

SPURION CALCULATOR

A utility in DAVE for TAS users called SPURION CALCULATOR allows one to calculate both elastic incoherent and inelastic scattering processes that can give rise to apparent inelastic processes one observes in a measurement.

1.1 Getting started

First, launch DAVE and select the Tools→TAS Tools→Spurion calculator. You should see a screen like the one shown in figure 1.

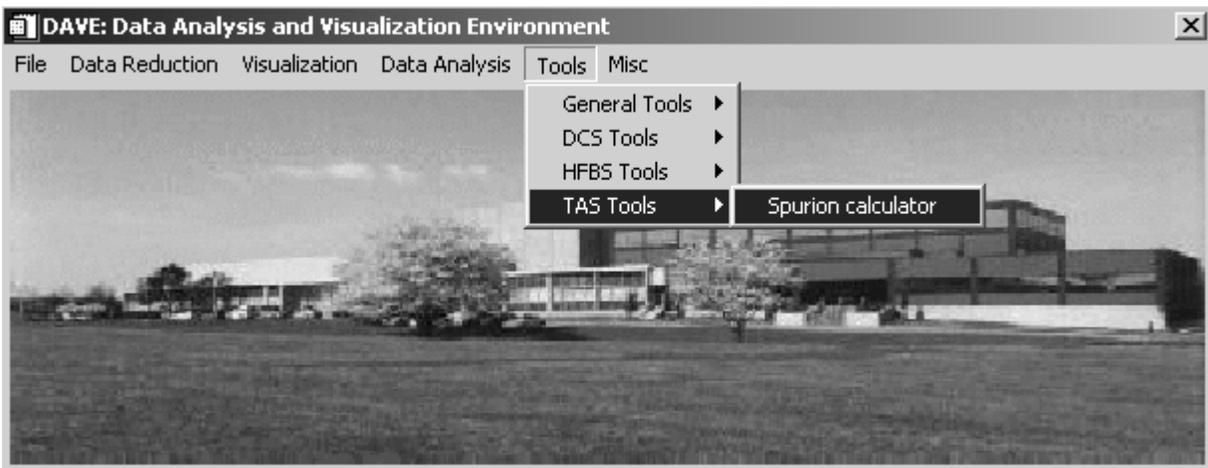


Figure 1 Opening screen of DAVE showing location of Spurion calculator.

Launch the program. You will see the spurion calculator main screen as shown in figure 2.

1.2 Using Spurion Calculator

When initially launched the program is configured to display the apparent excitation energy, $\Delta E_{\text{apparent}}$ (meV) vs. the final energy, E_{final} (meV). There are two types of line drawn in the plot window: solid and broken. Both line types correspond to elastic incoherent scattering processes in which a harmonic of the wavelength is elastically scattered from the monochromator and/or analyzer, resulting in an apparent inelastic peak. The solid lines correspond to the apparent energy transfer for that particular final energy and the broken lines correspond to the absolute value of the negative apparent energy transfers. As you move the cursor around the plot window, the values in the text field labeled *Fixed energy* and *Apparent energy transfer (meV)* update to reflect the current position of the

cursor. Since the E_f radio button is selected in the *Fixed energy* selection, the fixed energy is the final energy. You can select E_i so that the initial energy is fixed depending on the spectrometer configuration.

