $E = 0$.

[In earlier versions of SAMMY (prior to the 2006 release, sammy-7.0.0), studies suggested that results obtained for *very* low energies (well below thermal) were not completely accurate; specifically, Doppler-broadened $1/v$ cross sections did not retain the $1/v$ shape at these very low energies, and the step size ΔT was critically important. This was found to be due to a mistake in the coding, which was corrected for the sammy-7.0.0 release.]

To minimize the number of points required for use in the auxiliary grid, SAMMY users are encouraged to rely on the FGM (see Section III.B.1) for most calculations. The Leal-Hwang model is useful for double-checking results at low energies, and in other situations that call for accurate calculation of Doppler broadening of smooth cross sections.

To use the Leal-Hwang Doppler broadening, include in your INPut file a line which reads

USE LEAL,HWANG DOPPLER BROADENING

and specify the step size ΔT on card set 5 of the INPut file, Table VIA.1.