III.E.8. Energy-Scale Dependence on t_0 and L

When analyzing two or more independent data sets, the problem of displacement between energy scales often arises. Proper alignment of energy scales has traditionally been a task for the analyst; however, help is available from SAMMY. Two methods are described here.

First method:

In time-of-flight measurements, the energy of the incident neutron is determined from the flight-path length L, the flight time t, and the initial time t_0 as

$$E = \frac{m}{2}\frac{L^2}{\left(t-t_0\right)^2} \quad . \tag{III E8.1}$$

By treating L and t_0 as variables (parameters) and searching for those values of L and t_0 which provide the best fit of experimental measurement to the calculated cross section, it is possible to adjust the energy scales to provide agreement between different data sets. See card set 11, line 6, of the PARameter file, Section VI, for input details.

Derivatives of the cross section with respect to flight-path length L and initial time t_0 are given in terms of the derivative with respect to energy as

$$\frac{\partial\sigma}{\partial t_0} = \frac{\partial E}{\partial t_0}\frac{\partial\sigma}{\partial E} = \frac{2E}{\left(t-t_0\right)}\frac{\partial\sigma}{\partial E} \tag{III E8.2}$$

and

$$\frac{\partial\sigma}{\partial L} = \frac{\partial E}{\partial L}\frac{\partial\sigma}{\partial E} = \frac{2E}{L}\frac{\partial\sigma}{\partial E} \quad . \tag{III E8.3}$$

Recall that the cross section σ is given in terms of the scattering matrix U. The energy-dependence of σ is therefore that of U (via ρ) and of the $\left(1/k^2\right)$ multiplicative factor. That is, this derivative is given by

$$\frac{\partial\sigma}{\partial E} = \frac{\partial\sigma}{\partial\rho}\frac{\partial\rho}{\partial k}\frac{\partial k}{\partial E} - \frac{2}{k}\sigma\frac{\partial k}{\partial E} \quad , \tag{III E8.4}$$

which can be rewritten as

$$\frac{\partial\sigma}{\partial E} = \left(\frac{\partial\sigma}{\partial\rho}a - \frac{2}{k}\sigma\right)\frac{k}{2E} \quad . \tag{III E8.5}$$

Combining this equation with Eqs.(III E8.2) and (III E8.3) gives

$$\frac{\partial\sigma}{\partial t_0} = \frac{\rho}{(t-t_0)}\frac{\partial\sigma}{\partial\rho} - \frac{2}{(t-t_0)}\sigma \qquad \text{(III E8.6)}$$

and

$$\frac{\partial\sigma}{\partial L} = \frac{\rho}{L}\frac{\partial\sigma}{\partial\rho} - \frac{2}{L}\sigma \quad . \qquad \text{(III E8.7)}$$

The derivative of the cross section with respect to ρ is again, as in Section II.D.1.c, found by substituting Eq. (II D1 c.9) into Eq. (II D1 c.6).

Note that relativistic corrections are often added to the expression in Eq. (III E8.1); such corrections are ignored in SAMMY's treatment of the t_0 dependence.

Within SAMMY the value of L is not varied directly; rather, L is set equal to the product of the "initial" value L_i times a dimensionless quantity L_0. This dimensionless multiplier is generally given an initial value of 1.0, and the value is varied in the SAMMY run.

In preliminary studies, what has been found practical is to use this option somewhat apart from the mainstream of SAMMY analyses. The procedure that worked best in our trials was to first obtain a reasonably good fit to the "best" data set (the data set which, in the analyst's judgment, has the "most correct" energy scale), with particular emphasis on obtaining accurate resonance energies. Next, modify the parameter file to vary only L_0 and t_0 (i.e., do not vary resonance energies or other resonance parameters) and make a SAMMY run to determine the best values for L_0 and t_0 for the data set in which the energy scale is "wrong." Once those values have been determined, generate a modified data set which has the corrected energy scale and use the modified set in subsequent work. The code SAMFTZ, described in Section X.G of this manual, can be used to generate the modified data set.

Second method:

Begin by fitting each data set separately from the others, establishing in particular appropriate energies for the largest resonances. Choose one data set (probably the transmission measurement with the longest flight path) as the standard. For each other data set, compare energies for individual resonances to those in the standard data set. By considering the relative energy difference as a function of resonance energy, a fit can be made to the functional form

$$\frac{E'-E}{E} = \frac{\Delta E}{E} = a + b\sqrt{E} \quad , \qquad \text{(III E8.8)}$$

in which E is the energy of the resonance in the standard data set, and E' the energy in the other data set. Equation (III E8.8) is the appropriate functional form, as can be seen by taking increments of Eq. (III E8.1),

$$\Delta E = \frac{\partial E}{\partial L}\Delta L + \frac{\partial E}{\partial t_0}\Delta t_0 = \frac{2E}{L}\Delta L + \frac{2E}{\left(t - t_0\right)}\Delta t_0 \quad , \qquad \text{(III E8.9)}$$

or

$$\frac{\Delta E}{E} = \frac{2\Delta L}{L} + \frac{2\sqrt{2E/m}}{L}\Delta t_0 = \frac{2\ \Delta L}{L} + \left(\frac{2\Delta t_0\sqrt{2/m}}{L}\right)\sqrt{E} \quad . \qquad \text{(III E8.10)}$$

Once appropriate values are determined for a and b, all energies in the non-standard data set can be modified by replacing the original (incorrect) energy E' by E'', where

$$E' = E'' + \left(a + b\sqrt{E''}\right)E'' \quad . \qquad \text{(III E8.11)}$$

Solution of this equation for E'' can be done iteratively, with $E'' \approx E'$ as starting value.