Fitting in CASSIS

Introduction

Sandrine BOTTINELLI, 2014-03-07

Introduction

- Fit tab allows baseline and line fitting with two different algorithms: Amoeba fitter and Levenberg-Marquardt fitter.
- In what follows, 'x' is the variable represented on the bottom x-axis of the displayed spectrum.
- Possible types of baselines are :
  - polynomial of order n: $\sum_{i=0}^{n} a_i \, x^i$
  - sinusoidal, parameterized with I_0, ω, φ: $I_0 \sin(\omega \, x + \varphi)$

Introduction

- All line profiles are parameterized with I_0 (intensity at x_0), x_0, FWHM (= full width at half maximum ; hereafter γ).
  Possible types of lines are :
  - Gaussian (produced by thermal Doppler broadening):

$$I_0 \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]$$

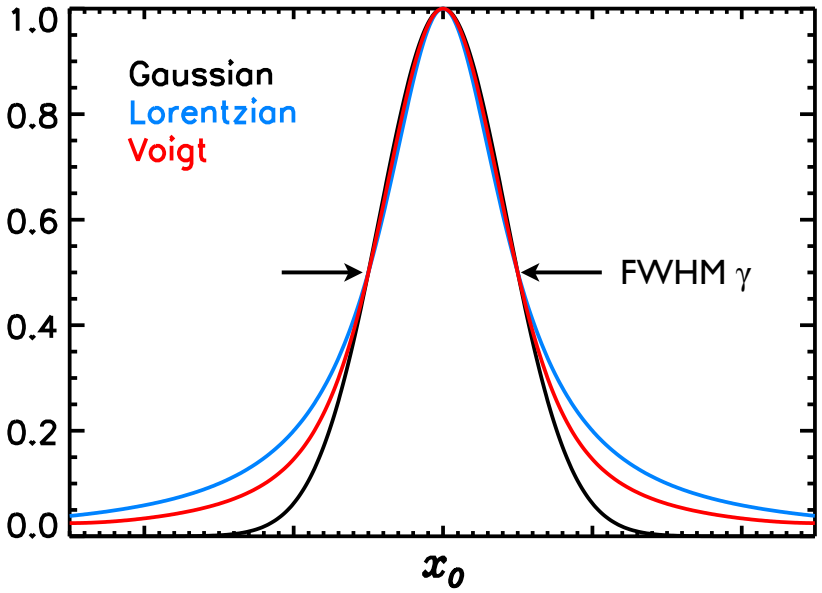
    where σ and γ are related by: $\gamma = 2\sigma\sqrt{2\ln 2} \approx 2.355\sigma$
  - Lorentzian (produced by natural and/or pressure broadening):

$$I_0 \frac{(\gamma/2)^2}{(x-x_0)^2 + (\gamma/2)^2}$$

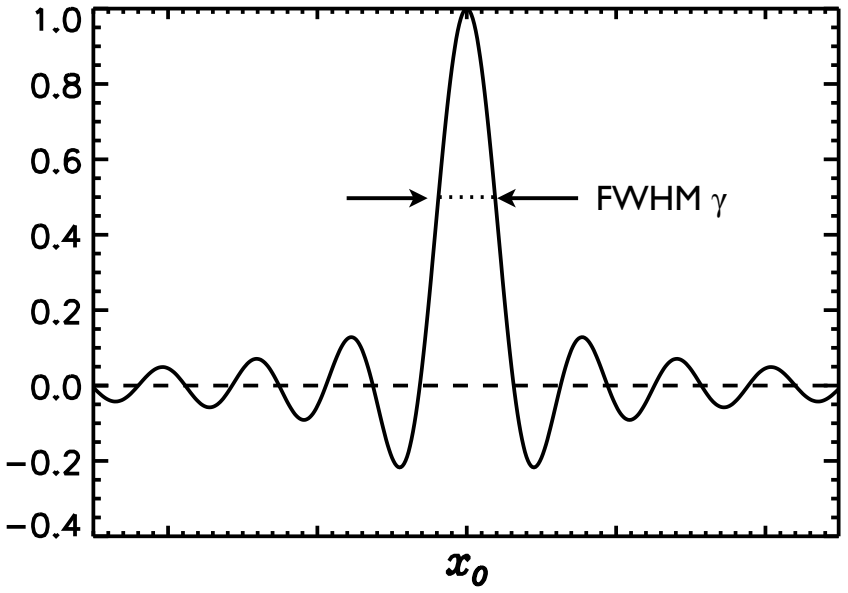
  - Voigt: the convolution of a Gaussian and a Lorentzian profile
  - Sinc (instrumental response):

$$I_0 \frac{\sin\left(\frac{x-x_0}{\gamma/3.75}\right)}{\frac{x-x_0}{\gamma/3.75}}$$

Introduction



Gaussian (black), Lorentzian (blue) and Voigt (red) profiles, normalized to 1. All profiles have the same FWHM (i.e., the Voigt profile is not calculated from the plotted Gaussian and Lorentzian)



Sinc profile, normalized to 1.