SAMMY Workshop Part 4.2a

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Part 4.2a, Derivation of Free Gas Model

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DERIVATION OF THE FREE GAS MODEL

<u>Definitions</u>:

- a parallel beam of monoenergetic particles with lab velocity $\bar{v}$
- target nuclei whose velocities $\bar{W}$ are distributed in such a way that $p(\bar{W})\, d^3W$ is the fraction with velocities in a small three-dimensional region d^3W around $\bar{W}$
- ρ_1 and ρ_2 are the densities of beam and target particles, respectively
- $\sigma(E)$ is unbroadened cross section
- $\tilde{\sigma}(m v^2/2)$ is the effective or Doppler-broadened cross section for incident particles with speed v [laboratory energy $m\, v^2 / 2$]

Then:

- the number of reactions occurring per unit time and unit volume is

$$\rho_1 \, \rho_2 \int d^3W \; p(\bar{W}) \; |\bar{v} - \bar{W}| \; \sigma(m|\bar{v} - \bar{W}|^2/2) \equiv$$
$$\rho_1 \, \rho_2 \; v \, \tilde{\sigma}(m v^2/2)$$

Assume:

- target nuclei have same velocity distribution as atoms of ideal [monatomic] gas, i.e. the Maxwell-Boltzmann distribution,

$$p(\bar{W}) \, d^3W = \frac{1}{\pi^{3/2}} \exp\left(- \frac{W^2}{u^2} \right) \frac{d^3W}{u^3}$$

with

$$\frac{M}{2} u^2 = k T$$

where M = nuclear mass and k = Boltzmann's constant, T = temperature

Then:

- The Doppler-broadened cross section is given by

$$v\,\tilde{\sigma}(m v^2/2) = \frac{1}{\pi^{3/2} u^3} \int_{\text{all } \bar{W}} d^3W \; \exp\left(- \frac{W^2}{u^2} \right) \; |\bar{v} - \bar{W}| \; \sigma(m|\bar{v} - \bar{W}|^2/2)$$

Simplify:

- change integration variable from $\bar{W}$ to $\bar{w} = \bar{v} - \bar{W}$

- choose spherical coordinates

$$v\tilde{\sigma}\left(\frac{m v^2}{2}\right) = \frac{1}{\pi^{3/2} u^3} \int_{\text{all } \bar{w}} d^3w \; \exp\left(- \frac{(v^2 - 2vw\cos\theta + w^2)}{u^2} \right) \; w\,\sigma\left(\frac{m w^2}{2}\right)$$

$$= \frac{1}{\pi^{3/2} u^3} \int_0^{2\pi} d\varphi \int_0^{inf} w^2\,dw \int_{-1}^{+1} d(\cos(\theta)) \; \exp\left(- \frac{(v^2 - 2vw\cos\theta + w^2)}{u^2} \right) \; w\,\sigma\left(\frac{m w^2}{2}\right)$$

$$= \frac{1}{\pi^{3/2} u^3} \int_0^{2\pi} d\varphi \int_0^{inf} dw\, w^3\, \sigma\left(\frac{m w^2}{2}\right) \exp\left(-\frac{(v^2+w^2)}{u^2}\right) \int_{-1}^{+1} d\mu\, \exp\left(-\frac{2 v w \mu}{u^2}\right)$$

$$= \frac{2\pi}{\pi^{3/2} u^3} \int_0^{inf} dw\, w^3\, \sigma\left(\frac{m w^2}{2}\right) \exp\left(-\frac{(v^2+w^2)}{u^2}\right)\left(\frac{-u^2}{2 v w}\right)\left[\exp\left(-\frac{2 v w}{u^2}\right) - \exp\left(+\frac{2 v w}{u^2}\right)\right]$$

$$= \frac{1}{v\sqrt{\pi}\, u} \int_0^{inf} dw\, w^2\, \sigma\left(\frac{m w^2}{2}\right) \left[\exp\left(-\frac{(v-w)^2}{u^2}\right) - \exp\left(-\frac{(v+w)^2}{u^2}\right)\right] .$$

which may be more familiar as:

$$\tilde{\sigma}\left(E = \frac{m v^2}{2}\right) = \frac{1}{v^2\sqrt{\pi}\, u} \int_0^{inf} dw\, w^2\, \sigma\left(\frac{m w^2}{2}\right) \exp\left(-\frac{(v-w)^2}{u^2}\right)$$

$$- \frac{1}{v^2\sqrt{\pi}\, u} \int_0^{inf} dw\, w^2\, \sigma\left(\frac{m w^2}{2}\right) \exp\left(-\frac{(v+w)^2}{u^2}\right)$$

Define pseudo cross section s:

$$s(w) = \sigma(m(w)^2/2) \quad \text{for } w > 0$$
$$= -\sigma(m(-w)^2/2) \quad \text{for } w < 0 \ .$$

Simplify:

- Free gas model of Doppler broadening can be written

$$\bar{\sigma}\left(\frac{m v^2}{2}\right) = \frac{1}{v^2 \sqrt{\pi}\, u} \int_{-inf}^{inf} dw\, w^2\, s(w) \exp\left(-\frac{(v-w)^2}{u^2}\right)$$