

III. B. DOPPLER BROADENING

Four options are available within SAMMY to accomplish Doppler broadening; three are based on the free-gas model (FGM), and the fourth is a solid-state model.

SAMMY's free-gas model is described in Section III.B.1. This model was introduced into SAMMY in order to overcome shortcomings of the two earlier versions (Sections III.B.2 and III.B.3), and is now the default method. This is the option that should be used for most calculations. For additional details, see [NL98].

A second method, described in Section III.B.2, is an elegant and rigorous adaptation of the FGM based on work by Leal and Hwang [LL85]. This method works best with smooth cross sections, and thus has limitations for use in the resonance region.

SAMMY's original method, a high-energy Gaussian approximation (HEGA) to the FGM, is based on an adaptation of the method used by George Auchampaugh in his code MULTI [GA74]. This method is described in Section III.B.3. Because this is a high-energy approximation, it cannot be used for very low-energy computations.

A fourth option is available for use in those situations in which the FGM is inadequate. The crystal-lattice model (CLM) of Doppler broadening, added to SAMMY for Release M6 of the code, is described in Section III.B.4. SAMMY's implementation is based on the DOPUSH model of Naberejnev [DN99, DN99a].