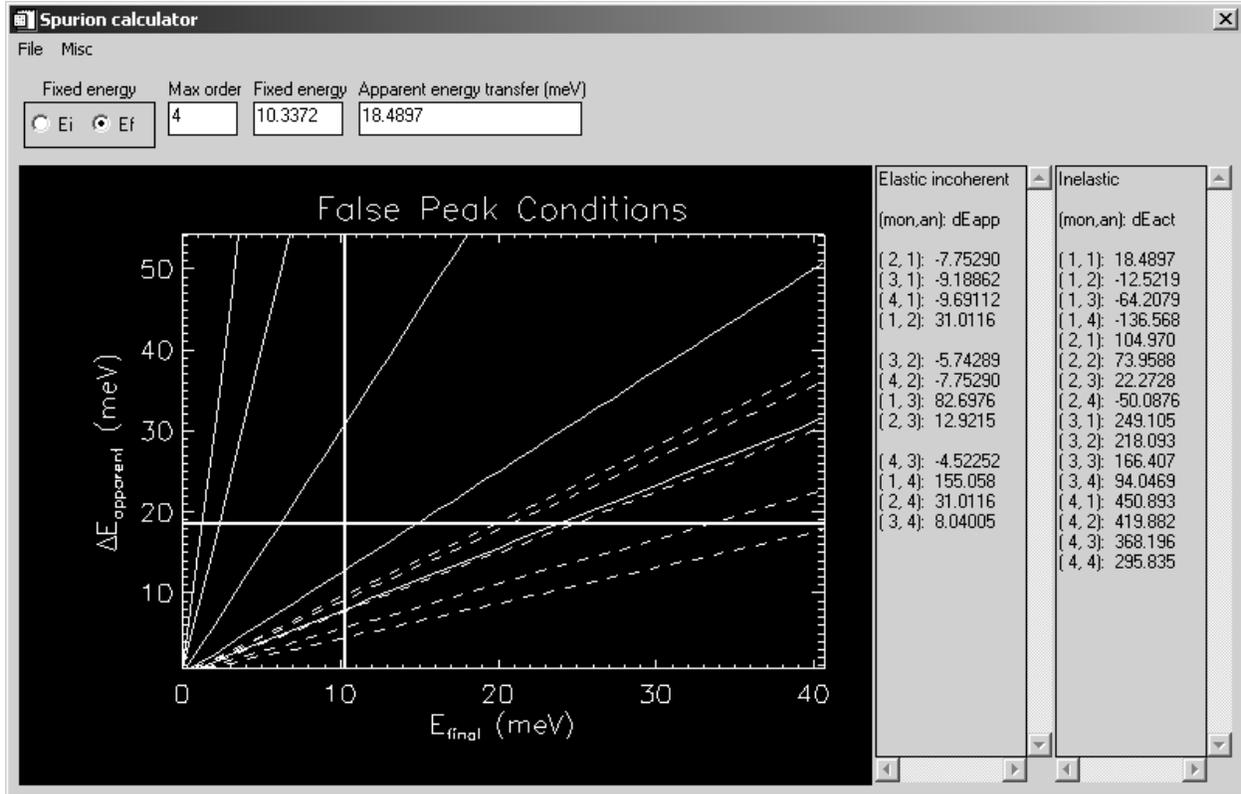


Figure 2 Screen shot of spurion calculator.

When you move the cursor around the screen, you also see that the values in the two text panels in the right hand side of the application update. The first text panel lists the elastic incoherent scattering processes for the various harmonics, (mon,an), where mon is the harmonic of the reflection at the monochromator and an is the harmonic of the reflection at the analyzer. The quantity, dEapp, is the apparent energy of the reflection.

Example: As shown above, the elastic incoherent process **(2,3): 12.9215** means that for a fixed final energy of 10.3372 meV, the second-order reflection from the monochromator and third-order reflection from the analyzer results in an apparent energy transfer of 12.9215 meV.

The elastic incoherent processes are a function of the fixed final (initial) energy, E_{final} (E_{initial}) and the orders of reflection from the monochromator and analyzer, n_m

and n_a . This means, for instance, that you can type in a final energy in the text field labeled *Fixed energy* and hit enter. The values in the text column showing the elastic incoherent processes are updated based on this fixed (final) energy.

The equations that define the elastic incoherent scattering processes are displayed below:

$$\begin{aligned}\Delta E_{\text{actual}} &= 0 \\ \Delta E_{\text{apparent}} &= \left(\left(\frac{n_a}{n_m} \right)^2 - 1 \right) E_{\text{final}} \\ \Delta E_{\text{apparent}} &= \left(1 - \left(\frac{n_m}{n_a} \right)^2 \right) E_{\text{initial}}\end{aligned}\tag{1.3}$$

where n_m and n_a are the order of the reflection from the monochromator and analyzer respectively.

In addition to elastic scattering processes causing spurious peaks to appear in the inelastic spectrum, inelastic scattering processes can cause peaks to appear at the incorrect location in the inelastic spectrum. In this case ΔE_{actual} represents the real inelastic scattering process that gives rise to an apparent energy transfer, $\Delta E_{\text{apparent}}$.

The equations that define the inelastic scattering processes are displayed below:

$$\begin{aligned}\Delta E_{\text{actual}} &= n_m^2 \Delta E_{\text{apparent}} + (n_m^2 - n_a^2) E_{\text{final}} \\ \Delta E_{\text{actual}} &= n_a^2 \Delta E_{\text{apparent}} + (n_m^2 - n_a^2) E_{\text{initial}}\end{aligned}\tag{1.4}$$

where n_m and n_a are the order of the reflection from the monochromator and analyzer respectively.

The actual energy transfer, ΔE_{actual} , is a function of $\Delta E_{\text{apparent}}$, E_{final} (or E_{initial}) depending on which radio button you checked in the *Fixed energy selection*, and the order of reflection from the monochromator and analyzer, n_m and n_a . The values in the right-most text panel update as you move the cursor around the plot window.

Example: As shown in figure 2 above, the inelastic process **(2,1): 104.970** means that for a fixed final energy of 10.3372 meV, the second-order reflection from the monochromator and first-order reflection from the analyzer results in an apparent energy transfer of 18.4897 meV only if there is a real process present (e.g. a phonon) with energy 104.970 meV.

In order to perform this calculation for a specific fixed final (initial) energy and apparent energy transfer, you can type in a final energy in the text field labeled *Fixed energy*, an apparent energy transfer in the text field labeled *Apparent energy transfer (meV)* and hit enter. The values in the text column showing the elastic incoherent processes are updated based on this fixed (final) energy.