FITEDGE User's Guide v1.11

For use with FITEDGE 1.11+

Recent changes

version 1.11: This is the inaugural version, at least to get a manual. The main change to this version over previous ones is that this version uses a formula-based constraint system, and so I (Corwin) now judge it ready for others to use.

Quick start

FITEDGE requires an input file named `inparam.dat`. The syntax is simply

fitedge

At the minimum, inparam.dat should contain roughly the following

```
************************************************************
#Sample input file
#Required parameters only not commented out
DATAFILE /home/hahn/exafs/exdata/hf37/es/096b2e_pre
FITRANGE  8900 9010.
MAXITER 200
#SKIPFIT
#Parameter names:
#       C1:     constant
#       Ai:     amplitude of peak i
#       Ei:     energy of peak i
#       Si:     sigma of peak i
#       Gi:     gamma of peak i
#       Ri:     gaussian/lorentzian ratio of peak i
#CONSTRAINTS
#S2=S1
#S3=S2
#S4=S1
#G2=G1
#G3=G1
#G4=G1
#E1=(A2*S2*E2 + A3*S3*E3)/(A2*S2+S3*A3)
OFFSET   0.000
OFFVAR 0
```

```
PEAKTYPE EDGESTEP
PEAKVALUES    0.0646  8940.17  8.082  4.200 0.500
PEAKVAR  1 0 1 0 0
PEAKTYPE RESONANCE
PEAKVALUES    1.3065  8939.20  2.540  4.200 0.500
PEAKVAR  1 1 1 0 0
PEAKTYPE RESONANCE
PEAKVALUES    0.3800  8945.54  1.568  4.200 0.500
PEAKVAR  1 1 1 0 0
PEAKTYPE RESONANCE
PEAKVALUES   -0.1292  8954.54 -2.207  4.200 1.000
PEAKVAR  1 0 1 0 0
*******************************************************
```

As can be seen in the example above, fits can include an overall OFFSET, but otherwise are the sum of different kinds of peaks. The variables can be turned on and off in the fit using the appropriate "VAR "command and setting a flag to 1 or 0, respectively.

Each `PEAK` is either of `PEAKTYPE EDGESTEP` or `RESONANCE`. A RESONANCE peak is defined as a pseudo-Voigt. The parameters are given on the PEAKVALUES line as follows:

`PEAKVALUES` $\quad <I_i>,<E_i>,<\sigma_i>, <\Gamma_i>,<r_i>$

where I_i is the peak intesity of peak i, E_i is the energy of the peak, σ_i is the Gaussian half-width of the peak, Γ_i is the Lorentzian half-width of the peak, and r_i is the Gaussian-to-Lorentzian ratio of this pseudo-Voigt.

An `EDGESTEP` peak-type is simply a `RESONANCE` peak (same `PEAKVALUE` definitions) that is integrated from E=0 to E=E_i. For example, in the case of r_i=0.0, this integrated Lorentzian would be an arctan.

Any number of peaks can be defined, but the number of lines in an inputfile must come in threes in the order `PEAKTYPE, PEAKVALUES, PEAKVAR`.

Constraints are very important when fitting multiple XANES peaks. Parameter names are defined in the example above. Note the commented example:
`E1=(A2*S2*E2 + A3*S3*E3)/(A2*S2+S3*A3)`
This example is an important one as it sets the position of the edge in a 2-peak fit to be at the weighted mean of the total area under the two peaks.

ISSUES/PROBLEMS

It is fairly common for the integration routine (qromo, from Numerical Recipes) to have issues when integrating the pseudo-Voigt for the `EDGESTEP` peak type. The problem

manifests as a lumpy edge step, but the calculation of chi^2 reflects the fit result. Proceed with moderate caution. I've noticed sometimes I do better after varying r_i.

The Gaussian/Lorentzian ratio, r_i, can be varied, but it is often better to simply fix this parameter.

Standard output is to `fitedge.dat` and `results.dat`. Parameters are not overwritten in `results.dat`.

Command summaries

Overview

Syntax is `fitedge`
Output: `fitedge.dat, results.dat`

Required input file commands are `DATAFILE, FITRANGE`

Starting values for pair parameters are set either with `OFFSET, PEAKTYPE` followed by `PEAKVALUES` followed by `PEAKVAR`.

Fit behavior is set by `SKIPFIT` or `MAXITER`.

Constraints begin with a `CONSTRAINTS` line with following constraint formulas, using parameter defined above. The dependent variable is set always on the left hand side of the equation, as in `G3=G1` (Gamma of third peak is fixed to the value from the first peak).

Error analysis uses the `RESOLUTION` command line to determine the number of independent data points in the fit. The default is "`RESOLUTION 1.0`", which sets the resolution to 1.0 eV.

Details

`MAXITER <`n_{max}`>`

n_{max} is the maximum number of fitting iterations before forcing output. Default is 999.

`SKIPFITPEAK`

Equivalent to MAXITER 0. Useful for seeing calculation of result from a given input.

`RESOLUTION <res>`

`<res>` is the energy resolution of the data set. This parameter is only used for calculating the number of independent data points when performing the error analysis. The default is 1.0 eV.

`LABEL <label>`

Alternate string besides `filename` to use in `results.dat`.