III.A.1. Analyst's Responsibility for Auxiliary Energy Grid

In SAMMY, the user/analyst (*not* the author) is responsible for being sure that the numerical integrations are performed properly. That is to say, the auxiliary energy grid (discussed in detail in Section III.A.2) must be sufficiently dense so that the numerical integration scheme produces the correct results.

Why must the grid be dense? Unbroadened cross sections would not be well defined on a sparse grid. Hence, the integrations would not be accurate. This is illustrated in Figures III A1.1 – 4, which are greatly exaggerated for demonstration purposes. In the first figure, red dots indicate the default grid points on which the unbroadened cross section might be calculated. The dashed curve represents the actual unbroadened cross section, while the solid curve represents the approximate cross section found by interpolating between grid points. With this sparse grid, agreement between the two curves in poor.

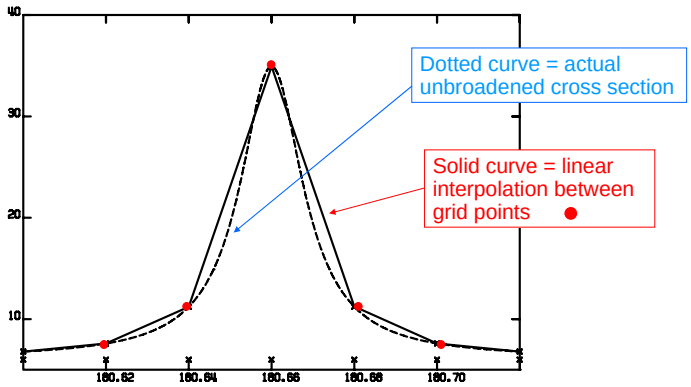

Figure III A1.1. Unbroadened cross section calculated using too few points in the auxiliary grid.

Figure III A1.2 shows the Doppler-broadened cross section (solid curve) that would result from using the auxiliary grid of Figure III A1.1 to perform the numerical integration. The calculated Doppler-broadened cross section is significantly larger than the actual Doppler-broadened cross section.

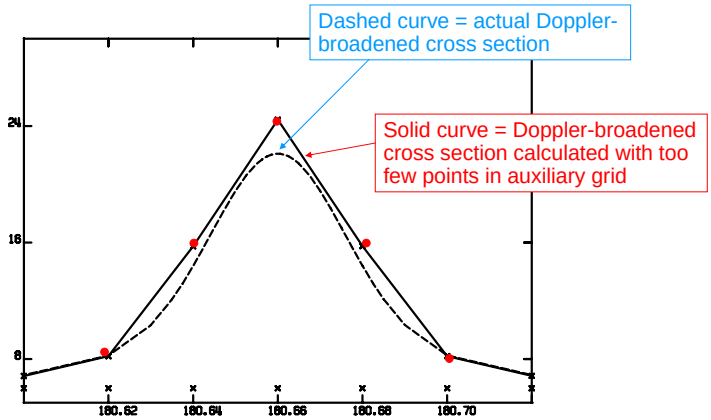

Figure III A1.2. Incorrect Doppler-broadened cross section calculated with too few points in the auxiliary grid.

In contrast, Figure III A1.3 shows a denser auxiliary grid, one which adequately describes the unbroadened cross section. The Doppler-broadened cross section calculated with this grid is shown in Figure III A1.4, in which the actual and the calculated Doppler-broadened cross sections are indistinguishable. (Note that the "experimental" grid is the same in Figures III A1.2 and III A1.4.)

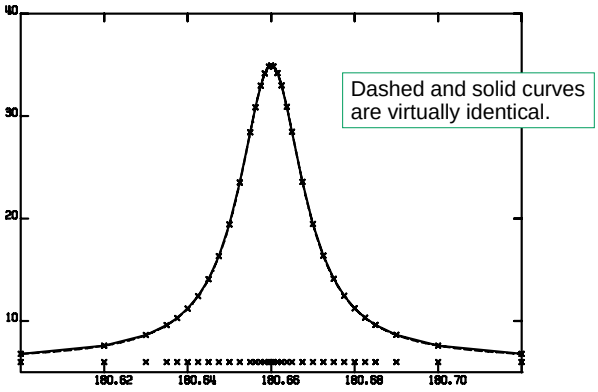

Figure III A1.3. Unbroadened cross section calculated using an adequate number of points in the auxiliary grid.

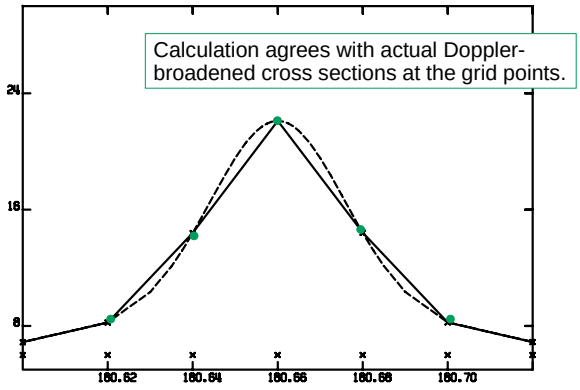

Figure III A1.4. Doppler-broadened cross section calculated with an adequate number of points in the auxiliary grid.

The reader may ask why SAMMY does not automatically check to be certain that the auxiliary grid is adequate, especially since this is done by other codes (e.g., processor codes such as AMPX [MD02] or NJOY [RM82]) which calculate Doppler-broadened cross sections. Significant amounts of computation time are required for such checks. With processor codes, the Doppler-broadened cross section is generally calculated only once, and then used many times, so accuracy is far more important than speed of computation. With analysis codes such as SAMMY, the Doppler-broadened cross section is recalculated whenever new resonance parameters are used, so speed of computation can be an issue. During initial stages of an analysis, the user may wish to sacrifice accuracy to gain speed. During later stages of the analysis, the user will want to test whether there is sufficient accuracy.

Options for increasing the density of points in the auxiliary grid are given in line 2 of the INPut file, Table VI A.1. These should be used to make comparisons between Doppler- and resolution-broadened results from dense vs. sparse grids. (For example, if the number of points is doubled by setting NXTRA = 1, and broadened cross sections are nearly the same as with NXTRA = 0, then the sparser grid is adequate.) Early in the analysis, it is probably sufficient to use the sparsest grid that gives reasonable results. Near the end of the project, a denser grid might be used to ensure greater accuracy.